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Evaluation of Nuclear Moments

IAEA Consultants Meeting
27 – 30 March 2017

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Abstract

A summary is given of an IAEA Consultancy Meeting on Evaluation of Nuclear Moments which was held from 27 to 30 March 2017 at the IAEA,Vienna. Participants reviewed the current status of measurements and methods applied to extract the magnetic dipole and electric quadrupole moments of the nucleus, and discussed the corrections necessary to obtain a set of consistent data for evaluation. Agreement on the treatment of diamagnetism, hyperfine anomaly, time-dependent measurements of short-lived states and the electric field gradient for quadrupole moments was reached and a plan of action for producing a table of recommended best values was adopted.

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Contents

ANNEXES

1. Introduction

Nuclear electromagnetic moments carry information on the interaction of the electromagnetic field with the nucleus and allow us to draw conclusions on basic structure properties of the nucleus such as the angular momentum, parity, excitation energies and matrix elements of the stationary states of the nucleus. As such, they are important for basic nuclear physics studies, as well as for a range of applied sciences based on atomic physics, chemistry, and solid state physics. The electric Quadrupole Moment (QM) is directly related to the shape of the nuclear charge distribution, while the magnetic Dipole Moment (DM) is intimately related to the way the nucleus carries its angular momentum as it originates with the intrinsic spins and orbital angular momentum of the nucleons.

Different measurement techniques have been developed over the years to produce experimental values of QM and DM for stable and more exotic nuclides in their ground and excited states. Many of these methods for the DM require corrections for the effect of the medium upon an applied magnetic field (diamagnetism and/or the Knight shift) and for the non-point-like nature of the nucleus (the hyperfine anomaly). Careful comparison and assessment of the different measured values needs to take these factors into consideration to arrive at a best value of the DM. All QM results depend upon a calculation of the electric field gradient acting at the nucleus in the experimental environment. Computation techniques to deliver this vital parameter have made great strides in recent decades and a consistent set of QM's needs to utilise the latest results.

Compilations of the available experimental information on QM/DM began in the early 1950s and recent years have seen publications of listings of results as published, with little or no additional analysis. The evaluated QMs of P. Pyykkö (Refs [1.1], [1.2]) have been widely used as standards for subsequent measurements and evaluations (Refs [1.3] to [1.5]). Tabulated compilations of both QM and DM results have been published by N.J. Stone (Refs [1.6], [1.7], [1.8]) and are now also available online from the Nuclear Moments Database [1.9].

The compilations mentioned above are widely used by evaluators of the Nuclear Structure and Decay Data (NSDD) network as the main source of data on electric quadrupole and magnetic dipole moments for inclusion in the Evaluated Nuclear Structure Data File (ENSDF) [1.10]. ENSDF is one of the most widely consulted databases for nuclear structure data for basic and applied sciences, therefore it is important that it contains reliable and up-to-date information.

It has been suggested by the NSDD network as well as by members of the broader scientific community that the existing compilations of QM/DM require further scrutinizing and processing that should involve (i) critical assessment of the measurement techniques, (ii) revision of the corrections and other input data to account for progress achieved in the various fields of nuclear and atomic physics as well as nuclear chemistry. This evaluation procedure should lead to recommendations of the best values of QM/DM for adoption by the scientific user community.

The evaluation of the electromagnetic nuclear moments requires expertise from different fields as mentioned above, and contributions from experts from all over the world. In response to this, the IAEA organised a Consultancy Meeting on Evaluation of Nuclear Moments, from 27 to 30 March 2017, at the IAEA Headquarters in Vienna. Nine scientists from eight countries attended: M. Bissell (Switzerland), K. Jackowski (Poland), F. Kondev (USA), T.J. Mertzimekis (Greece), G. Neyens (Belgium), J.R. Persson (Norway), P. Pyykkö (Finland), N.J Stone (UK), A.E. Stuchbery (Australia). The Scientific Secretary of the meeting was P. Dimitriou (IAEA).

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[1.4] M. De Rydt et al., Atomic Data and Nuclear Data Tables **99** (2013) 391–415.

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[1.9] T.J. Mertzimekis, Development of a dedicated database for nuclear moments data, IAEA report INDC(NDS)-0704, Vienna (2016).

[1.10] Evaluated Nuclear Structure Data File (ENSDF), http://www.nndc.bnl.gov/ensdf/

2. Objective

The objective of the meeting was to review the current status of measurements and methods used to extract QM/DM, and to propose methods for evaluating the existing data and providing recommended values for QM and DM.

3. Scope

The scope of the meeting covered all the existing measurement techniques for extracting DMs such as Nuclear Magnetic Resonance (NMR), β-NMR, Atomic Beam experiments, Laser spectroscopy, Time-Differential and Time Integral Perturbed Angular Correlation and Distribution methods, Transient Field methods, and Recoil in Vacuum, as well as improvements in calculations of the Electric Field Gradient for the determination of the QM.

To address the corrections and evaluation principles required for the above-mentioned techniques, the meeting was organised in four separate sessions dealing with the four main types of corrections that need to be considered:

- Diamagnetism (corrections for the chemical shift induced by the external magnetic field of the surrounding material-insulators, gases, liquids, solids)
- Hyperfine Anomaly (for non-uniform distribution of charge and spin/angular momentum within the nucleus)
- Treatment of short-lived states (requires consideration of half-lives of short-lived states, and parameterizations of the magnetic field applied in the Transient Field measurements)
- Electric Quadrupole Moments (require precise calculations of Electric Field Gradient)

This report covers a summary of the meeting presentations (Section 4) and technical discussions (Section 5) and the conclusions drawn (Section 6). A List of Actions arising from this meeting is provided in Annex 1.

4. Presentation summaries

4.1 The Structure and Objectives of the Meeting, N.J. Stone

Following a brief summary of the range of methods employed in the measurement of nuclear magnetic dipole and electric quadrupole moments, this talk concentrated on problem areas concerning the preparation of a listing of recommended values which, having emerged over a long period, define the personnel and objectives of this meeting.

It is recognized that preparation of such a listing is a fundamentally different proposition from compiling a record of measurements as they are made. Many of the most precise measurements, on stable isotopes by the Nuclear Magnetic Resonance (NMR) technique, were made more than half a century ago, yet such results form a framework to which very many more recent measurements refer. The NMR frequency measured in an applied magnetic field has to be corrected for diamagnetism – also known as the chemical shift – in insulators, liquids and gases. Accurate calculation of these corrections is not straightforward and developments in recent decades have led to serious revision of older values. These revisions need to be propagated throughout the full range of results by all methods.

Somewhat less precise than the best conventional NMR measurements, beta-NMR results on polarized radioactive isotopes also require use of a host material and an applied magnetic field to conserve the polarization whilst the resonance is studied. Correction has to be made for diamagnetism in insulators and, in some cases where a metal host is employed, for the Knight shift caused by conduction electron polarization. These corrections have been made with varying degrees of sophistication and need to be checked to yield the best moment values.

A second broad class of measurements utilizes the strong magnetic interactions produced by s- and relativistic p-electrons at the nucleus (the Fermi contact term). Yet these interactions are not uniform over the nuclear volume due to both the Breit-Rosenthal effect, which describes the non-point-like nature of the nuclear charge distribution and the Bohr-Weisskopf effect which relates to the distribution over the nuclear volume of the spin and orbital angular momentum contributions to the nuclear moment. The common practice of determining moments by ratios of the magnetic hyperfine interaction constant *A* renders the values found liable to correction for the so-called hyperfine anomaly. However this correction is frequently neglected.

Thirdly, magnetic moment measurements on nuclear levels of lifetime $< 10^{-8}$ s are frequently performed by one of two methods which, despite their considerable achievements, each have distinct problems stemming from the challenges of measuring the moments of such short-lived states. Among the various techniques based on perturbation of the angular distribution of nuclear decay products, integral methods (those which measure the average effect observed in all decays in the sample, IPAC, IPAD, IMPAC etc.) in general suffer from uncertainty concerning the uniformity of the site in the sample occupied by the decaying nucleus and the variation of fields the ensemble of nuclei may experience. A second method, using the transient field (TF) experienced by the nuclei of energetic ions moving through a polarized ferromagnetic metal, requires calibration of these fields. In cases where there is no well measured moment involved in the experiment, calibration may depend upon the state of knowledge at the time of measurement. All such results require expert review.

