Almanac 2012

Analytical Tables and Product Overview

Innovation with Integrity

Analytical Solutions

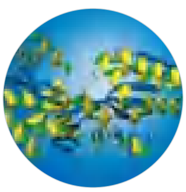
Bruker – the performance leader in life science and analytical systems.

Right from the beginning, which is now more than fifty years ago, Bruker has been driven by a single idea: to provide the best technological solution for each analytical task.

Today, worldwide, more than 5,400 employees in over 70 locations on all continents are focusing their efforts on this permanent challenge. Bruker systems cover a broad spectrum of applications in all fields of research and development and are used in all industrial production processes for the purpose of ensuring quality and rocess reliability. Bruker continues to build upon its extensive range of products and solutions, expand its broad base of installed systems and maintain a strong reputation amongst its customers. As one of the world's leading analytical instrumentation companies, Bruker remains focused on developing state-of-the-art technologies and innovative solutions for today's ever complex analytical questions.

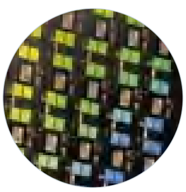
Bruker – Innovation with Integrity

Life Science



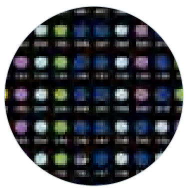
Quality & Process Control

Materials Research

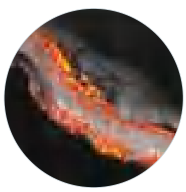


Food & Environment

Pharma & Biotech



Clinical Research



ISBN-13 978-3-929431-25-4

X-Ray and Elemental Analysis

- X-Ray Fluorescence (XRF)
- X-Ray Diffraction (XRD)
- Crystallography
- Energy Dispersive X-Ray Spectroscopy (EDS)
- Optical Emission Spectroscopy (OES)
- CS/ONH Analysis

Magnetic Resonance

- Nuclear Magnetic Resonance (NMR)
- Magnetic Resonance Imaging (MRI)
- Electron Paramagnetic Resonance (EPR)

Mass Spectrometry and Chemical Analysis

- FT-Mass Spectrometry (FTMS)
- MALDI
- Liquid Chromatography – Mass-Spectrometry (LC-MS)
- Inductively Coupled Plasma – Mass-Spectrometry (ICP-MS)
- Gas Chromatography – Mass Spectrometry (GC-MS)
- CBRNE Detection

Optical Vibrational Spectroscopy

- FT-Infrared Spectroscopy (FT-IR)
- Raman Spectroscopy
- Near Infrared Spectroscopy (NIR)

Microanalysis

- Atomic Force Microscopy (AFM)
- Scanning Probe Microscopy (SPM)
- Stylus and Optical Metrology
- Tribology

● Bruker offices

www.bruker.com/map

Bruker Corporation

The Bruker name has become synonymous with the excellence, innovation and quality that characterizes our comprehensive range of scientific instrumentation. Our trusted solutions encompass a wide number of analytical techniques ranging from Magnetic Resonance to Mass Spectrometry and Gas Chromatography, to Microanalysis, Optical, and X-Ray Spectroscopy. These market- and technology -leading products are driving and facilitating many key application areas such as life science research, pharmaceutical analysis, applied analytical chemistry applications, materials research and nanotechnology, clinical research, molecular diagnostics and homeland defense. Visit our website to discover more about our technologies and solutions.

www.bruker.com

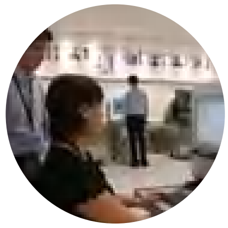
Karlsruhe, Germany

Fällanden, Switzerland

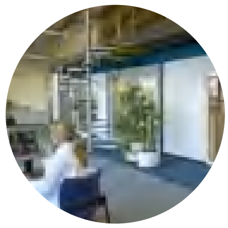
Bremen, Germany

Rheinstetten, Germany

Bruker – analytical excellence, acknowledged expertise and global presence.



Application lab
in Singapore



MR Imaging labs
in Ettlingen, Germany

Magnet Production
in Wissembourg, France

Santa Barbara, USA

Shanghai, China

Wissembourg, France

Singapore

Yokohama, Japan

Fremont, USA

Content:

Tables

2012 Monthly Calendar

Participation at Exhibitions and Conferences

Bruker Users Meetings worldwide

Training Courses

⬭ Represents public holidays.

Nuclear Magnetic Resonance

Solutions for Life Sciences
and Analytical Research

Innovation with Integrity

NMR

Fourier

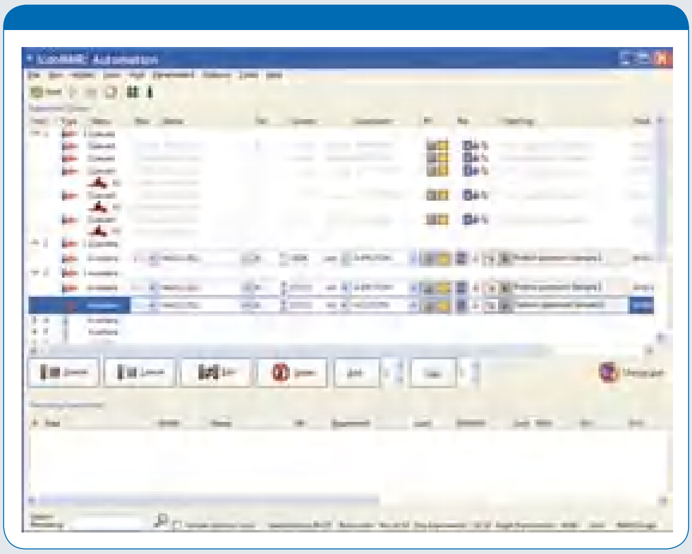
Dedicated high-resolution NMR spectrometer delivers affordable NMR for all your common applications in education and routine chemistry research

Fourier brings NMR within everyone's reach. It delivers powerful performance at extremely compact size, low weight and most importantly, minimal cost. With its new Fourier probe technology and a unique push-button, power on/off concept, ease of siting and handling is guaranteed. Designed and built by the world's NMR market leader, Fourier unique qualities include the industry standard operating software, TopSpin™. TopSpin's various tools for exploring the world of NMR make Fourier the ideal solution for chemistry education and routine analysis. Researchers have access to numerous pre-defined 1D and 2D experiments and interactive, automated processing tools help to transfer spectroscopic data into a corresponding report.

Easy sample loading on the SampleXpress Lite

Benefits

- Affordable NMR spectrometer for Chemistry Education and Small Molecule Analysis
- Industry Standard TopSpin software
- Providing higher throughput with the SampleXpress Lite 16 position sample changer
- Proven IconNMR software for automation control
- New robust Fourier NMR probe for easiest handling
- 1D/2D Proton and Carbon NMR for every Chemist

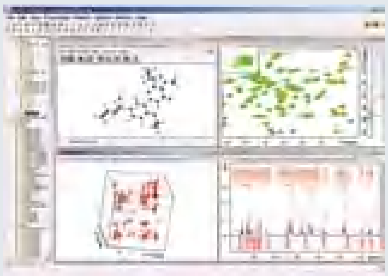


Sample setup with the intuitive IconNMR interface

Avance III NanoBay

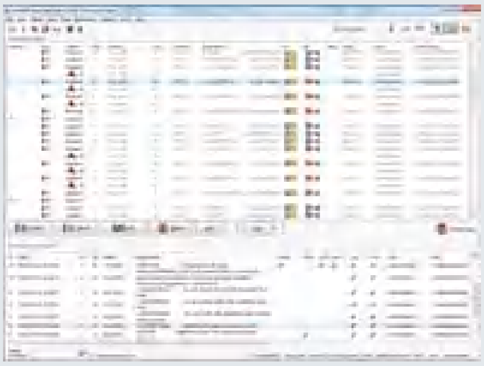
The Most Fully Integrated State-of-the-Art NMR Spectrometer Ever

The Avance™ III NanoBay is the most comprehensively integrated, state-of-the-art NMR spectrometer ever produced. The NanoBay's innovative design sees Bruker's high-performance Avance III NMR spectrometer technology boldly held within an exceptionally compact enclosure.



Amix™ provides a collection of powerful tools that enable statistical and spectroscopic analyses of your NMR data. For a wide variety of applications, such as metabolomics, small molecules research and mixture analysis an increase in productivity can be achieved.

It delivers high-productivity with highest quality NMR information for pharmaceutical and industrial chemists, as well as food analysis, diagnostics research and other small molecule applications.



IconNMR™ is the graphical user interface for fully automated acquisition and processing. This productivity tool excels whenever large numbers of samples accrue, or where multiple users access your spectrometer.

Benefits

- Ultra compact, innovative design high-end NMR spectrometer
- Available at 300 and 400 MHz
- Featuring UltraShield™ Plus magnet technology
- Easy siting in small analytical laboratories
- TopSpin™ - Intuitive routine user interface
- Based on well-proven Avance™ III spectrometer technology
- High-fidelity NMR information for a wide range of chemical applications

Avance III NanoBay 400 MHz spectrometer

Avance III

The Avance™ III is the ultimate NMR platform for life-sciences and materials research. Robust, automated and easy-to-use it is the ideal NMR analysis system for the pharmaceutical, biotech, and chemical industries, for metabonomics, materials science, molecular diagnostics, and much more.

The Avance III is the newest generation in the very successful Avance series, which has established Bruker as the clear technological and market leader in NMR and pre-clinical MRI worldwide. The Avance III spectrometer architecture is designed around an advanced digital concept which provides an optimized pathway for high-speed RF generation and data acquisition with highly modular and scalable transmitters and multiple receiver channels.

The Avance III platform provides 25 ns event timing (12.5 ns clock), and simultaneous phase, frequency and amplitude switching with capabilities that exceed the requirements of even the most demanding solid-state NMR experiments. The second-generation digital receiver technology delivers high dynamic range, high digital resolution and large-bandwidth digital filtering. The unique digital lock system provides the utmost in field/frequency stability.

Benefits

- Patented Direct Digital Synthesis
- One-chip RF generation
- Timing Resolution: 12.5 ns
- Minimum event time: 25 ns
- High-speed RF generation and data acquisition
- Scalable transmitters and multiple receiver channels
- High-dynamic range and digital resolution
- Large-bandwidth digital filtering

Ultra-High Field Avance III 850 MHz NMR system

Avance 1000

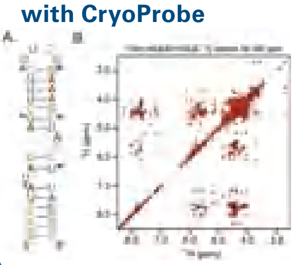
Bruker is proud to provide the world's highest field NMR system of highest sensitivity and dispersion to the scientific research community. With this instrument, research in biochemistry, structural biology and other molecular research will be pushed to new frontiers.

The first Avance 1000 NMR system equipped with a CryoProbe has been installed at the new 'Centre de RMN à Très Haut Champs' in Lyon, France.

- 1 GHz NMR system with 23.5 T persistent superconducting magnet
- Standard bore, 54 mm diameter
- UltraStabilized™ sub-cooling technology, achieving the highest field and most compact magnet coil at this field strength
- Proprietary jointing technology enabling high current and high-field joints with minimum resistance for maximum field stability
- 5-mm triple-resonance CryoProbe, enabling unique 1 GHz NMR applications
- 1.3-mm, 2.5-mm & 3.2-mm double and triple resonance MAS probes, enabling unique 1 GHz NMR solids applications

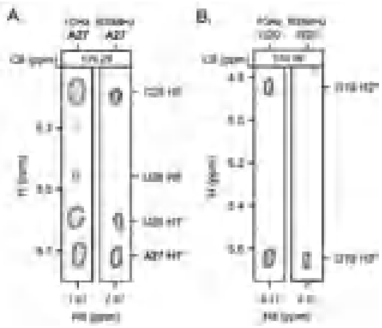
1GHz (23.5 T) UltraStabilized magnet installed at Centre de RMN à Très Haut Champs, Lyon, Fr. Courtesy: Prof. L. Emsley.

RNA, 3D NOESY-(^{13}C)-HSQC at 1 GHz with CryoProbe



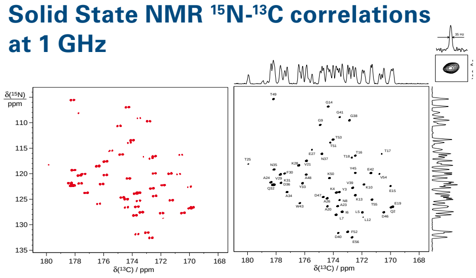
NMR structure determination of the conserved secondary structural motif of 23S rRNAs by John King, Christos Shammas and Vasudevan Ramesh, (University of Manchester).

RNA, 1 GHz vs 800 MHz



Comparison of ^{13}C planes of the 1 GHz and 800 MHz 3D NOESY-(^{13}C)-HSQC spectra. (**A**) (139.29ppm) (A27) (**B**) (138.96 ppm) arising from G20 H8 proton and the NOEs observed thereof to G19.

Solid State NMR ^{15}N-^{13}C correlations at 1 GHz



NCO correlation recorded on U[^{15}N,^{13}C]-microcrystalline GB1 without (left) and with (right) a S3E J-decoupling block; 60 kHz MAS, T1max=40 ms, T2max=50 ms, NS=48, exp. time=17 hrs.

Acknowledgements:

Dr. Moreno Lelli, Dr. Józef Lewandowski, Dr. Guido Pintacuda, Dr. Anne Lesage, Dr. Benedicte Elena, and Prof. Lyndon Emsley with CRMN, Lyon, France.

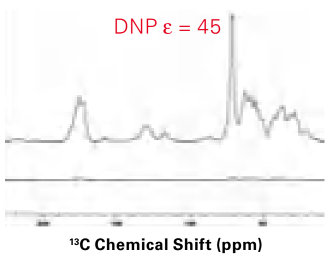
DNP-NMR Spectrometer

Sensitivity Boost for Biomolecular NMR

263 GHz DNP - NMR Spectrometer

Dynamic Nuclear Polarization (DNP) experiments transfer polarization from electron to nuclear spins enhancing sensitivity and dramatically reducing signal averaging time. Bruker Avance DNP-NMR Spectrometers are designed specifically for solid-state NMR, delivering unsurpassed sensitivity for exciting new applications.

DNP CPMAS of ^{13}C-Proline



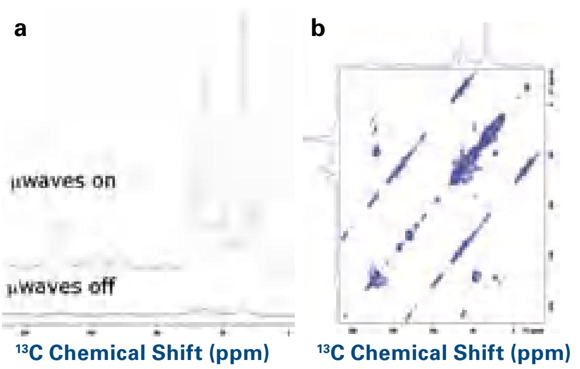
Courtesy of Prof. Ann McDermott, Columbia University

^{13}C CPMAS spectra with and without microwaves irradiation of a micro-crystalline yeast Triose Phosphate Isomerase (TIM) frozen solution with 20 mM TOTAPOL. 32 scans, 2 s recycle delay, 9 kHz MAS, 100 K sample temperature, 400 MHz ^{1}H frequency.

Benefits

- DNP-enhanced solid-state NMR experiments at high field
- Polarization enhancement yields up to a factor of 80 gain in sensitivity, to date
- Unique high power 263 GHz micro-wave source with easy-to-use software-controlled high-power gyrotron (9.7 T)
- Microwave transmission line designed for optimum beam propagation to the sample
- Low-temperature MAS probe technology with cold spinning gas supply and built-in wave guide
- 395 GHz (600 MHz ^{1}H) and 528 GHz (800 MHz ^{1}H) spectrometers in development

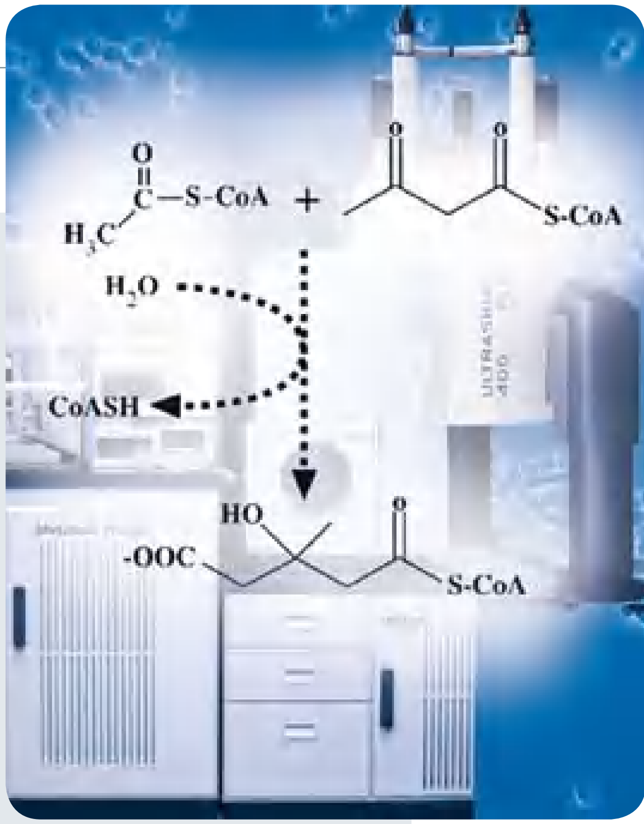
DNP on membrane proteins



Courtesy of Prof. David Weliky, Michigan State University

DNP experiments on membrane-associated HIV gp41protein with uniform ^{13}C,^{15}N labeling at Ala-6 and Gly-10. (**a**) ^{13}C CPMAS spectra with and without µwaves showing a factor of 22 DNP signal enhancement at 100 K, 8 kHz MAS, 32 scans, 5 s recycle delay. (**b**) DNP-enhanced DARR ^{13}C-^{13}C correlation experiment with 15 ms mixing time, 32 scans, 8 kHz MAS, and 200 points in f1.

Metabolic Profiler



Metabolic profiling and finger printing is a key process in the pharmaceutical industry for studying drug efficacy or toxicology. In clinical research, metabolic profiling helps to identify biomarker compounds for early disease detection and monitoring, and enables researchers to study the effects of drugs in biological systems in a rapid and robust method.

Integrated Analysis

The Metabolic Profiler™ is a dedicated, integrated LC-NMR/MS solution for metabolic analysis featuring an Avance NMR spectrometer and a micrOTOF-Q II™. This system provides a simple, easy to use and inexpensive base for acquiring the spectroscopic data needed for basic metabolic profiling. The system delivers the integration of automated sample handling, acquisition, collection and archiving of your data, and enables the comparative and statistical analysis needed for your research.

Data Management

SampleTrack™ is an Oracle®-based information system that utilizes SQL tools for organizing, searching and archiving sample information, which can simplify experimental control of large sample sets.

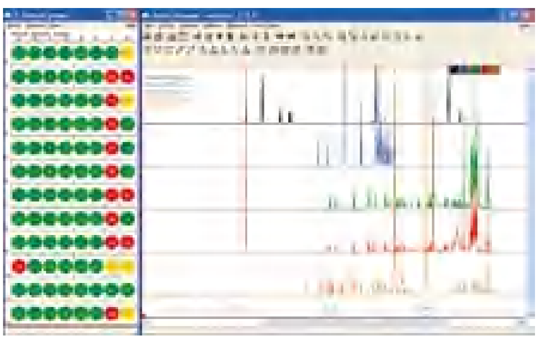
Statistical Analysis

The AMIX program provides a comprehensive range of powerful tools that enable statistical and spectroscopic analyses of both your NMR and MS data. AMIX features Pattern Match - which can define spectral patterns in multiple ways and project these to spectra. In addition, the Multi-Integration features can be used to identify and quantify metabolites in complex mixtures.

Reference Compound Spectral Database

The most complete metabolite NMR spectral database available which contains over 17,000 spectra of the most common endogenous metabolites.
By taking into account the effects of pH, field strength and by using one as well as two dimensional NMR data, the database enables the assignment of metabolites in biofluids, cell extracts and tissues in a unique and unambiguous way. Linking the database to AMIX enables automatic investi-gations, such as matching to mixture spectra. Direct integration into statistical data evaluation is also possible.

Analysis with AMIX



AMIX™ analyzes data and is linked to the Spectral Database for further comparative analysis.

Magnets

Bruker has specialized in the design and production of magnets and cryogenic systems for a wide range of applications, becoming the world's largest manufacturer of superconducting magnets for NMR. Bruker is engaged in every aspect of the magnet business including research and development, production and testing, individual site planning, as well as service and support.

UltraStabilized

UltraStabilized™ is our innovative magnet technology for Ultra-High Field NMR up to 1000 MHz. This proprietary technology provides reliable, stable operation at reduced helium bath temperature and ambient pressure.

US²

The US² represents the efficient combination of Bruker's renowned magnet technologies (UltraStabilized™ and UltraShield™) for enhanced system performance and siting flexibility at Ultra-High Field strength.

Ascend

This new magnet line at 400 to 850 MHz incorporates the key technologies of the well-established UltraShield™ Plus magnets, with new innovations for superior performance. The Ascend™ magnet design features advanced superconductor technology, enabling the design of smaller magnet coils, resulting in a significant reduction in the size of the cryostat. Ascend magnets are therefore easier to site, safer to run and have lower operational costs. These high-performance systems are ideal for structural biology research and materials research applications.

Ascend 500, 600, and 700 MHz systems

Probes

X Observe Probes

These probes are optimized for observation of X-nuclei. They are available in selective or broadbanded versions for double, triple and quadruple resonance experiments, including automated tuning and matching.

^{1}H Inverse Probes

The inner coil of these versatile probes, in multinuclear or selective configuration, is fully optimized for ^{1}H observation at highest sensitivity with optimal lineshape. The available configurations and choices of X-nuclei are identical to those for X Observe Probes.

Inverse MicroProbes

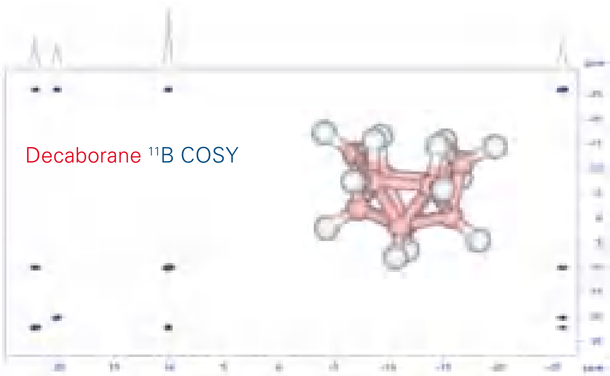
For highest ^{1}H sensitivity per mole of substance, e.g. in natural products applications, Bruker offers 1- and 1.7-mm ^{1}H/^{13}C/^{15}N fixed-frequency probes.

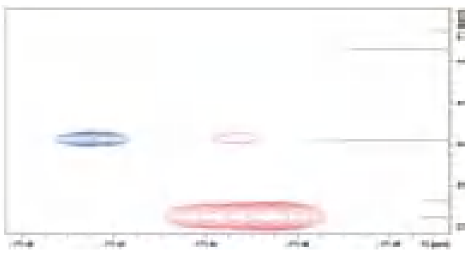
SmartProbe

SmartProbe

The SmartProbe™ delivers highest sensitivity on both the multinuclear and proton channel. The SmartProbe design exclusively features a broadband frequency channel enabling fully automated applications on protons and the widest range of X-nuclei. This unique probe technology enables fluorine applications including ^{19}F observe with ^{1}H decoupling and vice versa.

SmartProbe Applications with X-nuclei





Comparison of the 19F, 1H HOESY and HMBC experiment. While the HOESY spectrum has a correlation to the proton of the heterocycle, the HMBC shows a correlation to the NH protons.

CryoProbes & Prodigy

CryoProbe Prodigy

CryoProbe™ technology has delivered the single largest increase in detection sensitivity ever achieved in the evolution of NMR equipment. The factor 3-4 jump in sensitivity enables the use of correspondingly smaller sample quantities that are impractical with conventional probes, or enables the user to increase sample throughput up to 16-fold.

Product Lines

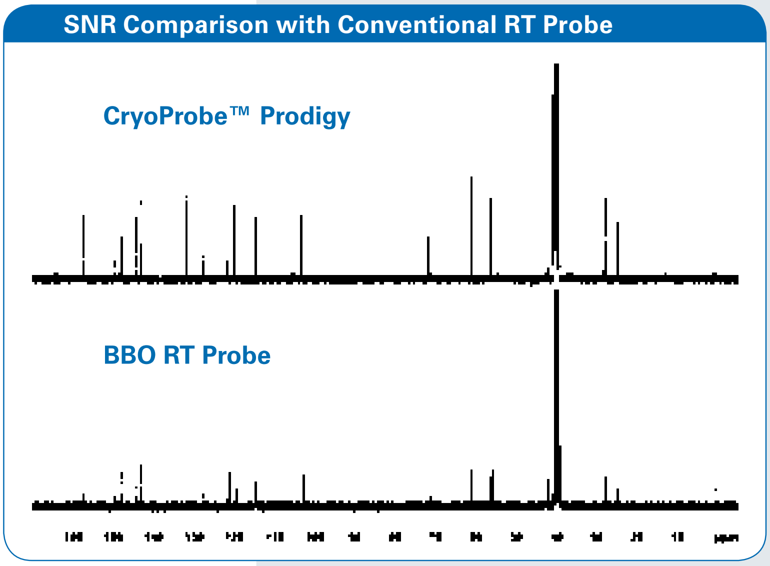
Bruker offers the largest range of CryoProbe configurations from 400 MHz to 1000 MHz, including proton optimized probes such as our 1.7- and 5-mm inverse triple-resonance probes, as well as 10-mm dual ^{13}C observe probes.

The 1.7-mm Micro-CryoProbe offers an increase in sensitivity per mole of more than an order of magnitude compared to a conventional 5-mm probe. For optimal X-nucleus detection we offer the 5-mm Quad CryoProbe in ^{13}C/^{31}P/^{19}F/^{1}H and ^{15}N/^{13}C/^{31}P/^{1}H versions. All high-resolution CryoProbes are equipped with a ^{2}H lock and a Z-gradient. A ^{1}H micro-imaging CryoProbe is also offered to enhance the study of sample structure and properties in the micrometer range.

CryoProbe Prodigy with pump and control unit

Prodigy

CryoProbe Prodigy, a new, revolutionary CryoProbe that delivers tremendous boosts in sensitivity at an affordable price. Costing significantly less than a conventional CryoProbe, the broadband CryoProbe Prodigy uses nitrogen-cooled RF coils and preamplifiers to deliver a sensitivity enhancement over room temperature (RT) probes of a factor of 2 to 3 for X-nuclei from ^{15}N to ^{31}P. The sensitivity gain on the proton channel exceeds standard probe performance by a factor of 2 or more.



Comparison of the 13C-sensitivity of a standard BBO probe with the CryoProbe Prodigy at 400 MHz. Sample: 50 mM quinine, 32 scans each.

Solid Probes

Our comprehensive range of the most advanced solids probes are ideal for inorganic and biological samples using experiments such as CP, d.CP, MQMAS, or REDOR.

Maximal spinning rates are 70 kHz for the ultra-high speed 1.3-mm MAS probe for materials science, 30 kHz for the 3.2-mm triple-resonance E^{free} MAS probe for protein research, and 15 kHz for the 4-mm HR-MAS probe with Z gradient for metabolomics studies.

The BioSolids probe product line is based on one of two technologies, TL_2 or E^{free}. For optimum performance these probes are configured as fixed frequency triple resonance probes, most often requested for proton, carbon and nitrogen. TL_2 probes yield the best overall sensitivity with high ^1H sensitivity for inverse detection experiments.

E^{free}

E^{free} probes are specifically designed to minimize RF heating. The two coil configuration provides enhanced sensitivity for ^{13}C and ^{15}N and the highest tuning and matching stability for safe, long term experiments. Minimized RF heating ensures the integrity of your protein, even while operating at room temperature.

1.3-mm MAS

The 1.3-mm probe product line provides the highest spinning speeds coupled with high-sensitivity and RF fields. Where sample heating might become an issue, convenient low power decoupling can be employed.

Efree probe

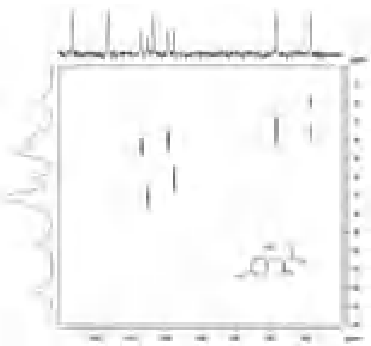
TL_2

TL_2 technology is the choice when high-decoupling fields are needed for optimum decoupling in J-coupling based experiments and when sample heating is not an issue. TL_2 probes are best used for dry and non-salty samples, or samples that are kept in a frozen state.

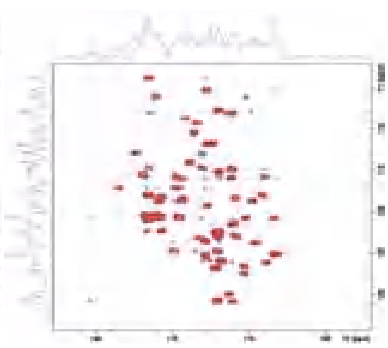
1.9-mm MAS

The new 1.9-mm MAS probe now enables fast spinning of nuclei less sensitive than ^{19}F and ^1H, offering 42 kHz spinning frequency at 10 µL active sample volume.

NMR using fast magic angle spinning



700 MHz 2D FSLG-HETCOR of L-tyrosine-HCl. Spinning frequency was 42 kHz, RF field for FSLG was 140 kHz. Projections are 1D ^{13}C CP/ MAS and ^1H wPMLG-5 spectra, respectively. Note that only directly bonded ^1H – ^{13}C correlations are visible.



NCO PAIN CP with ultrafast sample rotation. Spectra with 3 ms (red) and 6ms (blue) mixing time for long distance contacts in GB1 at 60 kHz rotation, 5°C with 75–80 kHz, ^{13}C, ^{15}N and 15 kHz on ^1H. (Lewandowski et al. JACS 129, 728 (2007))

TopSpin

Ideal for first-time spectrometer users as well as routine users, TopSpin's different acquisition tools make it easy for both beginner and expert to find their way to an NMR spectrum.

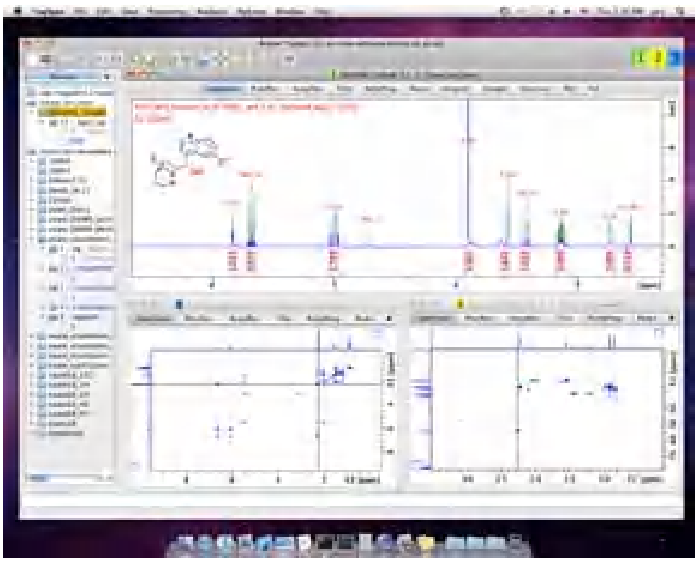
TopSpin provides a wealth of data processing visualization and administration features, including:

- Comprehensive set of functionalities for dealing with 1D to 5D data including automatic forward/backward or delayed linear prediction
- Inverse Fourier transform processing of rows, columns, planes and subcubes of nD datasets
- Interactive and automatic multi-dimensional peak picking and integration..

Features

- PC-standard user interface offers easy accessibility for Windows® and Linux® users
- Comprehensive functionalities for processing, displaying and analyzing single and multi-dimensional spectra
- Intuitive acquisition
- Non-uniform sampling
- Small molecule characterization
- BioTools™ - Biomolecular NMR made easy
- Method development environment
- Result publishing, predefined and user-defined layouts
- Lineshape analysis for solid-state NMR, including dynamic NMR
- Regulatory compliance support tools (audit trailing, electronic signature, autoarchiving)
- Special licenses for students and universities

TopSpin User Interface



TopSpin 3.1 on Mac

TopSpin for Mac OS X

Entirely programmed in the native Apple Mac OS X environment, the new TopSpin software caters to MAC users' familiarity with the unique and intuitive characteristics of that operating system, while maintaining the proven capabilities, look and feel of TopSpin. Incorporating a comprehensive range of NMR data analysis, processing and simulation features, TopSpin includes modules for efficient small molecule characterization and structural biology research.

Automation

Avance™ NMR systems meet the most demanding of automation needs by streamlining every aspect of NMR analysis, including sample submission, sample preparation, automatic probe tuning, data acquisition, processing, data distribution and archiving. Depending upon the laboratory's needs or goals, automation may involve high-throughput screening, overnight automation or multi-user open access.

IconNMR

This productivity tool excels whenever large numbers of samples are submitted for standardized experiments, or when many users access the spectrometer. IconNMR™ supports sample changers and sample preparation robots. The user can set up or supervise measurements remotely via a Web browser from a desktop or pocket PC.

SampleJet

SampleJet™ changer for 300-700 MHz NMR systems offers both high-throughput as well as individual sample capabilities in a single NMR sample changer. Its versatile design can accept samples from five 96-position racks, allowing batch analysis of up to 480 tubes. In addition, the SampleJet easily accepts single tube samples via a separate carousel that can hold up to forty-seven 1-, 1.7-, 3- and 5-mm tubes.

SampleCase

SampleCase™ is the first NMR automation solution that provides easy, safe and convenient access to fully-fledged NMR automation at user height. Ensuring simple random access automation without the need for steps or ladders, it also enables manual insertion and ejection of samples with the simple push of a button. The user-friendly system can be fitted to almost any Bruker NMR magnet.

SampleXpress

SampleXpress

Bruker's easy-to-use, cost effective solution for medium-throughput automation in NMR routine and research applications. Its compact, exceptionally integrated design drastically reduces sample exchange times to just a few seconds, making SampleXpress™ ideal for optimizing throughput in standard NMR service laboratories running 30-100 samples per day. In addition, efficiency is maximised thanks to interchangeable, easy-fill cassette modules that can be loaded off-system and in parallel with current experiments. The system is also equipped with integrated bar code reader for automatic sample identification.

SampleCase

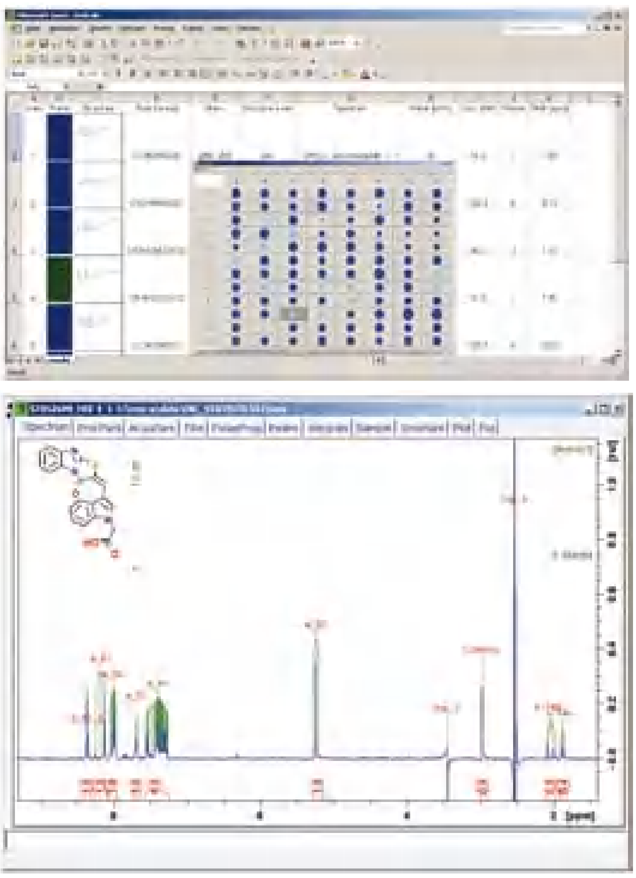
Complete Molecular Confidence (CMC™)

CMC-i: Structure Consistency Analysis

Only complete computational NMR spectral analysis provides a safe assessment of the consistency between a given structure and its ^{1}H NMR spectrum. Finally overcoming tedious manual procedures, optimizing predicted spectral parameters to match experimental data using iterative spectral analysis is now possible in full automation.

- Complete NMR spectral analysis yielding fully assigned spectra and highly accurate spectral parameters extracted from data, even for overlapping signals and strongly coupled spin systems
- Benefits from PERCH's highly sophisticated algorithms for predicting chemical shifts and couplings and optimizing them to match the experimental data using iterative quantum mechanical spectral analysis
- Extremely safe assessment of the consistency between a given structure and its ^{1}H NMR spectrum data based upon the quality of the fit and the similarity between predicted and actual spectral parameters, with optional use of HSQC information
- Accurate estimation of sample purity

CMC-q



Single and multiple result view

CMC-q: Absolute Quantification

Complete Molecular Confidence for quantification (CMC-q) is a complete workflow solution that facilitates automatic NMR-based quality assurance in batches.

- CMC-q provides quick access to automated NMR quality assurance and quantification of larger batches of samples. Delivering accurate, precise information on sample concentration and water content in typical screening samples, CMC-q also marks questionable structures and provides a suggestion for spectral assignment. This is ideally complemented with LC-MS information such as that derived from Bruker's SmartFormula program.
- Operating on a file-in, file-out basis, the user supplies an input file describing the samples to be measured, and receives an output file of results.
- The spectra interpretation function can also analyze individual datasets and prepare spectra for publication or for further analysis.

CMC-assist: Data Interpretation and Workflow Steamlining

The most powerful software tool for interactive, assisted NMR data analysis is now available. Designed for NMR end-users, CMC-assist efficiently extracts information from complex NMR data, conducts assessments and generates detailed reports for direct transfer to publications, patents and lab journals. CMC-assist not only excels as an off-line analysis interface but its automatied NMR interpretation power can also be used to generate results directly at any Bruker NMR instrument equipped with the latest control software, making it the most efficient and streamlined NMR workflow on the market.

- Seamless integration with Bruker spectrometers
- State-of-the-art analysis engine, powered by modern human logic emulation algorithms
- Automatic results may be refined manually
- Automatic data analysis includes:
  - Integration and ^{1}H number determination
  - Multiplet analysis
  - Structural assignment
  - Consistency statement
  - Concentration
- Reports include detailed PDF and multiplet string in different journal formats
- Windows, Linux or Mac operation systems are fully supported

CMC-assist & CMC-se

CMC-assist User Interface

CMC-se: Structure Elucidation

CMC-se is an NMR software package for simple and efficient structure elucidation of small molecules. With its innovative approach, CMC-se accelerates the spectroscopist's workflow during the elucidation process by automating many of the key analysis and interpretation steps. In combination with Bruker's Avance™ NMR spectrometer product line, CMC-se is the only elucidation tool that integrates high-quality NMR data acquisition with sophisticated software analysis. CMC-se is available for the major operating systems: Windows®, Linux® and Mac OS® X.

- Simple and efficient structure elucidation of small molecules in drug discovery and natural products research
- Automates many of the necessary analysis and interpretation steps
- Seamless integration of NMR acquisition and sophisticated software analysis
- Enables both accomplished researchers and beginners to expedite the elucidation of unknown substances in diverse pharmaceutical and chemical applications
- Organizes the data for a molecule into a single project, and provides unique graphical tools for data visualization and interpretation

Assure

Assure RMS-Raw Material Screening

Impurities and adulterants in starting materials pose potential health threats when present in the manufacturing of pharmaceutical APIs and drug products. These same impurities and adulterants may also result in lower production yields and increased product purification. Screening starting materials by NMR using Assure - Raw Material Screening identifies problem samples prior to use and prevents costly manufacturing mistakes. Designed for GMP and GLP environments, Assure - Raw Material Screening provides a traceable record of sample analysis and results. Applications include pharmaceutical and chemical production and analytical reference standards.

Quantification

Category	Concentration	Status	Match
Active Ingredient	99.64%	✓	✓
Adulterant	0.36%	✗	✓
Impurity	0.00%	○	
Unknowns	-		

Fail — % relative to total integral

Compound	Concentration	Status
Hydrocodone	99.64%	quantified
Phenetole	0.36%	quantified
Solvent	0.00%	Not quantified

Quantification results of main components and impurities are reported in a simple to read format with a user defined 'pass/fail' threshold.

Features

- System Suitability Test for GMP/GLP Labs
- Automated Data Acquisition
- Automated Quantitative and Qualitative Analysis
- Automated Report Generation
- QC Report - a 'pass' or 'fail' report
- Detailed Expert Report - total analysis
- Lock-out mode for access-limited users
- Convenience Features
- Sample SBASE/KBASE
- Customizable

Assure SST - System Suitability

Assure-System Suitability Test (SST) is the ideal tool for any NMR spectroscopy laboratory. In full automation, the NMR spectrometer is validated regularly for instrument performance and optimized before you run your samples.

Choose from a list of available individual tests to perform lineshape and sensitivity measurements on your liquid-state NMR spectrometer that will run at a time convenient for your facility.

Probe-specific parameter settings enable use on practically any liquid-state NMR probe.

Assure-SST's Temperature Calibration feature calibrates AND adjusts the temperature of the sample to the actual desired value. Accuracy in temperature provides optimal results for spectral reproducibility from instrument to instrument.

- Fully Automated Performance Validation
- Instrument Optimization
- Monitors performance of 'walk-up' instruments
- Enables NMR specialist to produce more results
- Improves data quality
- Meets GLP requirements

FoodScreener

The JuiceScreener™, combined with its SGF Profiling™ technique, can deliver huge amounts of information derived from one single experiment, instead of multiple individual analysis steps. This provides higher throughput and reliability than conventional techniques, leading to a significant reduction in cost per sample. This enables up to 5 times more sample investigations with no change in budget, resulting in an improved and more comprehensive quality control screening program.

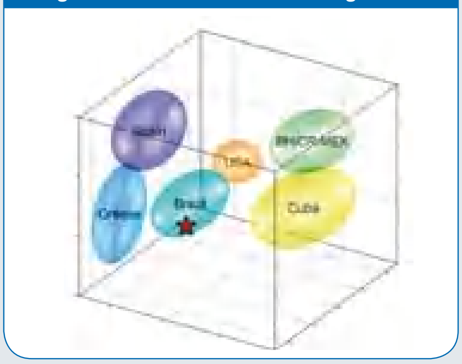
Push-Button Routine

SGF Profiling is a fully automated push-button routine that needs no interaction from the operator. From sample bar code registration, preparation and handling, to data acquisition and statistical evaluation, all steps are under the control of SampleTrack™, Bruker's laboratory information system.

Spectroscopic Database

Screening is based on a constantly updated, extensive spectroscopic database that includes thousands of NMR spectra from mainly authentic juices. Currently the data base includes about 40 different fruit types from more than 50 production sites worldwide. In addition, the database also provides access to hundreds of small molecule compounds for further analysis of unknown ingredients.

Origin Authentification of Orange Juice



Features

- Fully automated push-button NMR solution including evaluation and reporting
- Simultaneous absolute quantification of all relevant organic ingredients for juice assessment
- High-throughput with minimal sample preparation
- Reduced cost per sample
- Reliable screening method providing targeted and non-targeted multi-marker analyses
- Enables the detection of unexpected fraud
- Screening is based on an extensive NMR spectroscopic database of more than 8000 reference juices, obtained from production sites all over the world
- Complex statistical models enable the analysis of: origin authenticity, species purity, fruit content, false labeling, production process control and sample similarity

Hyphenation

Major tools for small molecule research and mixture analysis include HPLC, SPE, NMR and MS. Bruker offers hyphenated systems to meet various research needs. While NMR can be used to investigate the complete mixture, LC-NMR can analyse the individual compounds separated by the chromatography. An LC-NMR interface can easily be added to any NMR system from Bruker thereby also enabling hyphenated LC-(SPE)-NMR(/MS) applications. By combining the structural resolving power of NMR for the separated compounds with the mass accuracy of the micrOTOF, we can offer the most complete system for structural analysis available today.

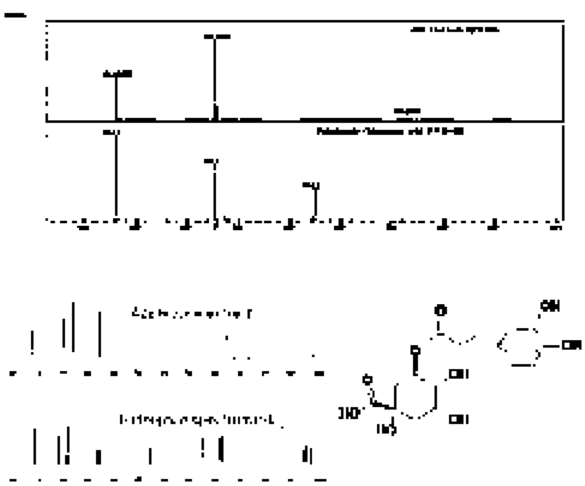
Hyphenated system including sample preparation, NMR, LC and MS

LC-(SPE)-NMR

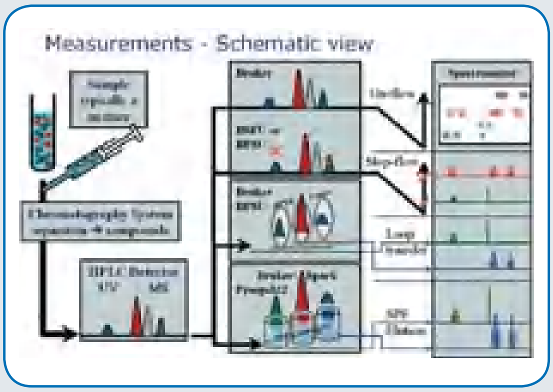
Two different methods for coupling are possible: either by coupling the chromatography system directly to the NMR spectrometer, or by the intermediate collection of the samples. Direct coupling can be performed as stopflow or on-flow analysis. For intermediate collection loop-storage or collection on solid phase extraction (SPE)-cartridges is possible.

The use of SPE provides an efficient interface between chromatography and NMR even enabling the analysis of low level metabolites.

LC-SPE-NMR-MS Results



LC-(SPE)-NMR-MS of Apple Juice high resolution mass spectra from m/z 355.1034 (upper part) of chlorogenic acid and the comparison with ion trap library (lower part) [1]H NMR spectrum of chlorogenic acid and the comparison with reference compound commercially available.



Immediate Access to Latest Technologies

Contract Bruker Analytical Services

Everyone can now benefit from Bruker's latest technologies, instrumentation, and unmatched experience in analytical applications. We offer supporting services that include advanced high-resolution NMR and mass spectrometry applications. Our customers can benefit from access to the latest developments in the field through Bruker's cooperations with academic and industrial research labs. Our experts can also assist you with special customized projects.

Benefits

- Short and long term support increases project handling capacity
- Latest, most advanced Bruker technologies
- Unique analytical expertise and knowledge
- Method development and feasibility studies

Advanced NMR Services

- Structure verification and elucidation
- Reaction and purity control
- Quantitative analysis
- Variable temperature experiments
- Screening methods for pharmaceutical and clinical research
- Food quality control
- Juice analysis using SGF-profiling
- Metabonomics studies
- Natural product analysis

Additional Analytical Services

- Mass Spectrometry & Imaging
- EPR (ESR) Spectroscopy
- TD (Time Domain) NMR Spectroscopy
- X-ray Diffraction, Crystallography & Fluorescence
- FT-IR Spectroscopy & Microscopy
- Raman Spectroscopy & Microscopy
- LC-(SPE)-NMR/MS

Customized Projects

When additional measures are needed, our technical experts will discuss the range of special capabilities available to you. Whether it is a short term project where specialized equipment is a necessity, method development is required or feasibility studies are needed, we can help you with our extensive resources.

High-Performance Power Supplies

High-Voltage Power Supplies

Bruker high-voltage power supplies find their main applications in IOT- and Klystron-based RF transmitters in Particle Physics. Our power supplies provide high-voltages of up to 50 kV at broad range, from 1 kW up to several Megawatts. The compact solid-state design is based either on the latest switch mode technique or, in the case of highest power applications, based on SCR (Thyristor) control.

Klystron power supply for the MAMI C race track microtron, Mainz University, Germany.

High-Current Power Supplies

Bruker high-current power supplies are employed in industry and particle physics research worldwide. Our high-current power supplies, available for pulsed or DC, monopolar, bipolar or four-quadrant operation, deliver high-currents of up to 30.000 A. Based on the latest switch mode technology they ensure optimum efficiency and enable stand-alone, fail-safe operation. The option of linear mode regulation provides maximum stability and minimum noise and fluctuations from 1% to better than 1 ppm (part per million).

For high-power applications our high-current power supplies benefit from SCR (Thyristor) control. We offer single- and multi-channel supplies starting in the 100 Watt range going up to several Megawatts.

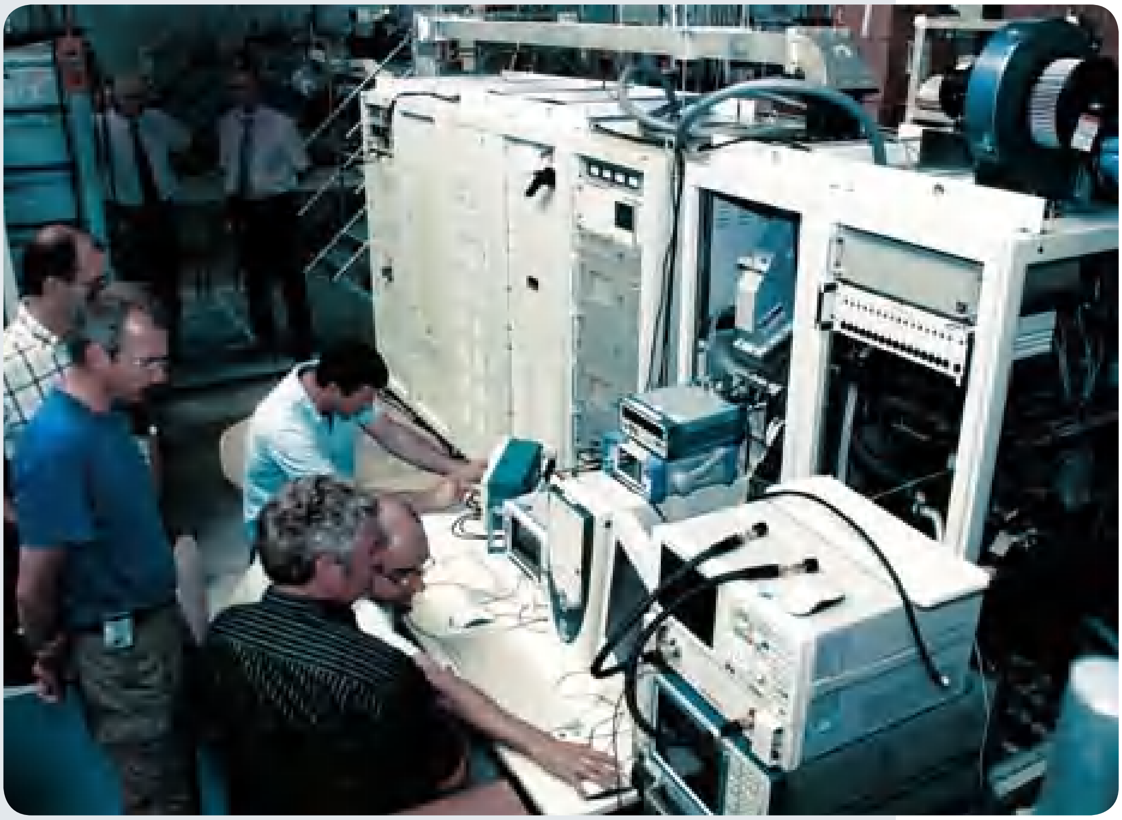
RF Transmitters

Bruker Radio Frequency Transmitters are established in nuclear physics applications all over the world. Our high-voltage power supplies, capable of emitting power from 100 Watt up to 300 kW and more, benefit from modern switch mode design for optimum efficiency and feature SCR (Thyristor) control to handle the highest power applications.

Choose from single or stacked solid-state amplifiers, whilst IOT amplifiers deliver optimum peak power conversion efficiency.

For arc protection our emitter tubes operate with defined stored energy, with optional solid-state crowbar circuits to protect the sensitive elements.

Start-up and operating procedures are handled automatically ensuring stand-alone, fail-safe operation, while a solid-state safety system ensures maximum protection for the transmitter elements and the user applications.



RF IOT high-power transmitter at ELBE FZD Rossendorf, Dresden, Germany.

Content:

TD-NMR Products

Time Domain NMR

Time Domain Benchtop NMR Analyzers

Innovation with Integrity

TD-NMR

the minispec TD-NMR Analyzers

The minispec benchtop product lines utilize Time-Domain (TD-)NMR spectroscopy, a method related to High-Resolution NMR and Magnetic Resonance Imaging MRI. Unique permanent magnet and radio frequency (RF) technologies are applied to investigate the sample as a whole, non-destructive and non-invasive.

Turnkey solutions for Quality Control (QC) are offered with straight-forward calibrations comprising well-known international recognized standard methods according to ISO, ASTM and AOCS. the minispec series provide also a sound of basis for R&D applications like MRI contrast agent research, determination of droplet size distribution in emulsions and obesity research.

the minispec mq Series

the minispec mq Series

The award winning mq series covers a wide range of applications for both R&D and routine quality control and offers multiple expansion capabilities.

With the addition of innovative accessories and readily exchangeable probe assemblies, the mq Series is suited for a full range of time domain NMR measurements. Typical applications are:

Food Industry

- Solid Fat Content in fat compositions (AOCS Cd 16b-93, ISO 8292 & IUPAC 2.150 methods)
- Oil and moisture in seeds and oil seed residues (AOCS Ak4-95, ISO 10565 & 10632 methods, USDA GIPSA approved)
- Solid Fat Content as well as total fat content in chocolate and chocolate related products
- Droplet size analysis in O/W and W/O emulsions Oil, water and protein in dry and wet food and feed

Textile Industry

- Spin Finish on Fibres (OPU)
- Coatings on Polymers

Polymer Industry

- Xylene soluble content in polypropylene
- Density and crystallinity in polyethylene
- Rubber content in polymers like ABS or polystyrene
- Cross-link density of elastomers

Petrochemical Industry

- Hydrogen content in hydrocarbons (ASTM D 7171 method)
- Oil content in paraffin and wax

Pharmaceutical Industry

- Fat and lean in live mice and rats
- Contactless weight determination
- Moisture and solvents in powders and tablets
- Contrast agent investigations near MRI fields: 0.25 T, 0.5 T, 0.75 T, 1.0 T and 1.5 T

Healthcare Industry

- Fluorine content in toothpaste
- Melting properties of cosmetics

R&D and Academics

- All types of temperature dependent relaxation time studies
- Diffusion experiments
- Single-Sided NMR

Dedicated Solutions for Industrial Quality Control

the minispec Plus multi-lingual software including 3 user levels

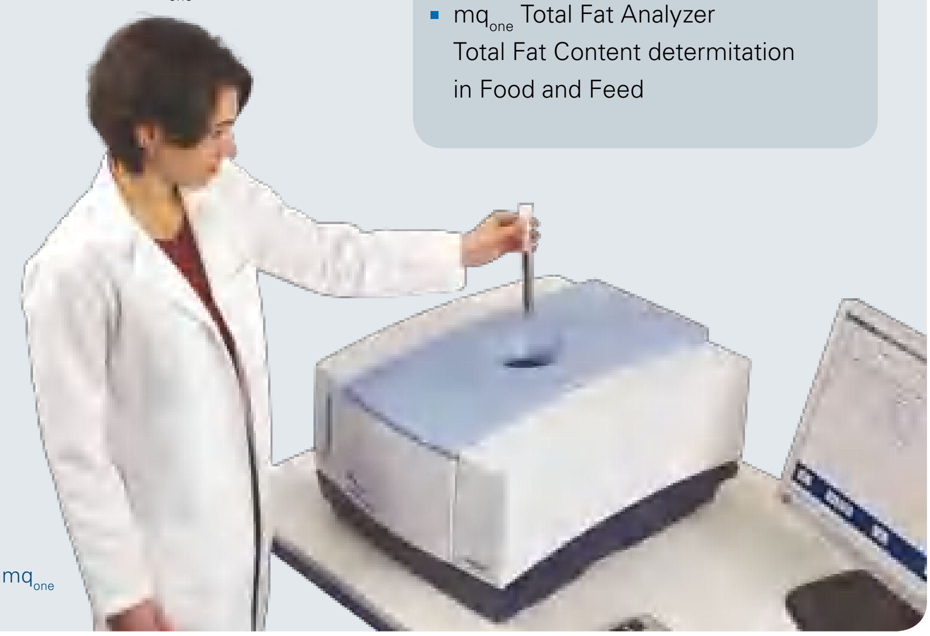
the minispec turnkey analysis workflow

Readily available calibration standards, such as Bruker's certified SFC samples

No sample preparation, just insert sample into the minispec mq$_{one}$

the minispec mq$_{one}$ Series

The mq$_{one}$ Analyzer is not just an analytical device. It offers a dedicated solution for the analytical task of daily quality control (QC) in the industry. The simple calibration, the intuitive workflow and the multilingual software allow the operation of the mq$_{one}$ Analyzer by everybody. The three user levels and compliance to 21CFR part 11 lead to safe and fully traceable data. The high performance of the mq$_{one}$ Analyzer guarantees high result quality and the well known Bruker quality ensures a long lifetime of your mq$_{one}$ Analyzer.



the minispec mq$_{one}$

the minispec mq$_{one}$ Analyzers

- mq$_{one}$ SFC Analyzer
  Solid-Fat Content (ISO, AOCS)
- mq$_{one}$ Seed Analyzer and
  mq$_{one}$ Seed Analyzer XL
  Oil and Moisture in Seeds, press cake, residues (ISO, IUPAC, AOCS)
- mq$_{one}$ Hydrogen Analyzer
  Hydrogen in Fuels (ASTM)
- mq$_{one}$ Spin Finish Analyzer
  Finish on Fibre, Oil-Pick-Up (OPU)
- mq$_{one}$ Polymer Analyzer
  Xylene-soluble content in PP
- mq$_{one}$ Total Fat Analyzer
  Total Fat Content determitation
  in Food and Feed

the minispec LF Series

the minispec LF90 II

the minispec LF series

Bruker's minispec LF Series of whole Body Composition Analyzers provides a precise method for measurement of Lean Tissue, Fat, Free Fluid and Total Body Fluid in live mice and rats. Longitudinal studies are possible as the animal is carefully handled without the need of anaesthesia. Measurements with the LF Series are done in minutes without the need for any sample preparation. With the new minispec LF110 also rats with mass >= 1kg can be analysed.

the minispec LF50 H

the mq-ProFiler

The mq-ProFiler is a compact NMR analyzer equipped with a single-sided magnet and RF probes capable of performing ^{1}H-NMR experiments on the surface or surface near volume elements. This device is a portable TD-NMR analyzer without any sample size restriction for industrial process/ quality control and research.

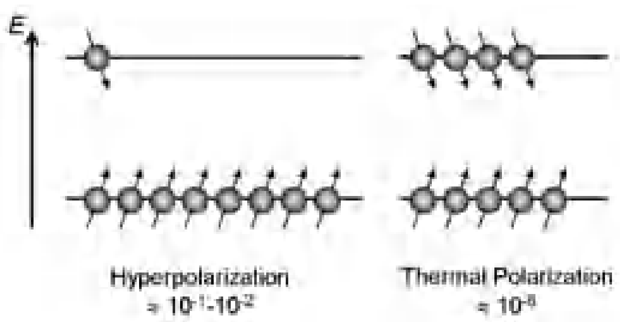
Typical applications of the mq-ProFiler are:

- Cross link density, filler materials, aging in tires (even with steel bars) and other polymers
- In-package food analysis: Fat content extent of gel formation, etc.
- Moisture content, porosity, and effect of hydrophobic treatments in building materials
- Fast monitoring of Fat content in high moisture foods like fresh salmon fish
- Porosity, separation of oil from water signal and drainage/absorption/drying study in rocks and other porous materials
- Contamination (oil) in moisture-free soil
- Skin hydration study

HyperQuant

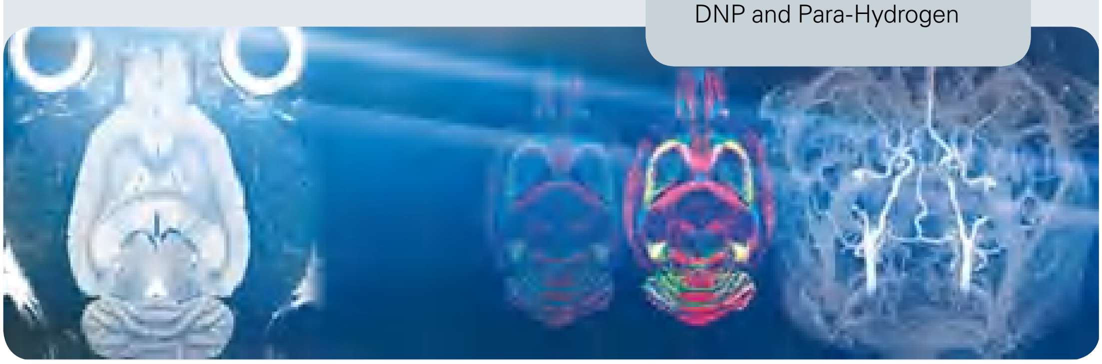
HyperQuant™ is a benchtop time-domain NMR reader that precisely and quantitatively delivers both the magnetic hyperpolarization and thermal polarization status of a sample. This proprietary solution applies a unique permanent 0.94 Tesla magnet system combined with an innovative MR probe design and novel NMR pulse sequence capabilities. This unique combination enables quantification of the thermal polarization level of ^{13}C-labeled samples using volumes as low as 1 ml. The hyperpolarization enhancement factors can be obtained directly on the sample of interest, without the need for a separate calibration reference.

Effect of Hyperpolarization



Features

- Direct quantification of magnetic hyperpolarization and thermal polarization levels
- Calibration-free technology based on direct comparison of hyperpolarized and thermally polarized state
- Turn-key ^{13}C application
- Proven bench-top TD-NMR design
- Unique 0.94 T permanent magnet system
- Only 1 ml of sample volume required
- Tracing of the ^{13}C hyperpolarization decay
- Thermal signal determination with 99% accuracy
- Quantifying concentrations of fully labeled ^{13}C samples
- External trigger interface to HyperSense™
- Applicable to all hyperpolarization methods including DNP and Para-Hydrogen



Content:

MRI Products

Magnetic Resonance Imaging

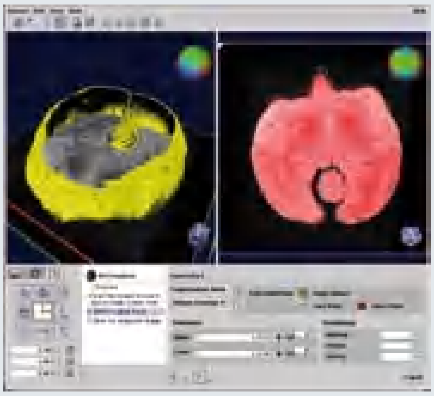
Solutions for Molecular Imaging and Preclinical Research

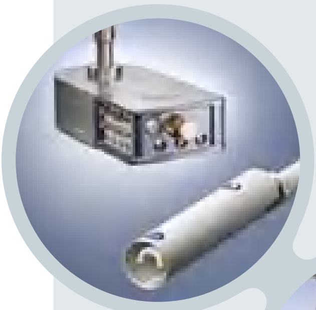
MRI

Innovation with Integrity

BioSpec

The BioSpec® series is designed for the emerging market of preclinical and molecular MRI. State-of-the-art MRI CryoProbe™ technology together with ultra-high field USR magnets deliver high spatial resolution *in vivo* enabling customers to come closer to the molecular and cellular level. Thanks to its innovative modular concept, virtually any small animal MR imaging application in life science, biomedical and preclinical research can be conducted. Whatever your application is, the BioSpec series will deliver the optimum solution, will perfectly equip you for the most demanding tasks and challenges.





Standard and optional Product Features

- High-end UltraShield™ Refrigerated (USR) magnets from 4.7 up to 15,2 Tesla
- A wide range of bore sizes (11 to 40 cm) for investigations on any kind of animals
- Helium zero-boil-off and nitrogen free magnets for reduced service costs
- Scalable Avance III architecture with up to 16 receiver and 6 transmitter channels
- Parallel imaging (GRAPPA) for almost all applications including EPI
- Multiple transmit imaging applications
- BGA-S gradients with highest amplitudes, slew rates, shim strengths, and duty cycles
- Motorized animal positioning for increased throughput
- IntraGate™ - Self gated steady-state cardiac imaging (no external triggering devices)
- Phased-array RF coil technology for maximum sensitivity and minimum scan times
- MRI CryoProbe™ delivers an exceptional increase in sensitivity to 250 %
- ParaVision® - Intuitive software package, for multi-dimensional MRI/MRS data acquisition,reconstruction, analysis and visualization

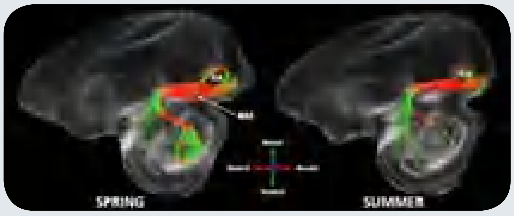
Innovative Animal MRI Solutions for Molecular and Preclinical Imaging

BioSpec benefits from the excellence of Bruker BioSpin, the global market and technology leader in analytical magnetic resonance instruments including NMR, preclinical MRI and EPR. With an install base of over 500 MRI systems worldwide and more than 40 local Bruker offices on all continents, you can rely on our long term expertise and dedicated after sales support.

DTI of the Song Control System (SCS) of Starlings

DTI is used to quantify seasonal changes in the SCS. The density of axonal connections changes under hormonal influences.

Courtesy: De Groof, A. Van der Linden, RUCA, Antwerp, Belgium.



Mouse Abdomen

T2 RARE abdominal mouse imaging with excellent contrast.

Courtesy: D. Elverfeldt, B. Kreher, J. Hennig et al., University Hospital Freiburg, Germany.

Cardiac Angiography

Visualization of coronary arteries *in vivo* (mice) using IntraGate.

ClinScan

With the ClinScan® you enter the field of translational research and molecular imaging. The ClinScan, a 7 T animal MRI and MRS scanner is designed to further facilitate translational research from 'mice to men' in the field of pre-clinical and molecular imaging.

ClinScan is Bruker BioSpin's solution for an emerging market of research MRI systems that allows a direct and fast transfer of preclinical studies on animal models to clinical studies on humans.

By virtue of the strategic alliance with Siemens Medical Solutions on human high-field MR systems, ClinScan uses the clinical user interface *syngo*® MR. Its operation is identical to that of Siemens Magnetom TIM systems.

Diffusion imaging (DTI)

Product Description

- 7 T Bruker USR magnet (Ultra Shielded Refrigerated, bore size 20 cm or 30 cm)
- Bruker gradient and shim coil (gradient strength of 290 mT/m or 630 mT/m, slew rate of 1160 T/m/s or 6300 T/m/s)
- Bruker RF array coil technology in combination with numerous animal handling accessories
- Siemens Magnetom Avanto technology with up to 32 receive channels
- Clinical routine user interface *syngo* MR to enable efficient workflow and highly automated state-of-the-art MRI and MRS applications on small animals

Multi Modality Imaging - MRI/PET

Simultaneous *in vivo* imaging of a F-18-FDG labeled mouse heart at 7 T. PET and MRI acquisition was done in parallel without interference between the two modalities.

Courtesy: B. Pichler, H. Wehrl, M. Judenhofer et al., Laboratory for Preclinical Imaging University Tübingen, Germany.

ClinScan systems are designed for translational molecular MRI and provide the clinical routine user interface *syngo* MR that facilitates straightforward transfer of protocols from benchtop to bedside and vice-versa.

Application Packages

Application packages for animal MRI resemble the application packages you already know from clinical MRI. Sequences and protocols are optimized for the specific needs in animal MRI.

Standard Imaging

The application suite is a full set of programs and protocols optimized for a wide range of high-field applications.

Parallel Imaging

- iPAT (integrated parallel Imaging) techniques including GRAPPA & mSENSE
- Higher speed and temporal resolution

Diffusion and Perfusion Imaging Echo Planar Imaging (EPI)

- Multi directional diffusion weighting
- Tensor calculation including tractography
- Perfusion applications including processing

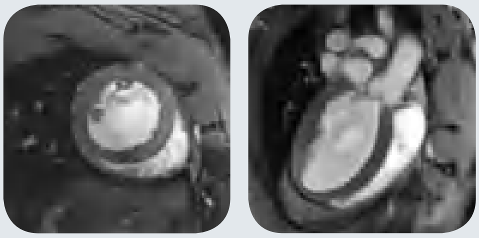
Cardiac Imaging

- True FISP & 2D/3D FLASH segmented
- Prospective triggering & retrospective gating
- Retrospectively gated cine imaging BOLD Imaging
- Single Shot EPI with PACE for BOLD-Imaging
- Automatic image reconstruction as well as on-the-fly t-test calculation in real-time for variable paradigms

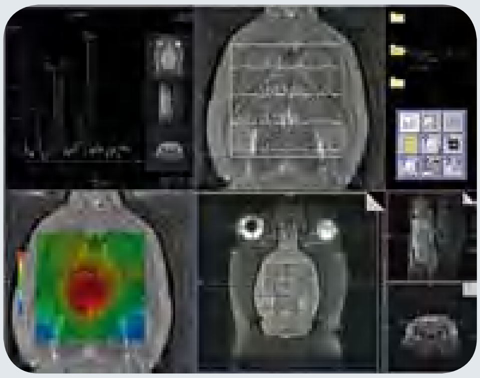
Spectroscopic Imaging & Spectroscopy

- Spin Echo & STEAM, PRESS and CSI
- Hybrid CSI technique including volume selection and FoV encoding
- Multi-nuclei option

Rat brain, BOLD fMRI



Cardiac imaging



Chemical shift imaging with outer volume suppression

Cartilage of rat knee (DESS) and rat brain, inner ear (CISS 3D)

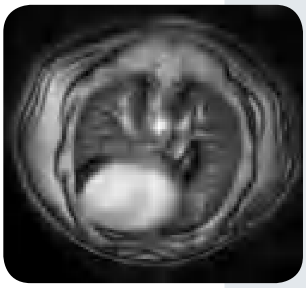
PharmaScan

Dedicated MR Scanner for Pharmaceutical, Biomedical and Molecular Imaging Research

The PharmaScan® is a high-field, easy-to-use and at the same time easy-to-install and very cost-effective MR-system. It is designed for MRI applications on small animals such as mice and rats in the field of routine pharmaceutical, biomedical and molecular imaging research. With the integrated automatic image acquisition and analysis, fast and reliable results can be obtained by simple operation of the system by non-academic personnel, without compromising full flexibility for the MR expert.

High-Resolution DTI

Coronal map of the major principle diffusion direction of a rat brain. The diffusion tensor imaging, with 30 diffusion directions, is acquired by the segmented echo planar imaging technique.



Mouse Lung Imaging using Ultra Short TE (UTE) Imaging

Radial scan with ultra short TE enables the visualization of detailed lung structures without using expensive hyperpolarized helium techniques.

Standard and optional Product Features

- ^{1}H MRI and MRS routine system, optimized for small rodents (such as rats, mice, gerbils)
- Actively shielded magnets at 4.7 T and 7 T allows easy and cost-efficient siting
- 16 cm clear bore size with 72 mm free access for the animal
- Parallel imaging (GRAPPA)
- High-performance BGA-9 or BGA-9S (as an option) gradients with highest amplitude, slew rates, shim strengths, and duty cycles optimized for small animal imaging
- No Faraday cage required
- 25 m² floor space required
- Scalable Avance III architecture incorporates up to 4 receivers
- AutoPac™ - Motorized, positioning system for routine animal handling and increased animal throughput
- IntraGate™ - Self gated steady-state cardiac imaging requiring no external trigger devices
- Phased-array RF coil technology for increased sensitivity and reduced scan times
- MRI CryoProbe™ - Sensitivity increase up to a factor of 2.5
- ParaVision® - Fully intuitive software package for multi-dimensional MRI/MRS data acquisition, reconstruction, analysis and visualization

Icon

Icon™ is a compact and easy-to-use 1 T permanent magnet high-performance MRI desktop system for preclinical and molecular imaging in biomedical and pharmaceutical research

Designed and built by the world's pre-clinical MRI market leader, Icon's unique qualities include the industry standard MRI software ParaVision.

ParaVision® offers a workflow-oriented routine user interface, enabling a wide range of small rodent and material science MRI applications.

Operators and researchers have access to numerous optimized measurement protocols and powerful interactive processing and analysis tools to deliver immediate results. Optional software packages enable Icon to perform the latest MRI applications, such as pulsed arterial spin tagging, fast echo-planar image read-out, or ultra-short echo time techniques. The optional DataManager facilitates efficient data management and archiving.

As an education tool, students will find the ParaVision software intuitive, whether it is used to perform research imaging protocols, or to learn programming of new MRI methods.

Ultra-fast relaxometry in mouse brain (*in vivo*) using a Look-Locker type EPI. The color-coded parametric T_1 map was laid over the anatomical image. This method enables fast contrast agent tracing in the brain with a temporal resolution of of 1:20 min.

BGA-S Gradient Series

Maximum Gradient and Shim Performance in Animal MRI

The Bruker gradient series BGA-S™ delivers unsurpassed performance for the whole range of animal MRI applications. The unique design provides highest gradient strengths and slew rates required for high-field animal imaging. The high cooling efficency results in unmatched duty cycles and as a consequence of it, modern imaging sequences with minimum field of view and a high number of slices for long experiment times can easily be performed. The integrated shim coils add up to ultra-strong shim capabilities. The BGA-S gradients can be operated as inserts and are easily exchangeable for maximum flexibility.

Specifications

	BGA-6S	BGA-9S	BGA-12S	BGA-20S
Outer diameter [mm]	113	150	198	303
Inner diameter [mm]	60	90	114	200
Strength* [mT/m] at I_{max}	1000	760	660	300
Slew rate* [T/m/s] at U_{max}	11250	6840	4570	1100
Gradient linearity/DSV [% / mm]	± 5 / 35	± 5 / 60	± 4 / 80	± 3 / 130
Number of RT Shims	9	11	11	9
Max. cont. gradient all axis [mT/m each axis]	500	190	330	87
Max. continous gradient one axis [mT/m]	350	130	220	60
U_{max} [V]/I_{max} [A]	300/100	300/200	500/300	500/300

* Output values have been measured on MRI system

Product Description

- Highest gradient strengths up to 1000 mT/m
- Highest slew rates
- Excellent duty cycle specifications
- Very high gradient linearity
- Optimal gradient shielding
- Maximum shim performance

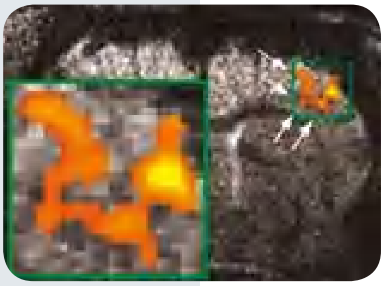
USR Magnets

Combining High-Field Magnet Performance with Easy Handling and Siting

The UltraShielded Refrigerated (USR) horizontal bore magnet product line features ultra-high magnetic fields and variable bore sizes in combination with easy handling and siting. Field strengths offered from 4.7 up to 11.7 T deliver optimum sensitivity for high-resolution MRI and MRS. The various bore diameters from 11 to 40 cm ensure optimal experimental performance on a wide range of animal MRI applications. Active shielding based on our well-proven UltraShield™ technology provides minimum stray fields. For ease of operation all USR™ magnets are nitrogen-free and include helium refrigeration for zero boil-off and minimum service intervals.

Features

- Ultra-high magnetic fields
- Variable bore sizes
- Highest field homogeneity
- Compact magnet design
- Excellent field stability
- Optimum external disturbance suppression
- Minimum stray fields
- Easy and cost efficient siting
- Nitrogen free
- Helium refrigeration (zero boil-off[1])
- Longer service intervals (two years)
- Cold delivery and fast installation
- Over 180 USR installations worldwide



High-resolution BOLD activation measured at 11.7 T USR magnet.

Courtesy: J.Seehafer, M.Hoehn, MPI for Neurological Research, Cologne, Germany

USR Magnet Product Line for a wide range of applications

	47/40 USR	70/20 USR	70/30 USR	94/20 USR	94/30 USR	117/16 USR
^1H Frequency (MHz)	200	300	300	400	400	500
Field Strength (T)	4.7	7.0	7.0	9.4	9.4	11.7
Bore Diameter (cm)	40	20	30	20	30	16
Length (m)	1.49	1.31	1.49	1.49	2.01	1.46
Width (m)	1.65	1.12	1.65	1.65	1.71	1.65
Ceiling height (m)	2.85	2.60	2.85	2.85	2.90	2.85
Field Drift (ppm/h)	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
Weight (kg)	4.700	2.500	5.000	5.500	11.500	7.000
Stray Field (radial x axial) (m x m)	2 x 3	1.5 x 1.5	2 x 3	2.0 x 3.0	2.3 x 3.3	1.7 x 2.8
Service Interval (year)	2	2	2	2	2	2
Zero Boil-off	Yes[1]	Yes[1]	Yes[1]	Yes[1]	Yes[1]	Yes[1]

USR systems are available with field strengths ranging from 4.7 to 11.7 T and bore sizes of 16, 20, 30 or 40 cm as shown in the table.

