Year-2008 nuclear quadrupole moments

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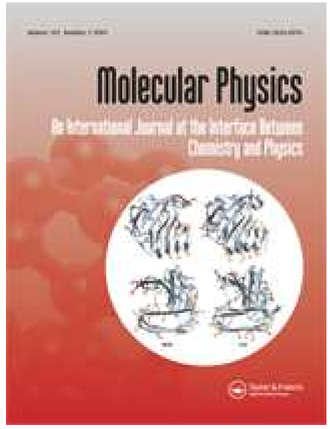

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Year-2008 nuclear quadrupole moments

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Abstract

A "year-2008" set of nuclear quadrupole moments, Q, is presented. Compared to the previous, "year-2001" set, a major revision of the value or an improvement of the accuracy is reported for $_{38}$Sr, $_{49}$In, $_{50}$Sn(Mössbauer state), $_{51}$Sb, $_{55}$Cs, $_{57}$La, $_{80}$Hg and $_{88}$Ra. Slight improvements or valuable reconfirmations exist for $_{7}$N, $_{11}$Na, $_{13}$Al, $_{53}$I, $_{71}$Lu .

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1 Introduction

Atomic nuclei with the nuclear spin $I \geq 1$ have nuclear electric quadrupole moments. As emphasized in the previous reviews [1,2], the currently best way to determine such quadrupole moments, eQ, at least for light elements, is to combine nuclear quadrupole coupling constants, (NQCC), ν^{X} (also denoted e^2qQ/h, eqQ/h or eqQ, or for atoms B, all in frequency units), with careful ab initio calculations of the electric field gradient, q, at this nucleus. The atomic, molecular or solid-state calculation methods and the computer hardware are steadily improving and new experimental spectroscopic data are appearing. The main competitor of this method, at least for the heavier nuclei, is the 'mesonic' way, based on measuring the hyperfine structure of essentially Coulombic energy levels of muons or π mesons near the nucleus studied. No such experiments have been published for a couple of decades and the apparatus has been demounted. Low-precision determinations of Q are available from nuclear Coulomb scattering, nuclear rotational energy levels and from nuclear theory. The knowledge of the nuclear quadrupole moments is important in nuclear physics for testing nuclear models.

In contrast to the absolute value of the nuclear quadrupole moment, which can hence not be directly measured, isotopic ratios between the quadrupole coupling constants for two isotopes of the same element can be directly measured by spectroscopic methods. Such ratios are available from optical spectroscopy, radiofrequency measurements on atomic and molecular beams, as well as nuclear magnetic resonance, nuclear quadrupole resonance or Mössbauer spectroscopy and from perturbed angular correlation (PAC) measurements. Such ratios are also being measured for a number of exotic isotopes.

The knowledge of reliable Q is also important in chemical spectroscopy. Spectroscopic quadrupole splittings act as a gauge of the electron distribution, and studies of molecular dynamics require Q in systems where nuclear quadrupole effects determine the spin-lattice relaxation time, T_1. That is usually the case for the NMR of quadrupolar nuclei and sometimes the case for spin-$\frac{1}{2}$ nuclei scalar-coupled to quadrupolar nuclei.

In addition to composite nuclei, the Ω^- hyperon can have a quadrupole moment whose magnitude, however, is unknown [3].

2 Background

2.1 Earlier compilations

The available nuclear quadrupole moments were reviewed in 1969 by Fuller and Cohen [4], in 1976 by Fuller [5], in 1978 by Lederer and Shirley [6], and in 1989 by Raghavan [7].

The reviews by the present author include the "year-1992" set ($Z \leq 20$ from [1], $Z > 20$ from [7]) and the "year-2001" set [2]. Another recent compilation of both magnetic and electric nuclear moments is that by Stone [8]. The main secondary sources are the CRC Handbook of Chemistry and Physics [9] - [10] and the IUPAC compilations [11]- [12]. Note also the WebElements [13]. The Table of Isotopes [14] partially includes these Q changes, to the extent they have been further quoted in *Nuclear Data Sheets*.

2.2 Improvements in electronic calculations

Basis sets. It is important to go to the basis-set limit to get stable electric field gradients, q. As a recent example, van Stralen and Visscher [15] were still able to change the iodine quadrupole moment for ^{127}I to -696(12) mb from the previous, year-2001 value of -710(10) mb [16].

Electron correlation. In certain cases, like the Al atom [17], it is found that triple excitations are still able to influence the calculated electric field gradient, q, if a one-per-cent level of accuracy is aimed at. These triple excitations are perturbatively included in the CCSD(T) method ('Coupled clusters with single and double excitations and perturbative treatment of triple excitations'). For molecules, CCSD(T) calculations can be performed using several existing programs.

The accuracy of density-functional theory ('DFT') is difficult to assess but it may be as good as a few per cent. Examples are shown below.