Finally, concerning nuclear electric quadrupole moments, although a listing of recommended values was published recently, the existence of more than a few problem elements for which no standard reference value exists prompted the inclusion of this topic in the programme of the meeting,

The programme has four main sessions devoted to the topics outlined above (see Section 5 Technical Discussions). The considerations described led to the selection of the members of the meeting, the invitees including experts in both the nuclear physics and the atomic physics aspects of the corrections and calculations required as well as experts in the more prominent measurement techniques.

4.2 Nuclear Magnetic Dipole Moments from Gas Phase NMR Spectra, K. Jackowski

Nuclear Magnetic Resonance (NMR) spectroscopy is widely used in chemistry, biology and medicine. Unfortunately, the standard NMR method permits only for the relative measurements of shielding parameters (chemical shifts). The chemical shifts which represent the effects of diamagnetism, are separately defined for each magnetic nucleus and as a result NMR spectroscopy is fragmented into approximately 100 different experimental methods. This problem does not exist if the nuclear magnetic moments are known with sufficient accuracy because then the shielding constants are determined directly from NMR spectra and their measurement does not depend on the observed nucleus.

Nuclear magnetic shielding in molecules is described by the σ parameter in the equation:

$B_{eff} = (1 - \sigma)\, B_0$ where B_0 is the external magnetic field and B_{eff} is the magnetic field interacting with a nucleus. At present the σ values, known as the shielding constants, can be accurately calculated for small molecules including the corrections for elevated temperature to 300 K. At the same time, the same isolated molecules can be observed by NMR experiments in the gas phase and their resonance frequencies are accurately determined. It gives us an opportunity to perform the comparison of the nuclear magnetic moments of two different nuclei in the same molecule where one nucleus (usually a proton) is used as the reference.

This method was applied for the following nuclei: ^{13}C, ^{14}N, ^{15}N, ^{17}O, ^{19}F, ^{29}Si, ^{31}P, ^{33}S, ^{35}Cl, ^{37}Cl, ^{73}Ge and ^{207}Pb. Some other nuclei (i.e. ^{10}B, ^{11}B, ^{83}Kr, ^{129}Xe and ^{131}Xe) were studied with a small addition of helium-3 which was used here as the external reference of a nuclear magnetic moment. The ^{3}He magnetic moment was carefully verified when we measured its value relative to ^{1}H and ^{2}H in gaseous mixtures of helium-3 with HD molecules.

The new values of nuclear magnetic dipole moments appear to be much more accurate than the previous data obtained using the similar NMR comparison for molecules in liquids or solids for two reasons: First, because new NMR measurements in the gas phase deliver the resonance frequencies exactly for the same molecular objects which were used in the calculations of magnetic shielding. Second, because the present state-of the-art ab initio calculations of shielding are more reliable than the usually crude estimates of shielding available 50 or even 60 years ago.

4.3 Hyperfine Anomaly, J.R. Persson

The hyperfine anomaly was observed when accurate measurements of both the hyperfine interaction constant *A* and the nuclear magnetic moment became available with the advent of the Atomic Beam Magnetic Resonance (ABMR) method in the 1940s. The anomaly arises from two effects; the Bohr-Weisskopf (BW) effect (extended magnetisation) and Breit-Rosenthal (BR) (extended charge distribution) affecting s- and $p_{1/2}$-electrons.

The anomaly is normally defined as: $\frac{a_1}{a_2}\frac{\mu_2/I_2}{\mu_1/I_1} = 1 + {}^{1}\Delta^{2}$

It should be noted that the anomaly is both nuclear and atomic state-dependent. On the atomic side, the different electrons contribute differently to the hyperfine interaction in different atomic states, and on the nuclear side, the distribution of magnetism in the nucleus varies from state to state.

The effect of the extended charge distribution (BR) can attain values up to 25% in absolute value, however, the differential effects between two neighbouring isotopes (historically they have been calculated for isotopes with N = 2) are on the order of 2×10^{-4} (for the heaviest elements, i.e. from Pb to U) which explains why it has generally been neglected. The BW- effect is normally on the order of $10^{-2} - 10^{-3}$ (1 – 0.1%), with exceptions up to 10%.

The classical method to determine the hyperfine anomaly has been to combine independent measurements of the hyperfine interaction constant *A* and the nuclear magnetic moment. The size of the anomaly has for a long time caused the effect to be neglected, or included as an increase of error, in the determination of the nuclear magnetic moment, especially in the case of laser spectroscopy.

From an atomic physics point of view

The development of laser spectroscopy with higher resolution has reached levels of accuracy where the hyperfine anomaly can no longer be ignored. Theoretical developments and calculations in atomic physics have made it feasible to calculate the atomic contributions to the anomaly with high accuracy. This is especially true for the Breit-Rosenthal effect, where it is possible to calculate the contribution for different atomic states and between different isotopes using measurements of the change in mean charge radius. This is something that is important in the case of long isotope chains and highly deformed nuclei. It is therefore possible to separate the two effects better today. Semi-empirical methods have been devised to deduce the anomaly, without requiring accurate knowledge of the nuclear magnetic moment, by using the *A* constant from more than two atomic states with different contributions to the anomaly. The different atomic contributions may be determined either using a known anomaly as calibration, or through analysis of the hyperfine structure or by calculation of the ratio of the contact contributions to the hyperfine structure.

This procedure has enabled the determination of the hyperfine anomaly in new isotopes (^{143,145}Nd, ^{155,157}Gd and ^{191,193,195,195}Pb).

The determination of the anomaly has given improved values of the nuclear magnetic moment in the case of Pb. The theoretical models for calculating the BW-effect are, to this day, too crude and lack the accuracy needed for useful comparisons. However, it is possible to express the BW-effect in terms of changes in the magnetisation radius, which might be a more useful way making it possible to compare with the change in charge radius.

4.4 Introduction on short-lived states, A.E. Stuchbery

Short-lived states here means lifetimes below a few nanoseconds, and typically in the picoseconds range. The methodology is perturbed angular correlations or distributions (typically observing gamma rays). The measurements may be time-dependent (= time differential) or time-integral methods.

The Time Differential (TD) measurements are generally reliable, giving good precision and accuracy. Examples are TDPAC, TDPAD, and TDRIV, where PAC is Perturbed Angular Correlations, PAD is Perturbed Angular Distributions, and RIV is Recoil in Vacuum.

Time-Integral measurements are usually the only option for picosecond states and are more prone to be problematic. Examples are RIV, IPAC (Radioactivity), IMPAC/IMPAD, and Transient-Field.

The methods, and their limitations which impact on the evaluation of data, may be summarized under the type of hyperfine interaction used to perturb the nuclear moment:

Free-ion hyperfine interactions - Recoil in Vacuum (RIV)

For low-Z elements ($Z < 12$) TDRIV is possible with ps states, using hydrogen-like hyperfine fields. For higher-Z ions, the RIV method has used complex fields from many-electron ions and is usually a time-integral method. Evaluation of these data is likely to be relatively straight-forward.

Static internal field in ferromagnetic host

Radioactivity (TDPAC/IPAC) and Implantation (IMPAC = online & integral) methods use the hyperfine fields at dilute impurities in a ferromagnetic host, which can be prepared as an alloy or by ion-implantation. Evaluation of these data will be more problematic, particularly for integral methods. The measurement can be adversely affected by the sample preparation (IPAC), by the magnitude of the polarizing field, and in the case of in-beam methods (IMPAC) by pre-equilibrium effects on the time-scale of picoseconds associated with the dynamics of the ion-implantation process.

Transient field in ferromagnetic host

The transient-field method is a time-integral measurement, with the time range determined by either the stopping time of the ion in the ferromagnetic host or the time the ion takes to transit a ‘thin’ ferromagnetic foil (of order 1 ps in both cases). The TF method provides excellent relative g-factor values. The problem for experimenters, and hence evaluators, concerns the absolute values of the g factors, which must be determined relative to independently known g factors. In the best cases calibration is possible using a known g factor of a neighbouring isotope of the same (or close-by) Z. In many cases, however, experimenters have used a ‘universal’ parametrization of the transient field. The widely used parametrizations were developed around 1980 and need to be re-evaluated. Sometimes uncertainties on the TF calibration are not included in reported g factors. Careful evaluation is needed.

