The Nuclear Quadrupole Moments of the 20 First Elements: High-Precision Calculations on Atoms and Small Molecules *

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The available values of the nuclear quadrupole moments for the elements H–Ca are reviewed and related to recent advances in numerical methods in quantum chemistry. For Li the quantum chemical and nuclear Coulomb scattering values now agree. For Mg, also the muonic result agrees with them. For Na and Al, the new, accurate atomic values deviate from the earlier muonic values.

1. Introduction

Nuclear quadrupole moments, Q, can be determined in several independent ways:

1. A combination of observed nuclear quadrupole coupling constants (NQCC), eqQ/h, in atoms, molecules or solids with a calculated or estimated value of the electric field gradient, q.

a) If no reliable theoretical values can be produced, a rough way is to deduce the q values from magnetic hyperfine $\langle r^{-3} \rangle$ values, or valence-only calculations. Sternheimer correction factors are then needed.

b) If the q are obtained from more fundamental calculations, allowing for deformation of core orbitals, no such corrections are needed.

2. Observation of nuclear quadrupole splittings in muonic atoms. In this case most of the field gradient comes from the muon, which simplifies the calculation of q. Corrections for finite nuclear size and nuclear polarizability are needed, however.

3. Nuclear Coulomb scattering experiments.

In principle a fourth, independent method exists:

4. Nuclear theoretical calculations. Their reliability, however, seems to be, at best, 10–20 per cent.

The "standard values" of Q, even for most of the light elements, have been surprisingly inaccurate. Their development can be followed from the compilations by Fuller and Cohen [1] in 1969, Fuller [2] in 1976, Lederer and Shirley [3] in 1978 and Raghavan in 1989 [4]. For a general discussion of the lighter nuclei, see also the reviews by Ajzenberg-Selove and others [5–7]. The 1990-91 Handbook of Chemistry and Physics contains both an up-to-date table by Holden [8] in Section 11 and a totally outdated 1967 table in Section 9!

The central point of this lecture is that considerable progress has recently been made in the method 1 b, making it one of the best sources for Q values for the lighter elements. We here review the available data for the 20 first elements.

2. A Review of the Data

Hydrogen: For deuterium, the clearly best determination remains that of Bishop and Cheung [9], based on the experimental splittings in HD and D_2. The value is $+2.860(15)$ mb (millibarn $= 10^{-31}$ m^2), the "conservative" [9] error limits coming from the theoretical calculations. An identical value was obtained earlier by Reid and Vaida [10]. The error limits are determined by the calculation of q; the experiments are more accurate.

Helium: No isotopes or nuclear states are known with $I > 1/2$ and lifetimes long enough for nuclear quadrupole coupling to be seen.

Lithium: Focussing first on ^{7}Li, Green [11] obtained in 1971 a value of $-36.6(3)$ mb using experimental splittings in the LiH molecule. This value remained the "standard" one for some time [2, 3]. In 1984, using fully numerical quantum chemical methods we [12] found that the field gradient in LiH was extraordinarily sensitive to the basis set used, Green's basis being far too small, and obtained a LiH-based Q-value of -40.6 mb. Four years later we confirmed that value

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from a different molecule, LiF, obtaining −40.55(80) mb [13]. The LiH value was confirmed by Karna and Grein (−39.6 mb) [14]. The latest value is −40.1 mb, comprising a fit to the molecular data for LiH, LiF and LiCl [15].

Atomic calculations on Li have been performed. The q values for the 2p state by Blundell et al. [16] and by Sundholm and Olsen [17] are −0.02270(1) and −0.02253(8) a.u., respectively. The problem is that both the 2p [18] and 3p [19] states have lifetimes broadening comparable to the nuclear quadrupole splitting, making the experimental errors too large.

An independent source would be nuclear Coulomb scattering. The early German values, however, agreed with the old LiH value [20], until an improved fit to the same data [21, 22] gave a $Q(^7\mathrm{Li})$ of −40.0(6) mb, in agreement with the molecular values. Australian data (−40(11) mb [23], later improved to −40.3 mb [24]) agreed with the new molecular values, but were of lower claimed accuracy. The entire story is summarised in Figure 1. The earlier controverses seem now to be resolved.