[1]With a valid service contract

MRI CryoProbe

New Signal-to-Noise Horizons in Small Animal MRI

Bruker now offers a new series of MRI CryoProbes for MRI systems. They feature very low temperature, closed cycle cooled RF-coils and preamplifiers offering an increase in signal-to-noise ratio (SNR) to a factor of 2.5 over standard room temperature RF-coils in routine MRI applications. The use of the MRI CryoProbe™ in routine imaging of the mouse brain *in vivo* at 9.4 T delivers outstanding image quality. The increased signal-to-noise ratio enables one to acquire high-resolution images of the microscopic structures in the mouse brain down to the cellular level.

Product Features

- Increase in sensitivity to more than 250 %
- Flexible design for easy siting
- Standardized interface allowing different MRI CryoProbes to be used with one cooling system
- Efficient design allows minimal distances between RF-coil and object
- Carefully controlled thermal environment with no cold surfaces in contact with animal
- Cooling down outside the magnet possible

Comparison with Nissle staining

Comparison of micro-structures in the mouse cerebellum with histological Nissle staining (left). Identification of anatomical structures like white matter, granular layers, molecular layers and Purkinje cell layers are possible.
Courtesy: Rudin M., Baltes C. et al., ETH Zurich, Switzerland

MRI CryoProbe™ at 11.7 T

Ultra-high resolution (35 × 35 × 200) µm³ mouse brain imaging *in vivo* acquired in 20 minutes.

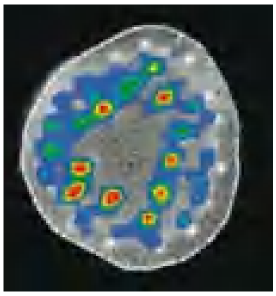
Courtesy: V. Rasche
University of Ulm, Germany

Micro-imaging

CryoProbe for Micro-imaging

The extension of Bruker's cryogenic NMR probe expertise into the field of MRI microscopy leads to new and exciting opportunities. Micro-imaging techniques for small samples with diameters up to 5 mm benefit from CryoProbe™ technology and a factor 4 improvement in sensitivity. The result is improved image quality, increased spatial resolution and/or reduced scan times. The MIC CryoProbes for ^{1}H at 400-600 MHz offer variable temperature operation over the range from 0 to 80 °C and are used with a Bruker BioSpin Micro2.5 gradient system in vertical wide-bore magnets with bore sizes of 89 mm or larger. The newly developed dual $^{1}H/^{13}C$ micro-imaging CryoProbe is also available.

^{13}C Chemical Shift Imaging



Detection of sugar transport. An Angiocanthos plant was fed with ^{13}C labelled glucose. The C1-^{13}C bound protons (coloured) overlayed to a proton image of the system cross-section C1 α-Glucose (93 ppm (^{13}C), 5.42 ppm (^{1}H)), system field strength 9.4 T, cyclic J cross polarization method in-plane resolution of ^{13}C image: 156 x 156 µm², slice thickness: 5 mm total scan time 4:00 h.

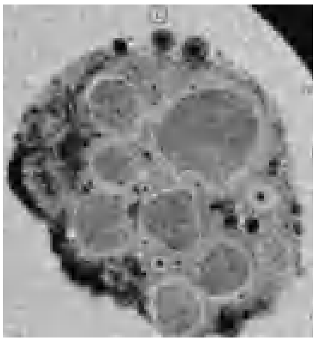
Courtesy of M. Wenzler, Max Planck Institut für chemische Ökologie, Jena, Germany

Research Possibilities

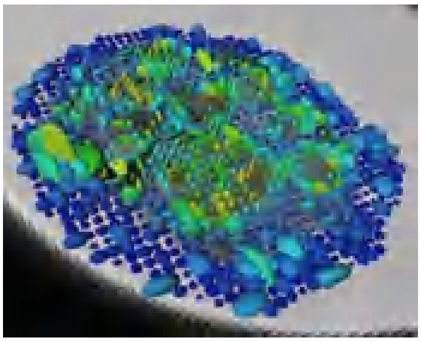
- Investigations on plants, insects and other small animals, embryos, or histological tissue samples.
- Studies of porous and inhomogeneous objects at intermediate field strengths with minimum susceptibility distortions and highest sensitivity.
- Studies of fast dynamic processes.
- Microliter spectroscopy.

Diffusion Tensor Imaging on excised human nerve cord

Excised human nerve cord



Multi Gradient Echo Imaging, TR 600 ms, TE 5 ms, 10 µm x 10 µm x 120 µm



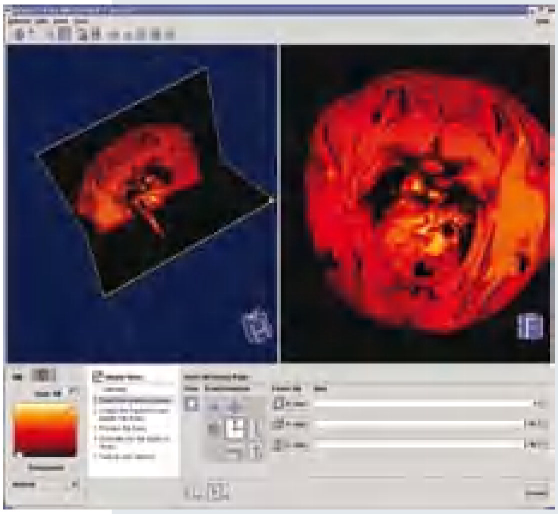
Diffusion Tensor Imaging, TR 2.7 s, TE 14.34 ms, δ 2.5 ms, Δ 7.0 ms, 31 µm x 31 µm x 1 mm, effectiv B values 1310 s/mm² - 1704 s/mm², Diffusion Tensor Visualization by AVIZO FIRE

Sample provided by
Dr. Joerg Raczkowsky, Karlsruhe Institute of Technology, Institute for Process Control and Robotics, Karlsruhe, Germany
Dr. med. Ralph König, Neurochirurgische Klinik University Ulm, BKH Günzburg, Germany

ParaVision 5.1

Ultimate MR-Acquisition and Processing in Preclinical Research and Life Science

ParaVision® is Bruker's software package for multi-dimensional MRI/MRS data acquisition, reconstruction, analysis and visualization for its BioSpec®, PharmaScan® and Micro-imaging product lines. It offers an intuitive routine user interface and cutting-edge techniques for animal MR imaging and spectroscopy - including a rich palette of powerful image evaluation and visualization tools.

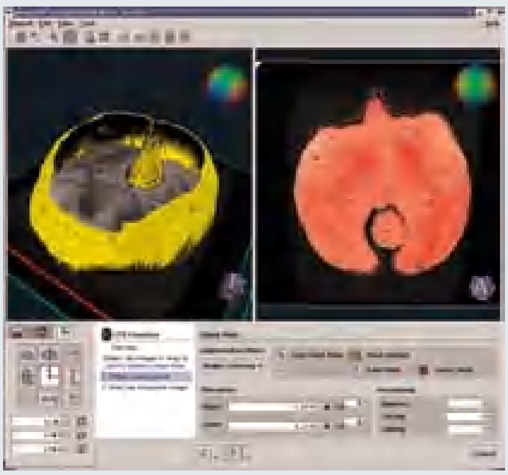


New Reconstruction and Processing Features

- Push-button GRAPPA reconstruction
- Sum of squares and phase-sensitive phased-array reconstruction
- Phased-array spectroscopy reconstruction
- Partial Fourier reconstruction
- EPI reconstruction with efficient ghost suppression
- Navigator techniques to reduce motion artifacts in EPI and SPIRAL
- 2D and 3D region growing
- Display and analysis of time-course data with the fitting tool "ISA"
- Frame-selective loading of image sequences for display, e.g. either timecourse frames or slices for a multi-slice movie dataset
- 3D visualization with surface rendering
- Image mask inversion

Product Description

- Intuitive routine workflow
- Application-oriented, ready-to-use protocols
- Self-acting, method-specific scanner adjustments
- Automatic instrumentation recognition
- Parallel imaging option for all suitable acquisition techniques with automatic generation of composed images/ spectra
- Half-Fourier (Partial-Fourier) encoding
- Real-time display of acquired and reconstructed data
- Data archiving including DICOM export
- Development environment with powerful tools for rapid prototyping of user-defined experiments and professional method implementation



Beyond Standard BioSpecs

Vertical BioSpec

The vertical BioSpec® has been engineered for MR research investigations of non-human primates. It enables specifically fMRI studies on monkeys as they are particularly receptive to behavioral conditioning while sitting in upright position. The vertical BioSpecs are offered with two different magnet types operating at 4.7 T and 7 T which both have a high-magnetic field stability and excellent homogeneity. The actively shielded gradient coil with integrated shims is especially designed for a vertically oriented magnet.

FLASH imaging on BioSpec 170/25, in-plane resolution: (80 × 80) μm^2

Courtesy: D. Le Bihan , NeuroSpin, Paris, France

Ultra-High Field MRI

Bruker is offering up to 17 T horizontal MRI BioSpec, enabling high-resolution *in vivo* preclinical MRI on small animals at a microscopic scale. The magnet with a bore size of 25 cm is based on Bruker's UltraStabilized™ subcooling technology offering excellent field homogeneity and stability.

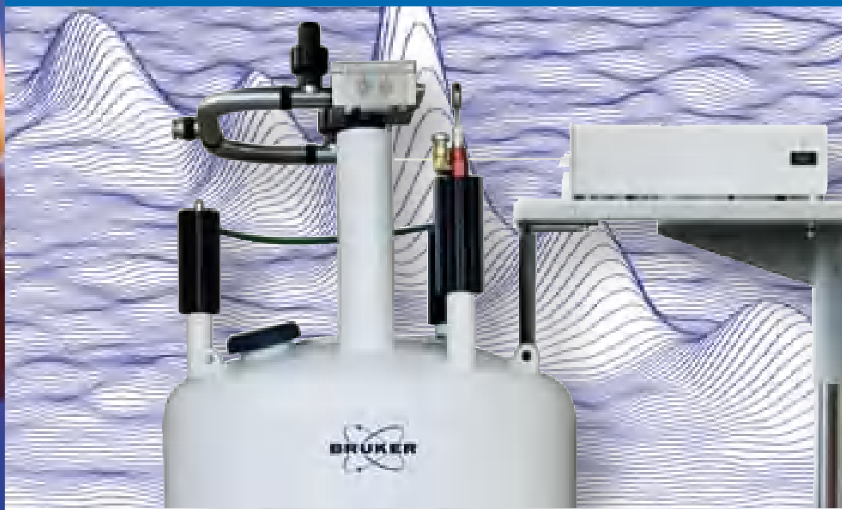
A new BGA-S™ gradient coil with unsurpassed specifications regarding gradient field strength, gradient slew rate, and gradient duty cycle provides best MRI performance.

These innovations will push the current limits of animal MR imaging towards higher spatial and spectral resolution, enabling new applications in the field of molecular imaging and preclinical research.

Content:

EPR Products





Electron Paramagnetic Resonance

Solutions for Life Science and Analytical Research

Innovation with Integrity

EPR

ELEXSYS-II E780

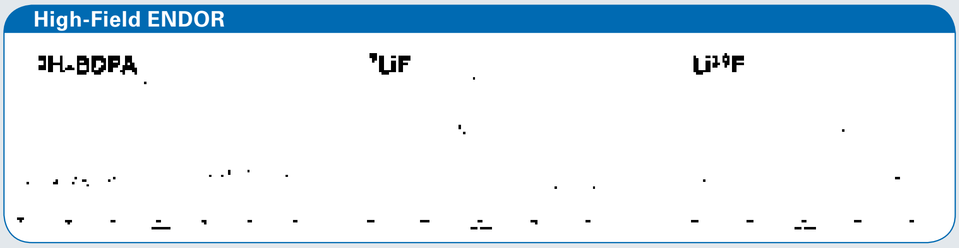
The World's First Commercial mm-wave 263 GHz EPR Spectrometer

Bruker has pioneered the world's first commercial mm-wave 263 GHzEPR spectrometer, ELEXSYS-II E780, representing a first step for Bruker's EPR division into quasi-optical microwave technology. It incorporates a unique cryo-free superconducting magnet that can be ramped up to 12 T and is combined with new probe technology for optimum sensitivity, even on large samples up to 5 mm. Based on the well-proven Bruker ELEXSYS concept it provides multiple turn-key operation modes including,

CW-, Pulse-EPR, ENDOR and ELDOR, thus enabling research groups for the first time, to routinely use very high-frequency EPR technology.

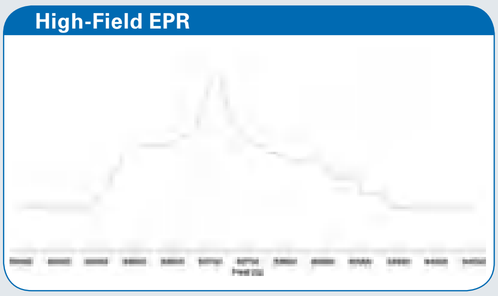
Features

- Enables mm-wave very high-field EPR at 263 GHz
- Quasi optical front-end featuring reflection and induction detection
- Cryogen free superconducting EPR magnet incorporating 12 T main coil and 0.2 T high-resolution sweep coil
- Multiple turn-key operation modes including CW-, Pulse-EPR, ENDOR and ELDOR
- High-sensitivity single mode resonator
- Non-resonant probe for samples up to 5 mm
- Variable sample temperature from 4 to 300 K
- Safe and robust operation
- Runs routine software package Xepr

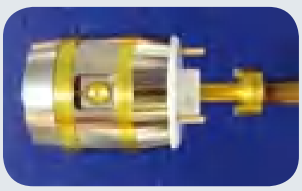


Multinuclear pulsed ENDOR

Non-Resonant Probe



TEMPOL Echo Detected Field Swept at 50K



Single Mode Resonator TE011

ELEXSYS-II E500 CW-EPR

Redefining research level EPR

Introduced in 1997 the ELEXSYS has become the renowned research platform for modern EPR. Over the years a constant technical evolution has assured to keep track with new emerging demands of the EPR society. The second generation of the pulse devices SpecJet-II and PatternJet-II have been launched in 2006 and just recently DICE-II has become available.

Yet another major development step has now created ELEXSYS-II. The OS9 acquisition server has been replaced and the SuperX microwave bridge has been redesigned with improved specifications. The new multi-purpose signal processing unit (SPU) plays a central role in the expanded capabilities of the ELEXSYS-II, replacing the signal channel, fast digitizer, and rapid scan with a single integrated unit offering unprecedented performance and specifications.

Standard super-high-Q cavity for ELEXSYS Systems

ELEXSYS-II: The only commercial spectrometer series which covers all EPR techniques

	L-Band	*S-Band*	*X-Band*	*K-Band*	*Q-Band*	*W-Band*	*mm-wave*
CW-EPR	•	•	•	•	•	•	•
FT-EPR	•	•	•		•	•	•
CW-ENDOR			•		•		
Pulse-ENDOR			•		•	•	•
Pulse-ELDOR	•	•	•		•	•	•
Imaging	•	•	•				
Saturation recovery	•	•	•		•		
Rapid scan	•	•	•	•	•		
Transient EPR			•		•	•	
ODMR			•		•		

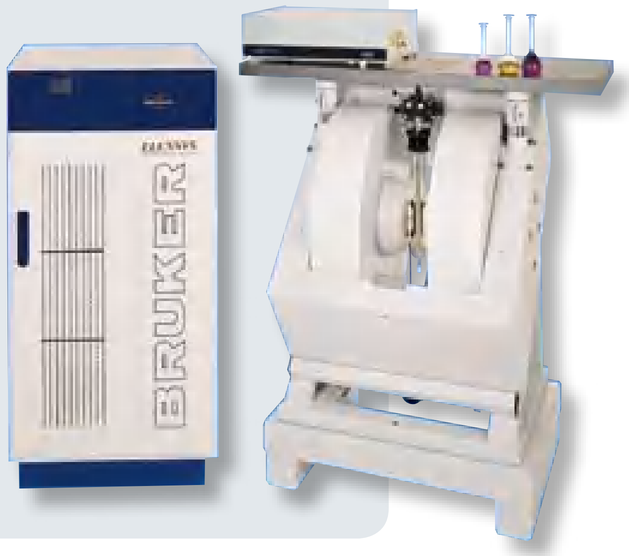
E500 Accessories

- Teslameter
- Field-Frequency lock
- N_2 and Helium VT systems
- automated goniometer
- DICE-II ENDOR system
- microwave frequencies from L- to W-Band
- numerous dedicated probeheads
- large selection of magnet systems

E500 Highlights

- SuperX microwave units of world record sensitivity weak-pitch signal-to-noise of 3000:1
- rapid scan module
- stationary and time resolved experiments
- multi purpose signal processing unit
- reference free spin counting

Cu^{2+} histidine at 20 K and 20 dB power



ELEXSYS-II E580 FT/CW

With the recent introduction of the second generation pulse programmer and transient recorder, PatternJet-II and SpecJet-II, improvements in digital resolution and averaging capabilities have again pushed up the performance level of the E580.

- **zero overhead for 1D phase cycling**
- **zero overhead for 2D blocks**
- **zero overhead for time evolution averaging (e.g. ESEEM)**

PatternJet-II

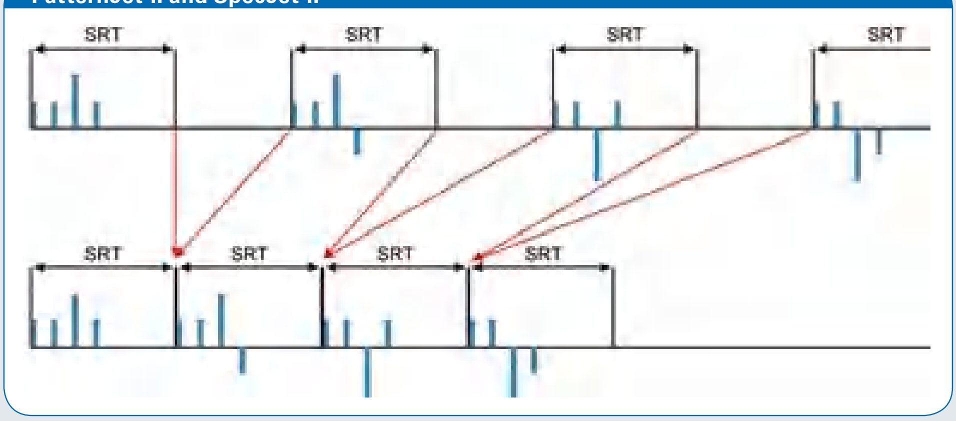
Virtually no experimental limits are imposed by the PatternJet Series of pulse programmers. Designed for the needs of EPR this pulse programmer features a dynamic range of 10^9, i.e. ns resolution over a time scale of up to one second. The well established concept of our first generation PatternJet has been technically enhanced and carried on to the second generation PatternJet-II with a 1 GHz clock.

SpecJet II

With the first generation of SpecJet a dramatic improvement in pulse-EPR sensitivity could be achieved by high-speed signal averaging. The SpecJet-II with 1 GHz sampling rate now further enhances the abilities to capture fast and short lived transient signals. The real time display of the averaged echo/FID can now be toggled between time and FT mode and greatly facilitate spectrometer handling and signal optimization.

The extended memory of PatternJet-II and SpecJet-II allow now overhead free direct phase cycling even for 2D data acquisition. A considerable measuring time saving is achieved with this new feature.

PatternJet-II and SpecJet-II



Direct On-Board Phase Cycling

ELEXSYS-II Imaging Unit

Biomedical research and material science applications by EPR imaging is a rapidly growing field. Bruker's response to this development is the E540 imaging accessory. Based on the proven ELEXSYS architecture, this instrument operates at L- or X-Band and provides the seamless integration of imaging techniques into EPR spectroscopy. The imaging accessory comprises 2D or 3D water cooled gradient coils, power supplies, gradient controller, acquisition and processing software for up to 4D imaging.

Imaging accessory for biomedical application E540GCL

3D gradients with 40 G/cm for imaging in L- and X-Band

E540R36 and E540R23

the 36-mm and 23-mm access L-Band probes for animal research

E540SC

the surface coil L-Band probe for animal research

High-power gradient accessory for X-Band imaging

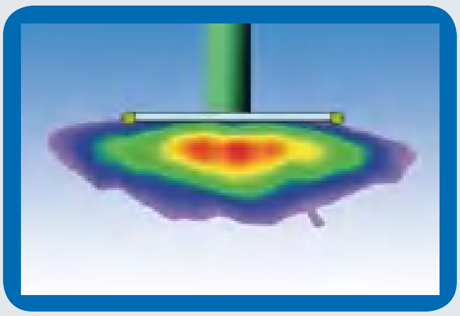
E540GCX2

- 2D gradients with 200 G/cm
- Compatible with ER 073 magnet
- 25 mm air gap
- ER4108TMHS resonator
- Compatible with ER 4112HV Helium system

ER4108TMHS

Image of two DPPH crystals with 25 µm pixel resolution

E540R36



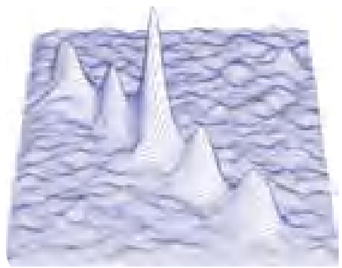
Sensitivity profile of L-Band surface coil

ELEXSYS-II Multi-Frequency and Multi-Resonance Accessories

Multi-frequency EPR is commonly understood in terms of its relation to CW-EPR spectroscopy. Bruker's commercial Multi-frequency/Multi-resonance EPR covers both, CW-EPR and FT-EPR as well as Pulse-ENDOR and Pulse-ELDOR at a multitude of microwave frequencies. Thanks to the ELEXSYS platform design and the advantageous intermediate frequency (IF) concept, every ELEXSYS spectrometer can be expanded for state-of-the-art multi-frequency experiments; now and in the future. All features of the X-Band CW/FT microwave bridge are transferred to the new operating frequency. For each frequency band a dedicated probe provides a maximum of sensitivity and ease of use.

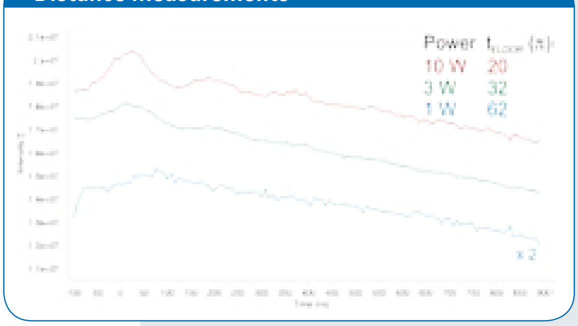
Flexline Pulse-ENDOR Resonator EN4118X-MD4

ESEEM Application



S-Band HYSCORE of BDPA

Distance Measurements



Q-Band 4 Pulse - DEER

High-Frequency/High-Field EPR and ENDOR at 94 GHz

The ELEXSYS family of EPR spectrometers includes two W-band systems, the E600 and E680. The former is optimized for CW-EPR experiments at 94 GHz, while the E680 operates in both CW and FT-mode. The instrument is equipped with a 6 T super conduction magnet featuring an additional high-resolution sweep coil with 2 kG range.

Multi Frequency Options

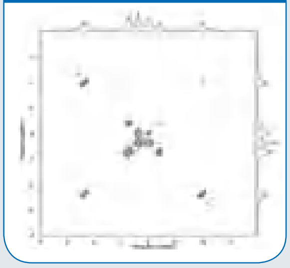
The Bruker IF Concept allows to add a second or third microwave frequency to the X-band E 580 instrument. These upgrades are available for Q-Band (34 GHz), S-Band (3.4 – 3.8 GHz) and L-Band (0.8 – 1.4 GHz). The upgrade comprises the microwave unit and a dedicated probe for variable temperature operation.

Multi Resonance Options

Electron-Nuclear Double Resonance (ENDOR) accessories are available for the EMX-series in CW mode and for the ELEXSYS series in CW and pulse mode. The frequency range is 1 – 100 MHz for the EMX and 1 – 650 MHz for ELEXSYS. Dedicated ENDOR resonators for CW and pulse operation at variable temperature complete the ENDOR accessory.

Electron-Electron Double Resonance (ELDOR) is a pulse technique and can be added to all pulse spectrometers of the ELEXSYS line. The most popular distance measurement technique is supported by specialized probes of the Flexline series.

Q-Band HYSCORE



^{2}H Q-Band single crystal HYSCORE

EMX*plus*

The foundation of EPR

The EMXplus is the next generation of Bruker's successful EMX spectrometer line, well-known for its premium performance in CW-EPR research. The design of the EMXplus reflects its dedication to the heart of the matter: rapid and high-quality data.

Simply power-on the EMXplus and start your EPR journey. Following self-validation procedures, the EMXplus is ready to use via Bruker's WIN-ACQ software.

The Perfect Duo I

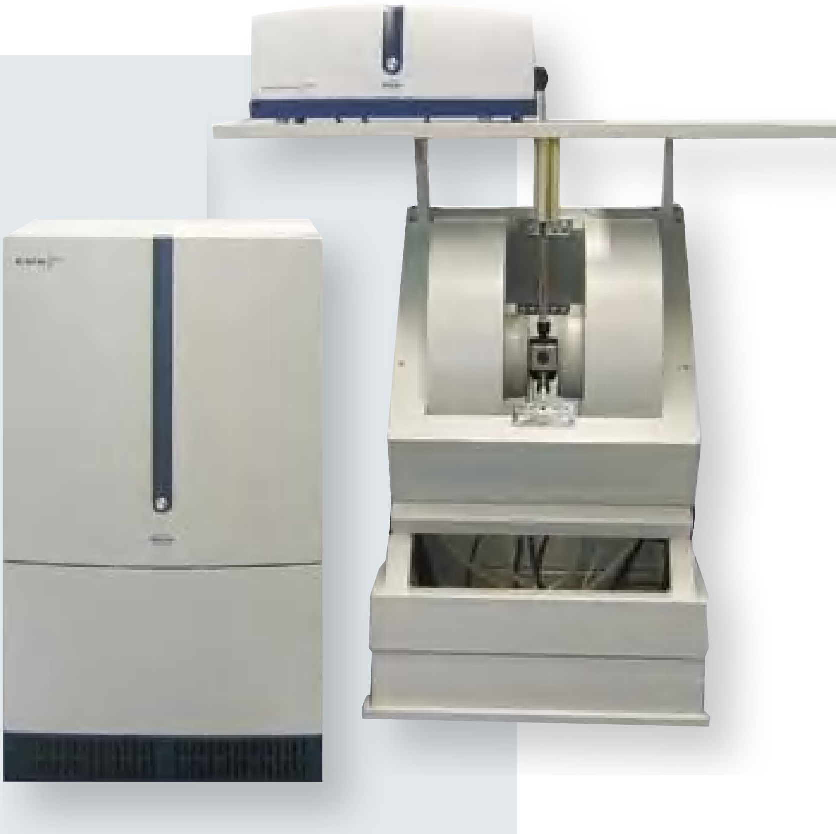
The Signal Channel and Field Controller work together seamlessly to provide practically unlimited resolution on both axes: field and signal intensity.

The Perfect Duo II

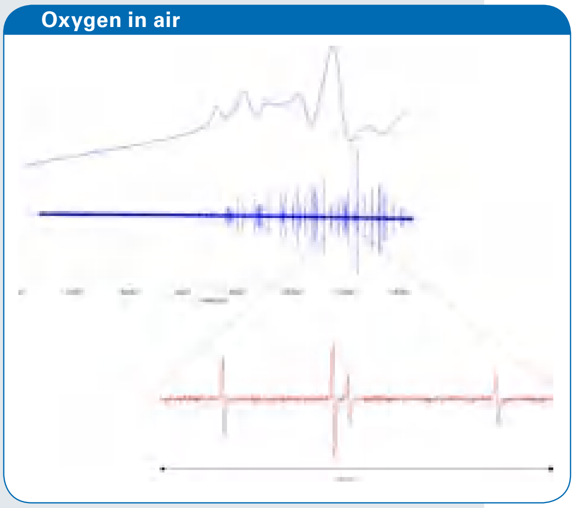
The EMXplus Signal Channel now offers two detection channels in one. Simultaneous quadrature and 1st & 2nd harmonic detection schemes are just a mouse click away.

Accessories & Options

- The PremiumX microwave package for enhanced sensitivity
- The Variable Temperature Controller can be incorporated into the EMXplus console
- The ER036TM Teslameter ensures precise g-factor determination in combination with the integrated microwave counter
- The EMX-ENDOR package allows CW-ENDOR experiments to be performed on EMXplus Systems
- The full range of microwave frequencies from L- to Q-Band



Ultra-high-resolution over large sweep

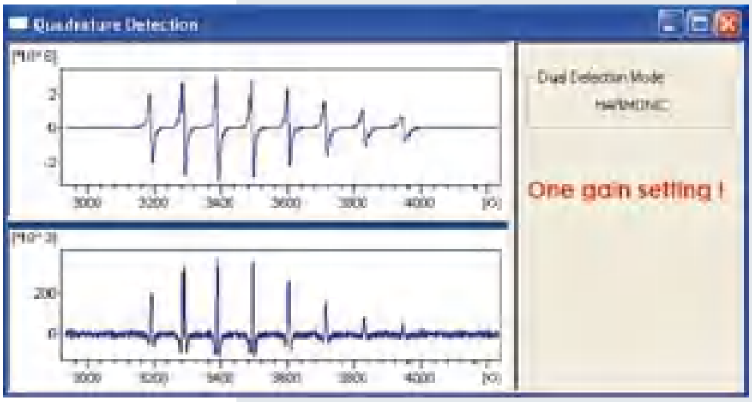


The spectra show oxygen in air at ambient pressure (top) and reduced pressure (middle) measured at Q-Band. A sweep range of 14 kG was recorded with 180000 points, resulting in a resolution of 80 mG, sufficient for the line width of 300 mG at reduced pressure.

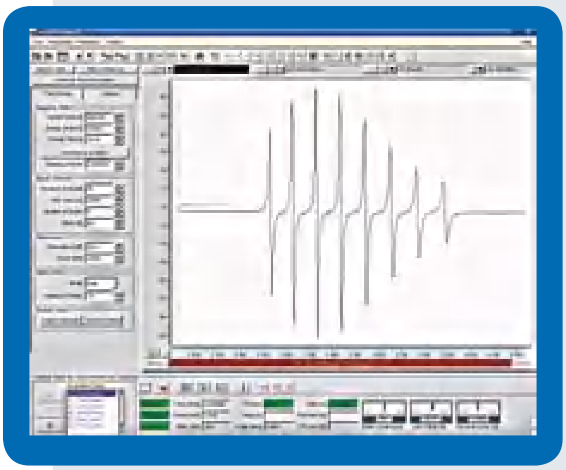
EMX*micro*

The EMXmicro completes the EMX family and features an electronics cabinet with the footprint of a PC tower. The instruments micro cabinet can be combined with all electromagnets and microwave bridges from L- to Q-Band.

The standard software of the EMX series for data acquisition and processing is provided by WinACQ and WinEPR.



Dual-mode simultaneous detection of 1st and 2nd harmonic EPR spectrum of a vanadyl sample



Xenon user interface

Xenon

This new software package is an option for the EMXmicro/plus series. It features a Linux® front end PC with a new graphical user interface integrating acquisition and processing in an user friendly environment. Xenon features numerous novel tools for data acquisition and processing, e.g. the direct spin counting method without reference sample.

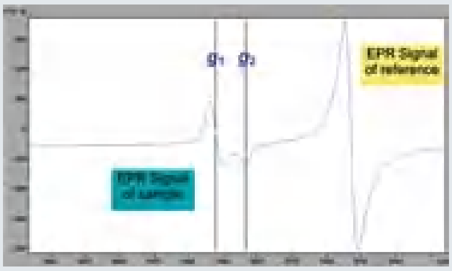
e-scan

Bruker's e-scan product line of table-top EPR (ESR) readers offer dedicated and tailored turn-key systems for specific Quality Control applications as well as systems for medical and pharmaceutical R&D applications of Reactive Oxygen Species (ROS) and Reactive Nitrogen Species (RNS). All e-scan systems have been designed for and have proven rock-solid in 24/7 operation with the best possible price-performance ratio available today.

A few example application fields for e-scan:

- Irradiation Dosimetry with Alanine Dosimeters (ISO/ASTM method)
- Food Irradiation Control (EU standard methods)
- Beer Shelf Life: flavour stability and antioxidant stability (patented application)
- Biomedical EPR research: ROS and RNS detection and quantification

e-scan food control inserts (left) and the cavity template. (right).

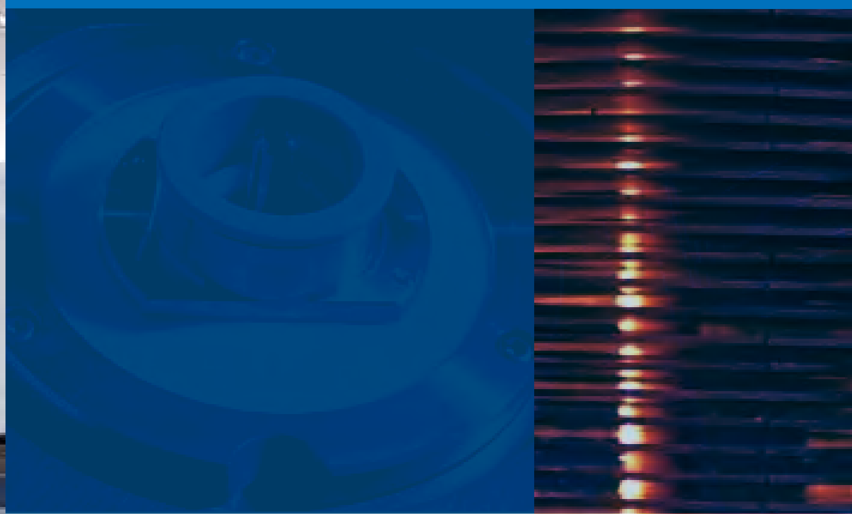


EPR spectrum of an irradiated chicken bone recorded with the e-scan Food Analyzer.

Content:

GC/LC/MS-Products

For research use only.
Not for use in diagnostic procedures.



GC/LC and MS-Systems

Research and Analytical System Solutions

Innovation with Integrity

GC/LC/MS-Systems

MALDI-TOF Mass Spectrometers

Bruker's FLEX Series of MALDI based mass spectrometers are industry leaders whose performance level can be easily matched to almost any application need.

Composed of three increasingly powerful systems; microflex™, autoflex speed™ and ultrafleXtreme™, these flexible, powerful, and reliable systems can deliver answers for a wide range of applications such as the MALDI Biotyper solution used in clinical biology to identify microorganisms through characteristic peak patterns; their unique molecular fingerprints.

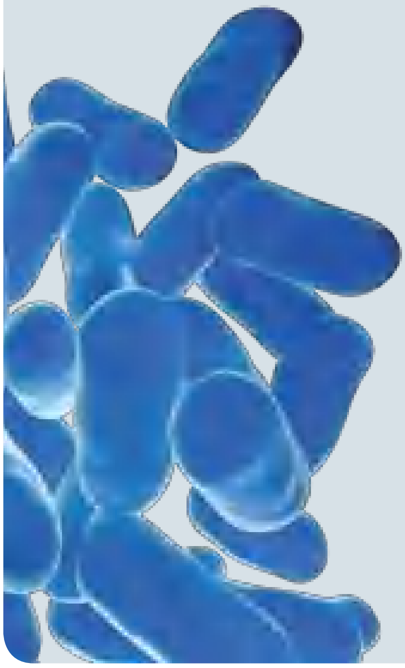
Capable of utilizing a number of intuitive software packages, the FLEX Series brings the power of MALDI mass spectrometry to any level of user.

ultrafleXtreme

The pinnacle of the FLEX series, the ultrafleXtreme is built to deliver the highest levels of performance in sensitivity, resolution, and mass accuracy for a MALDI instrument.

Highly flexible, the ultrafleXtreme is especially effective in proteomics, molecular imaging and protein analysis settings as it can utilize the full power of patented 1 kHz smartbeam™ laser technology.

Other cutting edge MALDI technology enhancements such as PAN™ resolution for broad mass range measurements and LIFT™ technology to enhance sensitivity, allow the use of the ultrafleXtreme in top-down or bottom-up protein analysis utilizing gel or LC-based workflows. Outstanding in both quanitiative and qualitative applications, the ultrafleXtreme represents the ultimate in MALDI instrument design and performance capabilities.



ultrafleXtreme

microflex LT

microflex LT/microflex

The entry level member of the FLEX product family is the microflex series. However, there's nothing minimal about the performance of these instruments. Designed to be compact, affordable, and easy-to-use, the microflex series packs a lot of power into its excellent design. Fully capable of providing answers to a wide range of analytical challenges with its 15k resolution, the microflex series can be scaled to fit many needs with either linear or reflectron based options. The innovative microflex series can bring the value and performance of MALDI mass spectrometry to any laboratory, including those who may have thought mass spectrometry was out of reach.

autoflex speed

The workhorse of the FLEX Series, the autoflex speed has a number of exciting hardware options to deliver a very powerful, yet easy to master, platform for many MALDI based applications. Incorporating proprietary smartbeam 1kHz laser technology, the autoflex speed delivers unrivalled speed, sensitivity, and resolution for an instrument in its class. Hardware options include either MALDI-TOF or MALDI TOF/TOF configurations. The autoflex speed can also be equipped with a number of specially designed software packages to create a customized instrument for key applications like molecular imaging or protein sequencing and analysis.

autoflex speed

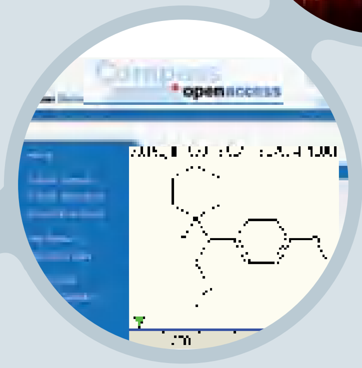
LC-MS

Bruker's novel amaZon ion trap family of mass spectrometers utilize a unique spherical ion trap architecture that delivers exceptional performance for many analytical tasks.
This design, in combination with an ingenious detector and dual ion funnel transfer technology, offers:

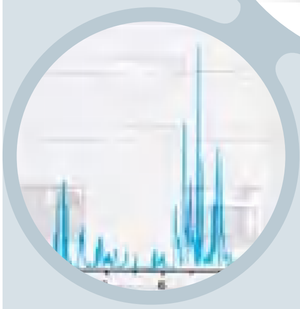
- dramatically improved sensitivity (by a factor of 10x),
- speed up to 52,000 μ/sec
- dynamic range over 4 orders of magnitude
- mass resolution up to 30,000
- high-mass range of 50-3,000 m/z

ProteinScape 3.0 bioinformatics database system

amaZon ion trap for analytical power and utility



Fully automated screening for toxins/drugs based on MS/MS library search. Push button solution in open access environment.



Support of all widely used HPLC, CapLC, nanoLC, and UHPLC systems

Ion Trap Mass Spectrometers

The amaZon series of ion traps are equipped with instantaneous polarity switching capabilities for dealing with a variety of analytes. Capable of MS^n analysis, ion traps provide the analytical power necessary for very complex samples.

Some members of the amaZon ion trap instrument family can utilize ancillary chemistries and techniques ETD (Electron Transfer Dissociation) and PTR (Proton Transfer Reaction) to aid in the analysis of proteins and their posttranslational modifications. Bruker's family of ion trap instruments is represented by the amaZon speed, amaZon speed ETD, and amaZon SL instruments.

amaZon SL

A solid, robust, high value platform for fast LC/MS^n applications, the amaZon SL is designed to increase productivity for routine analyses such as chemistry support, quality and process control, and other small molecule analysis applications.

The amaZon SL comes equipped with the SmartLine software suite which provides particularly quick and easy access to analytical workflows to help generate reliable results. The amaZon SL is designed for reliable 24/7 operation, even in an open access environment.

amaZon speed

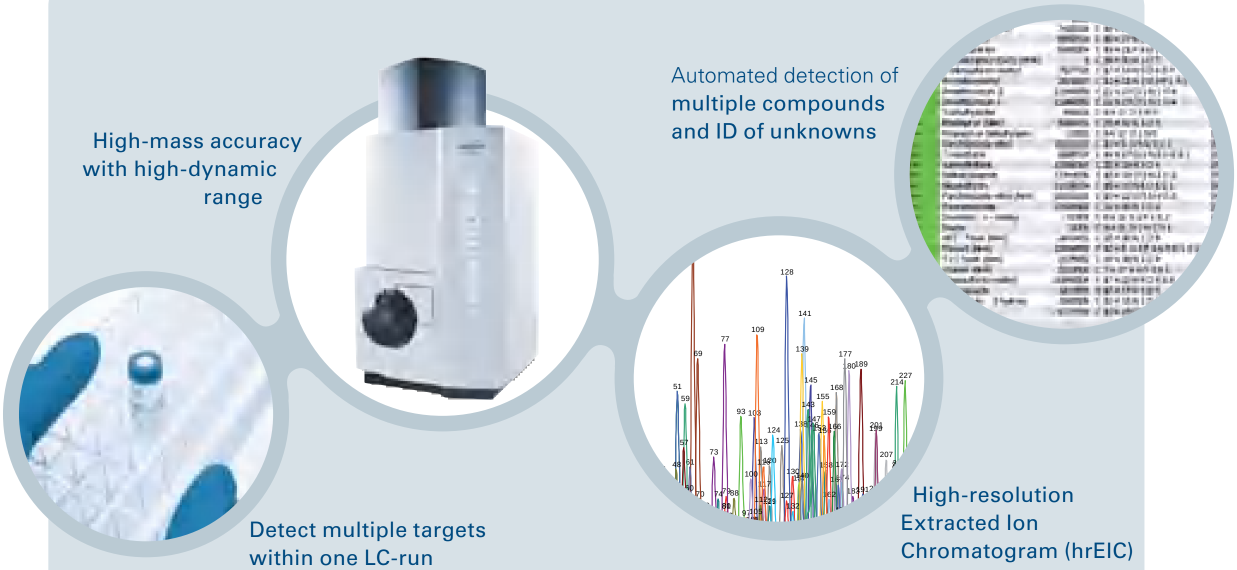
Representing the latest developments in ion trap technology, the amaZon speed provides most of the capabilities of the amaZon family. With greatly enhanced sensitivity, MS/MS speed and „Zero-Delay Alternating" polarity switching, the amaZon speed is an excellent choice for the analysis of complex samples when more in depth and detailed analysis of molecular structure is needed. Supported by spectral MS^n libraries, the amaZon speed is the ultimate mass spectrometer for MS/MS based multi-compound screening.

amaZon speed ETD

Designed especially for the analysis of proteins and their post-translational modifications (phosphorylation, glycosylation, etc.), the amaZon speed ETD is the latest generation instrument for the analysis of post translational modifications (PTMs) and proteomics. Incorporating ETD and PTR molecular fragmentation technologies, the amaZon speed ETD system provides extremely valuable information about the location and nature of various PTMs, as well as very useful de novo sequencing power leading e.g. to full coverage of the protein N- and C-terminal sequence.

amaZon speed ETD

LC-MS



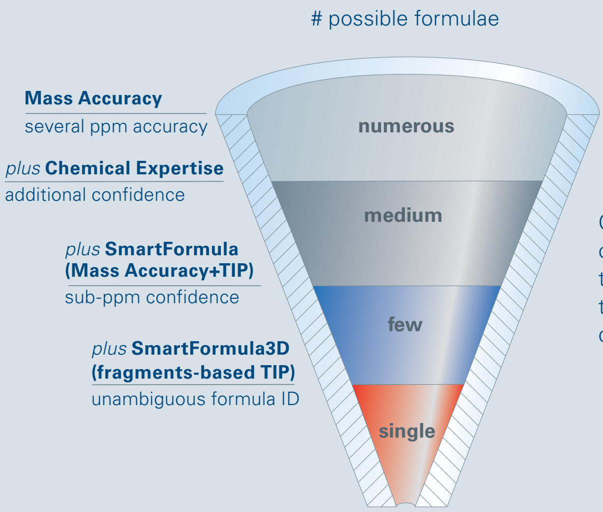
Bruker's TOF and quadrupole TOF mass spectrometers feature some of the very latest developments in o-TOF technology to provide maximum confidence for accurate mass molecular formula determination.

Capable of delivering hyper-accurate results, Bruker's o-TOF platforms combine numerous hardware innovations with unique software packages that deliver industry leading sensitivity, 5 orders of magnitude dynamic range, ppm or better mass accuracy and up to 60,000 resolution for the analysis of small molecules and many types of biomolecules.

micrOTOF focus II

An outstanding high-performance system, the micrOTOF II benefits from years of experience in LCMS design, and features an excellent combination of resolution and mass accuracy to deliver outstanding results.

The perfect choice for straight forward molecular formula determination of small molecules, proteins, or small molecule metabolites, the micrOTOF II can help solve some very tough analytical challenges.



Confident determination of the elemental composition of a LC-MS peak. Isotopic pattern information - SmartFormula3D - reduces the number of molecular formula candidates dramatically.

micrOTOF-Q II

A high-performance hybrid mass spectrometry system, the micrOTOF-Q II combines the very latest in ESI-qTOF technology in MS and MS/MS modes to enable very high levels of confidence in many applications.

Whether used with direct infusion or with UHPLC, Fast Chromatography, or other separation techniques, the micrOTOF-Q II delivers some of the best results in molecular formula determination available on the market today. When exact molecular formula determination is the goal, the micrOTOF-Q II is the answer.

micrOTOF-Q II

UHR-TOF Mass Spectrometers

maXis impact

maXis impact

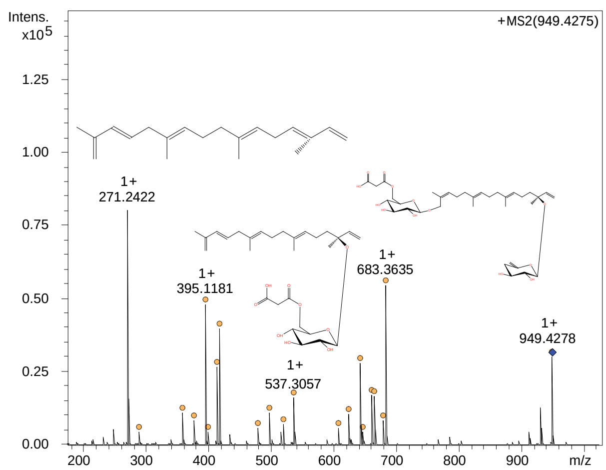
There is no need to make compromises in mass spectrometry anymore. The maXis impact™ sets a new technology standard where industry leading performance values are all simultaneously available in a single acquisition at full sensitivity.

Powered by a series of patented technology innovations, the maXis impact simply provides the very best results without compromise in a cost effective, benchtop format.

maXis 4G

The maXis 4G, with Full Sensitivity Resolution, continues to advance the performance level and capabilities of this revolutionary series of instruments. With significant enhancements in mass accuracy and resolution, and unparalleled sensitivity and speed, the maXis 4G offers the confidence to measure and identify small molecules, proteins and intact large molecules, such as antibodies, with unprecedented levels of certainty in both MS and MS/MS modes.

Compound identification and structure confirmation



FTMS Mass Spectrometers

solariX ®

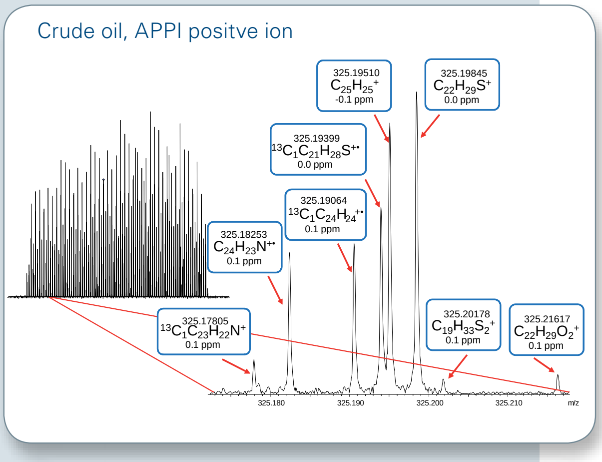
solariX, the next-generation hybrid Qq-FTMS, is an easy to use, high-performing system that is equipped to address the most challenging proteomics and complex mixture applications.

The broad-band, ultrahigh-resolving power (> 1,000,000 @ m/z 400, 7 T) is essential for tackling complex mixtures, especially those that are not amenable to on-line separation techniques such as; hydrocarbon related analysis ("petroleomics"), environmental analysis, and metabolomics.

For applications that require high-performance LC-MS or LC-MS/MS, the solariX is ideally suited. New functionality provides more resolution when it is needed most and with optional, faster acquisitions for MS/MS data.

Added top-down versatility is provided with fully enabled Electron Transfer Dissociation (ETD). This exciting new technique, combined with FTMS performance, is superb for the comprehensive analysis of proteins and peptides and their subtle, posttranslational modifications.

The solariX can be configured with Dual ESI/MALDI (based on advanced ion funnel technology) and a range of API source options (APCI, GC-APCI, APPI). Low maintenance, refrigerated magnets are standard with solariX and can be configured with one of several magnetic field options (7T, 9.4T, 12T and 15T).



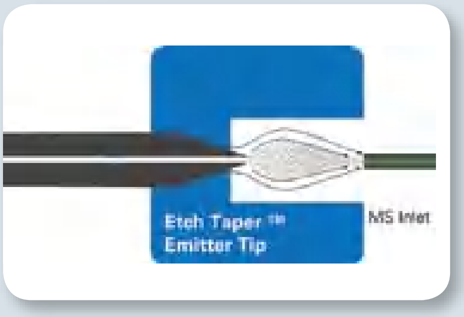
solariX

Ion Sources

CaptiveSpray

Nanoflow LC-MS in daily laboratory work is still one of the bigger challenges in proteomics. The Bruker CaptiveSpray source is a revolutionary ion source with a patented design that provides easier operation than even standard electro spray. CaptiveSpray delivers nanospray sensitivity, resists plugging, and provides reproducible uninterrupted flow for even the most complex proteomics samples.

The CaptiveSpray can be used also at low µL flow rates to allow the use of larger ID columns. It fits all current Bruker ESI-MS systems.



Vortex around spray concentrates and focuses spray into the MS source

CaptiveSpray LC-MS source

DirectProbe DIP: Instant answers from solid samples with APCI or APPI

The DirectProbe (DIP) add-on for the Bruker APCI II and APPI II ion source allows direct analysis of liquid and solid samples without tedious sample preparation. In routine organic synthesis analyses, it simplifies identification and characterization of chemical reaction products without compromising sensitivity.

DirectProbe

Software & Application Directed Solutions

Compass & Bioinformatics

Bruker software solutions are designed to provide maximum information with minimal effort. Highly intuitive and extremely user friendly, our software solutions are all designed and delivered with the user and their application in mind:

- Compass™: Bruker's unified software environment for intuitive mass spectrometric instrument control and data processing.
- Compass OpenAccess™: Automated walk-up LC/MS chemical formula generation
- Compass Security Pack
- ProteinScape™ – the bioinformatics platform for ID and quantitation
- BioTools™:Interactive protein analysis
- flexImaging™: Comprehensive and powerful MALDI Imaging
- MALDI Biotyper™: The easy software for microbial ID
- GenoTools™: Software solution for the analysis of genomics data
- MetaboliteTools™: Identification and confirmation of metabolites
- ProfileAnalysis™: Comprehensive statistical evaluation of LC-MS data
- TargetAnalysis™: Unambigous molecular formula identification
- PolyTools™: Interpretation of MALDI polymer spectra

Your choice of HPLC

Bruker supports all major vendor HPLC systems for LC-MS applications.
Our flexible software plug-in architecture allows for fully integrated HPLC support and method development. Other HPLC systems can be integrated with a simple contact closure.

HPLC Vendors supported by Bruker Compass with full software plug-ins are: Dionex, Waters, Agilent, Hitachi, Thermo/Proxeon, CTC/PAL Autosamplers, Shimadzu and Eksigent.

Applications-Software

Bruker offers dedicated software packages and solutions for various application areas:

- **Life Science Research and Clinical Application Solutions**
  PRIME: Proteomics through Integrated MALDI and ESI
  MALDI Molecular Imaging
  Identification of Microorganisms
  Lipidomics
  Nucleic Acid Analysis
  LC-MS based Metabolomics
  Metabolite Profiling with LC-MS and NMR
- **Pharmaceutical and Applied Analytical Application Solutions Identification of Unknowns**
  Pesticide, Toxin, and Pollutant Screening
  Drug Metabolite Identification
  Open Access Chemistry Support
  Petroleomics
  Polymer Analysis

ICP-MS

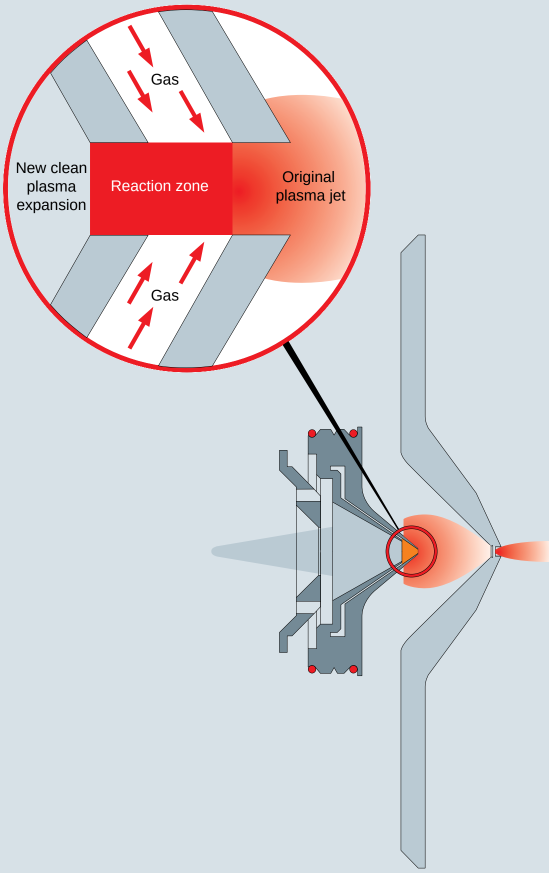
Bruker innovation, making ICP-MS easier

If you've ever wished that ICP-MS could be simpler, wish no more. The aurora M90 makes light work of it. No matter what your requirements, with a Bruker ICP-MS, you can tackle any application with ease.

The aurora M90 delivers industry leading detection limit performance. Collision/reaction interface (CRI) technology makes setup of complex cell systems a thing of the past. Simply turn on the gas flow to remove interferences. It's that simple.

Let Bruker Quantum work for you

If your goal is to spend less time creating methods and optimizing conditions, and more time running samples, Bruker's Quantum software delivers. Enjoy accurate results in less time with an intuitive yet flexible user interface that takes the hard work out of ICP-MS.



The CRI injects helium (He) and hydrogen (H_2) collision and reaction gasses directly into the plasma as it passes through the orifice of the skimmer cone. This innovative approach suppresses interferences before the analytes are extracted into the ion optics.

aurora M90

Gas Chromatograph Mass Spectrometers

Scion SQ

Bruker's long traditions of innovation and product reliability have combined to create a new industry standard for gas chromatography single quadrupole mass detection – the SCION SQ. By understanding, and then designing to exceed the most critical performance and reliability needs of GC users, Bruker has delivered a system that is especially for, and all about, the ultimate success of the GC user. The SCION SQ detector is designed to meet many important user specified requirements – reliable performance, ease of use and simple maintenance-all in a small instrument footprint that saves valuable bench space.

Scion TQ

The SCION triple quadrupole (TQ) detector is a comprehensive solution for your most demanding gas chromatography applications. It delivers unrivalled bench-space savings, the result of an innovative 'lens-free', elliptical ion-path design that delivers ultra-high sensitivity and chemical noise reduction – performance you would expect when innovation merges with a legacy of reliability.

scion TQ

Gas Chromatographs

Laboratory gas chromatography systems (GC)

The 400 Series consists of two gas chromatographs and an associated range of analyzers and solutions designed for leading applications. These systems allow chemists and engineers to employ standard methods and/or high-quality trace sample analysis, in the petrochemical, agrochemical and environmental industries.

The 450-GC is a highly affordable and powerful analytical instrument that offers robust operation in an easy-to-use package. The system gives users a broad choice of injectors, detectors, switching and sampling valves up to three channels. The high-resolution color touch screen is intuitive and supports local languages. The Bruker 430-GC offers the same outstanding performance as the 450-GC but in a compact, single channel package that occupies about half the bench space of conventional multi-channel GC.

450-GC + CP-8400

Gas Chromatograph Accessories

Injector, Autosampler and Detector Options

Bruker 400-GC Series GC Accessories represent significant value and upgrade instrument performance and efficiency. The 400-GC Series has been designed to allow the incorporation of a wide range of options to expand the performance and enhance the capabilities of the system. These options include:

Autosamplers

The CP-8400 range of AutoSamplers combines unattended system operation features with high-throughput and sample capacity, virtually without sample carry over. These systems can be configured for:

- High-sample throughput with dual and duplicate modes of injection
- Automatic access to two injectors with a single tower to double analysis output
- Liquid, ambient headspace, and SPME sampling
- Pre-programmed injection modes to minimize method development time and guesswork

The SHS-40 Automated Headspace Sampler is designed to take maximum advantage of the productivity and cost benefits of Headspace – Gas Chromatography (HS-GC). Powerful and robust, the SHS-40 enhances the capabilities of any analytical laboratory to comprehensively and efficiently measure volatile organic compounds (VOCs) from a variety of sources.

- Fully Automated: Minimal Operator Intervention
- Highly Productive: Simplified Method Development
- Easily Integrated: Ready to Use with Bruker GC and GC-MS Systems
- Flexible: Use for Direct Analysis or "React and Analyze" Chemistries
- Robust: Very Low Maintenance Requirements and guesswork

Combi PAL/CTC

For Laboratories requiring even greater sample throughput or more extensive sample preparation automation options, Bruker offers the Combi PAL/CTC.

Gas Chromatograph Consumables

Bruker's commitment to providing the very best in analytical systems extends beyond providing great instrumentation. In most cases, a good analytical system encompasses instrument, software and high-quality consumables. Bruker applies the same demanding standards of quality to its wide range of GC consumables. From septa, ferrules and injector liners to vials and tools, we have the parts and consumables to complete the analytical solution. Our latest and newly launched comprehensive range of GC columns and Super Clean^{TM} Gas filters shows our commitment to providing the latest and best in technology.

A Selection of GC Columns to Meet Your Needs

Bruker GC columns span a broad range of column diameters, stationary phases, and capillary column materials: Fused Silica (FS) and Inert Steel (IS). Ideal for either routine or research type analyses. Bruker GC column offerings bridge across many important applications and include a number of offerings such as:

- Standard WCOT (Wall Coated Open Tubular)
- Small internal diameter
- Solid stationary phase PLOT (Porous Layer Open Tubular)
- Inert steel micro-packed an packed colums

Super Clean™ Gas Filters

Innovative design with product reliability has produced an extensive range of gas filters configured for the most demanding applications. Bruker Gas Purification Systems have the range to satisfy your needs from individual to combination filters, from Ultra purity combined with Ultra capacity, to all in one solution kits. Innovative features designed into the product yield extensive benefits to the user.

- Ultra-high capacity for long life, less change and improved productivity
- High-purity output ensures 99.9999% Pure Gas
- "Quick connect" fittings for easy, leak-tight filter changes
- Glass internals prevent diffusion; plastic externally for safety
- Easy-to-read indicators for planned maintenance and improved up-time

MALDI Biotyper Consumables

Added Convenience Enhances Assay Productivity

To make it easier and cost effective to routinely use the MALDI Biotyper, Bruker offers a number of kits and accessories designed and tested to maximize the performance and productivity of the MALDI Biotyper system.

Bacterial Test Standard

The Bacterial Test Standard is a typical *E.coli* extract, containing some additional proteins which can be used for instrument mass calibration as well as a performance verification standard.

HCCA (alpha-Cyano-4-hydroxycinnamic acid) Matrix

The matrix is supplied as solid and should be rehydrated using organic solvent ‘OS’ solution. Typically 1 ul of matrix is added to each sample prior to analysis.

MALDI Sepsityper™ Kit 50

The MALDI Sepsityper Kit is for the analysis of microorganisms from positive blood cultures. The process typically takes no longer than 20 minutes.

MALDI Biotyper Targets

Bruker offers the widest range of MALDI targets available, including reusable and disposable targets with and without barcodes.

Reusable Polished Steel Targets - 96 Positions

This most common and widely used Assay target provides excellent performance for all sample types. These targets can be cleaned and re-used literally thousands of times.

Disposable Biotargets - 48 Positions

The disposable Biotargets are supplied individually bar-coded in boxes of 25 each. Each target contains 48 positions and 5 additional calibration positions. The silicon-based Biotarget can be re-analyzed as often as necessary until all 48 spots have been used.

BigAnchorChip™ Targets

The Bruker patented BigAnchorChip targets are especially designed for handling liquid samples. They are specially prepared with a hydrophobic coating which surrounds hydrophilic sample positions.

Content:

CBRN Products

CBRNE

Chemical, Biological, Radiological, Nuclear and Explosives Detection

Innovation with Integrity

CBRNE Detection

Prepared for a changing World of Threats

Bruker Daltonics – since 30 years a trusted manufacturer of CBRNE detection equipment – offers and constantly improves their sophisticated CBRNE product line and this way tries to help counter chemical, biological, radiological, nuclear and explosive threats. State-of-the-art technology, ruggedized design and modular accessories allow flexible and extensive applications.

The complete product line for CBRNE detection

CBRNE technology has always been the core competence of Bruker Daltonics. We were the first supplier who covered the complete range of chemical, biological and nuclear detection. Bruker is specialized in development, engineering and manufacturing of military hardened and easy-to-use analytical systems and is ISO9001 certified. The product line supports all possible use cases for the detection of various threats.

Systems for CBRNE Defence

Bruker solutions includes personal and handheld point detectors as well as detection systems for reconnaissance vehicles, battle tanks, shipboardor stationary use. Bruker provides sophisticated CBRNE software solutions for instrument control and systems integration.

Safety & Security

Bruker equipment supports not only the response teams from Fire Departments, Police, Customs and Civil Defence in addition, major events such as summits, concerts, parades and sporting events can be targets for terrorist attacks. Harbours, ports, airports and public buildings are also sensitive to the release of hazardous agents. Bruker detection equipment can be integrated into monitoring systems for these critical infrastructures using combinations of both static and mobile detection systems.

Bruker offers a wide product range including

- Mobile Mass Spectrometers
- Ion Mobility Spectrometers
- Stand-off detectors based on passiv FTIR
- FTIR ATR ruggedized Spectrometers
- Radiation Meters
- Neutron Induced Gamma Spectrometry
- Generic Biological Aerosol detectors
- PCR and ELISA based biological identifiers

Bruker CBRNE equipment is in service with armed and naval forces, civil defence and first responders worldwide. Our instruments are part of major reconnaissance vehicles in the world like the CBRNRS Fox or the Korean K-216 and part of the chemical and/or radiological detection system of ships like the German frigate F123/124 and the MEKO 100. The systems are also an integrated part of the protection system within German and Swedish Coast Guard ships.

Chemical Hazardous Agent Detection

RAID series

A series of chemical monitors, covering multiple tasks including monitoring of collective protection facilities and CBRN filter stations, as well as handheld or personal point detection for protection purposes. Based on the well-established Ion Mobility Spectrometry, all important CWA and Toxic Industrial Chemicals (TIC) can be monitored in realtime.

The µRAID; the first personal chemical agent detector based on Brukers field proven IMS technology; provides unmatched overall sensitivity in this class of instruments. The expandable TIC capability is organised into five libraries that can be tailored with the relevant instrument dataset to meet your specific requirement.

The innovative RAID-XP combines chemical and radiological detection into one system.

The RAID-M 100 is distinguished by its flexible and easy use for portable and hand-held deployment. It is designed for fast and sensitiv detection and identification of CWA and TICs.

The RAID-S2 is specially designed for long term operations. The instrument can either be operated separately, or several instruments can be connected in networks.

RAID-AFM can be deployed for stationary chemical detection in vulnerable areas such as air and sea ports and public facilities such as sports arenas. The innovations of a non-radioactive ionisation source or a gamma radiation detector option makes it the most flexible stationary solution in the world.

RAID-AFM (NC version)

Integrated RAID-S2 sensors

RAID-XP

µRAID

RAID-M 100

Chemical & Radiation Detection

Stand-off detector for atmospheric pollutants

A compact, mobile infrared detector for real-time remote sensing of chemical agent clouds. All known CWA and important Toxic Industrial Chemicals (TICs) can be automatically identified and monitored over a distance of several kilometres – either stationary or on the move. Latest developments have resulted in linking two ore more RAPID's to setup a triangulation system and allowing tomographic reconstruction of chemical clouds.

Monitoring of public events with stand off detection of chemical clouds.

RAPID

MM2

The MM2 sets a milestone in GC/MS technology with a volume of 43 litres and a weight of 35 kg. Equipped with improved Gas Chromatography/ Mass Spectrometry technique it represents the new generation of quadrupole mass spectrometers. The MM2 is optimized for long-term chemical reconnaissance in various armoured vehicles, as well as for mobile chemical agent inspection and detection missions.

MM2

SVG 2

Hand-held, hardened radiation detector, based on state-of-the-art semiconductor technology. Equipped with integrated sensors for gamma and neutron radiation detection, and an external $\alpha/\beta/\gamma$-probe.

SVG2

Biological Detection

VeroTect a generic detector for biological aerosol uses the combination of fluorescence and aerosol shape and size sensors for the detection of biological aerosol clouds.

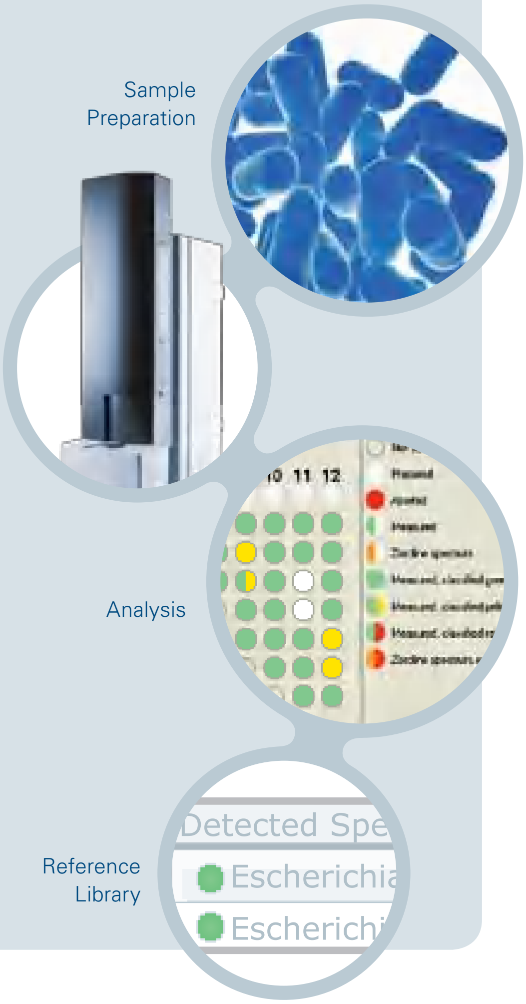
pTD is a fully automated ELISA based on-site identifier for toxins using the unique electrical biochip technology in a disposable consumable.

M-BL, the mobile biological lab, offers PCR based detection of pathogens with integrated sample preparation in a ruggedized, easy to use format.

VeroTect

pTD

M-BL



MALDI Biotyper

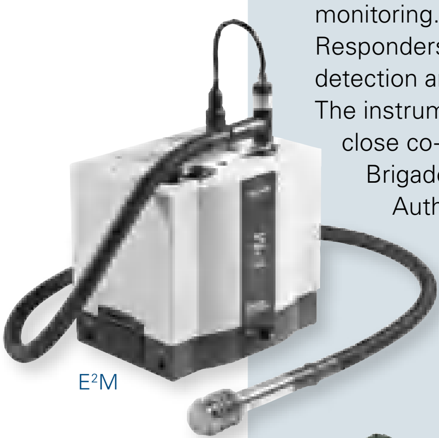
The MALDI Biotyper allows fast and reliable identification and classification of microorganisms, such as bacteria, archaea, yeasts or fungi. There is neither a need for any prior PCR amplification, nor for the usage of selective growth media nor for any other pre-assumptions, which may influence the outcome of the analysis. The MALDI Biotyper software identifies microorganisms by the species-specific signal patterns contained in their respective molecular profiles.

For research use only. Not for use in diagnostic procedures.

First Responders & Environmental Protection

E^{2}M

The enhanced environmental mass spectrometer E^{2}M is a mobile, compact and lightweight GC/MS system for fast, reliable onsite identification of organic chemicals from any medium (soil, water, air) within 20 minutes via complementary sampling techniques. Typical fields of application are environmental protection, mobile on-site analysis and event monitoring. The E^{2}M fully supports First Responders and Homeland Security detection and identification activities. The instrument has been developed in close co-operation with German Fire Brigades and Disaster Management Authorities.



E^{2}M

RAID-M 100

DE-tector

RAID-M 100

The RAID-M 100 is outside the military used by civil defense forces, first responders and fire fighters to challenge the threat of toxic industrial compounds.

DE-tector

The third generation of IMS based trace detectors is formed with the Drugs Explosive detector of Bruker. The twin-tube IMS design means no split of the sample before it will be ionised with a non radioactive source. CHIRP and IMS-Profiler gives unmatched sensitivity and false alarm suppression.

Mobile-IR in use

Mobile-IR

Most chemical substances have their own infrared signature; just like a fingerprint. With the new Mobile-IR, it is easy to identify unknown chemicals in just a few seconds, by comparing the fingerprint of the substance with included data bases. Unlike other portable instruments, the Bruker Mobile-IR is designed to be used under adverse conditions. It is waterproof to IP67 standards, and offers a high degree of shock protection.

NIGAS

NIGAS

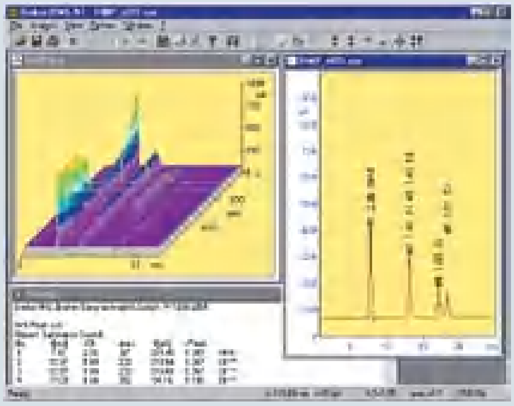
System for automated, non-invasive detection of chemical warfare agents in ammunition, using Neutron Activation Analysis with a non-radioactive source. The instrument is transportable and can be used even under field conditions.

Software Solutions

System Integration

Our CBRNE detectors can be easily integrated into any kind of CBRN detection platform. The systems are deployed under various environmental conditions. Ruggedised design and sophisticated accessories allow flexible and extensive applications for the detection of hazardous compounds by mounting the systems on vehicles, ships, helicopters, shelters or by hand-held use under field conditions. Sophisticated software supports the integration of our CBRNE detectors. Bruker has over thirty years of experience in systems integration.

RAPID Control software with alarm window, on-line video picture and function keys for fast access to all system operation parameters.



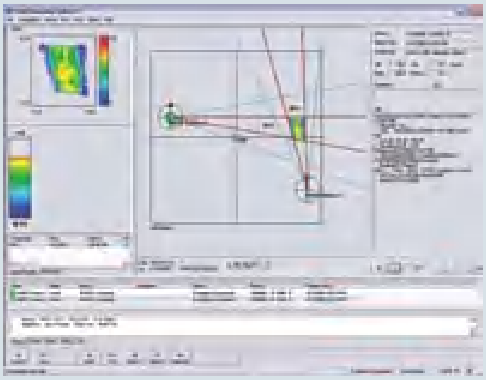
Bruker XIMS software family are control and data systems for the Bruker Ion Mobility Spectrometers (IMS). They are assigned for instrument control of the detector, for data acquisition and analysis of two- and three-dimensional IMS spectra on a PC.

Analytical support tool XIMS NT

Bruker offers analytical software packages to support the use of their hand-held and personal detection equipment in order to get deeper insight into the threat situation and to tailor the instruments to customer specific needs.

CPS – Cloud positioning system

CPS collects data from two ore more RAPID systems. It offers triangulation and tomographic reconstruction of detected chemical clouds.



Content:

Optical Vibrational Spectroscopy

Optical Vibrational Spectroscopy

Advanced Research and QA/QC Solutions
Based on Infrared and Raman Spectroscopy

IR/NIR/FT-RAMAN

Innovation with Integrity

FT-IR

Bruker Optics has the industry's most comprehensive FT-IR product-line; from the very compact FT-IR spectrometer to the world's highest resolution.

ALPHA with ATR Sampling Module

ALPHA

About the size of a lab book, the very compact FT-IR spectrometer Alpha will play a big part in your daily routine. Plug & play set-up, easy-to-use software, combined with QuickSnap™ sampling modules assure powerful and reliable FT-IR analysis you expect from Bruker. Alpha is ideal for academic teaching and routine industrial applications.

Mobile-IR

Mobile-IR Portable FT-IR

Material Identification Anywhere! Bruker's Mobile-IR is a self-contained, rugged portable FT-IR spectrometer that provides benchtop performance, wider spectral coverage and higher spectral resolution. It's ideal for crime scene investigation, environmental monitoring and hazardous material identification applications.

TENSOR 27 FT-IR Spectrometer

TENSOR Series

If you need a FT-IR spectrometer that can rapidly identify, quantify and verify your routine samples, Tensor is the right tool for your laboratory. It combines the highest performance and outstanding flexibility with ease of use. A full line of sample compartment and external FT-IR accessories enable it to be used for various challenging applications.

Most Comprehensive FT-IR Product Line; from the Smallest in Size to the Highest in Resolution

VERTEX Series

The VERTEX Series is built on a fully upgradeable optics platform that is designed with the utmost flexibility in mind. Multiple input and exit ports allows users to connect various external and internal accessories and components to customize the instrument based on applications. Vertex spectrometers share a wide range of features and utilize patented RockSolid™ and Ultra-Scan™ interferometer designs.

VERTEX 70 FT-IR Spectrometer

Vacuum Optics

With the vacuum models, peak sensitivity in the mid-, near- and far IR regions is obtained without the fear of masking very weak spectral features by air water vapor absorptions.For the VERTEX 80v vacuum spectrometer a unique option is available: The new automatic beamsplitter exchange unit BMS-c for automatic spectral range selection without the need of venting the spectrometer vacuum optics.

VERTEX 80v Vacuum FT-IR Spectrometer

IFS 125 Series

The IFS 125 is built for performance with each instrument component optimized to approach the theoretical limit of sensitivity. It offers the highest spectral resolution available down to 0,001 cm^{-1}, a resolving power of up to 10^6 and the wide wavelength range from 5 cm^{-1} in the far-IR/THz to 50,000 cm^{-1} in the UV. The mobile IFS 125/M is dedicated to gas phase absorption studies, requently applicable to atmospheric research.

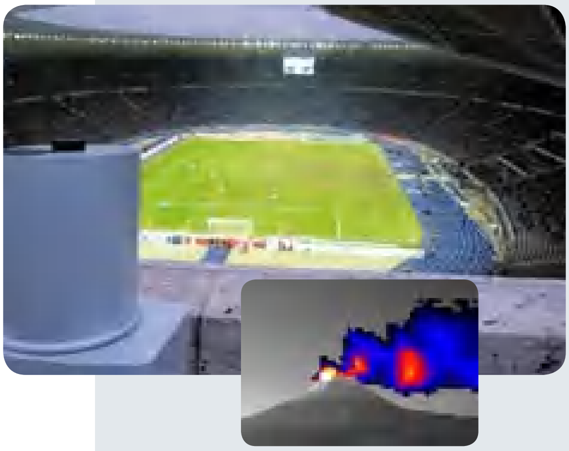
IFS 125HR

Remote Sensing

HI 90
Hyperspectral Imaging
System

HI 90 Hyperspectral Imaging System

Atmospheric, environmental research, volcanology, industrial surveillance and homeland security outline the wide range of applications of the new HI 90, Hyperspectral Imaging system. The HI 90 is ideally suited for real-time identification, quantification, and visualization of gas clouds. In addition, algorithms based on a combination of image processing and spectral analysis can be applied allowing for the system to be used in a range of imaging applications for solids and liquids.



SIGIS 2
Scanning Imaging Remote
Sensing System

SIGIS 2 Scanning Imaging Remote Sensing System

SIGIS 2 is a remote sensing system that allows identification, quantification, and visualization of gas clouds from long distances. The system maps a predefined area and results of the analysis are visualized by the video image, overlaid by a chemical image.

The SIGIS 2 can be used for environmental applications, atmospheric research, volcanology, and industrial facility surveillance. The SIGIS 2 is currently being deployed by emergency response forces in Austria, Denmark, Germany, and Italy.

EM 27 Remote Sensing FT-IR

EM 27 Remote Sensing FT-IR

Providing laboratory grade performance, the EM27 remote sensing FT-IR can easily be deployed in the field for various environmental air monitoring applications. Emissions from smoke stacks and waste disposals, hazardous emissions from chemical accidents can be observed with an operating range of up to several kilometers.

FT-Raman

The Raman effect is based on the inelastic scattering of monochromatic light with matter. As the complementary vibrational technique of IR spectroscopy Raman provides detailed molecular structure information.

Bruker Optics added FT-Raman capabilities to its product line shortly after the technique was first reported in late 1980s.

MultiRam

The MultiRAM is a stand-alone high-performance FT-Raman spectrometer. It has a large sample compartment to utilize an extensive range of pre-aligned sampling accessories.