4.5 Electric Quadrople Moments, P. Pyykkö

The 2001 and 2008 summaries by the author were found to be acceptable by the other participants, with only occasional remarks. It was found to be desirable that a similar 2017 version be produced and that it could serve as the basis of further tables by the IAEA (N.J. Stone and others).

A brief list of at least 16 elements, where new data is available, was given.

Concerning errors, or averaging, a distinction was made between cases, where the change has a clear physical or methodological reason, and the others with statistical deviations.

One anomalous case was Q(Bi) where the 'atomic' and 'molecular' results differ for an unknown reason.

A general introduction was made to the methods of relativistic quantum chemistry and their credibility. They are needed for obtaining the q of the measured eqQ/h.

4.6 Measurements of Magnetic Moments using Collinear Laser Spectroscopy, M. Bissell

In this contribution recent measurements of bismuth isotopes by collinear laser spectroscopy were presented. The case was shown as an example of how magnetic moments determined from laser spectroscopy may be influenced by the hyperfine anomaly (HFA). It was stated that in this specific instance the objective of the experiment was not the measurement of moments, but rather the investigation and characterization of the differential HFA's, in order to ascertain their influence on previous measurements using in-source laser spectroscopy. The potential interest in the differential hyperfine anomaly, not only as a means to correct magnetic moments, but also as an independent nuclear structure observable was presented. The key indication that laser spectroscopy data had been influenced by this effect, a non-constant ratio of hyperfine A factors between different atomic levels was shown for the case in question. Subsequently, it was demonstrated that isotopes with similar underlying configurations have consistent A ratios and thus for these measurement the ratios of magnetic moments would not be affected by the hyperfine anomaly at a level which is statistically significant. The applicability of the extreme single particle model to measurements such as this, in proximity to major shell-closures was demonstrated by plotting the observed A factor ratio against the predicted nuclear magnetization part of the HFA calculation. It was shown in this way that we can be certain of the origin of the discrepancies and thus attention should concentrate on measurements displaying a large change from spin to orbital nuclear magnetization. As the gradient of such a plot can only give information on the difference in differential hyperfine anomaly between two levels, reliable correction of magnetic moments will require the appropriate atomic calculations. Future directions in the study of HFA's were then briefly described along with the next steps in addressing the specific case of Bi.

4.7 Evaluation of selected Electric Quadrupole Moments: ^{8,9}Li and isotopes with protons in the sd-shell, G. Neyens

D. Borremans et al., Physical Review C 72, 044309 (2005)

Based on new measurements of Q(^{8}Li, ^{9}Li) in Zn, $LiNbO_3$, $LiTaO_3$ and all previously available quadrupole frequency measurements in different crystals, recommended Q-moments are given for ^{8}Li and ^{9}Li, relative to the reference value for ^{7}Li, Q(^{7}Li) = -40.0(3) mb. The latter has been recommended in the evaluation of stable isotope quadrupole frequency measurements by P. Pyykkö, Mol. Phys. 99, 1617 (2001).

These recommended values can now serve as input to extract the quadrupole moment of ^{11}Li, which has been measured by different groups in independent experiments, relative to that of ^{9}Li, *M. De Rydt et al., Atomic Data and Nuclear Data Tables 99 (2013) 391–415*

Based on the recommended Q-moment values for stable isotopes of O, F, Ne, Na, Mg, Al, S, Cl, Ar, K and Ca, all measured quadrupole frequencies of unstable isotopes (and one isomer) of these lighter elements have been compiled and evaluated. From the available weighted mean values of quadrupole frequencies, quadrupole moments have been extracted relative to that of the stable reference.

In some cases there is no direct link between the unstable and stable reference frequency as they have been measured in different crystals. Thus in the Na isotopes, ^{28}Na has only been measured in the same crystal as ^{23}Na, however ^{22}Na has been measured with the same laser transition as both of the other isotopes. This allows us to link the moments of ^{22,28}Na to the reference ^{23}Na quadrupole moment.

For other isotopes, e.g. ^{26,27,29}Na, the quadrupole frequency has been measured in another crystal along with ^{28}Na. This links their moments to that of ^{28}Na and thus indirectly also to that of ^{23}Na.

For all isotopes of the proton sd-shell elements, a similar analysis has been made, leading to a table with 43 new evaluated quadrupole moments.

4.8 Directly Measured Spins and Nuclear Moments, F.G. Kondev

The basic nuclear ground-state and isomer properties, such as branching ratios, masses, half-lives, quantum numbers and their projections, magnetic and quadrupole moments, and charge radii are anchor points in understanding the structure of nuclei and the validity of various nuclear models. In general, information about these properties can be found in the ENSDF database, but the actual evaluations are completed elsewhere by experts in the field. While several compilations exist on directly measured spin values, the complete and reliable evaluation is still absent. A wealth of new data on directly measured spin values is expected at the existing and future rare-isotope beam facilities in conjunction with the laser spectroscopy techniques. Given the mutual connection between magnetic and quadrupole moments and nuclear spin, such evaluation would be a valuable tool to specialists in the field of nuclear structure and it would allow information on the nuclear state parity to be obtained. An example was presented for the odd-Z Eu (Z = 63) deformed nuclei, where the knowledge of the magnetic moment would allow to distinguish between the 5/2[413] and 5/2[532] Nilsson orbitals, located near the proton Fermi surface.

4.9 Overview of the Online Nuclear EM Moments Database, T.J. Mertzimekis

The IAEA Online Nuclear Moments database (http://www-nds.iaea.org/nuclearmoments) was presented in some detail. The database has been developed to its full extent under the auspices of the IAEA and a technical report has been published (INDC(NDS)-0704, 2016). The database builds upon earlier printed compilations, but extends the available information through frequent updates scanning about 30 peer-reviewed journals and conference proceedings volumes. In its current state, the database has more than 5300 bibliographical entries referring to experimentally deduced nuclear magnetic dipole and electric quadrupole moments.

The user interfaces, the searching capabilities and the description of provided information to the user were presented in some detail during this meeting. Besides the fact that new data are added every three months, the database provides direct links to the original citations using the well-established schemes of Nuclear Science References (NSR) and Digital Object Identifiers (DOI). Elementary particle data are also available, taken directly from the Particle Data Group Evaluations (PDG). A detailed help file contains explanations of annotations and additional useful information, such as references to earlier compilations, list of techniques etc.

4.10 A Way To Evaluate Moments Based On Buck-Perez Scheme, T.J. Mertzimekis

In the extreme single particle shell model the symmetry of mirror nuclei is reflected in the magnetic moment. The spin expectation value is related to the magnetic moments of mirror partners having the same isospin value. In the Buck-Perez scheme, a simple consideration of mirror nuclei with T = 1/2 uses experimental data of magnetic dipole moments to produce a well-defined linear relationship between the odd-proton and odd-neutron g factors for all available mirror pairs.

A recent update of the Buck-Perez scheme for T = 1/2 and T = 3/2 has been used to predict moments in nuclei with T = 5/2, having their mirror partners already measured (T. Mertzimekis, Phys. Rev. C. 94, 064313 (2016); 10.1103/PhysRevC.94.064313). From the application of the method, both magnitude and sign of the magnetic moment can be estimated, but also measurements with contradictory results can be resolved in a straightforward way. This evaluation technique was applied successfully to the ground-state magnetic moment of ^{57}Cu, which had been measured independently by the MSU and KU Leuven groups resulting in significantly different values. Additional comments on the case and the resolution of the ^{57}Cu problem were provided by Gerda Neyens.

5. Technical discussions

The technical discussions focussed on four different topics in separate dedicated sessions. A convenor was assigned to each session with the task of giving an overview of the status of the measurements, the methods of introducing corrections and the quality of the data, as well as recommendations for the evaluation procedure. The four topics:

1. Corrections for diamagnetism for precise Nuclear Magnetic Dipole Moments (DM): Karol Jackowski, Convenor
2. Corrections for Hyperfine Anomaly: Jonas Persson, Convenor
3. DMs for short-lived states: Andrew Stuchbery, Convenor
4. Quadrupole Moments (QM): Pekka Pykkö, Convenor

A summary of the convenors' overviews and the ensuing discussions are given in the following sections.