Most of the lithium in the universe comes from the Big Bang. It turned out that the obtained $Q(^7\mathrm{Li})$ was indirectly of interest in this context, the various nuclear properties (Q, the nuclear E1 polarizability and the astrophysical S factor), being related to each other [22, 25].

Values of 0.0205(20) and 0.0204(10) for the ratio of the ^{6}Li and ^{7}Li quadrupole moments are obtained from LiF [26] and LiBr [27], respectively. Thus the ^{6}Li value has a considerably lower accuracy than the ^{7}Li one. The ^{8}Li and ^{9}Li NQCC in $LiNbO_3$ of 42.5(6) and 37.4(1.1) kHz, respectively, combined with the known ^{7}Li value of 54.7(3) kHz [28], together with the present recommended value of $Q(^7\mathrm{Li})$ [15], give the ^{8}Li and ^{9}Li values in Table 1. Comparison with nuclear theory suggests for them the signs + and −, respectively [29].

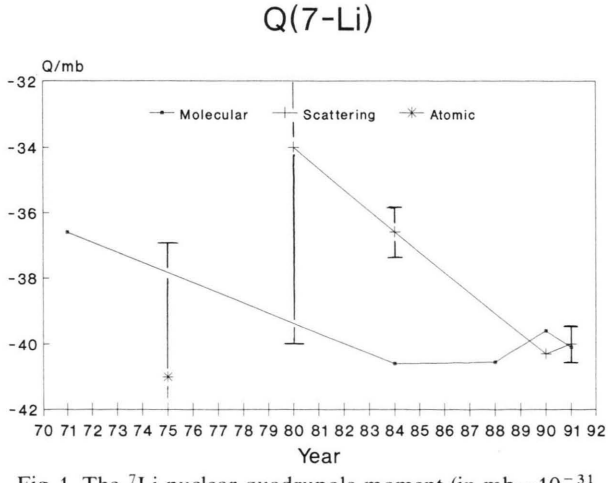

Fig. 1. The ^{7}Li nuclear quadrupole moment (in mb = 10^{-31} m^2) from three different methods as function of year, 1971 to 1991.

Beryllium: For the 2s 2p $^3P_2$ state of ^{9}Be, a quadrupole coupling constant, B_j, of 1.429(8) MHz is available [30]:

$$B_j = D\,[(2j-1)/(2j+2)]\,(\langle r^{-3}\rangle_{nl}/\mathrm{a.u.})\,(Q/\mathrm{barn}) \quad (1)$$

with $D = 234.9647$ MHz.

Combined with the calculation of Sundholm and Olsen [31], it yields a Q of 52.88(38) mb, the error limits arising from the experiment. The old standard value of 53(3) mb [3, 4, 30] uses an empirical q with a Sternheimer correction. The q calculation of Ray et al. [32] ($Q = 52.5(3)$ mb agrees with the present one; there is no controversy for Be.

A calculation for BeH^+ is already available [33] but the experimental NQCC is missing.

Boron: In this case the $2s^2\,2p^1\ ^2P_{3/2}$ ground state quadrupole coupling constant, B_j, of ^{11}B is known as 2.6927(10) MHz [34]. For ^{10}B, no direct atomic measurement is available and the NQR ratio $Q(^{10}\mathrm{B})/Q(^{11}\mathrm{B})$ of 2.0837(7) [35, 36] must be used. The $Q(^{11}\mathrm{B})$ of 40.59(10) mb, obtained by Sundholm and Olsen [37] is very close to the 1970 Bethe-Goldstone one by Nesbet [38]. The error limits depend on both theoretical and experimental inaccuracy.

The ratio $|Q(^{12}\mathrm{B})/Q(^{11}\mathrm{B})|$ is 0.33(3) [39]. For ^{13}B, see [40].