Atomic codes. Most existing standard data for the Q of light elements from atomic data were produced by the multiconfiguration Hartree-Fock (MCHF) code LUCAS [18]. For heavier elements, fairly large multiconfiguration Dirac-Fock (MCDF) expansions can now be used. Examples on such large Multiconfiguration Dirac-Fock calculations from the present period are those on Hg [19] and Ra [20] atoms. Because the former method can use much larger expansions and the latter takes full account of relativity, cross-checks between the two methods were useful [16]. For very large expansions, the Complete Active Space (CASSCF) limit would be approached.

Perhaps the most accurate 'atomic' or 'molecular' Q value remains the ^{14}N one of 20.44(3) mb from Tokman et al. [17]. It was obtained using the N^{2+} $2p\ ^2P_{3/2}$ state, a system with only one valence electron.

Solid-state calculations, notably using Linearized Augmented Plane Wave (LAPW) codes, such as WIEN97, include electron correlation via density functionals and are variationally sufficiently flexible to yield electric field gradients for determination of nuclear quadrupole moments [21]. Relativistic effects can be included using quasirelativistic approximations. One new Q value for antimony [22] came from this source during the review period. It was, however, refuted by later molecular work.

Relativistic effects. The simplest way to roughly estimate the size of relativistic effects is to use multiplicative correction factors. Such tables of both H-like or Dirac-Fock-level correction factors were published for the elements 1-93 by Pyykkö and Seth [23].

Approximate relativistic Hamiltonians require a 'picture-change' correction before expectation values are calculated. Two such methods are the Douglas-Kroll (DK) transformation [24] and the 'Zeroth order regularized approximation' (ZORA) [25]. With full-Dirac wave functions the expectation value can be calculated directly. Analytic high-order Douglas-Kroll-Hess electric field gradients were calculated by Mastalerz et al. [26] with the hydrogen halides HX, X=F-At as examples.

Special tricks. Because the total energy of the approximate relativistic Hamiltonians is obtained without further corrections, Schwerdtfeger's group (see ref. [24]) introduced a 'Point-Charge Nuclear Quadrupole Moment' (PCNQM) method where q is extracted from a finite-field approach. For technical checks on it, see Kellö and Sadlej [27].

Finally we repeat that in all-electron calculations, with sufficiently large basis sets for the core shells, the Sternheimer-type polarization [28] is automatically included.

A review on calculations of nuclear quadrupole coupling constants was published by Schwerdtfeger et al. [29].

The Q values below are quoted in barn (1 b = 10^{-28} m^2) or in millibarn (1 mb = 10^{-31} m^2). An alternative unit is Fermi (10^{-15} m) squared, 1 fm^2 = 10 mb.

2.3 Recent experimental data

Magnetic resonance or microwave studies of atomic or molecular electronic ground states can yield a very high accuracy for the quadrupole coupling constants. Very accurate atomic data – quote Br or I as examples – have existed for almost 50 years. If the atomic ground state has spherical symmetry, an excited state must be used in the measurements and then lifetime broadening may become a problem. A classical example are the np states of alkali metals. With considerable experimental ingenuity, quadrupole coupling constants can still be obtained. A recent example is the improved measurement for the Na atom $3p$ state by Das et al. [30]. The recent molecular data are discussed below under the relevant elements.

3 Review of new data

Lithium. The Q values of ^{8}Li($I = 2$) and ^{9}Li($I = \frac{3}{2}$) were measured by Borremans et al. [31]. The results were +31.4(2) and -30.6(2) mb, using as primary value a $Q(^7\text{Li})$ of -40.0(3) mb.

Boron. Sumikama et al. [32] produce for the proton-halo nucleus ^{8}B a Q value of +64.5(1.4) mb, using as primary standard the $Q(^{11}\text{B})$ value of 40.65(26) mb of Nesbet.

Nitrogen. The $Q(^{14}N)$ of Tokman et al. [17] was 20.44(3) mb from a $2p$ state of N^{2+}. A major part of the estimated error came from the experiment. This Q value was confirmed by Kellö and Sadlej [33], who obtain 20.46 mb by considering the diatomic NP molecule. Relativistic effects were included at the IOTP level.

Sodium. Das et al. [30] reported an improved measurement for the Na atom $3p$ state B. The result of 2.721(8) MHz can be combined here with the calculation of Sundholm and Olsen [34] to get a new 'atomic' $Q(^{23}Na)$ of 104(1) mb, which is in perfect agreement with the currently used molecular value of 104(1) mb, based on NaF and NaCl [35].