5.1 Corrections for Diamagnetism, Convenor: K. Jackowski

Accurate treatment of diamagnetism in Gas Phase NMR Spectra

As described in Sect. 4.2, the shielding constant (σ) or chemical shift, is the most important spectral parameter of molecules in the uniform NMR method. In recent years, the availability of enhanced computing capabilities has allowed the use of advanced quantum mechanical methods for reliable and accurate calculations of the shielding constants which include the electron correlation effects (e.g. CCSD(T)), as well as the temperature effects (ZPV and 300K corrections) and the relativistic effects (treated e.g. using DFT or DHF theory).
The results of such calculations are then combined with the NMR resonance frequencies for isolated molecules which are available from gas phase measurements.

This method has been applied extensively by the Warsaw group to obtain accurate DM values for a range of elements. They have measured NMR frequencies of molecules in the gas phase, in the range of linear dependence of frequency on density where the data can be extrapolated to zero density. At zero density intermolecular interactions are absent and the obtained results are valid for isolated molecules. Then they have compared the calculated shielding constants and the resonance frequencies for two different nuclei in the same experiment, where one nucleus (usually ^{1}H or ^{3}He) is treated as the reference. This allows the determination of an unknown nuclear magnetic moment. This method has been used to determine DMs of the ground states of the following nuclei: ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{15}N, ^{17}O, ^{19}F, ^{29}Si, ^{31}P, ^{33}S, ^{35}Cl, ^{37}Cl, ^{73}Ge, ^{83}Kr, ^{129}Xe, ^{131}Xe and ^{207}Pb.

The uncertainties in the new data have been carefully examined by the group. As shown in the presentation, the error bar of the ^{13}C DM is negligibly small when the measurements of resonance frequency are considered and becomes more significant when the calculations of shielding constants are analysed. It is worth noting that all the shielding data can be additionally verified by comparing them with similar results for other molecules, because the chemical shifts are well known for numerous different chemical compounds. Altogether, the analysis of error bars of the new results of the Warsaw group reveals that the values of their DMs are significantly improved in comparison to the old values available in the widely used tables [5.1].

The calculations of shielding constants were extended by Antušek et al. [5.2] to hydrated ions of various metals and were subsequently used for the determination of DMs for nuclei of elements such as: Li, Na, K, Rb, and many others. Experimental frequencies for the measurements were adopted from the data of reference standards used in NMR spectroscopy, as given by Harris et al. in the IUPAC recommendation of 2001 [5.3]. The shielding calculations for large molecular objects (hydrated metal ions) are expected to be of somewhat lower accuracy than the calculations for small isolated molecules like CH_4 or H_2O. Also, the experimental frequencies were measured for solutions of different concentrations, whatever was suitable for the referencing of chemical shifts. Nevertheless, the new results for metal nuclei are consistent with the atomic beam values, in contrast to the previous estimates of magnetic moments made with the application of similar NMR methods. It is clear that this improvement is mostly due to more accurate calculations of shielding constants, though the error bars are estimated to be larger in this case.

It was also mentioned that although the method has been extensively applied to gas phase molecules, it can in principle be extended to liquids (see hydrated ions) and solids. The latter case would be more challenging than the former.

Applied field correction in techniques other than simple NMR, N.J. Stone

Corrections to beta-NMR experiments

Another technique that involves an applied magnetic field and provides data of sufficient precision to require correction for diamagnetism/chemical shift is beta-NMR. In this technique nuclear polarization is produced in a fragmentation reaction and the polarized nuclei are stopped in a cubic environment which can be an insulating single crystal or a metal. A well measured static magnetic field is applied to produce a nuclear Zeeman splitting. NMR is detected through resonant destruction of the asymmetry of decay of the nuclear polarization.

This technique has been used to determine the DMs of more than 50 nuclear ground and long lived excited states, mainly in nuclei of mass < 50. Most reports of these experiments in the literature make some attempt to correct the applied field for diamagnetism/the chemical shift and also, if a metal stopper is used, for conduction electron electron paramagnetism/the Knight shift. The correction, up to several hundred ppm, is significant given the resonance precision of ~ 1 in 10^5.

This short presentation showed examples of these corrections which, as applied, varied widely. Many used outdated estimates of the chemical shift based on Feiock and Johnson's work [5.4] for atoms from the 1960's. It is important that an effort be made to improve these corrections to provide better moment values.

Corrections to experiments by NMR on nuclei oriented at mK temperatures

This technique has been applied to measure magnetic moments in over 100 nuclear ground states and long-lived isomers. When resonance is being sought the ferromagnetic metal sample into which the nuclei under study are introduced by co-melting, diffusion or implantation is magnetized by an applied field of order 0.1 T. The field is produced by a small superconductive coil carrying a current measured to better than 1% and is uniform to 1 – 2%. The field is calculated from the geometry of the coil and is checked against current measurement when the magnet is installed in the equipment.

The total field at the nuclei under study is made up of this applied field, subject to correction, and the internal hyperfine field generated within the ferromagnetic metal, which is of order 10 – 100 T. The detected NMR resonances are typically in the frequency range 50 – 500 MHz with linewidths of 1 – 2 MHz fitted to give center frequency to 0.1 – 0.2 MHz, that is 1 in 10^4.

The applied field in these measurements is thus a few % of the total field and the uncertainty in its value constitutes only 1 in 10^4 of the measured result. For this reason usually no correction is made to the applied field as calculated.

In certain circumstances changes in the applied field are used to shift the observed resonance and the magnetic moment is determined from the slope of frequency versus field. In these experiments also any applied field correction and uncertainly is smaller than other contributions to estimated experimental errors.

Discussion Actions

It is obvious that the new DMs determined by the Warsaw group using more accurate shielding constant calculations and gas phase NMR measurements are more accurate and reliable and therefore an effort should be made to replace the previous data in the widely used compilation tables [5.1].

This has however, further implications in that many other types of measurements have used the NMR moments of certain elements as reference values, and therefore these DM values will also have to be re-adjusted to take account of the more recent and accurate NMR measurements.

The extent of such a revision of the DMs table needs to be assessed by Stone and Jackowski.

Action 1 (Jackowski, Stone): to replace old NMR measurements that were inconsistent with the more consistent and precise values from gas-phase NMR measurements performed by the Polish group (list nuclides). **Estimated deadline: May – June 2017**

Action 2 (Jackowski): to consult with Antušek on validity of results for liquid phase NMR and ab initio calculations, especially regarding the large uncertainties, to decide whether these data should also be added to the tables (in consultation with Stone). **Estimated deadline: May – June 2017**

Action 3 (Jackowski): to go through the beta-NMR measurements (to be provided by Stone) and explore possible ways to introduce diamagnetism corrections, where needed. **Estimated deadline: end of 2017**

Action 4 (Stone): to look into the TDPAC/PAD measurements which may require corrections for diamagnetism and Knight shift, and single out those that need to be further treated for these corrections, and refer them to Jackowski. **Estimated deadline: end of 2017**

Action 5 (Stone): to investigate the possible methods of introducing Knight shift corrections (Chalk River publications, contact J. Beene, D. Ward). **Estimated deadline: May – June 2017**

Recommendation: For diamagnetism corrections, Jackowski will be contacting also K. Ruud (Tromsǿ, Norway), Juha Vaara (Oulu, Finland).

5.2 Hyperfine Anomaly, Convenor: J.R. Persson

In the table of Nuclear Moments, the correction of hyperfine anomaly is limited to a few cases where high accuracy measurements have been done. As the effect is normally on the order of 0.1 – 1% this is expected to be sufficient in most cases. However, in the case of long isotopic chains the BR-effect may attain large values. If the nuclei are deformed or when the spin changes are large a substantial BW-effect is expected. When the orbital and spin interactions in the nucleus almost cancel, the BW may also be substantial, for example in gold isotopes. In these cases, it should be possible to use different nuclear models to identify nuclei that might have a large hyperfine anomaly, thus making it possible to treat these nuclei with caution when determining the nuclear magnetic moment from measurements of the hyperfine interaction constants.

In addition to identifying vulnerable nuclei it is also important to study the atomic structure and determine how sensitive different atomic states are to the hyperfine anomaly. It is also important to obtain a parametrisation so that the BR-effect can be related to the change in charge radius.

$$^{1}\varDelta_{BR}^{2} = \lambda_c \delta\langle r_c^2\rangle$$

The anomaly will affect the tabulated nuclear magnetic moments as demonstrated in the presentation in the case of I = 13/2 states in isotopes in Pb isotopes. Experimental determination of the anomaly in $^{191-197}$Pb gave a value of about 2% for these isotopes. Assuming that all 13/2 isotopes have a similar anomaly compared with ^{207}Pb(I = 1/2), it is possible to find the size of the moment correction which, was a deduction of about 0.012 nuclear magnetons, from the values of μ_I given in the original publication. This reduction is of the same order or larger than the errors given in the original. Hence the corrected values should be adopted.