Carbon: The 20.38 minute isotope ^{11}C has $I = 3/2$ and a B of (−) 4.949(28) MHz was measured by Haberstroh et al. [41] for the $^3P_2$ atomic state. A later calculation gave the previous "standard" Q of 34.26 mb [42]. Combined with the calculation by Sundholm and Olsen [43], it gives 33.27(24) mb, most of the error being experimental.

For the first excited state of the ^{12}C isotope, nuclear Coulomb scattering gives the rather imprecise value of 60(30) mb [44].

Nitrogen: The common ^{14}N isotope has $I = 1$. The archaic molecular Q values of about 16 mb from the late 1960ies (e.g. [45, 46], see [3]) were based on small basis sets and large, polyatomic molecules, treated at SCF level. Curiously, these results are still often quoted in papers on nuclear theory (e.g. [47, 48]). A

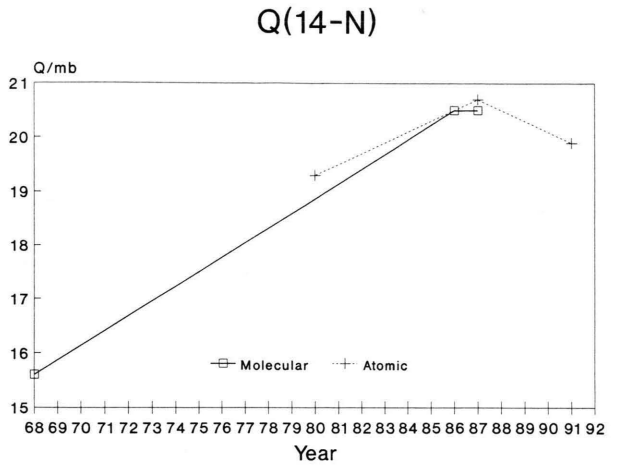

Fig. 2. The ^{14}N nuclear quadrupole moment (in mb = 10^{-31} m^2) from atomic and molecular sources, 1968–1991. The references are [49, 54, 55] and [45, 50, 53], respectively. The nuclear theories (see [48]) give values below the figure.

measurement on the 2p 3p $^1P_1$ state of the N^+ ion [49] gave a B of −4.58(5) MHz and, combined with a semiempirical q, a $Q(^{14}N)$ of 19.3(8) mb. Our fully numerical calculations, combined with basis-set results, gave in 1986 the value of 20.5 mb [50], both gas-phase NO^+ and vibrationally corrected solid-state N_2 data giving the same result. Later basis-set calculations [51–54] cluster around this value. The numerical N^+ MCHF calculation [55] gives a Q of 20.1(2) mb, the uncertainty arising from the experiment. These developments are shown in Figure 2.

For the 11 ms isotope ^{12}N, pionic nuclear reactions give a value of 26 mb [56].

Oxygen: The B value of the $2p^4$ $^3P_2$ ground state of the stable ^{17}O isotope has been measured to be 10.438(30) MHz [57] and the q calculations [42, 58] gave a Q of −25.78 and −26.3 mb, respectively. Numerical MCHF calculations by Sundholm and Olsen [44] refine the atomic value to −25.58(22) mb.

The molecular value of −26.4(3) mb [59] agrees well with it. It is based on the measurement on CO, although initially the four molecules, CO, OH^-, H_2O and CH_2O were considered. Their experimental NQCC are 4.337(56), −7.6(1), 10.175(67) and 12.37(1) MHz, respectively. The OH^- value is a solid-state one; a gas-phase value would be valuable.

Fluorine: Perturbed angular distribution measurements gave a NQCC of 12.4(6) MHz for solid FCl ($^{19}F^*$ (197 keV)) [62]. The $^{20}F/^{19}F$ ratio in MgF_2 was measured to be 5.77(2)/9.95(30) = 0.580(19) [63]. Combined with an SCF-level basis-set calculation on FCl [64], the values of 72(4) and 42(3) mb obtain for $Q(^{19}F)$ and $Q(^{20}F)$, respectively. These values could be improved by better molecular calculations. A NQCC of 127.2(10) MHz for solid F_2 is also available [65]. Librational corrections for the solids should be included.