Aluminium. The 2001 standard value was that of Kellö et al. [36] of $Q(^{27}Al) = 146.6(1.0)$ mb. It was confirmed by Pernpointner and Visscher [37], who obtain 146.0(4) mb using fully relativistic CCSD(T) calculations on AlX, X=F, Cl, Br. The later work of Sur et al. [38] gave alternative values of 141.5 or 142.5 mb but had no triplet virtual excitations and is therefore of inferior accuracy to previous work.

Kameda et al. [39] reported for $Q(^{32}Al)$ a value of 24(2) mb, using the earlier, Sundholm-Olsen [34] primary ^{27}Al value of 140.2(10) mb. The later, '2001' value of 146.6 mb would yield 25(2) mb.

Sulphur. The $Q(^{33}S)$ of -67.8(13) mb was erroneously reproduced in Table 2 of ref. [2] as 767.8(13) mb. Figure 2 was correct. This error is now rectified.

Chlorine. In the 1992 and 2001 compilations we have used the 'atomic' $Q(^{35}Cl)$ value of -81.65(80) mb from Sundholm and Olsen [40]. It is further supported by the atomic calculations of Yakobi et al. [41], giving -81.1(1.2) mb. The revised solid-state value of Alonso et al. [42] is 85.0(11) mb. [CHECK THAT 'note' IS REPRODUCED BY BIBTEX]

The previous value is kept.

Alonso [42] produced a less accurate value of 85.5(1.1) mb. Their solid-state-based values for Cl, Br and I were later withdrawn.

Potassium. B values of 2.786(71), -3.445(90) and 3.351(71) MHz were reported by Falke et al. [43]. for the 4 $^2P_{3/2}$ states of the three isotopes $^{39,\ 40,\ 41}K$, respectively.

Calcium. The '2001' value of $Q(^{43}Ca)$ was -40.8(8) mb. The primary source is Sundholm and Olsen [40]. Yu et al. [44] obtained using Ca^+ a less accurate result of -44(9) mb.

Benhelm et al. [45] measured for the Ca^+ $D_{5/2}$ state a B of 4.241(4) MHz.

Chromium. The 'atomic' table value of $Q(^{53}Cr)$ of -150(50) mb is very inaccurate. Jarosz [46] proposes a new value of -220(10) mb. The value is still based on semiempirical q values.

Iron. The '2001' value of the ^{57}Fe 14.41 keV $I = \frac{3}{2}$ Mössbauer state Q is 160 mb [47]. Note that it was nearly doubled from the previous value. The new value is qualitatively supported by the less accurate value of 140(20) mb by Schwerdtfeger et al. [48]. It is also supported by the value of 150(20) mb from nuclear theory [49] and by the FLAPW calculations of Wdowik and Ruebenbauer [50], giving 170(10) mb.

Copper. Thierfelder et al. [51] obtain at four-component DFT level a $Q(^{63}\mathrm{Cu})$ of -208 mb, in good agreement with the table value of -220(15) mb.

Zinc. The B for the $4s4p\ ^3P_1$ states of $^{65,\ 67}$Zn were measured by Byron et al. [52] to be +2.870(5) and -18.782(8) MHz, respectively. A $Q(^{65}\mathrm{Zn})$ of 24(2) mb was deduced. The 65/67 ratio of -0.1528(3) was also reported. A recent theoretical calculation by Liu et al. [53].

Bromine. The previous 'atomic + molecular' $Q(^{79}\mathrm{Br})$ value of 313(3) mb [16] appeared after [2]. It is reasonably close to the new 'atomic' value of 302(5) mb by Yakobi et al. [41] and is kept so far.

The revised solid-state value of Alonso et al. [42] is 318(5) mb. [CHECK THAT 'note' IS REPRODUCED BY BIBTEX]

Strontium. The previous, atomic standard value for $Q(^{87}\mathrm{Sr})$ was 335(20) mb. New atomic values of 327(24) mb and 305(2)mb were obtained by Mårtensson-Pendrill [54] and Sahoo [55], respectively. The systems were the $5p$ and $4d\ ^2D_{5/2}$ states [56] of Sr^+, respectively. We take the Sahoo value of 305(2) mb as the new standard value. It would be interesting to confirm it by using the measured b for diatomic SrO [57].

Yu et al. [44] obtained a $Q(^{87}\mathrm{Sr})$ of 323(20) mb using the $P_{3/2}$ state of Sr^+.

The agreement of the Sr^+ $B(^2D)$ of Itano [58] with experiment is clearly improved if the new Q of 305 mb is used.

Indium. van Stralen and Visser [59] obtain from diatomic InX, X=F-I the $Q(^{115}\mathrm{In})$ of 770(8) mb, compared with the old atomic value of 810 mb. The new calculations were four-component CCSD(T) ones. The basis-set convergence was slow and the largest indium basis was of [25s23p15d9f9g] quality. This value is accepted as the new standard value. The isotopic ratio 113/115 = 0.986362(15) yields a $Q(^{113}\mathrm{In})$ of 759(8) mb. These are taken as the new values for indium.