In order to obtain accurate values of the nuclear magnetic moment using the hyperfine structure the following precautions should be taken.

- In order to find an experimental value of the (contact) hyperfine anomaly, at least 2 (preferably more) states have to be measured in different isotopes.
- A survey on problematic regions (isotopes) should be done, to identify nuclei with large differential BW-effect.
- Where a large BW-effect is suspected a thorough study should be done.
- When measuring long isotopic chains the BR-effect must be considered.
- A study of the effects of the BR correction should be done (in progress).

The terminology used in connection with the hyperfine anomaly is generally inconsistent, with different authors using the same term when describing different things. In order to overcome these ambiguities, clear definitions should be made and used properly:

- Hyperfine anomaly – the effect in general.
- Differential hyperfine anomaly – the general effect between two isotopes.
- State hyperfine anomaly – experimental anomaly for a specific atomic state, different degree of contact interaction.
- Contact hyperfine anomaly – the effect due to contact interaction, valid for a specific isotope and nuclear state.
- Bohr-Weisskopf effect – BW effect compared with a point dipole (nucleus).
- Differential Bohr-Weisskopf effect - BW effect between two isotopes.
- Breit-Rosenthal (Crawford-Schawlow) effect - BR effect compared with a point charge (nucleus).
- Differential Breit-Rosenthal (-Crawford-Schawlow) effect - BR effect between two isotopes.

Note on Atomic Beam Magnetic Resonance

The ABMR method while suitable for measurements of the g_J-factor and hyperfine interaction constants, is not directly suitable for measurements of the nuclear g_I- factor. This is due to the fact that the detection (with magnets) is best suited for sub-states that change the sign of the effective magnetic moment, something that is not affected by the nuclear g_I - factor. In order to get an accurate measurement of nuclear g_I - factor the transitions should be $\Delta m_J = 0$, $\Delta m_I = \pm 1$, in other words the quantum number m_F should not be a good quantum number. This means that high applied magnetic fields are needed. In order to overcome this it is possible to use the triple-resonance method [5.5], where transitions (A & B in figure 1) in the low-field regions are applied to populate/depopulate suitable sublevels. In this case, a transition(C) in the high field region will be a direct measurement of the nuclear g_I- factor.

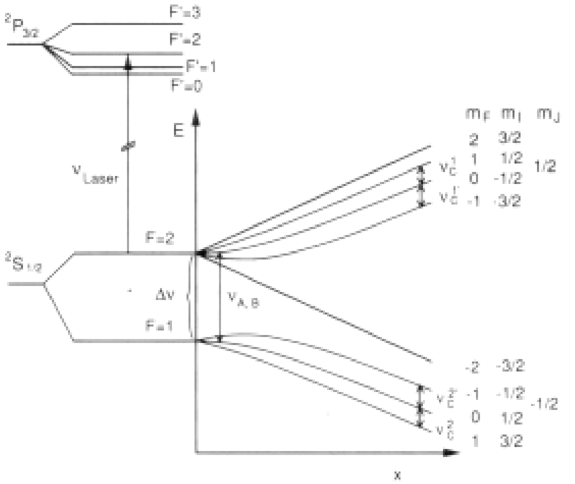

Fig. 1. Hfs energy levels in a magnetic field B for ^{39}K ($I = 3/2$) in the ground $^2S_{1/2}$ state. Low field m_F and high field m_J, m_I quantum numbers are indicated, as are the transitions used for the triple resonance method and for the optical pumping via the excited $^2P_{3/2}$ state. The magnetic field parameter $x \propto B$.

Figure from *An atomic-beam magnetic resonance (ABMR) apparatus for systematic measurements of the hyperfine anomaly [5.6].*

Even if this is a direct measurement, corrections due to off-diagonal hyperfine interactions from neighbouring atomic states may be substantial. In practice this means that the accuracy of direct measurements is limited to elements where the atomic structure is quite simple with atomic states well separated, i.e. alkalis. The relatively large errors in direct measurements with ABMR of the nuclear g_I-factor is due to the off-diagonal hyperfine interaction which puts a limitation to this method for complex atoms.

It should also be noted that there are some errors in the designated method used in the table of nuclear moments [5.1], where it is stated that the measurement is direct, but from the paper it is clearly not. These cases should be amended.

Correction for the hyperfine anomaly – a situation of almost universal neglect, N.J. Stone

This short contribution served to highlight the fact that in many long chain measurements by laser methods all results are determined by ratio to a single, well measured, reference moment through the hyperfine *A* parameter. Although the reference moment is frequently derived from conventional NMR and is thus not subject to a Bohr-Weisskopf correction, any anomaly between that moment and any other in the chain is frequently neglected.

Sizeable hyperfine anomalies, > 0.2%, are relatively rare, but are expected when the nuclear single particle configuration changes between a state of spin I = L + S and one having I = L – S, especially if the latter has a small resultant moment as in the case of $p_{1/2}$ and $d_{3/2}$ proton states. The hypothetical case of perfect spin and orbital moment cancellation was invoked, where variation of the electron wave-function over the nucleus will give rise to a non-zero hyperfine interaction and hence an infinite Bohr-Weisskopf effect and hyperfine anomaly.

In order to be aware of any potentially more important cases where the hyperfine anomaly correction may be significantly greater than the experimental error, it would be valuable to survey the whole range of measured moments to seek such cases and, if possible, to make a best estimate of the correction. It is not likely that a more general attempt to estimate the correction is worthwhile at this time, given the reported experience of difficulty in obtaining agreement with existing anomaly measurements.

The fact that the magnitude of the anomaly between any pair of nuclear states depends not only upon their moment distribution but also upon the fractional contact term contribution to the hyperfine interaction was recognized. Not only does this render the correction variable between different electronic states, as referred to by the Convenor, J. Persson, but also produces differences in the anomaly between different solid state systems. Examples were cited where this has been used to separate s-electron and non-s-electron hyperfine interactions in ferromagnetic metals.

Discussion-Actions

The basic points that emerged from the discussion were that

i) hyperfine anomalies are of the order of 0.1 – 1% and therefore smaller than the precision of the measurements themselves in many cases. However, in cases where they are comparable with the precision of the measurements, they should be estimated and taken into account.

ii) Cases where hyperfine anomalies are expected to be significant can be identified by a change in the single particle configuration between a state of spin I = L+S and one having I = L – S.

iii) Nuclear structure models can also be invoked to calculate the hyperfine anomaly. Cases where different models give sizeable hyperfine anomalies should also be considered for corrections.

Action 6 (Persson): to survey the table of magnetic dipole moments (INDC(NDS)-0658) and flag those cases where BR effect may be non-negligible and should be considered. **Estimated deadline: August 2017**

Action 7 (Persson and Bissell): to survey the table of magnetic dipole moments (INDC(NDS)-0658) and flag those cases where BW effect could be significant and merit further investigation, i.e. additional measurements, improvement of accuracy. **Estimated deadline: end of 2017**

Action 8 (Persson): to provide the IAEA with the table of isotopes for which experimental evidence of significant BW effect exists. **Deadline: end of meeting**

5.3 Measurements on short-lived excited states, Convenor: A.E. Stuchbery

Recoil in Vacuum, Static-Field and Transient-Field measurements

Evaluation of TDRIV or RIV/D

About 20 cases up to Z = 12. Overall, these TDRIV data can be accepted at face value, particularly if at least one period is observed.

Evaluation of RIV

Most RIV measurements are recent work from HRIBF, Oak Ridge National Laboratory, on Sn and Te isotopes, especially on excited states of radioactive beams. All are referenced to radioactivity measurements on the Te isotopes via transient-field measurements. The papers report $g\tau$ or $g^2\tau$, so re-evaluation for new lifetimes would be straight forward. Evaluation of a change in calibration g factors, however, would require specialist knowledge, but uncertainties in field-calibrations are generally small cf. the error on these radioactive beam g-factor measurements. Need for revision is not likely in the near future, so these measurements can in all likelihood be adopted as reported.