MultiRam Stand-Alone FT-Raman

RAM II FT-Raman Module

Designed as an add-on module, Bruker's RAM II is a dual-channel FT-Raman unit that can be coupled to the VERTEX series multi range FT-IR spectrometers.

RAM II coupled to VERTEX 70 FT-IR

Low Temperature Silicon QC

The CryoSAS is a high-sensitivity system for the quality control of solar and electronic grade silicon material according to international standards. Although sample cooling to very low temperatures is required, the fully automated system is easy to operate, and does not require cryogenic liquids.

CryoSAS

FT-IR & Raman Microscopy

Sample visualization is the important first step in the analysis of almost any sample. Infrared and Raman spectroscopy are versatile and powerful analytical techniques that can be applied to micro-analysis. Bruker's FT-IR and Raman microscopes are built on state-of-the-art optical microscopy platforms that provide optimal sample visualization and also feature chemical imaging and mapping. Areas of applications include material science, forensics, mineralogy, failure analysis, content uniformity, sample homogeneity and quality control.

HYPERION 2000
coupled to TENSOR 27

SENTERRA Raman Microscope

HYPERION Series

Featuring full automation, infrared chemical imaging, crystal-clear sample viewing and a wide variety of IR and visible objectives, the HYPERION™ series provide everything needed to conduct the most demanding micro-analysis easily and efficiently. It can be coupled to TENSOR and VERTEX Series FT-IR Spectrometers.

The HYPERION™ 3000 represents the pinnacle of infrared microspectroscopy, incorporating state-of-the-art Focal Plane Array detectors for the most demanding infrared imaging applications. High-resolution chemical images can be collected in a matter of seconds.

SENTERRA

Bruker's SENTERRA™ is an easy to use Raman microscope that combines many novel features such as the patented SureCal permanent calibration, fluorescence rejection and on-demand confocal depth profiling. With a wide variety of excitation lasers providing high-spectral resolution, it is ready to challenge any microanalysis research applications.

RamanScopeIII

When sample fluorescence is a problem, FT-Raman microscopy with near infrared 1064 nm excitation is frequently the only solution. RamanScopeIII can be coupled to Bruker's FT-Raman spectrometers, and be combined with the SENTERRA™ dispersive Raman microscope as a hybrid solution.

FT-NIR

Discover the flexibility of Near Infrared Spectroscopy

NIR spectroscopy has largely replaced a number of wet chemical analysis methods. With the fiber optics and the integrating sphere sampling techniques, NIR spectroscopy does not require any sampling preparation. It is a fast and precise tool for the nondestructive analysis of liquids, solids and paste-like materials, saving costs by reducing time and reagent use.

TANGO

Faster, simpler, more secure - with TANGO your NIR analysis speeds up. The new TANGO from Bruker Optics has exactly what users require of an FT-NIR spectrometer suitable for food analysis: Robustness, high precision and straightforward operator guidance. The proven FT-NIR technology by Bruker was combined with an easy-to-use touch screen operation and a small footprint, perfect for those laboratories with limited space.

TANGO

MPA Multi Purpose Analyzer

Bruker's dedicated FT-NIR spectrometer MPA offers everything you need for the analysis of liquids, solids, powders and tablets. Selection of the different measurement accessories is completely software controlled and validated, without the need for any manual exchange.

MPA

MATRIX Series

The award winning MATRIX™ series process-ready FT-NIR Spectrometers incorporate state-of-the-art optics for outstanding sensitivity and stability. Available configurations include fiber optic coupling up-to 6 probes and integrating sphere.

MATRIX-I

Process Analytical Technologies

Today, many companies are not only striving to manufacture high-quality products, but also increase production efficiency by installing the analytical systems directly into their production plants. This improves process verifiability and gives the company the opportunity to optimize material use.

Bruker's technology base includes FT-IR, FT-NIR, dispersive NIR and Raman Spectroscopy. This allows us to offer a choice of analytical solutions based on applications or sampling points. The robust design of our spectrometers enable use in tough conditions in the production plant.

MATRIX-F duplex FT-NIR Spectrometer

MATRIX-F FT-NIR Spectrometers

The award winning MATRIX-F FT-NIR spectrometers allow the direct measurement in process reactors and pipelines, leading to a better understanding and control of the process. Its innovative design provides consistent high-quality results, less downtime and direct method transfer. ATEX **II 2G EEx p II T6** version available.

MATRIX-MF FT-IR Reaction Monitoring

MATRIX-MF FT-IR Spectrometers

Utilizing the information rich mid-IR region for use in both laboratory and process environments, the MATRIX-MF is a process ready spectrometer that is ideal for real-time monitoring and analysis of chemical and biological reactions. ATEX **II 2G Ex px II T6** version available.

MATRIX-F ex for hazardous environments

FT-NIR measurement heads and probes

A wide range of fiber optic probes is available for the MATRIX-F series – from immersion probes for liquids to reflection probes for solid materials. For contactless measurements, Bruker offers emission heads which collect the reflected light from the sample, also as fully ATEX certified version for gas and dust Ex-zones.

OPUS – Spectroscopy Software

"All-in-one" IR and Raman spectroscopy software consisting of a suite of software packages that cover both standard and specialized applications.

Features

- Running under Windows XP and Windows 7 operating system
- Supporting the demands of 21 CFR Part 11"Electronic Records, Electronic Signatures"
- Manipulating multiple spectra and 3D files at the same time
- Providing comprehensive spectra processing routines e.g. integration and baseline correction
- Providing easy to use, intuitive application-specific software interfaces for complete routine analysis tasks

Display and Processing of 3D files

OPUS-VIDEO

- Wizard guides the operator through the full procedure of data acquisition
- Powerful autofocus functionality
- Acquisition of spectral data up to 10 Giga Byte

OPUS-3D

- IR and Raman images may be combined with high-resolution visible images and shown as 2D contour plots or as 3D topography plots
- Multiple data analysis functions from simple "Integration" to "Cluster Analysis", "Spectral Similarity" or "Factorization"

Quantitative Analysis and Quality Control, Process Control

QUANT

- PLS tools box to setup quantitative analytical methods
- Automatic method development and optimization
- Automatic outlier recognition and removal

IDENTIFICATION

- Complete tools box of algorithms for substance identifications
- PCA including visualization by 2D and 3D score plots
- Hierarchical multi-level libraries to separate even similar substances
- Validation with independent samples: positive and negative samples

PROCESS and REACTION MONITORING

- Real time evaluation using multivariate methods and on-line trending
- Communication protocols to DCS (OPC, Profibus DP, Modbus, 4-20 mA, …)
- Interactive setup of integration methods during reaction monitoring
- Automatic end point detection based on PCA or integration results

Content:

Advanced Analytical Solutions

XRD, XRF, SC-XRD, AFM, OIM
MA, OES, CS/ONH

X-RAY, AFM, OES

Innovation with Integrity

X-ray Powder Diffraction

Table-top, automated, or scientific workshorse instrumentation

D8 ADVANCE

X-ray diffraction expands analytical capabilities down to the nanometer range. Our highly accurate, reliable and fast diffraction solutions are accompanied by an intuitive and clearly laid-out user interface, easy handling, and individual data presentation, as well as perfect integration and communication capabilities.

Applications

- Crystalline phase identification
- Crystalline phase quantification
- % crystallinity
- Crystallite size determination
- Crystal structure analysis
- Texture and preferred orientation
- Microstrain
- Residual stress
- Depth profiling
- Polymorph screening
- High temperature
- Low temperature
- Humidity
- Phase transition
- Nanoparticles

D4 ENDEAVOR

D2 PHASER

... with TURBO X-RAY SOURCE

Thin Film X-ray Diffraction

Quick-Change Artists without Limits

With the capabilities provided by the D8 DISCOVER, laboratory X-ray diffraction enters new frontiers in the nano-world and materials research so that synchrotron measurement campaigns become obsolete in many cases.

... for XRD^2

Applications

- Crystalline phase identification
- Crystalline phase quantification
- % crystallinity
- Crystallite size determination
- Crystal structure analysis
- Texture and preferred orientation
- Microstrain and relaxation
- Residual stress
- Layer thickness
- Layer roughness
- Lattice parameter
- Chemical composition
- Lateral structures
- Defects
- Depth profiling
- Real space mapping
- Microdiffraction
- Polymorph screening
- High and low temperature
- Humidity
- Phase transition
- Nanoparticles

D8 DISCOVER

D2 CRYSO

Small Angle X-ray Scattering and X-ray Metrology

Enter the Universe of Nanostructure Analysis

SAXS²

NANOSTAR U

The innovative Small Angle X-ray Scattering System NANOSTAR is the ideal tool for investigating precipitants in bulk materials and macromolecules like protein solutions with a size on the order of 10 to 1000 Ångstrom.

Applications

- Small Angle X-ray Scattering (SAXS)
- Grazing-incidence SAXS (GISAXS)
- Wide Angle X-ray Scattering (WAXS)
- BioSAXS
- Nanography
- Particle size
- Particle size distribution
- Particle shape
- Orientation distribution
- Particle distances
- High and low temperature
- Subsurface structure
- Roughness
- Molecular volume and mass

D8 FABLINE

The D8 FABLINE is the only X-ray metrology instrument with four combined applications:

- High-Resolution X-Ray Diffraction (HRXRD)
- X-ray Reflectivity (XRR)
- Micro X-ray Fluorescence (µXRF)
- Grazing incidence Diffraction (GID)

X-ray Fluorescence Analysis

Defining the World of Elements in Seconds

X-ray fluorescence spectrometry is the most effective way to perform multi-elemental analysis determining concentrations in all forms of samples: solids, powders and liquids. Based on the renowned XFlash® silicon drift detector technology Bruker AXS energy dispersive X-ray fluorescence (EDXRF) systems offer highest analytical precision and stability. The S2 PICOFOX allows the analysis of thin films as well as the analysis of traces down to 0.1 ppb using total reflection X-ray fluorescence (TXRF). The S2 RANGER with TouchControl™ provides you with instant answers for element concentrations from Na to U in unknown samples.

S2 PICOFOX: True Trace Element Analysis by TXRF

Applications

- Fresh water, sea water
- Sewage, sludge
- Pharmaceuticals
- Blood, urine
- Proteins, macromolecules
- Food, dietary supplements
- Wine, beverages
- Nanoparticles
- Washcoats
- Contaminations
- Aerosols
- Thin films

S2 RANGER: EDXRF with TouchControl™

Applications

- Petrochemicals
- Minerals and mining
- Slags
- Cement
- Geology
- Pharmaceuticals
- Metals and alloys
- Soil, sediments and waste

Unrivalled

Excellence in WDXRF: S8 TIGER - S8 LION - S8 DRAGON

Our wavelength dispersive X-ray fluorescence (WDXRF) systems provide you with excellent analytical results for elements from Be to U in your samples. They feature high-accuracy and the best achievable precision for effective process and quality control. They are reliable and robust for all industrial applications, yet flexible and powerful for all non-routine applications in research and development.

Get in touch with the power

S8 TIGER: TouchControl™ and SampleCare™

S8 LION and S8 DRAGON Ultimate Analytical Speed Best Precision

Applications

- Cement
- Ferrous and Non-Ferrous Metals
- Industrial Minerals
- Mining

Applications

- Petrochemicals
- Plastics and polymers
- Cement
- Geology
- Metals and alloys
- Precious metals
- Minerals and mining
- Glass and ceramics
- Chemicals and catalysts
- Pharmaceuticals
- Soil, sediments and waste
- Foods

Micro-X-ray Fluorescence Analysis

M1 and M4 Tabletop Micro-XRF Spectrometer Series

M4 TORNADO

µ-XRF is the method of choice for the elemental analysis of inhomogeneous or irregularly shaped samples as well as small samples or even inclusions. Bruker's M1 and M4 tabletop spectrometers offer maximum versatility for all applications, whether for routine analysis in quality control or for individual setups analyzing special samples.

Applications

- Minerals
- Metals and alloys
- Electronic components (RoHS)
- Particles
- Forensics
- Layers
- Art conservation, archeology

M1 MISTRAL and M1 ORA

Applications

- Jewelry
- Metals and alloys
- Layers (M1 MISTRAL)

ARTAX

Applications

- Non-destructive element analysis in
- Art conservation, archeology and archeometry
- Metals, alloys, sheet metal
- Thin layers

S1 TURBO^{SD}

The Bruker handheld XRF analyzers provide quick and easy non-destructive analysis. The S1 TURBO^{SD} and S1 SORTER enable fast analysis and ID of most alloys. The TRACER III-V and III-SD tube based systems include the Bruker /NASA joint patented vacuum system and high-resolution detector allows for laboratory grade results of elements from Mg to U.

Optical Emission Spectrometry

Spark optical emission spectrometers (S-OES) are the ideal instruments for all types of metals. From pure metal trace analysis to high alloyed grades, spark OES covers the complete range from sub-ppm to percentage levels. All relevant elements can directly be analyzed simultaneously.

Spark spectrometer instruments cover all types of metal applications. Our range of high-end instruments allows our customers to elevate their business into new levels of quality and process control.

Q4 TASMAN / Q2 ION – Benchtop metals analyzer

Q4 TASMAN (CCD)

Applications

- Iron and steel and its alloys
- Aluminium and its alloys
- Copper and its alloys
- Nickel and its alloys
- Cobalt and its alloys
- Magnesium and its alloys
- Lead and its alloys
- Tin and its alloys
- Titanium and its alloys
- Zinc and its alloys

Measuring results

Photomultiplier optic

Channel photomultiplier (CPM)

Pneumatic sample clamp

Metal samples

Q2 ION - Ultra compact Spark-OES

Q8 CORONADO – Analysis automation

Applications

- Process analysis of steels
- Process analysis of cast iron
- Process analysis of aluminum
- Process analysis of copper

Q8 MAGELLAN – Stationary vacuum spectrometer

Applications

Elemental analysis of:

- Iron and steel alloys and its traces
- Nitrogen in steel
- Aluminium alloys and its traces
- Copper alloys and its traces
- Oxygen in copper
- Nickel alloys and its traces
- Cobalt alloys and its traces
- Magnesium alloys and its traces
- Tin alloys and its traces
- Lead alloys and its traces
- Titanium alloys and its traces

Q6 COLUMBUS (CPM)

CS / ONH Analysis in Solids

Our innovative analysis instruments allow automatic and fast determination of Carbon, Sulfur, Oxygen, Nitrogen and Hydrogen in solids. Our instruments provide highly accurate measurement within a short analysis time and are highly reliable and userfriendly.

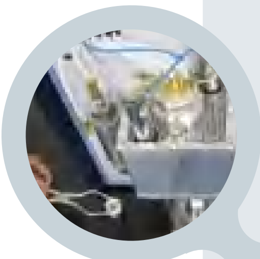
The state-of-the-art technology allows not only the use for quality control but also in the various fields of material development. The "One-4-All" analysis software is clear and simply structured and universal for all instruments.

G4 ICARUS HF

CS analyzer with high-frequency furnace

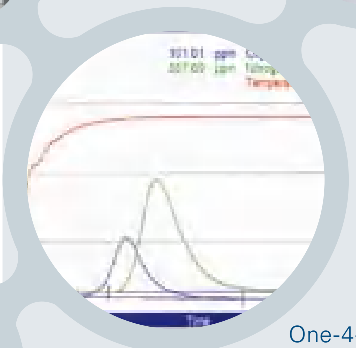
G4 ICARUS TF

CS analyzer with high-temperature tube furnace

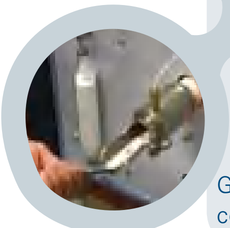


G4 ICARUS HF
ceramic crucible

G4 PHOENIX DH
tube Ø 30 mm



One-4-All
software



G4 ICARUS TF
ceramic boat

Applications

- Iron, steel and alloys
- Aluminum and alloys
- Titanium and alloys
- Zirconium and alloys
- Ores, minerals
- Coal, coke and ash
- Catalysts

G8 GALILEO

O, N, H analyzer

Applications

- Iron, steel and alloys
- Aluminum and alloys
- Copper and alloys
- Titanium and alloys
- Zirconium and alloys
- Ores
- Ceramics
- Minerals

G4 PHOENIX

Determination of diffusible hydrogen

Applications

- Steel
- Aluminum
- Weld material
- Weld seams

Microanalysis (EDS) and Electron Backscatter Diffraction (EBSD)

Accurate, Fast and Easy to Use

The QUANTAX EDS microanalysis system works in conjunction with Scanning Electron Microscopes, as well as Transmission Electron Microscopes (TEM) with the worldwide first SDD series designed for TEM. In addition QUANTAX also provides the option of EBSD analysis with the fully integrated QUANTAX CrystAlign.

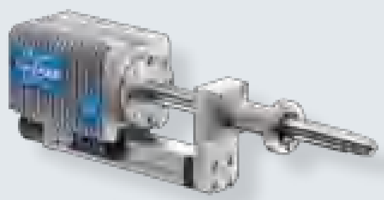
Applications

- Metals and alloys
- Semiconductors
- Layers and coatings
- Minerals
- Glasses
- Nano-materials
- Plastics and organic solids
- Biological samples
- Forensics

QUANTAX 800

e-Flash detector series

XFlash® 5030/5060 T for TEM



XFlash® 5000 series for SEM

Chemical Crystallography

Systems as individual as your research

Single Crystal X-ray diffraction is the method of choice for determining the 3-dimensional structure of any kind of chemical compound. The method provides accurate and precise measurements of molecular dimensions in a way that no other investigative technique can begin to approach.

Our D8 Crystallography Solutions, the D8 QUEST and the D8 VENTURE, are designed to offer highest standards of quality, performance, and reliability. Both feature the new PHOTON 100 detector, a 10x10-cm^2 CMOS active pixel sensor X-ray detector. This new air-cooled detector is combined with the most flexible and precise sample motion available. A wide selection of dedicated X-ray sources including sealed tube, microfocus tube and rotating anodes completes these systems to give you the best structure possible.

The compact D8 QUEST hosts single source and is setup for excellent sample access and reachability.

The D8 VENTURE provides a more spacious enclosure, which also allows for solutions including two X-ray sources. This highly versatile setup enables the scientist to switch between Mo- or Cu-radiation, e.g. for absolute structure determination just with a mouse click.

D8 VENTURE

Applications

- Structure determination of new molecules and minerals
- Absolute structure determination on molybdenum and copper radiation
- Integrated treatment of twinned samples
- Electron charge-density studies by high-anglediffraction
- Structural investigation of high-pressure phases
- Modulated structures
- Diffuse scattering

D8 QUEST

Automated Crystal-Structure Analysis

Walk-up X-ray Structure Determination for Chemists

Bruker AXS' SMART X2S is the first benchtop X-ray crystallography system for fully automated 3D chemical structure determination. It is designed for use by chemists, who need unambiguous answers to their structural questions.

The SMART X2S takes small molecule structure determination to the next level of convenience by automating the previously difficult aspects of X-ray structure determination, from sample loading through data collection all the way to report generation and data archiving. Its compact design, low maintenance, low cost of ownership, easy and intuitive operation through a touch screen graphical interface are truly groundbreaking.

SMART X2S

Features

- Structural information for routine samples when you need it – quickly, reliably and cost effectively
- Crystal-in, Structure-out Automation
- Unambiguous synthesis control for working chemists
- Perfectly complements MS, NMR, FT-IR and Raman

Biological Crystallography

Best in-house data - guaranteed

Modern beamlines are designed to collect data from large numbers of ever smaller crystals, and facilitate data collection from crystals with very large unit cell dimensions. These requirements are similarly driving the development of the D8 Structural Biology for the home-lab solutions in the same direction, where X-ray flux on the crystal is comparable with that achieved at bending magnet beamlines. The high X-ray flux sources are combined with highly precise and easy to use sample stages and rounded up by the new, air-cooled CMOS-based PHOTON 100 detector. The D8 QUEST features a new generation of IµS sealed tube microfocus source, while the more spacious D8 VENTURE hosts the TURBO X-RAY SOURCE (TXS) microfocus rotating anode in addition. Demanding SAD-phasing experiments, measuring even an extremely small anomalous signal can be carried out routinely, while high-throughput crystal screening is more efficient than ever before.

D8 VENTURE with microfocus TXS

Features

- High-intensity microfocus TXS or
- High-brilliance IµS microfocus source
- Large 100-cm^2 PHOTON CMOS-detector
- KAPPA goniostat for easy sample mounting and high-data multiplicity
- Three years of warranty on the IµS and the PHOTON 100
- Completely air-cooled configurations available
- Minimal down-time
- Lowest cost of ownership
- Excellent sample access and sample visibility
- Intuitive PROTEUM2 software package

Atomic Force and Scanning Probe Microscopy

Analyze Nanometer Size Surface Structures within Minutes

Bruker's atomic force microscopes (AFMs) drive the world's leading-edge research in life science, materials science, semiconductor, electrochemistry, and many other applications. The MultiMode® 8 and Dimension® Icon® systems are the latest generation of the world's most widely selected AFMs, offering true atomic resolution for materials research in air or liquids. The BioScope™ Catalyst™ features the most complete integration available between AFMs and high-end inverted and confocal microscopes, and has been specifically engineered to image samples under biologically relevant conditions.

DIMENSION Icon

The N8 range of instruments provides a complete set of solutions for atomic force and scanning probe microscopy (SPM). All systems are based on the unique NANOS SPM head, which uses an interferometric detection principle, enabling optically navigated AFM.

New N8 NEOS, AFM and optical microscope

Automated AFM / AFP Systems

Automated atomic force microscopy and atomic force profiling (AFP) support routine analysis in many different industrial applications, like in-line semiconductor, data storage and MEMS. The systems provide the highest level of measurement performance for a variety of automated and semi-automated metrology applications, performing Atomic Force Profilometry, Critical Dimension AFM scanning, TappingMode™ for roughness metrology, and deep trench AFM scan modes.

InSight 3DAFM

Stylus and Optical Metrology

Optical Interferometric Profilers

White light interferometric (WLI) optical profilers from Bruker are optimized to address a wide range of advanced production QA/QC and R&D precision machining and manufacturing applications within the high-brightness LED, solar, ophthalmic, semiconductor, medical device and academic research markets. Based on ten generations of proprietary technology advances, Bruker's WLI profilers feature patented, higher brightness dual-LED illumination that, when combined with the systems' superior vertical resolution, provide the high-sensitivity and stability necessary for precision, non-contact 3D surface metrology in applications and environments that are challenging for other metrology systems.

CONTOUR GT-K1

NP*FLEX*

Dektak® 150

Stylus Profilers

Bruker's stylus profilers are the culmination of four decades of proprietary stylus profiler technology. These surface profilers provide repeatable, accurate measurements on varied surfaces, from traditional 2D roughness surface characterization and step height measurements to advanced 3D mapping and film stress analyses.

Trademarks

Amix™	trademark of Bruker
Ascend™	trademark of Bruker
Assure™	trademark of Bruker
Avance™	trademark of Bruker
B-ACS™	trademark of Bruker
BGA-S™	trademark of Bruker
BioSpec®	reg. trademark of Bruker
ClinScan®	reg. trademark of Bruker
CMC™	trademark of Bruker
CryoPlatform™	trademark of Bruker
CryoProbe™	trademark of Bruker
DICE™	trademark of Bruker
ELEXSYS™	trademark of Bruker
EMXmicro™	trademark of Bruker
EMXplus™	trademark of Bruker
e-scan™	trademark of Bruker
HyperQuant™	trademark of Bruker
HyperSense™	trademark of Bruker
Icon NMR™	trademark of Bruker
IntraGate™	trademark of Bruker
JuiceScreener™	trademark of Bruker
LINUX®	reg. trademark of Linus Torvalds
Metabolic Profiler™	trademark of Bruker
OS X®	reg. trademark of MacIntosh
ParaVision®	reg. trademark of Bruker
PatternJet™	trademark of Bruker
PharmaScan®	reg. trademark of Bruker
SampleCase™	trademark of Bruker
SampleJet™	trademark of Bruker
SampleTrack™	trademark of Bruker
SampleXpress™	trademark of Bruker
SFG Profiling™	trademark of Bruker
SmartProbe™	trademark of Bruker
SpecJet™	trademark of Bruker
SuperX-FT™	trademark of Bruker
Syngo®	reg. trademark of Siemens
TopSpin™	trademark of Bruker
UltraShield™	trademark of Bruker
UltraStabelized™	trademark of Bruker
USR™	trademark of Bruker
WINDOWS NT®	reg. trademark of Microsoft
WINDOWS 2000®	reg. trademark of Microsoft
Xenon™	trademark of Bruker
amaZon ETD™	trademark of Bruker Daltonik
autoflex speed™	trademark of Bruker Daltonik
BigAnchorChip™	trademark of Bruker Daltonik
BioTools™	trademark of Bruker Daltonik
Biotyper™	trademark of Bruker Daltonik
Compass™	trademark of Bruker Daltonik
Compass OpenAccess™	trademark of Bruker Daltonik
GenoTools™	trademark of Bruker Daltonik
LIFT™	trademark of Bruker Daltonik
maXis impact™	trademark of Bruker Daltonik
MetaboliteTools™	trademark of Bruker Daltonik
microflex™ LT	trademark of Bruker Daltonik
micrOTOF ™ II	trademark of Bruker Daltonik
micrOTOF-Q ™ II	trademark of Bruker Daltonik
PAN™	trademark of Bruker Daltonik
PolyTools™	trademark of Bruker Daltonik
Profile Analysis™	trademark of Bruker Daltonik
ProteinScape™	trademark of Bruker Daltonik
Sepsityper™	trademark of Bruker Daltonik
Smartbeam™	trademark of Bruker Daltonik
solariX®	reg. trademark of Bruker Daltonik
Super Clean™	trademark of Bruker Daltonik
TargetAnalysis™	trademark of Bruker Daltonik
ultrafleXtreme™	trademark of Bruker Daltonik
HYPERION™	trademark of Bruker Optics
MATRIX™	trademark of Bruker Optics
QuickSnap™	trademark of Bruker Optics
RockSolid™	trademark of Bruker Optics
SENTERRA™	trademark of Bruker Optics
UltraScan™	trademark of Bruker Optics
D8™	trademark of Bruker AXS
DIFFRAC™	trademark of Bruker AXS
SampleCare™	trademark of Bruker AXS
TouchControl™	trademark of Bruker AXS
TOPAS™	trademark of Bruker AXS
XFlash®	reg.trademark of Bruker AXS
QUANTAX®	reg.trademark of Bruker AXS
BioScope™	trademark of AFM system
Catalyst™	trademark of AFM system
Icon®	reg. trademark of AFM system
MultiMode®	reg. trademark of AFM system
Dimension®	reg. trademark of AFM system brand
TappingMode™	trademark of AFM technique
Dektak®	reg. trademark of SOM system brand

Tables and Others Useful Information

NMR

IR Spectroscopy

Mass Spectrometry

Chemical Tables

Physical Tables

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted by increasing atomic number

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
1	H	1/2	99.9885	5.87E+03	**1.00E+00**	**300.130**	**400.130**	**500.130**	**600.130**	**700.130**	**750.130**	**800.130**	**850.130**	**900.130**	**950.130**	**1000.130**
2	H	1	0.0115	6.52E−03	9.65E−03	46.072	61.422	76.773	92.124	107.474	115.150	122.825	130.500	138.175	145.851	153.526
3	H	1/2		-	1.21E+00	320.131	426.795	533.459	640.123	746.786	800.118	853.450	906.782	960.114	1013.446	1066.778
3	He	1/2	1.34E-04	3.48E−03	4.42E−01	228.636	304.815	380.994	457.173	533.352	571.441	609.531	647.620	685.710	723.799	761.889
6	Li	1	7.59	3.79E+00	8.50E−03	44.167	58.883	73.600	88.316	103.032	110.390	117.748	125.106	132.464	139.822	147.180
7	Li	3/2	92.41	1.59E+03	2.94E−01	116.642	155.506	194.370	233.233	272.097	291.529	310.961	330.393	349.825	369.257	388.688
9	Be	3/2	100.0	8.15E+01	1.39E−02	42.174	56.226	70.277	84.329	98.381	105.407	112.433	119.459	126.485	133.510	140.536
10	B	3	19.9	2.32E+01	1.99E−02	32.245	42.989	53.732	64.476	75.220	80.591	85.963	91.335	96.707	102.079	107.451
11	B	3/2	80.1	7.77E+02	1.65E−01	96.294	128.378	160.462	192.546	224.630	240.672	256.714	272.755	288.797	304.839	320.881
13	C	1/2	1.07	**1.00E+00**	1.59E−02	75.468	100.613	125.758	150.903	176.048	188.620	201.193	213.765	226.338	238.910	251.483
14	N	1	99.636	5.90E+00	1.01E−03	21.688	28.915	36.141	43.367	50.594	54.207	57.820	61.433	65.046	68.659	72.273
15	N	1/2	0.364	2.23E−02	1.04E−03	30.423	40.560	50.697	60.834	70.971	76.039	81.107	86.176	91.244	96.312	101.381
17	O	5/2	0.038	6.50E−02	2.91E−02	40.687	54.243	67.800	81.356	94.913	101.691	108.469	115.248	122.026	128.804	135.582
19	F	1/2	100.0	4.89E+03	8.32E−01	282.404	376.498	470.592	564.686	658.780	705.827	752.874	799.921	846.968	894.015	941.062
21	Ne	3/2	0.27	3.91E−02	2.46E−03	23.693	31.587	39.482	47.376	55.270	59.217	63.165	67.112	71.059	75.006	78.953
23	Na	3/2	100.0	5.45E+02	9.27E−02	79.390	105.842	132.294	158.746	185.198	198.424	211.650	224.876	238.101	251.327	264.553
25	Mg	5/2	10.00	1.58E+00	2.68E−03	18.373	24.494	30.616	36.738	42.859	45.920	48.981	52.042	55.103	58.163	61.224
27	Al	5/2	100.0	1.22E+03	2.07E−01	78.204	104.261	130.318	156.375	182.432	195.460	208.489	221.517	234.546	247.574	260.602
29	Si	1/2	4.685	2.16E+00	7.86E−03	59.627	79.495	99.362	119.229	139.096	149.030	158.963	168.897	178.831	188.764	198.698
31	P	1/2	100.0	3.91E+02	6.65E−02	121.495	161.976	202.457	242.938	283.419	303.659	323.900	344.140	364.380	384.621	404.861
33	S	3/2	0.75	1.00E−01	2.27E−03	23.038	30.714	38.390	46.066	53.742	57.580	61.418	65.256	69.094	72.932	76.770
35	Cl	3/2	75.76	2.10E+01	4.72E−03	29.406	39.204	49.002	58.800	68.598	73.497	78.396	83.295	88.194	93.093	97.992
37	Cl	3/2	24.24	3.88E+00	2.72E−03	24.478	32.634	40.789	48.945	57.101	61.179	65.256	69.334	73.412	77.490	81.568
39	K	3/2	93.258	2.79E+00	5.10E−04	14.005	18.672	23.338	28.004	32.671	35.004	37.337	39.670	42.003	44.337	46.670
41	K	3/2	6.730	3.34E−02	8.44E−05	7.687	10.249	12.810	15.371	17.932	19.213	20.494	21.774	23.055	24.336	25.616
43	Ca	7/2	0.135	5.10E−02	6.43E−03	20.199	26.929	33.659	40.389	47.119	50.484	53.849	57.214	60.579	63.944	67.309
45	Sc	7/2	100.0	1.78E+03	3.02E−01	72.907	97.199	121.490	145.782	170.074	182.220	194.366	206.511	218.657	230.803	242.949
47	Ti	5/2	7.44	9.18E−01	2.10E−03	16.920	22.557	28.195	33.833	39.470	42.289	45.108	47.926	50.745	53.564	56.383
49	Ti	7/2	5.41	1.20E+00	3.78E−03	16.924	22.563	28.203	33.842	39.481	42.300	45.120	47.939	50.759	53.578	56.398
50	V	6	0.250	8.18E−01	5.57E−02	29.924	39.894	49.865	59.835	69.805	74.790	79.775	84.761	89.746	94.731	99.716
51	V	7/2	99.750	2.25E+03	3.84E−01	78.943	105.246	131.549	157.852	184.155	197.306	210.458	223.609	236.761	249.912	263.064
53	Cr	3/2	9.501	5.07E−01	9.08E−04	16.965	22.617	28.270	33.922	39.575	42.401	45.227	48.054	50.880	53.706	56.532
55	Mn	5/2	100.0	1.05E+03	1.79E−01	74.400	99.189	123.978	148.768	173.557	185.951	198.346	210.741	223.135	235.530	247.924
57	Fe	1/2	2.119	4.25E−03	3.42E−05	9.718	12.955	16.193	19.431	22.669	24.288	25.906	27.525	29.144	30.763	32.382
59	Co	7/2	100.0	1.64E+03	2.78E−01	71.212	94.939	118.666	142.393	166.120	177.984	189.847	201.711	213.575	225.438	237.302
61	Ni	3/2	1.1399	2.40E−01	3.59E−03	26.820	35.756	44.692	53.628	62.564	67.032	71.500	75.968	80.436	84.904	89.372
63	Cu	3/2	69.15	3.82E+02	9.39E−02	79.581	106.096	132.612	159.127	185.643	198.901	212.158	225.416	238.674	251.931	265.189
65	Cu	3/2	30.85	2.08E+02	1.15E−01	85.248	113.652	142.055	170.459	198.863	213.065	227.266	241.468	255.670	269.872	284.074
67	Zn	5/2	4.102	6.92E−01	2.87E−03	18.779	25.035	31.292	37.549	43.806	46.934	50.063	53.191	56.319	59.448	62.576
69	Ga	3/2	60.108	2.46E+02	6.97E−02	72.035	96.037	120.038	144.039	168.041	180.041	192.042	204.043	216.043	228.044	240.045
71	Ga	3/2	39.892	3.35E+02	1.43E−01	91.530	122.026	152.523	183.020	213.517	228.765	244.013	259.262	274.510	289.758	305.007

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted by increasing atomic number

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
73	Ge	9/2	7.76	6.44E−01	1.41E−03	10.469	13.958	17.446	20.934	24.423	26.167	27.911	29.655	31.399	33.144	34.888
75	As	3/2	100.0	1.49E+02	2.54E−02	51.390	68.513	85.635	102.758	119.881	128.442	137.003	145.564	154.126	162.687	171.248
77	Se	1/2	7.63	3.15E+00	7.03E−03	57.239	76.311	95.382	114.454	133.525	143.061	152.597	162.133	171.668	181.204	190.740
79	Br	3/2	50.69	2.37E+02	7.94E−02	75.195	100.248	125.302	150.356	175.410	187.937	200.464	212.991	225.518	238.045	250.572
81	Br	3/2	49.31	2.88E+02	9.95E−02	81.055	108.061	135.068	162.074	189.081	202.584	216.087	229.591	243.094	256.597	270.100
83	Kr	9/2	11.500	1.28E+00	1.90E−03	11.548	15.395	19.243	23.091	26.938	28.862	30.786	32.710	34.633	36.557	38.481
85	Rb	5/2	72.17	4.50E+01	1.06E−02	28.977	38.632	48.287	57.942	67.597	72.425	77.252	82.080	86.907	91.735	96.562
87	Rb	3/2	27.83	2.90E+02	1.77E−01	98.204	130.924	163.645	196.365	229.086	245.446	261.806	278.166	294.527	310.887	327.247
87	Sr	9/2	7.00	1.12E+00	2.72E−03	13.007	17.341	21.675	26.009	30.342	32.509	34.676	36.843	39.010	41.177	43.344
89	Y	1/2	100.0	7.00E−01	1.19E−04	14.707	19.607	24.507	29.408	34.308	36.758	39.208	41.658	44.108	46.558	49.008
91	Zr	5/2	11.22	6.26E+00	9.49E−03	27.901	37.197	46.494	55.790	65.086	69.734	74.382	79.031	83.679	88.327	92.975
93	Nb	9/2	100.0	2.87E+03	4.88E−01	73.460	97.936	122.413	146.889	171.365	183.603	195.841	208.079	220.317	232.555	244.794
95	Mo	5/2	15.90	3.06E+00	3.27E−03	19.559	26.076	32.593	39.110	45.627	48.885	52.144	55.402	58.661	61.919	65.178
97	Mo	5/2	9.56	1.96E+00	3.49E−03	19.970	26.623	33.277	39.931	46.585	49.911	53.238	56.565	59.892	63.219	66.546
99	Tc	9/2		-	3.82E−01	67.554	90.063	112.571	135.079	157.588	168.842	180.096	191.350	202.604	213.858	225.113
99	Ru	5/2	12.76	8.46E−01	1.13E−03	13.821	18.427	23.032	27.637	32.242	34.545	36.847	39.150	41.452	43.755	46.057
101	Ru	5/2	17.06	1.58E+00	1.57E−03	15.491	20.652	25.814	30.975	36.136	38.717	41.298	43.878	46.459	49.040	51.620
103	Rh	1/2	100.0	1.86E−01	3.17E−05	9.563	12.750	15.936	19.123	22.309	23.902	25.496	27.089	28.682	30.275	31.869
105	Pd	5/2	22.33	1.49E+00	1.13E−03	13.734	18.310	22.886	27.463	32.039	34.327	36.615	38.903	41.191	43.479	45.767
107	Ag	1/2	51.839	2.05E−01	6.74E−05	12.149	16.197	20.244	24.292	28.340	30.364	32.388	34.412	36.436	38.460	40.483
109	Ag	1/2	48.161	2.90E−01	1.02E−04	13.967	18.620	23.274	27.927	32.581	34.908	37.234	39.561	41.888	44.215	46.541
111	Cd	1/2	12.80	7.27E+00	9.66E−03	63.674	84.890	106.105	127.320	148.536	159.144	169.751	180.359	190.967	201.575	212.182
113	Cd	1/2	12.22	7.94E+00	1.11E−02	66.608	88.802	110.995	133.188	155.381	166.478	177.574	188.671	199.767	210.864	221.961
113	In	9/2	4.29	8.85E+01	3.51E−01	65.626	87.491	109.357	131.223	153.089	164.022	174.954	185.887	196.820	207.753	218.686
115	In	9/2	95.71	1.99E+03	3.53E−01	65.766	87.679	109.592	131.504	153.417	164.373	175.330	186.286	197.242	208.198	219.155
115	Sn	1/2	0.34	7.11E−01	3.56E−02	98.199	130.918	163.636	196.355	229.074	245.433	261.793	278.152	294.511	310.871	327.230
117	Sn	1/2	7.68	2.08E+01	4.60E−02	106.943	142.575	178.208	213.840	249.472	267.288	285.104	302.921	320.737	338.553	356.369
119	Sn	1/2	8.59	2.66E+01	5.27E−02	111.920	149.211	186.502	223.792	261.083	279.728	298.374	317.019	335.664	354.309	372.955
121	Sb	5/2	57.21	5.48E+02	1.63E−01	71.823	95.753	119.684	143.615	167.545	179.510	191.476	203.441	215.406	227.372	239.337
123	Sb	7/2	42.79	1.17E+02	4.66E−02	38.894	51.854	64.813	77.772	90.731	97.211	103.691	110.170	116.650	123.129	129.609
123	Te	1/2	0.89	9.61E−01	1.84E−02	78.543	104.713	130.883	157.052	183.222	196.307	209.392	222.477	235.562	248.647	261.731
125	Te	1/2	7.07	1.34E+01	3.22E−02	94.690	126.240	157.790	189.340	220.889	236.664	252.439	268.214	283.989	299.764	315.539
127	I	5/2	100.0	5.60E+02	9.54E−02	60.048	80.056	100.063	120.071	140.078	150.082	160.086	170.090	180.093	190.097	200.101
129	Xe	1/2	26.4006	3.35E+01	2.16E−02	83.467	111.277	139.087	166.897	194.707	208.613	222.518	236.423	250.328	264.233	278.138
131	Xe	3/2	21.2324	3.51E+00	2.82E−03	24.742	32.986	41.230	49.474	57.718	61.840	65.962	70.084	74.206	78.328	82.450
133	Cs	7/2	100.0	2.84E+02	4.84E−02	39.365	52.482	65.598	78.714	91.830	98.388	104.946	111.504	118.062	124.620	131.178
135	Ba	3/2	6.592	1.94E+00	5.01E−03	29.816	39.751	49.685	59.620	69.554	74.521	79.489	84.456	89.423	94.390	99.357
137	Ba	3/2	11.232	4.62E+00	7.00E−03	33.353	44.466	55.579	66.692	77.805	83.361	88.918	94.474	100.031	105.587	111.144
138	La	5	0.090	4.97E−01	9.40E−02	39.600	52.794	65.989	79.183	92.377	98.974	105.572	112.169	118.766	125.363	131.960
139	La	7/2	99.910	3.56E+02	6.06E−02	42.395	56.521	70.647	84.772	98.898	105.961	113.023	120.086	127.149	134.212	141.275
141	Pr	5/2	100.0	1.97E+03	3.35E−01	91.89	122.51	153.12	183.74	214.36	229.67	244.97	260.28	275.59	290.90	306.21

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted by increasing atomic number

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
143	Nd	7/2	12.2	2.43E+00	3.39E−03	16.35	21.80	27.25	32.69	38.14	40.86	43.59	46.31	49.04	51.76	54.48
145	Nd	7/2	8.3	3.87E−01	7.93E−04	10.07	13.43	16.78	20.14	23.49	25.17	26.85	28.53	30.20	31.88	33.56
147	Sm	7/2	14.99	1.34E+00	1.52E−03	12.51	16.68	20.84	25.01	29.18	31.26	33.35	35.43	37.52	39.60	41.68
149	Sm	7/2	13.82	6.92E−01	8.52E−04	10.31	13.75	17.18	20.62	24.06	25.77	27.49	29.21	30.93	32.64	34.36
151	Eu	5/2	47.81	5.04E+02	1.79E−01	74.62	99.48	124.34	149.20	174.06	186.49	198.92	211.35	223.78	236.22	248.65
153	Eu	5/2	52.19	4.73E+01	1.54E−02	32.94	43.91	54.88	65.86	76.83	82.32	87.80	93.29	98.78	104.26	109.75
155	Gd	3/2	14.80	1.26E−01	1.45E−04	9.21	12.28	15.35	18.42	21.49	23.03	24.56	26.10	27.63	29.17	30.70
157	Gd	3/2	15.65	3.00E−01	3.26E−04	12.08	16.11	20.13	24.16	28.19	30.20	32.21	34.22	36.24	38.25	40.26
159	Tb	3/2	100.0	4.08E+02	6.94E−02	72.14	96.18	120.22	144.26	168.29	180.31	192.33	204.35	216.37	228.39	240.41
161	Dy	5/2	18.889	5.26E−01	4.74E−04	10.32	13.75	17.19	20.63	24.07	25.78	27.50	29.22	30.94	32.66	34.38
163	Dy	5/2	24.896	1.91E+00	1.31E−03	14.46	19.28	24.10	28.92	33.74	36.15	38.56	40.97	43.38	45.79	48.20
165	Ho	7/2	100.0	1.16E+03	1.98E−01	63.43	84.57	105.71	126.84	147.98	158.54	169.11	179.68	190.25	200.82	211.38
167	Er	7/2	22.869	6.77E−01	5.04E−04	8.66	11.54	14.42	17.31	20.19	21.63	23.08	24.52	25.96	27.40	28.85
169	Tm	1/2	100.0	3.32E+00	5.66E−04	24.82	33.10	41.37	49.64	57.91	62.04	66.18	70.32	74.45	78.59	82.72
171	Yb	1/2	14.28	4.63E+00	5.52E−03	52.521	70.020	87.519	105.019	122.518	131.268	140.017	148.767	157.517	166.266	175.016
173	Yb	5/2	16.13	1.28E+00	1.35E−03	14.61	19.48	24.35	29.22	34.09	36.52	38.96	41.39	43.83	46.26	48.69
175	Lu	7/2	97.41	1.79E+02	3.13E−02	34.27	45.69	57.11	68.53	79.94	85.65	91.36	97.07	102.78	108.49	114.20
176	Lu	7	2.59	6.05E+00	3.98E−02	24.33	32.43	40.53	48.64	56.74	60.80	64.85	68.90	72.95	77.01	81.06
177	Hf	7/2	18.60	1.53E+00	1.40E−03	12.18	16.24	20.30	24.36	28.42	30.45	32.48	34.51	36.53	38.56	40.59
179	Hf	9/2	13.62	4.38E−01	5.47E−04	7.65	10.20	12.75	15.30	17.85	19.13	20.40	21.68	22.95	24.23	25.50
181	Ta	7/2	99.988	2.20E+02	3.74E−02	35.984	47.974	59.964	71.953	83.943	89.938	95.932	101.927	107.922	113.917	119.912
183	W	1/2	14.31	6.31E−02	7.50E−05	12.505	16.671	20.837	25.004	29.170	31.253	33.337	35.420	37.503	39.586	41.669
185	Re	5/2	37.40	3.05E+02	1.39E−01	67.603	90.128	112.652	135.177	157.701	168.964	180.226	191.488	202.751	214.013	225.275
187	Re	5/2	62.60	5.26E+02	1.43E−01	68.284	91.036	113.788	136.539	159.291	170.667	182.042	193.418	204.794	216.170	227.546
187	Os	1/2	1.96	1.43E−03	1.24E−05	6.850	9.132	11.415	13.697	15.979	17.120	18.262	19.403	20.544	21.685	22.826
189	Os	3/2	16.15	2.32E+00	2.44E−03	23.306	31.072	38.837	46.602	54.368	58.251	62.133	66.016	69.899	73.781	77.664
191	Ir	3/2	37.3	6.38E−02	2.91E−05	5.40	7.20	9.00	10.79	12.59	13.49	14.39	15.29	16.19	17.09	17.99
193	Ir	3/2	62.7	1.37E−01	3.73E−05	5.86	7.82	9.77	11.73	13.68	14.66	15.63	16.61	17.59	18.56	19.54
195	Pt	1/2	33.832	2.07E+01	1.04E−02	64.518	86.015	107.512	129.009	150.505	161.254	172.002	182.751	193.499	204.247	214.996
197	Au	3/2	100.0	1.62E−01	2.76E−05	5.31	7.08	8.84	10.61	12.38	13.26	14.15	15.03	15.92	16.80	17.69
199	Hg	1/2	16.87	5.89E+00	5.94E−03	53.756	71.667	89.577	107.488	125.399	134.354	143.310	152.265	161.221	170.176	179.132
201	Hg	3/2	13.18	1.16E+00	1.49E−03	19.843	26.455	33.067	39.678	46.290	49.595	52.901	56.207	59.513	62.819	66.124
203	Tl	1/2	29.52	3.40E+02	1.96E−01	171.444	228.567	285.690	342.813	399.937	428.498	457.060	485.621	514.183	542.745	571.306
205	Tl	1/2	70.48	8.36E+02	2.02E−01	173.127	230.810	288.494	346.178	403.862	432.704	461.546	490.388	519.230	548.071	576.913
207	Pb	1/2	22.1	1.18E+01	9.06E−03	62.789	83.710	104.630	125.551	146.471	156.932	167.392	177.852	188.313	198.773	209.233
209	Bi	9/2	100.0	8.48E+02	1.44E−01	48.229	64.298	80.367	96.437	112.506	120.541	128.575	136.610	144.644	152.679	160.714
209	Po	1/2		-	1.44E−02	73.08	97.42	121.77	146.12	170.47	182.64	194.81	206.99	219.16	231.34	243.51
231	Pa	3/2	100.0	4.06E+02	6.90E−02	72.00	95.99	119.98	143.97	167.96	179.96	191.95	203.94	215.94	227.93	239.93
235	U	7/2	0.7204	6.53E−03	1.54E−04	5.527	7.368	9.209	11.051	12.892	13.813	14.734	15.654	16.575	17.496	18.416

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope		Spin	Nat. Abund. (%)	Receptivity Natural rel. ^{13}C	Receptivity Molar rel. ^{1}H	Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments 7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
3	H	1/2		–	1.21E+00	320.131	426.795	533.459	640.123	746.786	800.118	853.450	906.782	960.114	1013.446	1066.778
1	H	1/2	99.9885	5.87E+03	**1.00E+00**	**300.130**	**400.130**	**500.130**	**600.130**	**700.130**	**750.130**	**800.130**	**850.130**	**900.130**	**950.130**	**1000.130**
19	F	1/2	100.0	4.89E+03	8.32E–01	282.404	376.498	470.592	564.686	658.780	705.827	752.874	799.921	846.968	894.015	941.062
3	He	1/2	1.34E–04	3.48E–03	4.42E–01	228.636	304.815	380.994	457.173	533.352	571.441	609.531	647.620	685.710	723.799	761.889
205	Tl	1/2	70.48	8.36E+02	2.02E–01	173.127	230.810	288.494	346.178	403.862	432.704	461.546	490.388	519.230	548.071	576.913
203	Tl	1/2	29.52	3.40E+02	1.96E–01	171.444	228.567	285.690	342.813	399.937	428.498	457.060	485.621	514.183	542.745	571.306
31	P	1/2	100.0	3.91E+02	6.65E–02	121.495	161.976	202.457	242.938	283.419	303.659	323.900	344.140	364.380	384.621	404.861
7	Li	3/2	92.41	1.59E+03	2.94E–01	116.642	155.506	194.370	233.233	272.097	291.529	310.961	330.393	349.825	369.257	388.688
119	Sn	1/2	8.59	2.66E+01	5.27E–02	111.920	149.211	186.502	223.792	261.083	279.728	298.374	317.019	335.664	354.309	372.955
117	Sn	1/2	7.68	2.08E+01	4.60E–02	106.943	142.575	178.208	213.840	249.472	267.288	285.104	302.921	320.737	338.553	356.369
87	Rb	3/2	27.83	2.90E+02	1.77E–01	98.204	130.924	163.645	196.365	229.086	245.446	261.806	278.166	294.527	310.887	327.247
115	Sn	1/2	0.34	7.11E–01	3.56E–02	98.199	130.918	163.636	196.355	229.074	245.433	261.793	278.152	294.511	310.871	327.230
11	B	3/2	80.1	7.77E+02	1.65E–01	96.294	128.378	160.462	192.546	224.630	240.672	256.714	272.755	288.797	304.839	320.881
125	Te	1/2	7.07	1.34E+01	3.22E–02	94.690	126.240	157.790	189.340	220.889	236.664	252.439	268.214	283.989	299.764	315.539
141	Pr	5/2	100.0	1.97E+03	3.35E–01	91.89	122.51	153.12	183.74	214.36	229.67	244.97	260.28	275.59	290.90	306.21
71	Ga	3/2	39.892	3.35E+02	1.43E–01	91.530	122.026	152.523	183.020	213.517	228.765	244.013	259.262	274.510	289.758	305.007
65	Cu	3/2	30.85	2.08E+02	1.15E–01	85.248	113.652	142.055	170.459	198.863	213.065	227.266	241.468	255.670	269.872	284.074
129	Xe	1/2	26.4006	3.35E+01	2.16E–02	83.467	111.277	139.087	166.897	194.707	208.613	222.518	236.423	250.328	264.233	278.138
81	Br	3/2	49.31	2.88E+02	9.95E–02	81.055	108.061	135.068	162.074	189.081	202.584	216.087	229.591	243.094	256.597	270.100
63	Cu	3/2	69.15	3.82E+02	9.39E–02	79.581	106.096	132.612	159.127	185.643	198.901	212.158	225.416	238.674	251.931	265.189
23	Na	3/2	100.0	5.45E+02	9.27E–02	79.390	105.842	132.294	158.746	185.198	198.424	211.650	224.876	238.101	251.327	264.553
51	V	7/2	99.750	2.25E+03	3.84E–01	78.943	105.246	131.549	157.852	184.155	197.306	210.458	223.609	236.761	249.912	263.064
123	Te	1/2	0.89	9.61E–01	1.84E–02	78.543	104.713	130.883	157.052	183.222	196.307	209.392	222.477	235.562	248.647	261.731
27	Al	5/2	100.0	1.22E+03	2.07E–01	78.204	104.261	130.318	156.375	182.432	195.460	208.489	221.517	234.546	247.574	260.602
13	C	1/2	1.07	**1.00E+00**	1.59E–02	75.468	100.613	125.758	150.903	176.048	188.620	201.193	213.765	226.338	238.910	251.483
79	Br	3/2	50.69	2.37E+02	7.94E–02	75.195	100.248	125.302	150.356	175.410	187.937	200.464	212.991	225.518	238.045	250.572
151	Eu	5/2	47.81	5.04E+02	1.79E–01	74.62	99.48	124.34	149.20	174.06	186.49	198.92	211.35	223.78	236.22	248.65
55	Mn	5/2	100.0	1.05E+03	1.79E–01	74.400	99.189	123.978	148.768	173.557	185.951	198.346	210.741	223.135	235.530	247.924
93	Nb	9/2	100.0	2.87E+03	4.88E–01	73.460	97.936	122.413	146.889	171.365	183.603	195.841	208.079	220.317	232.555	244.794
209	Po	1/2		–	1.44E–02	73.08	97.42	121.77	146.12	170.47	182.64	194.81	206.99	219.16	231.34	243.51
45	Sc	7/2	100.0	1.78E+03	3.02E–01	72.907	97.199	121.490	145.782	170.074	182.220	194.366	206.511	218.657	230.803	242.949
159	Tb	3/2	100.0	4.08E+02	6.94E–02	72.14	96.18	120.22	144.26	168.29	180.31	192.33	204.35	216.37	228.39	240.41
69	Ga	3/2	60.108	2.46E+02	6.97E–02	72.035	96.037	120.038	144.039	168.041	180.041	192.042	204.043	216.043	228.044	240.045
231	Pa	3/2	100.0	4.06E+02	6.90E–02	72.00	95.99	119.98	143.97	167.96	179.96	191.95	203.94	215.94	227.93	239.93
121	Sb	5/2	57.21	5.48E+02	1.63E–01	71.823	95.753	119.684	143.615	167.545	179.510	191.476	203.441	215.406	227.372	239.337
59	Co	7/2	100.0	1.64E+03	2.78E–01	71.212	94.939	118.666	142.393	166.120	177.984	189.847	201.711	213.575	225.438	237.302
187	Re	5/2	62.60	5.26E+02	1.43E–01	68.284	91.036	113.788	136.539	159.291	170.667	182.042	193.418	204.794	216.170	227.546
185	Re	5/2	37.40	3.05E+02	1.39E–01	67.603	90.128	112.652	135.177	157.701	168.964	180.226	191.488	202.751	214.013	225.275
99	Tc	9/2		–	3.82E–01	67.554	90.063	112.571	135.079	157.588	168.842	180.096	191.350	202.604	213.858	225.113
113	Cd	1/2	12.22	7.94E+00	1.11E–02	66.608	88.802	110.995	133.188	155.381	166.478	177.574	188.671	199.767	210.864	221.961
115	In	9/2	95.71	1.99E+03	3.53E–01	65.766	87.679	109.592	131.504	153.417	164.373	175.330	186.286	197.242	208.198	219.155

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope		Spin	Nat. Abund. (%)	Receptivity Natural rel. ^{13}C	Receptivity Molar rel. ^{1}H	Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments 7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
113	In	9/2	4.29	8.85E+01	3.51E–01	65.626	87.491	109.357	131.223	153.089	164.022	174.954	185.887	196.820	207.753	218.686
195	Pt	1/2	33.832	2.07E+01	1.04E–02	64.518	86.015	107.512	129.009	150.505	161.254	172.002	182.751	193.499	204.247	214.996
111	Cd	1/2	12.80	7.27E+00	9.66E–03	63.674	84.890	106.105	127.320	148.536	159.144	169.751	180.359	190.967	201.575	212.182
165	Ho	7/2	100.0	1.16E+03	1.98E–01	63.43	84.57	105.71	126.84	147.98	158.54	169.11	179.68	190.25	200.82	211.38
207	Pb	1/2	22.1	1.18E+01	9.06E–03	62.789	83.710	104.630	125.551	146.471	156.932	167.392	177.852	188.313	198.773	209.233
127	I	5/2	100.0	5.60E+02	9.54E–02	60.048	80.056	100.063	120.071	140.078	150.082	160.086	170.090	180.093	190.097	200.101
29	Si	1/2	4.685	2.16E+00	7.86E–03	59.627	79.495	99.362	119.229	139.096	149.030	158.963	168.897	178.831	188.764	198.698
77	Se	1/2	7.63	3.15E+00	7.03E–03	57.239	76.311	95.382	114.454	133.525	143.061	152.597	162.133	171.668	181.204	190.740
199	Hg	1/2	16.87	5.89E+00	5.94E–03	53.756	71.667	89.577	107.488	125.399	134.354	143.310	152.265	161.221	170.176	179.132
171	Yb	1/2	14.28	4.63E+00	5.52E–03	52.521	70.020	87.519	105.019	122.518	131.268	140.017	148.767	157.517	166.266	175.016
75	As	3/2	100.0	1.49E+02	2.54E–02	51.390	68.513	85.635	102.758	119.881	128.442	137.003	145.564	154.126	162.687	171.248
209	Bi	9/2	100.0	8.48E+02	1.44E–01	48.229	64.298	80.367	96.437	112.506	120.541	128.575	136.610	144.644	152.679	160.714
2	H	1	0.0115	6.52E–03	9.65E–03	46.072	61.422	76.773	92.124	107.474	115.150	122.825	130.500	138.175	145.851	153.526
6	Li	1	7.59	3.79E+00	8.50E–03	44.167	58.883	73.600	88.316	103.032	110.390	117.748	125.106	132.464	139.822	147.180
139	La	7/2	99.910	3.56E+02	6.06E–02	42.395	56.521	70.647	84.772	98.898	105.961	113.023	120.086	127.149	134.212	141.275
9	Be	3/2	100.0	8.15E+01	1.39E–02	42.174	56.226	70.277	84.329	98.381	105.407	112.433	119.459	126.485	133.510	140.536
17	O	5/2	0.038	6.50E–02	2.91E–02	40.687	54.243	67.800	81.356	94.913	101.691	108.469	115.248	122.026	128.804	135.582
138	La	5	0.090	4.97E–01	9.40E–02	39.600	52.794	65.989	79.183	92.377	98.974	105.572	112.169	118.766	125.363	131.960
133	Cs	7/2	100.0	2.84E+02	4.84E–02	39.365	52.482	65.598	78.714	91.830	98.388	104.946	111.504	118.062	124.620	131.178
123	Sb	7/2	42.79	1.17E+02	4.66E–02	38.894	51.854	64.813	77.772	90.731	97.211	103.691	110.170	116.650	123.129	129.609
181	Ta	7/2	99.988	2.20E+02	3.74E–02	35.984	47.974	59.964	71.953	83.943	89.938	95.932	101.927	107.922	113.917	119.912
175	Lu	7/2	97.41	1.79E+02	3.13E–02	34.27	45.69	57.11	68.53	79.94	85.65	91.36	97.07	102.78	108.49	114.20
137	Ba	3/2	11.232	4.62E+00	7.00E–03	33.353	44.466	55.579	66.692	77.805	83.361	88.918	94.474	100.031	105.587	111.144
153	Eu	5/2	52.19	4.73E+01	1.54E–02	32.94	43.91	54.88	65.86	76.83	82.32	87.80	93.29	98.78	104.26	109.75
10	B	3	19.9	2.32E+01	1.99E–02	32.245	42.989	53.732	64.476	75.220	80.591	85.963	91.335	96.707	102.079	107.451
15	N	1/2	0.364	2.23E–02	1.04E–03	30.423	40.560	50.697	60.834	70.971	76.039	81.107	86.176	91.244	96.312	101.381
50	V	6	0.250	8.18E–01	5.57E–02	29.924	39.894	49.865	59.835	69.805	74.790	79.775	84.761	89.746	94.731	99.716
135	Ba	3/2	6.592	1.94E+00	5.01E–03	29.816	39.751	49.685	59.620	69.554	74.521	79.489	84.456	89.423	94.390	99.357
35	Cl	3/2	75.76	2.10E+01	4.72E–03	29.406	39.204	49.002	58.800	68.598	73.497	78.396	83.295	88.194	93.093	97.992
85	Rb	5/2	72.17	4.50E+01	1.06E–02	28.977	38.632	48.287	57.942	67.597	72.425	77.252	82.080	86.907	91.735	96.562
91	Zr	5/2	11.22	6.26E+00	9.49E–03	27.901	37.197	46.494	55.790	65.086	69.734	74.382	79.031	83.679	88.327	92.975
61	Ni	3/2	1.1399	2.40E–01	3.59E–03	26.820	35.756	44.692	53.628	62.564	67.032	71.500	75.968	80.436	84.904	89.372
169	Tm	1/2	100.0	3.32E+00	5.66E–04	24.82	33.10	41.37	49.64	57.91	62.04	66.18	70.32	74.45	78.59	82.72
131	Xe	3/2	21.2324	3.51E+00	2.82E–03	24.742	32.986	41.230	49.474	57.718	61.840	65.962	70.084	74.206	78.328	82.450
37	Cl	3/2	24.24	3.88E+00	2.72E–03	24.478	32.634	40.789	48.945	57.101	61.179	65.256	69.334	73.412	77.490	81.568
176	Lu	7	2.59	6.05E+00	3.98E–02	24.33	32.43	40.53	48.64	56.74	60.80	64.85	68.90	72.95	77.01	81.06
21	Ne	3/2	0.27	3.91E–02	2.46E–03	23.693	31.587	39.482	47.376	55.270	59.217	63.165	67.112	71.059	75.006	78.953
189	Os	3/2	16.15	2.32E+00	2.44E–03	23.306	31.072	38.837	46.602	54.368	58.251	62.133	66.016	69.899	73.781	77.664
33	S	3/2	0.75	1.00E–01	2.27E–03	23.038	30.714	38.390	46.066	53.742	57.580	61.418	65.256	69.094	72.932	76.770
14	N	1	99.636	5.90E+00	1.01E–03	21.688	28.915	36.141	43.367	50.594	54.207	57.820	61.433	65.046	68.659	72.273
43	Ca	7/2	0.135	5.10E–02	6.43E–03	20.199	26.929	33.659	40.389	47.119	50.484	53.849	57.214	60.579	63.944	67.309

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
97	Mo	5/2	9.56	1.96E+00	3.49E–03	19.970	26.623	33.277	39.931	46.585	49.911	53.238	56.565	59.892	63.219	66.546
201	Hg	3/2	13.18	1.16E+00	1.49E–03	19.843	26.455	33.067	39.678	46.290	49.595	52.901	56.207	59.513	62.819	66.124
95	Mo	5/2	15.90	3.06E+00	3.27E–03	19.559	26.076	32.593	39.110	45.627	48.885	52.144	55.402	58.661	61.919	65.178
67	Zn	5/2	4.102	6.92E–01	2.87E–03	18.779	25.035	31.292	37.549	43.806	46.934	50.063	53.191	56.319	59.448	62.576
25	Mg	5/2	10.00	1.58E+00	2.68E–03	18.373	24.494	30.616	36.738	42.859	45.920	48.981	52.042	55.103	58.163	61.224
53	Cr	3/2	9.501	5.07E–01	9.08E–04	16.965	22.617	28.270	33.922	39.575	42.401	45.227	48.054	50.880	53.706	56.532
49	Ti	7/2	5.41	1.20E+00	3.78E–03	16.924	22.563	28.203	33.842	39.481	42.300	45.120	47.939	50.759	53.578	56.398
47	Ti	5/2	7.44	9.18E–01	2.10E–03	16.920	22.557	28.195	33.833	39.470	42.289	45.108	47.926	50.745	53.564	56.383
143	Nd	7/2	12.2	2.43E+00	3.39E–03	16.35	21.80	27.25	32.69	38.14	40.86	43.59	46.31	49.04	51.76	54.48
101	Ru	5/2	17.06	1.58E+00	1.57E–03	15.491	20.652	25.814	30.975	36.136	38.717	41.298	43.878	46.459	49.040	51.620
89	Y	1/2	100.0	7.00E–01	1.19E–04	14.707	19.607	24.507	29.408	34.308	36.758	39.208	41.658	44.108	46.558	49.008
173	Yb	5/2	16.13	1.28E+00	1.35E–03	14.61	19.48	24.35	29.22	34.09	36.52	38.96	41.39	43.83	46.26	48.69
163	Dy	5/2	24.896	1.91E+00	1.31E–03	14.46	19.28	24.10	28.92	33.74	36.15	38.56	40.97	43.38	45.79	48.20
39	K	3/2	93.258	2.79E+00	5.10E–04	14.005	18.672	23.338	28.004	32.671	35.004	37.337	39.670	42.003	44.337	46.670
109	Ag	1/2	48.161	2.90E–01	1.02E–04	13.967	18.620	23.274	27.927	32.581	34.908	37.234	39.561	41.888	44.215	46.541
99	Ru	5/2	12.76	8.46E–01	1.13E–03	13.821	18.427	23.032	27.637	32.242	34.545	36.847	39.150	41.452	43.755	46.057
105	Pd	5/2	22.33	1.49E+00	1.13E–03	13.734	18.310	22.886	27.463	32.039	34.327	36.615	38.903	41.191	43.479	45.767
87	Sr	9/2	7.00	1.12E+00	2.72E–03	13.007	17.341	21.675	26.009	30.342	32.509	34.676	36.843	39.010	41.177	43.344
147	Sm	7/2	14.99	1.34E+00	1.52E–03	12.51	16.68	20.84	25.01	29.18	31.26	33.35	35.43	37.52	39.60	41.68
183	W	1/2	14.31	6.31E–02	7.50E–05	12.505	16.671	20.837	25.004	29.170	31.253	33.337	35.420	37.503	39.586	41.669
177	Hf	7/2	18.60	1.53E+00	1.40E–03	12.18	16.24	20.30	24.36	28.42	30.45	32.48	34.51	36.53	38.56	40.59
107	Ag	1/2	51.839	2.05E–01	6.74E–05	12.149	16.197	20.244	24.292	28.340	30.364	32.388	34.412	36.436	38.460	40.483
157	Gd	3/2	15.65	3.00E–01	3.26E–04	12.08	16.11	20.13	24.16	28.19	30.20	32.21	34.22	36.24	38.25	40.26
83	Kr	9/2	11.500	1.28E+00	1.90E–03	11.548	15.395	19.243	23.091	26.938	28.862	30.786	32.710	34.633	36.557	38.481
73	Ge	9/2	7.76	6.44E–01	1.41E–03	10.469	13.958	17.446	20.934	24.423	26.167	27.911	29.655	31.399	33.144	34.888
161	Dy	5/2	18.889	5.26E–01	4.74E–04	10.32	13.75	17.19	20.63	24.07	25.78	27.50	29.22	30.94	32.66	34.38
149	Sm	7/2	13.82	6.92E–01	8.52E–04	10.31	13.75	17.18	20.62	24.06	25.77	27.49	29.21	30.93	32.64	34.36
145	Nd	7/2	8.3	3.87E–01	7.93E–04	10.07	13.43	16.78	20.14	23.49	25.17	26.85	28.53	30.20	31.88	33.56
57	Fe	1/2	2.119	4.25E–03	3.42E–05	9.718	12.955	16.193	19.431	22.669	24.288	25.906	27.525	29.144	30.763	32.382
103	Rh	1/2	100.0	1.86E–01	3.17E–05	9.563	12.750	15.936	19.123	22.309	23.902	25.496	27.089	28.682	30.275	31.869
155	Gd	3/2	14.80	1.26E–01	1.45E–04	9.21	12.28	15.35	18.42	21.49	23.03	24.56	26.10	27.63	29.17	30.70
167	Er	7/2	22.869	6.77E–01	5.04E–04	8.66	11.54	14.42	17.31	20.19	21.63	23.08	24.52	25.96	27.40	28.85
41	K	3/2	6.730	3.34E–02	8.44E–05	7.687	10.249	12.810	15.371	17.932	19.213	20.494	21.774	23.055	24.336	25.616
179	Hf	9/2	13.62	4.38E–01	5.47E–04	7.65	10.20	12.75	15.30	17.85	19.13	20.40	21.68	22.95	24.23	25.50
187	Os	1/2	1.96	1.43E–03	1.24E–05	6.850	9.132	11.415	13.697	15.979	17.120	18.262	19.403	20.544	21.685	22.826
193	Ir	3/2	62.7	1.37E–01	3.73E–05	5.86	7.82	9.77	11.73	13.68	14.66	15.63	16.61	17.59	18.56	19.54
235	U	7/2	0.7204	6.53E–03	1.54E–04	5.527	7.368	9.209	11.051	12.892	13.813	14.734	15.654	16.575	17.496	18.416
191	Ir	3/2	37.3	6.38E–02	2.91E–05	5.40	7.20	9.00	10.79	12.59	13.49	14.39	15.29	16.19	17.09	17.99
197	Au	3/2	100.0	1.62E–01	2.76E–05	5.31	7.08	8.84	10.61	12.38	13.26	14.15	15.03	15.92	16.80	17.69

NMR Properties of Selected Isotopes

Z = proton number, **A** = mass number, **Half-Life** where appropriate in years (y), days (d), hours (h), minutes (m); ***I*** = spin quantum number; **NA** = natural abundance (IUPAC 2003); $\boldsymbol{\mu_z}$ = z-component of nuclear magnetic moment in units of the nuclear magneton (μ_N); ***Q*** = electric quadrupole moment in units of fm² = 10^{-30} m² (1 fm² = 0.01 barns); calc. magnetogyric ratio $\gamma = \mu_z/\hbar\ I$. Note: for $\boldsymbol{\mu_z}$ and ***Q*** the experimental uncertainty begins with the last significant digit.

			Isotope (half-life)	**Spin**	**Nat. Abund. 2003** (TICE 2001)	**Rel. Nucl. Magn. Mom.** (measured)	**Quadrupole Moment**	**Magnetogyric Ratio** (calc., free atom)
Z	**A**	**Sym**	**Name**	***I***	**NA** (%)	μ_z / μ_N	***Q*** [fm²]	γ [10^7 rad s^{-1} T^{-1}]
0	1	n	Neutron	1/2		-1.9130427		-18.3247183
1	1	H	Hydrogen	1/2	99.9885	2.79284734		26.7522208
	2	H (D)	Deuterium	1	0.0115	0.857438228	0.286	4.10662919
	3	H (T)	Tritium (12.32 y)	1/2		2.97896244		28.5349865
2	3	He	Helium	1/2	0.000134	-2.12749772		-20.3789473
3	6	Li	Lithium	1	7.59	0.8220473	-0.0808	3.937127
	7	Li	Lithium	3/2	92.41	3.2564625	-4.01	10.397704
4	9	Be	Beryllium	3/2	100	-1.17749	5.288	-3.75966
5	10	B	Boron	3	19.9	1.80064478	8.459	2.87467955
	11	B	Boron	3/2	80.1	2.688649	4.059	8.584707
6	13	C	Carbon	1/2	1.07	0.702412		6.728286
7	14	N	Nitrogen	1	99.636	0.40376100	2.044	1.9337798
	15	N	Nitrogen	1/2	0.364	-0.28318884		-2.7126189
8	17	O	Oxygen	5/2	0.038	-1.89379	-2.558	-3.62806
9	19	F	Fluorine	1/2	100	2.626868		25.16233
10	21	Ne	Neon	3/2	0.27	-0.661797	10.155	-2.113081
11	23	Na	Sodium (Natrium)	3/2	100	2.2176556	10.4	7.0808516
12	25	Mg	Magnesium	5/2	10.00	-0.85545	19.94	-1.63884
13	26	Al	Alumin(i)um (7.17E5 y)	5		2.804	27	2.686
13	27	Al	Alumin(i)um	5/2	100	3.6415069	14.66	6.9762780
14	29	Si	Silicon	1/2	4.685	-0.55529		-5.31903
15	31	P	Phosphorus	1/2	100	1.13160		10.8394
16	33	S	Sulfur	3/2	0.75	0.643821	-6.78	2.055685
17	35	Cl	Chlorine	3/2	75.76	0.8218743	-8.165	2.6241991
	37	Cl	Chlorine	3/2	24.24	0.6841236	-6.435	2.1843688
18	39	Ar	Argon (269 y)	7/2		-1.59		-2.17
19	39	K	Potassium (Kalium)	3/2	93.258	0.3915073	5.85	1.2500612
	40	K	Potassium (1.248E9 y)	4	0.0117	-1.298100	-7.3	-1.554286
	41	K	Potassium	3/2	6.730	0.21489274	7.11	0.68614062
20	41	Ca	Calcium (1.02E5 y)	7/2		-1.594781	-6.7	-2.182306
	43	Ca	Calcium	7/2	0.135	-1.317643	-4.08	-1.803069
21	45	Sc	Scandium	7/2	100	4.756487	-22.0	6.508800
22	47	Ti	Titanium	5/2	7.44	-0.78848	30.2	-1.51054
	49	Ti	Titanium	7/2	5.41	-1.10417	24.7	-1.51095
23	50	V	Vanadium (1.4E17 y)	6	0.250	3.345689	21	2.670650
	51	V	Vanadium	7/2	99.750	5.1487057	-5.2	7.0455139
24	53	Cr	Chromium	3/2	9.501	-0.47454	-15	-1.51518
25	53	Mn	Manganese (3.74E6 y)	7/2		*5.024*		6.875
	55	Mn	Manganese	5/2	100	3.46871790	33	6.64525453
26	57	Fe	Iron, Ferrum	1/2	2.119	0.09062300		0.8680627
	59	Fe	Iron (44.507 d)	3/2		-0.3358		-1.0722
27	59	Co	Cobalt	7/2	100	4.627	42 s	6.332
	60	Co	Cobalt (1925.2 d)	5		3.799	44	3.639
28	61	Ni	Nickel	3/2	1.1399	-0.75002	16.2	-2.39477
29	63	Cu	Copper, Cuprum	3/2	69.15	2.227346	-22.0	7.111791
	65	Cu	Copper, Cuprum	3/2	30.85	2.3816	-20.4	7.6043
30	67	Zn	Zinc	5/2	4.102	0.8752049	15.0	1.6766885
31	69	Ga	Gallium	3/2	60.108	2.01659	17.1	6.43886
	71	Ga	Gallium	3/2	39.892	2.56227	10.7	8.18117
32	73	Ge	Germanium	9/2	7.76	-0.8794677	-19.6	-0.9360306
33	75	As	Arsenic	3/2	100	1.43947	31.4	4.59615
34	77	Se	Selenium	1/2	7.63	0.5350743		5.125388

NMR Properties of Selected Isotopes

BRUKER

Theor. NMR freq. ν_o calc. from γ and scaled to ^1H = 100.0 MHz; Molar Receptivity $\mathbf{R_M(H)}$ relative to equal number of protons is proportional to $\gamma^3\ I\ (I+1)$; Receptivity at nat. abundance $\mathbf{R_{NA}(C)}$ relative to ^{13}C; recommended Reference sample (IUPAC 2001); *experimental* reson. freq. of ref. sample on the unified Ξ scale (at B_0 where TMS (^1H) = 100.0 MHz).
Numbers containing E are in exponential format.

