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Published online: 13 Feb 2018.

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RESEARCH ARTICLE

Year-2017 nuclear quadrupole moments

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ABSTRACT

A 'year-2017' set of nuclear quadrupole moments, Q, is presented. Compared to the previous, 'year-2008' set, a major revision of the value, or an improvement of the accuracy is reported for $_1^2$H, $_{18}^{37,39}$Ar, $_{19}^{39,40,41}$K, $_{30}^{67}$Zn, $_{48}$Cd, $_{49}$In, $_{50}$Sn (Mössbauer state), $_{51}$Sb, $_{87}$Fr and $_{90}$Th. Slight improvements or valuable reconfirmations exist for $_4$Be, $_6$C, $_{16}$S, $_{17}$Cl, $_{33}$As, $_{35}$Br, $_{53}$I, $_{54}$Xe, $_{56}$Ba, $_{57}$La and $_{72}$Hf.

$$Q\left(_1^2\mathrm{H}\right) \text{ to } Q\left(_{90}^{229}\mathrm{Th}\right) \text{ changed since 2008.}$$

1. Introduction

Atomic nuclei with the nuclear spin $I \geq 1$ have nuclear electric quadrupole moments. As emphasised in the previous reviews [1–3], 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, eqQ, B or 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 the essentially Coulombic energy levels of muons or π mesons. Due to their high masses, their orbits are near the nucleus studied, where the potential is nearly Coulombic. No such experiments have been published for about three 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. Although most nuclei are axially symmetric, triaxial nuclear shapes also occur [4].

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 in the same system can be directly measured by spectroscopic methods. Such ratios are available from optical spectroscopy, radio frequency 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. As a counterexample, if a Mössbauer experiment can be performed only on one isotope in one system, but an atomic experiment can be performed on another isotope in a different system, the ratio cannot be experimentally determined.

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 Nuclear Magnetic Resonance (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 [5].

2. Background

2.1. Earlier compilations

The available nuclear quadrupole moments were reviewed in 1969 by Fuller and Cohen [6], in 1976

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by Fuller [7], in 1978 by Lederer and Shirley [8] and in 1989 by Raghavan [9].

The reviews by the present author include the 'year-1992' set ($Z \leq 20$ from [1], $Z > 20$ from [9]), the 'year-2001' set [2] and the 'year-2008' set [3]. A recent compilation of both magnetic and electric nuclear moments is that by Stone [10]. A later summary of the Q by Stone is the ref. [11]. It already includes many items from the present update. A publicly available International Atomic Energy Agency (IAEA) web data base with the Stone data is published by Mertzimekis *et al.* [12]. Further, secondary sources are the CRC Handbook of Chemistry and Physics [13–15] and the IUPAC compilations [16,17]. Note also the WebElements [18]. The Table of Isotopes [19] partially includes these Q changes, to the extent they have been further quoted in *Nuclear Data Sheets*.

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.

2.2. Improvements in electronic calculations

Molecular theory. A *tour de force* was the treatment of HD and D$_2$ (hydrogen deuteride and deuterium molecules) by Adamowicz' group [20], yielding for the deuteron a new Q of 2.85783(30) mb. The claimed error limit is entirely coming from the experimental uncertainty of the $J = 1$ HD coupling constant. Born–Oppenheimer (BO) surfaces and a set of explicitly correlated shifted Gaussians were used. The BO calculation included relativistic corrections.

Basis sets. For hydrogen molecule isotopomers, see the previous subsection. For these systems, the basis-set limit to get stable electric field gradients, q, could be reached.

A recent example of a heavier atom was iodine. van Stralen and Visscher [21] were still able to change the 'molecular' iodine quadrupole moment for ^{127}I to $-696(12)$ mb from the previous, year-2001 value of $-710(10)$ mb [22]. The currently chosen $Q(^{127}$I$)$ of -688.22 mb comes from the atomic ground state [23].