Evaluation of Radioactivity IPAC

These measurements can vary widely. We therefore need to set criteria for selecting or rejecting IPAC data. Matters of relevance include: sample preparation and annealing, impurity concentration, impurity sites and alloy formation between impurity and host, the magnitude of the polarizing field, and whether Ge or NaI detectors were used to measure the perturbed angular correlation.

Critique and Evaluation of IMPAC (Static field)

These measurements were designed as an in-beam version of the IPAC, using simultaneous excitation and implantation of impurity nuclei into a ferromagnetic host by a nuclear reaction, usually Coulomb excitation. It was discovered in 1968 that there is in fact a combined transient- and static-field precession effect, which can sometimes add and sometimes (partially) cancel. After 1975 the method was largely replaced by the transient-field method. Results from the IMPAC method must be treated with a high degree of caution. A major concern is the existence of pre-equilibrium effects after ion implantation, which may last for 5 to 10 ps. These measurements were included in the early transient-field parametrizations – before the existence of pre-equilibrium effects in the static field had been identified – clearly they should not be relied upon for TF calibration. Critical IMPAC cases for TF calibration are ^{56}Fe and ^{82}Se.

Nevertheless, we can distinguish cases where the IMPAC data can be used. On one hand, if the static field contribution is negligible, the measurement can be treated as a transient-field measurement. On the other hand, if the static field dominates and $\tau \gg 10$ ps, the measurement can be treated as a static field measurement like IPAC.

We also need to distinguish in-beam IMPAC from implantation followed by decay, which is like the radioactivity method (i.e. pre-equilibrium effects associated with the ion implantation are not applicable).

Evaluation of Transient Field Measurements

As noted in the introduction, the TF method is excellent for relative g-factor measurements. The issues we have to face in evaluation concern the absolute g-factor values, and particularly the accuracy of the various ‘global’ parametrizations. These parametrizations of the transient-field strength in terms of the velocity and Z of the ion were introduced in the early 1980s and have been widely used since. The parametrizations that have survived are: (i) the ‘linear’ parametrization, introduced by Eberhardt et al in 1977, which has the TF strength increase linearly in both velocity and Z. It is still used in a modified form by the Bonn group (Speidel et al.); (ii) the Rutgers parametrization has a near square-root dependence on ion velocity but retains a near linear dependence on Z; the Chalk-River parametrization likewise retains a strict dependence on Z and modifies the linear velocity dependence by multiplying by an exponential factor which decreases as the ion velocity increases. Despite their differences, the 3 parametrizations (Rutgers, Bonn, Chalk River) are broadly in agreement with each other.

Several problems with attempts to parametrize the TF strength can be noted: (i) There is good calibration data for $82 > Z > 46$, but for $12<Z<46$ the data from IMPAC measurements need to be re-evaluated if not discarded, (ii) For iron hosts discontinuities in the TF strength have been found. These occur at low ion velocities (about $2v_0$) when the 1s, 2s, 3s, or 4s shell of the moving ion matches the energy of the 2p orbit in iron. The most complete data on this effect are for the 1s orbit (between O and F) and for the 4s orbit (between Os and Ir/Pt). Fortunately the effect is not applicable for gadolinium hosts, and most g-factor measurements have used gadolinium hosts (Broadly speaking level matching effects do not occur because the level-matching conditions are outside the velocity range relevant to experiments), (iii) Parametrizations based largely on iron-host data can fail when extrapolated to gadolinium. For example the TF strength for Pd ions in gadolinium is a factor of 1.4 times the Rutgers parametrization (This difference might arise from the atomic level matching of the ion 3s orbit with the iron 2p as noted in the previous point), (iv) Generally ANU and Rutgers have agreed when they happened to measure the same ion-host combination under similar experimental conditions. This statement can be generalized to other groups too. However ANU could not reproduce the Chalk River parametrization on the ^{169}Tm case which CR used to establish their parametrization. It was speculated that this difference might stem from the fact that CR calculated rather than measured their angular correlations.

The following questions were proposed in anticipation of the formulation of a set of guidelines and policies for evaluating TF measurements:

i) Was it a thick-foil (IMPAC) or thin-foil measurement?
ii) If thin-foil, did the recoils all get out of the ferromagnetic layer (typically, was $v > \sim 2 v_0$)?
iii) What was the TF calibration?

iv) If relative to an independently known g factor – OK (if same/neighbouring Z and not near one of the danger zones for iron hosts).

v) If relative to a parametrization – the measurement needs further scrutiny.

vi) The evaluator must check if the authors included the TF strength uncertainty in the quoted g factors. If the level is very short lived (< 1 ps) – hence lifetime dependent, it may need revision to be consistent with the lifetime in ENSDF.

As a general task, we must evaluate the uncertainty associated with the TF parametrization. We need to develop a policy/method to present data with appropriate uncertainties, perhaps separating statistical and systematic errors.

Comment on averaging

Discussion was opened on procedures and policies for averaging data, in anticipation of this being essential for a large fraction of the IPAC and transient-field measurements.

Notes regarding contribution on calibration problems in TF measurements, N.J. Stone

The problem relating to the lack of any theory and the existence of multiple empirical calibrations of the TF acting at nuclei in ions moving through ferromagnetic metals is central to attempts to produced recommended values of magnetic moments of many short-lived excited states. This contribution discussed the difficulty of establishing any improved uniform calibration as explored by an attempt made some years ago. More details are to be seen in the slides and are available. The work should be checked but the conclusions are likely to stand. In some areas a local standard exists which reduces the dependence upon the adopted calibration, but this is not always the case. As noted above, some of these results show little or no allowance for uncertainty in the TF fields based on the adopted calibration.

The essential problem is the low number and limited quality of existing input reference moment data, necessary to underpin the relationship between the TF field and the nuclear g-factor/magnetic moment. These input data are mainly from IMPAC or IPAC experiments of limited accuracy which are themselves subject to limitations of reliability because of their integral nature. The work on setting up the calibrations was done around 1980 (refs in slides). Here reference is made to the Rutgers calibration, but equivalent comment could be made concerning the others from Chalk River and Bonn. All were bold attempts to set their work on a better footing, but now, nearly 40 years later, some examination and possible re-evaluation is needed.

The work done by two Oxford students under my direction in 2005 was to use the Rutgers calibration to estimate the rotation to be observed in a series of published experiments and compare their results with the reported observations. What was found was a wide scatter with an RMS deviation of close to 20%. This scatter was found both using the data available to the experimenters who set up the adopted calibration in 1980 and the larger number of input data available in 2005. In very few cases did the prediction and observation agree within 10%.

Very similar scatter and RMS deviation figures were found when the same analysis was made using the Chalk River calibration.

It is also relevant to point out that whilst the Rutgers group have used the same calibration, with the same parameters, to describe TF in Fe and Gd host, the Chalk River group report finding a 42% difference between the fields experience in the two metals under the same experimental conditions.

This analysis serves to emphasize the need to undertake a full appraisal of results which depend, to varying degrees, upon the adopted calibrations of the TF field.

Discussion-Actions

Action 9 (Stuchbery and Stone): to pick out cases that probably do not require close scrutiny and can be accepted as they are. **Deadline: May-June 2017.**

Action 10 (Stuchbery and Stone): to quantify the uncertainty on the parameterization in TF method and see whether an improved parameterization is feasible. **Deadline: end of 2017.**

Action 11 (Stuchbery): to look into more detail in the evaluation of first 2+ states for consistent treatment of TF and IPAC methods, including updating half-lives (Kondev). **Deadline: April 2018.**

Action 12 (Stuchbery): to look into higher excited states and odd-A nuclei (short-lived states) (for TF method), including updating half-lives (Kondev). **Deadline: June 2018.**

Action 13 (Stuchbery and Stone): to follow up on those cases that require some attention and do not fall under above Actions 10-12, including updating half-lives (Kondev). **Deadline: tbd.**

Action 14 (Neyens): to contribute to the evaluation of beta-NMR data after they have been corrected (accordingly). **Upon request.**

Action 15 (Neyens and Bissell): to advise on cases of Laser Spectroscopy measurements that require special attention. **Upon request.**

Action 16 (Persson): bring Ekstrøm in contact with Stone to advise on Atomic Beam Magnetic Resonance measurements. **After meeting.**

5.4 Electric Quadrupole Moments, Convenor: P. Pyykkö

The list of 16 elements for which new data have become available since the last evaluation by Pyykkö [5.7] is given in the table below. (Note that not all the results for Au are listed in the table below).

