Recommended Values of nuclear moments: the input from improved calculation involving multi-electron configurations.

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IAEA
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The Project

In ~ 1995 Dick Meyer requested I undertake to provide listings of recommended values of nuclear magnetic dipole and electric quadrupole moments.

Confession

Only in 2020 was this objective achieved!

Why did it take so long and what is the current position?
Tabulations of Measurements vs Recommended Values

Tabulation

A listing of published results – a useful resource for researchers.

Recommended values

Give a single number as being the best estimate we have of the true value.

This imposes a duty on the reviewer to select/average available results and update where necessary.
Outline

Electric quadrupole moments
1. Review of situation:
   Updated Table published in 2019.
2. Major changes and problem elements

Magnetic dipole moments
1. What’s involved: measurements and corrections
2. Reference moment values
   Tables published in 2019-21
4. Very recent developments
Electric Quadrupole Moments

TABLE OF NUCLEAR ELECTRIC QUADRUPOLE MOMENTS

Issued October 2021: references to April 2021. Recommended values only.
Changes and problem elements

All Table entries have been adjusted to the adopted standards wherever necessary. Often these changes are very minor, but in some cases they are not:

1. Values
2. Uncertainties
3. Problems
1. Values.

Elements for which **new efgs have produced considerable change** in the extracted quadrupole moments as **compared to most recent previous listing [N.J.S. IAEA 2011]**.

<table>
<thead>
<tr>
<th>Element</th>
<th>Change from 2011 listing (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>-22</td>
</tr>
<tr>
<td>Ca</td>
<td>-26.1</td>
</tr>
<tr>
<td>Ge</td>
<td>+15.3</td>
</tr>
<tr>
<td>Se</td>
<td>-30.9</td>
</tr>
<tr>
<td>Sr</td>
<td>-7.6</td>
</tr>
<tr>
<td>In</td>
<td>-5.1</td>
</tr>
<tr>
<td>Sn</td>
<td>+25.7</td>
</tr>
<tr>
<td>Sb</td>
<td>+52</td>
</tr>
<tr>
<td>Cs</td>
<td>-6.0</td>
</tr>
<tr>
<td>Ba</td>
<td>+9.6</td>
</tr>
<tr>
<td>Gd</td>
<td>-5.0</td>
</tr>
</tbody>
</table>
2. Uncertainties

Elements for which recent improved efg calculations have reduced uncertainties by a substantial factor.

<table>
<thead>
<tr>
<th>Element</th>
<th>Error reduction factor</th>
<th>Element</th>
<th>Error reduction factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.10 (i.e x 10)</td>
<td>Sr</td>
<td>0.10</td>
</tr>
<tr>
<td>F</td>
<td>0.25</td>
<td>In</td>
<td>0.4</td>
</tr>
<tr>
<td>Ge</td>
<td>0.03</td>
<td>Sn</td>
<td>0.7</td>
</tr>
<tr>
<td>Se</td>
<td>0.14</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Exception to minimum uncertainty

The quadrupole moment of the deuteron has been recently recalculated using new methods to estimate the efg in HD and D$_2$ molecules, the result

\[ Q(2H) = +0.0028578(3) \]

compared to the previous best \(+0.00286(2)\)

claims accuracy of **0.01%** and uncertainty reduced by a factor of **50**.

3. Elements for which adopted efg inaccuracy causes large (>9%) quadruple moment uncertainty.

<table>
<thead>
<tr>
<th>Element</th>
<th>Error (%) in best efg value</th>
<th>Element</th>
<th>Error (%) in best efg value</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>20</td>
<td>Sm</td>
<td>10</td>
</tr>
<tr>
<td>Cr</td>
<td>33</td>
<td>Rn</td>
<td>10</td>
</tr>
<tr>
<td>Zn</td>
<td>10</td>
<td>Ac</td>
<td>12</td>
</tr>
<tr>
<td>Nd</td>
<td>10</td>
<td>Th</td>
<td>21</td>
</tr>
<tr>
<td>Pm</td>
<td>27</td>
<td>Es</td>
<td>12</td>
</tr>
</tbody>
</table>

Recall also

Elements **without adopted standards** are;

**Si, P, Cd, Te, Ce, Tm, W, Pt, Po, At.**

All of these 20 elements have some problems or conflicts and would benefit from detailed theoretical effort.
Magnetic dipole moments
Magnetic dipole moments – some basic statistics

The NJS INDC(NDS)-0658 (2014) report contained results on ~2200 magnetic moments of nuclear states.

longer lived:

- Laser Resonant spectroscopy 547
- NMR on LT oriented nuclei 143
- Atomic beam resonance 106
- Conventional NMR (stable isotopes) 103
- Integral NO 56
- Mossbauer Effect 54
- Optical Pumping 32

shorter lived:

- TDPAC/TDPAD 446
- Integral PAC 218

Less than 10^-8 s

- Transient Field 393
- Recoil in Vacuum 46

Several methods offer results to 1 in 10^3 or better so small corrections are important.
Hierarchy of Reference Moments.