Electron correlation. In certain cases, like the Al atom [24], 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. Even CCSDTQ data (Coupled clusters with single, double, triple and quadruple excitations) occasionally exist; see 'Sulphur' below.

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 in the following. In exceptional cases, like the diatomic coinage-metal halides, DFT can even produce a wrong sign [25].

Atomic codes. Most of the early existing standard values for the Q of light elements from atomic data were produced by the multi-configuration Hartree–Fock (MCHF) code LUCAS [26]. Another method for the 17 first elements, or so, is the large-scale MCHF code of Froese Fischer and coworkers [27]. For reviews, see [28,29]. Relativistic effects were included at the Breit–Pauli level or, later, four-component relativistic level.

For heavier elements, fairly large multi-configuration Dirac–Fock (MCDF) expansions can now be used. Examples on such large MCDF calculations from the present period are those on Hg [30] and Ra [31] 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 [22]. For very large expansions, the Complete Active Space Self-Consistent Field (CASSCF) limit would be approached.

Perhaps the most accurate 'atomic' or 'molecular' Q value, except for the deuteron one, remains that for the ^{14}N of 20.44(3) mb from Tokman *et al.* [24]. It was obtained using the N^{2+} $2p^1$ $^2P_{3/2}$ state, a system with only one valence electron.

Solid-state calculations, notably using linearised 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 [32]. Relativistic effects can be included using quasi relativistic approximations.

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 [33].

Approximate relativistic Hamiltonians require a 'picture-change' correction before expectation values are calculated. Two such methods are the Douglas–Kroll (DK) transformation [34] and the 'Zeroth order regularised approximation' (ZORA) [35]. 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.* [36] 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. [34]) introduced a 'Point-Charge Nuclear Quadrupole Moment' method where q is extracted from a finite-field approach. For technical checks on it, see Kellö and Sadlej [37].

Finally, we repeat that in all-electron calculations, with sufficiently large basis sets for the core shells,

the Sternheimer-type polarisation [38] is automatically included.

A review on calculations of NQCC was published by Schwerdtfeger *et al.* [39]. The effects of the electron penetration to the nucleus were considered by Koch *et al.* [40].

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. Such data – quote Br or I as examples – have existed for almost 70 years [41]. 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.* [42]. The recent molecular data are discussed below under the relevant elements.

2.4. Nuclear physics aspects and further methodological comments

A nuclear physics review of the π(sd) nuclei, up to $Z = 20$, was published by De Rydt *et al.* [43]. For the nuclear physics of quadrupole moments, see Neyens [44].

As already commented [2] on Eu isotopes, the ratio of the 'muonic' $Q(^{151}\text{Eu})/Q(^{153}\text{Eu})$ of 0.3744(53) is not in perfect agreement with the corresponding ratio of the observed B parameters for a number of atomic states [45], or 0.39184(22). The reasons are still not understood. The experiments may require further consideration. For summaries on the muonic approach, see [46] or the review of Powers [47].

3. Review of new data

Deuterium. Much improved calculations on both HD and D_2 were reported by Pavanello *et al.* [20]. The results on HD, $J = 1$, yielded a new Q of 2.85783(30) mb. The error limit entirely came from the experimental uncertainty. Note that the measurement was less accurate for D_2 than for HD. The D_2 data were still sufficiently accurate for the previous determination [48].

Beryllium. The calculations of Nemouchi *et al.* [49] on $2s2p^2$ ^4P states of Be$^-$, giving a $Q(^9\text{Be})$ of 52.77 mb, do not contradict the $Q(^9\text{Be})$ of 52.88(38) mb, obtained from a $2s2p$ ^3P state of the Be atom by Sundholm and Olsen [50]. The $Q(^7\text{Be})$ of -64.5 mb was also discussed. This forms a valuable confirmation.