The $^{17}F/^{19}F^*$ ratio of Minamisono et al. [60] in MgF_2 is 0.806(39), yielding a $Q(^{17}F)$ of ±58(4) mb. They further quote a $^{18}F^*/^{19}F^*$ ratio of 1.07(4) by Morgenstern [61], yielding a $Q(^{18}F^*)$ of ±77(7) mb.

Neon: Nuclear MCHF calculations predict for $Q(^{21}Ne)$ a value of 120 mb [66]. The B in the $2p^5 3s$ $^3P_2$ state of ^{21}Ne (0.27% abundance) has been measured to be −111.55(10) MHz [67]. Combined with later measurements for $2p^{-1}$ hole states and Sternheimer corrected, it gave a Q of 102.9(75) mb [68]. Numerical MCHF calculations by Sundholm and Olsen [43] land at the close-lying value of 101.55(75) mb. Knowledge of $Q(^{21}Ne)$ may become important in NMR [69].

Scattering values are available for ^{20}Ne (−230(30)) and ^{22}Ne (−190(40) mb [70]).

Sodium: The common iotope is ^{23}Na ($I = 3/2$) and the a priori best Q is the 1983 muonic value of 100.6(20) mb [71], close to the Sternheimer atomic value of 101(8) mb [72], based on $B = 2.82(30)$. Measurements of the atomic B exist for several isotopes ($A = 21–29$) [73]. The values, for the 3p [74–76] and 4p [74] states, however show a great variation. A recent calculation by Salomonsson and Ynnerman [77], choosing the experimental B of 2.90(21) MHz [74], would give 111 mb, 10% above the muonic value. Numerical MCHF calculations by Sundholm and Olsen [78], assuming a 3p state B of 2.77(6) MHz [75], gives a Q(Na) of 108.9(32) mb. That B value and the calculation by Salomonsson and Ynnerman [77] would give a Q of 105.9 mb.

Sundholm and Olsen [78] include triple excitations. Their error limit includes both theoretical and experimental errors. Salomonsson and Ynnerman [77] used a CCSD (Coupled Cluster Singles and Doubles) approach.

The situation concerning $Q(^{23}Na)$ appears unsettled. Molecular values based on the accurate experimental NaF NQCC [79] or the accurate theoretical NaH q [80] would be interesting.

Magnesium: The ^{25}Mg 3s 3p $^3P_1$ NQCC was measured by Lurio [81] to be −8.308(5) MHz. Combined with the FEM-MCHF calculation [82] it gives the

current atomic Q value of +199.4(20) mb, which agrees well with the Coulomb scattering [83] and muonic [84] values of +196(4) and +201(3) mb, respectively.

Aluminium: For the $^2P_{3/2}$ state of the Al atom, Harvey et al. [34] give an experimental B of 18.91526(70) MHz. Combined with the FEM-MCHF q value [78], it gives a $Q(^{27}Al)$ of 140.3(10) mb.

The muonic value is 150(6) mb [84]. The ratio $|Q(^{28}Al)/Q(^{27}Al)|$ is measured to be 1.17(8) [85].

Silicon: The 4.2 second ^{27}Si has $I=5/2$ but apparently no quadrupole coupling data are available [3]. The isotopes $^{28,30,32}Si$ have $I=2$ excited states with lifetimes of 0.32–0.70 ps, for which Q-values from Coulomb excitation are quoted [4].

Phosphorus has no stable $I>1/2$ isotopes, either. The 14.28 day ^{32}P has $I=1$ but no quadrupole data are quoted for any state of any phosphorus isotope in [4].