A	Sym	**Theoretical NMR Freq.** (free atom) ν_o [MHz]	**Molar Receptivity** (rel. ^1H) $R_M(H)$	**Receptivity at Nat. Abund.** (rel. ^{13}C) $R_{NA}(C)$	**Reference Sample** Reference	**Measured. NMR Freq.** (rel. ^1H ref.) Ξ [MHz]
1	n	68.4979	3.21E–01			
1	H	100.0000	**1.00E+00**	5.87E+03	1% Me_4Si in $CDCl_3$	100.000000
2	D	15.3506	9.65E–03	6.52E–03	$(CD_3)_4Si$ neat	15.350609
3	T	106.6640	1.21E+00		TMS-T_1	106.663974
3	He	76.1767	4.42E–01	3.48E–03	He gas	76.178976
6	Li	14.7170	8.50E–03	3.79E+00	9.7 m LiCl in D_2O	14.716086
7	Li	38.8667	2.94E–01	1.59E+03	9.7 m LiCl in D_2O	38.863797
9	Be	14.0536	1.39E–02	8.15E+01	0.43 m $BeSO_4$ in D_2O	14.051813
10	B	10.7456	1.99E–02	2.32E+01	15% $BF_3.Et_2O$ in $CDCl_3$	10.743658
11	B	32.0897	1.65E–01	7.77E+02	15% $BF_3.Et_2O$ in $CDCl_3$	32.083974
13	C	25.1504	1.59E–02	**1.00E+00**	1% Me_4Si in $CDCl_3$	25.145020
					DSS in D_2O	25.144953
14	N	7.2285	1.01E–03	5.90E+00	$MeNO_2$ + 10% $CDCl_3$	7.226317
15	N	10.1398	1.04E–03	2.23E–02	$MeNO_2$ + 10% $CDCl_3$	10.136767
					liquid NH_3	10.132767
17	O	13.5617	2.91E–02	6.50E–02	D_2O	13.556457
19	F	94.0570	8.32E–01	4.89E+03	CCl_3F	94.094011
21	Ne	7.8987	2.46E–03	3.91E–02	Neon gas, 1.1 MPa	7.894296
23	Na	26.4683	9.27E–02	5.45E+02	0.1 M NaCl in D_2O	26.451900
25	Mg	6.1260	2.68E–03	1.58E+00	11 M $MgCl_2$ in D_2O	6.121635
26	Al	10.0399	4.05E–02			
27	Al	26.0774	2.07E–01	1.22E+03	1.1 m $Al(NO_3)_3$ in D_2O	26.056859
29	Si	19.8826	7.86E–03	2.16E+00	1% Me_4Si in $CDCl_3$	19.867187
31	P	40.5178	6.65E–02	3.91E+02	H_3PO_4 external	40.480742
					$(MeO)_3PO$ internal	40.480864
33	S	7.6842	2.27E–03	1.00E–01	$(NH_4)_2SO_4$ in D_2O (sat.)	7.676000
35	Cl	9.8093	4.72E–03	2.10E+01	0.1 M NaCl in D_2O	9.797909
37	Cl	8.1652	2.72E–03	3.88E+00	0.1 M NaCl in D_2O	8.155725
39	Ar	8.1228	1.13E–02			
39	K	4.6727	5.10E–04	2.79E+00	0.1 M KCl in D_2O	4.666373
40	K	5.8099	5.23E–03	3.59E–03	0.1 M KCl in D_2O	5.802018
41	K	2.5648	8.44E–05	3.34E–02	0.1 M KCl in D_2O	2.561305
41	Ca	8.1575	1.14E–02			
43	Ca	6.7399	6.43E–03	5.10E–02	0.1 M $CaCl_2$ in D_2O	6.730029
45	Sc	24.3299	3.02E–01	1.78E+03	0.06 M $Sc(NO_3)_3$ in D_2O	24.291747
47	Ti	5.6464	2.10E–03	9.18E–01	$TiCl_4$ neat + 10% C_6D_{12}	5.637534
49	Ti	5.6479	3.78E–03	1.20E+00	$TiCl_4$ neat + 10% C_6D_{12}	5.639037
50	V	9.9829	5.57E–02	8.18E–01	$VOCl_3$ + 5% C_6D_6	9.970309
51	V	26.3362	3.84E–01	2.25E+03	$VOCl_3$ + 5% C_6D_6	26.302948
53	Cr	5.6638	9.08E–04	5.07E–01	K_2CrO_4 in D_2O (sat.)	5.652496
53	Mn	25.6983	3.56E–01			
55	Mn	24.8400	1.79E–01	1.05E+03	0.82 m $KMnO_4$ in D_2O	24.789218
57	Fe	3.2448	3.42E–05	4.25E–03	$Fe(CO)_5$ + 20% C_6D_6	3.237778
59	Fe	4.0079	3.22E–04			
59	Co	23.6676	2.78E–01	1.64E+03	0.56 m $K_3[Co(CN)_6]$ in D_2O	23.727074
60	Co	13.6026	1.01E–01			
61	Ni	8.9517	3.59E–03	2.40E–01	$Ni(CO)_4$ + 5% C_6D_6	8.936051
63	Cu	26.5839	9.39E–02	3.82E+02	$[Cu(CH_3CN)_4][ClO_4]$ in CH_3CN (sat.) + 5% C_6D_6	26.515473
65	Cu	28.4250	1.15E–01	2.08E+02	$[Cu(CH_3CN)_4][ClO_4]$ in CH_3CN (sat.) + 5% C_6D_6	28.403693
67	Zn	6.2675	2.87E–03	6.92E–01	$Zn(NO_3)_3$ in D_2O (sat.)	6.256803
69	Ga	24.0685	6.97E–02	2.46E+02	1.1 m $Ga(NO_3)_3$ in D_2O	24.001354
71	Ga	30.5813	1.43E–01	3.35E+02	1.1 m $Ga(NO_3)_3$ in D_2O	30.496704
73	Ge	3.4989	1.41E–03	6.44E–01	Me_4Ge + 5% C_6D_6	3.488315
75	As	17.1804	2.54E–02	1.49E+02	0.5 M $NaAsF_6$ in CD_3CN	17.122614
77	Se	19.1587	7.03E–03	3.15E+00	Me_2Se + 5% C_6D_6	19.071513

NMR Properties of Selected Isotopes

Z	A	Sym	Name	*I*	NA (%)	μ_z / μ_N	*Q* [fm^2]	γ [10^7 rad s^{-1} T^{-1}]
	79	Se	Selenium (2.95E5 y)	7/2		-1.018	80	-1.393
35	79	Br	Bromine	3/2	50.69	2.106400	30.5	6.725619
	81	Br	Bromine	3/2	49.31	2.270562	25.4	7.249779
36	83	Kr	Krypton	9/2	11.500	-0.970669	25.9	-1.033097
37	85	Rb	Rubidium	5/2	72.17	1.3533515	27.6	2.5927059
	87	Rb	Rubidium (4.81E10 y)	3/2	27.83	2.751818	13.35	8.786403
38	87	Sr	Strontium	9/2	7.00	-1.093603	33.5	-1.163938
39	89	Y	Yttrium	1/2	100	-0.1374154		-1.316279
40	91	Zr	Zirconium	5/2	11.22	-1.30362	-17.6	-2.49743
41	93	Nb	Niobium	9/2	100	6.1705	-32	6.5674
42	95	Mo	Molybdenum	5/2	15.9	-0.9142	-2.2	-1.7514
	97	Mo	Molybdenum	5/2	9.56	-0.9335	25.5	-1.7884
	99	Mo	Molybdenum (65.924 h)	1/2		*0.375*		3.59
43	99	Tc	Technetium (2.1E5 y)	9/2		5.6847	-12.9	6.0503
44	99	Ru	Ruthenium	5/2	12.76	-0.641	7.9	-1.228
	101	Ru	Ruthenium	5/2	17.06	-0.716	45.7	-1.372
45	103	Rh	Rhodium	1/2	100	-0.08840		-0.84677
46	105	Pd	Palladium	5/2	22.33	-0.642	66	-1.230
47	107	Ag	Silver, Argentum	1/2	51.839	-0.1136797		-1.088918
	109	Ag	Silver	1/2	48.161	-0.13069		-1.2519
48	111	Cd	Cadmium	1/2	12.80	-0.5948861		-5.698315
	113	Cd	Cadmium (7.7E15 y)	1/2	12.22	-0.6223009		-5.960917
49	113	In	Indium	9/2	4.29	5.5289	79.9	5.8845
	115	In	Indium (4.41E14 y)	9/2	95.71	5.5408	81	5.8972
50	115	Sn	Tin	1/2	0.34	-0.91883		-8.8013
	117	Sn	Tin	1/2	7.68	-1.00104		-9.58880
	119	Sn	Tin (Stannum)	1/2	8.59	-1.04728		-10.0317
51	121	Sb	Antimony (Stibium)	5/2	57.21	3.3634	-36	6.4435
	123	Sb	Antimony	7/2	42.79	2.5498	-49	3.4892
	125	Sb	Antimony (2.7586 y)	7/2		*2.63*		3.60
52	123	Te	Tellurium (9.2E16 y)	1/2	0.89	-0.7369478		-7.059101
	125	Te	Tellurium	1/2	7.07	-0.8885051		-8.510843
53	127	I	Iodine	5/2	100	2.81327	-71	5.38957
	129	I	Iodine (1.57E7 y)	7/2		2.6210	-48	3.5866
54	129	Xe	Xenon	1/2	26.4006	-0.777976		-7.45210
	131	Xe	Xenon	3/2	21.2324	0.691862	-11.4	2.209077
55	133	Cs	C(a)esium	7/2	100	2.582025	-0.343	3.533256
56	135	Ba	Barium	3/2	6.592	0.838627	16.0	2.677690
	137	Ba	Barium	3/2	11.232	0.93734	24.5	2.99287
57	137	La	Lanthanum (6E4 y)	7/2		2.695	26	3.688
57	138	La	Lanthanum (1.05E11 y)	5	0.090	3.713646	45	3.557240
	139	La	Lanthanum	7/2	99.910	2.7830455	20	3.808333
58	139	Ce	Cerium (137.64 d)	3/2		*1.06*		3.38
	141	Ce	Cerium (32.508 d)	7/2		*1.09*		1.49
59	141	Pr	Praeseodymium	5/2	100	4.2754	-5.89	8.1907
60	143	Nd	Neodymium	7/2	12.2	-1.065	-63	-1.4574
	145	Nd	Neodymium	7/2	8.3	-0.656	-33	-0.898
61	145	Pm	Promethium (17.7 y)	5/2		3.8	21	7.3
62	147	Sm	Samarium (1.06E11 y)	7/2	14.99	-0.8148	-25.9	-1.115
	149	Sm	Samarium	7/2	13.82	-0.6717	7.5	-0.9192
63	151	Eu	Europium	5/2	47.81	3.4717	90.3	6.6510
	153	Eu	Europium	5/2	52.19	1.5324	241	2.9357
64	155	Gd	Gadolinium	3/2	14.80	-0.2572	127	-0.8212
	157	Gd	Gadolinium	3/2	15.65	-0.3373	135	-1.0770
65	159	Tb	Terbium	3/2	100	2.014	143.2	6.431
66	161	Dy	Dysprosium	5/2	18.889	-0.480	251	-0.920
	163	Dy	Dysprosium	5/2	24.896	0.673	265	1.289
67	163	Ho	Holmium (4570 y)	7/2		4.23	360	5.79
	165	Ho	Holmium	7/2	100	4.132	358	5.654
	166	Ho	Holmium (1200 y)	7		*3.60*	-340	2.46
68	167	Er	Erbium	7/2	22.869	-0.5639	357	-0.7716
	169	Er	Erbium (9.40 d)	1/2		0.4850		4.646
69	169	Tm	Thulium	1/2	100	-0.231		-2.21
	171	Tm	Thulium (1.92 y)	1/2		-0.228		-2.18
70	171	Yb	Ytterbium	1/2	14.28	0.49367		4.7288
	173	Yb	Ytterbium	5/2	16.13	-0.67989	280	-1.30251
71	175	Lu	Lutetium	7/2	97.41	2.232	349	3.0547

NMR Properties of Selected Isotopes

A	Sym	ν_o [MHz]	R_M(H)	R_{NA}(C)	Reference	Ξ [MHz]
79	Se	5.2072	2.97E–03			
79	Br	25.1404	7.94E–02	2.37E+02	0.01 M NaBr in D_2O	25.053980
81	Br	27.0997	9.95E–02	2.88E+02	0.01 M NaBr in D_2O	27.006518
83	Kr	3.8617	1.90E–03	1.28E+00	Kr gas	3.847600
85	Rb	9.6916	1.06E–02	4.50E+01	0.01 M RbCl in D_2O	9.654943
87	Rb	32.8436	1.77E–01	2.90E+02	0.01 M RbCl in D_2O	32.720454
87	Sr	4.3508	2.72E–03	1.12E+00	0.5 M $SrCl_2$ in D_2O	4.333822
89	Y	4.9203	1.19E–04	7.00E–01	$Y(NO_3)_3$ in H_2O/D_2O	4.900198
91	Zr	9.3354	9.49E–03	6.26E+00	$Zr(C_5H_5)_2Cl_2$ in CH_2Cl_2 (sat.) + 5% C_6D_6	9.296298
93	Nb	24.5488	4.88E–01	2.87E+03	$K[NbCl_6]$ in CH_3CN / CD_3CN (sat.)	24.476170
95	Mo	6.5467	3.27E–03	3.06E+00	2 M Na_2MoO_4 in D_2O	6.516926
97	Mo	6.6849	3.49E–03	1.96E+00	2 M Na_2MoO_4 in D_2O	6.653695
99	Mo	13.4272	2.42E–03			
99	Tc	22.6161	3.82E–01		NH_4TcO_4 in H_2O / D_2O	22.508326
99	Ru	4.5903	1.13E–03	8.46E–01	0.3 M $K_4[Ru(CN)_6]$ in D_2O	4.605151
101	Ru	5.1274	1.57E–03	1.58E+00	0.3 M $K_4[Ru(CN)_6]$ in D_2O	5.161369
103	Rh	3.1652	3.17E–05	1.86E–01	$Rh(acac)_3$ in $CDCl_3$ (sat.)	3.186447
105	Pd	4.5975	1.13E–03	1.49E+00	K_2PdCl_6 in D_2O (sat.)	4.576100
107	Ag	4.0704	6.74E–05	2.05E–01	$AgNO_3$ in D_2O (sat.)	4.047819
109	Ag	4.6795	1.02E–04	2.90E–01	$AgNO_3$ in D_2O (sat.)	4.653533
111	Cd	21.3003	9.66E–03	7.27E+00	Me_2Cd neat liq.	21.215480
113	Cd	22.2820	1.11E–02	7.94E+00	Me_2Cd neat liq.	22.193175
113	In	21.9963	3.51E–01	8.85E+01	0.1 M $In(NO_3)_3$ in D_2O + 0.5 M DNO_3	21.865755
115	In	22.0436	3.53E–01	1.99E+03	0.1 M $In(NO_3)_3$ in D_2O + 0.5 M DNO_3	21.912629
115	Sn	32.8994	3.56E–02	7.11E–01	Me_4Sn + 5% C_6D_6	32.718749
117	Sn	35.8430	4.60E–02	2.08E+01	Me_4Sn + 5% C_6D_6	35.632259
119	Sn	37.4986	5.27E–02	2.66E+01	Me_4Sn + 5% C_6D_6	37.290632
121	Sb	24.0858	1.63E–01	5.48E+02	$KSbCl_6$ in CH_3CN / CD_3CN (sat.)	23.930577
123	Sb	13.0425	4.66E–02	1.17E+02	$KSbCl_6$ in CH_3CN / CD_3CN (sat.)	12.959217
125	Sb	13.4527	5.11E–02			
123	Te	26.3870	1.84E–02	9.61E–01	Me_2Te + 5% C_6D_6	26.169742
125	Te	31.8136	3.22E–02	1.34E+01	Me_2Te + 5% C_6D_6	31.549769
127	I	20.1462	9.54E–02	5.60E+02	0.01 M KI in D_2O	20.007486
129	I	13.4067	5.06E–02			
129	Xe	27.8560	2.16E–02	3.35E+01	$XeOF_4$ neat liq.	27.810186
131	Xe	8.2575	2.82E–03	3.51E+00	$XeOF_4$ neat liq.	8.243921
133	Cs	13.2073	4.84E–02	2.84E+02	0.1 M $CsNO_3$ in D_2O	13.116142
135	Ba	10.0092	5.01E–03	1.94E+00	0.5 M $BaCl_2$ in D_2O	9.934457
137	Ba	11.1874	7.00E–03	4.62E+00	0.5 M $BaCl_2$ in D_2O	11.112928
137	La	13.7852	5.50E–02			
138	La	13.2970	9.40E–02	4.97E–01	$LaCl_3$ in D_2O / H_2O	13.194300
139	La	14.2356	6.06E–02	3.56E+02	0.01 M $LaCl_3$ in D_2O	14.125641
139	Ce	12.6514	1.01E–02			
141	Ce	5.5755	3.64E–03			
141	Pr	30.6168	3.35E–01	1.97E+03		
143	Nd	5.4476	3.39E–03	2.43E+00		
145	Nd	3.3555	7.93E–04	3.87E–01		
145	Pm	27.2124	2.35E–01			
147	Sm	4.1678	1.52E–03	1.34E+00		
149	Sm	3.4358	8.52E–04	6.92E–01		
151	Eu	24.8614	1.79E–01	5.04E+02		
153	Eu	10.9737	1.54E–02	4.73E+01		
155	Gd	3.0697	1.45E–04	1.26E–01		
157	Gd	4.0258	3.26E–04	3.00E–01		
159	Tb	24.0376	6.94E–02	4.08E+02		
161	Dy	3.4374	4.74E–04	5.26E–01		
163	Dy	4.8195	1.31E–03	1.91E+00		
163	Ho	21.6369	2.13E–01			
165	Ho	21.1356	1.98E–01	1.16E+03		
166	Ho	9.2072	5.83E–02		(+6 keV excited state)	
167	Er	2.8842	5.04E–04	6.77E–01		
169	Er	17.3658	5.24E–03			
169	Tm	8.2711	5.66E–04	3.32E+00		
171	Tm	8.1637	5.44E–04			
171	Yb	17.6762	5.52E–03	4.63E+00	0.171 M $Yb(\eta\text{-}C_5Me_5)_2(THF)_2$ in THF	17.499306
173	Yb	4.8688	1.35E–03	1.28E+00		
175	Lu	11.4185	3.13E–02	1.79E+02		

NMR Properties of Selected Isotopes

Z	A	Sym	Name	*I*	NA (%)	μ_z / μ_N	*Q* [fm^2]	γ [10^7 rad s^{-1} T^{-1}]
	176	Lu	Lutetium (3.78E10 y)	7	2.59	3.169	497	2.168
72	177	Hf	Hafnium	7/2	18.60	0.7935	337	1.0858
	179	Hf	Hafnium	9/2	13.62	-0.641	379	-0.682
73	179	Ta	Tantalum (1.82 y)	7/2		2.289	337	3.132
	180	Ta	Tantalum (1.2E15 y)	9	0.012	4.825	495	2.568
	181	Ta	Tantalum	7/2	99.988	2.3705	317	3.2438
74	183	W	Tungsten (Wolfram)	1/2	14.31	0.11778476		1.1282407
75	185	Re	Rhenium	5/2	37.40	3.1871	218	6.1057
	187	Re	Rhenium (4.35E10 y)	5/2	62.60	3.2197	207	6.1682
76	187	Os	Osmium	1/2	1.96	0.06465189		0.6192897
	189	Os	Osmium	3/2	16.15	0.659933	85.6	2.107130
77	191	Ir	Iridium	3/2	37.3	0.1507	81.6	0.4812
	193	Ir	Iridium	3/2	62.7	0.1637	75.1	0.5227
78	195	Pt	Platinum	1/2	33.832	0.60952		5.8385
79	197	Au	Gold, Aurum	3/2	100	0.148158	54.7	0.473060
80	199	Hg	Mercury, Hydrargyrum	1/2	16.87	0.5058855		4.845793
	201	Hg	Mercury	3/2	13.18	-0.560226	38.6	-1.788770
81	203	Tl	Thallium	1/2	29.52	1.6222579		15.539339
	205	Tl	Thallium	1/2	70.48	1.6382146		15.692186
82	205	Pb	Lead (1.73E7 y)	5/2		0.7117	23	1.3635
	207	Pb	Lead (Plumbum)	1/2	22.1	0.58219		5.5767
83	209	Bi	Bismuth	9/2	100	4.1103	-51.6	4.3747
84	209	Po	Polonium (102 y)	1/2		0.68		6.51
86	211	Rn	Radon (14.6 h)	1/2		0.601		5.76
87	212	Fr	Francium (19.3 m)	5		4.62	-10	4.43
88	225	Ra	Radium (14.9 d)	1/2		-0.734		-7.03
89	227	Ac	Actinium (21.77 y)	3/2		1.1	170	3.5
90	229	Th	Thorium (7.34E3 y)	5/2		0.46	430	0.88
91	231	Pa	Protactinium (3.25E4 y)	3/2	100	*2.01*	-172	6.42
92	233	U	Uranium (1.592E5 y)	5/2		*0.59*	366.3	1.13
	235	U	Uranium (7.04E8 y)	7/2	0.7204	-0.38	493.6	-0.52
	238	U	Uranium (4.468E9 y)	0	99.274		1390	
93	237	Np	Neptunium (2.14E6 y)	5/2		3.14	386.6	6.02
94	239	Pu	Plutonium (2.410E4 y)	1/2		0.203		1.94
	241	Pu	Plutonium (14.4 y)	5/2		-0.68	560	-1.30
95	241	Am	Americium (432.7 y)	5/2		1.58	314	3.03
	243	Am	Americium (7.37E3 y)	5/2		1.50	286	2.87
96	243	Cm	Curium (29.1 y)	5/2		*0.41*		0.79
	245	Cm	Curium (8.48E3 y)	7/2		*0.5*		0.68
	247	Cm	Curium (1.56E7 y)	9/2		*0.37*		0.39
97	247	Bk	Berkelium (1.4E2 y)	(3/2)		*no data*		
	249	Bk	Berkelium (320 d)	7/2		*2.0*		2.7
98	251	Cf	Californium (9.0E2 y)	1/2		*no data*		
99	252	Es	Einsteinium (472 d)	(5)		*no data*		
	253	Es	Einsteinium (20.47 d)	7/2		4.10	670	5.61
100	253	Fm	Fermium (3.0 d)	(1/2)		*no data*		
	257	Fm	Fermium (100.5 d)	(9/2)		*no data*		

This Table (updated Oct. 2009) was assembled and calculated by W.E. Hull using information from the following sources:

De Laeter et al. *Pure Appl Chem* 75 (2003) 683-800. (isotope abundances)

Harris RK, et al. *Pure Appl Chem* 73 (2001) 1795-1818 and 80 (2008) 59-84. (shift references)

Mills I, et al. *Quantities, Units and Symbols in Physical Chemistry* (IUPAC recommendations 1993, corrections 1995). Blackwell Scientific (1993, 1995).

Pyykkö P. Spectroscopic nuclear quadrupole moments. Mol. Phys. 99 (2001) 1617-1629.

NMR Properties of Selected Isotopes

A	Sym	ν_o [MHz]	R_M(H)	R_{NA}(C)	Reference	Ξ [MHz]
176	Lu	8.1049	3.98E–02	6.05E+00		
177	Hf	4.0588	1.40E–03	1.53E+00		
179	Hf	2.5502	5.47E–04	4.38E–01		
179	Ta	11.7085	3.37E–02			
180	Ta	9.5979	1.06E–01	7.48E–02	(+77 keV excited state)	
181	Ta	12.1254	3.74E–02	2.20E+02	$KTaCl_6$ in CH_3CN (sat.)	11.989600
183	W	4.2174	7.50E–05	6.31E–02	1 M Na_2WO_4 in D_2O	4.166387
185	Re	22.8233	1.39E–01	3.05E+02	0.1 M $KReO_4$ in D_2O	22.524600
187	Re	23.0568	1.43E–01	5.26E+02	0.1 M $KReO_4$ in D_2O	22.751600
187	Os	2.3149	1.24E–05	1.43E–03	0.98 M OsO_4 in CCl_4	2.282331
189	Os	7.8765	2.44E–03	2.32E+00	0.98 M OsO_4 in CCl_4	7.765400
191	Ir	1.7986	2.91E–05	6.38E–02		
193	Ir	1.9538	3.73E–05	1.37E–01		
195	Pt	21.8243	1.04E–02	2.07E+01	1.2 M Na_2PtCl_6 in D_2O	21.496784
197	Au	1.7683	2.76E–05	1.62E–01		
199	Hg	18.1136	5.94E–03	5.89E+00	Me_2Hg neat liq. (toxic!)	17.910822
201	Hg	6.6864	1.49E–03	1.16E+00	Me_2Hg neat liq. (toxic!)	6.611583
203	Tl	58.0862	1.96E–01	3.40E+02	$Tl(NO_3)_3$	57.123200
205	Tl	58.6575	2.02E–01	8.36E+02	$Tl(NO_3)_3$	57.683838
205	Pb	5.0966	1.54E–03			
207	Pb	20.8458	9.06E–03	1.18E+01	Me_4Pb + 5% C_6D_6	20.920599
209	Bi	16.3525	1.44E–01	8.48E+02	$Bi(NO_3)_2$ sat. in conc. HNO_3 + 50% D_2O	16.069288
209	Po	24.3479	1.44E–02			
211	Rn	21.5193	9.97E–03			
212	Fr	16.5423	1.81E–01			
225	Ra	26.2814	1.82E–02			
227	Ac	13.1288	1.13E–02			
229	Th	3.2941	4.17E–04			
231	Pa	23.9899	6.90E–02	4.06E+02		
233	U	4.2251	8.80E–04			
235	U	1.9437	1.54E–04	6.53E–03	UF_6 + 10% C_6D_6	1.841400
238	U					
237	Np	22.4860	1.33E–01			
239	Pu	7.2686	3.84E–04			
241	Pu	4.8696	1.35E–03			
241	Am	11.3146	1.69E–02			
243	Am	10.7417	1.45E–02			
243	Cm	2.9361	2.95E–04			
245	Cm	2.5576	3.51E–04			
247	Cm	1.4720	1.05E–04			
249	Bk	10.2302	2.25E–02			
253	Es	20.9719	1.94E–01			

Stone NJ. *Table of Nuclear Magnetic Dipole and Electric Quadrupole Moments (2001)* [http://www.nndc.bnl.gov/nndc/stone_moments/nuclear-moments.pdf].
LBNL Isotopes Project Nuclear Data Dissemination Home Page. *Table of Nuclear Moments* [http://ie.lbl.gov/toipdf/mometbl.pdf].
NUDAT 2 half-life data: http://www.nndc.bnl.gov/

NMR Tables

Isotopes sorted according to spin and nucleon numbers

Isotope			Spin	Isotope			Spin	Isotope			Spin
1	H	Hydrogen	1/2	39	K	Potassium	3/2	173	Yb	Ytterbium	5/2
3	H	Tritium *	1/2	41	K	Potassium	3/2	185	Re	Rhenium	5/2
3	He	Helium	1/2	53	Cr	Chromium	3/2	187	Re	Rhenium	5/2
13	C	Carbon	1/2	61	Ni	Nickel	3/2	229	Th	Thorium *	5/2
15	N	Nitrogen	1/2	63	Cu	Copper	3/2	237	Np	Neptunium *	5/2
19	F	Fluorine	1/2	65	Cu	Copper	3/2	241	Am	Americium *	5/2
29	Si	Silicon	1/2	69	Ga	Gallium	3/2	243	Am	Americium *	5/2
31	P	Phosphorus	1/2	71	Ga	Gallium	3/2	10	B	Boron	3
57	Fe	Iron	1/2	75	As	Arsenic	3/2	39	Ar	Argon *	7/2
77	Se	Selenium	1/2	79	Br	Bromine	3/2	43	Ca	Calcium	7/2
89	Y	Yttrium	1/2	81	Br	Bromine	3/2	45	Sc	Scandium	7/2
103	Rh	Rhodium	1/2	87	Rb	Rubidium	3/2	49	Ti	Titanium	7/2
107	Ag	Silver	1/2	131	Xe	Xenon	3/2	51	V	Vanadium	7/2
109	Ag	Silver	1/2	135	Ba	Barium	3/2	59	Co	Cobalt	7/2
111	Cd	Cadmium	1/2	137	Ba	Barium	3/2	123	Sb	Antimony	7/2
113	Cd	Cadmium	1/2	139	Ce	Cerium *	3/2	133	Cs	C(a)esium	7/2
115	Sn	Tin	1/2	155	Gd	Gadolinium	3/2	139	La	Lanthanum	7/2
117	Sn	Tin	1/2	157	Gd	Gadolinium	3/2	143	Nd	Neodymium	7/2
119	Sn	Tin	1/2	159	Tb	Terbium	3/2	145	Nd	Neodymium	7/2
123	Te	Tellurium	1/2	189	Os	Osmium	3/2	147	Sm	Samarium	7/2
125	Te	Tellurium	1/2	191	Ir	Iridium	3/2	149	Sm	Samarium	7/2
129	Xe	Xenon	1/2	193	Ir	Iridium	3/2	165	Ho	Holmium	7/2
169	Tm	Thulium	1/2	197	Au	Gold	3/2	167	Er	Erbium	7/2
171	Yb	Ytterbium	1/2	201	Hg	Mercury	3/2	175	Lu	Lutetium	7/2
183	W	Tungsten	1/2	227	Ac	Actinium *	3/2	177	Hf	Hafnium	7/2
187	Os	Osmium	1/2	231	Pa	Protactinium *	3/2	181	Ta	Tantalum	7/2
195	Pt	Platinum	1/2	17	O	Oxygen	5/2	235	U	Uranium *	7/2
199	Hg	Mercury	1/2	25	Mg	Magnesium	5/2	245	Cm	Curium *	7/2
203	Tl	Thallium	1/2	27	Al	Alumin(i)um	5/2	249	Bk	Berkelium *	7/2
205	Tl	Thallium	1/2	47	Ti	Titanium	5/2	253	Es	Einsteinium *	7/2
207	Pb	Lead	1/2	55	Mn	Manganese	5/2	73	Ge	Germanium	9/2
209	Po	Polonium *	1/2	67	Zn	Zinc	5/2	83	Kr	Krypton	9/2
211	Rn	Radon *	1/2	85	Rb	Rubidium	5/2	87	Sr	Strontium	9/2
225	Ra	Radium *	1/2	91	Zr	Zirconium	5/2	93	Nb	Niobium	9/2
239	Pu	Plutonium *	1/2	95	Mo	Molybdenum	5/2	99	Tc	Technetium *	9/2
251	Cf	Californium *	1/2	97	Mo	Molybdenum	5/2	113	In	Indium	9/2
2	H	Deuterium	1	99	Ru	Ruthenium	5/2	115	In	Indium	9/2
6	Li	Lithium	1	101	Ru	Ruthenium	5/2	179	Hf	Hafnium	9/2
14	N	Nitrogen	1	105	Pd	Palladium	5/2	209	Bi	Bismuth	9/2
7	Li	Lithium	3/2	121	Sb	Antimony	5/2	138	La	Lanthanum	5
9	Be	Beryllium	3/2	127	I	Iodine	5/2	212	Fr	Francium *	5
11	B	Boron	3/2	141	Pr	Praeseodymium	5/2	50	V	Vanadium	6
21	Ne	Neon	3/2	145	Pm	Promethium *	5/2	176	Lu	Lutetium	7
23	Na	Sodium	3/2	151	Eu	Europium	5/2				
33	S	Sulfur	3/2	153	Eu	Europium	5/2				
35	Cl	Chlorine	3/2	161	Dy	Dysprosium	5/2				
37	Cl	Chlorine	3/2	163	Dy	Dysprosium	5/2				

* Unstable isotope with lifetime suitable for NMR.

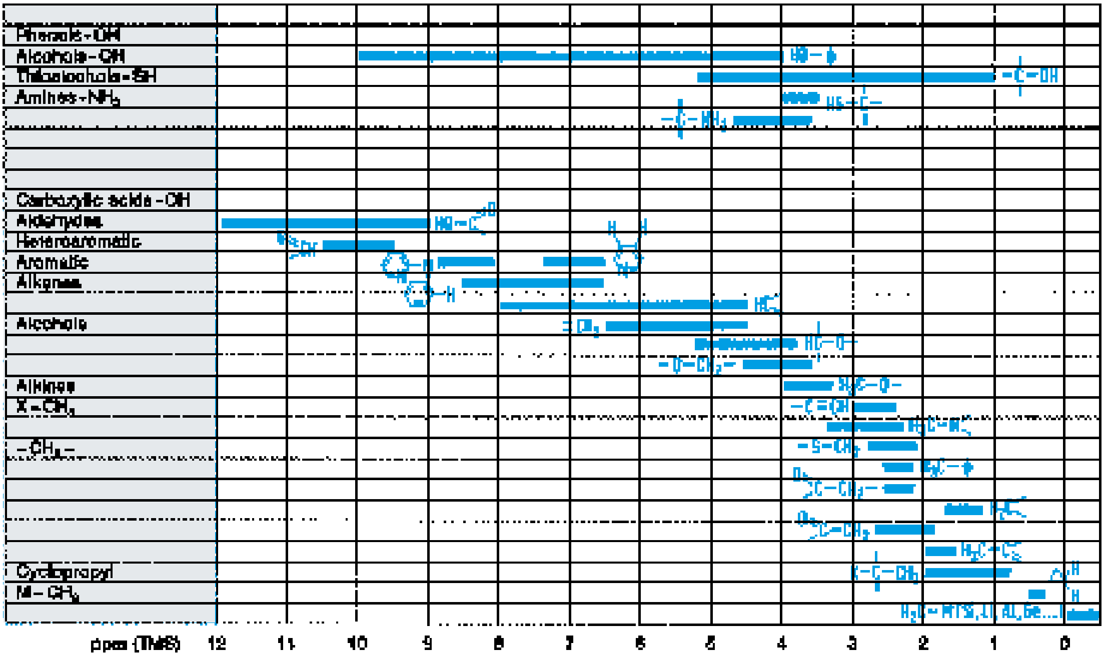
Properties of Selected Deuterated Solvents for NMR

Solvent	Formula	MW_{ave}	Density [d_4^{20}]	MP [°C]	BP [°C]	RI [n_D^{20}]	Dielec. [ε]	^{1}H shift (Mult.) [ppm]	J(HD) [Hz]	^{13}C Shift (Mult.) [ppm]	J(CD) [Hz]	H_2O/HDO Shift [ppm]
Acetic Acid-d4	$C_2D_4O_2$	64.08	1.119	15.9	115.5	1.368	6.1	11.65 2.04 (5)	2.2	178.99 20 (7)	20	11.5
Acetone-d6	C_3D_6O	64.12	0.872	–93.8	55.5	1.3554	20.7	2.05 (5)	2.2	29.92 (7) 206.68 (13)	19.4 0.9	2.84/ 2.81
Acetonitrile-d3	C_2D_3N	44.07	0.844	–46	80.7	1.3406	37.5	1.94 (5)	2.5	1.39 (7) 118.69	21	2.12
Benzene-d6	C_6D_6	84.15	0.950	6.8	79.1	1.4986	2.3	7.16		128.39 (3)	24.3	0.4
Chloroform-d1	$CDCl_3$	120.38	1.500	–64.1	60.9	1.4445	4.8	7.24		77.23 (3)	32	1.55
Cyclohexane-d12	$C_6D_{12}O$	96.24	0.890	7	78		2	1.38		26.43 (5)	19	0.80
Deuterium oxide	D_2O	20.03	1.107	3.8	101.4	1.328	78.5	4.81				
1,2-Dichloroethane-d4	$C_2D_4Cl_2$	102.99	1.307	–35	83	1.443		3.72 (5)		43.6 (5)	23.5	
Dichloromethane-d2	CD_2Cl_2	86.95	1.362	–97	39.5	1.362		5.32 (3)	1.1	54 (5)	27.2	1.52
Diethylether-d10	$C_4D_{10}O$	84.19	0.78	–116.3	34.6			3.34 (m) 1.07 (m)		65.3 (5) 14.5 (7)	21 19	
Diethylene glycol dimethyl ether-d14 (diglyme-d14)	$C_6D_{14}O_3$	148.26	0.95	–68	162			3.49 (br) 3.40 (br) 3.22 (5)	1.5	70.7 (5) 70 (5) 57.7 (7)	21 21 21	
1,2-Dimethoxyethane-d10 (glyme-d10)	$C_4D_{10}O_2$	100.18	0.86	–58	83			3.40 (m) 3.22 (5)	1.6	71.7 (5) 57.8 (7)	21 21	
N,N-Dimethyl-formamide-d7	C_3D_7NO	80.14	1.04	–60	153	1.428	36.7	8.03 2.92 (5) 2.75 (5)	1.9 1.9	163.15 (3) 34.89 (7) 29.76 (7)	29.4 21.0 21.1	3.45
Dimethyl sulfoxide-d6	$C_2D_6O_S$	84.17	1.190	20.2	190	1.4758	46.7	2.50 (5)	1.9	39.51 (7)	21.0	3.3
1,4-Dioxane-d6	$C_4D_8O_2$	96.16	1.129	12	99	1.4198	2.2	3.53 (m)		66.66 (5)	21.9	2.4
Ethanol-d6	C_2D_6O	52.11	0.888	–114.5	78	1.358	24.5	5.29 3.56 1.11 (m)		56.96 (5) 17.31 (7)	22 19	5.2
Methanol-d4	CD_4O	36.07	0.89	–99	65	1.3256	32.7	4.87 3.31 (5)	1.7	49.15 (7)	21.4	4.86
Methyl cyclohexane-d14	C_7D_{14}	112.27	0.77	–126	101	1.4189						
Nitrobenzene-d5	$C_6D_5NO_2$	128.14	1.253	6	211	1.5498		8.11 (br) 7.67 (br) 7.50 (br)		148.6 134.8 (3) 129.5 (3) 123.5 (3)	24.5 25 26	2.42
Nitromethane-d3	CD_3NO_2	64.06	1.19	–26	100	1.3795		4.33 (5)		62.8 (7)	22	2.2
2-Propanol-d8	C_3D_8O	68.15	0.786	–89.5	82.4	1.3728		5.12 3.89 (br) 1.10 (br)		62.9 (3) 24.2 (7)	21.5 19	
Pyridine-d5	C_5D_5N	84.13	1.02	–41	114	1.5079	12.4	8.74 7.58 7.22		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 25	4.97
Tetrachloroethane-d2	$C_2D_2Cl_4$	169.86	1.7	–43	146	1.493		5.91 (5)		74.2 (5)		1.5
Tetrahydrofuran-d8	C_4D_8O	80.16	0.99	–108	64	1.4035	7.6	3.58 1.73		67.57 (5) 25.37 (5)	22.2 20.2	2.42
Toluene-d8	C_7D_8	100.19	0.94	–85	109	1.4932	2.4	7.09 (m) 7.00 6.98 (m) 2.09 (5)	2.3	137.86 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	23 24 24 19	0.45
2,2,2-Trifluoroacetic Acid-d1	$C_2DF_3O_2$	115.03	1.50	–15	71	1.30		11.50		164.2 (4) 116.6 (4)		11.5
2,2,2-Trifluoroethanol-d3	$C_2D_3F_3$	87.06	1.42	–44	77	1.30		5.02 3.88 (4x3)	2 (9)	126.3 (4) 61.5 (4x5)	22	5

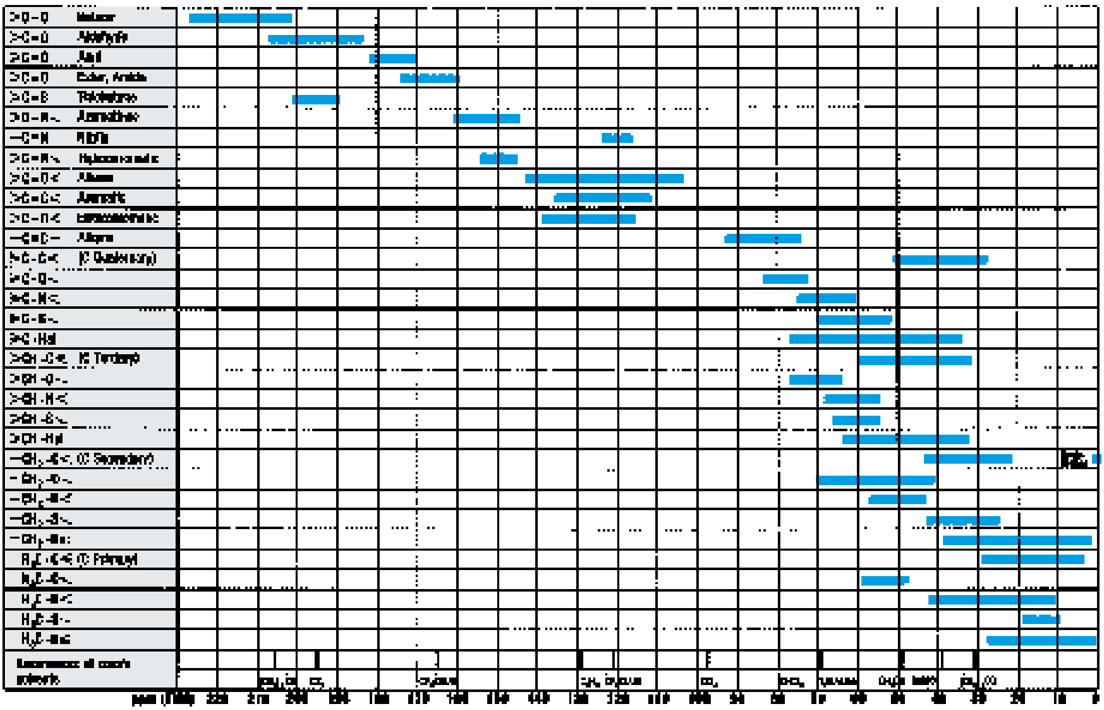
This Table summarizes the physical properties of deuterated solvents and the chem. shifts (rel. to TMS) and deuterium couplings for the solvent signals and the approximate shifts for residual water (last column).

NMR Tables

[1]H Chemical Shifts in Organic Compounds



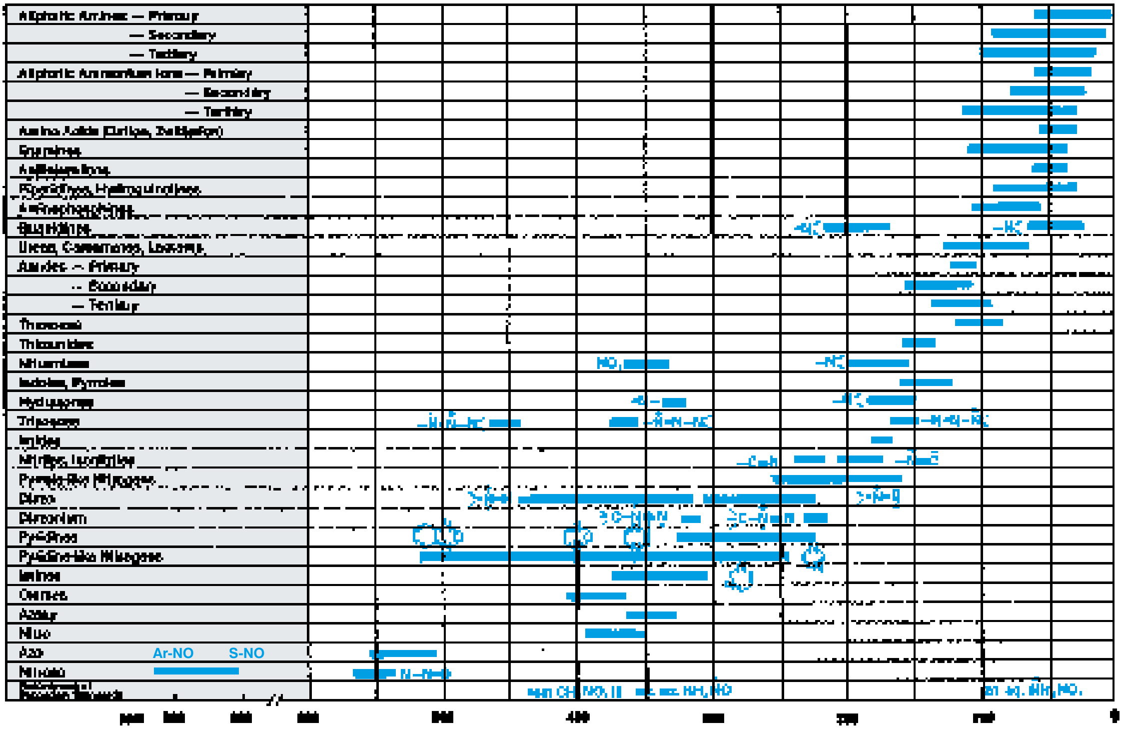
[13]C Chemical Shifts in Organic Compounds*



* Relative to internal tetramethylsilane.

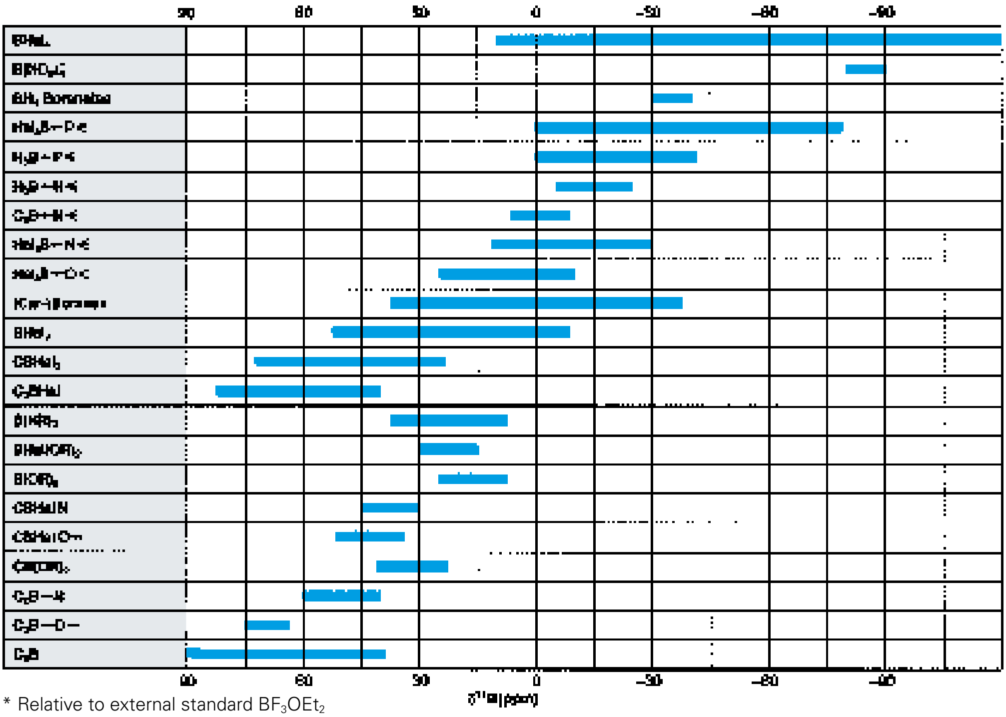
NMR Tables

^{15}N Chemical Shifts in Organic Compounds*



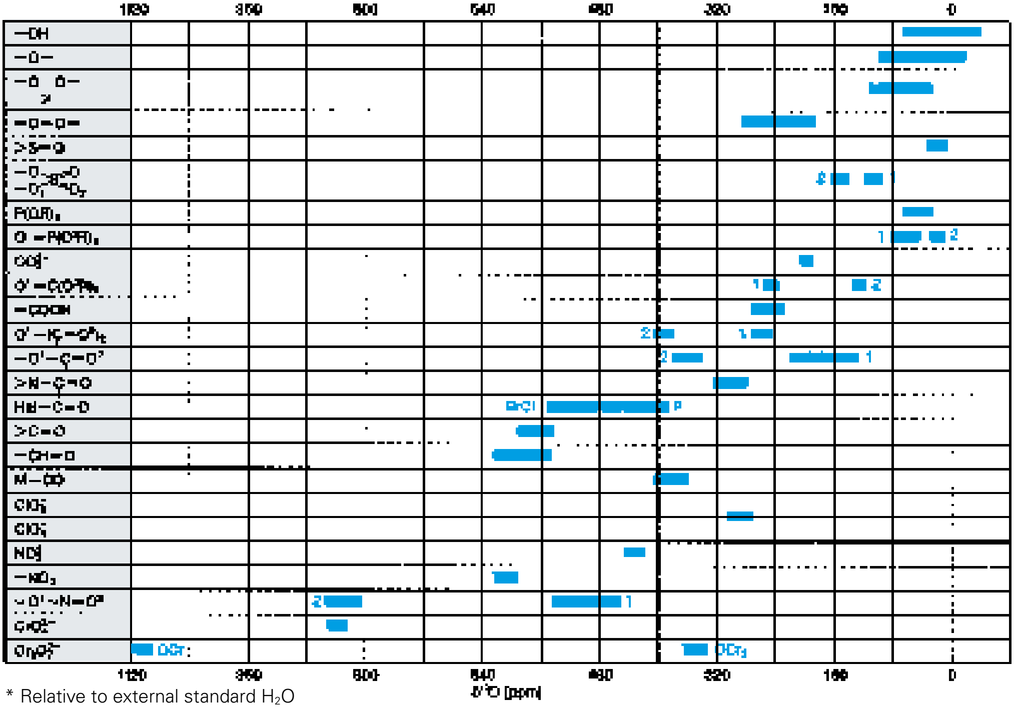
* Relative to external liquid ammonia at 25°C. Data taken from: G. C. Levy and R. L. Lichter: "Nitrogen-15 Nuclear Magnetic Resonance Spectroscopy", J. Wiley, 1979.

^{11}B Chemical Shifts*



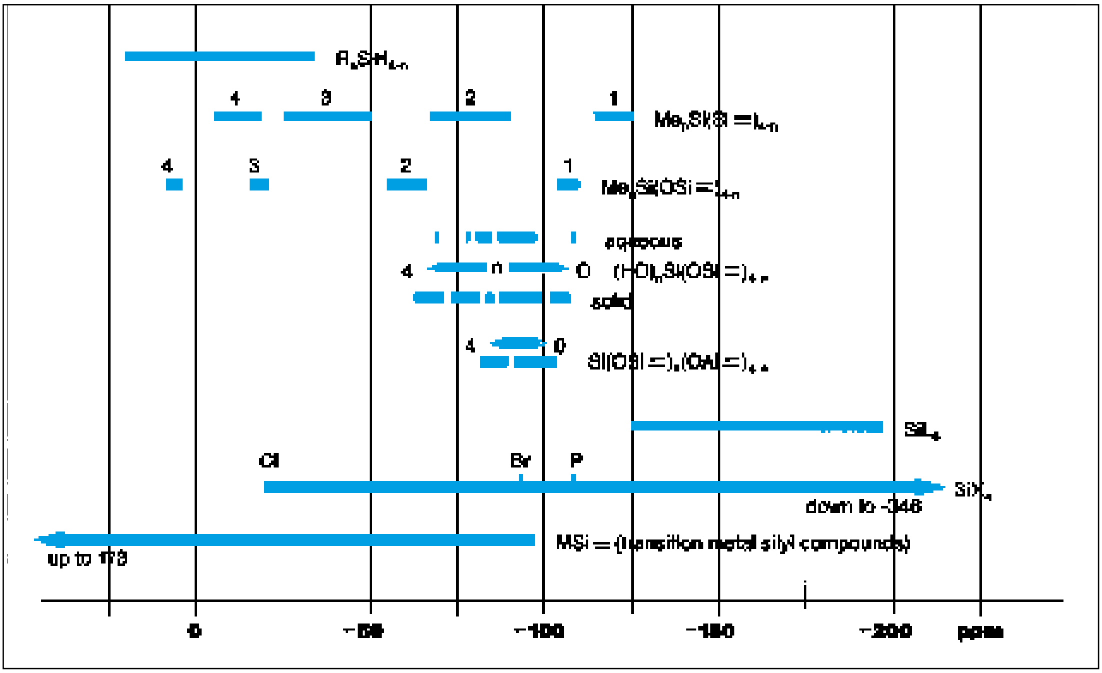
* Relative to external standard BF_3OEt_2

[17]O Chemical Shifts*



* Relative to external standard H_2O

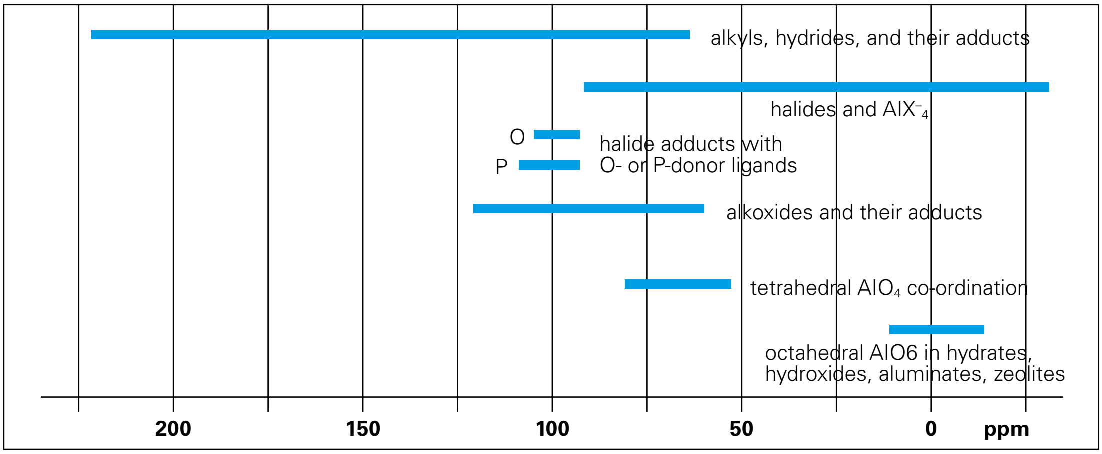
[29]Si Chemical Shifts*



* Relative to $Si(CH_3)_4$.

NMR Tables

^{27}Al Chemical Shifts*



* Relative to $Al(H_2O)^{3+}_6$.

MRI Tables

Abbreviations and Acronyms Used in Magnetic Resonance Imaging

Method	Description	Equivalent acronyms
SINGLEPULSE	Basic pulse-and-acquire spectroscopy	FID
NSPECT	Non-localized spectroscopy with NOE and decoupling options	FID
CSI	Chemical shift imaging with optional PRESS localization	
PRESS	Localized MRS with double spin echo	
STEAM	Localized MRS with stimulated echo (for short TE)	
ISIS	Localized MRS with inversion-based voxel definition	OSIRIS
DtiEpi	Diffusion tensor imaging with EPI (SE and STE)	PGSE-EPI
DtiStandard	Diffusion tensor imaging with 2DFT (SE and STE)	PGSE
EPI	Echo-Planar Imaging (GE and SE), single-shot or interleaved, with navigator-based phase stabilization and automatic ghost correction	
FAIR_EPI	Pulsed arterial spin labelling-based perfusion imaging with EPI	
FC2D_ANGIO	Time-of-flight angiography flow-compensated	TOF-angio
FL2D_ANGIO	Time-of-flight angiography w/o flow-comp. (short TE)	
FISP	Fast gradient echo with steady state signal selection (FID, echo or fully balanced), and optional inversion recovery for T1 mapping.	FLASH, FAST, FISP, PSIF, CE-FAST, SSFP, GRASS, TrueFISP
FLASH	Gradient echo	FISP, GRASS, FAST
GEFC	Gradient echo with flow compensation	
MDEFT	T1-weghted hi-res imaging with inversion-recovery preparation	MPRAGE
MGE	Multiple gradient echo	
MSME	Multiple spin echo including T2 mapping	
RARE	Fast spin echo based on CPMG sequence	FSE, TSE
RAREVTR	RARE with variable TR for simultaneous T1&T2 mapping	
RAREst	Fast spin echo for short TE using slew-rate-optimized gradients	HASTE
FLOW_MAP	Quantitative flow mapping and PC-angio	
UTE	Ultra-short TE radial scan	
FieldMap	Quantitative B0 mapping, part of the MAPSHIM tool for localized high-order shimming	
SPIRAL	Fast MRI with spiral k-space scan	
IntraGate-FLASH	Cardiac and respiration-cine with retrospective (trigger-free) gating	

NMR Tables

Additivity Parameters for ^{13}C Chemical Shifts in Substituted Benzenes

$\delta_i = 128.5 + S_i(\delta_j)$, $S_i(\delta_I)$ refers to the carbon atom bearing the substituent

Substituent	$S_i(\delta_I)$	$S_i(\delta_o)$	$S_i(\delta_m)$	$S_i(\delta_p)$	Substituent	$S_i(\delta_I)$	$S_i(\delta_o)$	$S_i(\delta_m)$	$S_i(\delta_p)$
–H	0.0	0.0	0.0	0.0	**–I**	–32.3	9.9	2.6	–0.4
–CH_3	9.3	0.6	0.0	–3.1	**–OH**	26.9	–12.7	1.4	–7.3
–CH_2CH_3	15.7	–0.6	–0.1	–2.8	**–OCH_3**	30.2	–14.7	0.9	–8.1
–$CH(CH_3)_2$	20.1	–2.0	0.0	–2.5	**–NH_2**	19.2	–12.4	1.3	–9.5
–$C(CH_3)_3$	22.1	–3.4	–0.4	–3.1	**–$N(CH_3)_2$**	22.4	–15.7	0.8	–11.8
–Cyclopropyl	15.1	–3.3	–0.6	–3.6	**–$N(C_6H_5)_2$**	19.3	–4.4	0.6	–5.9
–CH_2Cl	9.1	0.0	0.2	–0.2	**–NO_2**	19.6	–5.3	0.8	6.0
–CH_2Br	9.2	0.1	0.4	–0.3	**–CN**	–16.0	3.5	0.7	4.3
–CF_3	2.6	–2.2	0.3	3.2	**–NCO**	5.7	–3.6	1.2	–2.8
–CH_2OH	13.0	–1.4	0.0	–1.2	**–$SC(CH_3)_3$**	4.5	9.0	–0.3	0.0
–$CH=CH_2$	7.6	–1.8	–1.8	–3.5	**–COH**	9.0	1.2	1.2	6.0
–C≡CH	–6.1	3.8	0.4	–0.2	**–$COCH_3$**	9.3	0.2	0.2	4.2
–C_6H_5	13.0	–1.1	0.5	–1.0	**–COOH**	2.4	1.6	–0.1	4.8
–F	35.1	–14.3	0.9	–4.4	**–COO^-**	7.6	0.8	0.0	2.8
–Cl	6.4	0.2	1.0	–2.0	**–$COOCH_3$**	2.1	1.2	0.0	4.4
–Br	–5.4	3.3	2.2	–1.0	**–COCl**	4.6	2.9	0.6	7.0

Some Representative ^{19}F Chemical Shifts Referenced to $CFCl_3$

	δ / ppm		δ / ppm		δ / ppm
MeF	-271.9	$CFBr_3$	7.4	$FCH=CH_2$	-114
EtF	-213	CF_2Br_2	7	$F_2C=CH_2$	-81.3
CF_2H_2	-1436	CFH_2Ph	-207	$F_2C=CF_2$	-135
CF_3R	-60 to -70	CF_2Cl_2	-8	C_6F_6	-163
AsF_5	-66	$[AsF_6]^-$	-69.5	$[BeF_4]^-$	-163
BF_3	-131	ClF_3	116; -4	ClF_5	247; 412
IF_7	170	MoF_6	-278	ReF_7	345
SeF_6	55	$[SbF_6]^-$	-109	SbF_5	-108
$[SiF_6]^{2-}$	-127	TeF_6	-57	WF_6	166
XeF_2	258	XeF_4	438	XeF_6	550

Some Representative ^{31}P Chemical Shifts Referenced to 85 % H_3PO_4

(a) Phosphorus (III) compounds			
	δ / ppm		δ / ppm
PMe_3	-62	$PMeF_2$	245
PEt_3	-20	$PMeH_2$	-163.5
$P(n\text{-}Pr)_3$	-33	$PMeCl_2$	192
$P(i\text{-}Pr)_3$	-19.4	$PMeBr_2$	184
$P(n\text{-}Bu)_3$	-32.5	PMe_2F	186
$P(i\text{-}Bu)_3$	-45.3	PMe_2H	-99
$P(s\text{-}Bu)_3$	7.9	PMe_2Cl	96.5
$P(t\text{-}Bu)_3$	63	PMe_2Br	90.5

(b) Phosphorus (V) compounds			
	δ / ppm		δ / ppm
Me_3PO	36.2	Me_3PS	59.1
Et_3PO	48.3	Et_3PS	54.5
$[ME_4P]^+$	24.4	$[Et_4P]^+$	40.1
$[PO_4]^{3-}$	6.0	$[PS_4]^{3-}$	87
PF_5	-80.3	$[PF_6]^-$	-145
PCl_5	-80	$[PCl_4]^+$	86
$MePF_4$	-29.9	$[PCl_6]^-$	-295
Me_3PF_2	-158	Me_2PF_3	8.0

NMR Tables

Some Important Silylated Compounds Used as ^{1}H Shift References

Name	Chemical formula	Abbre-viation	Mole-cular weigth	Boiling or melting point (°C)	δ ^{1}H ppm rel. TMS
Tetramethylsilane	$(CH_3)_4Si$	TMS	88.2	BP = 26.3	0
Hexamethyldisilane	$(CH_3)_3Si–Si(CH_3)_3$	HMDS	146.4	BP = 112.3	0.037
Hexamethyldisiloxane	$(CH_3)_3Si–O–Si(CH_3)_3$	HMDSO	162.4	BP = 100	0.055
Hexamethyldisilazane	$(CH_3)_3Si–NH–Si(CH_3)_3$	HMDSA	161.4	BP = 125	0.042
3-(trimethylsilyl)propane sulfonic acid soduim salt 4,4-dimethyl-4-silapentane sodium sulfonate	$(CH_3)_3Si(CH_2)_3SO_3Na$	TSPSA DSS	218.3	MP = 200	0.015
3-(trimethylsilyl)propionic acid sodium salt 4,4-dimethyl-4-silapentane sodium carboxylate	$(CH_3)_3Si(CH_2)_2COONa$	TSP DSC	168.2	MP > 300	0.000
3-(trimethylsilyl) 2,2,3,3-tetra-deuteropropionic acid sodium salt	$(CH_3)_3Si(CD_2)_2COONa$	TSP-d_4	172.2	MP > 300	0.000
Octamethylcyclotetrasiloxane	$(CH_3)_2Si[O–Si(CH_3)_2]_3–O$ (ring)	OCTS	296.8	BP = 175 MP = 16.8	0.085
1,1,3,3,5,5-hexakis-(trideutero-methyl)-1,3,5-trisilacyclohexane	$(CD_3)_2Si–CH_2–Si(CD_3)_2$ $CH_2–Si(CD_3)_2–CH_2$ (ring)	CS-d_{18}	216.6	BP = 208	-0.327
Tetrakis-(trimethylsilyl)-methane	$[(CH_3)_3Si]_4C$	TTSM	304.8	MP = 307	0.236

Enhancement Factors η_{NOE} and η_{INEPT} for X {^{1}H} Nuclear Overhauser and INEPT Experiments

X	^{19}F	^{31}P	^{11}B	^{13}C	^{15}N	^{29}Si	^{57}Fe	^{103}Rh	^{109}Ag	^{119}Sn	^{183}W
η_{NOE} [a]	0.53	1.24	1.56	1.99	–4.93	–2.52	15.41	–15.80	–10.68	–1.33	11.86
η_{INEPT} [b]	1.06	2.47	3.12	3.98	–9.86	–5.03	30.82	–31.59	–21.37	–2.67	23.71

[a] The maximum possible intensity enhancement is equal to $1 + \eta_{NOE}$ in the extreme narrowing limit.
[b] For ^{19}F or ^{31}P as polarization source (irradiated nucleus) the factors η_{NOE} and η_{INEPT} are reduced by the factor 0.941 $[\gamma(^{19}F)/\gamma(^1H)]$ and 0.405 $[\gamma(^{31}P)/\gamma(^1H)]$

Relevant Properties of Cryogenic Fluids

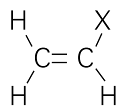
(Liquid helium and nitrogen are used in supercon magnets)

Cryogen	Normal Boiling Point (K)	Latent Heat (J/g)	Amount of Liquid Evaporated by 1 Watt (l/hour)	Liquid Density (g/ml)	Gas Density at NTP (g/ml)	Liquid to NTP Gas Volume Ratio	Enthalpy Change (gas) B.P. to 77 K (J/mole)	Enthalpy Change (gas) 77 to 300 K (J/mole)
Liquid Helium	4.2	20.9	1.038	0.125	1.79×10^{-4}	1 : 700	384	1157
Liquid Hydrogen	20.39	443	0.115	0.071	8.99×10^{-5}	1 : 790	590	2900
Liquid Nitrogen	77.55	198	0.023	0.808	1.25×10^{-3}	1 : 650	–	234
Liquid Oxygen	90.19	212.5	0.015	1.014	1.43×10^{-3}	1 : 797	–	From BP: 193

NTP = normal room temperature and atmospheric pressure

NMR Tables

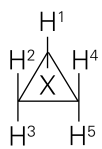
^{1}H, ^{1}H Coupling Constants in Selected Organic Molecules



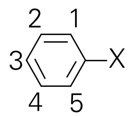
X	$^3J_{cis}$	$^3J_{trans}$	^2J
H	11.6	19.1	2.5
Li	19.3	23.9	7.1
COOH	10.2	17.2	1.7
CN	11.75	17.92	0.91
C_6H_5	11.48	18.59	1.08
CH_3	10.02	16.81	2.08
OCH_3	7.0	14.1	-2.0
Cl	1.3	14.6	-1.4
Br	7.1	15.2	-1.8
F	4.65	12.75	-3.2

H_3C-CH_2-X

X	^3J
Li	8.90
$Si(C_2H_5)_3$	8.0
H	7.5
C_6H_5	7.62
CN	7.60
I	7.45
Br	7.33
CH_3	7.26
Cl	7.23
$N(C_2H_5)_2$	7.13
OC_2H_5	6.97
$^+O(C_2H_5)_2$	4.7



X	$^3J(1,2)$	$^3J(1,3)$	$^3J(2,4)$	$^3J(3,5)$	$^3J(2,5)$	$^2J(2,3)$
H	8.97	5.58	8.97	8.97	5.58	-4.34
Cl	7.01	3.58	10.26	10.58	7.14	-6.01
Br	7.13	3.80	10.16	10.45	7.01	-6.12
I	7.51	4.37	9.89	9.97	6.63	-5.94
NH_2	6.63	3.55	9.65	9.89	6.18	-4.29
CN	8.43	5.12	9.18	9.49	7.08	-4.72
COOH	8.04	4.57	9.26	9.66	7.14	-4.00
COCl	7.88	4.43	9.19	9.99	7.59	-4.46
$COCH_3$	7.96	4.55	8.76	9.60	6.94	-3.41



X	$^3J(1,2)$	$^4J(1,3)$	$^5J(1,4)$	$^4J(1,5)$	$^3J(2,3)$	$^4J(2,4)$
H	7.54	1.37	0.66	1.37	7.54	1.37
Li	6.73	1.54	0.77	0.74	1.42	1.29
CH_3	7.64	1.25	0.60	1.87	7.52	1.51[a]
$COOCH_3$	7.86	1.35	0.63	1.79	7.49	1.31
I	7.93	1.14	0.47	1.88	7.47	1.75
Br	8.05	1.12	0.46	2.1	7.44	1.78
Cl	8.05	1.13	0.48	2.27	7.51	1.72
NH_2	8.02	1.11	0.47	2.53	7.39	1.60
$N(CH_3)_2$	8.40	1.01	0.43	2.76	7.29	1.76
$N(CH_3)_3$	8.55	0.92	0.48	3.05	7.46	1.69
NO_2	8.36	1.18	0.55	2.40	7.47	1.48
OH	8.17	1.09	0.49	2.71	7.40	1.74
OCH_3	8.30	1.03	0.44	2.94	7.36	1.76
F	8.36	1.07	0.43	2.74	7.47	1.82[b]

[a] $^4J(1, CH_3)$ -0.75
$^5J(2, CH_3)$ 0.36
$^6J(3, CH_3)$ -0.62

[b] $^3J(1, F)$ 8.91
$^4J(2, F)$ 5.69
$^5J(3, F)$ 0.22

Substituent Effect S(*i,j*) for J_{HH} in Monosubstituted Benzenes

pos. *i,j*	F	Cl	Br	I	NO_2	OCH_3
1,2	+0.81	+0.61	+0.53	+0.39	+0.77	+0.79
1,3	−0.34	−0.23	−0.27	−0.25	−0.20	−0.32
1,4	−0.24	−0.16	−0.20	−0.19	−0.16	−0.22
1,5	+1.21	+0.87	−0.71	+0.51	+1.02	+1.33
2,3	−0.04	+0.03	−0.05	−0.04	−0.07	−0.16
2,4	+0.39	+0.34	+0.36	+0.37	+0.08	+0.38

Typical Stray Field Data for NMR Magnet Systems

Magnet System ^{1}H MHz/mm Bore	Axial Distance (m) from Magnet Center to 5 Gauss (0.5 mT) Line	Radial Distance (m) from Magnet Center to 5 Gauss (0.5 mT) Line
200 MHz/154 mm US PLUS LH	1.80	0.90
300 MHz/54 mm US LH	0.90	0.60
300 MHz/54 mm Fourier US LH	0.90	0.60
300 MHz/54 mm Ascend ULH	0.90	0.60
300 MHz/89 mm Ascend	1.10	0.55
300 MHz/154 mm US PLUS LH	2.00	1.00
400 MHz/54 mm Ascend	1.00	0.50
400 MHz/54 mm Ascend ULH	1.00	0.50
400 MHz/54 mm Ascend RS	1.00	0.50
400 MHz/89 mm Ascend	1.20	0.60
400 MHz/89 mm Ascend DNP	1.50	1.10
400 MHz/154 mm US PLUS LH	2.55	1.50
500 MHz/54 mm Ascend	1.20	0.60
500 MHz/54 mm Ascend ULH	1.20	0.60
500 MHz/54 mm Ascend RS	1.20	0.60
500 MHz/89 mm Ascend	1.20	0.60
500 MHz/154 mm US PLUS LH	2.55	1.50
600 MHz/54 mm Ascend	1.40	0.70
600 MHz/54 mm Ascend ULH	1.40	0.70
600 MHz/89 mm Ascend	2.00	1.00
600 MHz/89 mm Ascend DNP	2.00	1.00
700 MHz/54 mm Ascend	1.60	0.80
750 MHz/54 mm Ascend	2.00	1.00
750 MHz/89 mm Ascend	2.80	1.40
800 MHz/54 mm Ascend	2.50	1.50
850 MHz/54 mm Ascend	2.70	1.60
850 MHz/89 mm US^2 WB	4.60	3.30
900 MHz/54 mm US^2	4.60	3.30
900 MHz/89 mm US^2 WB	4.60	3.30
950 MHz/54 mm US^2	4.60	3.30
1000 MHz/54 mm UltraStabilized	15.00	12.00

LH = Long Hold, ULH = Ultra Long Hold

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

2D	Two-Dimensional
3D	Three-Dimensional
ACCORDION	2D technique, simultaneous incrementing of evolution and mixing times
ADA	Alternated Delay Acquisition
ADC	Analog-to-Digital Converter, Apparent Diffusion Constant
ADEQUATE	Astonishingly Sensitive DoublE QUAntum Transfer Experiment
ADLF	Adiabatic Demagnetization in the Laboratory Frame
ADRF	Adiabatic Demagnetization in the Rotating Frame
A.E.COSY	Alternative Exclusive COSY
AFP	Adiabtic Fast Passage
AHT	Average Hamiltonian Theory
AJCP	Adiabatic J Cross Polarization
AMCP	Amplitude-Modulated Cross Polarization
ANGIO	MR ANGIOgraphy
APHH-CP	Adiabatic-Passage Hartmann-Hahn Cross Polarization
APT	Attached Proton Test
AQ	AcQuisition
ARP	Adiabatic Rapid Passage
ASIS	Aromatic Solvent-Induced Shift
ASL	Arterial Spin Labeling
ASTM	American Society for Testing and Materials
BASE	BAsis imaging with SElective-inversion preparation
BB	BroadBand, as in decoupling
BDR	Broadband Dipolar Recoupling
bEPI	blipped EPI
bFFE	balanced Fast-Field Echo
BIRD	BIlinear Rotation Decoupling
BIRD/2	half BIRD, bilinear $\pi/2$ pulse
BLEW	A windowless multiple-pulse decoupling sequence
BLEW-*n*	Burum-Linder-Ernst Windowless homonuc. dipolar dec. sequence of *n* pulses
BMS	Bulk Magnetic Susceptibility
BOLD	Blood Oxygenation Level-Dependent contrast (MRI)
BOSS	BimOdal Slice-Selective
BP	BiPhasic
BPP	Bloembergen/Purcell/Pound (theory)
BR-*n*	Burum-Rhim homonuclear dipolar decoupling sequence of *n* pulses
BSP	Bloch-Siegert Phase
BURP	Band-selective Uniform Response Pure-phase pulse
bTFE	balanced Turbo Field Echo
BW	BandWidth
BWR	Bloch-Wangsness-Redfield theory
CA	Contrast Agent
CAMELSPIN	Cross-relaxation Appropriate for Minimolecules Emulated by Locked SPINs
CBCA(CO)NH	$C\beta(i\text{-}1)$ and $C\alpha(i\text{-}1)$, $N(i)$, $H_N(i)$ 3D correl.
CBCANH	$C\beta(i,i\text{-}1)$ and $C\alpha(i,i\text{-}1)$, $N(i)$, $H_N(i)$ 3D correl.
CCPPA	Coupled Cluster Polarization Propagator Approximation
CE	Contrast-Enhanced
CEST	Chemical Exchange Saturation Transfer
CH-COSY	Carbon-Hydrogen COrrelation SpectroscopY
CHESS	CHEmical Shift Selective Imaging Sequence
CHIRP	rf pulse with linear freq. modulation
CIDEP	Chemically Induced Dynamic Electron Polarization
CIDNP	Chemically Induced Dynamic Nuclear Polarization
CINE	"movie-like" MRI
CISS	Constructive Interference Steady State
CNR	Contrast-to-Noise Ratio
COLOC	COrrelated Spectroscopy via LOng-Range Coupling
COLOC-S	COLOC with Suppression of one-bond correlations
CONOESY	Combined COSY/NOESY
CORMA	COmplete Relaxation Matrix Analysis
CORY-*n*	CORY modification of BR-*n*
COSS	COrrelation with Shift Scaling
COSY	COrrelated SpectroscopY
COSY-45	COSY with 45° mixing pulse
COSYDEC	COSY with F_1 DECoupling
COSYLR	COSY for Long-Range couplings
CP	Cross Polarization, Circular Polarization
CPD	Composite-Pulse Decoupling
CPMAS	Cross Polarization Magic-Angle Spinning
CPMG	Carr-Purcell-Meiboom-Gill Sequence
CRAMPS	Combined Rotation And Multiple Pulse Spectroscopy
CRAZED	Correlated Spectroscopy Revamped by Asymmetric Z-gradient Echo Detection
CRINEPT	Cross-correlated Relaxation-enhanced INEPT
CS	Contiguous Slice
CSA	Chemical Shift Anisotropy
CSCM	Chemical Shift Correlation Map
CSI	Chemical Shift Imaging
CT	Constant Time
CW	Continuous Wave
CYCLCROP	CYCLic CROss Polarization
CYCLOPS	CYCLically Ordered Phase Sequence
CYCLPOT	CYCLic POlarization Transfer
DAC	Digital-to-Analog Converter
DAISY	Direct Assignment Interconnection SpectroscopY
DANTE	Delay Alternating with Nutation for Tailored Excitation
DAS	Dynamic Angle Spinning
DCNMR	NMR in Presence of an Electric Direct Current
DD	Dipole-Dipole
DE	Dual Echo, Driven Equilibrium

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

DECSY	Double-quantum Echo Correlated SpectroscopY
DEFT	Driven Equilibrium Fourier Transform
DEPT	Distortionless Enhancement by Polarization Transfer
DEPTH	spin-echo sequence for spatial localization
DEPTQ	DEPT including quaternary carbons
DFT	Discrete Fourier Transformation
DICE	DIrect Connectivity Experiment
DICOM	Digital Imaging and COmmunications in Medicine
DIGGER	Discreet Isolation from Gradient-Governed Elimination of Resonances
DIPSI	Composite-pulse Decoupling In the Presence of Scalar Interactions
DISCO	DIfferences and Sums within COSY
DLB	Differential Line Broadening
DNMR	Dynamic NMR
D.NOESY	Direct cross-relaxation NOESY
DNP	Dynamic Nuclear Polarization
DOC	Double COnstant-Time sequence
DOPT	Dipolar Order Polarization Transfer
DOR	Double-Orientation Rotation
DOSY	Diffusion-Ordered SpectroscopY
DOUBTFUL	DOUBle Quantum Transition for Finding Unresolved Lines
DPFGSE	Double Pulsed Field Gradient Spin Echo
DQ	Double Quantum
DQC	Double Quantum Coherence
DQF	Double Quantum Filter
DQF-COSY	Double Quantum Filtered COSY
DQSY	Double-Quantum COSY
DQ/ZQ	Double Quantum/Zero Quantum Spectroscopy
DRAMA	Dipolar Recovery At the Magic Angle
DREAM	Double-quantum Relay Enhancement by Adiabatic Mixing
DRESS	Depth RESolved Spectroscopy
DRIVE	DRIVen Equilibrium
DRYCLEAN	Diffusion-Reduced water signals in spectroscopY of moleCules moving sLowEr thAN water
DSA	Data-Shift Acquisition
DSC	Dynamic Susceptibility Contrast
DSE	Dual Spin Echo
DTI	Diffusion Tensor Imaging
DTRCF	Double Tilted Rotating Coordinate Frame
DTSE	Double Turbo Spin Echo
DUMBO	Decoupling Using Mind-Boggling Optimization – a numerically optimized phase-modulated homonuc. dipolar dec. sequence
DWI	Diffusion-Weighted Imaging
E-BURP	Excitation BURP pulse
EC	Eddy Currents
E.COSY	Exclusive COrrelation SpectroscopY
ECO-WURST	WURST decoupling with Elimination of Cycling Oscillations
EFG	Electric Field Gradient
EM	Exponential Multiplication
EMF	ElectroMagnetic Field ElectroMotive Force
ENDOR	Electron-Nuclear DOuble Resonance
ENMR	Electrophoretic NMR
EPI	Echo-Planar Imaging
EPR	Electron Paramagnetic Resonance
EPS	Echo-Planar Spectroscopy
ES, ESP	Echo Spacing
E-SHORT	Enhanced SHORT repetition MRI
ESR	Electron Spin Resonace
E.TACSY	Exclusive TACSY
EXORCYCLE	4-step phase cycle for spin echoes
EXSY	EXchange SpectroscopY
FA	Flip Angle
FADE	FASE Acq. with Double Echo
FAIR	Flow-sensitive Alternating Inversion Recovery
FASE	Fast Advanced Spin Echo
FAST	Fourier-Acquired STeady State
FASTMAP	FAST B_0 Field MAPping for shimming
FATE	FAst Turbo Echo
FC	Flow Compensation
FC2D_ANGIO	Flow-Compensated time-of-flight 2D ANGIOgraphy
FE	Field Echo, Frequency Encoding
FFE	Fast Field Echo
FFLG	Flip-Flop Lee-Goldburg decoupling
FFT	Fast Fourier Transform
FGRE	Fast Gradient-Recalled Echo
FID	Free Induction Decay
FIDS	FItting of Doublets and Singlets
FieldMap	B_0 Field Mapping for localized shimming
FIRFT	Fast Inversion-Recovery Fourier Transform
FISP	Fast Imaging with Steady-state Precession
FL2D_ANGIO	FLow-sensitive 2D ANGIOgraphy
FLAIR	FLuid Attenuation Inversion-Recovery
FLASH	Fast Low-Angle SHot imaging
FLOCK	Long-range HETCOR using 3 BIRD pulses
FLOPSY	Flip-FlOP SpectroscopY
FLOW_MAP	Quantitative FLOW MAPping and PC-angiography
FMP	Fast MultiPlanar
fMRI	functional MRI
FOCSY	FOldover-Corrected SpectrospcopY
FONAR	Field-focusing MRI
FOV	Field Of View
FPT	Finite Perturbation Theory
FR	Frequency Encoding
FS	Fat Saturation, Fast Scan

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

FSE	Fast Spin Echo
FSLG	Frequency-Switched Lee-Goldburg – a homonuc. dipolar dec. scheme
FSPGR	Fast SPoiled GRadient Echo
FT	Fourier Transform
FUCOUP	FUlly COUPled Spectroscopy
FWHM	Full (line) Width at Half Maximum
GARP	Globaly Optimized Alternating Phase Rectangular Pulses
GE	Gradient Echo
GEFC	Gradient Echo with Flow Compensation
gem-COSY	geminal-filtered COSY
GES	Gradient-Echo Spectroscopy
GFE	Gradient Field Echo
GRASE	GRAdient and Spin Echo
GRASP	GRadient-Accelerated SPectroscopy
GRASS	Gradient-Recalled Acquisition in the Steady State
GRE	Gradient-Recalled Echo
GRECCO	GRadient-Enhanced Carbon COupling
GROESY	Gradient-Enhanced Selective 1D ROESY
GROPE	Generalized compensation for Resonance Offset and Pulse length Errors
GS	Gradient Spectroscopy
gs- ...	gradient-selected ... (e.g. gs-COSY)
H,X-COSY	H,X shift correlation (X-detected)
HASTE	Half-Fourier Acquisition Single-shot Turbo spin Echo
HBHA (CBCA CO) NH	$H\beta(i\text{-}1)$ and $H\alpha(i\text{-}1)$, $N(i)$, $H_N(i)$ 3D correl.
HCACO	$H\alpha(i)$, $C\alpha(i)$, $C'O(i)$ 3D correl.
HCACON	$H\alpha(i)$, $C\alpha(i)$, $C'O(i)$, $N(i+1)$ 4D correl.
HCA(CO)N	$H\alpha(i)$, $C\alpha(i)$, $N(i+1)$ 3D correl.
HCA(CO) NNH	$H\alpha(i)$, $C\alpha(i)$, $N(i+1)$, $H_N(i+1)$ 4D correl.