The ratios B_J/Q for the Be-like to Ne-like ions at the Dirac-Fock-Breit (DFB) level are listed by Verdebout *et al.* [29].

Carbon. Carette and Godefroid [51] obtain for $Q(^{11}\text{C})$ a value of 33.36(19) mb in a ^2D state of C$^-$, compared with 33.27(24) mb in case of Sundholm and Olsen [52] in a ^3P state of C. The latter Q value was used as the standard value since ref. [1]. The relativistic corrections in [52] were estimated by multiplicative correction factors while in [51] both Breit–Pauli and Dirac–Fock (DF) functions at MCHF-CI level were used. The newer Q value could be considered 'valuable confirmation' of the previous one.

Sulphur. The 'molecular'[53] $Q(^{33}\text{S})$ and $Q(^{35}\text{S})$ of $-69.4(4)$ and 48.3(3) mb, respectively, were determined from CS and SiS. They are close to the '2008' value of $-67.8(13)$ mb but had improved error limits. The experimental errors on the molecular coupling constants were negligible and in the calculations, both relativistic effects, Gaunt-level corrections, and full triple and quadruple excitations, up to CCSDTQ level were considered.

For reference, the ^{33}S value from S$^-$ was $-65.7(6)$ mb [54].

Chlorine. In the 1992 and 2001 compilations, we have used the 'atomic' $Q(^{35}\text{Cl})$ value of $-81.65(80)$ mb from Sundholm and Olsen [55]. It is supported by the atomic calculations of Yakobi *et al.* [56], giving $-81.1(1.2)$ mb. Chaudhuri *et al.* [23] further find -81.12 mb. We take this value. The ratio 35/37 of 1.26889(3) (see ref. [2]) gives $Q(^{37}\text{Cl}) = -63.93$ mb.

Carette and Godefroid [54] obtain for $Q(^{35}\text{Cl})$ and $Q(^{37}\text{Cl})$ values of -81.764 and -64.438 mb, respectively, as valuable confirmation.

Argon. The most stable quadrupolar isotopes of argon are the 35.0d Ar-37 and the 269y Ar-39. The latest B-values for the excited states of these atoms are reported by Williams *et al.* [57]. The q calculations were so far missing. The 4s[3/2]$_2$ ($3p^54s$; ^3P_o) and 4p[5/2]$_3$ ($3p^54p$; ^3D_e) states of Ar-39 were remeasured, and those of Ar-37 quoted, by Williams *et al.* In a previous study on $^{32-40, 46}$Ar, Klein *et al.* [58] deduced the q from the magnetic hyperfine coupling and obtained a $Q(^{37, 39}\text{Ar})$ of 76.2(1.6) and $-117(20)$ mb, respectively. The Sternheimer corrections were not included. The $Q(^{37, 39}\text{Ar})$ of Sundholm and Pyykkö [59] are 76(3) and $-116(2)$ mb, respectively.

Our first review [1] moreover quotes rough, Coulomb excitation Q for $^{36, 40}$Ar.

Potassium. The latest experimental B of ^{39}K($4P_{3/2}$) is 2.786(71) MHz [60]. The calculation by Singh *et al.* [61] and that experiment [60] yield an atomic $Q(^{39}\text{K})$ of 61.4(6) mb, compared with the 2001 and: 2008 standard value of 58.5 mb. The available ratios would yield

for the isotopes K-40 and K-41 a Q of $-76.4(8)$ and $74.7(7)$ mb, respectively. These values are supported by the new molecular calculations of Teodoro *et al.* [62] of Q, $60.3(6)$, $-75.0(8)$ and $73.4(7)$ mb for K-39, K-40 and K-41, respectively. Note that the molecular measurements for KF, KCl and KBr were very accurate, while the supposed uncertainty of the experimental $B(4P_{3/2})$ was 2.5% for the potassium atom. These molecular calculations used a quadruple-ζ basis and a DC+G-CCSD-T approach. Thus, the new atomic [61] and molecular [62] values support each other and we choose the new molecular ones as the next standard Q values. Its deviations from the molecular values of Kellö and Sadlej [63] were attributed by Teodoro *et al.* to improved basis-sets, deep-core correlation and a more complete inclusion of relativistic effects.