Previous solid-state measurements and new WIEN97 FLAPW calculations by Errico and Rentería [60] on metallic indium gave independent $Q(^{115}\mathrm{In})$ values of 760(20) and 780(20) mb, depending on whether LDA or GGA functionals were used. The average of these values would be in perfect agreement with the new molecular value.

A new measurement of a b of -607.3234(22) MHz for diatomic InI appeared [61].

Tin. For the $I =$ Mössbauer state of ^{119}Sn, Krogh et al. [62] report a new Q value of 119(1) mb. The previous value was 109(8) mb.

New isotopic B ratios for the tin isotopes $^{126-132}$Sn were measured by Le Blanc et al. [63]. The primary values from Eberz et al. [64] were used for these radioactive isotopes.

Antimony. The old, atomic standard values for ^{121,123}Sb were -360(40) and -490(50) mb. The original source is [65]. Solid-state calculations by Svane [22] first suggested that the ^{121}Sb value should be changed to -669 mb. Then molecular calculations by Demovič et al. [66] and Haiduke et al. [67] produced mutually consistent values of -556(24) and -543(11) mb, respectively. Both determinations were based on recent diatomic data for SbN, SbP, SbF and SbCl by Cooke and coworkers. As the Haiduke work is fully relativistic and has a lower error limit, we choose it as the new standard value. The $Q(^{121,123}$Sb) thus become -543(11) and -692(14) mb, respectively [67]. As pointed out by Svane [22], the 123/121 ratio was established by Wang as 1.2747 [68]. Amusingly, already in 1955 Murakawa [69] obtained the atomic values of -530(100) and -680(100) mb for ^{121,123}Sb, respectively. Later 'atomic' values were those by Ruby et al. [70] and Dembczynski [71]. The reported values of the antimony quadrupole moment as function of time are showed in Figure 1. The earliest atomic values in it come from ref. [72, 73]. The early molcular value comes from a measurement on gaseous SbH_3, combined with a semiempirical q estimate [74].

Iodine. The previous standard value for $Q(^{127}$I) of -710(10) mb [16] appeared after [2]. It was obtained using data for the I atom and the HI molecule. By further increasing the basis, van Lenthe and Visscher [15] lowered the value to -696(12) mb. Although the two values are within each other's error limits, we now choose the latter as the new standard value. The new atomic value of Yakobi et al. [41] would be -680(10) mb, further down.

The revised solid-state value of Alonso et al. [42] is 722(21) mb. [CHECK THAT 'note' IS REPRODUCED BY BIBTEX]

^{127}I has a 58 keV $I = \frac{7}{2}$ Mössbauer state. The ratio between the excited-state and ground-state quadrupole moments has been measured as $Q^*/Q = 0.896(2)$ [75]. The new primary value Q = -696(12) mb thus gives $Q(^{127}\mathrm{I}(58\ \mathrm{keV}, I = \frac{7}{2}))$ = -624(11) mb The long-lived $^{129}\mathrm{I}(I = \frac{7}{2}, 1.6{\cdot}10^7$ y) has a ratio $Q(^{129}\mathrm{I})/Q(^{127}\mathrm{I}) = 0.701213(15)$ [76], yielding a $Q(^{129}$I) of -488(8) mb. The same isotope has a 28 keV $I = \frac{5}{2}$ Mössbauer state. The ratio $Q(^{129}\mathrm{I}^*)/Q(^{129}\mathrm{I})$ has been measured as 1.2385(11) [77], yielding $Q(^{129}\mathrm{I}^*)$ = -604(10) mb.

Caesium. ^{133}Cs has a very small quadrupole moment. A recent measurement [78] of the coupling constant in diatomic CsF, combined with a field-gradient calculation by Pernpointner et al. [24] yields a Q value of -3.43(10) mb, used in the '2001' set. Since then, Gerginov et al. [79] measured for the atomic $6p\ ^2P_{3/2}$ state of ^{133}Cs a B of -0.4934 MHz and used calculated q to deduce a new Q of -3.55(4) mb.

Barium. The old table values of $Q(^{135,\ 137}$Ba) are 160(3) and 245(4) mb. New calculations are reported for the d states of Ba^+ by Sahoo [80] and yield the Q value of 246(1) mb for ^{137}Ba, thus supporting the previous value.

Again, a molecular reconfirmation using the data for diatomic BaO [] would be interesting.

Lanthanum. The diatomic data for LaX; X = F-I yielded a $Q(^{139}\mathrm{La})$ of 200(6) mb, compared with the earlier atomic value of 200(10) mb [81]. The new molecular value is accepted as the new standard value.

Samarium. The $Q(^{149}\mathrm{Sm})$ in Table 1 should read +75(7) mb. It was erroneously given as +74(7) mb in [2].