HCANNH	$H\alpha(i)$, $C\alpha(i)$, $N(i)$, $H_N(i)$ 3D correl.
(H)CC(CO) NH	$C\alpha,\beta,...(i)$, $N(i+1)$, $H_N(i+1)$ 3D correl.
HCCH-COSY	$H\alpha(i)$, $C\alpha(i)$, $H\beta(i)$ 3D correl.
HCCH-TOCSY	total correlation of side-chain H and C
HDQC	Heteronuclear Double-Quantum Correlation
HEED	Hahn spin-Echo ExtendeD sequence
HET2DJ	HETeronuclear 2D J-correlated
HETCOR	HETeronuclear CORrelation Spectroscopy
HETLOC	HETeronuclear LOng-range Couplings
HEHAHA	HEteronuclear HArtmann HAhn
HMBC	Heteronuclear Multiple-Bond Correlation
HMQ	Heteronuclear Multiple-Quantum
HMQC	Heteronuclear Multiple-Quantum Coherence
HMSC	Heteronuclear Multiple- and Single-bond Correlation
HNCA	$H_N(i)$, $N(i)$, $C\alpha(i)$ and $C\alpha(i\text{-}1)$ 3D shift correlation
HNCA-J	3D HNCA to measure $^3J(H_N,H\alpha)$
HN(CA)NNH	$H_N(i)$, $N(i)$, $N(i+1)$ and $N(i\text{-}1)$ 3D correl.
HN(CA)CO	$H_N(i)$, $N(i)$, $C'O(i)$, and $C'O(i\text{-}1)$ 3D shift correlation
H(N)CACO	$H_N(i)$, $C\alpha(i)$, $C'O(i)$ 3D shift correlation
HNCAHA	$H_N(i)$, $N(i)$, $C\alpha(i)$, $H\alpha(i)$ 4D shift correlation
HNCO	$H_N(i)$, $N(i)$, $C'O(i\text{-}1)$ 3D shift correlation
HN(CO)CA	$H_N(i)$, $N(i)$, $C\alpha(i\text{-}1)$ 3D shift correlation
H(N)COCA	$H_N(i+1)$, $C'O(i)$, $C\alpha(i)$ 3D shift correlation
HN(CO) CAHA	$H_N(i+1)$, $N(i+1)$, $C\alpha(i)$, $H\alpha(i)$ 4D shift correlation
HOESY	Heteronuclear Overhauser Effect SpectroscopY
HOHAHA	HOmonuclear HArtmann-HAhn Spectroscopy

HORROR	double-quantum HOmonucleaR ROtary Resonance
HQQC	Heteronuclear Quadruple-Quantum Correlation
HR	High Resolution
HRPA	Higher Random Phase Approximation
HS	HomoSpoil
HSL	Heteronuclear Spin Lock
HSQC	Heteronuclear Single-Quantum Coherence
HTQC	Heteronuclear Triple-Quantum Correlation
I-BURP	Inversion BURP pulse
ICE	Indirect Connectivity Experiment
IDESS	Improved DEpth Selective single surface coil Spectroscopy
IDR	Inverted Direct Response
IEPI	Interleaved EPI
IFT	Inverse FT
IGLO	Individual Gauge for different Localized Orbitals
INADE-QUATE	Incredible Natural Abundance DoublE QUAnatum Transfer Experiment
INAPT	INEPT with selective 1H excitation
INDOR	INternuclear DOuble Resonance
INEPT	Insensitive Nuclei Enhanced by Polarization Transfer
INEPT+	INEPT with refocusing period for in-phase multiplets
INEPT-R	INEPT Refocused for 1H-dec. spectra
INSIPID	INadequate Sensitivity Improvement by Proton Indirect Detection
IntraGate-FLASH	Cardiac and respiration cine MRI with retrospective (trigger-free) gating
INVERSE	H, X correlation via ^1H detection
IPAP	In-Phase Anti-Phase (in 2D)
IR	Inversion-Recovery
IRMA	Iterative Relaxation Matrix Analysis
ISECR	In-phaSE CRoss peaks (method)

Abbreviations and Acronyms Used in Magnetic Resonance

ISIS	Image-Selected In-vivo Spectroscopy (single-voxel)
IST	Irreducible Spherical Tensor
IVIM	IntraVoxel Incoherent Motion
JCP	J Cross-Polarization
J-mod	J modulation
JR	Jump-and-Return sequence (90_y-τ-90_{-y})
J-res	J-resolved 2D
LAS	Laboratory Axis System
LASE	Low-Angle SE
LB	Line Broadening (via EM)
LG	Lorentz-Gauss window function
LIS	Lanthanide Induced Shift
LORG	Local ORiGin
LOSY	LOcalized SpectroscopY
LP	Linear Polarization, Linear Prediction
LPSVD	Linear Prediction using Singular Value Decomposition
LSR	Lanthanide Shift Reagent
LUT	LookUp Table
MAGROFI	MAgnetization Grid ROtating-Frame Imaging
MARCO POLO	Multiple Analysis by Reduction of Cross peaks and Ordering of Patterns in an Overdetermined Library Organization
MARDI-GRAS	Matrix Analysis of Relaxation for DIstance GeometRy of an Aqueous Structure
MARF	Magic Angle in the Rotating Frame
MAS	Magic-Angle Spinning
MASS	Magic-Angle Sample Spinning
MAST	Motion Artifact Suppression Technique
MDEFT	Modified Driven Equilibrium FT method
ME	MultiEcho
MEDUSA	Technique for the Determination of Dynamic Structures
MEM	Maximum Entropy Method
MEMP	MultiEcho MultiPlanar
MESS	MultiEcho Single Shot
MFISP	Mirrored FISP (PSIF)
MGE	Multiple Gradient Echo
MINIP	MINinmum Intensity Projection
MIP	Maximum Intensity Projection
MLEV	M. Levitt's CPD sequence
MLM	Maximum Likelihood Method
MOTSA	Multiple Overlapping Thin Slab(Slice) Acquisition
MP	Multiple Pulse, MultiPlanar, Magnetization-Prepared
MPF*n*	Multiple-Pulse Decoupling with Phase and Frequency Switching with *n* offsets
MP-GR	MultiPlanar Gradient-Recalled Acq. in Steady State
MPR	MultiPlanar Reconstruction
MP-RAGE	Magnetization-Prepared RApid Gradient Echo (MP-GRE)
MQ	Multiple-Quantum
MQC	Multiple-Quantum Coherence
MQF	Multiple-Quantum Filter
MQHPT	Multiple-Quantum Heteronuclear Polarization Transfer
MQS	Multiple-Quantum Spectroscopy
MR	Magnetic Resonance
MRA	MR Angiography
MREV-*n*	Mansfield-Rhim-Elleman-Vaughan homonuc. dipolar dec. cycle of *n* pulses
MRV	MR Venography
MRI	Magnetic Resonance Imaging
MRS	Magnetic Resonance Spectroscopy
MRSI	Magnetic Resonance Spectroscopic Imaging
MRT	Magnetic Resonance Tomography
MS	MultiSlice
mSENSE	modified SENSE
MS-EPI	MultiShot EPI
MSHOT-*n*	Magic Sandwich High-Order Truncation homonuc. dipolar decoupling sequence with *n* TREV-4 sandwiches
MSME	MultiSlice MultiEcho (T2 mapping)
MSOFT	MultiSlice Off-resonance FaT Suppression
MSP	Multiple Sensitive Point
MSPGSE	Multiple-Stepped PGSE
MT	Magnetization Transfer
MTC	Magnetization Transfer Contrast
MTSA	Multiple Thin-Slab Acquisition
MUSIC	MUltiplicity-Selective In-phase Coherence transfer
MVS	Multiple Volume Spectroscopy
NEDOR	Nuclear Electronic DOuble Resonance
NERO	Nonlinear Excitation with Rejection on Resonance
NEWS	Narrow-gap non-Excitation for Water Suppression
NEX	Number of EXcitations
NMR	Nuclear Magnetic Resonance
NOE	Nuclear Overhauser Effect
NOE-DIFF	NOE-DIFFerence spectroscopy
NOESY	NOE-based 2D shift correlation
NOVEL	Nuclear Orientation Via Electron spin Locking
NPW	No Phase Wrap
NQCC	Nuclear Quadrupole Coupling Constant
NQR	Nuclear Quadrupole Resonance
NQS	Non-Quaternary Suppression
NSPECT	Non-localized SPECTroscopy
OBTUSE	Offset Binomial Tailored for Uniform Spectral Excitation
OCS	Optimized Cosine-Sine pulse
ODMR	Optically Detected Magnetic Resonance
OS	Overcontiguous Slices
OSIRIS	Outer-Volume-Suppressed Image-Related In vivo Spectroscopy – a modification of ISIS
PACE	Prospective Acquisition CorrEction
PAR	Phase-Alternated Rotation of magnetization

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

PARACEST	PARAmagnetic Chemical Exchange Saturation Transfer
PAS	Principal Axis System
PC	Phase Contrast
PCA	Phase Contrast Angio-graphy
P.COSY	Purged COSY
PD	Proton Density
PDLF	Proton-Detected Local Field
PE	Phase Encoding
P.E.COSY	Primitive E.COSY, Purged Exclusive COSY
PEDRI	Proton-Electron Double Resonance Imaging
PELF	Proton-Encoded Local Field
PENDANT	Polarization ENhancement During Attached Nucleus Testing
PEP	Preservation of Equivalent Pathways
PFG	Pulsed Field Gradient
PFGSE	Pulsed Field Gradient Spin Echo
PGSE	Pulsed Gradient Spin Echo
PISEMA	Polarization Inversion with Spin Exchange at the Magic Angle
PITANSEMA	Polarization Inversion Time Averaged Nutation Spin Exchange at the Magic Angle
PJR	Power-adapted Jump and Return
PMFG	Pulsed Magnetic Field Gradient
PMLG	Phase-Modulated Lee-Goldburg dipolar decoupling
PMRFI	Phase-Modulated Rotating-Frame Imaging
POF	Product Operator Formalism
POMMIE	Phase Oscillations to MaxiMIze Editing
POST	Permutationally Offset-STabilized
PRE	Proton Relaxation Enhancement
Presat	Presaturation (usually of solvent)
PRESS	Point-RESolved Spectroscopy
PRFT	Partially Relaxed Fourier Transform
PROPELLER	Periodically Rotated Over-lapping ParallEL Lines with Enhanced Reconstruction
PS	Partial Saturation
PS-COSY	Phase-Sensitive COSY
PSD	Phase-Sensitive Detection
PSIF	mirrored FISP (SE acquisition)
PT	Polarization Transfer
PW	Pulse Width
PWI	Perfusion-Weighted Imaging
Q	Quality Factor (of RF coil/circuit) Quantitative … (e.g. QMRI, QCSI)
QF	Quadrupole moment/Field gradient (interaction or relaxation mechanism)
Q Flow	Flow Quantification
QPD	Quadrature Phase Detection
QUEST	QUick Echo Split Imaging Technique
QUIPSS	QUantitative Imaging of Perfusion using a Single Subtraction
RAM	Rapid Acquisition Matrix
RARE	Rapid Acquisition Relaxation Enhanced
RAREst	RARE with short tE using slew-rate-optimized gradients
RAREVTR	RARE with Variable TR (simultaneous T_1 & T_2 mapping)
RASE	Rapid Acquisition Spin Echo
RBW	Receiver BandWidth
RCF	Rotating Coordinate Frame
RCT	Relayed Coherence Transfer
RE	Rapid Excitation (MRI)
REAPDOR	Rotational Echo Adiabatic Passage DOuble Resonance
RE-BURP	Refocused Band-selective Uniform Response Pure phase
RECSY	Multistep RElayed Coherence SpectroscopY
REDOR	Rotational Echo DOuble Resonance
RELAY	RELAYed Correlation Spectroscopy
REPAY	Reverse Editing of Protons According to multiplicitY
REREDOR	Rotor-Encoded REDOR
REST	REgional Saturation Technique
RF	Radio Frequency
RFDR	RF-Driven Recoupling
RF-FAST	RF-spoiled FAST
RFOV	Rectangular FOV
RICE	Rapid Imaging using Com-posite Echo
RIDE	RIng Down Elimination
RINEPT	Reverse INEPT
RISE	Rapid Imaging using Spin Echo
RMSD	Root-Mean-Square Deviation
ROAST	Resonant Offset Averaging in the STeady State
RODI	ROtatin-grame relaxation Dispersion Imaging
ROE	Rotating-frame Overhauser Effect
ROESY	ROE-based 2D shift correlation
ROI	Region Of Interest
ROPE	Respiratory Ordered PE
ROTO	ROESY-TOCSY Relay
RPA	Random Phase Approximation
RR	Rotational Resonance
RSSARGE	RF-Spoiled SARGE
RT	Respiratory Trigger
RUFIS	Rotating UltraFast Imaging Sequence
SA	Shielding Anisotropy
SAR	Specific Absorption Rate (RF)
SARGE	Spoiled steady-state Acquisition with Rewinded Gradient Echo
SAT	SATuration
SB	Sine-Bell window function
SC	Scalar Coupling
S.COSY	COSY with shift Scaling in F1
SCT	SCan Time
SCUBA	Stimulate Cross peaks Under Bleached Alphas
SD	Spin Dipolar

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

SDDS	Spin Decoupling Difference Spectroscopy
SDEPT	Selective DEPT
SE	Spin Echo
SECSY	Spin-Echo Correlated SpectroscopY
SEDOR	Spin-Echo DOuble Resonance
SEDRA	Simple Excitation for Dephasing of Rotational echo Amplitudes
SEDUCE	SElective Decoupling Using Crafted Excitation
SEFT	Spin-Echo Fourier Transform Spectroscopy (with J modulation)
SELCOSY	SELective COSY
SELTICS	Sideband ELimination by Temporary Interruption of the Chemical Shift
SELINCOR	SELective INverse CORrelation
SELINQUATE	SELective INADEQUATE
SELRESOLV	SELective RESolution of C,H Coupling
SEMS	Spin-Echo MultiSlice
SEMUT	Subspectral Editing Using a MUltiple-Quantum Trap
SENSE	SENSitivity Encoding
sEPI	spiral EPI
SEPT	Selective INEPT
SERF	SElective ReFocussing
SESAM	SEmi-Selective Acquisition Modulated (Decoupling)
SFAM	Simultaneous Freq. and Ampl. Modulation
SFORD	Single Frequency Off-Resonance Decoupling
SGSE	Steady-Gradient Spin-Echo
SHECOR	Selective HEteronuclear CORrelation
SHORT	SHORT repetition techniques
SI	Spectroscopic Imaging
SIAM	Simultaneous acq. of In-phase and Antiphase Multiplets
SIP	Saturation Inversion Projection
SIMBA	Selective Inverse Multiple-Bond Analysis
SINEPT	SINE-dependent PT
SINGLE PULSE	SINGLE PULSE-acquire spectroscopy
SIS	Substituent-Induced Shift
SJR	Second-order Jump and Return
SKEWSY	SKEWed Exchange SpectroscopY
SL	Spin-Lock pulse
SLF	Separated Local Field
SLITDRESS	SLIce inTerleaved Depth REsolved Surface coil Spectroscopy
SLOPT	Spin-LOcking Polarization Transfer
SMART	Shimadzu Motion Artifact Reduction Technique
SMASH	Short Minimum Angle SHot, SiMultaneous Acquisition of Spatial Harmonics
SNR or S/N	Signal-to-Noise Ratio
SOPPA	Second-Order Polarization Propagator Approach
SORS/STC	Slice-selective Off-Resonance Sinc Pulse / Saturation Transfer Contrast
SPACE	SPAtial and Chemical-Shift Encoded Excitation
SPAIR	SPectral Selection Attenuated Inversion Recovery
SPECIFIC-CP	SPECtrally Induced Filtering In Combination with Cross Polarization
SPEED	Swap PhasE-Encoded Data
SPGR	SPoiled Gradient-Recalled
SPI	Selective Population Inversion
SPIDER	Steady-state Projection Imaging with Dynamic Echo Train Readout
SPIO	SuperParamagnetic Iron Oxide
SPIR	Spectral Presaturation Inversion-Recovery
SPIRAL	MRI with SPIRAL *k*-space scan
SPRITE	Single-Point Ramped Imaging with T1 Enhancement
SPT	Selective Population Transfer
SQ	Single-Quantum
SQC	Single-Quantum Coherence
SQF	Single-Quantum Filter
SR	Saturation-Recovery
SRP	Self-Refocusing Pulse
SS	Slice Selection (gradient), Single Slice
SSB	Shifted Sine-Bell window function
SSFP	Steady-State Free Precession
SSFSE	Single-Shot FSE
SSI	Solid State Imaging
SSMP	Single-Slice Multiple-Phase
ssNMR	solid-state NMR
SSTSE/T2	Single-Shot TSE with T2 weighting
ST	Saturation Transfer, Slice Thickness
STAGE	Small Tip Angle GE
STE	STimulated Echo
STEAM	STimulated Echo Acquisition Mode for imaging
STEP	STE Progressive Imaging
STERF	Steady-State TEchnique with Refocused FID
STIR	Short T1 Inversion-Recovery
STREAM	Suppressed Tissue with REfreshment Angiography Method
STUD	Sech/Tanh Universal Decoupling – an adiabatic decoupling scheme
SUBMERGE	SUppression By Mistuned Echo and Repetitive Gradient Episodes
SUSAN	Spin decoupling employing Ultra-broadband inversion sequences generated via Simulated ANnealing
SWATTR	Selective Water Attenuation by T2 and T1 Relaxation
SVS	Single-Volume Spectroscopy
T1 ...	T1-weighted ... (method)
T1W	T1-Weighted
T2 ...	T2-weighted ... (method)
T2W	T2-Weighted
T2*W	T2*-Weighted
TACSY	TAylored Correlation SpectroscopY
TANGO	Testing for Adjacent Nuclei with a Gyration Operator

Abbreviations and Acronyms Used in Magnetic Resonance

TART	Tip Angle Reduced T_1 Imaging
TD	Trigger Delay, Time Difference
TCF	Time Correlation Function
TE	Time delay between excitation and Echo maximum
TEDOR	Transferred-Echo DOuble Resonance
TEI	TE Interleaved
TF	Turbo Factor
TFE	Turbo Field Echo
TGSE	Turbo Gradient Spin Echo
THRIVE	T1W High-Resolution Isotropic Volume Examination
TI	Time following Inversion
TIR	Turbo IR
TMR	Topical Magnetic Resonance
TOBSY	TOtal through-Bond correlation SpectroscopY
TOCSY	TOtal Correlation SpectroscopY
TOF	Time-Of-Flight
TOE	Truncated NOE
TONE	Tilt-Optimized Nonsaturated Excitation
TORO	TOCSY-ROESY Relay
TOSS	TOtal Suppression of Sidebands
TPPI	Time-Proportional Phase Incrementation
TPPM	Two-Pulse Phase Modulation
TPR	Time and Phase Reversal
TQ	Triple-Quantum
TQF	Triple-Quantum Filter
TR	Time for Repetition of excitation
T/R	Transmit/Receive
TRAPDOR	TRAnsfer of Populations in DOuble Resonance
TRCF	Tilted Rotating Coordinate Frame
TREV-*n*	Time-REVersal echo sequence of ***n*** pulses for homonuc. dipolar dec.
TRNOE	TRansferred NOE
TROSY	Transverse Relaxation Optimized SpectroscopY
T-ROESY	Transverse ROESY

TrueFISP	FISP with balanced gradient waveform
TS	Time of Saturation
TSE	Turbo Spin Echo
TSETSE	double-resonance Two-Spin Effect for correlation spectroscopy
TSR	Total SR
Turbo-FLASH	FLASH sequence during one IR period
U-BURP	Universal BURP pulse
UE	Unpaired Electron (relaxation mechanism)
UFSE	UltraFast SE
UNCOSY	UNiform excitation COSY
USPIO	UltraSmall Paramagnetic Iron Oxide
UTE	Ultra-short TE radial scan
UTSE	Ultra-short TSE
VAPRO	VAriable PROjection method
VAS	Variable Angle Spinning
VE	Velocity-Encoded
VEC	Velocity-Encoded Cine (MRI)
VEMP	Variable-Echo MultiPlanar
VENC	Velocity ENCoding value
VEST	Volume Excitation STimulated echoes
VIGRE	Volumetric Interpolated GRadient Echo
VOI	Volume Of Interest
VOSING	VOlume-selective Spectral editING
VOSY	VOlume-Selective SpectroscopY
VPS	Volumes Per Segment
VSOP	Very Small superparamagnetic iron Oxide Particles
WAHUHA	WAugh-HUber-HAeberlen Sequence
WALTZ	CPD Sequence Containing the Elements 1-2-3
WATERGATE	WATER suppression through GrAdient Tailored Excitation
WATR	Water Attenuation by Transverse Relaxation
WEFT	Water Eliminated Fourier Transform
WET	Water suppression Enhanced through T1 effects

WFOP	Water Fat Opposed Phase
WFS	Water Fat Separation (Shift Difference)
WHH-*n*	WAHUHA dec. cycle of ***n*** pulses
WIM-*n*	Windowless Isotropic Mixing dec. cycle of ***n*** pulses
WURST	Wideband, Uniform Rate, and Smooth Truncation – an adiabatic decoupling sequence
XCORFE	H, X CORrelation using a Fixed Evolution time
XD-NOESY	eXchange-Decoupled NOESY
X-FILTER	Selection of ^{1}H-^{1}H correlation when both H are coupled to X
X-HALF-FILTER	Selection of ^{1}H-^{1}H correlation when one H is coupled to X
Z-COSY	Z-filtered COSY
Z-FILTER	pulse sandwich for elimination of signal components with dispersive phase
ZECSY	Zero-Quantum-Echo Correlation SpectroscopY
ZIP	Zero-fill Interpolation Processing
ZQ	Zero Quantum
ZQC	Zero-Quantum Coherence
ZQF	Zero-Quantum Filter
ZZ-Spectroscopy	Selection of coherences involving ZZ or longitudinal two-spin order
ZZZ-Spectroscopy	Selection of coherences involving longitudinal 3-spin order
β-COSY	COSY with low-angle mixing pulse
Ψ-COSY	pseudo-COSY using incremented freq.-selective excitation

NMR Tables

Symbols for NMR and Related Quantities*

Roman alphabet	
a or A	Hyperfine (electron-nucleus) coupling constant
$A_q^{(l,m)}$	The *m*th component of an irreducible tensor of order *l* representing the nuclear spin operator for an interaction of type *q*
$\mathbf{B}$	Magnetic field (strictly the magnetic flux density or magnetic induction)
$\mathbf{B}_0$	Static magnetic field of an NMR spectrometer
$\mathbf{B}_1$, $\mathbf{B}_2$	Radiofrequency magnetic fields associated with frequencies ν_1, ν_2
$\mathbf{B}_L$	Local magnetic field of random field or dipolar origin
$\mathbf{C}$	Spin-rotation interaction tensor
C_X	Spin-rotation coupling constant of nuclide X
$\mathbf{D}$	Dipolar interaction tensor
$D_{i,j}$	Dipolar coupling constant between nuclei (*i* and *j*), in Hz
D^C	Nuclear receptivity relative to that of ^{13}C
D^P	Nuclear receptivity relative to that of ^{1}H
$\mathbf{E}$	Electric field strength
F	Spectral width
F_1, F_2 or f_1, f_2	The two frequency dimensions of a two-dimensional spectrum
$\hat{\mathbf{F}}_G$	Nuclear spin operator for a group, G, of nuclei
F_G	Magnetic quantum number associated with $\hat{\mathbf{F}}_G$
g	Nuclear or electronic *g* factor (Landé splitting factor)
G	Magnetic field gradient amplitude
$\hat{\mathbf{H}}$	Hamiltonian operator
$H_{i,j}$	Matrix element of Hamiltonian operator
$\hat{\mathbf{I}}_j$	Nuclear spin operator for nucleus *j*
$\hat{I}_{j+}$, $\hat{I}_{j-}$	'Raising' and 'lowering' spin operators for nucleus *j*
I_j	Magnetidc quantum number associated with $\hat{\mathbf{I}}_j$
$\mathbf{J}$	Indirect coupling tensor
$^nJ_{AB}$	Spin-spin coupling constant for nuclei A and B through *n* bonds in Hz
$J(\omega)$	Spectral density of fluctuations at angular frequency ω
$^nK_{AB}$	Reduced nuclear spin-spin coupling constant $K_{AB} = 4\pi^2 J_{AB}/h\gamma_A\gamma_B$) in T^2J^{-1}

$\mathbf{L}$	Angular momentum
m_j	Eigenvalue of $\hat{\mathbf{I}}_{jz}$ (magnetic component quantum number)
m_{tot}	Total magnetic component quantum number for a spin system (eigenvalue of $\Sigma_j \hat{\mathbf{I}}_{jz}$)
$m_{tot}(X)$	Total magnetic component quantum number for X-type nuclei
$\mathbf{M}_0$	Equilibrium macroscopic magnetization per unit volume in the presence of $\mathbf{B}_0$
M_x, M_y, M_z	Components of macroscopic magnetization per volume
M_n	*n*th moment of spectrum (M_2 = second moment, etc.)
n_α, n_β	Populations of the α and β spin states
N	Total number of nuclei of a given type per unit volume in the sample
$\mathbf{q}$	Electric field gradient tensor in units of the elementary charge
eQ	Nuclear quadrupole moment, *Q* is in m^2 and *e* is the elementary charge in *C*
R_1^X	Spin-lattice (longitudinal) relaxation rate constant for nucleus X
R_2^X	Spin-spin (transverse) relaxation rate constant for nucleus X
R_{1p}^X	Longitudinal relaxation rate constant for nucleus X in the reference frame rotating with $\mathbf{B}_1$
S	Signal intensity
$\hat{\mathbf{S}}$	Electron (or, occasionally, nuclear) spin operator; cf. $\hat{\mathbf{I}}$
t_1, t_2	Time dimensions for two-dimensional NMR
T_c	Coalescence temperature under chem. exchange for signals in an NMR spectrum
T_1^X	Spin-lattice (longitudinal) relaxation time of the X nucleus
T_2^X	Spin-spin (transverse) relaxation time of the X nucleus
T_2^*	Net dephasing time for M_x or M_y
T_{1p}^X	Longitudinal relaxation time for the X nucleus in the reference frame rotating with $\mathbf{B}_1$
T_d	Pulse (recycle) delay
T_{ac}	Acquisition time
$T_q^{(l,m)}$	The *m*th component of an irreducible tensor of order *l* representing the strength of an interaction of type *q*

* *IUPAC Recommendations: Magnetic Resonance in Chemistry, Vol. 36, 145-149 (1998)*

NMR Tables

Symbols for NMR and Related Quantities*

$\boldsymbol{V}$	Electric field gradient tensor. $\boldsymbol{V} = e\boldsymbol{q}$, where e is the elementary charge
$V_{\alpha\beta}$	Elements of Cartesian electric field gradient tensor
W_o, W_1, W_2	Relaxation rate constants (transition probabilities per time) between energy levels differing by 0, 1 and 2 in m_{tot}
W_{rs}	Transition probability between spin states r and s
Greek alphabet	
α	Nuclear spin wavefunction (eigenfunction of $\hat{\boldsymbol{I}}_z$) for the $m_I = +$ ½ state of a spin-½ nucleus
α_E	The Ernst angle (for optimum sensitivity)
β	Nuclear spin wavefunction (eigenfunction of $\hat{\boldsymbol{I}}_z$) for the $m_I = -$ ½ state of a spin-½ nucleus
γ_X	Magnetogyric ratio of nucleus X
δ_X	Chemical shift (for the resonance) of nucleus of element X, usually in ppm
Δn	Population difference between nuclear states (Δn_o at Boltzmann equilibrium)
$\Delta\delta$	Change or difference in δ
$\Delta\nu_{1/2}$	Full width in frequency units of a resonance line at half-height
$\Delta\sigma$	Anisotropy in σ [$\Delta\sigma = \sigma_{zz} - ½(\sigma_{xx} + \sigma_{YY})$]
$\Delta\chi$	(i) Susceptibility anisotropy ($\Delta\chi = \chi_{\parallel} - \chi_{\perp}$); (ii) difference in electronegativities
ε_o	Permittivity of the vacuum
ζ	Anisotropy in shielding, expressed as $\sigma_{zz} - \sigma_{iso}$
η	(i) Nuclear Overhauser enhancement; (ii) tensor asymmetry factor; (iii) viscosity
κ	Skew of a tensor
θ	Angle, especially for that between a given vector and $\boldsymbol{B}_o$
$\boldsymbol{\mu}$	(i) Magnetic dipole moment (component μ_z along $\boldsymbol{B}_o$); (ii) electric dipole moment
μ_o	Permeability of the vacuum
μ_B	Bohr magneton (earlier β_e)
μ_N	Nuclear magneton (earlier β_N)
ν_j	Larmor or resonance frequency of nucleus j (in Hz)
ν_o	(i) Spectrometer operating frequency; (ii) Basic Larmor or resonance frequency for a given isotope

ν_1	Frequency of primary RF magnetic field B_1 (excitation, detection)
ν_2	Frequency of secondary RF magnetic field B_2 (decoupling)
Ξ_X	Normalized resonance frequency for nucleus X relative to ν_H for tetramethylsilane (TMS) at the same $\boldsymbol{B}_O$ field; $\Xi_x = 100\ \nu_x/\nu_H$ (TMS)
ρ	Density matrix
$\hat{\rho}$	Density operator
ρ_{ij}	Element of matrix representation of $\hat{\rho}$
$\boldsymbol{\sigma}$	Shielding tensor
σ_j	(Isotropic) shielding constant of nucleus j
$\sigma_{\parallel}$, $\sigma_{\perp}$	Components of shielding tensor σ parallel and perpendicular to the symmetry axis
$\hat{\sigma}$	Reduced density operator
τ	(i) Time between RF pulses or recovery time following inversion (ii) lifetime in dynamic NMR studies
τ_c	Correlation time for molecular motion, especially for isotropic molecular tumbling
τ_d	Dwell time for data sampling
τ_{null}	Recovery time leading to null M_z after a 180° pulse
τ_p	Pulse duration
τ_{sc}	Correlation time for relaxation by the scalar mechanism
τ_{sr}	Correlation time for spin-rotation relaxation
$\tau_{\parallel}$, $\tau_{\perp}$	Correlation times for molecular tumbling parallel and perpendicular to the symmetry axis
χ	(i) Magnetic susceptibility; (ii) nuclear quadrupole coupling constant ($\chi = e^2 q_{zz} Q/h$)
$\omega_j, \omega_o, \omega_1, \omega_2$	As for ν_j, ν_o, ν_1, ν_2 but in angular frequency units (rad/s)
Ω	Span of a tensor
Ω_1, Ω_2	Angular frequency of RF fields $\boldsymbol{B}_1$, $\boldsymbol{B}_2$

* *IUPAC Recommendations: Magnetic Resonance in Chemistry, Vol. 36, 145-149 (1998)*

^{1}H Chemical Shifts for Common Contaminants in Deuterated Solvents

	Proton	mult., J	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
residual solvent H			7.26	2.05	2.50	7.16	1.94	3.31	4.79
H_2O		s	1.56	2.84 [a]	3.33 [a]	0.40	2.13	4.87	
acetic acid	CH_3	s	2.10	1.96	1.91	1.55	1.96	1.99	2.08
acetone	CH_3	s	2.17	2.09	2.09	1.55	2.08	2.15	2.22
acetonitrile	CH_3	s	2.10	2.05	2.07	1.55	1.96	2.03	2.06
benzene	CH	s	7.36	7.36	7.37	7.15	7.37	7.33	
t-butanol	CH_3	s	1.28	1.18	1.11	1.05	1.16	1.40	1.24
	OH[c]	s			4.19	1.55	2.18		
t-butyl methyl ether	CCH_3	s	1.19	1.13	1.11	1.07	1.14	1.15	1.21
	OCH_3	s	3.22	3.13	3.08	3.04	3.13	3.20	3.22
BHT[b]	ArH	s	6.98	6.96	6.87	7.05	6.97	6.92	
	OH[c]	s	5.01		6.65	4.79	5.20		
	$ArCH_3$	s	2.27	2.22	2.18	2.24	2.22	2.21	
	$ArC(CH_3)_3$	s	1.43	1.41	1.36	1.38	1.39	1.40	
chloroform	CH	s	7.26	8.02	8.32	6.15	7.58	7.90	
cyclohexane	CH_2	s	1.43	1.43	1.40	1.40	1.44	1.45	
1,2-dichloroethane	CH_2	s	3.73	3.87	3.90	2.90	3.81	3.78	
dichloromethane	CH_2	s	5.30	5.63	5.76	4.27	5.44	5.49	
diethyl ether	CH_3	t, 7	1.21	1.11	1.09	1.11	1.12	1.18	1.17
	CH_2	q, 7	3.48	3.41	3.38	3.26	3.42	3.49	3.56
diglyme	CH_2	m	3.65	3.56	3.51	3.46	3.53	3.61	3.67
	CH_2	m	3.57	3.47	3.38	3.34	3.45	3.58	3.61
	OCH_3	s	3.39	3.28	3.24	3.11	3.29	3.35	3.37
1,2-dimethoxyethane	CH_3	s	3.40	3.28	3.24	3.12	3.28	3.35	3.37
	CH_2	s	3.55	3.46	3.43	3.33	3.45	3.52	3.60
dimethylacetamide	CH_3CO	s	2.09	1.97	1.96	1.60	1.97	2.07	2.08
	NCH_3	s	3.02	3.00	2.94	2.57	2.96	3.31	3.06
	NCH_3	s	2.94	2.83	2.78	2.05	2.83	2.92	2.90
dimethylformamide	CH	s	8.02	7.96	7.95	7.63	7.92	7.97	7.92
	CH_3	s	2.96	2.94	2.89	2.36	2.89	2.99	3.01
	CH_3	s	2.88	2.78	2.73	1.86	2.77	2.86	2.85
dimethylsulfoxide	CH_3	s	2.62	2.52	2.54	1.68	2.50	2.65	2.71
dioxane	CH_2	s	3.71	3.59	3.57	3.35	3.60	3.66	3.75
ethanol	CH_3	t, 7	1.25	1.12	1.06	0.96	1.12	1.19	1.17
	CH_2	q, 7[d]	3.72	3.57	3.44	3.34	3.54	3.60	3.65
	OH	s[c,d]	1.32	3.39	4.63		2.47		
ethyl acetate	CH_3CO	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	CH_2CH_3	q, 7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	CH_2CH_3	t, 7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
ethyl methyl ketone	CH_3CO	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	CH_2CH_3	q, 7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	CH_2CH_3	t, 7	1.06	0.96	0.91	0.85	0.96	1.01	1.26
ethylene glycol	CH	s[e]	3.76	3.28	3.34	3.41	3.51	3.59	3.65
"grease"[f]	CH_3	m	0.86	0.87		0.92	0.86	0.88	
	CH_2	br s	1.26	1.29		1.36	1.27	1.29	
n-hexane	CH_3	t	0.88	0.88	0.86	0.89	0.89	0.90	
	CH_2	m	1.26	1.28	1.25	1.24	1.28	1.29	
HMPA[g]	CH_3	d, 9.5	2.65	2.59	2.53	2.40	2.57	2.64	2.61
methanol	CH_3	s[h]	3.49	3.31	3.16	3.07	3.28	3.34	3.34
	OH	s[c,h]	1.09	3.12	4.01		2.16		
nitromethane	CH_3	s	4.33	4.43	4.42	2.94	4.31	4.34	4.40
n-pentane	CH_3	t, 7	0.88	0.88	0.86	0.87	0.89	0.90	
	CH_2	m	1.27	1.27	1.27	1.23	1.29	1.29	

*Reprinted with permission from: J. Org. Chem. 1997, **62**, 7512-7515*

[1]H Chemical Shifts for Common Contaminants in Deuterated Solvents (continued)

	Proton	mult.	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
i-propanol	CH_3	d, 6	1.22	1.10	1.04	0.95	1.09	1.50	1.17
	CH	sep, 6	4.04	3.90	3.78	3.67	3.87	3.92	4.02
pyridine	CH(2)	m	8.62	8.58	8.58	8.53	8.57	8.53	8.52
	CH(3)	m	7.29	7.35	7.39	6.66	7.33	7.44	7.45
	CH(4)	m	7.68	7.76	7.79	6.98	7.73	7.85	7.87
silicone grease[i]	CH_3	s	0.07	0.13		0.29	0.08	0.10	
tetrahydrofuran	CH_2	m	1.85	1.79	1.76	1.40	1.80	1.87	1.88
	CH_2O	m	3.76	3.63	3.60	3.57	3.64	3.71	3.74
toluene	CH_3	s	2.36	2.32	2.30	2.11	2.33	2.32	
	CH(*o/p*)	m	7.17	7.1-7.2	7.18	7.02	7.1-7.3	7.16	
	CH(*m*)	m	7.25	7.1-7.2	7.25	7.13	7.1-7.3	7.16	
triethylamine	CH_3	t, 7	1.03	0.96	0.93	0.96	0.96	1.05	0.99
	CH_2	q, 7	2.53	2.45	2.43	2.40	2.45	2.58	2.57

[a] In these solvents the intermolecular rate of exchange is slow enough that a peak due to HDO is usually also observed; it appears at 2.81 and 3.30 ppm in acetone and DMSO, respectively. In the former solvent, it is often seen as a 1:1:1 triplet, with $^2J_{H,D}$ = 1 Hz. [b] 2,6-di-*tert*-butyl-4-methylphenol. [c] The signals from exchangeable protons were not always identified. [d] In some cases (see note *a*), the coupling interaction between the CH_2 and the OH protons may be observed (J = 5 Hz). [e] In CD_3CN, the OH proton was seen as a multiplet at δ = 2.69, and extra coupling was also apparent on the methylene peak. [f] Long-chain, linear aliphatic hydrocarbons. Their solubility in DMSO was too low to give visible peaks. [g] Hexamethylphosphoramide. [h] In some cases (see notes *a, d*), the coupling interaction between the CH_3 and the OH protons may be observed (J = 5.5 Hz). [i] Poly(dimethylsiloxane). Its solubility in DMSO was too low to give visible peaks.

[13]C Chemical Shifts for Common Contaminants in Deuterated Solvents

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
solvent signals		77.16	29.84	39.52	128.06	1.32	49.00	
			206.26			118.26		
acetic acid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH_3	20.81	20.51	20.95	20.37	20.73	20.56	21.03
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67	215.94
	CH_3	30.92	30.60	30.56	30.14	30.91	30.67	30.89
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06	119.68
	CH_3	1.89	1.12	1.03	0.20	1.79	0.85	1.47
benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34	
t-butanol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH_3	31.25	30.72	30.38	30.47	30.68	30.91	30.29
t-butyl methyl ether	OCH_3	49.45	49.35	48.70	49.19	49.52	49.66	49.37
	C	72.87	72.81	72.04	72.40	73.17	74.32	75.62
	CCH_3	26.99	27.24	26.79	27.09	27.28	27.22	26.60
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85	
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09	
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49	
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11	
	CH_3Ar	21.20	21.31	20.97	21.40	21.23	21.38	
	CH_3C	30.33	31.61	31.25	31.34	31.50	31.15	
	C	34.25	35.00	34.33	34.35	35.05	35.36	
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
cyclohexane	CH_2	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dichloroethane	CH_2	43.50	45.25	45.02	43.59	45.54	45.11	
dichloromethane	CH_2	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH_3	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH_2	65.91	66.12	62.05	65.94	66.32	66.88	66.42

^{13}C Chemical Shifts for Common Contaminants in Deuterated Solvents (continued)

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
diglyme	CH_3	59.01	58.77	57.98	58.66	58.90	59.06	58.67
	CH_2	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH_2	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH_3	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH_2	71.84	72.47	17.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH_3	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH_3	35.28	34.89	37.38	34.67	35.17	35.50	35.03
	NCH_3	38.13	37.92	34.42	37.03	38.26	38.43	38.76
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH_3	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH_3	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH_3	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH_2	67.14	67.60	66.36	67.16	67.72	68.11	67.19
ethanol	CH_3	18.41	18.89	18.51	18.72	18.80	18.40	17.47
	CH_2	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH_3CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH_2	60.49	60.56	59.74	60.21	60.98	61.50	62.32
	CH_3	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH_3CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.72	206.55	209.88	212.16	218.43
	$\mathit{CH_2}CH_3$	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	$CH_2\mathit{CH_3}$	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH_2	63.79	64.26	62.76	64.34	64.22	64.30	63.17
"grease"	CH_2	29.76	30.73	29.20	30.21	30.86	31.29	
n-hexane	CH_3	14.14	14.34	13.88	14.32	14.43	14.45	
	CH_2(2)	22.70	23.28	22.05	23.04	23.40	23.68	
	CH_2(3)	31.64	32.30	30.95	31.96	32.36	32.73	
HMPA[b]	CH_3	36.87	37.04	36.42	36.88	37.10	37.00	36.46
methanol	CH_3	50.41	49.77	48.59	49.97	49.90	49.86	49.50[c]
nitromethane	CH_3	62.50	63.21	63.28	61.16	63.66	63.08	63.22
n-pentane	CH_3	14.08	14.29	13.28	14.25	14.37	14.39	
	CH_2(2)	22.38	22.98	21.70	22.72	23.08	23.38	
	CH_2(3)	34.16	34.83	33.48	34.45	34.89	35.30	
i-propanol	CH_3	25.14	25.67	25.43	25.18	25.55	25.27	24.38
	CH	64.50	63.85	64.92	64.23	64.30	64.71	64.88
pyridine	CH(2)	149.90	150.67	149.58	150.27	150.76	150.07	149.18
	CH(3)	123.75	124.57	123.84	123.58	127.76	125.53	125.12
	CH(4)	135.96	136.56	136.05	135.28	136.89	138.35	138.27
silicone grease	CH_3	1.04	1.40		1.38		2.10	
tetrahydrofuran	CH_2	25.62	26.15	25.14	25.72	26.27	26.48	25.67
	CH_2O	67.97	68.07	67.03	67.80	68.33	68.83	68.68
toluene	CH_3	21.46	21.46	20.99	21.10	21.50	21.50	
	C(*i*)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(*o*)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH(*m*)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH(*p*)	125.33	126.12	125.29	125.68	126.28	126.29	
triethylamine	CH_3	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH_2	46.25	47.07	45.74	46.77	47.10	46.96	47.19

[a] See footnotes for Table 1. [b] $^2J_{PC}$ = 3 Hz. [c] Reference material; see text.

*Reprinted with permission from J. Org. Chem. 1997, **62**, 7512-7515*

NMR Formulae

Quantity	Formula (bold face = vectors)	Definitions (SI units) (see SI section for constants and units)
Magnetic Field Magnetic Force	$\boldsymbol{B} = \mu_o \boldsymbol{H}$ $\boldsymbol{F} = Q\, \boldsymbol{v} \times \boldsymbol{B}$	$\boldsymbol{B}$ = magn. flux density, magn. induction (T) $\boldsymbol{H}$ = magn. field strength (A m^{-1}) μ_o = permeability of vacuum ($4\pi \times 10^{-7}$ H m^{-1}) Q = elec. charge (C); v = velocity (m/s)
Nuclear Spin Spin Angular Mom. Magn. Moment	$\boldsymbol{I}$ $\hbar\, m_I$ $\boldsymbol{\mu}_I = \gamma_I \hbar_I \boldsymbol{I} = g_I \beta_N \boldsymbol{I}$	γ = magnetogyric ratio (rad s^{-1} T^{-1}); $\hbar = h/2\pi$ $\beta_N = \mu_B$ (nuclear magneton); g_I = nuclear g factor m_I = quantum no. ($-I$, $-I+1$, ...$+I$)
Zeeman Interaction Larmor Freq. Nutation Vector	$\mathrm{H} = -\boldsymbol{\mu}_I \cdot \boldsymbol{B}_0$, $E = -m_I\, \gamma_I\, \hbar\, B_0$ $\omega_0 = \gamma_I B_0$, $\nu_0 = \bar{\gamma}_I B_0$ $\boldsymbol{\omega} = -\gamma_I \boldsymbol{B}$	ω in rad s^{-1}, ν in Hz ($\Delta m_I = \pm 1$), $\bar{\gamma} = \gamma/2\pi$ (clockwise precession in lab frame for $\gamma > 0$)
Boltzmann Pop. Diff. Equil. Magn.	$\Delta N/N \sim \gamma_I\, \hbar/2kT$ ($\Delta m_I = \pm 1$) $M_0 = B_0\, [N\gamma_I^2 \hbar^2\, I(I+1) / 3kT]$	N = number of nuclei with spin I T = temperature (K)
Rotating Frame (r.f.) and residual field	$\gamma\, \Delta\boldsymbol{B}_0 = \gamma\, \boldsymbol{B}_0 + \boldsymbol{\omega}_{r.f.}$ $\boldsymbol{\Omega} = -\gamma\, \Delta\boldsymbol{B}_0 = \boldsymbol{\omega}_0 - \boldsymbol{\omega}_{r.f.}$	$\boldsymbol{\omega}_{r.f.}$ = rot. frame vector (detector freq.) in direction $\boldsymbol{\omega}_0$ ($-z$ axis for $\gamma > 0$) $\Delta\boldsymbol{B}_0$ = residual field in r.f. $\boldsymbol{\Omega}$ = precession freq. in r.f. (clockwise in r.f. for $\omega_0 > \omega_{r.f.}$)
Effective RF Field Amplitude and Tilt Nutation	$\omega_1 = -\gamma\, \boldsymbol{B}_1$, $\boldsymbol{B}_{eff} = \boldsymbol{B}_1 + \Delta\boldsymbol{B}_0$ $B_{eff} = [B_1^2 + \Delta B_0^2]^{1/2}$, $\tan\theta = \Delta B_0/B_1$ $\boldsymbol{\beta}_{eff}$ (in rad) $= -\gamma\, \boldsymbol{B}_{eff}\, \tau_p$ $\bar{\gamma}\, B_{eff}$ (in Hz) $= 1/(4\tau_{90})$	$\boldsymbol{B}_1$ = RF field vector in xy plane; nutation is ccw around $\boldsymbol{\omega}_{eff} = -\gamma\, \boldsymbol{B}_{eff}$; θ = tilt angle between $\boldsymbol{B}_{eff}$ and xy-plane; for $\Delta B_0/B_1 < 0.1$: $\theta < 6°$, $B_{eff} \approx B_1$ τ_p = RF pulse width (s); τ_{90} = 90° pulse
Optimum flip angle	$\cos\beta_{opt} = \exp(-TR/T_1)$	TR = pulse repetition time
Relaxation rates	spin-lattice: $R_1 = 1/T_1$ spin-spin: $R_2 = 1/T_2 = \pi\Delta\nu_o$	$\Delta\nu_o$ = natural Lorentzian linewidth at half-height
Bulk Susceptibility Correction	for cylindrical samples with external ref. in coaxial capillary $\delta_{corr} = \delta_{obs} + C\, (\chi_{ref} - \chi_{sample})$	$C = +2\pi/3$ (tube perpendicular to B_0) $C = -4\pi/3$ (tube parallel to B_0)
Spin-echo amplitude in constant B_0 gradient	$M(2\,\tau) =$ $M_0 \exp[-2\,\tau/T_2 - (2/3)(\gamma\, G)^2 D\tau^3]$	90-τ-180-τ Hahn echo with gradient G D = diffusion coeff. in gradient direction
Spin-echo attenuation in PFG-SE experiment	$\ln\, (S_{echo} / S_0) = -bD$ $b = (\gamma\delta\, G)^2(\Delta - \delta/3)$	G = B_0 gradient pulse amplitude (T/m) δ = pulse width; Δ = pulse spacing
Rotational Correlation Time	Stokes-Einstein Relation $\tau_c = (4\pi\eta\, r^3) / (3kT)$	τ_c = rot. correlation time for isotropic tumbling η = viscosity; r = molecular radius (sphere)
Nuclear Oberhauser Enhancement	$M_S\{I\}/M_S(0) = 1 + 0.5(\gamma_I/\gamma_S)(R_1^{IS}/R_1^S)$ (extreme narrowing; $\omega_S\tau_C << 1$)	enhancement of spin S due to continuous irradiation of spin I; R_1^{IS} = dipolar relaxation of S via I; R_1^S = relaxation of S via all mechanisms
Polarization Transfer	$M_S\{PT\}/M_S(0) = \gamma_I/\gamma_S$	PT from I to S via J_{IS}
Lorentzian Lineshape	$a(\omega) = R_2 / [R_2^2 + \Delta\omega^2]$ $d(\omega) = \Delta\omega / [R_2^2 + \Delta\omega^2]$	$a(\omega)$, $d(\omega)$ = absorption, dispersion signals $\Delta\omega = \omega - \Omega$

NMR Formulae

NMR Relaxation

Mechanisms (isotropic tumbling, SI units)	**Remarks**
Intramolecular Heteronuclear Dipole-Dipole Spin I relaxed by Spin S $R_1^I = E_{IS}\, r_{IS}^{-6}\, [(1/12)J_0(\omega_I - \omega_S) + (3/2)J_1(\omega_I) + (3/4)J_2(\omega_I + \omega_S)]$ $R_2^I = E_{IS}\, r_{IS}^{-6}\, [(1/6)J_0(0) + (1/24)J_0(\omega_I - \omega_S) + (3/4)J_1(\omega_I) +$ $(3/2)J_1(\omega_S) + (3/8)J_2(\omega_I + \omega_S)]$ where $E_{IS} = (\mu_0/4\pi)^2\, (\gamma_I\, \gamma_S\, \hbar)^2\, S(S + 1)$ Extreme narrowing: $R_1^I = (4/3)\, E_{IS}\, r_{IS}^{-6}\, \tau_c\, (\omega\tau_c << 1)$ For several spins S: use $\sum r_{IS}^{-6}$ NB: $T_1^I = 1/R_1^I$ only when S is saturated	Factor $(\mu_0/4\pi) = 10^{-7}$ is required for conversion from cgs-Gauss units to MKSA (SI) units. Spectral Densities for random isotropic rotation $J_q(\omega) = C_q\, [\tau_c/(1 + \omega^2\tau_c^2)]$ $(q = 0,1,2)$ $C_0 = 24/15;\ C_1 = 4/15;\ C_2 = 16/15$ extreme narrowing: $J_q(\omega) = C_q\, \tau_c$
Intramolecular Homonuclear Dipole-Dipole Spin I_k relaxed by Spin I_1 $R_1^I = E_I\, r_{kl}^{-6}\, (3/2)\, [J_1(\omega_I) + J_2(2\omega_I)]$ $R_{1\rho}^I = E_I\, r_{kl}^{-6}\, [(3/8)J_0(\omega_1) + (15/4)J_1(\omega_I) + (3/8)J_2(2\omega_I)]$ $R_2^I = E_I\, r_{kl}^{-6}\, [(3/8)J_0(0) + (15/4)J_1(\omega_I) + (3/8)J_2(2\omega_I)]$ where $E_I = (\mu_0/4\pi)^2\, \gamma_I^4\, \hbar^2\, I(I + 1)$ Extreme narrowing: $R_1^I = R_2^I = 2\, E_I\, r_{kl}^{-6}\, \tau_c\, (\omega\tau_c << 1)$ For several spins I: use $\sum r_{kl}^{-6}$	
Intermolecular Heteronuclear Dipole-Dipole Spin I on mol. A relaxed by Spin S on mol. B $(\omega\tau_C << 1)$ $R_1^I = 16\pi\, c_S\, E_{IS}\, /\, (27\, r_{IS}\, D_{trans})$ (pair distribution function = step function)	$E_{IS} = (\mu_0/4\pi)^2\, (\gamma_I\, \gamma_S\, \hbar)^2\, S(S + 1)$ c_S = conc. of spins S r_{IS} = distance of closest approach $D_{trans} = (D_A + D_B)\, /\, 2$
Intermolecular Homonuclear Dipole-Dipole Spin I on mol. A relaxed by Spin I on mol. B $(\omega\tau_C << 1)$ $R_1^I = 8\pi c_I\, E_I\, /\, (9\, r_{II}\, D_{trans})$ also found in the literature is: $R_1^I = (4\pi/3)\, c_I\, E_I\, (\tau/r_{II}^3)\, [1 + (2r_{II}^2/5\, D_{trans}\, \tau)]$	$E_I = (\mu_0/4\pi)^2\, \gamma_I^4\, \hbar^2\, I(I + 1)$ c_I = conc. of spins I r_{II} = distance of closest approach τ = mol. jump time

Spherical Harmonics

Spherical harmonics up to rank 2 expressed in polar and orthogonal Cartesian coordinates

$Y_{0,0}$	=	$\sqrt{\frac{1}{4\pi}}$		
$Y_{1,0}$	=	$\sqrt{\frac{3}{4\pi}}\cos\theta$	=	$\sqrt{\frac{3}{4\pi}}\,\frac{z}{r}$
$Y_{1,\pm1}$	=	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta\ e^{\pm i\varphi}$	=	$\mp\sqrt{\frac{3}{8\pi}}\,\frac{x\pm iy}{r}$
$Y_{2,0}$	=	$\sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta - 1)$	=	$\sqrt{\frac{5}{16\pi}}\,\frac{2z^2 - x^2 - y^2}{r^2}$
$Y_{2,\pm1}$	=	$\mp\sqrt{\frac{15}{8\pi}}\cos\theta\ \sin\theta\ e^{\pm i\varphi}$	=	$\mp\sqrt{\frac{15}{8\pi}}\,\frac{(x\pm iy)z}{r^2}$
$Y_{2,\pm2}$	=	$\sqrt{\frac{15}{32\pi}}\sin^2\theta\ e^{\pm 2i\varphi}$	=	$\sqrt{\frac{15}{32\pi}}\,\frac{(x\pm iy)^2}{r^2}$

NMR Formulae

Mechanisms (isotropic tumbling, SI units)	**Remarks**
Chemical Shift Anisotropy (CSA) molecular tumbling modulates the interaction of the chem. shift tensor with the B_0 field. $R_1 = (2/5)\ E_{CSA}\ [\tau_c / (1 + \omega^2\tau_c^2)]$ $R_2 = (1/90)\ E_{CSA}\ \{8\tau_c + [6\tau_c + (1 + \omega^2\tau_c^2)]\}$	predominant relaxation mech. for non-protonated X nuclei $E_{CSA} = \gamma^2\ B_0^2\ \Delta\sigma^2$ $\Delta\sigma = \sigma_\perp - \sigma_\parallel$ (in ppm) (assuming axial symmetry of tensor)
Quadrupole Relaxation ($I > 1/2$) $R_1 = R_2 = (3/40)\ C_I\ [1 + \eta^2/3]\ C_{QF}^2\ \tau_c \quad (\omega\tau_c << 1)$	$C_I = (2I + 3) / [I^2(2I - 1)]$ $C_{QF} = e^2\ Q\ q_{zz} / \hbar$ = quadrupolar coupling in Hz; η = asymmetry param.
Spin-Rotation Interaction (SR) Relaxation arises from the interaction of the nuclear spin with magnetic fields generated by the rotation of a molecular magnetic moment modulated by molecular collisions: $\left(\frac{1}{T_1}\right)_{SR} = \frac{2\ I_i\ kT}{3\ \hbar^2}\ C_{eff}^2\ \tau_J$ I_i = moment of inertia of the molecule C_{eff} = effective spin-rotational coupling constant τ_J = angular momentum correlation time With $\tau_c \cdot \tau_J = \frac{I_i}{6kT}$, we can introduce the reorientational correlation time and we obtain: $\left(\frac{1}{T_1}\right)_{SR} = \frac{I_i^2}{9\ \hbar^2}\ C_{eff}^2 \cdot \frac{1}{\tau_c}$	
Scalar Coupling (SC) This relaxation mechanism can occur if the nucleus I in question is scalar coupled (with coupling constant J) to a second spin ($S \geqq ½$) and the coupling is modulated by either chemical exchange (**SC relaxation of the first kind**) or the relaxation of spin S, e.g. if $S > ½$, (**SC relaxation of the second kind**). In this case spin splittings disappear and single lines are observed. $\left(\frac{1}{T_1}\right)_{SC} = \frac{8\pi^2\ J^2\ S\,(S+1)}{3}\left[\frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2\ \tau_{SC}^2}\right]$ $\left(\frac{1}{T_2}\right)_{SC} = \frac{4\pi^2\ J^2\ S\,(S+1)}{3}\left[\tau_{SC} + \frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2\ \tau_{SC}^2}\right]$ τ_{SC} = τ_e, if exchange time $\tau_e \ll T_1$ of either spin (first kind) τ_{SC} = T_1^S (the relaxation time of spin S) if $T_1^S \ll \tau_e$, $1/2\pi J$ (second kind) ω_I and ω_S are the resonance of I and S at the magnetic field in which $\left(\frac{1}{T_{1,2}}\right)_{SC}$ is measured.	

X-ray Diffractometry Tables

BRUKER

Bond Lengths of Main Group Elements

	H	B	C	N	O	F	Al	Si	P	S	Cl	Ga	Ge	As	Se	Br	In	Sn	Sb	Te	I
H	**68**	115	111	99	92	86	152	147	143	135	130	152	154	154	148	144	176	172	174	169	167
B	115	**162**	157	145	138	131	199	195	190	181	176	199	201	200	194	191	224	219	221	216	213
C	111	157	**158**	148	143	137	192	188	185	182	178	193	196	197	195	193	216	213	215	211	210
N	99	145	148	**146**	142	138	179	175	173	172	173	180	184	186	185	186	203	200	202	199	199
O	92	138	143	142	**144**	142	171	168	167	166	168	173	177	180	179	181	195	193	195	192	193
F	86	131	137	138	142	**148**	163	161	160	160	163	166	170	173	173	176	187	185	188	185	186
Al	152	199	192	179	171	163	**244**	236	227	217	210	239	238	237	229	225	268	261	261	253	249
Si	147	195	188	175	168	161	236	**230**	222	213	206	234	234	232	225	222	260	255	256	249	245
P	143	190	185	173	167	160	227	222	**218**	210	204	227	229	228	222	219	251	247	249	244	241
Si	135	181	182	172	166	160	217	213	210	**206**	202	218	220	222	219	216	241	238	240	235	235
Cl	130	176	178	173	168	163	210	206	204	202	**202**	211	215	217	215	216	234	231	233	230	230
Ga	152	199	193	180	173	166	239	234	227	218	211	**238**	238	237	230	226	263	259	260	253	250
Ge	154	201	196	184	177	170	238	234	229	220	215	238	**240**	239	233	230	263	258	260	255	252
As	154	200	197	186	180	173	237	232	228	222	217	237	239	**240**	235	231	261	257	259	254	253
Se	148	194	195	185	179	173	229	225	222	219	215	230	233	235	**232**	230	254	250	252	248	248
Br	144	191	193	186	181	176	225	222	219	216	216	226	230	231	230	**230**	249	246	248	245	245
In	175	223	216	202	195	187	268	260	251	241	234	263	262	260	253	249	**292**	285	285	277	273
Sn	172	219	213	200	193	185	261	255	247	238	231	259	258	257	250	246	285	**280**	281	273	270
Sb	174	221	215	202	195	188	261	256	249	240	233	260	260	259	252	248	285	281	**282**	275	272
Te	169	216	211	199	192	185	253	249	244	235	230	253	255	254	248	245	278	273	275	**270**	267
I	167	213	210	199	193	186	249	245	241	235	230	250	252	253	248	245	274	270	272	267	**266**

Bond valences *s* may be calculated from experimental bond lengths (*d*) after Pauling's correlation equation (Pauling, The Nature of Chemical Bond) using this single bond length (d_0). The constant *b* is commonly taken to be 37 pm.

$$s = \exp\left[(d_0 - d)/b\right] \qquad d = d_0 - (b \ln s)$$

The single bond lengths are listed in pm. They are calculated from the modified Schomaker-Stevenson equation (Blom, Haaland, *J. Mol. Struc.* 128 (1985) 21-27).

Laue Classes and Point Groups

Crystal System	Laue Class	Point Group
Triclinic	-1	*1* -1
Monoclinic	2/m	*2* m 2/m
Orthorhombic	mmm	*222* mm2 mmm
Tetragonal	4/m 4/mmm	*4* -4 4/m *422* -42m 4mm 4/mmm
Trigonal/Hexagonal	-3 -3m1 (-31m) 6/m 6/mmm	*3* -3 *321 (312)* 3m1 (31m) -3m1 (-31m) *6* -6 6/m *622* -62m 6mm 6/mmm
Cubic	m-3 m-3m	*23* m-3 *432* -43m m-3m

X-ray Diffractometry Tables

Space Groups

Point groups and space groups without centers of inversion or mirror planes are printed in italics. Those space groups which are uniquely determinable from the systematic absences and the symmetry of the diffraction pattern are printed in bold type.

Crystal System	Point Group	SG #	Condensed Symbol	Full Symbol
triclinic	*1*	*1*	*P1*	
	-1	2	P-1	
monoclinic	*2*	*3*	*P2*	*P 1 2 1*
		4	*P2(1)*	*P 1 2(1) 1*
		5	*C2*	*C 1 2 1*
	m	6	Pm	P 1 m 1
		7	Pc	P 1 c 1
		8	Cm	C 1 m 1
		9	Cc	C 1 c 1
	2/m	10	P2/m	P 1 2/m 1
		11	P2(1)/m	P 1 2(1)/m 1
		12	C2/m	C 1 2/m 1
		13	P2/c	P 1 2/c 1
		14	**P2(1)/c**	**P 1 2(1)/c 1**
		15	C2/c	C 1 2/c 1
orthorhombic	*222*	*16*	*P222*	*P 2 2 2*
		17	***P222(1)***	***P 2 2 2(1)***
		18	***P2(1)2(1)2***	***P 2(1)2(1) 2***
		19	***P2(1)2(1)2(1)***	***P 2(1) 2(1) 2(1)***
		20	***C222(1)***	***C 2 2 2(1)***
		21	*C222*	*C 2 2 2*
		22	*F222*	*F 2 2 2*
		23	*I222*	*I 2 2 2*
		24	*I2(1)2(1)2(1)*	*I 2(1) 2(1) 2(1)*
	mm2	25	Pmm2	P m m 2
		26	Pmc2(1)	P m c 2(1)
		27	Pcc2	P c c 2
		28	Pma2	P m a 2
		29	Pca2(1)	P c a 2(1)
		30	Pnc2	P n c 2
		31	Pmn2(1)	P m n 2(1)
		32	Pba2	P b a 2
		33	Pna2(1)	P n a 2(1)
		34	Pnn2	P n n 2
		35	Cmm2	C m m 2
		36	Cmc2(1)	C m c 2(1)
		37	Ccc2	C c c 2
		38	Amm2	A m m 2
		39	Abm2	A b m 2
		40	Ama2	A m a 2
		41	Aba2	A b a 2
		42	Fmm2	F m m 2
		43	**Fdd2**	**F d d 2**
		44	Imm2	I m m 2
		45	Iba2	I b a 2
		46	Ima2	I m a 2
	mmm	47	Pmmm	P 2/m 2/m 2/m
		48	**Pnnn**	**P 2/n 2/n 2/n**
		49	Pccm	P 2/c 2/c 2/m
		50	**Pban**	**P 2/b 2/a 2/n**
		51	Pmma	P 2(1)/m 2/m 2/a
		52	**Pnna**	**P 2/n 2(1)/n 2/a**
		53	Pmna	P 2/m 2/n 2(1)/a
		54	**Pcca**	**P 2(1)/c 2/c 2/a**
		55	Pbam	P 2(1)/b 2(1)/a 2/m
		56	**Pccn**	**P 2(1)/c 2(1)/c 2/n**
		57	Pbcm	P 2/b 2(1)/c 2(1)/m
		58	Pnnm	P 2(1)/n 2(1)/n 2/m
		59	Pmmn	P 2(1)/m 2(1)/m 2/n
		60	**Pbcn**	**P 2(1)/b 2/c 2(1)/n**
		61	**Pbca**	**P 2(1)/b 2(1)/c 2(1)/a**
		62	Pnma	P 2(1)/n 2(1)/m 2(1)/a

Crystal System	Point Group	SG #	Condensed Symbol	Full Symbol
		63	Cmcm	C 2/m 2/c 2(1)/m
		64	Cmca	C 2/m 2/c 2(1)/a
		65	Cmmm	C 2/m 2/m 2/m
		66	Cccm	C 2/c 2/c 2/m
		67	Cmma	C 2/m 2/m 2/a
		68	**Ccca**	**C 2/c 2/c 2/a**
		69	Fmmm	F 2/m 2/m 2/m
		70	**Fddd**	**F 2/d 2/d 2/d**
		71	Immm	I 2/m 2/m 2/m
		72	Ibam	I 2/b 2/a 2/m
		73	Ibca	I 2(1)/b 2(1)/c 2(1)/a
		74	Imma	I 2(1)/m 2(1)/m 2(1)/a
tetragonal	*4*	*75*	*P4*	*P 4*
		76	***P4(1)***	***P 4(1)***
		77	*P4(2)*	*P 4(2)*
		78	***P4(3)***	***P 4(3)***
		79	*I4*	*I 4*
		80	***I4(1)***	***I 4(1)***
	-4	81	P-4	P -4
		82	I-4	I -4
	4/m	83	P4/m	P 4/m
		84	P4(2)/m	P 4 (2)/m
		85	**P4/n**	**P 4/n**
		86	**P4(2)/n**	**P 4(2)/n**
		87	I4/m	I 4/m
		88	**I4(1)/a**	**I 4(1)/a**
	422	*89*	*P422*	*P 4 2 2*
		90	***P42(1)2***	***P 4 2(1) 2***
		91	*P4(1)22*	*P 4(1) 2 2*
		92	***P4(1)2(1)2***	***P 4(1) 2(1) 2***
		93	***P4(2)22***	***P 4(2)2 2***
		94	***P4(2)2(1)2***	***P 4(2) 2(1) 2***
		95	***P4(3)22***	***P 4(3) 2 2***
		96	***P4(3)2(1)2***	***P 4(3) 2(1) 2***
		97	*I422*	*I 4 2 2*
		98	***I4(1)22***	***I 4(1) 2 2***
	4mm	99	P4mm	P 4 m m
		100	P4bm	P 4 b m
		101	P4(2)cm	P 4(2) c m
		102	P4(2)nm	P 4(2) n m
		103	P4cc	P 4 c c
		104	P4nc	P 4 n c
		105	P4(2)mc	P 4(2) m c
		106	P4(2)bc	P 4(2) b c
		107	I4mm	I 4 m m
		108	I4cm	I 4 c m
		109	I4(1)md	I 4(1) m d
		110	**I4(1)cd**	**I 4(1) c d**
	-42m	111	P-42m	P -4 2 m
		112	P-42c	P -4 2 c
		113	P-42(1)m	P -4 2(1) m
		114	**P-42(1)c**	**P -4 2(1) c**
		115	P-4m2	P -4 m 2
		116	P-4c2	P -4 c 2
		117	P-4b2	P -4 b 2
		118	P-4n2	P -4 n 2
		119	I-4m2	I -4 m 2
		120	I-4c2	I -4 c 2
		121	I-42m	I -4 2 m
		122	I-42d	I -4 2 d
	4/mmm	123	P4/mmm	P 4/m 2/m 2/m
		124	P4/mcc	P 4/m 2/c 2/c
		125	**P4/nbm**	**P 4/n 2/b 2/m**

X-ray Diffractometry Tables

Crystal System	Point Group	SG #	Condensed Symbol	Full Symbol
		126	**P4/nnc**	**P 4/n 2/n 2/c**
		127	P4/mbm	P 4/m 2(1)/b 2/m
		128	P4/mnc	P 4/m 2(1)/n 2/c
		129	**P4/nmm**	**P 4/n 2(1)/m 2/m**
		130	**P4/ncc**	**P 4/n 2(1)/c 2/c**
		131	P4(2)/mmc	P 4(2)/m 2/m 2/c
		132	P4(2)mcm	P 4(2)/m 2/c 2/m
		133	**P4(2)/nbc**	**P 4(2)/n 2/b 2/c**
		134	**P4(2)/nnm**	**P 4(2)/n 2/n 2/m**
		135	P4(2)/mbc	P 4(2)/m 2(1)/b 2/c
		136	P4(2)/mnm	P 4(2)/m 2(1)/n 2/m
		137	**P4(2)/nmc**	**P 4(2)/n 2(1)/m 2/c**
		138	**P4(2)/ncm**	**P 4(2)/n 2(1)/c 2/m**
		139	I4/mmm	I 4/m 2/m 2/m
		140	I4/mcm	I 4/m 2/c 2/m
		141	**I4(1)/amd**	**I 4(1)/a 2/m 2/d**
		142	**I4(1)/acd**	**I 4(1)/a 2/c 2/d**
trigonal	*3*	*143*	*P3*	*P 3*
		144	*P3(1)*	*P 3(1)*
		145	*P3(2)*	*P 3(2)*
		146	*R3*	*R 3*
	-3	147	P-3	P -3
		148	R-3	R -3
	32	*149*	*P312*	*P 3 1 2*
		150	*P321*	*P 3 2 1*
		151	***P3(1)12***	***P 3(1) 1 2***
		152	***P3(1)21***	***P 3(1) 2 1***
		153	***P3(2)12***	***P 3(2) 1 2***
		154	***P3(2)21***	***P 3(2) 2 1***
		155	*R32*	*R 3 2*
	3m	156	P3m1	P 3 m 1
		157	P31m	P 3 1 m
		158	P3c1	P 3 c 1
		159	P31c	P 3 1 c
		160	R3m	R 3 m
		161	R3c	R 3 c
	-3m	162	P-31m	P -3 1 2/m
		163	P-31c	P -3 1 2/c
		164	P-3m1	P -3 2/m 1
		165	P-3c1	P -3 2/c 1
		166	R-3m	R -3 2/m
		167	R-3c	R -3 2/c
hexagonal	*6*	*168*	*P6*	*P 6*
		169	***P6(1)***	***P 6(1)***
		170	***P6(5)***	***P 6(5)***
		171	***P6(2)***	***P 6(2)***
		172	***P6(4)***	***P 6(4)***
		173	*P6(3)*	*P 6(3)*
	-6	174	P-6	P -6
	6/m	175	P6/m	P 6/m
		176	P6(3)/m	P 6(3)/m
	622	*177*	*P622*	*P 6 2 2*
		178	***P6(1)22***	***P 6(1)2 2***
		179	***P6(5)22***	***P 6(5) 2 2***
		180	***P6(2)22***	***P 6(2) 2 2***
		181	***P6(4)22***	***P 6(4) 2 2***
		182	***P6(3)22***	***P 6(3) 2 2***
	6mm	183	P6mm	P 6 m m
		184	P6cc	P 6 c c
		185	P6(3)cm	P 6(3) c m
		186	P6(3)mc	P 6(3) m c
	-6m	187	P-6m2	P -6 m 2
		188	P-6c2	P -6 c 2
		189	P-62m	P -6 2 m
		190	P-62c	P -6 2 c
	6/mmm	191	P6/mmm	P 6/m 2/m 2/m
		192	P6/mcc	P 6/m 2/c 2/c
		193	P6(3)/mcm	P 6(3)/m 2/c 2/m
		194	P6(3)/mmc	P 6(3)/m 2/m 2/c
cubic	*23*	*195*	*P23*	*P 2 3*
		196	*F23*	*F 2 3*
		197	*I23*	*I 2 3*
		198	***P2(1)3***	***P 2(1) 3***
		199	*I2(1)3*	*I 2(1) 3*
	m-3	200	Pm-3	P 2/m -3
		201	**Pn-3**	**P 2/n -3**
		202	Fm-3	F 2/m -3
		203	**Fd-3**	**F 2/d -3**
		204	Im-3	I 2/m -3
		205	**Pa-3**	**P 2(1)/a -3**
		206	**Ia-3**	**I 2(1)/a -3**
	432	*207*	*P432*	*P 4 3 2*
		208	***P4(2)32***	***P 4(2) 3 2***
		209	*F432*	*F 4 3 2*
		210	***F4(1)32***	***F 4(1) 3 2***
		211	*I432*	*I 4 3 2*
		212	***P4(3)32***	***P 4(3) 3 2***
		213	***P4(1)32***	***P 4(1) 3 2***
		214	*I4(1)32*	*I 4(1) 3 2*
	-43m	215	P-43m	P -4 3 m
		216	F-43m	F -4 3 m
		217	I-43m	I -4 3 m
		218	P-43n	P -4 3 n
		219	F-43c	F -4 3 c
		220	**I-43d**	**I -4 3 d**
	m-3m	221	Pm-3m	P 4/m -3 2/m
		222	**Pn-3n**	**P 4/n -3 2/n**
		223	Pm-3n	P 4(2)/m -3 2/n
		224	**Pn-3m**	**P 4(2)/n -3 2/m**
		225	Fm-3m	F 4/m -3 2/m
		226	Fm-3c	F 4/m -3 2/c
		227	**Fd-3m**	**F 4(1)/d -3 2/m**
		228	**Fd-3c**	**F 4(1)/d -3 2/c**
		229	Im-3m	I 4/m -3 2/m
		230	**Ia-3d**	**I 4(1)/a -3 2/d**

Periodic Table of Elements for X-ray Applications

35 — Atomic number
79.90 — Atomic weight
Br
Bromine — 3.12 — Density (g/cm³)
Kα 1.2 — Spectral line
11.9 — Energy (keV)
29.96 — Bragg angle (2 θ)