Moment values obtained by ratio with ‘fundamental reference’ moment’ which is used to establish the strength of a magnetic interaction, internal or applied field.

Different element data adopt as their fundamental reference moment:

- the proton moment
- the deuteron moment
- 11B
- 14N
- 17O
- 19F
- 23Na
- 35,37Cl
- 39K
- 45Sc
- 129Xe
- 137Ba

For each element a secondary (stable) reference moment is then chosen: results on isotopes from measured ratio to that chosen.

All these reference isotopes have quoted/author’s moment errors < 2 in 10^6 in 2014 Tabulation

Most precise is the proton: 3 in 10^9
Corrections to raw experimental data.

Focus on the diamagnetic correction which is required when a ‘known’ magnetic field is applied to the material in which the experimental nuclei are situated.

The most accurately measured results [NMR and atomic beam resonance] require this correction.

The correction is also known as the chemical shift particularly in liquid and gaseous samples.
Diamagnetic corrections since the 1940’s

1941  Willis Lamb, Phys Rev 60 817 found 0.0000319Z^4/3 giving 12% at Z = 80.
       N  1.000332  0.03%
       Ba 1.005549  0.5%
       Pb 1.017200  1.7%

1976  Gladys Fuller used Dickinson results in her tabulation allowing 10% error.
1989  Pramila Raghavan adopted Feiock and Johnson values, with no errors, for her ADNDT Moment Table.
2014  NJS in listings to 2014 followed the Raghavan practice.

This treatment resulted in an abundance of disturbing discrepancies in apparently highly accurate measurements by different groups and methods. Recommended values???
Diamagnetic factors from Feiock and Johnson (1969).

-the best available at the time of many measurements.

Valid only for closed sub-shell ions but used in chemical compounds, liquids, gases ..... 

Many NMR results claim to give results accurate to a few times $10^{-4}$ or (much) better. Requiring a diamagnetic correction of 1000 ppm to be accurate to better than 10%.
The diamagnetic correction is a multi-electron computation problem.

Comparable to electric field gradient calculations for electric quadrupole moments. Smaller but no less important for the most accurate results.

Great strides in such calculations have been possible in the last 10-15 years.

Effects are small, precision is difficult even with best methods. Problem is being tackled, easier (lighter) elements first.

32 elements recognised results (2019)

Gurus: Karol Jackowski and his Warsaw group [i.e. Antusek et al Chem Phys Lett 532 1 (2012) and later].
Changes produced by state-of-the-art screening calculations.

Examples in light, medium and heavy nuclei.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Correction</th>
<th>Moment</th>
</tr>
</thead>
<tbody>
<tr>
<td>F+J 7 N 14</td>
<td>1.000332</td>
<td>+0.40376100(6)</td>
</tr>
<tr>
<td>New</td>
<td>1.000224(5)</td>
<td>+0.403573(2)</td>
</tr>
<tr>
<td>F+J 56 Ba 137</td>
<td>1.007564</td>
<td>+0.937372(2)</td>
</tr>
<tr>
<td>New</td>
<td>1.00685(21)</td>
<td>+0.9375(2)</td>
</tr>
<tr>
<td>F+J 82 Pb 207</td>
<td>1.0172</td>
<td>+0.592583(9)</td>
</tr>
<tr>
<td></td>
<td>1.0129(13)</td>
<td>+0.5906(4)</td>
</tr>
</tbody>
</table>

Adjustments in 3rd/4th digit compared to precision of expt measurement $10^{-8}$!

Results: Moments are smaller and errors much larger.

Discrepancies shown to be related to differing samples.

Johnson and Feiock corrections generally too large by $\sim 25\%$. 
The Reference Moments

Adopted best reference moment values
(Source: K. Jackowski, at IAEA consultant meeting, 2017.) based on fully up-to-date diamagnetic corrections.)

