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

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IAEA

April 2022

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
3. Precise measurements: corrections in atoms, molecules, liquids. Solids

   Tables published in 2019-21

4. Very recent developments

Electric Quadrupole Moments

IAEA
International Atomic Energy Agency

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INDC International Nuclear Data Committee

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]**
.

Element	Change from 2011 listing (%)
F	-22
Ca	-26.1
Ge	+15.3
Se	-30.9
Sr	-7.6
In	-5.1
Sn	+25.7
Sb	+52
Cs	-6.0
Ba	+9.6
Gd	-5.0

2. Uncertainties

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

Element	Error reduction factor	Element	Error reduction factor
C	**0.10** (i.e x 10)	Sr	**0.10**
F	**0.25**	In	**0.4**
Ge	**0.03**	Sn	**0.7**
Se	**0.14**		

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.**

Ref M. Pavanello et al., Phys Rev A **81** 042526 (2010) .

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

Element	Error (%) in best efg value	Element	Error (%) in best efg value
V	**20**	Sm	**10**
Cr	**33**	Rn	**10**
Zn	**10**	Ac	**12**
Nd	**10**	Th	**21**
Pm	**27**	Es	**12**

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	12
the deuteron moment	31
11B	1
14N	2
17O	1
19F	1
23Na	6
35,37Cl	2
39K	1
45Sc	1
129Xe	1
137Ba	1

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

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

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.**

1950 **W.C.Dickinson, Phys Rev 80 563 Thomas-Fermi gave 6% at Z = 92.**

1969 **Feiock and Johnson, Phys Rev 187 39 (1969) made calculation giving**

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.

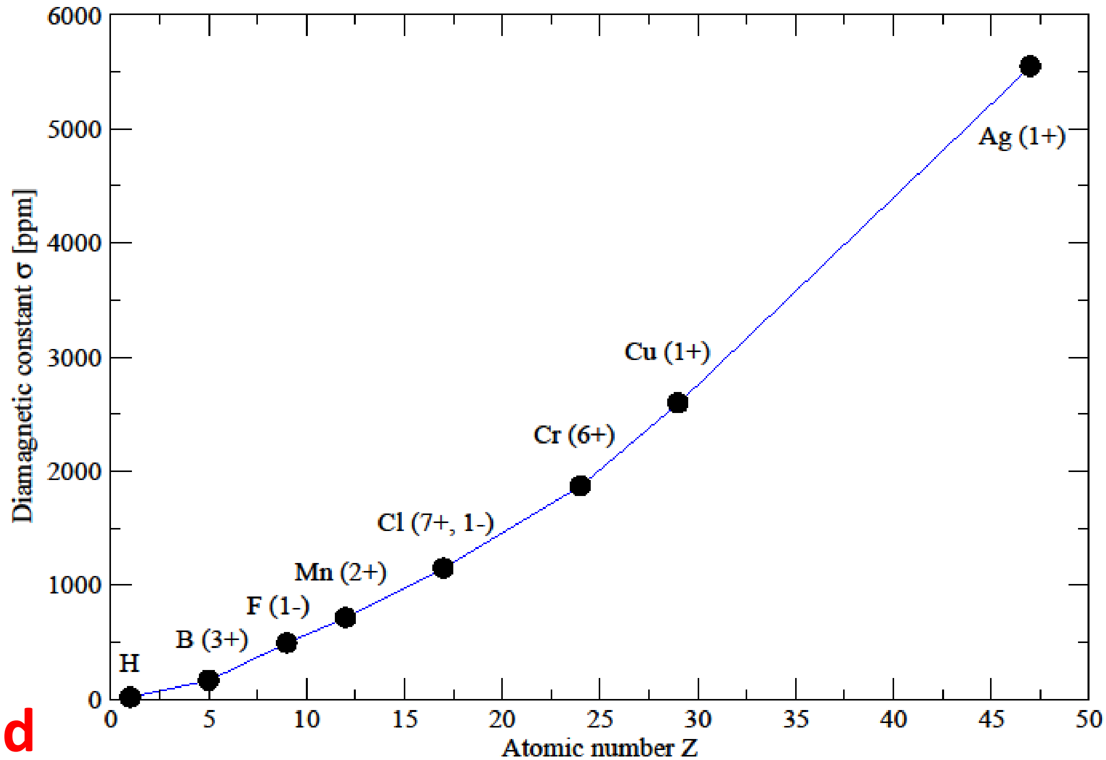
1989 Pramila Raghavan adopted Feiock and Johnson values, with no errors, for her ADNDT Moment Table.

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.