Scandium. The previous Q(Sc-45) was derived from monohalides. The B measurement for the ScN mononitride, reported by Zack *et al.* [64], would provide a further option for determining Q(Sc-45).

Chromium. The 'atomic' table value of $Q(^{53}\text{Cr})$ of $-150(50)$ mb is very inaccurate. Jarosz [65] proposes a new value of $-220(10)$ mb. The value is still based on semi-empirical q values.

Iron. The '2001' value of the ^{57}Fe 14.41 keV $I = \frac{3}{2}$ Mössbauer state Q is 160 mb [66]. 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.* [67]. It is also supported by the value of $150(20)$ mb from nuclear theory [68] and by the Full potential Linearized Augmented Plane Wave (FLAPW) calculations of Wdowik and Ruebenbauer [69], giving $170(10)$ mb. The most recent value of $Q(^{57}\text{Fe})$, 130 mb, is that of Cassassa *et al.* [70]. The previous value was the 160 mb, which we so far kept.

Copper. Thierfelder *et al.* [71] obtain at four-component DFT level a $Q(^{63}\text{Cu})$ of -208 mb, in good agreement with the table value of $-220(15)$ mb.

Santiago *et al.* [72] used molecular calculations on 14 linear molecules and obtained a $Q(^{63}\text{Cu})$ of $-198(10)$ mb, compared with the muonic value of $-220(15)$ mb, used previously, and so far kept.

Zinc. Collinear laser spectroscopic measurements were reported on a number of zinc isotopes with the odd $A = 63-79$ by Wraith *et al.* [73]. A detailed study of the excited $^3P_1$ and $^3P_2$ 4s4p states of the primary ^{67}Zn isotope yielded the Q value of $122(10)$ mb [74], notably close to the Mössbauer + DFT value of $125(5)$ mb of Haas *et al.* [75]. Its 5 mb error limit may be optimistic.

The earlier 1969 standard value from Laulainen and McDermott [76] was $150(15)$ mb. Their q was estimated from the magnetic hyperfine structure.

Gallium. The previous molecular $Q(^{69}\text{Ga})$ of $171(2)$ mb [77] was confirmed by an atomic calculation of Yakobi *et al.* [78], who obtain $174(3)$ mb. We keep the molecular value which has three data points and narrower error limits.

Arsenic. Demovič *et al.* [79] used molecular microwave data on AsP and quantum chemical calculations to obtain a $Q(^{75}\text{As})$ of $311(2)$ mb, compared to the previous muonic value, $314(6)$ mb. We take the new value and notice the agreement between the 'muonic' and 'molecular' values.

Bromine. The '2008' 'atomic + molecular' $Q(^{79}\text{Br})$ value was $313(3)$ mb [22]. Chaudhuri *et al.* [23] suggest an 'atomic' value of 307.98 mb, close to Stopkowicz *et al.* [80] who obtain a $Q(^{79}\text{Br})$ of 308.1 and 309.3 mb from the bromine atom and HBr, respectively. They suggest using the average value of $308.7(2)$ mb. We take this average. The 79/81 isotopic ratio of 1.19705 (see [2]) leads to $Q(^{81}\text{Br}) = 257.9(2)$ mb.

Rubidium. Das and Natarajan [81] report for $^{85,\,87}$Rb 5p $^2P_{3/2}$ states the B values of $26.0084(49)$ and $12.4970(35)$ MHz, respectively. Note that the 87/85 ratio is 0.48050, compared with the molecular ones of $0.4838301(18)$ and $0.483837(22)$ for RbF [82] and RbCl [83], respectively.

In the absence of improved q calculations, we keep the previous molecular Q values [2].