Lutetium. The muonic standard value for $Q(^{175}\mathrm{Lu})$ is +3.49(2) b [7]. The recent measurement on diatomic LuF and LuCl by Cooke et al. [82] provides an excellent source for a molecular value. The calculations of Haiduke et al. [83] yielded for $Q(^{175}\mathrm{Lu})$ a value of 3415(34) mb. The accuracy of the calculation was thought to be 1% or better. The same is true for the muonic value, yet the difference between the two values is 75 mb or 2%. As this was the first accurate cross-check between between muonic and molecular Q values, we still use the muonic standard value. The isotopic ratio of Cooke et al. [82] yields a 'molecular' $Q(^{176}\mathrm{Lu})$ of 4818(48) mb.

Further, accurate B values for the states $5d6s^2\ ^2D$, $5d6s6p\ ^4P$ and $6s^28p\ ^2P$ of the two isotopes $^{175,\ 176}\mathrm{Lu}$ were measured by Witte et al. [84].

Gold. The muonic $Q(^{197}\mathrm{Au})$ is 547(16) mb. Both atomic and molecular data suggest that the true value may be slightly lower. Yakobi et al. [85] obtain 521(7) mb using atomic data for the $5d^96s^2\ ^2D_{3/2,5/2}$ states. Four-component CCSD(T) calculations were performed. The results for the two J-states agreed within 0.1 %. Previous, relatively small MCDF atomic calculations by Itano [58] gave much larger Q values around 582-592 mb.

Molecular calculations were performed on diatomic AuF and triatomic linear NgAuF (Ng = Ar-Xe) systems by Belpassi et al. [86]. A comparison of these two systems improved the accuracy and gave a Q value of 510(15) mb for $Q(^{197}\mathrm{Au})$. The AuH molecule had to be omitted from the data set. The same idea was also tested at DFT level [87]. At four-component DFT level, Thierfelder et al. [51] obtain a Q of 526 mb.

Solid-state calculations using WIEN97 and their new measurements on gold-aluminium intermetallic compounds by Palade et al. [88] would yield for the nuclear ground state 560(30) mb. *Mercury.* Improved atomic calculations by Bieroń et al. [19] on the $^3P_1$ state of neutral mercury yield a $Q(^{201}\mathrm{Hg})$ of 387(6) mb. The value is close to the previous value of 386(49) mb but has much smaller error limits.

Fornal et al. [89] turned the trick around. If a theoretical Q value is accepted for the $^{206}\mathrm{Hg}$ isotope, the experimental 201/206 ratio would yield a value of 347(43) mb for $Q(^{201}\mathrm{Hg})$. The value is clearly smaller than that of Bieroń et al. [19].

Lead. Mao et al. [90] performed EFG calculations on solid $PbTiO_3$ and deduced a $Q(^{204m}\mathrm{Pb})$ of 0.62(1) b.

Radium. Improved MCDF calculations on the $7s7p\ ^3P_{1,2}$ and $^1P_1$ states of Ra yield a $Q(^{223}\mathrm{Ra})$

value of 1.21(3) b [20]. For other Ra isotopes, recall that isotopic ratios from the $7p\ ^2P_{3/2}$ states of Ra II are available [91].

The final values for all elements are given in Table 1. The changed values are summarised in Table 2.

4 Comparison of recent compilations

Certain differences exist between different recent compilations, see Table 3. The CRC Handbook [10] values agree with the present ones. So do the IUPAC [12] ones. The only exception is $_{51}$Sb, where the solid-state values were temporarily recommended by the present author. Stone [8] has a policy of giving several independent values without preference and did not include all the latest values. Like Raghavan [7], he gives the exact references of all data.

5 Conclusion

The study of nuclear quadrupole moments of the elements is in a sense a tiny science, having about hundred objects, each characterized by a single number, usually known with less than three-figure accuracy. Once a reliable value is available for one isotope, the isotopic ratios can usually be directly measured. Yet, an accurate knowledge of these numbers will help a surprisingly large section of Chemistry and Physics. During the reviewed period, new standard values were obtained for ´seven [CHECK AT END] elements. The present Table 1 is offered as the new standard set. It will have applications both in atomic and nuclear physics and in chemical and solid-state spectroscopy.