1	H	Hydrogen	1.01	0.0007			
3	Li	Lithium	6.94	0.534			
4	Be	Beryllium	9.01	1.85	Kα 1.2	0.108	74.34
11	Na	Sodium	22.99	0.97	Kα 1.2	1.0	25.00
					Kα 1.2	1.0	55.08
					Kβ 1	1.1	24.40
12	Mg	Magnesium	24.31	1.74	Kα 1.2	1.3	20.70
					Kα 1.2	1.3	136.72
					Kβ 1	1.3	20.00
19	K	Potassium	39.10	0.86	Kα 1.2	3.3	136.67
					Kα 1.2	3.3	50.69
					Kβ 1	3.6	118.10
20	Ca	Calcium	40.08	1.54	Kα 1.2	3.7	113.07
					Kα 1.2	3.7	45.20
					Kβ 1	4.0	100.21
					Lα 1	0.3	82.68
					Lβ 1	0.3	81.61
21	Sc	Scandium	44.96	2.99	Kα 1.2	4.1	97.68
					Kα 1.2	4.1	40.59
					Kβ 1	4.5	87.28
					Lα 1	0.4	69.50
					Lβ 1	0.4	68.67
22	Ti	Titanium	47.87	4.54	Kα 1.2	4.5	86.12
					Kα 1.2	4.5	36.67
					Kβ 1	4.9	77.25
					Lα 1	0.5	59.83
					Lβ 1	0.5	58.97
23	V	Vanadium	50.94	6.11	Kα 1.2	5.0	76.92
					Kα 1.2	5.0	123.17
					Kβ 1	5.4	69.12
					Lα 1	0.5	52.35
					Lβ 1	0.5	51.49
24	Cr	Chromium	52.00	7.15	Kα 1.2	5.4	69.34
					Kα 1.2	5.4	107.11
					Kβ 1	6.0	62.35
					Lα 1	0.6	46.33
					Lβ 1	0.6	45.49
25	Mn	Manganese	54.94	7.44	Kα 1.2	5.9	62.96
					Kα 1.2	5.9	95.20
					Kβ 1	6.5	56.63
					Lα 1	0.6	41.45
					Lβ 1	0.6	40.65
26	Fe	Iron	55.85	7.87	Kα 1.2	6.4	57.51
					Kα 1.2	6.4	85.73
					Kβ 1	7.1	51.72
					Lα 1	0.7	37.30
					Lβ 1	0.7	36.60
27	Co	Cobalt	58.93	8.56	Kα 1.2	6.9	52.79
					Kα 1.2	6.9	77.89
					Kβ 1	7.7	47.46
					Lα 1	0.8	33.77
					Lβ 1	0.8	33.12
37	Rb	Rubidium	85.47	1.53	Kα 1.2	13.4	26.61
					Kα 1.2	13.4	37.99
					Kβ 1	15.0	23.75
					Lα 1	1.7	113.68
					Lβ 1	1.8	108.08
					Kα 1.2	13.4	62.00
					Kβ 1	15.0	54.79
38	Sr	Strontium	87.62	2.64	Kα 1.2	14.1	25.15
					Kα 1.2	14.1	35.85
					Kβ 1	15.8	22.42
					Lα 1	1.8	103.45
					Lβ 1	1.9	98.53
					Kα 1.2	14.1	58.31
					Kβ 1	15.8	51.54
39	Y	Yttrium	88.91	4.47	Kα 1.2	14.9	23.79
					Kα 1.2	14.9	33.90
					Kβ 1	16.7	21.19
					Lα 1	1.9	95.07
					Lβ 1	2.0	90.57
					Kα 1.2	14.9	54.95
					Kβ 1	16.7	48.57
40	Zr	Zirconium	91.22	6.51	Kα 1.2	15.8	22.50
					Kα 1.2	15.8	32.04
					Kβ 1	17.7	20.07
					Lα 1	2.0	87.96
					Lβ 1	2.1	83.76
					Kα 1.2	15.8	51.75
					Kβ 1	17.7	45.28
41	Nb	Niobium	92.91	8.57	Kα 1.2	16.6	21.35
					Kα 1.2	16.6	30.38
					Kβ 1	18.6	19.03
					Lα 1	2.2	81.81
					Lβ 1	2.3	77.84
					Kα 1.2	16.6	48.95
					Kβ 1	18.6	43.39
42	Mo	Molybdenum	95.94	10.22	Kα 1.2	17.5	20.28
					Kα 1.2	17.5	28.84
					Kβ 1	19.6	18.06
					Lα 1	2.3	76.41
					Lβ 1	2.4	72.63
					Kα 1.2	17.5	46.39
					Kβ 1	19.6	41.11
43	Tc	Technetium	(98)	11.5	Kα 1.2	18.4	19.29
					Kα 1.2	18.4	27.42
					Kβ 1	20.6	17.17
					Lα 1	2.4	71.62
					Lβ 1	2.5	67.98
					Kα 1.2	18.4	44.03
					Kβ 1	20.6	39.01
44	Ru	Ruthenium	101.07	12.37	Kα 1.2	19.3	18.37
					Kα 1.2	19.3	26.10
					Kβ 1	21.7	16.34
					Lα 1	2.6	67.33
					Lβ 1	2.7	63.82
					Kα 1.2	19.3	41.84
					Kβ 1	21.7	37.07
45	Rh	Rhodium	102.91	12.41	Kα 1.2	20.2	17.51
					Kα 1.2	20.2	24.87
					Kβ 1	22.7	15.57
					Lα 1	2.7	63.46
					Lβ 1	2.8	60.05
					Kα 1.2	20.2	39.82
					Kβ 1	22.7	35.51
55	Cs	Caesium	132.91	1.87	Kα 1	30.9	16.16
					Lα 1	4.3	91.80
					Lβ 1	4.6	83.58
56	Ba	Barium	137.33	3.59	Kα 1	32.1	15.54
					Lα 1	4.5	87.16
					Lβ 1	4.8	79.24
57	La	Lanthanium	138.91	6.15	Kα 1	33.4	14.96
					Lα 1	4.7	82.90
					Lβ 1	5.0	75.27
72	Hf	Hafnium	178.49	13.31	Kα 1	55.8	8.95
					Lα 1	7.9	45.87
					Lβ 1	9.0	39.90
					Mα 1	1.6	119.17
					Lα 1	7.9	121.27
					Lβ 1	9.0	99.46
73	Ta	Tantalum	180.95	16.65	Kα 1	57.6	8.68
					Lα 1	8.2	44.41
					Lβ 1	9.3	38.47
					Mα 1	1.7	112.11
					Lα 1	8.1	115.36
					Lβ 1	9.3	94.92
74	W	Tungsten	183.84	19.25	Lα 1	8.4	43.01
					Lβ 1	9.7	37.12
					Mα 1	1.8	106.03
					Lα 1	8.4	110.13
					Lβ 1	9.7	90.75
75	Re	Rhenium	186.21	21.02	Lα 1	8.7	41.68
					Lβ 1	10.0	35.82
					Mα 1	1.8	100.66
					Lα 1	8.7	105.43
					Lβ 1	10.0	86.90
76	Os	Osmium	190.23	22.61	Lα 1	8.9	40.42
					Lβ 1	10.4	34.59
					Mα 1	1.9	95.64
					Lα 1	8.9	101.16
					Lβ 1	10.4	83.33
77	Ir	Iridium	192.22	22.65	Lα 1	9.2	39.21
					Lβ 1	10.7	33.42
					Mα 1	2.0	91.50
					Lα 1	9.2	97.24
					Lβ 1	10.7	80.01
87	Fr	Francium	(223)	1.87	Lα 1	12.0	29.65
					Lβ 1	14.8	24.06
88	Ra	Radium	(226)	5.5	Lα 1	12.3	28.89
					Lβ 1	15.2	23.31
89	Ac	Actinium	(227)	10.07	Lα 1	12.7	28.17
					Lβ 1	15.7	22.59

Lanthanides, Actinides:

58	Ce	Cerium	140.12	6.77	Lα 1	4.8	128.13
					Lα 1	4.8	79.00
					Lβ 1	5.3	71.61
59	Pr	Praseodymium	140.91	6.77	Lα 1	5.0	119.69
					Lα 1	5.0	75.41
					Lβ 1	5.5	68.23
60	Nd	Neodymium	144.24	7.01	Lα 1	5.2	112.66
					Lα 1	5.2	72.12
					Lβ 1	5.7	65.10
61	Pm	Promethium	(145)	7.26	Lα 1	5.4	106.48
					Lα 1	5.4	69.03
					Lβ 1	6.0	62.19
62	Sm	Samarium	150.36	7.52	Lα 1	5.6	101.12
					Lα 1	5.6	66.22
					Lβ 1	6.2	59.49
90	Th	Thorium	232.04	11.72	Lα 1	13.0	39.22
					Lα 1	13.0	27.46
					Lβ 1	16.2	21.90
					Lα 1	13.0	64.12
					Lβ 1	16.2	50.29
91	Pa	Protactinium	231.04	15.37	Lα 1	13.3	38.23
					Lα 1	13.3	26.79
					Lβ 1	16.7	21.24
					Lα 1	13.3	62.39
					Lβ 1	16.7	48.68
92	U	Uranium	238.03	18.45	Lα 1	13.6	37.29
					Lα 1	13.6	26.14
					Lβ 1	17.2	20.59
					Lα 1	13.6	60.75
					Lβ 1	17.2	47.13
93	Np	Neptunium	(237)	20.25	Lα 1	14.0	36.38
					Lα 1	14.0	25.51
					Lβ 1	17.8	19.96
94	Pu	Plutonium	(244)	19.84	Lα 1	14.3	35.50
					α	14.3	24.90
					Lβ 1	18.3	19.39

Analyser crystal	Name, material	2d-value (nm)
XS-B	La/B_4C multilayer	19.0
XS-C	$Ti0_2$/C multilayer	12.0
XS-N	Ni/BN multilayer	11.0
XS-55	W/Si multilayer	5.5
XS-CEM	Specific structure	2.75
TIAP	Thallium biphthalate	2.576
ADP	Ammonium dihydrogen phosphate	1.064
PET	Pentaerythrite	0.874
InSb	Indium antimonide	0.748
Ge	Germanium	0.653
LiF (200)	Lithium fluoride	0.403
LiF (220)	Lithium fluoride	0.285
LiF (420)	Lithium fluoride	0.180

Order Number DOC-P84-E00011 V3 © 2008 Bruker AXS GmbH. Printed in Germany.

$$\lambda\ (\mathrm{nm}) = \frac{1.24}{E\ (\mathrm{keV})}$$

$$n\lambda = 2d \sin\theta$$

2 4.00
He
Helium 0.0002

5 10.81	6 12.01	7 14.01	8 16.00	9 19.00	10 20.18
B	C	N	O	F	Ne
Boron 2.34	Carbon 2.27	Nitrogen 0.001	Oxygen 0.001	Fluorine 0.001	Neon 0.0009
Kα 1.2 0.18 42.51	Kα 1.2 0.28 107.24	Kα 1.2 0.39 70.14	Kα 1.2 0.53 50.90	Kα 1.2 0.68 38.91	Kα 1.2 0.85 30.8
	Kα 1.2 0.28 43.31	Kα 1.2 0.39 33.60	Kα 1.2 0.53 25.10	Kα 1.2 0.68 90.60	Kα 1.2 0.85 69.1

13 26.98	14 28.09	15 30.97	16 32.07	17 35.45	18 39.95
Al	Si	P	S	Cl	Ar
Aluminium 2.70	Silicon 2.33	Phosphorus 1.82	Sulphur 2.07	Chlorine 0.003	Argon 0.002
Kα 1.2 1.5 145.12	Kα 1.2 1.7 109.21	Kα 1.2 2.0 89.56	Kα 1.2 2.3 75.85	Kα 1.2 2.6 65.49	Kα 1.2 3.0 57.32
Kα 1.2 1.5 17.45	Kα 1.2 1.7 144.58	Kα 1.2 2.0 141.03	Kα 1.2 2.3 110.69	Kα 1.2 2.6 92.76	Kα 1.2 3.0 79.86
Kβ 1 1.5 131.86	Kβ 1 1.8 101.67	Kβ 1 2.1 83.20	Kβ 1 2.5 70.28	Kβ 1 2.8 60.49	Kβ 1 3.2 52.79
Kα 1 1.5 35.31	Kα 1 1.7 30.04	Kα 1 2.0 25.88	Kα 1 2.3 22.53		

28 58.69	29 63.55	30 65.41	31 69.72	32 72.64	33 74.92	34 78.96	35 79.90	36 83.80
Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Nickel 8.91	Copper 8.93	Zinc 7.13	Gallium 5.91	Germanium 5.32	Arsenic 5.78	Selenium 4.81	Bromine 3.12	Krypton 0.003
Kα 1.2 7.5 48.67	Kα 1.2 8.0 45.02	Kα 1.2 8.6 41.80	Kα 1.2 9.2 38.91	Kα 1.2 9.9 36.32	Kα 1.2 10.5 33.99	Kα 1.2 11.2 31.89	Kα 1.2 11.9 29.96	Kα 1.2 12.6 28.21
Kα 1.2 7.5 71.26	Kα 1.2 8.0 65.55	Kα 1.2 8.6 60.58	Kα 1.2 9.2 56.20	Kα 1.2 9.9 52.31	Kα 1.2 10.5 48.83	Kα 1.2 11.2 45.71	Kα 1.2 11.9 42.88	Kα 1.2 12.6 40.32
Kβ 1 8.3 43.72	Kβ 1 8.9 40.45	Kβ 1 9.6 37.52	Kβ 1 10.3 34.90	Kβ 1 11.0 32.56	Kβ 1 11.7 30.44	Kβ 1 12.5 28.52	Kβ 1 13.3 26.79	Kβ 1 14.1 25.20
Lα 1 0.9 30.70	Lα 1 0.9 28.06	Lα 1 1.0 25.74	Lα 1 1.1 23.69	Lα 1 1.2 21.88	Lα 1 1.3 20.25	Lα 1 1.4 18.82	Lα 1 1.5 17.52	Lα 1 1.6 126.81
Lβ 1 0.9 30.08	Lβ 1 1.0 27.45	Lβ 1 1.0 25.18	Lβ 1 1.1 23.12	Lβ 1 1.2 21.33	Lβ 1 1.3 19.71	Lβ 1 1.4 18.28	Lβ 1 1.5 16.99	Lβ 1 1.6 120.14
Kα 1.2 7.5 134.33	Kα 1.2 8.0 117.85	Kα 1.2 8.6 105.87	Kα 1.2 9.2 96.35	Kα 1.2 9.9 88.44	Kα 1.2 10.5 81.69	Kα 1.2 11.2 75.84	Kα 1.2 11.9 70.69	
Kβ 1 8.3 112.81	Kβ 1 8.9 101.26	Kβ 1 9.6 91.98	Kβ 1 10.3 84.24	Kβ 1 11.0 77.64	Kβ 1 11.7 71.90	Kβ 1 12.5 66.86	Kβ 1 13.3 62.39	

46 106.42	47 107.87	48 112.41	49 114.82	50 118.71	51 121.76	52 127.60	53 126.90	54 131.29
Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Palladium 12.02	Silver 10.55	Cadmium 8.69	Indium 7.31	Tin 7.29	Antimony 6.64	Tellurium 6.23	Iodine 4.93	Xenon 0.005
Kα 1.2 21.2 16.71	Kα 1.2 22.2 15.96	Kα 1.2 23.1 15.27	Kα 1.2 24.2 14.61	Kα 1.2 25.2 13.99	Kα 1.2 26.4 13.41	Kα 1.2 27.4 12.87	Kα 1.2 28.6 12.35	Kα 1.2 29.7 11.85
Kα 1.2 21.2 23.73	Kα 1.2 22.2 22.66	Kα 1.2 23.1 21.66	Kα 1.2 24.2 20.72	Kα 1.2 25.2 19.84	Kα 1.2 26.4 19.01	Kα 1.2 27.4 18.23	Kα 1.2 28.6 17.50	Kα 1.2 29.7 16.81
Kβ 1 23.8 14.85	Kβ 1 24.9 14.18	Kβ 1 26.1 13.55	Kβ 1 27.3 12.96	Kβ 1 28.5 12.41	Kβ 1 29.7 11.89	Kβ 1 31.0 11.40	Kβ 1 32.3 10.94	Kβ 1 33.6 10.50
Lα 1 2.8 59.95	Lα 1 3.0 56.75	Lα 1 3.1 53.82	Lα 1 3.3 51.12	Lα 1 3.4 48.64	Lα 1 3.6 46.34	Lα 1 3.8 44.20	Lα 1 3.9 42.22	Lα 1 4.1 40.37
Lβ 1 3.0 56.63	Lβ 1 3.2 53.50	Lβ 1 3.3 50.63	Lβ 1 3.5 47.99	Lβ 1 3.7 45.56	Lβ 1 3.8 43.31	Lβ 1 4.0 41.21	Lβ 1 4.2 39.27	Lβ 1 4.4 37.42
Kα 1.2 21.2 37.94	Kα 1.2 22.2 36.19	Kα 1.2 23.1 34.65	Kα 1.2 24.2 33.04	Kα 1.2 25.2 31.62	Kα 1.2 26.4 30.28	Kα 1.2 27.5 29.02	Kα 1.2 28.6 27.84	
Kβ 1 23.8 33.60	Kβ 1 24.9 32.04	Kβ 1 26.1 30.59	Kβ 1 27.3 29.24	Kβ 1 28.5 27.97	Kβ 1 29.7 26.78	Kβ 1 31.0 25.67	Kβ 1 32.3 24.62	

78 195.08	79 196.97	80 200.59	81 204.37	82 207.20	83 208.98	84 (209)	85 (210)	86 (222)
Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Platinum 21.46	Gold 19.28	Mercury 13.53	Thallium 11.86	Lead 11.34	Bismuth 9.81	Polonium 9.32	Astatine 7.00	Radon 0.01
Lα 1 9.4 38.06	Lα 1 9.7 36.96	Lα 1 10.0 35.90	Lα 1 10.3 34.92	Lα 1 10.6 33.93	Lα 1 10.8 33.00	Lα 1 11.1 32.11	Lα 1 11.4 31.26	Lα 1 11.7 30.44
Lβ 1 11.1 32.29	Lβ 1 11.4 31.22	Lβ 1 11.8 30.19	Lβ 1 12.2 29.20	Lβ 1 12.6 28.25	Lβ 1 13.0 27.34	Lβ 1 13.4 26.47	Lβ 1 13.9 25.64	Lβ 1 14.3 24.84
Mα 1 2.0 87.53	Mα 1 2.1 83.83	Mα 1 2.1 80.49	Mα 1 2.3 77.30	Mα 1 2.3 74.41	Mα 1 2.4 71.67			
Lα 1 9.4 93.62	Lα 1 9.7 90.27	Lα 1 10.0 87.13	Lα 1 10.3 84.20	Lα 1 10.6 81.45	Lα 1 10.8 78.86	Lα 1 11.1 76.41		
Lβ 1 11.1 76.91	Lβ 1 11.4 73.98	Lβ 1 11.8 71.22	Lβ 1 12.2 68.62	Lβ 1 12.6 66.16	Lβ 1 13.0 63.82	Lβ 1 13.4 61.59		

63 151.96	64 157.25	65 158.93	66 162.50	67 164.93	68 167.26	69 168.93	70 173.04	71 174.47
Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Europium 5.24	Gadolinium 7.90	Terbium 8.23	Dysprosium 8.55	Holmium 8.80	Erbium 9.07	Thulium 9.32	Ytterbium 6.97	Lutetium 9.84
Lα 1 5.9 96.23	Lα 1 6.1 91.87	Lα 1 6.3 87.87	Lα 1 6.5 84.15	Lα 1 6.7 80.73	Lα 1 7.0 77.58	Lα 1 7.2 74.63	Lα 1 7.4 71.89	Lα 1 7.7 69.31
Lα 1 5.9 63.55	Lα 1 6.1 61.09	Lα 1 6.3 58.78	Lα 1 6.5 56.59	Lα 1 6.7 54.53	Lα 1 7.0 52.60	Lα 1 7.2 50.78	Lα 1 7.4 49.06	Lα 1 7.7 47.42
Lβ 1 6.5 56.96	Lβ 1 6.7 54.59	Lβ 1 7.0 52.36	Lβ 1 7.2 50.27	Lβ 1 7.5 48.30	Lβ 1 7.8 46.43	Lβ 1 8.1 44.67	Lβ 1 8.4 42.99	Lβ 1 8.7 41.40
							Lα 1 7.4 136.36	Lα 1 7.7 128.12
							Lβ1 8.4 110.04	Lβ1 8.7 104.46

95 (243)	96 (247)	97 (247)	98 (251)	99 (252)	100 (257)	101 (258)	102 (259)	103 (262)
Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
Americium 13.69	Curium 13.51	Berkelium 14.79	Californium 15.1	Einsteinium 13.5	Fermium	Mendelevium	Nobelium	Lawrencium
Lα 1 14.6 34.65	Lα 1 15.0 33.84	Lα 1 15.3 33.04	Lα 1 15.7 32.38					
Lα 1 14.6 24.32	Lα 1 15.0 23.76	Lα 1 15.3 23.20	Lα 1 15.7 22.68					
Lβ 1 18.8 18.81	Lβ 1 19.4 18.26	Lβ 1 20.0 17.74	Lβ 1 20.6 17. 22					

Our Portfolio for Elemental Analysis

hydrogen 1 H									
lithium 3 Li	beryllium 4 Be								
sodium 11 Na	magnesium 12 Mg								
potassium 19 K	calcium 20 Ca		scandium 21 Sc	titanium 22 Ti	vanadium 23 V	chromium 24 Cr	manganese 25 Mn	iron 26 Fe	cobalt 27 Co
rubidium 37 Rb	strontium 38 Sr		yttrium 39 Y	zirconium 40 Zr	niobium 41 Nb	molybdenum 42 Mo	technetium 43 Tc	ruthenium 44 Ru	rhodium 45 Rh
caesium 55 Cs	barium 56 Ba	57-70 *	lutetium 71 Lu	hafnium 72 Hf	tantalum 73 Ta	tungsten 74 W	rhenium 75 Re	osmium 76 Os	iridium 77 Ir
francium 87 Fr	radium 88 Ra	89-102 **	lawrencium 103 Lr	rutherfordium 104 Rf	dubnium 105 Db	seaborgium 106 Sg	bohrium 107 Bh	hassium 108 Hs	meitnerium 109 Mt

lanthanum 57 La	cerium 58 Ce	praseodymium 59 Pr	neodymium 60 Nd	promethium 61 Pm	samarium 62 Sm	europium 63 Eu
actinium 89 Ac	thorium 90 Th	protactinium 91 Pa	uranium 92 U	neptunium 93 Np	plutonium 94 Pu	americium 95 Am

● Spark Spectrometers

● CS/ONH-Analyzers

								helium 2 He
			boron 5 B	carbon 6 C	nitrogen 7 N	oxygen 8 O	fluorine 9 F	neon 10 Ne
			aluminium 13 Al	silicon 14 Si	phosphorus 15 P	sulfur 16 S	chlorine 17 Cl	argon 18 Ar
nickel 28 Ni	copper 29 Cu	zinc 30 Zn	gallium 31 Ga	germanium 32 Ge	arsenic 33 As	selenium 34 Se	bromine 35 Br	krypton 36 Kr
palladium 46 Pd	silver 47 Ag	cadmium 48 Cd	indium 49 In	tin 50 Sn	antimony 51 Sb	tellurium 52 Te	iodine 53 I	xenon 54 Xe
platinum 78 Pt	gold 79 Au	mercury 80 Hg	thallium 81 Tl	lead 82 Pb	bismuth 83 Bi	polonium 84 Po	astatine 85 At	radon 86 Rn
ununnilium 110 Uun	unununium 111 Uuu	ununbium 112 Uub		ununquadium 114 Uuq				

gadolinium 64 Gd	terbium 65 Tb	dysprosium 66 Dy	holmium 67 Ho	erbium 68 Er	thulium 69 Tm	ytterbium 70 Yb
curium 96 Cm	berkelium 97 Bk	californium 98 Cf	einsteinium 99 Es	fermium 100 Fm	mendelevium 101 Md	nobelium 102 No

Handheld XRF-Analyzers ●

μ-XRF Spectrometers ●

Spectral Lines used for OES

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Ag	230,9644	231,0354	I
Ag	235,7920	235,8641	II
Ag	241,3184	241,3918	II
Ag	328,0683	328,1628	I
Ag	338,2890	338,3861	I
Al	256,7987	256,8757	I
Al	266,0386	266,1178	I
Al	305,9933	306,0823	I
Al	308,2153	308,3048	I
Al	394,4006	394,5122	I
Al	396,1520	396,2641	I
As	188,9789	189,0420	I
As	234,9840	235,0559	I
As	289,8710	289,9560	I
Au	242,7950	242,8687	I
Au	264,1480	264,2267	I
Au	267,5950	267,6745	I
B	182,5786	182,6410	I
B	208,9590	209,0255	I
B	249,6770	249,7523	I
B	345,1410	345,2399	II
Ba	455,4042	455,5319	II
Be	234,8610	234,9329	I
Be	298,6090	298,6910	I
Be	301,9330	302,0210	I
Be	313,0420	313,1327	II
Bi	306,7720	306,8612	I
Bi	351,0850	351,1854	I
C	133,5207	133,5708	II
C	165,7478	165,8122	I
C	193,0268	193,0905	I
Ca	393,3664	393,4778	II
Ca	396,8470	396,9593	II
Ca	422,6730	422,7920	I
Ca	443,4960	443,6205	I
Cd	214,4410	214,5085	II
Cd	228,8022	228,8728	I
Cd	308,0827	308,1722	II
Cd	346,6200	346,7193	I
Cd	361,0508	361,1538	I
Cd	467,8149	467,9458	I
Ce	399,9240	400,0371	II
Ce	401,2390	401,3524	II
Ce	413,7646	413,8813	II
Ce	418,6600	418,7780	II
Ce	446,0210	446,1462	II
Co	228,6156	228,6861	II
Co	258,0320	258,1093	II
Co	345,3505	345,4494	I
Cr	265,8590	265,9381	II
Cr	267,7160	267,7956	II

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Cr	286,2570	286,3411	II
Cr	298,9190	299,0062	II
Cr	425,4332	425,5529	I
Cu	200,0348	200,0996	II
Cu	224,2618	224,3314	II
Cu	296,1160	296,2025	I
Cu	324,7540	324,8477	I
Cu	327,3960	327,4904	I
Cu	453,0819	453,2089	I
Cu	510,5540	510,6963	I
Fe	187,6710	187,7340	II
Fe	249,3260	249,4012	II
Fe	259,9400	260,0177	II
Fe	271,4410	271,5215	II
Fe	273,0730	273,1538	II
Fe	281,3287	281,4116	I
Fe	360,8859	360,9888	I
Fe	371,9935	372,0993	I
Fe	238,2040	238,2767	II
Ga	417,2040	417,3216	I
Ge	303,9067	303,9951	I
H	121,5144	121,5668	I
Hf	277,3360	277,4179	II
Hg	253,6520	253,7282	I
Hg	435,8350	435,9575	I
Hg	579,0660	579,2266	I
In	260,1760	260,2538	I
In	293,2630	293,3488	I
In	451,1323	451,2588	I
Ir	380,0120	380,1199	I
K	766,4900	766,7010	I
La	412,3230	412,4393	II
La	433,3753	433,4972	II
Li	497,1750	497,3137	I
Li	610,3650	610,5340	I
Mg	279,0790	279,1613	II
Mg	279,5530	279,6354	II
Mg	285,2130	285,2968	I
Mg	291,5450	291,6304	I
Mg	382,9350	383,0437	I
Mg	383,8290	383,9379	I
Mg	448,1130	448,2387	II
Mg	517,2699	517,4140	I
Mn	257,6100	257,6872	II
Mn	263,8170	263,8956	II
Mn	293,3060	293,3918	II
Mn	346,0330	346,1321	II
Mn	403,3073	403,4213	I
Mn	403,4490	403,5630	I
Mo	202,0300	202,0952	II
Mo	277,5400	277,6219	II

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Mo	281,6150	281,6979	II
Mo	290,9120	290,9972	II
Mo	308,7620	308,8517	II
Mo	386,4110	386,5206	I
N	149,2192	149,2625	I
N	174,4631	174,5252	I
Na	588,9950	589,1583	I
Na	589,5920	589,7558	I
Nb	210,9420	211,0089	II
Nb	313,0790	313,1698	II
Nb	319,4980	319,5904	II
Nb	410,0400	410,1557	I
Nb	410,0920	410,2078	I
Nb	416,4660	416,5834	I
Nd	410,9460	411,0620	II
Ni	218,5500	218,6184	II
Ni	225,3850	225,4548	II
Ni	231,6040	231,6752	II
Ni	243,7890	243,8629	II
Ni	341,4760	341,5740	I
Ni	351,5054	351,6059	I
Ni	352,4540	352,5548	I
Ni	361,9392	362,0424	I
Ni	376,9455	377,0526	I
Ni	471,4420	471,5739	I
Ni	490,4413	490,5783	I
O	130,1661	130,2168	I
P	178,2249	178,2870	I
P	253,5650	253,6412	I
P	255,3262	255,4028	I
Pb	220,3505	220,4193	II
Pb	283,3052	283,3885	I
Pb	322,0538	322,1468	I
Pb	405,7820	405,8966	I
Pb	416,8033	416,9208	I
Pd	324,2700	324,3635	I
Pd	340,4580	340,5557	I
Pd	360,9550	361,0580	I
Pr	418,9480	419,0661	II
Pt	265,9450	266,0241	I
Pt	270,5890	270,6692	I
Pt	299,7970	299,8844	I
Rh	343,4890	343,5875	I
Ru	349,8940	349,9941	I
S	180,6688	180,7311	I
Sb	206,8341	206,9001	I
Sb	217,5810	217,6492	I
Sb	231,1470	231,2181	I
Sb	259,8050	259,8827	I
Sb	276,9950	277,0768	I
Sb	287,7920	287,8764	I

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Sb	326,7510	326,8452	I
Sc	361,3840	361,4871	II
Se	196,0259	196,0901	I
Si	212,4150	212,4821	I
Si	251,6123	251,6880	I
Si	288,1595	288,2440	I
Si	390,5523	390,6629	I
Sm	443,4320	443,5565	II
Sn	189,9278	189,9910	II
Sn	266,1248	266,2040	I
Sn	276,1780	276,2596	I
Sn	283,9990	284,0825	I
Sn	317,5050	317,5969	I
Sr	460,7330	460,8621	I
Sr	487,2490	487,3851	I
Ta	240,0630	240,1361	I
Ta	331,1160	331,2113	I
Te	169,9536	170,0000	I
Te	185,6573	185,7200	I
Te	214,2750	214,3425	I
Te	238,5780	238,6508	I
Th	401,9129	402,0265	II
Ti	311,2050	311,2953	II
Ti	324,1990	324,2926	II
Ti	337,2800	337,3769	II
Ti	365,3500	365,4541	I
Ti	367,1670	367,2716	I
Ti	368,5200	368,6249	II
Ti	498,1730	498,3120	I
Tl	351,9240	352,0246	I
Tl	377,5720	377,6792	I
V	214,0087	214,0761	II
V	288,2500	288,3345	II
V	311,0710	311,1612	II
V	369,2225	369,3276	I
V	437,9240	438,0471	I
W	209,8600	209,9266	II
W	220,4480	220,5168	II
W	400,8750	400,9883	I
Y	371,0300	371,1356	II
Y	464,3700	464,5000	II
Zn	206,1910	206,2569	II
Zn	213,8560	213,9234	I
Zn	250,2001	250,2755	II
Zn	334,5020	334,5982	I
Zn	481,0530	481,1875	I
Zr	332,6800	332,7757	II
Zr	343,8230	343,9216	II
Zr	349,6210	349,7210	II
Zr	357,2470	357,3490	II

X-ray Diffractometry Tables

BRUKER

Conversion from the 2Θ Bragg angle using Ag, Mo and Cu radiation to resolution and vice versa.

Calculations based on Bragg's Law: $2\ d \sin \Theta = n\ \lambda$

For λ, the mean of α_1 and α_2 ($2/3\ \alpha_1 + 1/3\ \alpha_2$) was taken, resulting in following wavelengths:

Ag	0.56083 Å
Mo	0.71073 Å
Cu	1.54178 Å

$2\Theta_{Ag}$ (°)	$2\Theta_{Mo}$ (°)	$2\Theta_{Cu}$ (°)	*d* (Å)	sin Θ/λ
3.21	4.07	8.84	**10.000**	0.050
3.63	4.61	**10.00**	8.845	0.057
6.43	8.15	17.74	**5.000**	**0.100**
7.24	9.18	**20.00**	4.439	0.113
7.89	**10.00**	21.80	4.077	0.123
10.00	12.68	27.73	3.217	0.155
10.73	13.61	29.78	**3.000**	0.167
10.80	13.70	**30.00**	2.979	0.168
12.88	16.34	35.92	2.500	**0.200**
14.29	18.14	**40.00**	2.254	0.222
15.75	**20.00**	44.26	2.046	0.244
16.12	20.47	45.34	**2.000**	0.250
17.69	22.47	**50.00**	1.824	0.274
19.37	24.62	55.10	1.667	**0.300**
20.00	25.43	57.03	1.615	0.310
20.96	26.65	**60.00**	1.542	0.324
21.55	27.41	61.85	**1.500**	0.333
23.57	**30.00**	68.31	1.373	0.364
24.09	30.66	**70.00**	1.344	0.372
25.93	33.03	76.15	1.250	**0.400**
27.04	34.47	**80.00**	1.199	0.417
29.81	38.05	**90.00**	1.090	0.459
30.00	38.29	90.72	1.083	0.461
31.31	**40.00**	95.80	1.039	0.481
32.36	41.36	**100.00**	1.006	0.497
32.57	41.63	100.87	**1.000**	**0.500**
34.67	44.37	**110.00**	0.941	0.531
36.72	47.06	**120.00**	0.890	0.562
38.50	49.39	**130.00**	0.851	0.588
38.96	**50.00**	132.92	0.841	0.595
39.33	50.48	135.36	0.833	**0.600**
39.97	51.34	**140.00**	0.820	0.609
40.00	51.37	140.19	0.820	0.610
41.04	52.75	149.00	**0.800**	0.625
41.14	52.88	**150.00**	0.798	0.626
41.98	54.00	**160.00**	0.783	0.639
42.49	54.67	**170.00**	0.774	0.646
42.66	54.90	**180.00**	0.771	0.649
46.23	59.67		0.714	**0.700**
46.48	**60.00**		0.711	0.704
47.23	61.02		**0.700**	0.714

$2\Theta_{Ag}$ (°)	$2\Theta_{Mo}$ (°)		*d* (Å)	sin Θ/λ
50.00	64.77		0.664	0.754
53.32	69.30		0.625	**0.800**
53.82	**70.00**		0.620	0.807
60.00	78.64		0.561	0.892
60.96	**80.00**		0.553	0.904
67.83	**90.00**		0.503	0.995
68.23	90.59		**0.500**	**1.000**
70.00	93.25		0.489	1.023
74.38	**100.00**		0.464	1.078
80.00	109.09		0.436	1.146
80.54	**110.00**		0.434	1.153
84.60	117.05		0.417	**1.200**
86.22	**120.00**		0.410	1.219
89.02	125.35		**0.400**	1.250
90.00	127.30		0.397	1.261
91.31	**130.00**		0.392	1.275
95.72	**140.00**		0.378	1.322
99.32	**150.00**		0.368	1.359
100.00	152.24		0.366	1.366
101.99	**160.00**		0.361	1.386
103.47	168.56		0.357	**1.400**
103.64	**170.00**		0.357	1.402
104.20	**180.00**		0.355	1.407
110.00			0.342	1.461
120.00			0.324	1.544
127.62			0.313	**1.600**
130.00			0.309	1.616
138.36			**0.300**	1.667
140.00			0.298	1.676
150.00			0.290	1.722
160.00			0.285	1.756
170.00			0.281	1.776
180.00			0.280	1.783

EPR/ENDOR Frequency Table

Z	A	E	Spin I	Nat. Abund. [%] (Half-life)	calc. X-Band ENDOR Freq. [MHz at 0.350 T] (free nucleus)	$g = \mu / (I\ \mu_N)$	$g\ \mu_N / g_e\ \mu_B$	Quadrupole Moment *Q* [fm² = 0.01 barn]
0	1	n	1/2		10.2076432	–3.8260854	1.040669 E–03	
1	1	H	1/2	99.9885	14.9021186	5.58569468	–1.519270 E–03	
	2	H	1	0.0115	2.28756617	0.857438228	–2.332173 E–04	0.286
	3	H	1/2	(12.32 y)	15.8951945	5.95792488	–1.620514 E–03	
2	3	He	1/2	0.000134	11.3519357	–4.25499544	1.157329 E–03	
3	6	Li	1	7.59	2.193146	0.8220473	–2.235912 E–04	–0.0808
	7	Li	3/2	92.41	5.791961	2.1709750	–5.904902 E–04	–4.01
4	9	Be	3/2	100.0	2.09429	–0.784993	2.13513 E–04	5.288
5	10	B	3	19.9	1.601318	0.600214927	–1.632543 E–04	8.459
	11	B	3/2	80.1	4.782045	1.792433	–4.875293 E–04	4.059
6	13	C	1/2	1.07	3.747940	1.404824	–3.821023 E–04	
7	14	N	1	99.636	1.077197	0.40376100	–1.098202 E–04	2.044
	15	N	1/2	0.364	1.511043	–0.56637768	1.540508 E–04	
8	17	O	5/2	0.038	2.02098	–0.757516	2.06039 E–04	–2.558
9	19	F	1/2	100.0	14.01648	5.253736	–1.428980 E–03	
10	21	Ne	3/2	0.27	1.177076	–0.441198	1.20003 E–04	10.155
11	22	Na	3	(2.6019 y)	1.5527	0.5820	–1.583 E–04	
	23	Na	3/2	100.0	3.944334	1.4784371	–4.021247 E–04	10.4
12	25	Mg	5/2	10.00	0.91290	–0.34218	9.3071 E–05	19.94
13	27	Al	5/2	100.0	3.886082	1.4566028	–3.961859 E–04	14.66
14	29	Si	1/2	4.685	2.96293	–1.11058	3.02070 E–04	
15	31	P	1/2	100.0	6.03801	2.26320	–6.15575 E–04	
16	33	S	3/2	0.75	1.145104	0.429214	–1.16743 E–04	–6.78
17	35	Cl	3/2	75.76	1.461790	0.5479162	–1.490294 E–04	–8.165
	36	Cl	2	(3.01 E5 y)	1.71476	0.642735	–1.748195 E–04	–1.80
	37	Cl	3/2	24.24	1.216786	0.4560824	–1.240513 E–04	–6.435
18	39	Ar	7/2	(269 y)	1.21	–0.454	1.234 E–04	
19	39	K	3/2	93.258	0.696337	0.2610049	–7.099152 E–05	5.85
	40	K	4	0.0117	0.865803	–0.324525	8.82686 E–05	–7.3
	41	K	3/2	6.730	0.382209	0.143261827	–3.896623 E–05	7.11
20	41	Ca	7/2	(1.02 E5 y)	1.215637	–0.4556517	1.239341 E–04	–6.7
	43	Ca	7/2	0.135	1.004386	–0.3764694	1.023971 E–04	–4.08
21	45	Sc	7/2	100.0	3.625677	1.358996	–3.696376 E–04	–22.0
22	47	Ti	5/2	7.44	0.84144	–0.31539	8.5784 E–05	30.2
	49	Ti	7/2	5.41	0.84166	–0.315477	8.58076 E–05	24.7
23	50	V	6	0.250	1.487665	0.5576148	–1.516674 E–04	21
	51	V	7/2	99.750	3.924649	1.4710588	–4.001178 E–04	–5.2
24	53	Cr	3/2	9.501	0.844019	–0.31636	8.6048 E–05	–15 or –2.8
25	53	Mn	7/2	(3.74 E6 y)	3.8296	1.4354	–3.9043 E–04	
	55	Mn	5/2	100.0	3.701688	1.38748716	–3.773869 E–04	33
26	57	Fe	1/2	2.119	0.483548	0.18124600	–4.92977 E–05	
27	59	Co	7/2	100.0	3.527	1.322	–3.596 E–04	42
	60	Co	5	(1925 d)	2.027	0.7598	–2.067 E–04	44
28	61	Ni	3/2	1.1399	1.33399	–0.50001	1.3600 E–04	16.2
29	63	Cu	3/2	69.15	3.961568	1.484897	–4.038817 E–04	–22.0
	65	Cu	3/2	30.85	4.2359	1.5877	–4.318525 E–04	–20.4
30	67	Zn	5/2	4.102	0.933986	0.35008196	–9.521988 E–05	15
31	69	Ga	3/2	60.108	3.58672	1.34439	–3.6567 E–04	17.1
	71	Ga	3/2	39.892	4.55726	1.70818	–4.6461 E–04	10.7
32	73	Ge	9/2	7.76	0.521409	–0.1954373	5.315759 E–05	–19.6
33	75	As	3/2	100.0	2.56025	0.959647	–2.61017 E–04	31.4
34	77	Se	1/2	7.63	2.855058	1.0701486	–2.910730 E–04	
	79	Se	7/2	(2.95 E5 y)	0.7760	–0.2909	7.911 E–05	80
35	79	Br	3/2	50.69	3.746454	1.404267	–3.819508 E–04	30.5
	81	Br	3/2	49.31	4.038433	1.513708	–4.117181 E–04	25.4
36	83	Kr	9/2	11.500	0.575479	–0.215704	5.86701 E–05	25.9
	85	Kr	9/2	(10.756 y)	0.596	–0.2233	6.075 E–05	43.3
37	85	Rb	5/2	72.17	1.444247	0.5413406	–1.472409 E–04	27.6
	87	Rb	3/2	27.83	4.894398	1.834545	–4.989836 E–04	13.35
38	87	Sr	9/2	7.00	0.648363	–0.243023	6.61005 E–05	33.5
39	89	Y	1/2	100.0	0.733223	–0.2748308	7.475208 E–05	

EPR/ENDOR Frequency Table

Z	A	E	Spin I	Nat. Abund. [%] (Half-life)	calc. X-Band ENDOR Freq. [MHz at 0.350 T] (free nucleus)	$g = \mu / (I\ \mu_N)$	$g\ \mu_N / g_e\ \mu_B$	Quadrupole Moment Q [fm^2 = 0.01 barn]
40	91	Zr	5/2	11.22	1.39118	–0.521448	1.41830 E–04	–17.6
41	93	Nb	9/2	100.0	3.6583	1.37122	–3.72963 E–04	–32
42	95	Mo	5/2	15.90	0.9756	–0.3657	9.9462 E–05	–2.2
	97	Mo	5/2	9.56	0.9962	–0.3734	1.016 E–04	25.5
43	99	Tc	9/2	(2.1 E5 y)	3.3703	1.2633	–3.4360 E–04	–12.9
44	99	Ru	5/2	12.76	0.684	–0.256	6.97 E–05	7.9
	101	Ru	5/2	17.06	0.764	–0.286	7.79 E–05	45.7
45	103	Rh	1/2	100.0	0.47169	–0.17680	4.8088 E–05	
	105	Rh	7/2	(35.36 h)	3.39	1.27	–3.46 E–04	
46	105	Pd	5/2	22.33	0.685	–0.257	6.98 E–05	66
47	107	Ag	1/2	51.839	0.606574	–0.2273593	6.184016 E–05	
	109	Ag	1/2	48.161	0.69734	–0.26138	7.1094 E–05	
48	111	Cd	1/2	12.80	3.174203	–1.1897722	3.236098 E–04	
	113	Cd	1/2	12.22	3.320483	–1.2446018	3.385231 E–04	
49	113	In	9/2	4.29	3.2779	1.2286	–3.3418 E–04	79.9
	115	In	9/2	95.71	3.2850	1.2313	–3.3490 E–04	81
50	115	Sn	1/2	0.34	4.9027	–1.8377	4.9983 E–04	
	117	Sn	1/2	7.68	5.34136	–2.00208	5.44552 E–04	
	119	Sn	1/2	8.59	5.5881	–2.09456	5.69706 E–04	
51	121	Sb	5/2	57.21	3.5893	1.34536	–3.65929 E–04	–36 or –45
	123	Sb	7/2	42.79	1.9436	0.72851	–1.9815 E–04	–49
	125	Sb	7/2	(2.75856 y)	2.00	0.75	–2.04 E–04	
52	123	Te	1/2	0.89	3.932218	–1.4738956	4.008894 E–04	
	125	Te	1/2	7.07	4.740899	–1.7770102	4.833345 E–04	
53	127	I	5/2	100.0	3.00222	1.125308	–3.060760 E–04	–71
	129	I	7/2	(1.57 E7 y)	1.9979	0.7489	–2.0368 E–04	–48
54	129	Xe	1/2	26.4006	4.15114	–1.555952	4.232082 E–04	
	131	Xe	3/2	21.2324	1.230549	0.461241	–1.254545 E–04	–11.4
55	133	Cs	7/2	100.0	1.968173	0.7377214	–2.006551 E–04	–0.343
	134	Cs	4	(2.0652 y)	1.9967	0.74843	–2.0357 E–04	38.9
	135	Cs	7/2	(2.3 E6 y)	2.0828	0.78069	–2.12341 E–04	5.0
	137	Cs	7/2	(30.07 y)	2.163	0.8109	–2.205 E–04	5.1
56	133	Ba	1/2	(10.51 y)	4.11749	–1.54334	4.19778 E–04	
	135	Ba	3/2	6.592	1.491586	0.559085	–1.520672 E–04	16.0
	137	Ba	3/2	11.232	1.66716	0.62489	–1.69967 E–04	24.5
57	137	La	7/2	(6 E4 y)	2.054	0.7700	–2.094 E–04	26
	138	La	5	0.090	1.981533	0.7427292	–2.020172 E–04	45
	139	La	7/2	99.910	2.121403	0.7951559	–2.1627690 E–04	20
59	141	Pr	5/2	100.0	4.5625	1.71016	–4.65152 E–04	–5.89
60	143	Nd	7/2	12.2	0.8118	–0.3043	8.2764 E–05	–63
	145	Nd	7/2	8.3	0.5000	–0.1874	5.0979 E–05	–33
61	147	Pm	7/2	(2.623 y)	1.97	0.737	–2.00 E–04	74
62	147	Sm	7/2	14.99	0.6211	–0.2328	6.332 E–05	–25.9
	149	Sm	7/2	13.82	0.5120	–0.1919	5.220 E–05	7.5
	151	Sm	5/2	(90 y)	0.3874	–0.1452	3.949 E–05	71
63	151	Eu	5/2	47.81	3.70487	1.38868	–3.77711 E–04	90.3
	152	Eu	3	(13.537 y)	1.7253	0.6467	–1.759 E–04	271
	153	Eu	5/2	52.19	1.6353	0.6130	–1.667 E–04	241
	154	Eu	3	(8.593 y)	1.783	–0.6683	1.818 E–04	280
	155	Eu	5/2	(4.753 y)	1.62	0.608	–1.65 E–04	240
64	155	Gd	3/2	14.80	0.4575	–0.1715	4.664 E–05	127
	157	Gd	3/2	15.65	0.5999	–0.2249	6.116 E–05	135
65	157	Tb	3/2	(71 y)	3.57	1.34	–3.64 E–04	141
	158	Tb	3	(180 y)	1.563	0.5860	–1.594 E–04	270
	159	Tb	3/2	100.0	3.5821	1.3427	–3.6520 E–04	143.2
66	161	Dy	5/2	18.889	0.512	–0.192	5.22 E–05	251
	163	Dy	5/2	24.896	0.718	0.269	–7.32 E–05	265
67	165	Ho	7/2	100.0	3.150	1.181	–3.211 E–04	358
68	167	Er	7/2	22.869	0.4298	–0.1611	4.382 E–05	357
69	169	Tm	1/2	100.0	1.23	–0.462	1.257 E–04	
	171	Tm	1/2	(1.92 y)	1.22	–0.456	1.240 E–04	
70	171	Yb	1/2	14.28	2.6341	0.98734	–2.6855 E–04	280
	173	Yb	5/2	16.13	0.72555	–0.27196	7.3970 E–05	

EPR/ENDOR Frequency Table

Z	A	E	Spin I	Nat. Abund. [%] (Half-life)	calc. X-Band ENDOR Freq. [MHz at 0.350 T] (free nucleus)	$g = \mu / (I\ \mu_N)$	$g\ \mu_N / g_e\ \mu_B$	Quadrupole Moment Q [fm^2 = 0.01 barn]
71	173	Lu	7/2	(1.37 y)	1.74	0.651	–1.772 E–04	
	174	Lu	1	(3.31 y)	5.1	1.9	–5.2 E–04	
	175	Lu	7/2	97.41	1.7016	0.6378	–1.735 E–04	349
	176	Lu	7	2.59	1.208	0.4527	–1.231 E–04	497
72	177	Hf	7/2	18.60	0.6049	0.2267	–6.166 E–05	337
	179	Hf	9/2	13.62	0.380	–0.142	3.87 E–05	379
73	181	Ta	7/2	99.988	1.8069	0.67729	–1.8422 E–04	317
74	183	W	1/2	14.31	0.628478	0.2355695	–6.407328 E–05	
75	185	Re	5/2	37.40	3.4012	1.2748	–3.4675 E–04	218
	187	Re	5/2	62.60	3.4359	1.2879	–3.5029 E–04	207
76	187	Os	1/2	1.96	0.344971	0.12930378	–3.516974 E–05	
	189	Os	3/2	16.15	1.173760	0.439955	–1.196648 E–04	85.6
77	191	Ir	3/2	37.3	0.26804	0.10047	–2.7326 E–05	81.6
	193	Ir	3/2	62.7	0.2912	0.1091	–2.9684 E–05	75.1
78	195	Pt	1/2	33.832	3.25229	1.21904	–3.31570 E–04	
79	197	Au	3/2	100.0	0.26351	0.098772	–2.6865 E–05	54.7
80	199	Hg	1/2	16.87	2.699312	1.011771	–2.751947 E–04	
	201	Hg	3/2	13.18	0.996420	–0.3734838	1.015850 E–04	38.6
81	203	Tl	1/2	29.52	8.656069	3.24451580	–8.824859 E–04	
	204	Tl	2	(3.78 y)	0.12	0.045	–1.22 E–05	
	205	Tl	1/2	70.48	8.741211	3.2764292	–8.911661 E–04	
82	207	Pb	1/2	22.1	3.1065	1.1644	–3.1670 E–04	
83	207	Bi	9/2	(32.9 y)	2.419	0.9069	–2.4667 E–04	–58
	209	Bi	9/2	100.0	2.437	0.9134	–2.4844 E–04	–51.6
84	209	Po	1/2	(102 y)	3.63	1.36	–3.70 E–04	
86	211	Rn	1/2	(14.6 h)	3.207	1.202	–3.269 E–04	
87	212	Fr	5	(20 min)	2.47	0.924	–2.51 E–04	–10
88	225	Ra	1/2	(14.9 d)	3.916	–1.468	3.993 E–04	
89	227	Ac	3/2	(21.77 y)	2.0	0.73	–1.99 E–04	170
90	229	Th	5/2	(7.34 E3 y)	0.491	0.184	–5.00 E–05	430
91	231	Pa	3/2	100.0 (3.25 E4 y)	3.57	1.34	–3.64 E–04	–172
92	233	U	5/2	(1.592 E5 y)	0.630	0.236	–6.42 E–05	366.3
	235	U	7/2	0.7204 (7.04 E8 y)	0.290	–0.109	2.95 E–05	493.6
93	237	Np	5/2	(2.14 E6 y)	3.351	1.256	–3.416 E–04	386.6
94	239	Pu	1/2	(2.410 E4 y)	1.08	0.406	–1.104 E–04	
	241	Pu	5/2	(14.4 y)	0.726	–0.272	7.40 E–05	560
95	241	Am	5/2	(432.7 y)	1.69	0.632	–1.72 E–04	314
	243	Am	5/2	(7.37 E3 y)	1.60	0.60	–1.63 E–04	286
96	243	Cm	5/2	(29.1 y)	0.438	0.164	–4.46 E–05	
	245	Cm	7/2	(8.48 E3 y)	0.38	0.14	–3.89 E–05	
	247	Cm	9/2	(1.56 E7 y)	0.22	0.082	–2.24 E–05	
97	249	Bk	3.5	(320 d)	1.5	0.6	–1.6 E–04	
99	253	Es	3.5	(20.47 d)	3.13	1.17	–3.19 E–04	670

revision 2009 based on NMR Properties Table, W. E. Hull; no. of decimal places reflects precision.

EPR Tables

Useful Relationships for EPR

Magn. Moment of the electron $\mu_e = g_e\ \mu_B\ S = g_e\ \mu_B / 2$ (g_e defined as negative) alternatively: $\mu_e = -g_e\ \mu_B / 2$ (with g_e positive) $\mu_B = \beta_e$ = Bohr magneton	**Magn. Moment for nucleus n** with spin I_n $\mu_n = g_n\ \mu_N\ I_n = \gamma_n\ \eta\ I_n$ $\mu_N = \beta_N$ = nuclear magneton
Resonance Condition - EPR $\nu_e = \lvert g \rvert\ \mu_B\ B_0 / h$ ν_e [GHz] = 13.996246 $\lvert g \rvert$ B_0 [T] B_0 [T] = 0.071447730 ν_e [GHz] / $\lvert g \rvert$ $\lvert g \rvert$ = 0.071447730 ν_e [GHz] / B_0 [T] $\lvert g \rvert$ = 3.04198626 ν_e [GHz] / ν_{H2O} [MHz]	**Resonance Condition - NMR** $\nu_n = \lvert g_n \rvert\ \mu_N\ B_0 / h = \lvert \gamma_n \rvert B_0 / 2\pi$ for ^{1}H: ν_{H2O} [MHz] = 42.5763875 B_0 [T] B_0 [T] = 0.0234871970 ν_{H2O} [MHz]
Hyperfine Coupling A [MHz] = 2.99792458 ×10^4 A [cm^{-1}] = 13.996246 $\lvert g \rvert$ A [mT] = 1.3996246 $\lvert g \rvert$ A [G]	A [cm^{-1}] = 0.333564095 × 10^{-4} A [MHz] = 4.6686451 × 10^{-4} $\lvert g \rvert$ A [mT] = 0.46686451 × 10^{-4} $\lvert g \rvert$ A [G]
Magnetic Field (flux density) = B_0 [in Tesla]	1 T = 10^4 G = 10 kG; 1 mT = 10 G; 1 G = 0.1 mT

see Physical Tables for Fundamental Constants

Skin Depth Table

Material	Specific Resistivity x 10^{-6} ohm-cm	Depth at 9.6 GHz		Depth at 100 kHz	
		µm	µin	mm	in
Silver	1.629	0.656	25.8	0.203	0.008
Copper. annealed	1.724	0.674	26.6	0.209	0.008
Gold	2.440	0.802	31.6	0.249	0.010
Aluminum	2.824	0.863	34.0	0.267	0.011
Rhodium	5.040	1.153	45.4	0.357	0.014
Tungsten	5.600	1.216	47.9	0.377	0.015
Molybdenum	5.700	1.226	48.3	0.380	0.015
Zinc	5.800	1.237	48.7	0.383	0.015
Brass	ca. 7.	1.359	53.5	0.421	0.017
Cadmium	7.600	1.416	55.8	0.439	0.017
Nickel	7.800	1.435	56.5	0.444	0.017
Platinum	10.000	1.624	64.0	0.503	0.020
Palladium	11.0	1.704	67.1	0.528	0.021
Tin	11.5	1.742	68.6	0.540	0.021
Lead	22.0	2.409	94.9	0.747	0.029

Table for Various Free Radicals Generated in Aqueous Solution

Radical	Sample solution	T (°C) *pH*	T_1 (µs)
$^{\bullet}CH_3$	0.1-0.5 M DMSO 1.0 M NaOH	19 *pH* = 14	0.2
$^{\bullet}CH_2COO^-$	0.5 M NaOAc 1.0 M NaOH	17-19 *pH* = 14	2.0
$^{\bullet}CH(COO^-)_2$	0.5 M malonic acid 2.0 M NaOH	18 *pH* = 14	2.9
$^-OC^{\bullet}(COO^-)_2$	0.1 M tartronic acid 1.2 M NaOH	17 *pH* = 14	3.6 $3.5 \leq T_1 < 4.0$
$^-OCH^{\bullet}COO^-$	0.1 M tartronic acid 1.2 M NaOH	17 *pH* = 14	1.4
$^{\bullet}CH_2O^-$	0.5 M CH_3OH 0.1 M NaOH	10 *pH* = 13	~0.1 $0.08 \leq T_1 < 0.15$
$^{\bullet}CH_3C^{\bullet}OH$	0.5 M CH_3CH_2OH 1.0 M NaOH	18 *pH* = 14	0.7
$(CH_3)_2CO^{\bullet-}$	0.5 M *i*-propanol 1.0 M NaOH	16 *pH* = 14	1.6

Radical	Sample solution	T (°C) *pH*	T_1 (µs)
$^{\bullet}CH_2OH$	0.5-1.0 M CH_3OH 1.0 M phosphate buffer	17 *pH* = 6.6-6.8	0.6
$CH_3C^{\bullet}HOH$	0.5 M CH_3CH_2OH 1.0 M phosphate buffer	18 *pH* = 6.6-6.8	1.3
$(CH_3)_2C^{\bullet}OH$	0.25 M *i*-propanol 0.5 M phosphate buffer	17 *pH* = 6.8	2.7
CH_2OD	0.5 M CH_3OH in D_2O acidif with H_2SO_4	9 *pD* = 3.6	0.72
		19 *pD* = 3.2	0.53
$(CH_3)_2C^{\bullet}OD$	0.5 M *i*-propanol in D_2O acidif with H_2SO_4	19 *pD* = 3.5	2.2
	0.5 M isopropanol in D_2O; 0.5 M phosphate buffer	19 *pD* = 7.0	2.5

Relaxation Times of Some Organic Free Radicals (Saturation-Recovery Method)

Radical	T_1 (µs)	T_2 (µs)
1,2-dicarboxylvinyl	9.0±1	7.0±2
chelidonic acid trianion	5.0±0.5	4.5±1
ascorbate radical	2.3±0.5	1.0±0.3
p-benzosemiquinone anion	2.0±0.3	1.8±0.5
2,5-di-*t*-butyl-benzosemiquinone anion	11.5±0.5	. . .

Values of T_2 for Various Organic Radicals at 77 K (ESE Method)

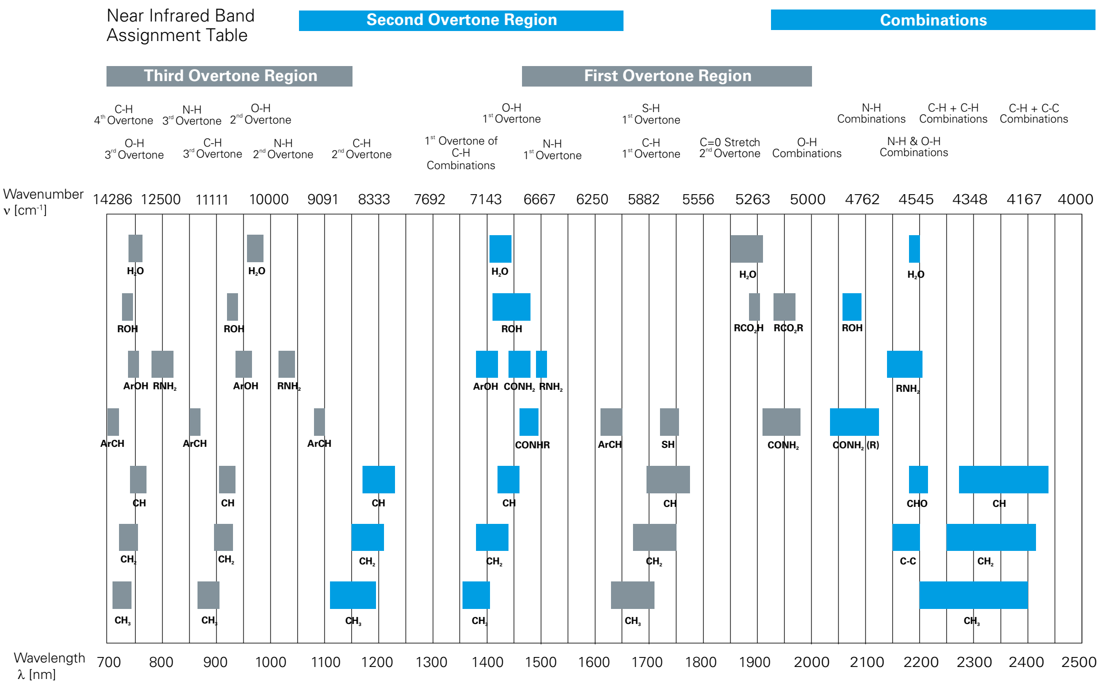
Radical	Matrix	T_2 (µs)
naphthalene anion	MTHF	3.4
naphtalene-d_8 anion	MTHF	3.2
1.3,5-triphenylbenzene anion	MTHF	3.2
triphenylene anion	MTHF	3.2
DPPH	MTHF	3.2
DPPH	fluorolube (FS-5)	10.0
perylene cation	sulfuric acid	10.4
anthracene cation	sulfuric acid	10.4
naphthacene cation	sulfuric acid	10.4
thianthrene cation	sulfuric acid	10.0
anthracene-d_{10} cation	sulfuric acid-d_2	200.0
anthracene cation	boric acid	14.6
biphenyl cation	boric acid	14.6
p-terphenyl cation	boric acid	14.2
naphthalene cation	boric acid	13.2
1,3,5-triphenylbenzene cation	boric acid	13.8
coronene cation	boric acid	10.0
triphenylene cation	boric acid	9.8
thianthrene cation	boric acid	10.0

IR Spectroscopy Tables

Conversion Table for Transmittance and Absorbance Units

Transmittance [%]	Absorbance	Transmittance [%]	Absorbance	Transmittance [%]	Absorbance	Transmittance [%]	Absorbance
1.0	2.000	26.0	.585	51.0	.292	76.0	.119
2.0	1.699	27.0	.569	52.0	.284	77.0	.114
3.0	1.523	28.0	.553	53.0	.276	78.0	.108
4.0	1.398	29.0	.538	54.0	.268	79.0	.102
5.0	1.301	30.0	.523	55.0	.260	80.0	.097
6.0	1.222	31.0	.509	56.0	.265	81.0	.092
7.0	1.155	32.0	.495	57.0	.244	82.0	.086
8.0	1.097	33.0	.481	58.0	.237	83.0	.081
9.0	1.046	34.0	.469	59.0	.229	84.0	.076
10.0	1.000	35.0	.456	60.0	.222	85.0	.071
11.0	.959	36.0	.444	61.0	.215	86.0	.066
12.0	.921	37.0	.432	62.0	.208	87.0	.060
13.0	.886	38.0	.420	63.0	.201	88.0	.056
14.0	.854	39.0	.409	64.0	.194	89.0	.051
15.0	.824	40.0	.398	65.0	.187	90.0	.046
16.0	.796	41.0	.387	66.0	.180	91.0	.041
17.0	.770	42.0	.377	67.0	.174	92.0	.036
18.0	.745	43.0	.367	68.0	.167	93.0	.032
19.0	.721	44.0	.357	69.0	.161	94.0	.027
20.0	.699	45.0	.347	70.0	.155	95.0	.022
21.0	.678	46.0	.337	71.0	.149	96.0	.018
22.0	.658	47.0	.328	72.0	.143	97.0	.013
23.0	.638	48.0	.319	73.0	.137	98.0	.009
24.0	.620	49.0	.310	74.0	.131	99.0	.004
25.0	.602	50.0	.301	75.0	.125	100.0	.000

Near-Infrared Table



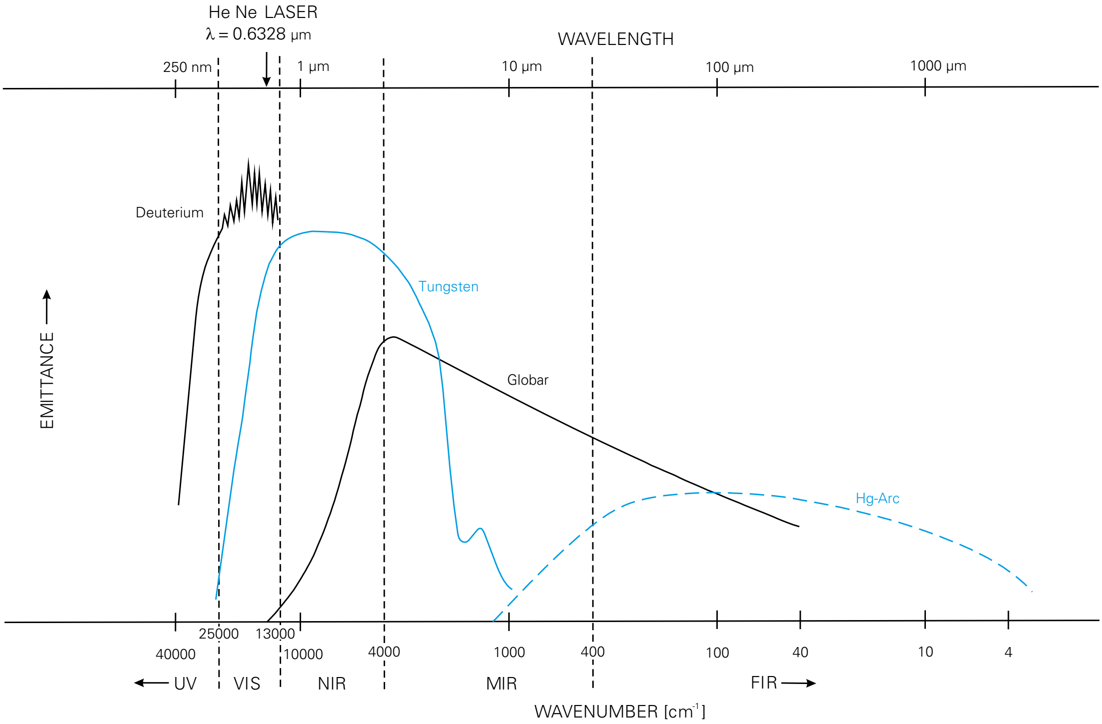
Conversion Table for Energy and Wavelength Units

Wavenumber [cm⁻¹]	Wavelength [µm]	Wavelength [nm]	Frequency [GHz]	Electron Volt [eV]
2.0	5 000.00	5 000 000	60	.00 025
4.0	2 500.00	2 500 000	120	.00 050
6.0	1 666.67	1 666 667	180	.00 074
8.0	1 250.00	1 250 000	240	.00 099
10.0	1 000.00	1 000 000	300	.00 124
12.0	833.33	833 333	360	.00 149
14.0	714.29	714 286	420	.00 174
16.0	625.00	625 000	480	.00 198
18.0	555.56	555 556	540	.00 223
20.0	500.00	500 000	600	.00 248
22.0	454.55	454 545	660	.00 273
24.0	416.57	416 667	719	.00 298
26.0	384.62	384 615	779	.00 322
28.0	357.14	357 143	839	.00 347
30.0	333.33	333 333	898	.00 372
32.0	312.50	312 500	959	.00 397
34.0	294.12	294 118	1 019	.00 422
36.0	277.78	277 778	1 079	.00 446
38.0	263.16	263 158	1 139	.00 471
40.0	250.00	250 000	1 199	.00 496
50.0	200.00	200 000	1 499	.00 620
60.0	166.67	166 667	1 799	.00 744
70.0	142.86	142 857	2 099	.00 868
80.0	125.00	125 000	2 398	.00 992
90.0	111.11	111 111	2 698	.01 116
100.0	100.00	100 000	2 988	.01 240
110.0	90.91	90 909	3 298	.01 364
120.0	83.33	83 333	3 597	.01 488
130.0	76.92	76 923	3 897	.01 612
140.0	71.43	71 429	4 197	.01 736
150.0	66.67	66 667	4 497	.01 860
160.0	62.50	62 500	4 797	.01 984
170.0	58.82	58 824	5 096	.02 108
180.0	55.56	55 556	5 396	.02 232
190.0	52.63	52 632	5 696	.02 356
200.0	50.00	50 000	5 996	.02 480
220.0	45.45	45 455	6 595	.02 728
240.0	41.67	41 667	7 195	.02 976
260.0	38.46	38 462	7 795	.03 224
280.0	35.71	35 714	8 394	.03 472
300.0	33.33	33 333	8 994	.03 720
320.0	31.25	31 250	9 593	.03 967
340.0	29.41	29 412	10 193	.04 215
360.0	27.78	27 778	10 792	.04 463
380.0	26.32	26 316	11 329	.04 711
400.0	25.00	25 000	11 992	.04 959
500.0	20.00	20 000	14 990	.06 199
600.0	16.67	16 667	17 987	.07 439
700.0	14.29	14 286	20 985	.08 679
800.0	12.50	12 500	23 983	.09 919
900.0	11.11	11 111	26 981	.11 159

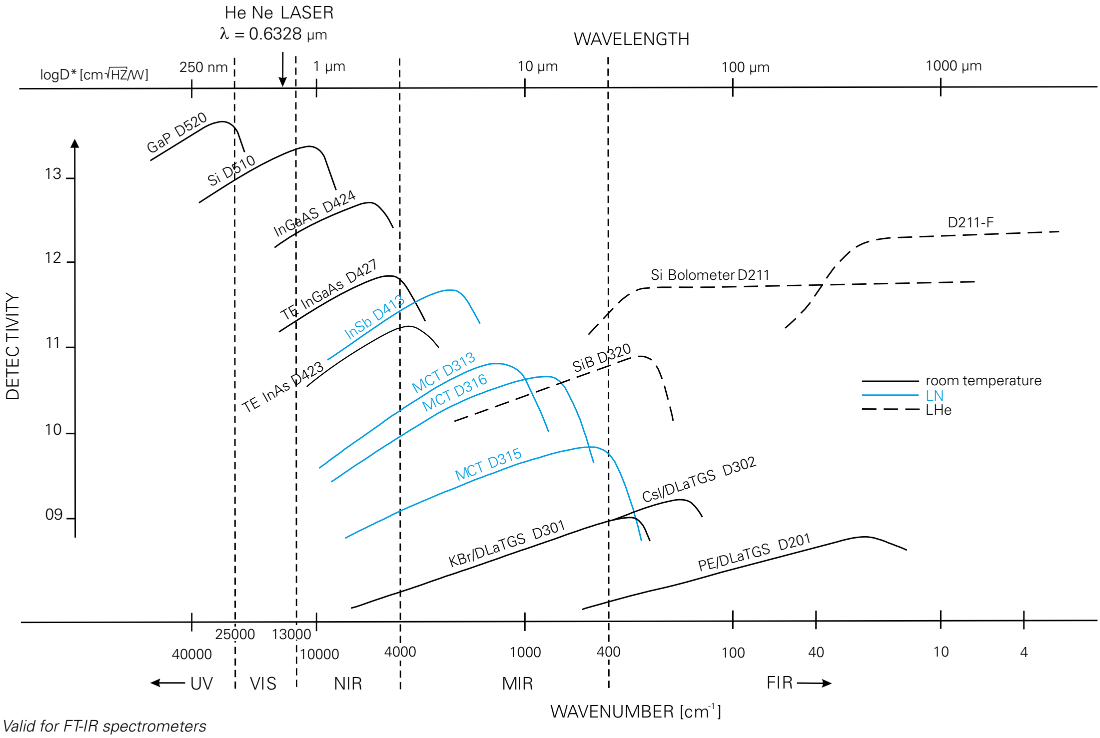
Wavenumber [cm⁻¹]	Wavelength [µm]	Wavelength [nm]	Frequency [GHz]	Electron Volt [eV]
1 000.0	10.00	10 000	29 979	.12 398
1 100.0	9.09	9 091	32 977	.13 638
1 200.0	8.33	8 333	35 975	.14 878
1 300.0	7.69	7 692	38 973	.16 118
1 400.0	7.14	7 143	41 971	.17 358
1 500.0	6.67	6 667	44 968	.18 598
1 600.0	6.25	6 250	47 966	.19 837
1 700.0	5.88	5 882	50 964	.21 077
1 800.0	5.56	5 556	53 962	.22 317
1 900.0	5.26	5 263	56 960	.23 557
2 000.0	5.00	5 000	59 958	.24 797
2 200.0	4.55	4 545	65 954	.27 276
2 400.0	4.17	4 167	71 950	.29 756
2 600.0	3.85	3 846	77 945	.32 236
2 800.0	3.57	3 571	83 941	.34 716
3 000.0	3.33	3 333	89 937	.37 195
3 200.0	3.13	3 125	95 933	.39 675
3 400.0	2.94	2 941	101 929	.42 155
3 600.0	2.78	2 778	107 924	.44 634
3 800.0	2.63	2 632	113 920	.47 114
4 000.0	2.50	2 500	119 916	.49 594
5 000.0	2.00	2 000	149 895	.61 992
6 000.0	1.67	1 667	179 874	.74 390
7 000.0	1.43	1 429	209 853	.86 789
8 000.0	1.25	1 250	239 832	.99 187
9 000.0	1.11	1 111	269 811	1.11 586
10 000.0	1.00	1 000	299 790	1.23 984
11 000.0	.91	909	329 769	1.36 382
12 000.0	.83	833	359 748	1.48 781
13 000.0	.77	769	389 727	1.61 179
14 000.0	.71	714	419 706	1.73 578
15 000.0	.67	667	449 685	1.85 976
16 000.0	.62	625	479 664	1.98 374
17 000.0	.59	588	509 643	2.10 773
18 000.0	.56	556	539 622	2.23 171
19 000.0	.53	526	569 601	2.35 570
20 000.0	.50	500	599 580	2.47 968
22 000.0	.45	455	659 538	2.72 765
24 000.0	.42	417	719 496	2.97 562
26 000.0	.38	385	779 454	3.22 358
28 000.0	.36	357	839 412	3.47 155
30 000.0	.33	333	899 370	3.71 952
32 000.0	.31	312	959 328	3.96 749
34 000.0	.29	294	1 019 286	4.21 546
36 000.0	.28	278	1 079 244	4.46 342
38 000.0	.26	263	1 139 202	4.71 139
40 000.0	.25	250	1 199 160	4.95 936
50 000.0	.20	200	1 498 950	6.19 921

IR Spectroscopy Tables

Sources



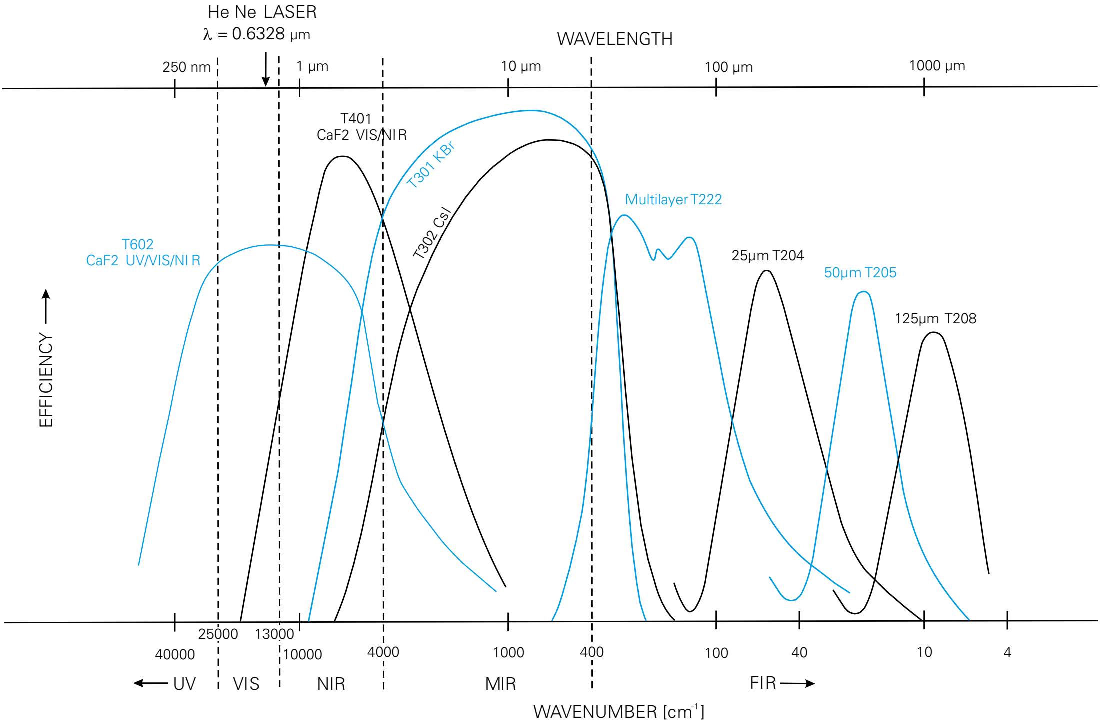
Detectors



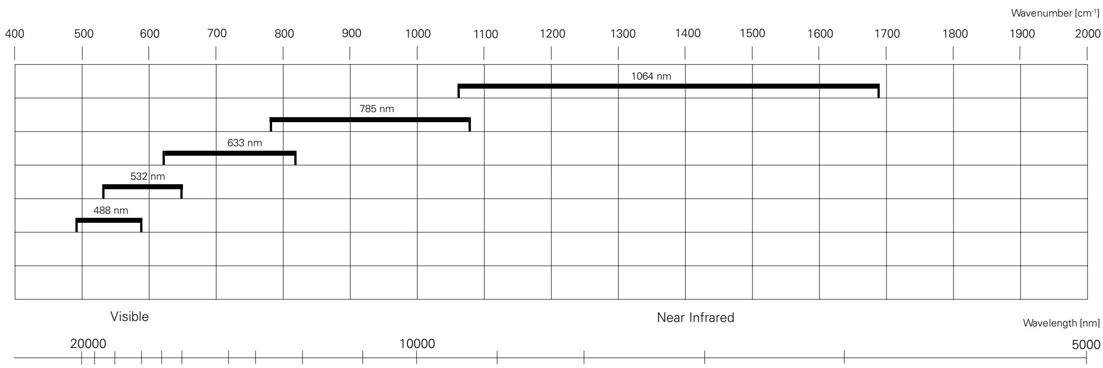
Valid for FT-IR spectrometers

IR Spectroscopy and Raman Tables

Beamsplitters



Stokes Shifts (0-3500 cm-1) of Various Laser Sources



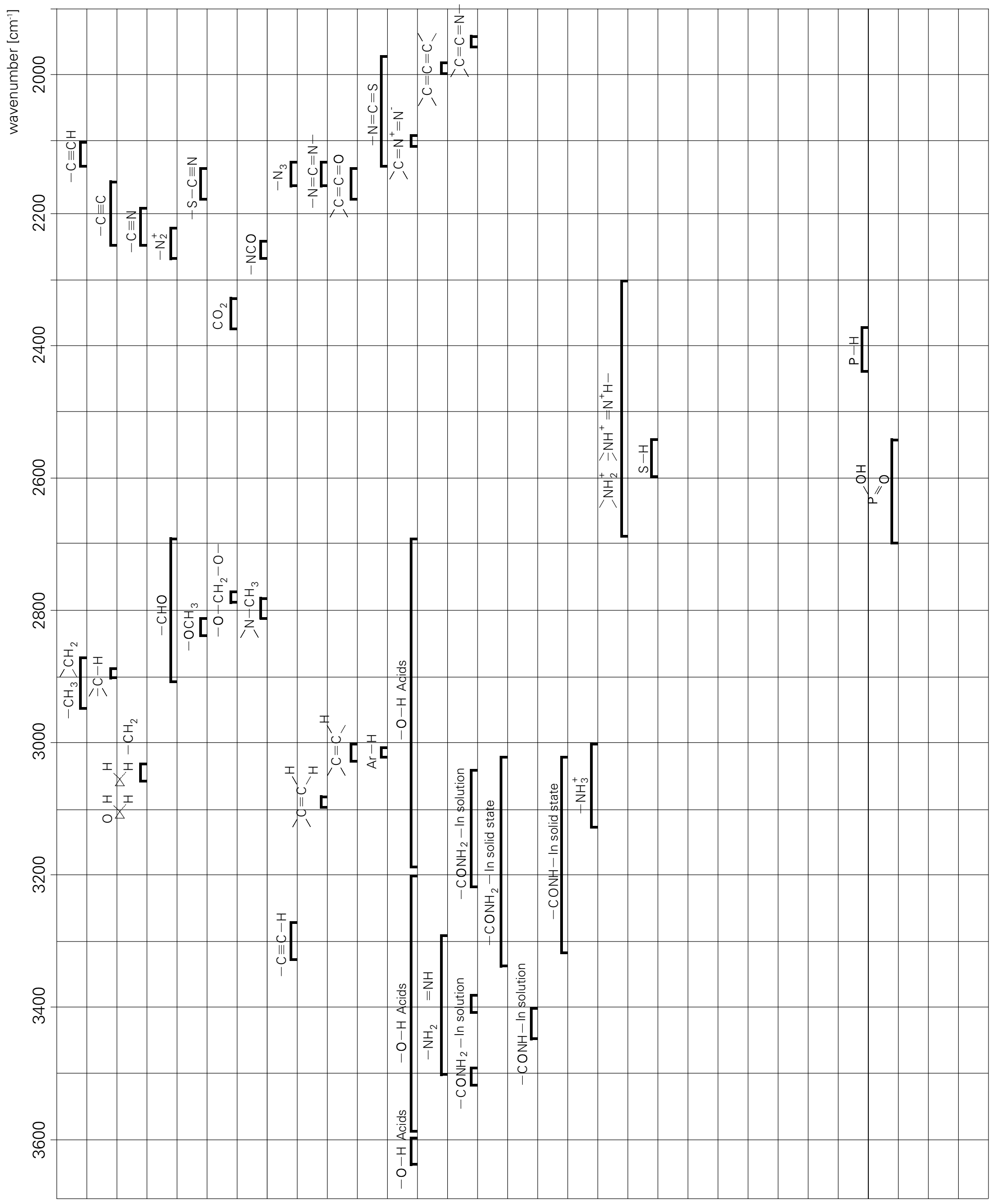
Vibrational Spectroscopy

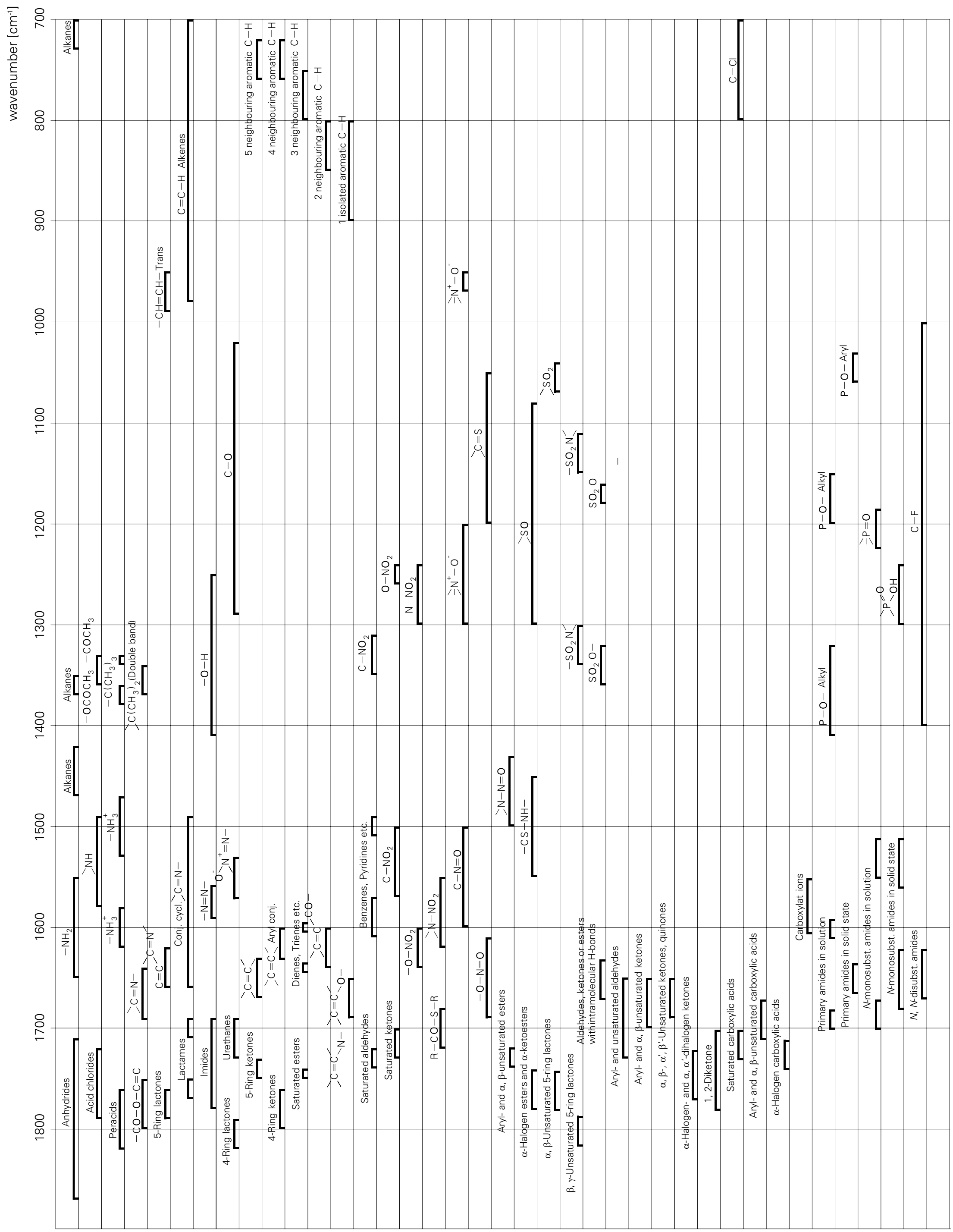
Selected Force Constants and Bond Orders of Organic and Inorganic Compounds (according to Siebert)