Strontium. Here, a measurement would be available on the $v = 0, 1, 2$ states of diatomic SrO [84], but the extraction of Q is missing. As said in the '2008' review, there also would be a SrS measurement [3].

Nuclear Physics studies on several states of $^{96,\,98}$Sr yielded Q values but not of high accuracy.

Rhodium. In the previous review, we cited for ^{100}Rh a Q value of 153 mb [32]. It should be added that this refers to a nuclear excited state in PAC studies. The nuclear ground state of $^{100}_{45}$Rh has $I = \frac{1}{2}$.

Palladium. The present $Q(^{105}\text{Pd})$ is muonic. High-precision atomic B-values would also be available [85].

Cadmium. For ^{111}Cd, the 245 keV 5/2$^+$ level is of interest for time-differential perturbed angular correlation spectroscopy. A value of $760(20)$ mb was obtained by Errico *et al.* [86] by combining DFT calculations and measurements on several non-cubic metals. The latest Haas [75] value for the same Q is smaller, $641(25)$ mb. It was obtained from Cd metal and solid dimethylcadmium. Nuclear theory yielded $636(45)$ mb. Hybrid functionals were used for the metals. The CCSD(T) molecular calculations were fully relativistic. The treatment of librations in the solid $Cd(CH_3)_2$ was roughly deduced from solid Br_2. If a librational frequency were known, the procedure of Pyykkö and Elmi [87] could be used. We are not aware of measurements that would interrelate these solid-state measurements to the following atomic ones.

The Q of a large number of isotopes, $107-123, 111m-123m$Cd were determined by Frömmgen et al. [88] using the 5s5p $^3P_2$ states of the Cd atom or the 5p $^2P_{3/2}$ state of the Cd$^+$ ion. The theoretical method for the q was MCDF. Their standard was the $Q(^{109}$Cd$) = 604(1)(25)$ mb.

For the metastable, 49 minute 396 keV $I = 11/2$ $Q(^{111m}$Cd$)$ Frömmgen et al. [88] obtain $-742(5)(31)$ and $-747(4)(30)$ mb from the atom and ion, respectively. The average would be -745 mb. If one would combine the experimental ratio of Laulainen and McDermott [76], $Q_{111m}/Q_{109} = -1.2250(30)$ with the $Q_{109} = 604$ mb used by Frömmgen et al. [88], one would obtain $Q(^{111m}$Cd$) = -740$ mb. An earlier report was that of Yordanov et al. [89]. For a summary, see Table 1.

Indium. van Stralen and Visser [90] obtained from diatomic InX, X=F-I the $Q(^{115}$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 Q value was accepted as the previous standard value. It is furthermore confirmed by the new atomic value of Yakobi et al. [78], who obtain 772(5) mb. The isotopic ratio 113/115 = 0.986362(15) yields a $Q(^{113}$In$)$ of 761(5) mb. These are taken as the current values for indium.

Previous solid-state measurements and new WIEN97 FLAPW calculations by Errico and Rentería [91] on metallic indium gave independent $Q(^{115}$In$)$ values of 760(20) and 780(20) mb, depending on whether Local Density Approximation (LDA) or Generalized Gradient Approximation (GGA) functionals were used. The average of these values would be in perfect agreement with the molecular value.

A new measurement of a B of $-607.3234(22)$ MHz for diatomic InI appeared [92].

Tin. For the 24 keV $I = \frac{3}{2}$ Mössbauer state of ^{119}Sn, Krogh et al. [93] report a Q value of $-119(1)$ mb. The '2001' value was $-128(7)$ mb. Barone et al. [94] performed a DFT study of 34 tin compounds, now including the 'picture-change' correction within the Douglas–Kroll–Hess approximation. Their final value is $-132(1)$ mb and this was taken as the '2008' standard value.