Sulphur: A scattering value exists for ^{32}S [86]. Earlier values for $Q(^{33}S)$ were obtained from SCF-level double-zeta calculations [87] on polyatomic molecules, from experiments on S^+ ($3p^2 3d$ or $3p^2 4d$, $B=56(7)$ and 50(7) MHz, respectively) [88] or from the experiment on the S^- ground state [89], combined with Sternheimer-corrected empirical q. These three values were −62, −84(8) and −74 mb, respectively. The numerical MCHF calculation [90] gives a $Q(^{33}S)$ of −67.8(13) mb. Combined with the experimental $Q(^{35}S)/Q(^{33}S)$ of −0.695 [91], the value for $Q(^{35}S)$ becomes 47.1(9) mb, both error limits being determined by the experimental B of S^-, 26.24(23) MHz [89].

Chlorine: The B of the $2p^5\ ^2P_{3/2}$ atomic ground state was measured to be 54.873(5) and 43.255(10) MHz for ^{35}Cl and ^{37}Cl, respectively [92]. From these values Sternheimer [93] deduced the "atomic" Q values of −82.49(2) and −64.93(2) mb, respectively.

The recent molecular values from HCl [59, 94] are −82 mb for Cl^{35}. The experimental values (for $v=0-2$ and $J=1-3$) are very accurate [79]. (The 1986 atomic value of −76(5) mb is deduced from a rough experimental B of −7.9(4) MHz for the $[3p^3(^2D)4p]\ ^3F_4$ state of Cl^+, attributing the semiempirically estimated q to the 4p electron only [88]. Thus this value is obviously less accurate).

The ratio $Q(^{37}Cl)/Q(^{35}Cl)$ is known to be 0.7880983(8) [79]. The ratio $Q(^{36}Cl)/Q(^{35}Cl)$ from the NQCC in ClCN was used by Townes and Aamodt in 1949 [95] to give the $Q(^{36}Cl)$ of −17.2(4) mb. As the basis apparently was a $Q(^{35}Cl)$ of −79.5 mb, compared to the current value of −82 mb, the result can be updated to −17.7(4) mb.

Argon: Rough Coulomb excitation values are available for excited states of the nuclei $^{36,40}Ar$, see Table 1 [96, 97]. The stable isotopes have $I=0$ and no data are available for the 269 year $I=7/2$ isotope ^{39}Ar.

Potassium: The stable isotopes are $^{39,41}K$. The radioactive ^{40}K also occurs in nature. Data are available for the atomic B of the 4p and 5p states [98, 99]. For them the error limits are rather large; Arimondo et al. [74] recommend for ^{39}K the values of 2.83(13) and 0.870(22) MHz, respectively. Sternheimer and Peierls [72] combined the data ($B(5p)=0.92(10)$ MHz [99, 100]) into $Q(^{39}K)=49(4)$ and $Q(^{41}K)=60(5)$ mb.

Svanberg [99b] obtained experimental B values of 2.77(10), 0.866(15) and 0.370(15) MHz for the 4p, 5p, and 6p states, respectively. The corresponding $Q(^{39}K)$ are 58.8, 59.6 and 57 mb and their weighted average 59(6) mb. Sternheimer corrected, magnetic hfs $\langle r^{-3}\rangle$ were used.

More accurate B data are available for the $3p^5 4s 3d\ ^4F$ and the $3p^5 4s 4p\ ^4D$ states, −78.86(80) and −78.5(32) MHz, respectively [101].

Accurate molecular data would be available for KF, which also gives a $Q(^{39}K)/Q(^{41}K)$ ratio of 0.8215(1) [100]. A solid-state value from $KClO_3$ is 0.8214(7), and the corresponding $^{40}K/^{39}K$ ratio 1.244(2) [102].

Calcium: The only stable isotope with $I>0$ is ^{43}Ca, while the radioactive ^{41}Ca also occurs in nature [103]. Accurate B values of −5.436(8) and −4.632(12) MHz, respectively, are available for the $4s4p\ ^3P_2$ [104] and $4s3d\ ^1D_2$ [105] states of the neutral atom. From them, Salomonsson [106, 107] finds through coupled-pair calculations of q a $Q(^{43}Ca)$ of −49(5) mb. The accuracy is limited by the calculation.