Bond A-B	Force Const. f (N cm^{-1})	Bond Order	Compound	Bond A-B	Force Const. f (N cm^{-1})	Bond Order	Compound
H-H	5.14	0.77	H_2	**C-S**	3.3	1.0	$S(CH_3)_2$
Li-Li	1.24	1.2	Li_2	**C-Cl**	3.12	0.93	CCl_4
B-B	3.58	1.2	B_2	**C-Ni**	2.91	1.2	Ni_4CO
C-C	16.5	3.2	HCCH	**C-Ni**	1.43	0.68	NiCO
N-N	22.42	3.2	N_2	**C-Se**	5.94	1.8	CSe_2
O-O	11.41	1.4	O_2	**C-Br**	2.42	0.86	CBr_4
F-F	4.45	0.58	F_2	**C-Rh**	2.4	1.2	$(Rh(CN)_6)^{3-}$
Na-Na	0.17	0.24	Na_2	**C-Ag**	2.0	0.99	$(Ag(CN)_2)^-$
Si-Si	4.65	2.0	Si_2	**C-I**	1.69	0.79	CI_4
Si-Si	~1.7	~0.9	Si_2H_6	**N-H**	7.05	1.1	NH_3
P-P	5.56	2.1	P_2	**N-B**	7.2	1.6	BN_2^{3-}
P-P	2.07	0.95	P_4	**N-C**	18.07	3.0	HCN
S-S	4.96	1.7	S_2	**N-N**	22.42	3.2	N_2
S-S	2.5	0.99	S_8	**N-N**	16.01	2.4	N-NNH
Cl-Cl	3.24	1.1	Cl_2	**N-N**	13.15	2.0	$N\text{-}N\text{-}N^-$
Ni-Ni	0.11	0.2	Ni solid	**N-O**	25.07	3.1	$N\text{-}O^+$
As-As	3.91	1.8	As_2	**N-O**	17.17	2.3	NO^+_2
Se-Se	3.61	1.6	$^{80}Se_2$	**N-O**	15.49	2.1	NO
Br-Br	2.36	1.1	Br_2	**N-O**	15.18	2.0	ONCl
Rb-Rb	0.08	0.2	Rb_2	**N-O**	11.78	1.7	NNO
Cd-Cd	1.11	1.0	Cd_2^{2+}	**N-F**	4.16	0.66	NF_3
Sb-Sb	2.61	1.9	Sb_2	**N-Si**	3.8	1.1	$((CH_3)_3Si)_2NH$
Te-Te	2.37	1.7	Te_2	**N-S**	12.54	2.5	NSF_3
I-I	1.70	1.2	I_2	**N-S**	8.3	1.9	HNSO
Hg-Hg	1.69	1.5	Hg_2^{2+}	**N-S**	3.1	0.87	$H_3N\text{-}SO_3$
Pb-Pb	4.02	3	Pb_2	**O-Li**	1.58	0.66	LiO
Bi-Bi	1.84	1.6	Bi_2	**O-Be**	7.51	1.8	BeO
H-B	2.75	0.68	BH_3	**O-B**	13.66	2.5	BO
H-C	5.50	1.0	CH_4	**O-B**	6.35	1.3	BO_3^{3-}
H-N	7.05	1.1	NH_3	**O-O**	16.59	2.0	O^+_2
H-O	8.45	1.1	H_2O	**O-O**	11.41	1.4	O_2
H-O	7.40	1.0	HO^-	**O-O**	6.18	0.89	O^-_2
H-F	8.85	1.1	HF	**O-O**	5.70	0.83	O_3
H-Al	1.76	0.60	AlH^-_4	**O-Na**	~3.2	~1.1	Na-OH
H-Si	2.98	0.84	SiH_4	**O-Mg**	3.5	1.1	MgO
H-P	3.11	0.82	PH_3	**O-Al**	5.66	1.5	AlO
H-S	4.29	1.0	H_2S	**O-Al**	3.8	1.1	$Al(OH)^-_4$
H-Cl	4.81	1.0	HCl	**O-Si**	9.25	2.1	SiO
H-Ge	2.81	0.82	GeH_4	**O-Si**	4.75	1.2	SiO^{-4}_4
H-As	2.85	0.81	AsH_3	**O-P**	9.41	2.0	PO
H-Se	3.51	0.93	H_2Se	**O-P**	6.16	1.4	PO^{3-}_4
H-Br	3.84	0.98	HBr	**O-S**	10.01	2.0	SO_2
H-Sn	2.03	0.76	SnH_4	**O-Cl**	4.26	1.0	ClO^-_2
H-Sb	2.09	0.77	SbH_3	**O-Cl**	3.30	0.82	ClO^-
H-I	2.92	0.97	HI	**O-Ca**	2.85	1.2	CaO
C-H	5.50	1.0	CH_4	**O-Ti**	7.19	2.4	TiO
C-B	3.82	1.1	$B(CH_3)_3$	**O-V**	7.36	2.3	VO
C-C	16.5	3.2	HCCH	**O-Cr**	5.82	1.9	CrO
C-C	9.15	1.9	H_2CCH_2	**O-Mn**	5.16	1.6	MnO
C-C	7.6	1.7	C_6H_6	**O-Fe**	5.67	1.7	FeO
C-C	4.4	1.1	H_3CCH_3	**O-Cu**	2.97	0.93	CuO
C-N	18.07	3.0	HCN	**O-Ge**	7.53	1.8	^{74}GeO
C-N	11.84	2.1	CN_2^{2-}	**O-Se**	6.45	1.5	SeO
C-N	6.54	1.3	$NNCH_2$	**O-Mo**	3.05	1.2	Ba_2CaMoO_6 (solid)
C-O	18.56	2.8	CO	**O-Ru**	6.70	2.2	RuO_4
C-O	15.61	2.4	CO_2	**O-Ag**	2.00	0.79	AgO
C-O	12.76	2.0	OCH_2	**O-Sn**	5.53	1.7	SnO
C-O	7.86	1.3	CO_3^{2-}	**O-Te**	5.31	1.6	TeO
C-O	5.1	0.96	$O(CH_3)_2$	**O-Ba**	3.79	1.8	BaO
C-F	6.98	1.1	CF_4	**O-Ce**	6.33	2.6	CeO
C-P	8.95	2.4	HCP	**O-Pr**	5.68	2.4	PrO
C-S	7.67	2.0	CS_2	**O-Nd**	3.5	1.6	$NdAc_3 \cdot H_2O$ (polymer)

IR Window Materials

Material	Transmission Range [cm^{-1}] ([micrometers])	Refractive Index n at 2000 cm^{-1}	Reflectance loss per surface	Hardness (Knoop)	Chemical Properties
Infrasil SiO_2	57,000-2,800 (0.175-3.6)	1.46	~ 3.3%	461	Insoluble in water; soluble in HF.
UV Sapphire AL_2O_3	66,000-2,000 (0.15-5.0)	1.75	~ 7.3%	1370	Very slightly soluble in acids and bases.
Silicon Si	10,000-100 (1.0-100)	3.42	~ 30%	1150	Insoluble in most acids and bases; soluble in HF and HNO_3.
Calcium Fluoride CaF_2	66,000-1,200 (0.15-8.0)	1.40	~ 2.8%	158	Insoluble in water; resists most acids and bases; soluble in NH_4 salts.
Barium Fluoride BaF_2	50,000-900 (0.2-11)	1.45	~ 3.3%	82	Low water solubility; soluble in acid and NH_4Cl.
Zinc Sulfide, Cleartran ZnS	22,000-750 (0.45-13.0)	2.25	~ 15%	355	Soluble in acid; insoluble in water.
Germanium Ge	5,000-600 (2.0-17)	4.01	~ 36%	550	Insoluble in water; soluble in hot H_2SO_4 and aqua regia.
Sodium Chloride NaCl	28,000-700 (0.35-15)	1.52	~ 4.5%	15	Hygroscopic; slightly soluble in alcohol and NH_3.
AMTIR GeAsSe Glass	11,000-900 (0.9-11)	2.50	~ 18%	170	Insoluble in water. Soluble in bases.
Zinc Selenide ZnSe	20,000-500 (0.5-20)	2.43	~ 17%	150	Soluble in strong acids; dissolves in HNO_3.
Silver Chloride AgCl	23,000-400 (0.42-25)	2.00	~ 11%	10	Insoluble in water; soluble in NH_4OH.
Potassium Bromide KBr	33,000-400 (0.3-25)	1.54	~ 4.5%	7	Soluble in water, alcohol, and glycerine; hygroscopic.
Cesium Iodide CsI	33,000-150 (0.3-70)	1.74	~ 7.3%	20	Soluble in water and alcohol; hygroscopic.
KRS-5 TlBr/I	16,000-200 (0.6-60)	2.38	~ 17%	40	Soluble in warm water; soluble in bases; insoluble in acids.
Polyethylene PE (high density)	600-10 (16-1,000)	1.52	~ 4.5%	5	Resistant to most solvents.
Diamond C	45,000-10 (0.22-1,000)	2.40	~ 17%	7000	Insoluble in water, acids, and bases.
TPX(TM) Methylpentene Resin	350-10 (28-1,000)	1.43	~ 3.3%		Similar to PE but transparent and more rigid.


wavenumber [cm⁻¹]
2000
2200
2400
2600
2800
3000
3200
3400
3600
—C≡CH
—C≡C
—C≡N
—N₂⁺
—S—C≡N
CO₂
—NCO
—N₃
—N=C=N—
C=C=O
—N=C=S
C=N⁺=N⁻
C=C=C
C=C=N—
NH₂⁺ NH⁺ ≡N⁺H—
S—H
P—H
P—OH =O
—CHO
—OCH₃
—O—CH₂—O—
N—CH₃
—CH₃ CH₂
C—H
O H H
H —CH₂
C=C H H
C=C H
Ar—H
—O—H Acids
—C≡C—H
—CONH₂—In solution
—CONH₂—In solid state
—CONH—In solid state
—NH₃⁺
—NH₂ =NH
—CONH—In solution


wavenumber [cm⁻¹]
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
Alkanes
Anhydrides
–NH2
Alkanes
Alkanes
Acid chlorides
NH
–OCOCH3 –COCH3
Peracids
–NH3+
–C(CH3)3
–CO–O–C=C
C=N
C=C
5-Ring lactones
C=C–H Alkenes
–CH=CH– Trans
Conj. cycl. C=N–
C(CH3)2 (Double band)
Lactames
Imides
–O–H
–N=N–
O–N+=N–
4-Ring lactones
Urethanes
C–O
5-Ring ketones
C=C
5 neighbouring aromatic C–H
4-Ring ketones
C=C Aryl conj.
4 neighbouring aromatic C–H
Saturated esters
Dienes, Trienes etc.
3 neighbouring aromatic C–H
2 neighbouring aromatic C–H
1 isolated aromatic C–H
Saturated aldehydes
Benzenes, Pyridines etc.
C–NO2
Saturated ketones
C–NO2
O–NO2
–O–NO2
N–NO2
R–CO–S–R
N–NO2
C–N=O
N+–O–
–O–N=O
Aryl- and α, β-unsaturated esters
N–N=O
C=S
α-Halogen esters and α-ketoesters
–CS–NH–
SO
α, β-Unsaturated 5-ring lactones
SO2
β, γ-Unsaturated 5-ring lactones
–SO2 N
Aldehydes, ketones or esters with intramolecular H-bonds
SO2 O–
SO2 O
Aryl- and unsaturated aldehydes
Aryl- and α, β-unsaturated ketones
α, β-, α', β'-Unsaturated ketones, quinones
α-Halogen- and α, α'-dihalogen ketones
1, 2-Diketone
Saturated carboxylic acids
C–Cl
Aryl- and α, β-unsaturated carboxylic acids
α-Halogen carboxylic acids
Carboxylat ions
Primary amides in solution
P–O– Alkyl
Primary amides in solid state
P–O– Aryl
N-monosubst. amides in solution
P=O
N-monosubst. amides in solid state
P=O OH
N, N-disubst. amides
C–F

MS: Exact Masses of the Isotopes

Atomic Masses and Representative Abundances of the Isotopes (NIST)

The masses and abundances of the isotopes we use for generating molecular formulas, simulating patterns and SNAP peak finding basically are taken from the National Institute of Standards and Technology (NIST).
Z = Atomic number, M = mass number; Ratios are calculated with most abundant isotope = 1.

Z	E	M	Exact Mass	Abund.	Valency
1	**H**	**1**	1.00782503207	0.999885	1
	D	**2**	2.0141017778	0.000115	
	T	**3**	3.0160492777		
2	**He**	**3**	3.0160293191	1.34e-6	0
		4	4.00260325415	0.99999866	
3	**Li**	**6**	6.015122795	0.0759	1
		7	7.01600455	0.9241	
4	**Be**	**9**	9.0121822	1	2
5	**B**	**10**	10.0129370	0.199	3
		11	11.0093054	0.801	
6	**C**	**12**	12 (by definition)	0.9893	4
		13	13.0033548378	0.0107	
		14	14.003241989		
7	**N**	**14**	14.0030740048	0.99636	3
		15	15.0001088982	0.00364	
8	**O**	**16**	15.99491461956	0.99757	2
		17	16.99913170	0.00038	
		18	17.9991610	0.00205	
9	**F**	**19**	18.99840322	1	1
10	**Ne**	**20**	19.9924401754	0.9048	0
		21	20.99384668	0.0027	
		22	21.991385114	0.0925	
11	**Na**	**23**	22.9897692809	1	1
12	**Mg**	**24**	23.985041700	0.7899	2
		25	24.98583692	0.1000	
		26	25.982592929	0.1101	
13	**Al**	**27**	26.98153863	1	3
14	**Si**	**28**	27.9769265325	0.92223	4
		29	28.976494700	0.04685	
		30	29.97377017	0.03092	
15	**P**	**31**	30.97376163	1	3
		32	31.97390727		
16	**S**	**32**	31.97207100	0.9499	2
		33	32.97145876	0.0075	
		34	33.96786690	0.0425	
		36	35.96708076	0.0001	
17	**Cl**	**35**	34.96885268	0.7576	1
		37	36.96590259	0.2424	
18	**Ar**	**36**	35.967545106	0.003365	0
		38	37.9627324	0.000632	
		40	39.9623831225	0.996003	
19	**K**	**39**	38.96370668	0.932581	1
		40	39.96399848	0.000117	
		41	40.96182576	0.067302	
20	**Ca**	**40**	39.96259098	0.96941	2
		42	41.95861801	0.00647	
		43	42.9587666	0.00135	
		44	43.9554818	0.02086	
		46	45.9536926	0.00004	
		48	47.952534	0.00187	
21	**Sc**	**45**	44.9559119	1	3
22	**Ti**	**46**	45.9526316	0.0825	4
		47	46.9517631	0.0744	
		48	47.9479463	0.7372	
		49	48.9478700	0.0541	
		50	49.9447912	0.0518	
23	**V**	**50**	49.9471585	0.00250	5
		51	50.9439595	0.99750	
24	**Cr**	**50**	49.9460442	0.04345	3
		52	51.9405075	0.83789	
		53	52.9406494	0.09501	
		54	53.9388804	0.02365	
25	**Mn**	**55**	54.9380451	1	2
26	**Fe**	**54**	53.9396105	0.05845	2
		56	55.9349375	0.91754	
		57	56.9353940	0.02119	
		58	57.9332756	0.00282	
27	**Co**	**59**	58.9331950	1	2
28	**Ni**	**58**	57.9353429	0.680769	2
		60	59.9307864	0.262231	
		61	60.9310560	0.011399	
		62	61.9283451	0.036345	
		64	63.9279660	0.009256	

MS: Exact Masses of the Isotopes

BRUKER

Atomic Masses and Representative Abundances of the Isotopes (NIST)

The masses and abundances of the isotopes we use for generating molecular formulas, simulating patterns and SNAP peak finding basically are taken from the National Institute of Standards and Technology (NIST).
Z = Atomic number, M = mass number; Ratios are calculated with most abundant isotope = 1.

Z	E	M	Exact Mass	Abund.	Valency
29	Cu	63	62.9295975	0.6915	1
		65	64.9277895	0.3085	
30	Zn	64	63.9291422	0.48268	2
		66	65.9260334	0.27975	
		67	66.9271273	0.04102	
		68	67.9248442	0.19024	
		70	69.9253193	0.00631	
31	Ga	69	68.9255736	0.60108	3
		71	70.9247013	0.39892	
32	Ge	70	69.9242474	0.2038	4
		72	71.9220758	0.2731	
		73	72.9234589	0.0776	
		74	73.9211778	0.3672	
		76	75.9214026	0.0783	
33	As	75	74.9215965	1	3
34	Se	74	73.9224764	0.0089	2
		76	75.9192136	0.0937	
		77	76.9199140	0.0763	
		78	77.9173091	0.2377	
		80	79.9165213	0.4961	
		82	81.9166994	0.0873	
35	Br	79	78.9183371	0.5069	1
		81	80.9162906	0.4931	
36	Kr	78	77.9203648	0.00355	0
		80	79.9163790	0.02286	
		82	81.9134836	0.11593	
		83	82.914136	0.11500	
		84	83.911507	0.56987	
		86	85.91061073	0.17279	
37	Rb	85	84.911789738	0.7217	1
		87	86.909180527	0.2783	
38	Sr	84	83.913425	0.0056	2
		86	85.9092602	0.0986	
		87	86.9088771	0.0700	
		88	87.9056121	0.8258	
39	Y	89	88.9058483	1	3

Z	E	M	Exact Mass	Abund.	Valency
40	Zr	90	89.9047044	0.5145	4
		91	90.9056458	0.1122	
		92	91.9050408	0.1715	
		94	93.9063152	0.1738	
		96	95.9082734	0.0280	
41	Nb	93	92.9063781	1	5
42	Mo	92	91.906811	0.1477	6
		94	93.9050883	0.0923	
		95	94.9058421	0.1590	
		96	95.9046795	0.1668	
		97	96.9060215	0.0956	
		98	97.9054082	0.2419	
		100	99.907477	0.0967	
43	Tc	97	96.906365		4
		98	97.907216		
		99	98.9062547		
44	Ru	96	95.907598	0.0554	3
		98	97.905287	0.0187	
		99	98.9059393	0.1276	
		100	99.9042195	0.1260	
		101	100.9055821	0.1706	
		102	101.9043493	0.3155	
		104	103.905433	0.1862	
45	Rh	103	102.905504	1	3
46	Pd	102	101.905609	0.0102	2
		104	103.904036	0.1114	
		105	104.905085	0.2233	
		106	105.903486	0.2733	
		108	107.903892	0.2646	
		110	109.905153	0.1172	
47	Ag	107	106.905097	0.51839	1
		109	108.904752	0.48161	
48	Cd	106	105.906459	0.0125	2
		108	107.904184	0.0089	
		110	109.9030021	0.1249	
		111	110.9041781	0.1280	
		112	111.9027578	0.2413	
		113	112.9044017	0.1222	
		114	113.9033585	0.2873	
		116	115.904756	0.0749	

MS: Exact Masses of the Isotopes

BRUKER

Atomic Masses and Representative Abundances of the Isotopes (NIST)

The masses and abundances of the isotopes we use for generating molecular formulas, simulating patterns and SNAP peak finding basically are taken from the National Institute of Standards and Technology (NIST).
Z = Atomic number, M = mass number; Ratios are calculated with most abundant isotope = 1.

Z	E	M	Exact Mass	Abund.	Valency
49	In	113	112.904058	0.0429	3
		115	114.903878	0.9571	
50	Sn	112	111.904818	0.0097	4
		114	113.902779	0.0066	
		115	114.903342	0.0034	
		116	115.901741	0.1454	
		117	116.902952	0.0768	
		118	117.901603	0.2422	
		119	118.903308	0.0859	
		120	119.9021947	0.3258	
		122	121.9034390	0.0463	
		124	123.9052739	0.0579	
51	Sb	121	120.9038157	0.5721	5
		123	122.9042140	0.4279	
52	Te	120	119.904020	0.0009	2
		122	121.9030439	0.0255	
		123	122.9042700	0.0089	
		124	123.9028179	0.0474	
		125	124.9044307	0.0707	
		126	125.9033117	0.1884	
		128	127.9044631	0.3174	
		130	129.9062244	0.3408	
53	I	127	126.904473	1	1
54	Xe	124	123.9058930	0.000952	0
		126	125.904274	0.000890	
		128	127.9035313	0.019102	
		129	128.9047794	0.264006	
		130	129.9035080	0.040710	
		131	130.9050824	0.212324	
		132	131.9041535	0.269086	
		134	133.9053945	0.104357	
		136	135.907219	0.088573	
55	Cs	133	132.905451933	1	1
56	Ba	130	129.9063208	0.00106	2
		132	131.9050613	0.00101	
		134	133.9045084	0.02417	
		135	134.9056886	0.06592	
		136	135.9045759	0.07854	
		137	136.9058274	0.11232	
		138	137.9052472	0.71698	

Z	E	M	Exact Mass	Abund.	Valency
57	La	138	137.907112	0.00090	3
		139	138.9063533	0.99910	
58	Ce	136	135.907172	0.00185	4
		138	137.905991	0.00251	
		140	139.9054387	0.88450	
		142	141.909244	0.11114	
59	Pr	141	140.9076528	1	3
60	Nd	142	141.9077233	0.272	3
		143	142.9098143	0.122	
		144	143.9100873	0.238	
		145	144.9125736	0.083	
		146	145.9131169	0.172	
		148	147.916893	0.057	
		150	149.920891	0.056	
61	Pm	145	144.912749		
		147	146.9151385		
62	Sm	144	143.911999	0.0307	2
		147	146.9148979	0.1499	
		148	147.9148227	0.1124	
		149	148.9171847	0.1382	
		150	149.9172755	0.0738	
		152	151.9197324	0.2675	
		154	153.9222093	0.2275	
63	Eu	151	150.9198502	0.4781	2
		153	152.9212303	0.5219	
64	Gd	152	151.9197910	0.0020	3
		154	153.9208656	0.0218	
		155	154.9226220	0.1480	
		156	155.9221227	0.2047	
		157	156.9239601	0.1565	
		158	157.9241039	0.2484	
		160	159.9270541	0.2186	
65	Tb	159	158.9253468	1	3
66	Dy	156	155.924283	0.00056	3
		158	157.924409	0.00095	
		160	159.9251975	0.02329	
		161	160.9269334	0.18889	
		162	161.9267984	0.25475	
		163	162.9287312	0.24896	
		164	163.9291748	0.28260	

MS: Exact Masses of the Isotopes

Atomic Masses and Representative Abundances of the Isotopes (NIST)

The masses and abundances of the isotopes we use for generating molecular formulas, simulating patterns and SNAP peak finding basically are taken from the National Institute of Standards and Technology (NIST).

Z = Atomic number, M = mass number; Ratios are calculated with most abundant isotope = 1.

Z	E	M	Exact Mass	Abund.	Valency
67	Ho	165	164.9303221	1	3
68	Er	162	161.928778	0.00139	3
		164	163.929200	0.01601	
		166	165.9302931	0.33503	
		167	166.9320482	0.22869	
		168	167.9323702	0.26978	
		170	169.9354643	0.14910	
69	Tm	169	168.9342133	1	3
70	Yb	168	167.933897	0.0013	2
		170	169.9347618	0.0304	
		171	170.9363258	0.1428	
		172	171.9363815	0.2183	
		173	172.9382108	0.1613	
		174	173.9388621	0.3183	
		176	175.9425717	0.1276	
71	Lu	175	174.9407718	0.9741	3
		176	175.9426863	0.0259	
72	Hf	174	173.940046	0.0016	4
		176	175.9414086	0.0526	
		177	176.9432207	0.1860	
		178	177.9436988	0.2728	
		179	178.9458161	0.1362	
		180	179.9465500	0.3508	
73	Ta	180	179.9474648	0.00012	5
		181	180.9479958	0.99988	
74	W	180	179.946704	0.0012	6
		182	181.9482042	0.2650	
		183	182.9502230	0.1431	
		184	183.9509312	0.3064	
		186	185.9543641	0.2843	
75	Re	185	184.9529550	0.3740	4
		187	186.9557531	0.6260	
76	Os	184	183.9524891	0.0002	3
		186	185.9538382	0.0159	
		187	186.9557505	0.0196	
		188	187.9558382	0.1324	
		189	188.9581475	0.1615	
		190	189.9584470	0.2626	
		192	191.9614807	0.4078	

Z	E	M	Exact Mass	Abund.	Valency
77	Ir	191	190.9605940	0.373	3
		193	192.9629264	0.627	
78	Pt	190	189.959932	0.00014	2
		192	191.9610380	0.00782	
		194	193.9626803	0.32967	
		195	194.9647911	0.33832	
		196	195.9649515	0.25242	
		198	197.967893	0.07163	
79	Au	197	196.9665687	1	1
80	Hg	196	195.965833	0.0015	2
		198	197.9667690	0.0997	
		199	198.9682799	0.1687	
		200	199.9683260	0.2310	
		201	200.9703023	0.1318	
		202	201.9706430	0.2986	
		204	203.9734939	0.0687	
81	Tl	203	202.9723442	0.2952	3
		205	204.9744275	0.7048	
82	Pb	204	203.9730436	0.014	4
		206	205.9744653	0.241	
		207	206.9758969	0.221	
		208	207.9766521	0.524	
83	Bi	209	208.9803987	1	5
90	Th	232	232.0380553	1	4
91	Pa	231	231.0358840	1	4
92	U	234	234.0409521	5.4e-05	3
		235	235.0439299	0.007204	
		238	238.0507882	0.992742	

References:

Coursey, J.S., Schwab, D.J., and Dragoset, R.A. (2003), Atomic Weights and Isotopic Compositions (version 3.0). [Online] Available: http://www.nist.gov/physlab/data/comp.cfm [2010, July 15]. National Institute of Standards and Technology, Gaithersburg, MD.

Originally published as M.E. Wieser and M. Berglund, Atomic Weights of the Elements 2007, Pure Appl. Chem. 81(11), 2131 (2009); J.K. Böhlke, J.R. de Laeter, P. De Bièvre, H. Hidaka, H.S. Peiser, K.J.R. Rosman, and P.D.P. Taylor, Isotopic Compositions of the Elements, 2001, J. Phys. Chem. Ref. Data 34(1), 57 (2005); and G. Audi, A.H. Wapstra, and C. Thibault, The 2003 Atomic Mass Evaluation, Nuclear Physics A 729(1), 337 (2003).

The following modifications/additions were made to the NIST Atomic Weights and Isotopic Compositions (version 3.0) table:

- Additional elements Ct, Nt and Ot were defined which have an abundance of 95 % of 13C, 15N and 18O and 5 % of 12C, 14N and 16O. These elements were added to calculate isotopically marked substances. Within the software the complete list of atoms and isotopes is available.
- Typical valencies of the atoms are listed additionally. For quickly inspecting the valencies used, please refer to the Table of Valencies.

Solid-Phase Peptide Synthesis

Mass Shift of Modifications, Protection Groups and Artifacts

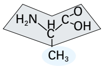
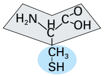
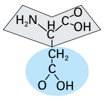
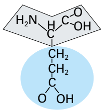
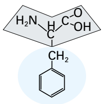
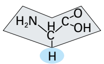
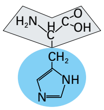
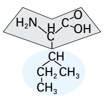
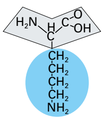
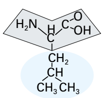
m/z shift [Da]	Modification	Abbreviation	Sum formula change	Valid residues	Origin
-186,07931	Trp->Null		$-C_{11}H_{10}N_2O$	W	Deletion
-163,06333	Tyr->Null		$-C_9H_9NO_2$	Y	Deletion
-156,10111	Arg->Null		$-C_6H_{12}N_4O$	R	Deletion
-147,06841	Phe->Null		$-C_9H_9NO$	F	Deletion
-137,05891	His->Null		$-C_6H_7N_3O$	H	Deletion
-131,04049	Met->Null		$-C_5H_9NOS$	M	Deletion
-129,04259	Glu->Null		$-C_5H_7NO_3$	E	Deletion
-128,09496	Lys->Null		$-C_6H_{12}N_2O$	K	Deletion
-128,05858	Gln->Null		$-C_5H_8N_2O_2$	Q	Deletion
-115,02694	Asp->Null		$-C_4H_5NO_3$	D	Deletion
-114,04293	Asn->Null		$-C_4H_6N_2O_2$	N	Deletion
-113,08406	Ile->Null		$-C_6H_{11}NO$	I	Deletion
-113,08406	Leu->Null		$-C_6H_{11}NO$	L	Deletion
-101,04768	Thr->Null		$-C_4H_7NO_2$	T	Deletion
-99,06841	Val->Null		$-C_5H_9NO$	V	Deletion
-97,05276	Pro->Null		$-C_5H_7NO$	P	Deletion
-87,03203	Ser->Null		$-C_3H_5NO_2$	S	Deletion
-71,03711	Ala->Null		$-C_3H_5NO$	A	Deletion
-57,02146	Gly->Null		$-C_2H_3NO$	G	Deletion
-16,01872	Pyro-glutamination (N-term)		$-NH_2$	Q	N-terminal
0,98402	Deamidation		$-NH_2+OH$	NQ	Artefact
14,01565	Methylation		$+CH_2$	DEKR	Chemical Modification
14,01565	Methylation	Me	$-H+CH_3$	Y	Fmoc
15,99492	Oxidation	Ox	$+O$	MW	Artefact
16,01872	Amidation (C-term)		$-O+NH_2O$	all Amino acids	C-terminal
27,99492	Formylation	For	$-H+CHO$	W	Boc
28,03130	Dimethylation		$+C_2H_4$	KR	Chemical Modification
28,03130	Ethylation	Et	$-H+C_2H_5$	Y	Boc
29,00274	Formyl (N-term)		$+CHO$	M	N-terminal
31,98983	Double Oxidation Tryptophane		$+O_2$	W	Artefact
42,01057	Acetylation	Ac	$-H+C_2H_3O$	K	Fmoc
42,04695	Trimethylation		$+C_3H_6$	KR	Chemical Modification
44,98508	Nitration	NO2	$-H+NO_2$	Y	Chemical Modification
44,98508	Nitration	NO2	$-H+NO_2$	R	Boc
47,94445	Selenocystein		$-S+Se$	C	Chemical Modification
56,06260	Diethylation		$+C_4H_8$	K	Chemical Modification
56,06260	tert.-Butyl	tBu	$-H+C_4H_9$	CSTY	Fmoc
56,06260	tert.-Butyl	tBu	$-H+C_4H_9$	STY	Boc
57,02146	Gly->GG		$+C_2H_3NO$	G	Double coupling
68,06260	Piperidine	Pip	$+C_5H_8$	DE	Artefact
71,03711	Propionamidation		$+C_3H_5NO$	C	Cys-State
71,03711	Ala->AA		$+C_3H_5NO$	A	Double coupling
71,03711	Acetamidomethyl	Acm	$-H+C_3H_6NO$	C	Fmoc/Boc
72,05752	tert.-Butoxy	OtBu	$-H+C_4H_9O$	DE	Fmoc/Boc
79,96633	Phosphorylation		$-H+PO_3H_2$	STY	Chemical Modification
86,07317	tert.-Butoxymethyl	Bum	$-H+C_5H_{11}O$	H	Fmoc
87,03203	Ser->SS		$+C_3H_5NO_2$	S	Double coupling
88,03467	tert.-Butylthio	tButhio	$-H+C_4H_9S$	C	Fmoc
90,04695	Benzyl	Bzl	$-H+C_7H_7$	CST	Fmoc
90,04695	Benzyl	Bzl	$-H+C_7H_7$	CSTY	Boc
95,98230	Trifluoroacetylation	Tfa	$-H+C_2F_3O$	K	Fmoc/Boc
97,05276	Pro->PP		$+C_5H_7NO$	P	Double coupling
99,06841	Val->VV		$+C_5H_9NO$	V	Double coupling
100,05243	tert.-Butoxycarbonyl	Boc	$-H+C_5H_9O_2$	all Amino acids	Boc

Solid-Phase Peptide Synthesis

Mass Shift of Modifications, Protection Groups and Artifacts

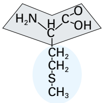
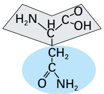
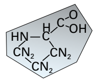
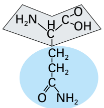
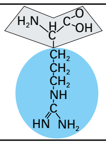
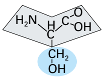
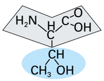
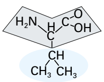
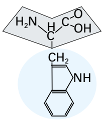
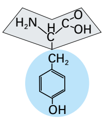
m/z shift [Da]	Modification	Abbreviation	Sum formula change	Valid residues	Origin
101,04768	Thr->TT		$+C_4H_7NO_2$	T	Double coupling
103,00918	Cys->CC		$+C_3H_5NOS$	C	Double coupling
104,06260	4-Methylbenzyl	MeBzl	$-H+C_8H_9$	C	Boc
106,04187	Benzyloxy	BzlO	$-H+C_7H_7O$	DE	Fmoc/Boc
113,08406	Ile->II		$+C_6H_{11}NO$	I	Double coupling
113,08406	Leu->LL		$+C_6H_{11}NO$	L	Double coupling
114,04293	Asn->NN		$+C_4H_6N_2O_2$	N	Double coupling
115,02694	Asp->DD		$+C_4H_5NO_3$	D	Double coupling
118,07825	2-Phenylisopropyl	O-2-PhiPr	$-H+C_9H_{11}$	DE	Fmoc
120,05752	4-Methoxybenzyl	MeOBzl	$-H+C_8H_9O$	C	Fmoc/Boc
120,05752	Benzyloxymethyl	Bom	$-H+C_8H_9O$	H	Boc
128,05858	Gln->QQ		$+C_5H_8N_2O_2$	Q	Double coupling
128,09496	Lys->KK		$+C_6H_{12}N_2O$	K	Double coupling
129,04259	Glu->EE		$+C_5H_7NO_3$	E	Double coupling
131,04049	Met->MM		$+C_5H_9NOS$	M	Double coupling
134,03678	Benzyloxycarbonyl	Z	$-H+C_8H_7O_2$	K	Fmoc/Boc
137,05891	His->HH		$+C_6H_7N_3O$	H	Double coupling
147,06841	Phe->FF		$+C_9H_9NO$	F	Double coupling
148,08882	Adamantyloxy	O-1-Ada	$-H+C_{10}H_{13}O$	D	Fmoc/Boc
148,08882	Adamantyloxy	O-2-Ada	$-H+C_{10}H_{13}O$	D	Boc
154,00885	Tosyl	Tos	$-H+C_7H_7O_2S$	HR	Fmoc/Boc
156,10111	Arg->RR		$+C_6H_{12}N_4O$	R	Double coupling
157,96901	2,6-Dichlorobenzyl	di-Cl-Bzl	$-H+C_7H_5Cl_2$	Y	Fmoc/Boc
163,06333	Tyr->YY		$+C_9H_9NO_2$	Y	Double coupling
164,08373	1-(4,4-Dimethyl-2,6-dioxo-cyclohexylidene)-ethyl	Dde	$-H+C_{10}H_{13}O_2$	K	Fmoc
166,00146	2,4-Dinitrophenyl	Dnp	$-H+C_6H_3N_2O_4$	H	Boc
167,99781	2-Chlorobenzyloxycarbonyl	2-Cl-Z	$-H+C_8H_6ClO_2$	K	Fmoc/Boc
180,05752	Xanthyl	Xan	$-H+C_{13}H_9O$	NQ	Boc
180,07864	2,4,6-Trimethoxybenzyl	Tmob	$-H+C_{10}H_{13}O_3$	N	Fmoc
182,04015	Mesitylene-2-sulfonyl	Mts	$-H+C_9H_{11}O_2S$	R	Fmoc
182,04015	Mesitylene-2-sulfonyl	Mts	$-H+C_9H_{11}O_2S$	RW	Boc
186,07931	Trp->WW		$+C_{11}H_{10}N_2O$	W	Double coupling
206,13068	1-(4,4-Dimethyl-2,6-dioxo-cyclohexylidene)-3-methylbutyl	ivDde	$-H+C_{13}H_{19}O_2$	K	Fmoc
211,94729	2-Bromobenzyloxycarbonyl	2-Br-Z	$-H+C_8H_6BrO_2$	Y	Boc
212,05072	4-Methoxy-2,3,6-trimethyl-benzenesulfonyl	Mtr	$-H+C_{10}H_{13}O_3S$	R	Fmoc/Boc
222,06808	Fluorenylmethoxycarbonyl	Fmoc	$-H+C_{15}H_{11}O_2$	all Amino acids	Fmoc
226,07760	Biotinylation		$+C_{10}H_{14}N_2S_1O_2$	K	Chemical Modification
226,09938	4,4'-Dimethoxybenzhydryl	Mbh	$-H+C_{15}H_{15}O_2$	NQ	Fmoc
242,10955	Trityl	Trt	$-H+C_{19}H_{15}$	CHNQST	Fmoc
242,10955	Trityl	Trt	$-H+C_{19}H_{15}$	CHNQ	Boc
252,08202	2,2,4,6,7-Pentamethyl-dihydrobenzofurane-5-sulfonyl	Pbf	$-H+C_{13}H_{17}O_3S$	R	Fmoc
256,12520	4-Methyltrityl	Mtt	$-H+C_{20}H_{17}$	HK	Fmoc
266,09767	2,2,5,7,8-Pentamethyl-chromane-6-sulfonyl	Pmc	$-H+C_{14}H_{19}O_3S$	R	Fmoc
272,12012	4-Methoxytrityl	Mmt	$-H+C_{20}H_{17}O$	C	Fmoc
276,07058	2-Chlorotrityl	2-Cl-Trt	$-H+C_{19}H_{14}Cl$	Y	Fmoc
327,18344	4{N-[1-(4,4-Dimethyl-2,6-dioxo-cyclohexylidene)-3-methylbutyl]-amino}benzyloxy	ODmab	$-H+C_{20}H_{26}NO_3$	DE	Fmoc
388,08211	Fluorescein		$+C_{22}H_{14}N_1O_6$	C	Chemical Modification
421,07324	Fluoresceinisothiocyanat	FITC	$+C_{21}S_1H_{15}N_3O_5$	CKRS	Chemical Modification
431,26920	Biotinylation		$-H+C_{20}H_{40}N_4O_4S$	K	Chemical Modification
672,29816	CyDye-Cy3		$+C_{37}H_{44}N_4S_1O_6$	C	Chemical Modification

Molecular Weights of Amino Acid Residues

Amino Acid Structure	Name	Symbol	1 Letter Code	Elemental Composition (Residue)	Monoisotopic Mass (Residue)	Averaged Mass (Residue)
	Alanine	Ala	A	C_3H_5NO	71.03712	71.08
	Cysteine	Cys	C	C_3H_5NOS	103.00919	103.15
	Aspartic acid	Asp	D	$C_4H_5NO_3$	115.02695	115.09
	Glutamic acid	Glu	E	$C_5H_7NO_3$	129.0426	129.12
	Phenylanaline	Phe	F	C_9H_9NO	147.06842	147.18
	Glycine	Gly	G	C_2H_3NO	57.02146	57.05
	Histidine	His	H	$C_6H_7N_3O$	137.05891	137.14
	Isoleucine	Ile	I	$C_6H_{11}NO$	113.08407	113.16
	Lysine	Lys	K	$C_6H_{12}N_2O$	128.09497	128.17
	Leucine	Leu	L	$C_6H_{11}NO$	113.08407	113.16

Masses of Terminal Groups

C-Terminal Groups	Composition	Monoisotopic Mass	Averaged Mass
Free Acid	OH	17.00274	17.00735
Amide	NH_2	16.01872	16.02262

Amino Acid Structure	Name	Symbol	1 Letter Code	Elemental Composition (Residue)	Monoisotopic Mass (Residue)	Averaged Mass (Residue)
	Methionine	Met	M	C_5H_9NOS	131.04049	131.20
	Asparagine	Asn	N	$C_4H_6N_2O_2$	114.04293	114.10
	Proline	Pro	P	C_5H_7NO	97.05277	97.12
	Glutamine	Gln	Q	$C_5H_8N_2O_2$	128.05858	128.13
	Arginine	Arg	R	$C_6H_{12}N_4O$	156.10112	156.19
	Serine	Ser	S	$C_3H_5NO_2$	87.03203	87.08
	Threonine	Thr	T	$C_4H_7NO_2$	101.04768	101.11
	Valine	Val	V	C_5H_9NO	99.06842	99.13
	Tryptophan	Trp	W	$C_{11}H_{10}N_2O$	186.07932	186.21
	Tyrosine	Tyr	Y	$C_9H_9NO_2$	163.06333	163.18

N-Terminal Groups	Composition	Monoisotopic Mass	Averaged Mass
Hydrogen	H	1.00783	1.0079
N-Formyl	HCO	29.00274	29.01808
N-Acetyl	CH_3CO	43.01839	43.04447

Amino Acid Calculator Table

Residues Sorted by Molecular Weight

Sums and Differences of 2 Amino Acid Residues   Residue Mass Differences

		G	A	S	P	V	T	C	I	L
		57.05203	71.07902	87.07832	97.11704	99.13299	101.10531	103.14344	113.15998	113.15998
G	57.05203	114.10406	14.02699	30.02629	40.06501	42.08097	44.05328	46.09141	56.10795	56.10795
A	71.07902	128.13105	142.15804	15.99931	26.03803	28.05398	30.02629	32.06442	42.08097	42.08097
S	87.07832	144.13035	158.15734	174.15665	10.03872	12.05467	14.02699	16.06512	26.08166	26.08166
P	97.11704	154.16907	168.19606	184.19537	194.23409	2.01595	3.98827	6.02640	16.04294	16.04294
V	99.13299	156.18502	170.21201	186.21132	196.25004	198.26599	1.97232	4.01045	14.02699	14.02699
T	101.10531	158.15734	172.18433	188.18363	198.22235	200.23831	202.21062	2.03813	12.05467	12.05467
C	103.14344	160.19547	174.22246	190.22176	200.26048	202.27644	204.24875	206.28688	10.01654	10.01654
I	113.15998	170.21201	184.23900	200.23831	210.27703	212.29298	214.26529	216.30342	226.31997	0.00000
L	113.15998	170.21201	184.23900	200.23831	210.27703	212.29298	214.26529	216.30342	226.31997	226.31997
N	114.10406	171.15609	185.18308	201.18238	211.22110	213.23705	215.20937	217.24750	227.26404	227.26404
D	115.08866	172.14069	186.16768	202.16699	212.20571	214.22166	216.19398	218.23211	228.24865	228.24865
Q	128.13105	185.18308	199.21006	215.20937	225.24809	227.26404	229.23636	231.27449	241.29103	241.29103
K	128.17468	185.22671	199.25370	215.25300	225.29172	227.30768	229.27999	231.31812	241.33466	241.33466
E	129.11565	186.16768	200.19467	216.19398	226.23270	228.24865	230.22096	232.25909	242.27564	242.27564
M	131.19742	188.24945	202.27644	218.27574	228.31446	230.33041	232.30273	234.34086	244.35740	244.35740
H	137.14152	194.19355	208.22054	224.21985	234.25857	236.27452	238.24684	240.28497	250.30151	250.30151
F	147.17714	204.22917	218.25616	234.25546	244.29418	246.31014	248.28245	250.32058	260.33712	260.33712
R	156.18813	213.24016	227.26714	243.26645	253.30517	255.32112	257.29344	259.33157	269.34811	269.34811
Y	163.17645	220.22848	234.25546	250.25477	260.29349	262.30944	264.28176	266.31989	276.33643	276.33643
W	186.21391	243.26594	257.29293	273.29224	283.33096	285.34691	287.31922	289.35735	299.37390	299.37390

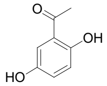
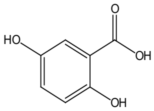
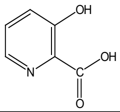
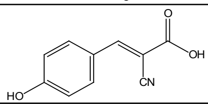
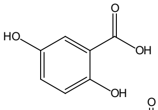
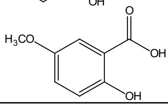
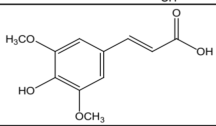
Amino Acid Calculator Table

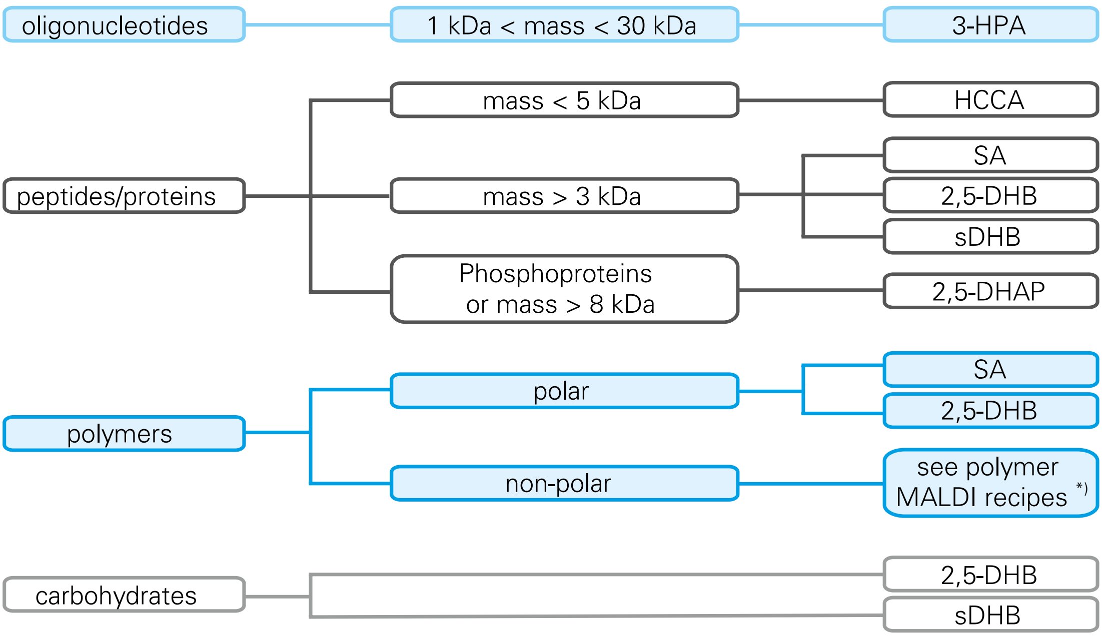
N	D	Q	K	E	M	H	F	R	Y	W
114.10406	**115.08866**	**128.13105**	**128.17468**	**129.11565**	**131.19742**	**137.14152**	**147.17714**	**156.18813**	**163.17645**	**186.21391**
57.05203	58.03664	71.07902	71.12265	72.06362	74.14539	80.08950	90.12511	99.13610	106.12442	129.16188
43.02504	44.00965	57.05203	57.09566	58.03664	60.11840	66.06251	76.09812	85.10911	92.09743	115.13490
27.02574	28.01034	41.05272	41.09636	42.03733	44.11910	50.06320	60.09882	69.10980	76.09812	99.13559
16.98702	17.97162	31.01400	31.05764	31.99861	34.08038	40.02448	50.06010	59.07108	66.05940	89.09687
14.97106	15.95567	28.99805	29.04169	29.98266	32.06442	38.00853	48.04415	57.05513	64.04345	87.08092
12.99875	13.98335	27.02574	27.06937	28.01034	30.09211	36.03621	46.07183	55.08282	62.07113	85.10860
10.96062	11.94522	24.98761	25.03124	25.97221	28.05398	33.99808	44.03370	53.04469	60.03301	83.07047
0.94407	1.92868	14.97106	15.01470	15.95567	18.03744	23.98154	34.01716	43.02814	50.01646	73.05393
0.94407	1.92868	14.97106	15.01470	15.95567	18.03744	23.98154	34.01716	43.02814	50.01646	73.05393
228.20812	0.98461	14.02699	14.07062	15.01160	17.09336	23.03747	33.07308	42.08407	49.07239	72.10985
229.19272	**230.17733**	13.04238	13.08602	14.02699	16.10875	22.05286	32.08848	41.09946	48.08778	71.12525
242.23510	243.21971	**256.26209**	0.04364	0.98461	3.06637	9.01048	19.04609	28.05708	35.04540	58.08287
242.27874	243.26335	256.30573	**256.34936**	0.94097	3.02274	8.96684	19.00246	28.01345	35.00176	58.03923
243.21971	244.20432	257.24670	257.29033	**258.23131**	2.08177	8.02587	18.06149	27.07247	34.06079	57.09826
245.30148	246.28608	259.32846	259.37210	260.31307	**262.39484**	5.94411	15.97972	24.99071	31.97903	55.01649
251.24558	252.23019	265.27257	265.31621	266.25718	268.33894	**274.28305**	10.03562	19.04660	26.03492	49.07239
261.28120	262.26581	275.30819	275.35182	276.29279	278.37456	284.31867	**294.35428**	9.01099	15.99931	39.03677
270.29219	271.27679	284.31917	284.36281	285.30378	287.38555	293.32965	303.36527	**312.37625**	6.98832	30.02579
277.28050	278.26511	291.30749	291.35113	292.29210	294.37386	300.31797	310.35359	319.36457	**326.35289**	23.03747
300.31797	301.30258	314.34496	314.38859	315.32957	317.41133	323.35544	333.39105	342.40204	349.39036	**372.42783**

Sum of 2 Residues

isobaric and close-to-isobaric mass differences are color coded
isobaric and close-to-isobaric substitutions by 2 residues are color coded

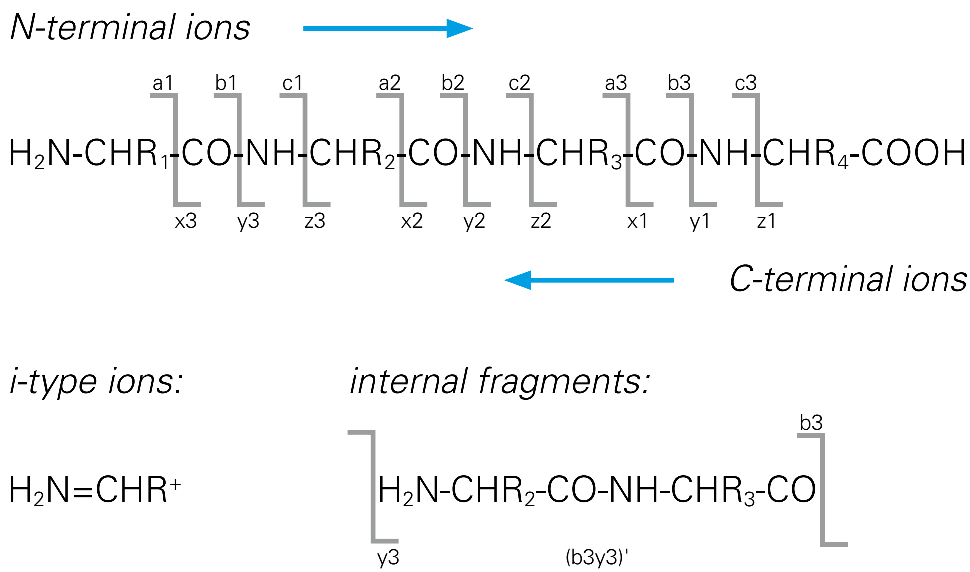
Matrices / Bruker Matrix Selection Guide

Matrix name	Elemental Composition	Structure	MH_{mono}^{+} [Th]	Average Mass	Order No.
2,5-Dihydroxyacetophenon (2,5-DHAP)	$C_8H_8O_3$		153,05462	152,20	**231829**
2,5-Dihydroxybenzoic acid (2,5-DHB)	$C_7H_6O_4$		155,03388	154,12	**201346**
3-Hydroxypicolinic acid (3-HPA), 1 g	$C_6H_5NO_3$		140,03422	139,11	**201224**
α-Cyano-4-hydroxycinnamic acid (HCCA)	$C_{10}H_7NO_3$		190,04987	189,17	**201344** **255344**
super 2,5-Dihydroxybenzoic acid (sDHB), 5 g	$C_7H_6O_4$ $C_8H_8O_4$	 		154,12 168,15	**209813**
Sinapinic acid (SA)	$C_{11}H_{12}O_5$		225,07575	224,22	**201345**



*) http://polymers.msel.nist.gov/maldirecipes

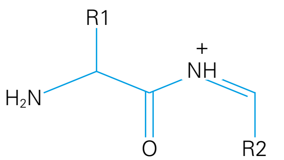
Peptide Fragmentation



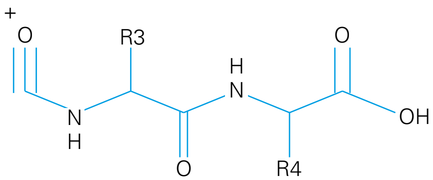
Typical fragment ions observed

- Low energy CID: b and y
- PSD: a, b, y and i, including neutral losses of NH_3 from a and b
- ISD: a, c, z+2, y
- ECD-FTICR: c and z

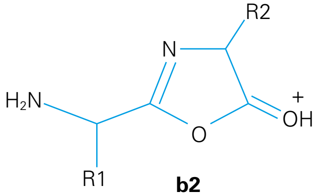
Structures of the fragments



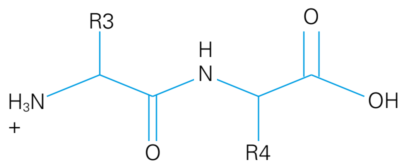
a2



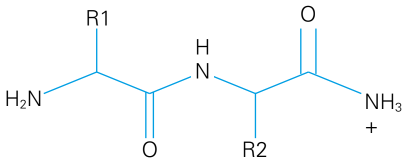
x2



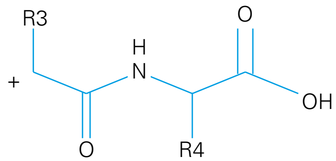
b2



y2



c2



z2

Relative Isotopic Abundance Table

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	
H	99.99	0.0115															H
He				100													He
Li						7.59	92.41										Li
Be									100								Be
B										19.9	80.1						B
C												98.93	1.07				C
N														99.64	0.36		N
O																99.76	O

	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	
O	0.04	0.21															O
F			100														F
Ne				90.48	0.27	9.25											Ne
Na							100										Na
Mg								78.99	10.00	11.01							Mg
Al											100						Al
Si												92.22	4.69	3.09			Si
P															100		P
S																94.99	S

	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	
S	0.75	4.25		0.01													S
Cl			75.76		24.24												Cl
Ar				0.34		0.06		99.60									Ar
K							93.26	0.01	6.73								K
Ca								96.94		0.647	0.135	2.086		0.004		0.187	Ca
Sc													100				Sc
Ti														8.25	7.44	73.72	Ti

	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	
Ti	5.41	5.18															Ti
V		0.25	99.75														V
Cr		4.345		83.79	9.501	2.365											Cr
Mn							100										Mn
Fe						5.845		91.75	2.11	0.28							Fe
Co											100						Co
Ni									68.08			26.22	1.14	3.63		0.93	Ni
Cu															69.15		Cu
Zn																48.27	Zn

	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	
Cu	30.85																Cu
Zn		27.98	4.10	19.02		0.63											Zn
Ga					60.11		39.89										Ga
Ge						20.38		27.31	7.76	36.72		7.83					Ge
As											100						As
Se												9.37	7.63	23.77		49.61	Se
Br															50.69		Br
Kr														0.36		2.29	Kr

	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	
Se		8.73															Se
Br	49.31																Br
Kr		11.59	11.50	56.99		17.28											Kr
Rb					72.17		27.83										Rb
Sr				0.56		9.86	7.00	82.58									Sr
Y									100								Y
Zr										51.45	11.22	17.15		17.38		2.80	Zr
Nb													100				Nb
Mo												14.77		9.23	15.90	16.68	Mo
Ru																5.54	Ru

	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	
Mo	9.56	24.19	9.67														Mo
Ru		1.87	12.76	12.60	17.06	31.55		18.62									Ru
Rh							100										Rh
Pd						1.02		11.14	22.33	27.33		26.46		11.72			Pd
Ag											51.84		48.16				Ag
Cd										1.25		0.89		12.49	12.80	24.13	Cd
Sn																0.97	Sn

Relative Isotopic Abundance Table

	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	
Cd	12.22	28.73		7.49													Cd
In	4.29		95.71														In
Sn		0.66	0.34	14.54	7.68	24.22	8.59	32.59		4.63		5.79					Sn
Sb									57.21		42.79						Sb
Te								0.09		2.55	0.89	4.74	7.07	18.84		31.74	Te
I															100		I
Xe												0.10		0.09		1.91	Xe

	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	
Te		33.8															Te
Xe	26.40	4.10	21.23	26.91		10.44		8.86									Xe
Cs					100												Cs
Ba		0.11		0.10		2.42	6.59	7.85	11.23	71.70							Ba
La										0.09	99.91						La
Ce								0.19		0.25		88.45		11.11			Ce
Pr													100				Pr
Nd														27.2	12.2	23.8	Nd
Sm																3.1	Sm

	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	
Nd	8.30	17.20		5.70		5.60											Nd
Sm			14.99	11.24	13.82	7.38		26.75		22.75							Sm
Eu							47.81		52.19								Eu
Gd								0.20		2.18	14.80	20.47	15.65	24.84		21.86	Gd
Tb															100		Tb
Dy												0.06		0.10		2.33	Dy

	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	
Dy	18.89	25.48	24.90	28.26													Dy
Ho					100												Ho
Er		0.14		1.60		33.50	22.87	26.98		14.91							Er
Tm									100								Tm
Yb								0.13		3.04	14.28	21.83	16.13	31.83		12.76	Yb
Lu															97.41	2.59	Lu
Hf														0.16		5.26	Hf

	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	
Hf	18.60	27.28	13.62	35.08													Hf
Ta				0.012	99.99												Ta
W				0.12		26.50	14.31	30.64		28.43							W
Re									37.4		62.60						Re
Os								0.02		1.59	1.96	13.24	16.15	26.26		40.78	Os
Ir															37.3		Ir
Pt														0.014		0.78	Pt

	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	
Ir	62.7																Ir
Pt		32.97	33.83	25.24		7.16											Pt
Au					100												Au
Hg				0.15		9.97	16.87	23.10	13.18	29.86		6.87					Hg
Tl											29.52		70.48				Tl
Pb												1.4		24.1	22.1	52.4	Pb

	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	
Bi	100																Bi

	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	
Th								100									Th
U										0.005	0.72			99.27			U

recommended mass number

recommended mass number for cool plasma

Molecular Weights

Molecular Weights of Selected Glycan Residues

Residue Name	Symbol	Elemental Composition	Monoisotopic Mass	Average Mass
Deoxyribose	dRib	$C_5H_8O_3$	116,04734	116,12
Arabinose	Ara	$C_5H_8O_4$	132,04226	132,11
Ribose	Rib	$C_5H_8O_4$	132,04226	132,11
Xylose	Xyl	$C_5H_8O_4$	132,04226	132,11
Fucose	Fuc	$C_6H_{10}O_4$	146,05791	146,14
Galactosamine	GalN	$C_6H_{11}NO_4$	161,06881	161,16
Glucosamin	GlcN	$C_6H_{11}NO_4$	161,06881	161,16
Galactose	Gal	$C_6H_{10}O_5$	162,05282	162,14
Glucose	Glc	$C_6H_{10}O_5$	162,05282	162,14
Mannose	Man	$C_6H_{10}O_5$	162,05282	162,14
Glucuronic acid	GlcA	$C_6H_8O_6$	176,03209	176,13
N-acetylgalactosamin	GalNAc	$C_8H_{13}NO_5$	203,07937	203,20
N-acetylglucosamin	GlcNAc	$C_8H_{13}NO_5$	203,07937	203,20
Muramic acid	Mur	$C_{11}H_{17}NO_7$	275,10050	275,26
N-acetylneuraminic acid	NANA	$C_{11}H_{17}NO_8$	291,09542	291,26

Molecular Weights of Nucleotide Residues (compatible to BioTools 3.2)

Nucleotide Residue	Elemental Composition	Monoisotopic Mass	Averaged Mass
AMP	$C_{10}H_{12}N_5O_6P$	329,05252	329,21
GMP	$C_{10}H_{12}N_5O_7P$	345,04744	345,21
UMP	$C_9H_{11}N_2O_8P$	306,02530	306,17
CMP	$C_9H_{12}N_3O_7P$	305,04129	305,18
dAMP	$C_{10}H_{12}N_5O_5P$	313,05761	313,21
dGMP	$C_{10}H_{12}N_5O_6P$	329,05252	329,21
dTMP	$C_{10}H_{13}N_2O_7P$	304,04604	304,20
dCMP	$C_9H_{12}N_3O_6P$	289,04637	289,18
Hypoxanthine	$C_{10}H_{11}N_4O_6P$	314,04162	314,19
7-deaza-dGMP	$C_{11}H_{13}N_4O_6P$	328,05727	328,22
7-deaza-dAMP	$C_{11}H_{13}N_4O_5P$	312,06236	312,22
2-amino-purine	$C_{10}H_{12}N_5O_5P$	313,05761	313,21
dAMP-thioCH3	$C_{11}H_{14}N_5O_4SP$	343,05041	343,30
dGMP-thioCH3	$C_{11}H_{14}N_5O_5SP$	359,04533	359,30
dTMP-thioCH3	$C_{11}H_{15}N_2O_6SP$	334,03885	334,29
dCMP-thioCH3	$C_{10}H_{14}N_3O_5SP$	319,03918	319,28
ddCMP	$C_9H_{12}N_3O_5P$	273,05146	273,19
ddAMP	$C_{10}H_{12}N_5O_4P$	297,06269	297,21
ddTMP	$C_{10}H_{13}N_2O_6P$	288,05112	288,20
ddGMP	$C_{10}H_{12}N_5O_5P$	313,05761	313,21

Chemical Tables

Important Abbreviations and Acronyms

A	adenine
AA	anisylacetone
AAO	acetaldehyde oxime
AC	acetate
Ac	acetyl [$CH_3C(0)-$]
acac	acetylacetone
ACTH	adrenocorticotropic hormone (corticotropin)
ADMA	alkyldimethylamine
ADP	adenosine 5′-diphosphate
AIBN	azobis(isobutyronitrile)
Ala	alanine (A)
Am	amyl
AMP	adenosine 5′-monophosphate
AN	acetonitrile
APS	adenosine 5′-phosphosulfate
Ar	aryl
Arg	arginine (R)
Asn	asparagine (N)
Asp	aspartic acid (D)
ATA	anthranilamide
ATP	adenosine 5′-triphosphate
BA	benzyladenine
BaP (BAP)	benzo[*a*]pyrene
BBP	benzyl butyl phthalate
BHC	benzene hexachloride
BHT	2,6-di-*t*-butyl-4-methylphenol
bipy	2,2'-bipyridyl
Bn	benzyl (also Bz, BZL, or Bnz)
BN	benzonitrile
Boc	t-butyloxycarbonyl
BOM	benzyloxymethyl [$PhCH_2OCH_2-$]
BON	*β*-oxynaphthoic acid
BPBG	butyl phthalyl butyl glycolate
Bs	brosylate [$BrC_6H_4SO_2-$]
BSA	*O*,*N*-bistrimethylsilyl acetamide
BTA	benzoyltrifluoroacetone
Bu	butyl
Bz	benzoyl
C	cytosine
p **CBA**	*p*-carboxybenzaldehyde
Cbz	carbobenzyloxy [$PhCH_2OC(O)-$]
CD	cyclodextrin
CDP	cytidine 5′-diphosphate

CE	cyanoethyl
CMP	cytidine 5′-monophosphate
CoA	coenzyme A
Cp (or cp)	cyclopentadiene
12-Crown-4	1,4,7,10-tetraoxacyclododecane
CTA	citraconic anhydride
Cys	cysteine (C)
DAA	diacetone acrylamide
DAP	dodecylammonium propionate
DCB	dicyanobenzene
DCEE	dichloroethyl ether
DDD	2,2′-dihydroxy-6,6′-dinaphthyl disulfide
DDH	1,3-dibromo-5,5-dimethylhydantoin
DDM	diphenyldiazomethane
DDT	1,1-bis(*p*-chlorophenyl)-2,2,2-trichloroethane
DEA	*N*,*N*-diethylaniline or diethyl amine
DEC	diethylaminoethyl chloride hydrochloride
DHA	dehydroacetic acid
DHP	dihydropyran
Diglyme	diethylene glycol dimethyl ether
Diox	dioxane
DMAc	*N*,*N*-dimethylacetamide
DMAA	*N*,*N*-dimethylacetoacetamide
DME	1,2-dimethoxyethane (glyme)
DMF	dimethylformamide
DML	dimyristoyl lecithin
DMS	dimethylsiloxane
DMSO	dimethyl sulfoxide
DMSO2	dimethyl sulfone
DMT	dimethyl terephthalate
DNA	deoxyribonucleic acid
DNF	2,4-dinitrofluorobenzene
DOCA	deoxycorticosterone acetate
DPG	2,3-diphosphoglycerate
DPL	dipalmitoyl lecithin
dpm	dipivaloylmethanato
DPPH	diphenylpicrylhydracyl
DST	disuccinimidyl tartrate
DTBN	di-t-butyl nitroxide
E	trans config. (entgegen)
EAA	ethyl acetoacetate
EAK	ethyl amyl ketone
EBA	*N*-ethyl-*N*-benzylaniline

Chemical Tables

Important Abbreviations and Acronyms

EBBA	*N*-(*p*-ethoxybenzylidene)-*p*-butylaniline
EDC	ethylene dichloride
EDTA	ethylenediaminetetraacetic acid
EGS	ethylene glycol bis(succinimidyl succinate)
en	ethylenediamine
Et	ethyl
EVA	ethylene vinyl acetate
FA	furfuryl alcohol
FAD	flavin adenine dinucleotide
FMA	fluoroscein mercuric acetate
Fmoc	9-fluorenylmethoxycarbonyl
Fuc	fucose
G	guanine
Gal	galactose
GDP	guanosine 5′-diphosphate
Glc	glucose
Gln	glutamine (Q)
Glu	glutamic acid (E)
Gly	glycine (G)
Glyme (glyme)	1,2-dimethoxyethane
HAB	4,4′-bis(heptyl)azoxybenzene
Hex	hexane (or hexyl) or hexose
HFA	hexafluoroacetone
His	histidine (H)
HMDS	hexamethyldisilazide
HMPA	hexamethylphosphoramide
HMPT	hexamethylphosphorous triamide
HOAB	*p*-*n*-heptyloxyazoxybenzene
HOAc	acetic acid
Hyp	hydroxyproline
IH	immobilized histamine
IHP	inositolhexaphosphate
Ile	isoleucine (I)
IMP	inosine 5′-monophosphate
IPN	isophthalonitrile
KDP	potassium dihydrogen phosphate
LAH	lithium aluminum hydride ($LiAlH_4$)
LAP	leucine aminopeptidase
LDH	lactic dehydrogenase
Leu	leucine (L)
Lys	lysine (K)
M	metal
MA	maleic anhydride

MAA	methoxyacetic acid
Man	mannose
MBBA	*N*-(*p*-methoxybenzylidene)-*p*-butylaniline
MCA	monochloroacetic acid
Me	methyl
MEM	*β*-methoxyethoxymethyl
Mes	mesityl = 2,4,6-trimethylphenyl
Met	methionine (M)
MMH	methylmercuric hydroxide
MOM	methoxymethyl
Ms	mesyl = methanesulfonyl = CH_3SO_2–
MSA	methanesulfonic acid
MTPA	*α*-methoxy-*α*-trifluoromethylphenylacetic acid
MVK	methyl vinyl ketone
NAC	*N*-acetyl
NAD(P)	nicotinamide adenine dinucleotide (phosphate)
NAD(P)H	nicotinamide adenine dinucleotide (phosphate)
NAI	*N*-acetylimidazole
NCA	*N*-chloroacetamide
Nf	nonaflate ($C_4F_9SO_2$–)
NM	nitromethane
NMA	*N*-methylacrylamide
NMF	*N*-methylformamide
Ns	*p*-nitrobenzenesulfonyl
NTA	nitrilotriacetic acid
OCBA	*o*-chlorobenzoic acid
OCT	*o*-chlorotoluene
ODCB	*o*-dichlorobenzene
P	polymer substituent
PAA	*p*-azoxyanisole
PAS	*p*-aminosalicylic acid
PBA	pyrene butyric acid
PBLG	poly(L-benzyl μ-glutamate)
PC	propylene carbonate
PCA	perchloric acid
PCB	polychlorinated biphenyl
PCP	pentachlorophenol
PDMS	poly(dimethylsiloxane)
PEG	polyethylene glycol
PET	
Ph	phenyl
Phe	phenylalanine (F)
phen	1,10-phenanthroline

Chemical Tables

Important Abbreviations and Acronyms

PMA	poly(methacrylic acid)
PMMA	poly(methyl methacrylate)
POC	cyclopentyloxycarbonyl
POM	poly(oxymethylene)
PPA	poly(phosphoric acid)
Pr	propyl
Pro	proline (P)
PS	polystyrene
PTFE	polytetrafluoroethylene
PVA	poly(vinyl alcohol)
PVC	poly(vinyl chloride)
PVF	poly(vinyl fluoride)
PVP	poly(vinyl pyrrolidone)
Pyr (or Py)	pyridine
RNA	ribonucleic acid
SDS	sodium dodecyl sulfate
Ser	serine (S)
SLS	sodium lauryl sulfate
T	thymine
TAB	trimethylammonium bromide (TMAB)
TBE	tetrabromoethane
TCA	trichloroacetic acid
TCNQ	tetracyanoquinodimethane
TEA	triethylamine
Tf	triflate [CF_3SO_2–]
TFA	trifluoroacetic acid

THF	tetrahydrofuran
THP	tetrahydropyran
Thr	threonine (T)
TIPS	triisopropylsilyl
TMB	*N,N,N′N′*-tetramethylbenzidine
TMM	trimethylenemethane
TMS	tetramethylsilyl
TMU	tetramethylurea
TNM	tetranitromethane
TNT	2,4,6-trinitrotoluene
Tol	p-tolyl
TP	thymolphthalein
TPC	thymolphthalein complexone
TPE	tetraphenylethylene
Tr	trityl = triphenylmethyl
Triglyme	triethylene glycol dimethyl ether
TRIS	tris(hydroxymethyl)aminomethane
Trp	tryptophan (W)
Ts	tosyl = *p*-toluenesulfonyl
Tyr	tyrosine (Y)
U	uracil
UTP	uridine 5′-triphosphate
Val	valine (V)
Xyl	xylose
Z	cis configuration (zusammen)

Concentration Units for Solutions

Name	Symbol	Definition
Weight percent	wt %	(Grams of solute per grams of solution) x 100
Mole fraction	X_A	Moles of A per total number of moles
Molar	*M*	Moles of solute per liter of solution
Normal	*N*	Equivalents of solute per liter of solution
Formal	*F*	Formula weights of solute per liter of solution
Molal	*m*	Moles of solute per kg of solvent
Weight formal	*f*	Formula weight of solute per kg of solvent

Chemical Tables

Acronyms and Abbreviations in Quantum Chemistry and Molecular Modeling

AEE	**A**verage **E**xcitation **E**nergy
AM1	**A**ustin **M**ethod **1**, a modified MNDO method (semi-empirical)
AMBER	**A**ssisted **M**odel **B**uilding and **E**nergy **R**efinement, P. Kollman's empirical force field for biopolymers
AMFI	**A**tomic **M**ean **FI**eld approximation for SO coupling
AO	**A**tomic **O**rbital
ARCS	**A**romatic **R**ing **C**urrent **S**hielding
BOMD	**B**orn-**O**ppenheimer **M**olecular **D**ynamics simulation
CC	**C**oupled **C**luster methods (ab initio)
CCSD(T)	**C**oupled **C**luster method at **S**ingles, **D**oubles, **T**riples level
CDFT	**C**urrent **D**ensity **F**unctional **T**heory (ab initio)
CFT	**C**rystal **F**ield **T**heory
CHARMM	**CH**emitry at **HAR**vard **M**acromolecular **M**echanics, empirical force field implementation of M. Karplus
CHF	**C**oupled **H**artree-**F**ock perturbation theory
CI	**C**onfiguration **I**nteraction
CNDO	**C**omplete **N**eglect of **D**ifferential **O**verlap (semi-empirical)
CNDO/*n*	**C**omplete **N**eglect of **D**ifferential **O**verlap (level ***n*** = 1 or 2)
CNDO/2H	CNDO/2 modified for hydrogen bonding
CPMD	**C**ar-**P**arrinello **M**olecular **D**ynamics simulation
CSGT	**C**ontinuous **S**et of **G**auge **T**ransformations (ab initio)
DFT	**D**ensity **F**unctional **T**heory (ab initio)
DFTB	**D**ensity **F**unctional **T**ight **B**inding method
DGEOM	**D**istance **GEOM**etry
DHF	relativistic four-component **D**irac-**H**artree-**F**ock method
DZ	**D**ouble **Z**eta, a basis set consisting of two STOs for each atomic orbital
EH	**E**xtended **H**ückel theory
EHT	**E**xtended **H**ückel MO **T**heory
EOM	**E**quation **O**f **M**otion
FEMO	**F**ree-**E**lectron **M**olecular **O**rbitals
FPT	**F**inite **P**erturbation **T**heory
GGA	**G**eneralized **G**radient **A**pproximation (DFT)
GIAO	**G**auge-**I**ncluding **A**tomic **O**rbitals, also used: **G**auge-**I**nvariant or **G**auge-**I**ndependent (ab initio)
GIPAW	**G**auge-**I**ncluding **P**rojector-**A**ugmented **W**aves (ab initio)
GTO	**G**aussian **T**ype atomic **O**rbital
HF	**H**artree-**F**ock method for self-consistent fields
HFC(C)	**H**yper**F**ine **C**oupling (**C**onstant)
HMO	**H**ückel **M**olecular **O**rbitals
HOMO	**H**ighest **O**ccupied **M**olecular **O**rbital
IGAIM	**I**ndividual **G**auge for **A**toms **I**n **M**olecules (ab initio)
IGLO	**I**ndividual **G**auge for **L**ocalized **O**rbitals (ab initio)
INDO	**I**ntermediate **N**eglect of **D**ifferential **O**verlap (semi-empirical)
INDO/S	**INDO** for **S**pectroscopy
JWKB	**J**effreys-**W**entzel-**K**ramers-**B**rillouin, a semiclassical approximation to quantum mechanics
K-LMG	split-valence basis set defined with K, L, M numbers of Gaussians