Reference	**Element**	**QEM (mb)**	**IAEA Tables (INDC(NDS)-0658) (mb)**
2009: Yakobi et al., CJC 87, 802.	Ga-69	174(3)	molecular 171(2)
	In-115	772(5)	molecular 770(8)
2010: Demovic et al., CPL 498, 10.	As-75	311(2)	314(6)
2010: Haas et al., HI 198, 133.	Zn, Cd	Review (Solids)	
2010: Pavanello et al., PRA 81, 042526.	H-2	2.85783(30)	2.860(15)
2011: Itkin et al., TCA 129, 409.	La-139	206(4)	molecular 200(6)
	Pb-197	347(15)	
2012: Haiduke, CPL 544, 13.	Hf-179	HfO, HfS 3750(37)	muonic 3793(33)
2012: Singh et al., PR A 86, 032509	K-39	61.4(6)	58.5
2012: Arcisauskaite et al., PCCP 14, 2651	Hg-199	675(12)	
2013: Chaudhuri et al., JPC A 117, 12616	Cl-35	-81.12	-81.65(80)
	Br-79	307.98	313(3)
	I-127	-688.22	-696(12)
2013: Stopkowicz	Br-79	308.7(20)	313(3)
2007: Yakobi	I-127	-680(10)	-696(12)
2013: Safronova, PR A 88, 060501	Th-229	3110(60)	
2013: Sahoo et al.	Ba-135	153(2)	160(3)
2013: Teodoro et al., PR A 88, 052504	Bi	-420(8)	-516(15) [Pyykkö, Mol. Phys. 106 (2008) 1965]

2014: Santiago et al., PCCP 16, 11590	Cu-63	-198(10)	muonic: -220(15), 211.4.
2014: Stopkowicz et al., PR A 90, 022507	S-33	-69.4(4)	-67.8(13)
2015: Sahoo, PR A 92, 052506	Fr-211	-210(20)	-190(30)
2015: Quevedo, PR A 91, 032516	K-39	60.3(6)	58.5 [Pyykkö, Mol. Phys. 106 (2008) 1965]
2015: Santiago et al., PR A 91, 042516	Au-197	515(15)	
2015: Frömmgen et al., EPJ D. 69, 164	Cd isotopes		
2016: Canella et al., CPL 660, 228	Xe-131	-114.6(1.1)	-114(1) [Kellö, et al, Chem. Phys. Lett. 346 (2001) 155.]
2016: Cassassa eta l., PCCP 18, 10201	Fe-57*	130	160 [Pyykkö, Mol. Phys. 106 (2008) 1965]
2016: Clément et al., PRL 116, 022701	Sr-96,-98		
2016: Errico et al., JPC C 120, 23111	Cd-111*, 245 keV, 5/2+	760(20)	-850(90), 740, 800 etc.

Discussion-Actions

The differences observed between the new measurements and the values included in the Tables of QEMs published by Stone (2015) [5.1] clearly indicate that these isotopes merit a further review and a new evaluation.

Action 17 (Stone): to provide to Pyykkö the list of disconnected sequences of QEMs and together with Pyykkö explore possibility of linking them to primary standards. **Deadline: end of 2017.**

Action 18 (Pyykkö): to update the 2008 evaluation of reference isotopes and to extend to include all available data on new isotopes. This will be limited to ground-states of stable isotopes and particular excited states. **Estimated deadline of preliminary draft: end of 2017.**

5.5 Other

The importance of spins of ground- and excited states in the determination of nuclear moments in certain cases was emphasized. As a result an action was placed on F. Kondev.

Action 19 (Kondev): to provide table of states with directly measured spins. **Deadline: by end of June 2018.**

Action 20 (Mertzimekis): to introduce ENSDF half-lives, spins-parities and energies of g.s. and excited states in the on-line Nuclear Moments Database, and two more fields: one for sending feedback and one for listing updates**. Deadline: By the end of 2017.**

Action 21 (IAEA-NDS): to make the Nuclear Moments Online Database more visible and accessible to the user community.

Action 22 (Dimitriou (IAEA)): to follow up progress of all actions listed above at regular intervals and ensure smooth and timely progress of the coordinated effort of establishing tables of recommended moments. **At regular intervals.**

Action 23 (All): Meeting participants to cite the meeting and meeting report in their future publications or conference presentations where it is relevant as indicated below:
[x] Summary Report of the IAEA Consultancy Meeting on Evaluation of Nuclear Moments, 27-30 March 2017, IAEA report INDC(NDS)-0732, Vienna 2017. (hyperlink)

References

[5.1] N.J. Stone, Tables of Nuclear Magnetic Dipole and Electric Quadrupole Moments, IAEA report INDC(NDS)-0658; Vienna (2014), N.J. Stone, Table of Nuclear Electric Quadrupole Moments, IAEA report INDC(NDS)-0650, Vienna (2013); N.J. Stone, Tables of nuclear magnetic dipole and electric quadrupole moments, ADNDT 90 (2005) pp 75-176.

[5.2] A. Antušek, M. Sulka, Chem. Phys. Lett., 660 (2016) 127 and references therein.

[5.3] R.K. Harris, et al., NMR Nomenclature. Nuclear Spin Properties and Conventions for Chemical Shifts (IUPAC Recommendations 2001), Pure Appl. Chem. **73/11** (2001) 1795.

[5.4] F.D. Feiock and W.R. Johnson, Phys. Rev**. 187** (1969) 39.

[5.5] W. Nierenberg & D. Brink, J. Phys. Radium **19**, 826 (1958).

[5.6] H.T. Duong et al., Nucl. Instr. and Meth. A**325 (1993)** 465.

[5.7] P. Pyykkö, Mol. Phys. **106** (2008) 1965.

6. Conclusions

The meeting reviewed the status of measurements of nuclear magnetic and quadrupole moments, in regards to the required corrections for the effect of diamagnetism, hyperfine anomaly (charge and magnetism), the half-life of the short-lived excited states, the parameterizations of the transient field adopted in transient-field methods.

Participants acknowledged that the improvements in quantum mechanical calculations and the treatment of various corrections have a significant impact on the precision of the determined nuclear moments. They agreed that the widely used compilations of experimental nuclear moment measurements produced by N.J. Stone under the auspices of the IAEA [5.1] need to be evaluated, taking into account all the necessary corrections, in order to produce a definitive table of recommended values. Details of the corrections and their implementation were presented in the four sessions dedicated to diamagnetism, hyperfine anomaly, short-lived excited states and electric quadrupole moments. Participants discussed the necessary steps that need to be taken to incorporate the corrections and evaluate the data in the compilation tables, and specific tasks were assigned.

Given the nature of the corrections and expertise required to produce tables of evaluated, recommended nuclear magnetic and quadruple moments, this work can only be carried out with significant contributions from an international group of experts in many fields of hyperfine interactions. This international effort would benefit from the coordination of the International Atomic Energy Agency.

APPENDIX I

List of Actions

Task	On	Timeline / Deadline
No. 1	Jackowski, Stone	May-June 2017
	replace old NMR measurements that were inconsistent with the more consistent and precise values from gas-phase NMR measurements performed by the Polish group (list nuclides).	
No. 2	Jackowski (in consultation with Stone)	May-June 2017
	consult with Antušek on validity of results for liquid phase NMR and ab initio calculations, especially regarding the large uncertainties, to decide whether these data should also be added to the tables.	
No. 3	Jackowski	By the end of 2017
	go through the beta-NMR measurements (to be provided by Stone) and explore possible ways to introduce diamagnetism corrections, where needed.	
No. 4	Stone	By the end of 2017
	look into the TDPAC/PAD measurements which may require corrections for diamagnetism and Knight shift, and single out those that need to be further treated for these corrections, and refer them to Jackowski.	
No. 5	Stone	May-June 2017
	investigate the possible methods of introducing Knight shift corrections (Chalk River publications, contact J. Beene, D. Ward).	
No. 6	Persson	August 2017
	survey the table of magnetic dipole moments (INDC(NDS)-0658) and flag those cases where BR effect may be non-negligible and should be considered.	
No. 7	Persson and Bissell	By the end of 2017
	survey the table of magnetic dipole moments (INDC(NDS)-0658) and flag those cases where BW effect could be significant and merit further investigation, i.e. additional measurements, improvement of accuracy.	
No. 8	Persson	At conclusion of this meeting
	provide the IAEA with the table of isotopes for which experimental evidence of significant BW effect exists.	
No. 9	Stuchbery and Stone	May - June 2017
	pick out cases that probably do not require close scrutiny and can be accepted as they are.	
No. 10	Stuchbery and Stone	By the end of 2017
	quantify the uncertainty on the parameterization in TF method and see whether an improved parameterization is feasible.	
No. 11	Stuchbery	By April 2018
	look into more detail in the evaluation of first 2+ states for consistent treatment of TF and IPAC methods, including updating half-lives (Kondev).	