Less accurate, and actually discordant, atomic B values are available for also the other odd Ca isotopes (41, 45, 47) in the $^3P_1$ [108] and $^1P_1$ [109] states. Scattering data exist for excited states of the even isotopes 42 and 44 [110].

3. Discussion

3.1. On the Reliability of the "Atomic" and "Molecular" q Values

The convergence of the calculated q as function of parameters of the calculation can be easily ascertained.

Table 1. Nuclear quadrupole moments, Q, in millibarn (10^{-31} m^2). An asterisk (*) indicates the "recommended" value.

Isotope	Method	System	Q	Year	Ref.
^{2}H	Molec.	HD, D_2	+2.860(15)*	1979	[9]
^{6}Li	Molec.	^{7}Li, LiBr	−0.82(4)*	1990	[15, 27]
^{7}Li	Molec.	LiH, LiF, LiCl	−40.1*	1990	[15]
	Molec.	LiH	−39.6	1990	[14]
	Scatt.		−40.3(6)	1990	[21]
	Scatt.		−40.0(6)	1991	[22]
^{8}Li	Solid	$LiNbO_3$	(+)31.1* [b]	1988, 1991	[15, 28]
^{9}Li	Solid	$LiNbO_3$	(−)27.4* [b]	1988, 1991	[15, 28]
^{9}Be	Atomic	Be 2s2p ^{3}P	52.88(38)*	1991	[31]
^{10}B	Atomic	B 2p ^{2}P	87.45	1969	[42]
		B 2p ^{2}P	84.72(56)	1970	[38]
		B 2p ^{2}P	84.59(24)*	1991	[37]
^{11}B	Atomic	B 2p ^{2}P	41.96	1969	[42]
		B 2p ^{2}P	40.65(26)	1970	[38]
		B 2p ^{2}P	40.59(10)*	1991	[37]
^{12}B	Atomic, solid	ZrB_2	13.4(14)	1978	[39]
^{13}B			37.4(40)	1973	[40]
^{11}C	Atomic	C $^3P_{1,2}$	30.8(6)	1964	[41]
		C $^3P_{1,2}$	34.26	1969	[42]
		C $^3P_{1,2}$	33.27(24)*	1992	[43]
^{12}C[a]	Scatt.		60(30)	1983	[44]
^{12}N	Pion reaction		26	1980	[56]
^{14}N	Atomic	N^+ 2p 3p ^{1}P	19.3(8)	1980	[49]
	Molec.	NO^+, N_2	20.5	1986	[50]
	Molec.	NO^+, N_2	20.5(10)	1986	[51]
	Molec.	HCN	20.0	1986	[52]
	Molec.		20.5(2)	1987	[53]
	Atomic	N^+ 2p 3p ^{1}P	20.7(4)	1987	[54]
	Atomic	N^+ 2p 3p ^{1}P	20.1(2)*	1992	[55]
^{17}O	Atomic	O 2p^4 $^3P_2$	−25.78	1969	[42]
	Molec.	CO	−26.4(3)	1987	[59]
	Atomic	O	−25.58(22)*	1992	[44]
^{18}O	See review				[4, 70]
^{17}F[b]	Solid	MgF_2, FCl	−58(4)		[60, 64]