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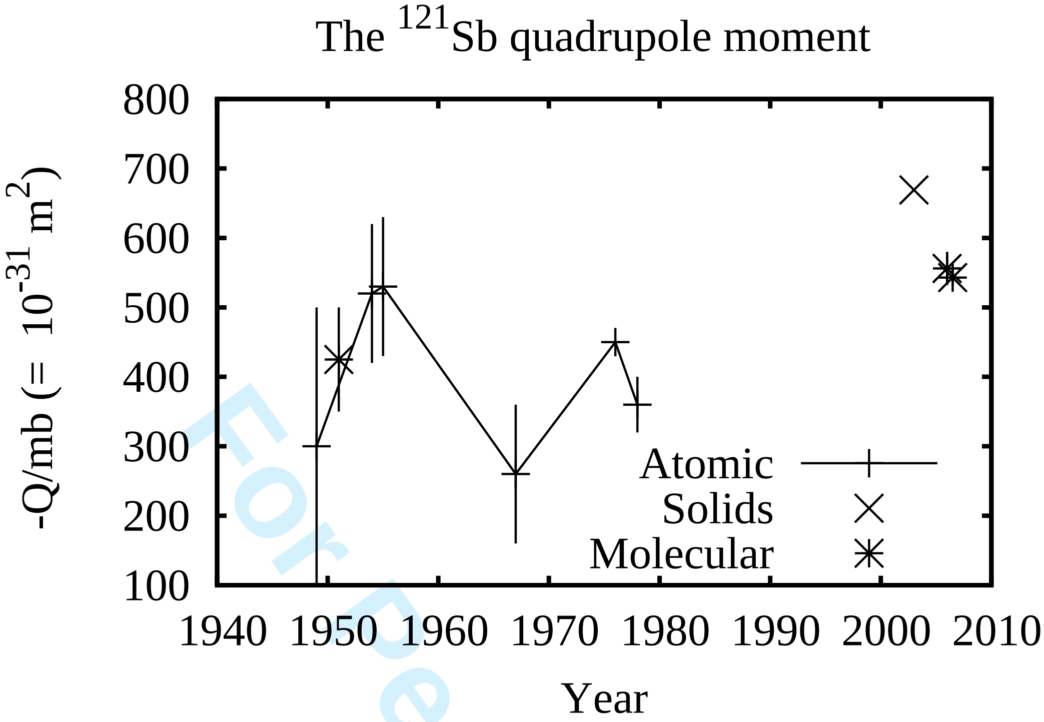


Figure 1: The obtained values of $Q(^{121}\mathrm{Sb})$ from various methods.

Table 1: "2008" Quadrupole Moments. New values are indicated by '•'. Unless otherwise mentioned, see [1] for $Z \leq 20$ and [2,7] for $Z > 20$. The original error limits are given but their meaning may vary. A star (*) indicates an excited nuclear state. Mössbauer states are underlined. Methods: 'a' atomic, 'm' molecular, 's' solid-state, 'μ' muonic, 'n' nuclear lifetime, 'π' pionic. 'XY': primary value from 'X', isotopic ratio from 'Y'. 'X+Y': both 'X' and 'Y'.

Nucleus	Q		Nucleus	Q		Nucleus	Q	
H-2	2.860(15)	m	Ga-69	171(2)	m	Gd-155	1270(30)	μ
Li-6	-0.808	m	Ga-71	107(1)	m	Gd-157	1350(30)	μ
Li-7	-40.1	m	Ge-73	-196	m	Tb-159	1432(8)	μ
Be-9	52.88(38)	a	As-75	314(6)	μ	Dy-161	2507	μa
			Se-77	760	s			
B-10	84.59(24)	a	Br-79	313(3)	a+m	Dy-163	2648(21)	μ
B-11	40.59(10)	a	Br-81	262(3)	a+m	Ho-165	3580(20)	π
C-11	33.27(24)	a	Kr-83	+259(1)	m	Er-167	3565(29)	μ
N-14	20.44(3)	a	Rb-85	276(1)	m	Yb-173	2800(40)	μ
O-17	-25.58(22)	a	Rb-87	133.5(5)	m	Lu-175	3490(20)	μ
F-19*	-94.2(9)	m+s	Sr-87	305(2)•	a			
Ne-21	101.55(75)	a	Y-90	-125(11)	a	Lu-176	4970(30)	μa
Na-23	104(1)	m	Zr-91	-176(3)	m	Hf-177	3365(29)	μ
Mg-25	199.4(20)	a	Nb-93	-320(20)	μ	Hf-179	3793(33)	μ
Al-27	146.6(10)	a+m	Mo-95	-22(1)	a	Ta-181	3170(20)	π
S-33	-67.8(13)	a	Mo-97	255(13)	a	Re-185	2180(20)	π
S-35	47.1(9)	a	Tc-99	-129(6)	a	Re-187	2070(20)	π
Cl-35	-81.65(80)	a	Ru-99	79(4)	a	Os-189	856(28)	μ
Cl-37	-64.35(64)	a	Ru-101	457(23)	a	Ir-191	816(9)	μ
			Rh-100	153	s			
K-39	58.5	m	Pd-105	660(11)	μ	Ir-193	751(9)	μ
K-40	-73	ms	In-113	799	a	Au-197	547(16)	μ
K-41	71.1	am	In-115	810	a	Hg-201	387(6)•	μ
			Sn-119	-128(7)	s			
Ca-41	-66.5(18)	a	Sb-121	-543(11)•	m	Pb-209	-269(165)	a
Ca-43	-40.8(8)	a	Sb-123	-692(14)•	m	Bi-209	-516(15)	a
Sc-45	-220(2)	m	I-127	-696(12)•	m	Rn-209	311(31)	a
Ti-47	302(10)	a	Xe-131	-114(1)	m	Fr-223	1170(10)	a
Ti-49	247(11)	a	Cs-133	-3.55(4)•	m	Ac-227	1700(200)	a
V-50	210(40)	a	Ba-135	160(3)	a	Th-229	4300(900)	a
V-51	-52(10)	a	Ba-137	245(4)	a	Pa-231	-1720(50)	n
Cr-53	-150(50)	a	La-138	450(20)	a	U-233	3663(8)	μ
Mn-55	330(10)	a	La-139	200(6)•	m	U-235	4936(6)	μ
Fe-57	160	s						
Co-59	420(30)	a	Pr-141	-58.9(42)	a	Np-237	3886(6)	μ
Ni-61	162(15)	a	Nd-143	-630(60)	a	Pu-241	5600(200)	a
Cu-63	-220(15)	μ	Nd-145	-330(30)	a	Am-243	4210	a
			Pm-147	+740(200)	a			
Cu-65	-204(14)	μs	Sm-147	-259(26)	μ	Es-253	6700(800)	a
Zn-67	150(15)	a	Sm-149	+75(7)	μa			
			Eu-151	903(10)	μ			
			Eu-153	2412(21)	μ			