No. 12	Stuchbery	By June 2018	look into higher excited states and odd-A nuclei (short-lived states) (for TF method), including updating half-lives (Kondev).
No. 13	Stuchbery and Stone	To be discussed	follow up on those cases that require some attention and do not fall under above Actions 10-12, including updating half-lives (Kondev).
No. 14	Neyens	Upon request	contribute to the evaluation of beta-NMR data after they have been corrected (accordingly).
No. 15	Neyens and Bissell	Upon request	advise on cases of Laser Spectroscopy measurements that require special attention.
No. 16	Persson	After this meeting	bring Eckstrøm in contact with Stone to advise on Atomic Beam Magnetic Resonance measurements.
No. 17	Stone	By the end of 2017	provide to Pyykkö the list of disconnected sequences of QEMs and together with Pyykkö explore possibility of linking them to primary standards.
No. 18	Pyykkö	Preliminary draft by the end of 2017	update the 2008 evaluation of reference isotopes and to extend to include all available data on new isotopes. This will be limited to ground-states of stable isotopes and particular excited states.
No. 19	Kondev	By end June 2018	provide table of states with directly measured spins.
No. 20	Mertzimekis	By the end of 2017	introduce ENSDF half-lives, spins-parities and energies of g.s. and excited states in the on-line Nuclear Moments Database, and two more fields: one for sending feedback and one for listing updates.
No. 21	IAEA NDS		make the Nuclear Moments Online Database more visible and accessible to the user community.
No. 22	Dimitriou	At regular intervals	follow up progress of all actions listed above at regular intervals and ensure smooth and timely progress of the coordinated effort of establishing tables of recommended moments.
No. 23	All	Continuous	cite the meeting and meeting report in their future publications or conference presentations where it is relevant.

APPENDIX II

Consultants' Meeting on

Evaluation of Nuclear Moments

27-30 March 2017

G0E85, IAEA Headquarters, Vienna, Austria

PROVISIONAL AGENDA

Monday, 27 March

09.00	Welcome and opening remarks	NDS Section Head
	Administrative matters	Dimitriou/Lidija
	Election of Chairman/Rapporteur	
	Adoption of Agenda	
09.15	*Objectives and outline of the meeting*	Dimitriou (15')
09.30 – 12.30		
	Table of recommended nuclear moments - what needs to be done	Stone (20')
	Online Database	Merztimekis (10')
	Spins and magnetic moments	Kondev (15')
	Nuclear Magnetic Dipole Moments from Gas Phase NMR Spectra	Jackowski (10')
	Hyperfine anomaly from an atomic physics view	Persson (10')
	Nuclear quadrupole interactions	Pyykkö (10')
	The challenge of short-lived states	Stuchbery (10')
	Collinear Laser spectroscopy at ISOLDE	Bissell (10')
	(Coffee break as needed)	

Session 1: The most precise moments.

	Corrections for diamagnetism	
	Introduction	Jackowski (30'+)
	Other contributions:	
	Corrections concerning applied fields in other techniques	Stone
	Discussion	
	(Coffee break as needed)	
12.30 – 14.00	Lunch	
14.00 – 17.30	**Session 1 cont'd**	

Tuesday, 28 March

09.00 – 12.30 **Session 2**

Methods to study moments and radii of long-lived (> 1 ms) and stable isotopes and isomers

Neyens (10')

Session 2: The hyperfine anomaly

Potential for, and interest in making, correction for this effect

Introduction	Persson (30'+)
Other contributions:	
Hyperfine anomalies in Bi	Bissell
Hyperfine anomalies in atoms and metals: experiments on Au isotopes	Stone
Discussion	

(Coffee break as needed)

12.30 – 14.00 Lunch

14.00 – 17.30 Continue session 2 / start session 3

Session 3: Measurements on short-lived excited states

Recoil in Vacuum, Static-Field and Transient Field measurements

Introduction	Stuchbery (30'+)
Other contributions:	
Calibration problems in the TF method	Stone
Discussion	

(Coffee break as needed)

19.00 Dinner at local restaurant

Wednesday, 29 March

09.00 – 12.30 **Session 3 cont'd**

Contributions regarding aspects of measurement of excited state moments

Other methods TDPAC, TDPAD, IPAC, Mossbaur effect …

Discussion

(Coffee break as needed)

12.30 – 14.00 Lunch

14.00 – 17.30 **Session 4: Nuclear electric quadrupole moments**

Introduction	Pyykkö (3030'+)
Other contributions:	
Evaluation of quadrupole moments in the sd-shell quadrupole moments of ^{8,9}Li isotopes	Neyens
Problem elements and secondary standards in Q extraction	Stone

Quadrupole interactions in 'cubic' ferromagnets – *a complication in NMR/ON'*	Stone
Discussion	

(Coffee break as needed)

Thursday, 30 March

09.00 – 12.30 Start wrap-up session with summaries

Session 1	Jackowski (30')
Session 2	Persson (30')
Session 3	Stuchbery (30')
Session 4: What is needed for QEM?	Pyykkö (30')

Discussion regarding next steps, actions and those involved.

(Coffee break as needed)

12.30 Closing of the meeting.

APPENDIX III

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Evaluation of Nuclear Moments

27-30 March 2017
G0E85, IAEA Headquarters, Vienna, Austria

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Presentation links

#	Author	Title	Link
1	M. Bissell	COLLINEAR LASER SPECTROSCOPY @ ISOLDE	PDF
2	M. Bissell	Bismuth at COLLAPS - An anomalous beam time	PDF
3	P. Dimitriou	Meeting on Evaluation of Nuclear Moments - Introduction	PDF
4	K. Jackowski	Nuclear Magnetic Dipole Moments from Gas Phase NMR Spectra	PDF
5	K. Jackowski	Nuclear Magnetic Dipole Moments from Gas Phase NMR Spectra(II)	PDF
6	K. Jackowski	Nuclear Magnetic Dipole Moments	PDF
7	F. Kondev	Directly Measured Spins & Nuclear Moments	PDF
8	T. Mertzimekis	The IAEA online database for nuclear EM moments	PDF
9	G. Neyens	Commonly used methods to study moments of exotic isotopes/isomers	PDF
10	G. Neyens	Evaluation of quadrupole moments: 1. the Li isotopes 2. the sd-shell nuclei	PDF
11	G. Neyens	Evaluation of quadrupole moments: 1. the Li isotopes 2. the sd-shell nuclei	PDF
12	J. Persson	Hyperfine Anomaly: A long and winding road	PDF
13	J. Persson	Hyperfine Anomaly: From an Atomic Physics View	PDF
14	J. Persson	Hyperfine Anomaly: Summary of hfa session	PDF
15	P. Pyykko	NUCLEAR QUADRUPOLE INTERACTIONS: A PERSONAL ITINERARY	PDF
16	P. Pyykko	NUCLEAR QUADRUPOLE MOMENTS: WHICH CHANGES SINCE 2008	PDF
17	N. Stone	Meeting to discuss preparation of recommended values of nuclear magnetic dipole [and electric quadrupole] moments	PDF
18	N. Stone	Corrections concerning applied fields in other techniques	PDF
19	N. Stone	Bohr-Weisskopf Effect and Hyperfine anomaly	PDF
20	N. Stone	Calibration Problems in Transient Field Measurements	PDF
21	N. Stone	Nuclear electric Quadrupole Moments: Problem elements and secondary standards	PDF
22	N. Stone	Quadrupole Interaction in ‘cubic’ ferromagnetic metal samples: a consideration in NMR/ON analysis	PDF
23	A. Stuchbery	Excited-state moments: the challenge of short-lived states. Introduction	PDF
24	A. Stuchbery	Excited-state moments: the challenge of short-lived states	PDF
25	A. Stuchbery	Excited-state moments: the challenge of short-lived states. Summing Up & Guidelines	PDF

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