Acronyms and Abbreviations in Quantum Chemistry and Molecular Modeling

LCAO	**L**inear **C**ombination of **A**tomic **O**rbitals (ab initio)
LDA	**L**ocal **D**ensity **A**pproximation (DFT)
LUMO	**L**owest **U**noccupied **M**olecular **O**rbital (see HOMO)
MCSCF	**M**ulti**C**onfiguration **S**elf **C**onsistent **F**ield (ab initio)
MD	**M**olecular **D**ynamics (with any method)
MINDO	**M**odified **I**ntermediate **N**eglect to **D**ifferential **O**verlap (semi-empirical)
MINDO/*n*	**M**odified **I**ntermediate Neglect of **D**ifferential **O**verlap (***n*** = 1-3, semi-empirical)
MINDO/3H	MINDO/3 modified for hydrogen bonding
MM	**M**olecular **M**echanics (with empirical force field)
MMn	N. L. Allinger's empirical force field for small molecules (n = integer)
MNDO	**M**odified **N**eglect of **D**ifferential **O**verlap (semi-empirical)
MNDO/H	MNDO modified for hydrogen bonding
MO	**M**olecular **O**rbital
MP2	**M**øller-Plesset 2nd-order perturbation calc. (ab initio)
MR-CI	**M**ulti-**R**eference **C**onfiguration **I**nteraction
NDDO	**N**eglect of **D**iatomic **D**ifferential **O**verlap
NICS	**N**ucleus-**I**ndependent **C**hemical **S**hift (aromaticity)
OPLS	**O**ptimized **P**otentials for **L**iquid **S**imulations, W. Jorgensen's empirical force field for biopolymers
PM3	**P**arameterized **M**ethod **3** (a modification of AM1)
PPP	**P**ariser-**P**arr-**P**ople method (semi-empirical)
QSAR	**Q**uantitative **S**tructure-**A**ctivity **R**elationship
REX	**R**elativistic **EX**tended Hückel MOs
RHF	**R**estricted **H**artee-**F**ock method (for SCF calculations)
SCF	**S**elf-**C**onsistent **F**ield
SCPT	**S**elf-**C**onsistent **P**erturbation **T**heory
SCRF	**S**elf-**C**onsistent **R**eaction **F**ield for free radicals
SD	**S**pin-**D**ipolar term
SO	**S**pin-**O**rbit coupling
SOMO	**S**ingly **O**ccupied **M**olecular **O**rbital
SOS	**S**um **O**ver **S**tates perturbation theory
STO	**S**later **T**ype **O**rbital basis set (ab initio)
STO-*n*G	**S**later **T**ype **O**rbitals as a sum of *n* Gaussians
TFD	**T**homas-**F**ermi-**D**irac method, a statistical treatment of electron density
UCHF	**U**n**C**oupled **H**artree-**F**ock perturbation method
UHF	**U**nrestricted **H**artee-**F**ock method for SCF calculations
VB	**V**alence **B**ond theory
VSEPR	**V**alence-**S**hell **E**lectron **P**air **R**epulsion, a theory of molecular geometry
VWN	**V**osko, **W**ilk, **N**usair parameterization for LDA
WKB	**W**entzel-**K**ramers-**B**rillouin method, a semiclassical approximation to quantum mechanics
ZDO	**Z**ero **D**ifferential **O**verlap (semi-empirical)
ZFS	**Z**ero-**F**ield **S**plitting
ZINDO	**Z**erner's **INDO** method
ZORA	**Z**ero-**O**rder **R**egular **A**pproximatio

IUPAC Periodic Table of Elements

BRUKER

Group

Element
K L M N O P Q E_{Z} M.P.° B.P.° C.P.° Ox.States At.Weight Abundance%

Key to Table

1 (IA)	2 (IIA)	3 (IIIB)	4 (IVB)	5 (VB)	6 (VIB)	7 (VIIB)	8 (VIII)	9 (VIII)
Hydrogen 1 H_{1} -259.34° -252.87° -240.18° +1-1 1.00794 91.0%								
Lithium 2 1 Li_{3} 180.5° 1342° +1 6.941 $1.86\cdot 10^{-7}$%	**Beryllium** 2 2 Be_{4} 1287° 2471° +2 9.012182 $2.38\cdot 10^{-9}$%							
Sodium 2 8 1 Na_{11} 97.80° 883° +1 22.98976928 0.000187%	**Magnesium** 2 8 2 Mg_{12} 650° 1090° +2 24.3050 0.00350%							
Potassium 2 8 8 1 K_{19} 63.38° 759° +1 39.0983 0.0000123%	**Calcium** 2 8 8 2 Ca_{20} 842° 1484° +2 40.078 0.000199%	**Scandium** 2 8 9 2 Sc_{21} 1541° 2836° +3 44.955912 $1.12\cdot 10^{-7}$%	**Titanium** 2 8 10 2 Ti_{22} 1668° 3287° +2+3+4 47.867 $7.8\cdot 10^{-6}$%	**Vanadium** 2 8 11 2 V_{23} 1910° 3407° +2+3+4+5 50.9415 $9.6\cdot 10^{-7}$%	**Chromium** 2 8 13 1 Cr_{24} 1907° 2671° +2+3+6 51.9961 0.000044%	**Manganese** 2 8 13 2 Mn_{25} 1246° 2061° +2+3+4+7 54.938045 0.000031%	**Iron** 2 8 14 2 Fe_{26} 1538° 2861° +2+3 55.845 0.00294%	**Cobalt** 2 8 15 2 Co_{27} 1495° 2927° +2+3 58.933195 $7.3\cdot 10^{-6}$%
Rubidium 2 8 18 8 1 Rb_{37} 39.31° 688° +1 85.4678 $2.31\cdot 10^{-8}$%	**Strontium** 2 8 18 8 2 Sr_{38} 777° 1382° +2 87.62 $7.7\cdot 10^{-8}$%	**Yttrium** 2 8 18 9 2 Y_{39} 1522° 3345° +3 88.90585 $1.51\cdot 10^{-8}$%	**Zirconium** 2 8 18 10 2 Zr_{40} 1855° 4409° +4 91.224 $3.72\cdot 10^{-8}$%	**Niobium** 2 8 18 12 1 Nb_{41} 2477° 4744° +3+5 92.90638 $2.28\cdot 10^{-9}$%	**Molybdenum** 2 8 18 13 1 Mo_{42} 2623° 4639° +6 95.96 $8.3\cdot 10^{-9}$%	**Technetium** 2 8 18 13 2 Tc_{43} 2157° 4265° +4+6+7 [98]	**Ruthenium** 2 8 18 15 1 Ru_{44} 2334° 4150° +3 101.07 $6.1\cdot 10^{-9}$%	**Rhodium** 2 8 18 16 1 Rh_{45} 1964° 3695° +3 102.90550 $1.12\cdot 10^{-9}$%
Cesium 2 8 18 18 8 1 Cs_{55} 28.44° 671° +1 132.9054519 $1.21\cdot 10^{-9}$%	**Barium** 2 8 18 18 8 2 Ba_{56} 727° 1897° +2 137.327 $1.46\cdot 10^{-8}$%	**Lanthanum** 2 8 18 18 9 2 La_{57} † 918° 3464° +3 138.90547 $1.45\cdot 10^{-9}$%	**Hafnium** 2 8 18 32 10 2 Hf_{72} 2233° 4603° +4 178.49 $5.02\cdot 10^{-10}$%	**Tantalum** 2 8 18 32 11 2 Ta_{73} 3017° 5458° +5 180.94788 $6.75\cdot 10^{-11}$%	**Tungsten** 2 8 18 32 12 2 W_{74} 3422° 5555° +6 183.84 $4.34\cdot 10^{-10}$%	**Rhenium** 2 8 18 32 13 2 Re_{75} 3186° 5596° +4+6+7 186.207 $1.69\cdot 10^{-10}$%	**Osmium** 2 8 18 32 14 2 Os_{76} 3033° 5012° +3+4 190.23 $2.20\cdot 10^{-9}$%	**Iridium** 2 8 18 32 15 2 Ir_{77} 2446° 4428° +3+4 192.217 $2.16\cdot 10^{-9}$%
Francium 2 8 18 32 18 8 1 Fr_{87} 27° +1 [223]	**Radium** 2 8 18 32 18 8 2 Ra_{88} 700° +2 [226]	**Actinium** 2 8 18 32 18 9 2 Ac_{89} ‡ 1051° 3198° +3 [227]	**Rutherfordium** 2 8 18 32 32 10 2 Rf_{104} +4 [267]	**Dubnium** 2 8 18 32 32 11 2 Db_{105} [268]	**Seaborgium** 2 8 18 32 32 12 2 Sg_{106} [271]	**Bohrium** 2 8 18 32 32 13 2 Bh_{107} [272]	**Hassium** 2 8 18 32 32 14 2 Hs_{108} [277]	**Meitnerium** 2 8 18 32 32 15 2 Mt_{109} [276]

† Lanthanides

Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium
2 8 18 19 9 2 Ce_{58} 798° 3443° +3+4 140.116 $3.70\cdot 10^{-9}$%	2 8 18 21 8 2 Pr_{59} 931° 3520° +3 140.90765 $5.44\cdot 10^{-10}$%	2 8 18 22 8 2 Nd_{60} 1021° 3074° +3 144.242 $2.70\cdot 10^{-9}$%	2 8 18 23 8 2 Pm_{61} 1042° 3000° +3 [145]	2 8 18 24 8 2 Sm_{62} 1074° 1794° +2+3 150.36 $8.42\cdot 10^{-10}$%	2 8 18 25 8 2 Eu_{63} 822° 1596° +2+3 151.964 $3.17\cdot 10^{-10}$%	2 8 18 25 9 2 Gd_{64} 1313° 3273° +3 157.25 $1.076\cdot 10^{-9}$%

‡ Actinides

Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium
2 8 18 32 18 10 2 Th_{90} 1750° 4788° +4 232.03806 $1.09\cdot 10^{-10}$%	2 8 18 32 20 9 2 Pa_{91} 1572° +5+4 231.03588	2 8 18 32 21 9 2 U_{92} 1135° 4131° +3+4+5+6 238.02891 $2.94\cdot 10^{-11}$%	2 8 18 32 22 9 2 Np_{93} 644° +3+4+5+6 [237]	2 8 18 32 24 8 2 Pu_{94} 640° 3228° +3+4+5+6 [244]	2 8 18 32 25 8 2 Am_{95} 1176° 2011° +3+4+5+6 [243]	2 8 18 32 25 9 2 Cm_{96} 1345° +3 [247]

Key to Table: The IUPAC Group Numbers 1 to 18 are used (CAS group numbering in parentheses). Information presented: E_{Z} = element symbol and nuclear charge (protons); melting, boiling, critical point (MP, BP, CP) in °C (sublimation or critical temp. marked with s or t); population of electron levels K - Q; possible oxidation states; **IUPAC mean atomic weights updated 2005** based on terrestrial isotope abundances (^{12}C = 12.0000); for unnatural elements atom. wt. of most abundant isotope is given in brackets; total element abundance (%) in the solar system.

10 (VIII)	11 (IB)	12 (IIB)	13 (IIIA)	14 (IVA)	15 (VA)	16 (VIA)	17 (VIIA)	18 (VIIIA)
								Helium He_2 2 -272.2° -268.93° -267.96° 0 4.002602 8.9%
			Boron B_5 2 3 2075° 4000° +3 10.811 $6.9\cdot 10^{-8}$%	**Carbon** C_6 2 4 4492t° 3642s° +2+4-4 12.0107 0.033%	**Nitrogen** N_7 2 5 -210.00° -195.79° -146.94° ±1±2±3+4+5 14.0067 0.0102%	**Oxygen** O_8 2 6 -218.79° -182.95° -118.56° -2 15.9994 0.078%	**Fluorine** F_9 2 7 -219.62° -188.12° -129.02° -1 18.9984032 $2.7\cdot 10^{-6}$%	**Neon** Ne_{10} 2 8 -248.59° -246.08° -228.7° 0 20.1797 0.0112%
			Aluminum Al_{13} 2 8 3 660.32° 2519° +3 26.9815386 0.000277%	**Silicon** Si_{14} 2 8 4 1414° 3265° +2+4-4 28.0855 0.00326%	**Phosphorus** P_{15} 2 8 5 44.15° 280.5° 721° +3+5-3 30.973762 0.000034%	**Sulfur** S_{16} 2 8 6 115.21° 444.60° 1041° +4+6-2 32.065 0.00168%	**Chlorine** Cl_{17} 2 8 7 -101.5° -34.04° 143.8° +1+5+7-1 35.453 0.000017%	**Argon** Ar_{18} 2 8 8 -189.35° -185.85° -122.28° 0 39.948 0.000329%
Nickel Ni_{28} 2 8 16 2 1455° 2913° +2+3 58.6934 0.000161%	**Copper** Cu_{29} 2 8 18 1 1084.62° 2562° +1+2 63.546 $1.70\cdot 10^{-6}$%	**Zinc** Zn_{30} 2 8 18 2 419.53° 907° +2 65.38 $4.11\cdot 10^{-6}$%	**Gallium** Ga_{31} 2 8 18 3 29.76° 2204° +3 69.723 $1.23\cdot 10^{-7}$%	**Germanium** Ge_{32} 2 8 18 4 938.25° 2833° +2+4 72.64 $3.9\cdot 10^{-7}$%	**Arsenic** As_{33} 2 8 18 5 817t° 614s° 1400° +3+5-3 74.92160 $2.1\cdot 10^{-8}$%	**Selenium** Se_{34} 2 8 18 6 221° 685° 1493° +4+6-2 78.96 $2.03\cdot 10^{-7}$%	**Bromine** Br_{35} 2 8 18 7 -7.2° 58.8° 315° +1+5-1 79.904 $3.8\cdot 10^{-8}$%	**Krypton** Kr_{36} 2 8 18 8 -157.36° -153.22° -63.74° 0 83.798 $1.5\cdot 10^{-7}$%
Palladium Pd_{46} 2 8 18 18 0 1554.9° 2963° +2+4 106.42 $4.5\cdot 10^{-9}$%	**Silver** Ag_{47} 2 8 18 18 1 961.78° 2162° +1 107.8682 $1.58\cdot 10^{-9}$%	**Cadmium** Cd_{48} 2 8 18 18 2 321.07° 767° +2 112.411 $5.3\cdot 10^{-9}$%	**Indium** In_{49} 2 8 18 18 3 156.60° 2072° +3 114.818 $6.0\cdot 10^{-10}$%	**Tin** Sn_{50} 2 8 18 18 4 231.93° 2602° +2+4 118.710 $1.25\cdot 10^{-8}$%	**Antimony** Sb_{51} 2 8 18 18 5 630.63° 1587° +3+5-3 121.760 $1.01\cdot 10^{-9}$%	**Tellurium** Te_{52} 2 8 18 18 6 449.51° 988° +4+6-2 127.60 $1.57\cdot 10^{-8}$%	**Iodine** I_{53} 2 8 18 18 7 113.7° 184.4° 546° +1+5+7-1 126.90447 $2.9\cdot 10^{-9}$%	**Xenon** Xe_{54} 2 8 18 18 8 -111.75° -108.04° 16.58° 0 131.293 $1.5\cdot 10^{-8}$%
Platinum Pt_{78} 2 8 18 32 16 2 1768.4° 3825° +2+4 195.084 $4.4\cdot 10^{-9}$%	**Gold** Au_{79} 2 8 18 32 18 1 1064.18° 2856° +1+3 196.966569 $6.1\cdot 10^{-10}$%	**Mercury** Hg_{80} 2 8 18 32 18 2 -38.83° 356.73° 1477° +1+2 200.59 $1.11\cdot 10^{-9}$%	**Thallium** Tl_{81} 2 8 18 32 18 3 304° 1473° +1+3 204.3833 $6.0\cdot 10^{-10}$%	**Lead** Pb_{82} 2 8 18 32 18 4 327.46° 1749° +2+4 207.2 $1.03\cdot 10^{-8}$%	**Bismuth** Bi_{83} 2 8 18 32 18 5 271.40° 1564° +3+5 208.98040 $4.7\cdot 10^{-10}$%	**Polonium** Po_{84} 2 8 18 32 18 6 254° 962° +2+4 [209]	**Astatine** At_{85} 2 8 18 32 18 7 302° [210]	**Radon** Rn_{86} 2 8 18 32 18 8 -71° -61.7° 104° 0 [222]
Darmstadtium Ds_{110} 2 8 18 32 32 16 2 [281]	**Roentgenium** Rg_{111} 2 8 18 32 32 17 2 [280]	**Copernicium** Cn_{112} 2 8 18 32 32 18 2 [285]						

Terbium Tb_{65} 2 8 18 27 8 2 1356° 3230° +3 158.92535 $1.97\cdot 10^{-10}$%	**Dysprosium** Dy_{66} 2 8 18 28 8 2 1412° 2567° +3 162.500 $1.286\cdot 10^{-9}$%	**Holmium** Ho_{67} 2 8 18 29 8 2 1474° 2700° +3 164.93032 $2.90\cdot 10^{-10}$%	**Erbium** Er_{68} 2 8 18 30 8 2 1529° 2868° +3 167.259 $8.18\cdot 10^{-10}$%	**Thulium** Tm_{69} 2 8 18 31 8 2 1545° 1950° +3 168.93421 $1.23\cdot 10^{-10}$%	**Ytterbium** Yb_{70} 2 8 18 32 8 2 819° 1196° +2+3 173.054 $8.08\cdot 10^{-10}$%	**Lutetium** Lu_{71} 2 8 18 32 9 2 1663° 3402° +3 174.9668 $1.197\cdot 10^{-10}$%

Berkelium Bk_{97} 2 8 18 32 27 8 2 1050° +3+4 [247]	**Californium** Cf_{98} 2 8 18 32 28 8 2 900° +3 [251]	**Einsteinium** Es_{99} 2 8 18 32 29 8 2 860° +3 [252]	**Fermium** Fm_{100} 2 8 18 32 30 8 2 1527° +3 [257]	**Mendelevium** Md_{101} 2 8 18 32 31 8 2 827° +2+3 [258]	**Nobelium** No_{102} 2 8 18 32 32 8 2 827° +2+3 [259]	**Lawrencium** Lr_{103} 2 8 18 32 32 9 2 1627° +3 [262]

Adapted by W. E. Hull from the Table prepared by Richard B. Firestone (rbf@lbl.gov), Isotopes Project, Lawrence Berkeley National Laboratory; see R. B. Firestone, C. M. Baglin, and S.Y. F. Chu, 1999 Update to the 8th Edition of the *Table of Isotopes*, John Wiley & Sons, (1999); for Atomic Wt. updates see T. B. Coplen, Pure Appl Chem 73 (2001) 667-683 and R. D. Loss, Pure Appl Chem 75 (2003) 1107-1122.

Chemical Tables

Properties of Selected Nondeuterated Solvents

Solvent	Formula	MW_{ave}	Density d_4^{20} [g/mL]	Viscosity η^{25} [mPa•s, cP]	MP [°C]	BP [°C]	Refrac. Index n_D^{20}	Dielec. Const. ε	Dipole Mom. [*D*]	Chemical Shift δ_H (ppm)	δ_C (ppm)
Acetic acid	$C_2H_4O_2$	60.05	1.049	1.13	16.5	118.1	1.3716	6.17	1.7	2.10 11.42	20.8 178.1
Acetone	C_3H_6O	58.08	0.788	0.306	–94.5	56.2	1.3587	20.7	2.8	2.05	30.50 205.4
Acetonitrile	C_2H_3N	41.05	0.784	0.35	–45.2	81.7	1.3441	37.5	3.44	1.93	1.6 117.8
Benzene	C_6H_6	78.11	0.8789	0.604	5.5	80.2	1.5011	2.29	0	7.16	128.5
1-Butanol	$C_4H_{10}O$	74.12	0.8097	2.55	–89.5	117.6	1.3993	17.7	1.70	1.0-1.5 3.5	14, 19 34, 63
2-Butanone (methyl ethyl ketone)	C_4H_8O	72.11	0.805	0.378	–86.7	79.6	1.3788	18.5	2.77	1.1, 2.2 2.5	7, 27.5 35, 207
Carbon disulfide	CS_2	76.14	1.270	0.363	–111.8	46.1	1.628	2.6	0		192.8
Carbon tetrachloride	CCl_4	153.82	1.590	0.908	–22.9	76.7	1.460	2.22	0		96.7
Chloroform	$CHCl_3$	119.38	1.480	0.537	–63.5	61.2	1.4458	4.81	1.08	7.26	77.2
Chloromethane	CH_3Cl	50.49	0.916	0.24	–97.5	–24.1	1.3389	12.6	1.87	3.06	25.6
Cyclohexane	C_6H_{12}	84.16	0.7786	0.894	6.5	80.8	1.4262	2.02	0	1.4	27.6
Cyclopentane	C_5H_{10}	70.13	0.745	0.44	–94.0	49.3	1.4065	1.94	0	1.5	26.5
Dibromomethane	CH_2Br_2	173.84	2.485		–52.7	96.9	1.5419	7.5	1.43	5.0	21.6
o-Dichlorobenzene	$C_6H_4Cl_2$	147.00	1.31	1.324	–17.2	180.3	1.5515	9.9	2.27	7.0-7.4	128-133
1,2-Dichloroethane	$C_2H_4Cl_2$	98.96	1.253	0.79	–35.7	83.4	1.4448	10.4	1.83	3.7	51.7
cis-1,2-Dichloroethylene	$C_2H_2Cl_2$	96.94	1.284		–80.0	60.6	1.4490	9.2	1.90	6.4	119.3
trans-1,2-Dichloroethylene	$C_2H_2Cl_2$	96.94	1.257		–49.8	47.7	1.4462	2.1	0	6.3	121.1
1,1-Dichloroethylene	$C_2H_2Cl_2$	96.94	1.213		–122.6	31.6	1.4254	4.6	1.34	5.5	115.5 128.9
Dichloromethane	CH_2Cl_2	84.93	1.326	0.41	–96.7	39.9	1.424	9.0	1.60	5.31	53.73
Diethylether	$C_4H_{10}O$	74.12	0.713	0.230	–116.3	34.6	1.3526	4.30	1.25	1.2 3.5	17.1 67.4
Diethylene glycol dimethyl ether (diglyme)	$C_6H_{14}O_3$	134.18	0.947	0.989	–64.1	162.0	1.407	7.1		3.3-3.6	59.0 70.5 72
1,2-Dimethoxyethane (glyme)	$C_4H_{10}O_2$	90.12	0.868	0.46	–69 –58	85	1.379	7.20	1.71	3.3 3.5	59 72
Dimethoxymethane	$C_3H_8O_2$	76.10	0.866		–105.2	42.3	1.3563	2.6		3.3 4.4	54.8 97.9
N,N-Dimethylacetamide	$C_4H_9N_O$	87.12	0.9415	2.14	–20	166	1.437	37.8	3.75	2.1 3	21.5 34, 38 169.6
Dimethylcarbonate	$C_3H_6O_3$	90.08	1.069		3	90.5	1.3688			3.65	54.8 156.9
Dimethylether	C_2H_6O	46.07			–139	–24.5				1.3	59.4
N,N-Dimethyl-formamide	C3H_7NO	73.10	0.9487	0.92	–60.5	152.9	1.4305	36.7	3.86	2.8 2.9 8.0	30.10 35.2 162.5
Dimethylsulfoxide	C_2H_6OS	78.14	1.100	1.987	18.5	189.5	1.4783	46.7	4.0	2.49	39.50
1,4-Dioxane	$C_4H_8O_2$	88.11	1.034	1.18	11.9	101.2	1.4224	2.25	0.45	3.53	67.30
Ethanol	C_2H_6O	46.07	0.789	1.074	–114.4	78.4	1.3614	24.5	1.69	1.10	17.20 56.70
Ethyl acetate	$C_4H_8O_2$	88.11	0.896	0.426	–83.8	77.1	1.3724	6.0	1.8	1.2 2.0 4.1	14.3 20.7 60.1 170.4
Ethylene carbonate	$C_3H_4O_3$	88.06	1.321	1.93	36.4	244	1.416	89.6	4.91	4.2	65.0 155.8
Ethylene glycol	$C_2H_6O_2$	62.07	1.115	21 (20 °C)	–12.6	197.5	1.431	37.7		3.7	63.4
Formamide	CH_3NO	45.04	1.133	3.3	2.6	210.5	1.4475	110	3.38	7.2 8.1	165.1
Glycerol	$C_3H_8O_3$	92.10	1.26	940	17.9	290.1	1.474	42.5		3.4 3.7	64.5 73.7

Chemical Tables

Properties of Selected Nondeuterated Solvents

Solvent	Formula	MW_{ave}	Density d_4^{20} [g/mL]	Viscosity η^{25} [mPa•s, cP]	MP [°C]	BP [°C]	Refrac. Index n_D^{20}	Dielec. Const. ε	Dipole Mom. [*D*]	Chemical Shift δ_H (ppm)	δ_C (ppm)
Hexamethyl-phosphoramide (HMPA)	$C_6H_{18}N_3OP$	179.20	1.027		7.2	233	1.4588	30.6	5.5	2.4 2.6	36.6
Hexane	C_6H_{14}	86.18	0.6594	0.294	−95.4	68.8	1.3749	1.89	0.08		
Methanesulfonic acid	CH_4O_3S	96.11	1.48	10.52	18	168	1.430			2.8	39.6
Methanol	CH_4O	32.04	0.791	0.544	−97.7	64.7	1.3284	32.6	1.70	3.31	49.0
Morpholine	C_4H_9NO	87.12	1.005	2.011	−3.1	128.9	1.4548	7.4	1.58	2.6 3.9	46.8 68.9
Nitromethane	CH_3NO_2	61.04	1.137	0.61	−28.7	100.9	1.3817	35.9	3.46	4.33	62.8
Pentane	C_5H_{12}	72.15	0.626	0.224	−129.7	36.1	1.3575	1.84	0.04		
2-Propanol	C_3H_8O	60.10	0.786	2.1	−87.9	82.4	1.3772	19	1.66	1.2 3.4	25.3 64.0
Pyridine	C_5H_5N	79.10	0.983	0.95	−41.8	115.4	1.510	12.4	2.3	7.21 7.57 8.72	123.5 135.5 149.5
Quinoline	C_9H_7N	129.16	1.098		−14.9	237.7	1.6293	9.0	2.2	7-8.8	121-151
1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$	167.85	1.60	1.58	−43.5	146.2	1.486	8.2	1.3	6.0	74.0
Tetrachloroethylene	C_2Cl_4	165.83	1.622	0.89	−22.2	121.1	1.504	2.3			120.4
Tetrahydrofuran	C_4H_8O	72.11	0.889	0.46	−108.6	66.0	1.407	7.5	1.68	1.72 3.57	25.26 67.2
Toluene	C_7H_8	92.14	0.867	0.56	−95.0	110.7	1.4969	2.38	0.36	2.09 7.01 7.09	21.3 138.5
Trichloroethylene	C_2HCl_3	131.39	1.465	0.545	−84.7	87.1	1.4767	3.4	0.81	6.4	116.7 124.0
Triethylamine	$C_6H_{15}N$	101.19	0.728	0.363	−114.7	89.2	1.401	2.42	0.87	1.0, 2.5	13, 51
Trifluoroacetic acid	$C_2HF_3O_2$	114.02	1.53	1.14	−15.4	72.5	1.285	42.1	2.26		115.7 163.8
2,2,2-Trifluoroethanol	$C_2H_3F_3O$	100.04	1.384	1.76	−44	74	1.291	8.55	2.52	3.9 5.0	62 126.3
Water	H_2O	18.02	0.9982	0.8909	0.0	100.0	1.3329	80.1	1.85	4.72	
o-Xylene	C_8H_{10}	106.17	0.88	0.76	−25.2	144.5	1.505	2.57	0.5	2.4 6.9	18 125-137

Data were revised 2006 from a variety of sources; density and refractive index are at 20°C, other parameters mainly at 25°C; exceptions occur when the solvent is not liquid at these temperatures; MP and BP are means or best values from the NIST Chem WebBook.

Electronegativities according to Pauling

Main group elements

H 2.20						
Li 0.98	Be 1.57	B 2.04	C 2.55	N 3.04	O 3.44	F 3.98
Na 0.93	Mg 1.31	Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16
K 0.82	Ca 1.10	Ga 2.01	Ge 2.01	As 2.18	Se 2.55	Br 2.96
Rb 0.82	Sr 0.95	In 1.78	Sn 1.96	Sb 2.05	Tr 2.1	I 2.66
Cs 0.7	Ba 0.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2

d-block elements

Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6
Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7
La 1.1	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9

f-block elements

All 1.1-1.3

Physical Tables

Fundamental Physical Constants (CODATA 2010) [a]

Quantity	Symbol	SI Value
Speed of Light (vacuum)	c, c_0	$2.997\,924\,58 \times 10^{8}$ m s^{-1} (defined)
Permeability of vacuum	μ_0	$4\pi \times 10^{-7}$ H m^{-1} or N A^{-2} (defined)
Permittivity of vacuum	$\varepsilon_0 = 1/(\mu_0 c_0^2)$	$8.854\,187\,817 .... \times 10^{-12}$ F m^{-1} (defined)
Planck Constant	h	$6.626\,069\,57\ (29) \times 10^{-34}$ J s
	$\hbar = h / 2\pi$ (au)	$1.0544\,571\,726\ (47) \times 10^{-34}$ J s
Elementary Charge (au)	e	$1.602\,176\,565\ (35) \times 10^{-19}$ C
Electron Rest Mass (au)	m_e	$9.109\,382\,91\ (40) \times 10^{-31}$ kg
Proton Rest Mass	m_p	$1.672\,621\,777\ (74) \times 10^{-27}$ kg
Proton/Electron Mass Ratio	m_p / m_e	1836.152 672 45 (75)
Neutron Rest Mass	m_n	$1.674\,927\,351\ (74) \times 10^{-27}$ kg
Deuteron Rest Mass	m_d	$3.343\,583\,48\ (15) \times 10^{-27}$ kg
Atomic Mass Unit (^{12}C/12)	m_u = 1 u = 1 Da	$1.660\,538\,921\ (73) \times 10^{-27}$ kg
Avogadro's Number	N_A	$6.022\,141\,29\ (27) \times 10^{23}$ mol^{-1}
Boltzmann Constant	k	$1.380\,6488\ (13) \times 10^{-23}$ J K^{-1}
Faraday Constant	F	$9.648\,533\,65\ (21) \times 10^{4}$ C mol^{-1}
Gas Constant	R	8.314 4621 (75) J mol^{-1} K^{-1}
Molar Volume of ideal gas [b]	$V_m = RT/p$	$22.413\,968\ (20) \times 10^{-3}$ m^3 mol^{-1}
Standard Atmosphere	atm	101.325 kPa (defined)
Fine Structure Constant	$\alpha = \mu_0 e^2 c_0 / 2h$	$7.297\,352\,5698\ (24) \times 10^{-3}$
Inverse Fine-Structure Constant	$1/\alpha$	137.035 999 074 (44)
Bohr Radius (au)	$a_0 = 4\pi\varepsilon_0\hbar^2 / m_e e^2$	$0.529\,177\,210\,92\ (17) \times 10^{-10}$ m
Hartree Energy (au)	$E_h = \hbar^2 / m_e a_0^2$	$4.359\,744\,34\ (19) \times 10^{-18}$ J
Rydberg Constant	$R_\infty = E_h / 2hc_0$	$10.973\,731\,568\,539\ (55) \times 10^{7}$ m^{-1}
Compton Wavelength (Electron)	$\lambda_C = h / m_e c_0$	$2.426\,310\,2389\ (16) \times 10^{-12}$ m
Bohr Magneton (β, β_e)	$\mu_B = e\hbar / 2m_e$	$927.400\,968\ (20) \times 10^{-24}$ J T^{-1}
Electron Magnetic Moment	μ_e	$-928.476\,430\ (21) \times 10^{-26}$ J T^{-1}
Electron Magnetogyric Ratio	$\gamma_e = 2\,\mu_e / \hbar$	$1.760\,859\,708\ (39) \times 10^{11}$ s^{-1} T^{-1}
	$\gamma_e / 2\pi$	28.024 952 66 (62) GHz T^{-1}
Free Electron Landé g factor	$g_e = 2\mu_e / \mu_B$	–2.002 319 304 361 53 (53)
Nuclear Magneton (β_N)	$\mu_N = (m_e / m_p)\,\mu_B$	$5.050\,783\,53\ (11) \times 10^{-27}$ J T^{-1}
Proton Magnetic Moment (free)	μ_p	$1.410\,606\,743\ (33) \times 10^{-26}$ J T^{-1}
(shielded, H_2O sphere, 25°C)	μ_p'	$1.410\,570\,499\ (35) \times 10^{-26}$ J T^{-1}
Proton Magnetogyric Ratio (free)	γ_p	$2.675\,222\,005\ (63) \times 10^{8}$ s^{-1} T^{-1}
(shielded, H_2O sphere, 25°C)	γ_p'	$2.675\,153\,268\ (66) \times 10^{8}$ s^{-1} T^{-1}
Proton MR freq. in H_2O	$\gamma_p' / 2\pi$	42.576 3866 (10) MHz T^{-1}
Electron/Proton Magn. Mom. Ratio	μ_e / μ_p	–658.210 6848 (54)
Deuteron Magnetic Moment	μ_d	$0.433\,073\,489\ (10) \times 10^{-26}$ J T^{-1}
Gravitation Constant (Newtonian)	G	$6.673\,84\ (80) \times 10^{-11}$ m^3 kg^{-1} s^{-2}
Standard Acceleration (Earth gravity)	g_n	9.806 65 m s^{-2} (defined)
π = 3.141 592 653 59	e = 2.7180281 828 46	ln 10 = 2.302 585 092 99

[a] au = atomic units; uncertainty of last digits shown in ( ); source: http://physics.nist.gov/constants
[b] at STP of 273.15 K and 101.325 kPa = 1 atm.

Physical Tables

SI Unit System (Système International) adapted from NIST Publication 330 (2001)

Fundamental SI Base Units	Unit Name	Symbol
length (l, λ)	meter	m
mass (m)	kilogram	kg
time (t)	second	s
electric current (I)	ampere	A
thermodynamic temperature (T)	kelvin	K
amount of substance (n)	mole	mol
luminous intensity (I_v)	candela	cd
SI-derived Quantities	**Unit Name**	**Symbol**
area (A)	square meter	m^2
volume (V)	cubic meter	m^3
speed, velocity ($\mathbf{v}$)	meter per second	m/s
acceleration ($\mathbf{a}$)	meter per second squared	m/s^2
momentum ($\mathbf{p} = m\mathbf{v}$)	kilogram meter per second	kg m/s
moment or inertia (I, J)	kilogram square meter	kg m^2
mass density (ρ)	kilogram per cubic meter	kg/m^3
specific volume (v)	cubic meter per kilogram	m^3/kg
molar mass (M)	kg per mole	kg/mol
molar volume (V_m)	cubic meter per mole	m^3/mol
concentration (c)	mole per cubic meter	mol/m^3
molal concentration (m)	mole per kilogram	mol/kg
kinematic viscosity (ν) diffusion coefficient (D)	square meter per second	m^2/s
electric current density (J)	ampere per square meter	A/m^2
magnetic field strength ($\mathbf{H}$) magnetization ($\mathbf{M} = \mathbf{B}/\mu_0 - \mathbf{H}$)	ampere per meter	A/m
magnetic dipole moment ($\mathbf{m}$, $\boldsymbol{\mu}$)	ampere square meter	A m^2
wave number ($\tilde{\nu}$)	reciprocal meter	m^{-1}
luminance (L_v)	candela per square meter	cd/m^2
refractive index (n)	(dimensionless)	

SI Prefix	Symbol	Factor
yocto	y	10^{-24}
zepto	z	10^{-21}
atto	a	10^{-18}
femto	f	10^{-15}
pico	p	10^{-12}
nano	n	10^{-9}
micro	µ	10^{-6}
milli	m	10^{-3}
centi	c	10^{-2}
deci	d	10^{-1}
deka	da	10^{1}
hecto	h	10^{2}
kilo	k	10^{3}
mega	M	10^{6}
giga	G	10^{9}
tera	T	10^{12}
peta	P	10^{15}
exa	E	10^{18}
zetta	Z	10^{21}
yotta	Y	10^{24}

Special SI-derived Quantities	Unit Name	Symbol	SI-derived and Base Units
plane angle ($\alpha = s/r$)	radian	rad	m m^{-1} = 1 [2π rad = 360°], 1 rad = 57.2957795°
solid angle ($\Omega = A/r^2$)	steradian	sr	m^2 m^{-2} = 1 [4π sr = sphere]
frequency (ν, f)	hertz	Hz	s^{-1}
force ($\mathbf{F} = m\mathbf{a}$)	newton	N	m kg s^{-2}
pressure, stress (p, P, $\sigma = \mathbf{F}/A$)	pascal	Pa	$N/m^2 = m^{-1}$ kg s^{-2}
energy, work, heat (E, W)	joule	J	N m = m^2 kg s^{-2}
power, radiant flux (P)	watt	W	J/s = m^2 kg s^{-3}
electric charge, quantity (Q), flux (ψ)	coulomb	C	s A
electric potential (V, ϕ), pot. difference (U), emf (E)	volt	V	W/A or J/C = m^2 kg s^{-3} A^{-1}
capacitance (C)	farad	F	C/V = m^{-2} kg^{-1} s^4 A^2
electric resistance (R), impedance (Z)	ohm	Ω	V/A = m^2 kg s^{-3} A^{-2}
electric conductance ($G = 1/R$)	siemens	S	A/V or Ω^{-1} = m^{-2} kg^{-1} s^3 A^2
magnetic flux (Φ)	weber	Wb	V s = m^2 kg s^{-2} A^{-1}
magnetic flux density, induction ($\mathbf{B}$)	tesla	T	Wb/m^2 = V s m^{-2} = kg s^{-2} A^{-1}
inductance (L)	henry	H	Wb/A or V s A^{-1} = m^2 kg s^{-2} A^{-2}
Celsius temperature (θ, t)	degree Celsius	°C	°C = K – 273.15

Physical Tables

Special SI-derived Quantities	Unit Name	Symbol	SI-derived and Base Units
luminous flux (*F*)	lumen	lm	cd sr = m^2 m^{-2} cd
illuminance (E_v)	lux	lx	lm/m^2 = m^2 m^{-4} cd = m^{-2} cd
activity, radioactive decay (*A*)	becquerel	Bq	s^{-1}
absorbed dose, specific energy	gray	Gy	J/kg = m^2 s^{-2}
dose equivalent (personal, organ)	sievert	Sv	J/kg = m^2 s^{-2}
catalytic activity	katal	kat	s^{-1} mol

Other SI-derived Quantities	Unit Name	SI Symbol	SI Base Units
angular velocity (ω)	radian per second	rad/s	s^{-1} [1 Hz = 2π rad s^{-1}]
angular acceleration	radian per second squared	rad/s^2	s^{-2}
moment of force (***M***), torque ($\boldsymbol{T} = \boldsymbol{r} \times \boldsymbol{F}$)	newton meter	N m	m^2 kg s^{-2}
dynamic viscosity (η, μ)	pascal second	Pa s	N s/m^2 = m^{-1} kg s^{-1}
surface tension (γ, σ)	newton per meter	N/m	kg s^{-2}
specific energy	joule per kilogram	J/kg	m^2 s^{-2}
molar energy	joule per mole	J/mol	m^2 kg s^{-2} mol^{-1}
energy density	joule per cubic meter	J/m^3	m^{-1} kg s^{-2}
heat flux density (*I*)	watt per square meter	W/m^2	kg s^{-3}
thermal conductivity (λ, *k*)	watt per meter kelvin	W/(m K)	m kg s^{-3} K^{-1}
heat capacity (C_v , C_p), entropy (*S*)	joule per kelvin	J/K	m^2 kg s^{-2} K^{-1}
specific heat capacity (*c*) or entropy	joule per kilogram kelvin	J/(kg K)	m^2 s^{-2} K^{-1}
molar entropy, molar heat capacity (C_m)	joule per mole kelvin	J/(mol K)	m^2 kg s^{-2} K^{-1} mol^{-1}
electric field strength (***E***)	volt per meter	V/m	m kg s^{-3} A^{-1}
electric field gradient (q_{ab})	volt per square meter	V/m^2	kg s^{-3} A^{-1}
electric charge density (ρ)	coulomb per cubic meter	C/m^3	m^{-3} s A
electric flux density (***D***)	coulomb per square meter	C/m^2	m^{-2} s A
electric polarization ($\boldsymbol{P} = \boldsymbol{D} - \varepsilon_0\boldsymbol{E}$)	coulomb per square meter	C/m^2	m^{-2} s A
electric dipole moment (μ)	coulomb meter	C m	m s A
electric polarizability (α)		C^2 m^2 J^{-1}	F m^2 = kg^{-1} s^4 A^2
electric quadrupole moment (*eQ*)	coulomb square meter	C m^2	m^2 s A
electric resistivity ($\rho = E / j$)	ohm meter	Ω m	m^3 kg s^{-3} A^{-2}
electric conductivity ($\kappa = 1 / \rho$)	siemens per meter	S/m	m^{-3} kg^{-1} s^3 A^2
molar conductivity (Λ)	siemens square meter		
permittivity (ε)	per mole farad per meter	S m^2/mol F/m	kg^{-1} s^3 A^2 mol^{-1} m^{-3} kg^{-1} s^4 A^2
permeability (μ = ***B/H***)	henry per meter	H/m	m kg s^{-2} A^{-2}
exposure (radiation), ion dose	coulomb per kilogram	C/kg	kg^{-1} s A
absorbed dose rate	gray per second	Gy/s	m^2 s^{-3}
rf specific absorption rate (SAR)	watt per kg	W/kg	m^2 s^{-3}
radiant intensity (*I*)	watt per steradian	W/sr	m^2 kg s^{-3}
radiance (*L*)	watt per square meter		
	steradian	W/(m^2 sr)	kg s^{-3}
irradiance (*E*) luminous energy (Q_v)	watt per square meter lumen second	W/m^2 lm s	kg s^{-3} s cd sr
catalytic activity concentration	katal per cubic meter	kat/m^3	m^{-3} s^{-1} mol

Physical Tables

Accepted non-SI units	Unit Name	Symbol	Value in SI units
length	astronomical unit	ua, AU	1 ua = 1.495 978 70 (30) × 10^{11} m
	nautical mile	nmi, NM	1 nautical mile = 1852 m
	Ångström	Å	1 Å = 10^{-10} m = 0.1 nm
area	are	a	1 a = 1 dam^2 = 10^2 m^2
	hectare	ha	1 ha = 1 hm^2 = 10^4 m^2
	barn	b	1 b = 100 fm^2 = 10^{-28} m^2
volume	liter	L (l)	1 L = 1 dm^3 = 10^{-3} m^3
concentration	moles per liter (molar, M)	mol/L	1 M = 1 mol/dm^3
time	minute	min	1 min = 60 s
	hour	h	1 h = 60 min = 3600 s
	day	d	1 d = 24 h = 86 400 s
angular measure	degree	°	1° = (π/180) rad = 60'
	minute	'	1' = (1/60)° = (π/10800) rad
	second	''	1'' = (1/60)' = (π/648000) rad
mass	atomic mass unit	u	1 u = 1.660 538 86 (28) × 10^{-27} kg
	metric ton	t	1 t = 1000 kg
velocity	knot = 1 naut. mile/h	kn	1 nmi/h = 0.514444444 m/s
energy	electronvolt	eV	1 eV = 1.602 176 53 (14) × 10^{-19} J
pressure	bar	bar	1 bar = 10^5 Pa = 1000 hPa
nat. log. intensity scale	neper	Np	1 Np = 1 (= 8.6858896 dB)
base-10 log. intensity scale	bel, decibel	B, dB	1 dB = (1n 10)/20 Np

CGS Units	Symbol	SI Value	CGS Units	Symbol	SI Value
erg	erg	1 g cm^2 s^{-2} = 10^{-7} J	dyne	dyn	1 g cm s^{-2} = 10^{-5} N
gal	Gal	1 cm/s^2 = 10^{-2} m/s^2	gauss	G	10^{-4} T = 0.1 mT
maxwell	Mx	10^{-8} Wb	oersted	Oe	(10^3/4π) A/m
phot	ph	10^4 lx	poise	P	1 dyn s /cm^2 = 10^{-1} Pa s
stilb	sb	1 cd/cm^2 = 10^4 cd/m^2	stokes	St	1 cm^2/s = 10^{-4} m^2 s^{-1}

non-SI Units	Symbol	SI Value	non-SI Units	Symbol	SI Value
acceleration	g_n	9.80665 m s^{-2}	atmosphere	atm	101325 Pa
bohr (au)	a_0, b	5.29177 × 10^{-11} m	calorie (therm.)	calth	4.184 J
calorie (intern.)	cal_{IT}	4.1868 J	carat (metric)	kt	200 mg
centipoise	cP	1 mPa s	curie	Ci	3.7 × 10^{10} Bq
dalton	Da, u	1.66053873 × 10^{-27} kg	debye	D	3.33564 × 10^{-30} C m
entropy unit	e.u.	4.184 J K^{-1} mol^{-1}	fermi	f, fm	1 fm = 10^{-15} m
footcandle		10.76391 lx	gamma	γ	1 nT = 10^{-9} T
horsepower	hp	745.6999 W	jansky	Jy	1 Jy = 10^{-26} W m^{-2} Hz^{-1}
lambert		$10^4/\pi$ = 3.183099 cd/m^2	light year	l.y.	9.46073047258 × 10^{15} m
mho		1 siemens	miles/gal. (US)	mpg	235.215/mpg = L/100 km
miles/h	mph	0.44704 m/s	parsec	pc	3.085677581 × 10^{16} m
point (1/72 in)	pt	0.3527778 mm	pound/in^2	psi	6.894757 kPa
quad (10^{15} Btu)		1.055056 × 10^{18} J	rad	rad	1 cGy = 10^{-2} Gy
rem	rem	1 cSv = 10^{-2} Sv	roentgen	R	1 R = 2.58 × 10^{-4} C/kg
svedberg	S, Sv	10^{-13} s	ton (TNT)		4.184 GJ
ton (register)		2.831685 m^3	torr (mm hg)	Torr	1/760 atm = 133.322 3684 Pa
X unit		ca. 1.002 × 10^{-4} nm	year (Gregorian)	a	365.2425 d 31 556 952 s

Physical Tables

SI Values of US and Imperial Measures

Linear Measures (1 m = 10^2 cm = 10^3 mm)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (m)**
mil; thou	mil	0.001 in	2.54 E-05
point (font sizes)	pt	1/72 in	3.527778 E-04
pica		12 pt	4.233333 E-03
inch (international)	**in**	**defined**	**0.0254**
inch (US survey)	in	defined: 39.3700 in = 1 m	0.0254000508001016
hand		4 in	0.1016
link (US survey)	li, lnk	33/50 ft	0.201168402336805
foot (int.)	**ft**	**12 in (int)**	**0.3048**
foot (US survey)	ft	defined: 1 ft = 12/39.37 m	0.304800609601219
yard (int.)	**yd**	**3 ft; 36 in (int)**	**0.9144**
yard (US survey)	yd	3 ft; 36 in	0.914401828803658
fathom (US survey)	fm	6 ft	1.82880365760732
rod (US survey)	rd	25 li; 5.5 yd; 16.5 ft	5.02921005842012
chain (US survey)	ch	4 rd; 100 li; 22 yd; 66 ft	20.1168402336805
furlong (US survey)	fur	10 ch; 40 rd; 220 yd; 660 ft	201.168402336805
cable (US survey)		120 fm; 720 ft	219.456438912878
mile (int.)	**mi**	**1760 yd; 5280 ft (int)**	**1609.344**
statute mile (US survey)	mi	25 rd; 80 ch; 5280 ft; 8000 li	1609.347219
nautical mile (int.)	**nmi**	**defined**	**1852**
sea mile (US survey)		6080.20 ft	1853.24866649733
league	lea	3 nautical miles	5556
Area Measures (1 m^2 = 10^4 cm^2 = 10^6 mm^2)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (m^2)**
square inch (int.)	sq in, in^2		6.4516 E-04
square foot (int.)	sq ft, ft^2	144 in^2	0.09290304
square yard (int.)	sq yd, yd^2	9 ft^2; 1296 in^2	0.83612736
square rod (US survey)	sq rd, rd^2	30.25 yd^2; 272.25 ft^2	25.2929538117141
acre (international)		4840 yd^2; 43560 ft^2; 0.40468564 ha	4046.8564224
acre (US survey)		10 ch^2; 160 rd^2; 4840 yd^2; 43560 ft^2	4046.87260987425
square mile (int.)	sq mi, mi^2	3097600 yd^2	2.589988110336 E+06
square mile (US survey)	sq mi, mi^2	640 acre	2.58999847031952 E+06
Volume Measures (1 L = 1 dm^3 = 10^{-3} m^3; 1 mL = 1 cm^3 = 10^{-6} m^3; 1 μl = 1 mm^3 = 10^{-9} m^3)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (L, dm^3)**
cubic inch (int.)	cu in, in^3	0.554 fl oz	0.016387064
cubic foot (int.)	cu ft, ft^3	1728 in^3	28.316846592
cubic yard (int.)	cu yd, yd^3	27 ft^3; 46656 in^3	764.554857984
displacement ton		defined as 35 ft^3	991.08963072
register ton		defined as 100 ft^3	2831.6846592
cubic mile (int.)	cu mi, mi^3	5.451776 E9 yd^3	4.168181825 E+12
Imperial dry and fluid measures (UK, Commonwealth)			
minim	min	1/480 fl oz	5.919388021 E-05
drop	gtt	1/288 fl oz; 5/3 min	9.865646701 E-05
dash		1/384 gi; 1/16 tsp	3.699617513 E-04
pinch		2 dash; 1/192 gi; 1/8 tsp	7.399235026 E-04
scruple	fl s	1/24 fl oz; 20 min	1.183877604 E-03
drachm	fl dr	1/8 fl oz; 60 min	3.551633000 E-03
teaspoon (Canada)	tsp	1/6 fl oz; 80 min	4.735510417 E-03
teaspoon	tsp	1/24 gi; 5/3 fl dr; 100 min	5.919388021 E-03
tablespoon (Canada)	tbsp	1/2 fl oz; 3 tsp; 240 min;	1.420653125 E-02
tablespoon	tbsp	1/8 gi; 5/8 fl oz; 3 tsp; 5 fl dr; 300 min	1.775816406 E-02
ounce (Imp)	**fl oz (Imp)**	**8 fl dr; 480 min**	**0.0284130625**
gill	gi (Imp)	5 fl oz	0.1420653125
cup (Canada)	c (CA)	8 fl oz	0.2273045

Imperial dry and fluid measures (UK, Commonwealth)			
Name	**Symbol**	**Equivalents**	**SI Value (L, dm³)**
pint	pt (Imp)	4 gill; 20 fl oz	0.56826125
quart	qt (Imp)	2 pt; 40 fl oz	1.1365225
gallon (Imperial)	**gal (Imp)**	**defined as 160 oz av water at 62 °F; 4 qt; 8 pt; 32 gi; 160 fl oz**	**4.54609**
peck	pk	2 gal	9.09218
bucket	bkt	4 gal	18.18436
bushel	bu	8 gal	36.36872
barrel	bl	36 gal	163.65924
US fluid measures			
minim	min	1/480 fl oz	6.161151992 E-05
drop	gtt	1/360 fl oz; 4/3 min	8.214869323 E-05
dash		1/96 fl oz; 1/16 tsp	3.080575996 E-04
pinch		2 dash; 1/48 fl oz; 1/8 tsp	6.161151992 E-04
dram	fl dr	1/8 fl oz; 60 min	3.696691195 E-03
teaspoon	tsp	1/6 fl oz	4.928921594 E-03
tablespoon	tbsp	1/2 fl oz; 4 fl dr; 0.5 fl oz	1.478676478 E-02
ounce (US)	**fl oz (US)**	**1/128 gal; 8 fl dr; 480 min**	**0.0295735295625**
jigger		1.5 fl oz; 12 fl dr	0.044360294
gill	gi (US)	4 fl oz	0.118294118
cup	c (US)	8 fl oz	0.236588
pint	pt (US)	2 c; 16 fl oz	0.473176473
quart	qt (US)	2 pt; 32 fl oz	0.946353
gallon (US)	**gal (US)**	**defined as 231 in³; 4 qt; 128 fl oz**	**3.785411784**
barrel	fl bl (US)	defined as 31.5 gal	119.240471196
barrel (oil)	bbl	defined as 42 gal (US)	158.987294928
US dry measures			
pint	pt	1/64 bu	0.5506104713575
quart	qt	1/32 bu; 2 pt	1.101220942715
board-foot	fbm	defined as 144 in³	2.359737216
gal	gal	1/8 bu; 4 qt	4.40488377086
peck	pk	1/4 bu; 8 qt	8.80976754172
bushel (dry level)	bu (US lvl)	defined as 2150.42 in³; 4 pk; 32 qt;	35.23907016688
barrel	bl	105 qt	115.628198985075
seam		8 bu	281.91256133504
cord	cd	128 ft³	3624.556363776

Mass (1 kg = 10³ g = 10⁶ mg)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (kg)**
avoirdupois	av		
grain	gr	1/7000 lb	6.479891 E-05
dram	dr av	1/256 lb; 7000/256 gr	1.7718451953125 E-03
ounce	oz av	1/16 lb; 16 dr	2.8349523125 E-02
pound	**lb av**	**defined**	**0.45359237**
stone (UK)		14 lb	6.35029318
quarter (UK)		2 stone; 28 lb	12.70058636
hundredweight (short, US)	net cwt	100 lb	45.359237
hundredweight (long, UK)	gross cwt	8 stone; 112 lb	50.80234544
short ton (US)	ton	20 cwt; 2000 lb	907.18474
long ton (UK)	ton	20 cwt (UK); 2240 lb	1016.0469088
troy or apothecary	t, ap		
grain	gr	same mass as in avoirdupois	6.479891 E-05
scruple	s ap	1/24 oz t; 20 gr	1.2959782 E-03
pennyweight	dwt, pwt	1/20 oz t; 24 gr	1.55517384 E-03
dram	dr t	1/8 oz t; 60 gr	3.8879346 E-03
ounce	oz t	1/12 lb t; 20 dwt; 8 dr t; 480 gr	3.11034768 E-02
pound	lb t	12 oz t; 96 dr t; 5760 gr	0.3732417216

Conversion Factors for Important Physical Units

Energy Equivalents

	Joule	Hertz	cm^{-1}	Kelvin	eV
Joule	1	1.5091905 E+33	5.03411762 E+22	7.242964 E+22	6.24150974 E+18
Hertz	6.62606876 E–34	1	3.335640952 E–11	4.7992374 E–11	4.13566727 E–15
cm^{-1}	1.98644544 E–23	2.99792458 E+10	1	1.4387752	1.239841857 E–04
Kelvin	1.3806503 E–23	2.0836644 E+10	0.6950356	1	8.6173432 E–05
eV	1.602176462 E–19	2.417989491 E+14	8.06554477 E+03	1.1604506 E+04	1

based on the Fundamental constants with $E = mc^2 = hc/\lambda = h\nu = kT$ and 1 eV = (e/C) J

Force Units: Si unit = Newton (N), cgs unit = dyne, Weight = mass×g_n

	N	p (pond)	kp	dyne
N	1	101.9716	0.1019716	1.0 E+05
p	0.00980665	1	1.00 E–03	980.665
kp	9.80665	1000	1	980665
dyne	1.0 E–05	1.019716 E–03	1.019716 E–06	1

Energy and Work Units: SI unit = Joule (J), cgs unit: 1 erg = 10^{-7} Joule

	J = N m	kp m	kWh	kcal	BTU	eV
J	1	0.101972	2.777778 E–07	2.390057 E–04	9.478134 E–04	6.241512 E+18
kp m	9.80665	1	2.724069 E–06	2.343846 E–03	9.294874 E–03	6.120832 E+19
kWh	3.600 E+06	3.670978 E+05	1	860.4207	3412.128	2.246944 E+25
kcal	4184	426.6493	1.162222 E–03	1	3.965651	2.611448 E+22
BTU	1055.06	1.075862 E+02	2.930722 E–01	2.521654 E–01	1	6.585169 E+21
eV	1.602176 E–19	1.633765 E–20	4.450489 E–26	3.829293 E–23	1.518564 E–22	1

Power Units: SI unit = Watt (W)

	W = J s^{-1}	kW	kpm/s	PS	cal/s	kcal/h
W	1	1.0 E–03	0.1019716	1.341022 E–03	0.2390057	0.8604207
kW	1.0 E+03	1	101.9716	1.341022	239.0057	860.4207
kpm/s	9.80665	9.80665 E–03	1	1.315093 E–02	2.343846	8.437844
PS	745.7	0.7457	76.04024	1	178.2266	641.6157
cal/s	4.184	4.184 E–03	0.4266493	5.610835 E–03	1	3.6
kcal/h	1.162222	1.162222 E–03	0.1185137	1.558565 E–03	0.2777778	1

Pressure Units: SI unit = Pascal

	Pa = N/m^2	kp/m^2	atm	bar	**Torr =** mmHg	**at =** kp/cm^2
Pa = N/m^2	1	0.1019716	9.86923 E–06	1.0 E–05	7.500617 E–03	1.019716 E–05
kp/m^2	9.80665	1	9.67841 E–05	9.80665 E–05	7.355592 E–02	1.0 E–04
atm	1.01325 E+05	1.033227 E+04	1	1.01325	760	1.033227
bar	1.0 E+05	1.019716 E+04	0.9869233	1	750.0617	1.019716
Torr	133.3224	13.59510	1.315789 E–03	1.333224 E–03	1	1.359510 E–03
at = kp/cm^2	9.80665 E+04	1.0 E+04	0.9678411	9.800665 E–01	735.5592	1

Time Units: SI unit = second

	s	min	h	d	week	year
s	1	1.666667 E–02	2.777778 E–04	1.157407 E–05	1.653439 E–06	3.168874 E–08
min	60	1	1.666667 E–02	6.944444 E–04	9.920635 E–05	1.901324 E–06
h	3600	60	1	4.166667 E–02	5.952381 E–03	1.140795 E–04
d	86400	1440	24	1	1.428571 E–01	2.737907 E–03
week	604800	10080	168	7	1	1.916535 E–02
year	31556952	525949.2	8765.82	365.2425	52.1775	1

Temperature Conversion: SI unit = Kelvin

	Kelvin (K)	Centigrade (°C)	Fahrenheit (°F)	Rankine (°R)
K	1	$T_C = T_K - 273.15$	$T_F = (9/5)T_K - 459.67$	$T_R = (9/5)T_K$
°C	$T_K = T_C + 273.15$	1	$T_F = (9/5)T_C + 32$	$T_R = (9/5)(T_C + 273.15)$
°F	$T_K = (5/9)(T_F + 459.67)$	$T_C = (5/9)(T_F - 32)$	1	$T_R = T_F + 459.67$
°R	$T_K = (9/5)T_R$	$T_C = (5/9)T_R - 273.15$	$T_F = T_R - 459.67$	1

Physical Tables

Colour, Wave Length, Frequency, Wave Number and Energy of Light

Colour	λ [nm]	ν [Hz]	ν [cm^{-1}]	E [eV]	E [kJ mol^{-1}]
Infrared	1000	$3.00 \cdot 10^{14}$	$1.00 \cdot 10^{4}$	1.24	120
Red	700	$4.28 \cdot 10^{14}$	$1.43 \cdot 10^{4}$	1.77	171
Orange	620	$4.84 \cdot 10^{14}$	$1.61 \cdot 10^{4}$	2.00	193
Yellow	580	$5.17 \cdot 10^{14}$	$1.72 \cdot 10^{4}$	2.14	206
Green	530	$5.66 \cdot 10^{14}$	$1.89 \cdot 10^{4}$	2.34	226
Blue	470	$6.38 \cdot 10^{14}$	$2.13 \cdot 10^{4}$	2.64	254
Violet	420	$7.14 \cdot 10^{14}$	$2.38 \cdot 10^{4}$	2.95	285
Near Ultraviolet	300	$1.00 \cdot 10^{15}$	$3.33 \cdot 10^{4}$	4.15	400
Far Ultraviolet	200	$1.50 \cdot 10^{15}$	$5.00 \cdot 10^{4}$	6.20	598

Density of Water (H_2O)

t [°C]	ρ [kg/dm³]	t [°C]	ρ [kg/dm³]	t [°C]	ρ [kg/dm³]
0	0.999841	11	0.999606	22	0.997772
1	0.999900	12	0.999498	23	0.997540
2	0.999941	13	0.999377	24	0.997299
3	0.999965	14	0.999244	25	0.997047
4	0.999973	15	0.999099	26	0.996785
5	0.999965	16	0.998943	27	0.996515
6	0.999941	17	0.998775	28	0.996235
7	0.999902	18	0.998596	29	0.995946
8	0.999849	19	0.998406	30	0.995649
9	0.999782	20	0.998205		
10	0.999701	21	0.997994		

Viscosity of Water, η in mPa · s (cP)

t [°C]	η	t [°C]	η	t [°C]	η	t [°C]	η
0	1.7865	**20**	1.0019	**50**	0.5477	**90**	0.3155
5	1.5138	**25**	0.8909	**60**	0.4674	**100**	0.2829
10	1.3037	**30**	0.7982	**70**	0.4048	**125**	0.2200
15	1.1369	**40**	0.6540	**80**	0.3554	**150**	0.1830

Physical Tables

Viscosities of Various Liquids, η in mPa · s (cP)

Liquid	0°C	10°C	20°C	30°C	40°C	50°C	60°C	70°C	100°C
Acetic acid	–	–	1.219	1.037	0.902	0.794	0.703	0.629	0.464
Acetone	0.397	0.358	0.324	0.295	0.272	0.251	–	–	–
Aniline	–	6.53	4.39	3.18	2.40	1.91	1.56	1.29	0.76
Benzene	–	0.757	0.647	0.560	0.491	0.435	0.389	0.350	–
Bromobenzene	1.556	1.325	1.148	1.007	0.889	0.792	0.718	0.654	0.514
Carbon disulfide	0.436	0.404	0.375	0.351	0.329	–	–	–	–
Carbon dioxide (liq.)	0.099	0.085	0.071	0.053	–	–	–	–	–
Carbon tetrachloride	1.348	1.135	0.972	0.845	0.744	0.660	0.591	0.533	0.400
Chloroform	0.704	0.631	0.569	0.518	0.473	0.434	0.399	–	–
Diethyl ether	0.294	0.267	0.242	0.219	0.199	0.183	0.168	0.154	0.119
Ethanol	1.767	1.447	1.197	1.000	0.830	0.700	0.594	0.502	–
Ethyl acetate	0.581	0.510	0.454	0.406	0.366	0.332	0.304	0.278	–
Ethyl formate	0.508	0.453	0.408	0.368	0.335	0.307	–	–	–
Formic acid	–	2.241	1.779	1.456	1.215	1.033	0.889	0.778	0.547
Mercury	1.681	1.661	1.552	1.499	1.450	1.407	1.367	1.327	1.232
Methanol	0.814	0.688	0.594	0.518	0.456	0.402	0.356	–	–
***n*-Octane**	0.710	0.618	0.545	0.485	0.436	0.494	0.358	0.326	0.255
Oil, castor	–	2420	986	451	231	125	74	43	16.9
Oil, olive	–	138	84	52	36	24.5	17	12.4	–
***n*-Pentane**	0.278	0.254	0.234	0.215	0.198	0.184	0.172	0.161	0.130
Sulfuric acid	56	49	27	20	14.5	11.0	8.2	6.2	–
Toluene	0.771	0.668	0.585	0.519	0.464	0.418	0.379	0.345	0.268

Self-Diffusion Coefficients *D* of Various Liquids at 25°C

Liquid	*D* [$10^{-9}m^2s^{-1}$]	Liquid	*D* [$10^{-9}m^2s^{-1}$]	Liquid	*D* [$10^{-9}m^2s^{-1}$]
Water (H_2O)	2.299	Acetonitrile	4.37	Cyclopentane	3.09
Water (D_2O)	1.872	Pyridine	1.54	Cyclooctane	0.55
Methanol (CH_3OH)	2.415	Nitromethane	2.39	*n*-Pentane	5.72
Methanol (CH_3OD)	2.30	Tetrahydrofuran	2.84	*n*-Hexane	4.26
Methanol (CD_3OH)	2.21	Benzene	2.21	*n*-Heptane	3.12
Methanol (CD_3OD)	2.11	Fluorobenzene	2.39	*n*-Octane	2.35_5
Ethanol	1.08	Hexafluorobenzene	1.46	*n*-Nonane	1.77
t-Butanol-d_1	0.28	Toluene	2.27	*N*-Decane	1.37
Formamide	0.55	Carbon disulfide	4.32	*n*-Undecane	1.07_6
N,N-Dimethylformamide	1.63	Carbon Tetrachloride	1.30	*n*-Dodecane	0.81
N,N-Dimethylacetamide	1.35	Chloroform	2.35	*n*-Tridecane	0.70
Dimethyl sulfoxide	0.73	Acetic acid	1.08	*n*-Tetradecane	0.52
Dioxane	1.09	Formic acid	1.08	Pentan-1-ol	0.29
Acetone	4.57	Cyclohexane	1.42	Octan-1-ol	0.14

Table by courtesy of Dr. M. Holz (Institute of Phys. Chem., University of Karlsruhe, FRG) and Prof. A Sacco (Dept. Chem., University of Bari, Italy).

Temperature Dependence of the Self-Diffusion Coefficient *D* of Water (H_2O)

t [°C]	*D* [$10^{-9}m^2s^{-1}$]	t [°C]	*D* [$10^{-9}m^2s^{-1}$]	t [°C]	*D* [$10^{-9}m^2s^{-1}$]	t [°C]	*D* [$10^{-9}m^2s^{-1}$]
-5	0.913	20	2.023	50	3.956	80	6.557
0	1.099	25	2.299	55	4.344	85	7.056
2.5	1.199	30	2.594	60	4.748	90	7.574
5	1.303	35	2.907	65	5.172	95	8.111
10	1.525	40	3.238	70	5.615	100	8.667
15	1.765	45	3.588	75	6.078		

Table by courtesy of Dr. M. Holz, Institute of Phys. Chem., University of Karlsruhe, FRG.

International Dialing Codes / World Time Zones

Time Zones are listed as increment in hour:min relative to UTC / GMT for ST = standard time; DST = Daylight Savings (Summer) Time (where used). Provences or Cities are listed for countries with more than one time zone.

NB: DST runs approximately from March to October in the northern hemisphere and October to March in the southern hemisphere; exact period depends on country and may change from year to year. (data adapted by W.E. Hull from www.happyzebra.com and www.worldtimezone.com)

Country (Code) - Provinces / Cities	ST	DST
Afghanistan (+93)	+4:30	
Albania (+355)	+1	+2
Algeria (+213)	+1	
Angola (+244)	+1	
Argentina (+54) DST only in Buenos Aires and some provinces in the northeast	–3	–2
Armenia (+374)	+4	+5
Australia (+61) - W. Austr. (Perth)	+8	
Australia (+61) - N. Terr. (Darwin),	+9:30	
Australia (+61) - Queensland (Brisbane)	+10	
Australia (+61) - Cap. Terr. (Canberra), N.S.W. (Sydney), Victoria (Melbourne), S. Austr. (Adelaide), Tasmania (Hobart)	+10	+11
Austria (+43)	+1	+2
Azerbaijan (+994)	+4	+5
Bahamas (+1)	–5	–4
Bahrain (+973)	+3	
Bangladesh (+880)	+6	+7
Barbados (+1)	–4	
Belarus (+375)	+2	+3
Belgium (+32)	+1	+2
Belize (+501)	–6	
Benin (+229)	+1	
Bermuda (UK)	–4	–3
Bhutan (+975)	+6	
Bolivia (+591)	–4	
Bosnia-Herzegovina (+387)	+1	+2
Botswana (+267)	+2	
Brazil (+55) / Rio Branco	–5	
Brazil (+55) / Manaus	–4	
Brazil (+55) / Salvador, Recife	–3	
Brazil (+55) / Brasilia, Rio de Janeiro, Porto Alegre, Sao Paulo	–3	–2
Brazil (+55) / Fernando de Noronha	–2	
Brunei (+673)	+8	
Bulgaria (+359)	+2	+3
Burkina Faso (+226)	0	
Burundi (+257)	+2	
Cambodia (+855)	+7	
Cameroon (+237)	+1	
Canada (+1) - Newfoundland & Labrador	–3:30	–2:30
Canada (+1) - Pr. Edward Island, Nova Scotia, New Brunswick	–4	–3
Canada (+1) - Ontario (Toronto, Ottawa), Quebec (Montreal, Quebec)	–5	–4
Canada (+1) - Manitoba (Winnipeg)	–6	–5
Canada (+1) - Alberta (Edmonton, Calgary), NW Territories	–7	–6
Canada (+1) - Saskatchewan	–7	
Canada (+1) - British Columbia (Vancouver), Yukon Terr.	–8	–7
Canary Islands (Spain)	0	+1
Central African Republic (+236)	+1	
Chad (+235)	+1	
Chile (+56)	–4	–3
China (+86)	+8	
Colombia (+57)	–5	
Congo, Repub. (+242) / Kinshasa	+1	
Congo, Dem. Repub. (+243) / Lubumbashi	+2	
Costa Rica (+506)	–6	
Cote dÍvoire (+225)	0	
Croatia (+385)	+1	+2
Cuba (+53)	–5	–4
Cyprus (+357)	+2	+3
Czech Republic (+420)	+1	+2
Denmark (+45)	+1	+2
Djibouti (+253)	+3	
Dominican Republic (+1)	–4	
Ecuador (+593)	–5	
Egypt (+20)	+2	+3
El Salvador (+503)	–6	
Eritrea (+291)	+3	
Estonia (+372)	+2	+3
Ethiopia (+251)	+3	
Fiji (+679)	+12	
Finland (+358)	+2	+3
France (+33)	+1	+2
French Guiana	–3	
Gabon (+241)	+1	
Galapagos Islands (Ecuador)	–6	
Gambia (+220)	0	
Gaza (+970)	+2	+3
Georgia (+995)	+4	
Germany (+49)	+1	+2
Ghana (+233)	0	
Gibraltar (UK)	+1	+2
Greece (+30)	+2	+3
Guatemala (+502)	–6	
Guadeloupe (France)	–4	
Guinea (+224)	0	
Guyana (+592)	–4	
Haiti (+509)	–5	
Honduras (+504)	–6	
Hungary (+36)	+1	+2
Iceland (+354)	0	
India (+91)	+5:30	
Indonesia (+62) - Papua	+9	
Indonesia (+62) - Bali, Kalimantan, Lombok, West Timor	+8	
Indonesia (+62) - Java, Sumatra	+7	
Iran (+98)	+3:30	+4:30
Iraq (+964)	+3	
Ireland (+353)	0	+1
Israel (+972)	+2	+3
Italy (+39)	+1	+2
Jamaica (+1)	–5	
Japan (+81)	+9	
Jordan (+962)	+2	+3
Kazakhstan (+7) / Almaty, Astana	+6	
Kazakhstan (+7) / Aqtau, Aqtobe	+5	
Kenya (+254)	+3	
Kosovo (+381)	+1	+2
Kuwait (+965)	+3	

International Dialing Codes / World Time Zones

Country (Code) - Provinces / Cities	ST	DST
Kyrgyzstan (+996)	+6	
Laos (+856)	+7	
Latvia (+371)	+2	+3
Lebanon (+961)	+2	+3
Lesotho (+266)	+2	
Liberia (+231)	0	
Libya (+218)	+2	
Liechtenstein (+423)	+1	+2
Lithuania (+370)	+2	+3
Luxembourg (+352)	+1	+2
Macedonia (+389)	+1	+2
Madagascar (+261)	+3	
Malawi (+265)	+2	
Malaysia (+60)	+8	
Maldives (+960)	+5	
Mali (+223)	0	
Malta (+356)	+1	+2
Martinique (France)	–4	
Mauritania (+222)	0	
Mauritius (+230)	+4	
Mexico (+52) - Aguascalientes, Fed. District (Mexico City), Guanajuato, Guerrero, Jalisco, Nuevo Leon, Quintana Roo, San Luis Potosi, Veracruz, Yucatan	–6	–5
Mexico (+52) - Chihuahua, Sinaloa	–7	–6
Mexico (+52) - Sonorro	–7	
Mexico (+52) - Baja California (Tijuana)	–8	–7
Moldova (+373)	+2	+3
Monaco (+377)	+1	+2
Mongolia (+976) / Choibalsan, Ulaanbaatar	+8	
Mongolia (+976) / Hovd	+7	
Montenegro (+382)	+1	+2
Morocco (+212)	0	+1
Mozambique (+258)	+2	
Myanmar (+95)	+6:30	
Namibia (+264)	+1	+2
Nepal (+977)	+5:45	
Netherlands (+31)	+1	+2
New Zealand (+64)	+12	+13
Nicaragua (+505)	–6	
Niger (+227)	+1	
Nigeria (+234)	+1	
North Korea (+850)	+9	
Norway (+47)	+1	+2
Oman (+968)	+4	
Pakistan (+92)	+5	+6
Panama (+507)	–5	
Papua New Guinea (+675)	+10	
Paraguay (+595)	–4	–3
Peru (+51)	–5	
Philippines (+63)	+8	
Poland (+48)	+1	+2
Portugal (+351)	0	+1
Puerto Rico (+1)	–4	
Qatar (+974)	+3	
Reunion (+262)	+4	
Romania (+40)	+2	+3
Russia (+7) / Kaliningrad	+2	+3
Russia (+7) / Kazan, Moscow, Murmansk, Novgorod, St. Petersburg	+3	+4
Russia (+7) / Samara	+4	+5
Russia (+7) / Chelyabinsk, Novosibirsk, Perm, Ufa, Yekaterinburg	+5	+6

Country (Code) - Provinces / Cities	ST	DST
Russia (+7) / Omsk	+6	+7
Russia (+7) / Krasnoyarsk	+7	+8
Russia (+7) / Irkutsk	+8	+9
Russia (+7) / Yakutsk	+9	+10
Russia (+7) / Vladivostok, Yuzhno-Sakhalinsk	+10	+11
Russia (+7) / Magadan	+11	+12
Russia (+7) / Anadyr, Kamchatka	+12	+13
Rwanda (+250)	+2	
Saudi Arabia (+966)	+3	
Senegal (+221)	0	
Serbia (+381)	+1	+2
Seychelles (+248)	+4	
Sierra Leone (+232)	0	
Singapore (+65)	+8	
Slovakia (+421)	+1	+2
Slovenia (+386)	+1	+2
Somalia (+252)	+3	
South Africa (+27)	+2	
South Korea (+82)	+9	
Spain (+34)	+1	+2
Sri Lanka (+94)	+5:30	
Sudan (+249)	+3	
Suriname (+597)	–3	
Swaziland (+268)	+2	
Sweden (+46)	+1	+2
Switzerland (+41)	+1	+2
Syria (+963)	+2	+3
Tahiti (France)	–10	
Taiwan (+886)	+8	
Tajikistan (+992)	+5	
Tanzania (+255)	+3	
Thailand (+66)	+7	
Timor-Leste (+670)	+9	
Togo (+228)	0	
Trinidad & Tobago (+1)	–4	
Tunisia (+216)	+1	
Turkey (+90)	+2	+3
Turkmenistan (+993)	+5	
UAE - Abu Dhabi, Dubai (+971)	+4	
Uganda (+256)	+3	
Ukraine (+380)	+2	+3
United Kingdom (+44) - England, Scotland, Wales, N. Ireland	0	+1
Uruguay (+598)	–3	–2
USA (+1) - Eastern Zone (New York, Boston, Miami, Philadelphia...)	–5	–4
USA (+1) - Central Zone (Chicago, Wichita, New Orleans, Pensicola)	–6	–5
USA (+1) - Mountain Zone (Helena, Denver, Santa Fe)	–7	–6
USA (+1) - Arizona	–7	
USA (+1) - Pacific Zone (Las Vegas, San Francisco, Los Angeles)	–8	–7
USA (+1) - Alaska (Anchorage)	–9	–8
USA (+1) - Hawaii (Honolulu)	–11	
Uzbekistan (+998)	+5	
Vatican City (+39)	+1	+2
Venezuela (+58)	–4:30	
Vietnam (+84)	+7	
Yemen (+967)	+3	
Zambia (+260)	+2	
Zimbabwe (+263)	+2	