<table>
<thead>
<tr>
<th>No</th>
<th>A</th>
<th>E</th>
<th>H</th>
<th>I</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>84</td>
<td>5 B 10</td>
<td>+1.8004636(8)</td>
<td>[3He]</td>
<td>NMR</td>
<td>JCP 130 044309 (09)</td>
</tr>
<tr>
<td>90</td>
<td>5 B 11</td>
<td>+2.688378(1)</td>
<td>[3He]</td>
<td>NMR</td>
<td>JCP 130 044309 (09)</td>
</tr>
<tr>
<td>131</td>
<td>6 C 13</td>
<td>+0.702369(4)</td>
<td>[1H]</td>
<td>NMR</td>
<td>Chem Phys Lett 411 111 (05)</td>
</tr>
<tr>
<td>153</td>
<td>7 N 14</td>
<td>+0.403573(5)</td>
<td>[1H]</td>
<td>NMR</td>
<td>Chem Phys Lett 411 111 (05)</td>
</tr>
<tr>
<td>162</td>
<td>7 N 15</td>
<td>-0.283057(1)</td>
<td>[1H]</td>
<td>NMR</td>
<td>Chem Phys Lett 411 111 (05)</td>
</tr>
<tr>
<td>195</td>
<td>8 O 17</td>
<td>-1.89354(1)</td>
<td>[1H]</td>
<td>NMR</td>
<td>Chem Phys Lett 411 111 (05)</td>
</tr>
<tr>
<td>229</td>
<td>9 F 19</td>
<td>+2.628 335(2)</td>
<td>[3He]</td>
<td>NMR</td>
<td>JCP 130 044309 (09)</td>
</tr>
<tr>
<td>436</td>
<td>14 Si 29</td>
<td>-0.555052(3)</td>
<td>[1H]</td>
<td>NMR</td>
<td>J Phys Chem A 110 11462 (06)</td>
</tr>
<tr>
<td>455</td>
<td>15 P 31</td>
<td>+1.130925(5)</td>
<td>[1H]</td>
<td>NMR</td>
<td>J Phys Chem A 115 10617 (11)</td>
</tr>
<tr>
<td>473</td>
<td>16 S 33</td>
<td>+0.64325(2)</td>
<td>[19F]</td>
<td>NMR</td>
<td>Chem Phys Lett 411 111 (05)</td>
</tr>
<tr>
<td>500</td>
<td>17 Cl 35</td>
<td>+0.82170(2)</td>
<td>[1H]</td>
<td>NMR</td>
<td>JCP 139 234402 (13)</td>
</tr>
<tr>
<td>512</td>
<td>17 Cl 37</td>
<td>+0.68400(1)</td>
<td>[1H]</td>
<td>NMR</td>
<td>JCP 139 234402 (13)</td>
</tr>
<tr>
<td>1338</td>
<td>32 Ge 73</td>
<td>-0.87824(5)</td>
<td>[1H]</td>
<td>NMR</td>
<td>J Phys Chem A 110 11462 (06)</td>
</tr>
<tr>
<td>1440</td>
<td>34 Se 77</td>
<td>+0.53356(5)</td>
<td>[1H]</td>
<td>NMR</td>
<td>Mol Phys 111 1355 (13)</td>
</tr>
<tr>
<td>1569</td>
<td>36 Kr 83</td>
<td>-0.970730(3)</td>
<td>[3He]</td>
<td>NMR</td>
<td>Magn Reson Chem 52 430 (14)</td>
</tr>
<tr>
<td>3369</td>
<td>54 Xe 129</td>
<td>-0.77796(2)</td>
<td>[3He]</td>
<td>NMR</td>
<td>Magn Reson Chem 53 273 (15)</td>
</tr>
<tr>
<td>3388</td>
<td>54 Xe 131</td>
<td>+0.69184(2)</td>
<td>[3He]</td>
<td>NMR</td>
<td>Magn Reson Chem 53 273 (15)</td>
</tr>
<tr>
<td>6221</td>
<td>82 Pb 207</td>
<td>+0.5906(4)</td>
<td>[1H]</td>
<td>NMR</td>
<td>Phys Chem Chem Phys 18 16483 (16)</td>
</tr>
</tbody>
</table>
Situation in 2019

Limited number of state-of-the-art calculations gave average reduction to 75(10)% of Feiock and Johnston corrections.
Where no new calculations existed, these reduced F+J corrections were applied, with their errors, in the 2019/20 Recommended Dipole Moment Tables.

INDC(NDS)-0794 NSR 2019STZV [states > 1ms lifetime]
and
INDC(NDS)-0816 NSR 2020STZY [states > 1 ms lifetime]

Nov 2019 ~2750 entries
Sept 2020 ~1150 entries

End of story?
Diamagnetism experts,
Nuclear Magnetic Moments
10 days ago discovered:

A. Antusek and M. Repisky  

Undetected by the NSR system (not surprisingly).

Content: state-of-the-art calculations for 24 transition metal elements with revised ‘reference’ stable dipole moments.
Transition metal element corrections compared to Feioch and Johnson. Results show significant paramagnetic effects across the d-subshells leading in some to reversal of sign of correction and requiring adjustments of as much as 2% in reference (stable) moments. This will lead to the same changes in moments of many other isotopes of these elements.

Examples:  
61Ni was -0.75002(4) now -0.7473(4)  
97Mo was -0.9335(1) now 0.9287(4)  
199Hg was +0.5058855(9) now +0.5059(5)
P.S. In addition to the published Reports the NDS On-line Moment Table already includes the Recommended Moments and the measurement listings are being updated.

Consequent upon the 24 element new reference moments many adjustments are necessary.
Nuclear electromagnetic moments form an active field of research, having multiple aspects and applications in nuclear physics and beyond.

Thank you