Table 2: Changes from the "2001" set. Mössbauer states are underlined.

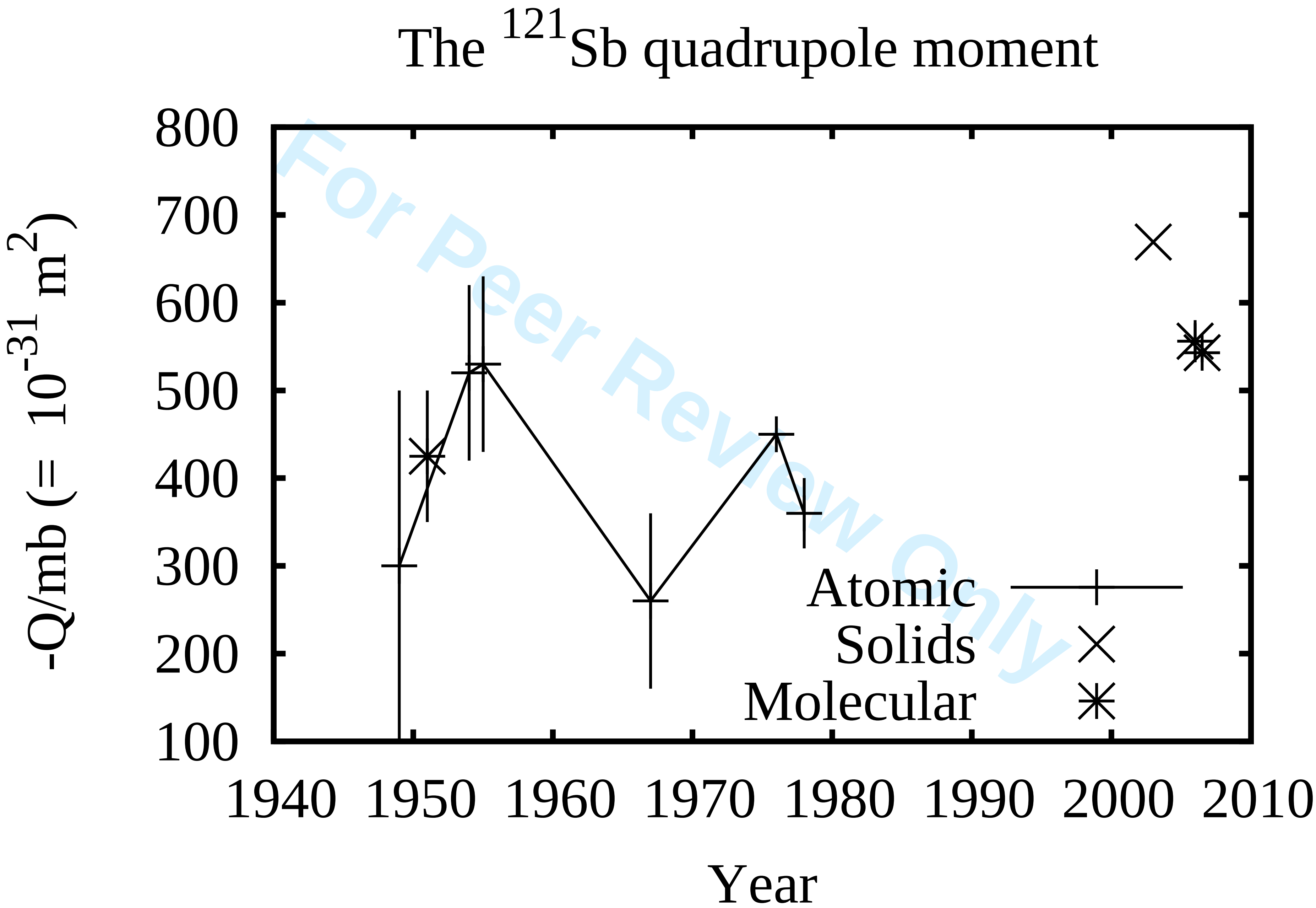
Nucleus	Value	Q/mb	Source	Ref.	Comments
Sr-87	Old	335(20)	Sr 5^3P_2, see [54]		
	New	305(2)	Sr^+ $4d$ $^2D_{5/2}$	[55]	
Sb-121	Old	-360(40)	Sb atom	[65]	
	New	-543(11)	SbN,SbP,SbF,SbCl	[67]	
Sb-123	Old	-490(50)	Sb atom	[65]	
	New	-692(14)		[67]	
I-127	Old	-710(10)	I $^2P_{3/2}$, HI	[16]	
	New	-696(12)	HI	[15]	
<u>I-127</u>	Old	-710			
	New	-624(11)			See text.
<u>I-129</u>	Old	-685			
	New	-604(10)			See text.
Cs-133	Old	-3.43(10)	CsF	[24, 78]	
	New	-3.55(4)		[79]	
La-139	Old	200(10)	a	[92]	
	New	200(6)	LaX; X=F-I	[81]	
Hg-201	Old	386(49)	Hg atom	[93]	
	New	387(6)	Hg($^3P_1$)	[19]	
Ra-223	Old	1221	Average atomic values.		
	New	1210(30)	Ra atom $7s7p$ $^3P_{1,2}$, $^1P_1$.	[20]	