^{18}F[b]	Solid	SiO_2:F	−77(5)		[61, 64]
^{19}F[a,b]	Molec.	FCl	−72(4)	1982	[64]
^{20}F[b]	Solid	MgF_2, FCl	+42(3)		[63, 64]
^{20}Ne[a]	Scatt.		−230(30)	1981	[70]
^{21}Ne	Atomic	Ne 2p^5 3s $^3P_2$	102.9(75)	1972	[68]
	Atomic	Ne 2p^5 3s $^3P_2$	101.55(75)	1992	[44]
^{22}Ne[a]	Scatt.		−190(40)	1981	[70]
^{21}Na	Atomic	Na 3p ^{2}P	50(37)	1982	[73]
^{23}Na	Muonic		100.6(20)*	1983	[71]
	Atomic	Na 2p ^{2}P	111	1991	[76, 77]
	Atomic	Na 2p ^{2}P	108.9(32)	1992	[78]
^{25}Na			−95(50)	1982	[63]
^{26}Na			−79(54)	1982	[73]
^{27}Na			−58(54)	1982	[73]
^{28}Na			−17(37)	1982	[73]
^{29}Na			25(54)	1982	[73]
^{24}Mg[a]	Scatt.		−180(20)	1981	[4, 70]
^{25}Mg	Coulomb scatt.		196(4)	1977	[83]
	Muonic		201(3)	1982	[84]
	Atomic	Mg 3s 3p ^{3}P	199.4(20)*	1991	[82]
^{26}Mg[a]	Scatt.		−130(40)	1981	[66]
^{27}Al	Atomic		140(2)	1972	[92]
	Muonic		150(6)	1982	[84]
	Atomic		140.3(1.0)*	1992	[78]
^{28}Al	Muonic, solid	Al_2O_3	175(14)	1978+	[85]
^{29}Al			180		[8]
^{28}Si[a]	Scatt.		160(30)	1981	[70]
^{30}Si[a]	Scatt.		−50(60)	1981	[70]
^{32}S[a]	Scatt.		−160(22)	1981	[86]
^{33}S	Atomic	S^- $^2P_{3/2}$	−67.8(13)*	1990	[90]
^{34}S[a]	Scatt.		40(30)	1981	[70]
^{35}S	Atomic	S^- $^2P_{3/2}$	47.1(9)*	1990	[90]
^{35}Cl	Atomic	Cl $^2P_{3/2}$	82.49(2)	1972	[92]
	Molec.	HCl	−82.	1987	[59]
	Molec.	HCl	−82.*	1990	[94]
^{36}Cl	Molec.	ClCN	−18.0(4)		[94, 95]
^{37}Cl	Atomic	Cl	−64.93(2)	1972	[93]
	Molec.	HCl	−64.6*		[94, 79]
^{38}Cl			−180		[8]
^{36}Ar[a]	Coulomb scatt.		110(60)	1971	[96]
^{40}Ar[a]	Coulomb scatt.		10(40)	1970	[97]
^{39}K	Atomic	K 5p $^2P_{3/2}$	+59(6)*	1971	[99b]
^{40}K	Atomic, solid	$KClO_3$	−73(7)*		[99b, 102]
^{41}K	Atomic, molec.	KF	72(7)*	1971	[99b, 100]
^{41}Ca	Atomic		−80(8)	1983	[103]
^{42}Ca[a]	Coulomb scatt.		−190(80)	1973	[110]
^{43}Ca	Atomic		−49(5)	1984	[104, 107]
^{44}Ca[a]	Coulomb scatt.		−140(70)	1973	[110]
^{45}Ca	Atomic		46(14)	1983	[104]
^{47}Ca	Atomic		21(4)	1982	[109]