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

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 ¬ 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.)

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

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]

IAEA International Atomic Energy Agency

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TABLE OF RECOMMENDED NUCLEAR MAGNETIC DIPOLE MOMENTS:
PART I, LONG-LIVED STATES

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TABLE OF RECOMMENDED NUCLEAR MAGNETIC DIPOLE MOMENTS:
PART II, SHORT-LIVED STATES

Nov 2019 **¬2750 entries** **Sept 2020** **¬1150 entries**

End of story?

Diamagnetism experts,
Nuclear Magnetic Moments

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Cite this: Phys. Chem. Chem. Phys., 2020, 22, 7065

NMR absolute shielding scales and nuclear magnetic dipole moments of transition metal nuclei

Andrej Antušek[*a] and Michal Repisky[b]

10 days ago discovered:

A. Antusek and M. Repisky **Phys Chem Chem Phys 22 7065 (Mar 2020)**

Undetected by the NSR system (not surprisingly).

Content: **state-of-the-art calculations for 24 transition metal elements with revised ‘reference’ stable dipole moments.**

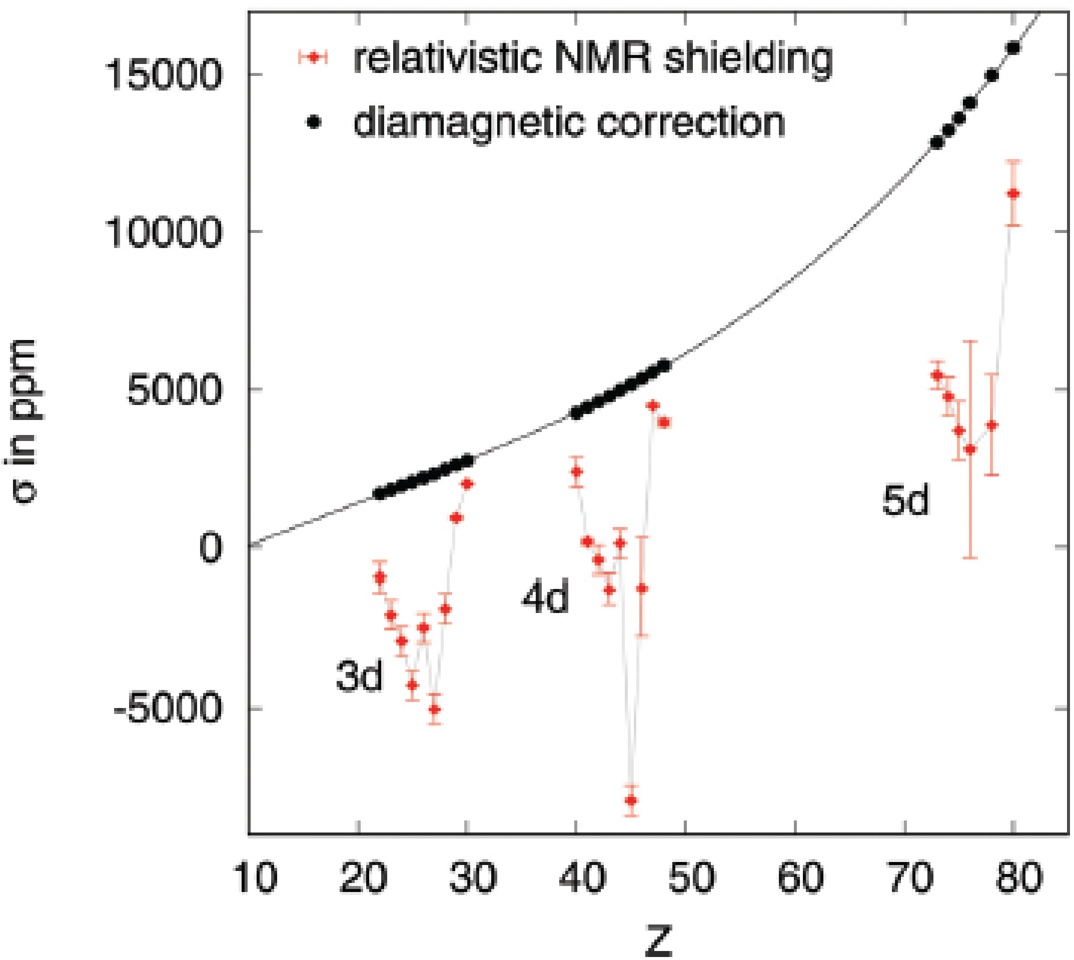
From Antusek 2020

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.

A major earthquake!



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