Table 3: Deviations of the present Q-values (in mb) from those in certain recent summaries. The values changed in the present, 'year-2008' summary are indicated by '•'. Excited states are Mössbauer states are underlined. Other excited states are indicated by a star.

Nucleus	Present	Stone [8]	CRC [10]	IUPAC [12]
Li-6	-0.808	-0.82	-0.808	-0.808
Li-7	-40.1	-40.6(8)	-40.1	-40.1
C-11	33.27(24)	32(2)	-	-
N-14	20.44(3)	20.01(10)	20.44	20.44(3)
O-17	25.58(22)	25.78	25.58	25.58(22)
F-19^{*,a}	-94.2(9)	72(4)	-	
Ne-21	101.55(75)	103(8)	101.55	101.55(75)
Ti-47	302(6)	300(20)	302	302(10)
Ti-49	247(11)	247(11)	247	247(11)
Cu-63	-220(15)	-220(15)	-220	-220(15)
Cu-65	-204(15)	-195(4)	-204	-204(15)
Ga-69	171(2)	165.0(8)	171	171(2)
Ga-71	107(1)	104.0(8)	107	107(1)
Ge-73	-196	-170(30)	-196	-196
<u>Se-77</u>	760	-	-	-
Rb-85	276(1)	277.1	276	276(1)
Rb-87	133.5(5)	134(1)	133.5	133.5(5)
Sr-87	305(2)•	330(2)	335	335(20)
Y-90	-125(11)	-155(3)	-	-
Rh-100	153	-	-	-
In-113	759(8)•	800(40)	799	799
In-115	770(8)•	810(50)	810	810
Sb-121	-543(11)•	-360(40)	-360	-669(15)

Nucleus	Present	Stone [8]	CRC [10]	IUPAC [12]
Sb-123	-692(14)•	-490(50)	-490	-853(19)
I-127	696(12)•	-710(10)	-710	-710(10)
La-138	•	450(20)	450	450(20)
La-139	200(6)•	200(10)	200	200(10)
Nd-143	-630(60)	-610(20)	-630	-630(60)
Nd-145	-330(30)	-314(12)	-330	-330(30)
Hg-201	387(6)•	380(40)	386	387(6)
Ra-223	1210(30)•	1250(70)	1250	-
Pa-231	-1720(50)	-	-1720	-1720(50)
Pu-241	5600(200)	6000(200)	-	-

[a] 197 keV, $I = \frac{5}{2}$ state.


The 121Sb quadrupole moment
800
700
600
500
400
300
200
100
-Q/mb (= 10-31 m2)
1940 1950 1960 1970 1980 1990 2000 2010
Year
Atomic
Solids
Molecular