[a] Excited nuclear state. – [b] Sign from nuclear theory [29].

Table 2. Agreement of calculated magnetic dipole hyperfine coupling constants, a_d (a.u.), with experiment.

System	Calc.	Exp.	Ref.
Li 2p ^{2}P	−0.01346(2)	−0.01357(9)	[17]
Be 2s 2p ^{3}P	−0.06569(10)	−0.06595	[31]
B 2p ^{2}P	−0.16749(30)	−0.1686(5)	[37]

As an example, the Hartree-Fock level q of LiH were given as function of the grid size in Table 1 of [12]. Similarly, the total, correlated q was studied as function of l_{max}, the highest one-electron orbital angular momentum, in the FEM-MCHF calculations by Sundholm and Olsen [17, 31, 37].

Are the converged values correct? A simple test on the routines is to run hydrogen-like systems, for which the value can be done analytically. A rather more convincing test is to obtain the nuclear quadrupole moment, Q, from several different molecules or several atomic states. This also checks the experimental atomic B_j or molecular NQCC.

Finally, for atoms, magnetic hyperfine coupling constants can be used as a test. The nuclear magnetic

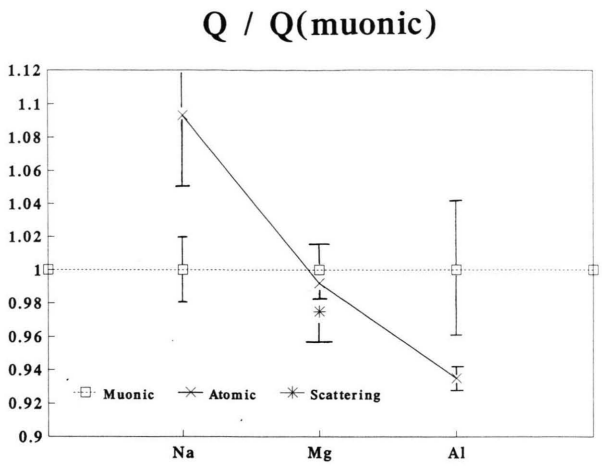

Fig. 3. "Atomic" and "Coulomb scattering" Q values for the elements Na–Al, expressed in terms of the "muonic" value. For references, see Table 1. Error limits for all three methods are given.

moments are known from NMR measurements, apart from small screening corrections, and the operator, especially for the magnetic spin-dipolar term, is of similar form $(P_2(\cos\Theta)/r^3)$ as the operator for q. Some examples on the obtained agreement are shown in Table 2. (It should be said that the separation of the magnetic orbital, dipolar and Fermi contact terms is not an exact process.)

3.2. Comparison with the Muonic Q Values

A priori, the muonic Q values had a high credibility. Our first test, $Q(^{25}\mathrm{Mg})$, was in an excellent agreement with the corresponding muonic value. Later we were surprised to find that the atomic $Q(^{23}\mathrm{Na})$ is about 10% larger, and the $Q(^{27}\mathrm{Al})$ some 7% lower than the muonic values, see Figure 3. The experimental sodium B values are rather scattered, but the aluminium one is very accurate. We therefore cannot escape the conclusion that the muonic Q values may actually be less accurate than originally thought.

Table 3. The estimated situation for the Q of the elements H–Ca. "Good accuracy" means error $\leq 1\%$.

Situation	Element
Good accuracy	H, ^{7}Li, Be, ^{11}B, C, N, O, Ne, Mg, Al, S
Atomic calc. needed	Cl, K, Ca (Ar)
Molec. calc. needed	F_2, FCl; NaF, NaCl; KF, KCl
Atomic exp. helpful	(^{10}B), ^{39}Ar, Na, (Na^+, Na^{2+}?)
NQR ratio helpful	^{6}Li/^{7}Li, (^{10}B/^{11}B)
No nuclei or no data	He, Si, P

3.3. Recommendations

The situation concerning the various nuclear quadrupole moments is roughly summarized in Table 3. Here an accuracy of about 1% or better is called "good". Sulfur is also near this level.

In particular it appears that the important nuclear quadrupole moment of Na is inaccurate due to experimental difficulties in accurately measuring B for the atomic np states. It is interesting to ask whether the $2p^5 3s 3p\ ^4D$ or $2p^5 3s 3d\ ^4F$ states of neutral Na or possibly the $2p^5 4s$ state of Na^+ or the $2p^5$ ground state of Na^{2+} would provide better experimental possibilities. For neutral K, the corresponding neutral-atom measurements exist and the calculations are underway. Alternatively, high-quality quantum chemical calculations on NaF or NaCl could provide a reliable $Q(^{23}\mathrm{Na})$.

The atomic calculations on Cl, K, and Ca atoms are being performed by Sundholm. For ^{39}Ar, both atomic measurements and calculations are still missing. The NQR community could somewhat improve $Q(^{6}\mathrm{Li})$ and $Q(^{10}\mathrm{B})$ by providing isotopic ratios of better accuracy.

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