New isotopic B ratios for the tin isotopes $^{126-132}$Sn were measured by Le Blanc et al. [95]. The primary values from Eberz et al. [96] were used for these radioactive isotopes.

Various isotopic combinations of diatomic SnS have been reported by Leung and Marshall [97]. The rotational constants of CS, SiS, GeS and SnS are now all known.

Iodine. The previous standard value for $Q(^{127}$I$)$ of $-696(12)$ mb[21] came from molecules. The newest atomic value of Chaudhuri et al. [23], -688.22 mb, which

we choose, is close to that of Yakobi et al. [56], $-680(10)$ mb. Note that for all halogen atoms the atomic hyperfine measurements were performed on the $P_{3/2}$ electronic ground state and, not suffering from lifetime broadening, were very accurate, like the molecular measurements.

^{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 $Q^*/Q = 0.896(2)$ [98]. The new primary value $Q = -688.22$ mb thus gives $Q(^{127}$I$(58$ keV$, I = \frac{7}{2})) = -616.6(1.4)$ mb. The long-lived ^{129}I$(I = \frac{7}{2}, 1.6 \cdot 10^7$ y$)$ has a ratio $Q(^{129}$I$)/Q(^{127}$I$) = 0.701213(15)$ [99], yielding a $Q(^{129}$I$)$ of -483 mb. The same isotope has a 28 keV $I = \frac{5}{2}$ Mössbauer state. The ratio $Q(^{129}$I$^*)/Q(^{129}$I$)$ has been measured as 1.2385(11) [100], yielding $Q(^{129}$I$^*) = -598$ mb.

Xenon. Canella et al. [101] redetermined $Q(^{131}$Xe$)$ using six molecular systems, obtaining $-114.6(1.1)$ mb. This supports the $-114(1)$ mb by Kellö et al. [102] using XeD$^+$. Because Canella et al. have more statistics and full Dirac relativity with a Gaunt correction, we take their value.

Barium. The previous, '2008' table values of $Q(^{135, 137}$Ba$)$ were 160(3) and 245(4) mb. The newest calculations by Sahoo et al. [103] for the d states of Ba$^+$ yield for the two isotopes the Q values of 153(2) and 236(3) mb, respectively. We choose these. The 137/135 isotopic ratio between these independent determinations is $236/153 = 1.542$ while a direct measurement gives 1.538485(95 [104]. A 2012 measurement [105] of $B(^{137}$Ba$^+(5d_{3/2}))$ is 44.538 793 6(10) MHz. Again, a molecular reconfirmation using the existing data for diatomic BaO [84] would be interesting.

Lanthanum. The diatomic data for LaX (X = F-I) yielded a $Q(^{139}$La$)$ of 200(6) mb, compared with the earlier atomic value of 200(10) mb [106]. The new molecular value was accepted as the new standard value in the 2008 summary. It is further reconfirmed by the atomic value of 206(4) mb of Itkin et al. [107] using the experimental data for a $^1D_2$ state. We now take that value. Not being aware of more accurate La-138/La-139 isotopic ratios, we leave the $Q(^{138}$La$)$ at its '2008' value [3].

Ytterbium. An interesting deviation of the calculated and experimental ^{173}Yb quadrupole coupling constant in two states of YbF was found by Pašteka et al. [108]. The experiments may require further attention.

Hafnium. Good B values for the lowest six vibrational levels of $^{177, 179}$Hf^{16}O exist [109]. Because the muonic Q values also have about 1% stated accuracy, this did provide an excellent test case to compare 'molecular' and 'muonic' values. Haiduke [110] used the HfO and HfS molecules and obtained a $Q(^{179}$Hf$)$ of 3750(37) mb, compared with the muonic value of 3793(33) mb. We note the agreement with satisfaction, and keep the previous muonic value.

Table 1. Changes from the '2008' set. Mössbauer states are underlined.

Nucleus	Value	Q/mb	Source	Ref.
H-2	Old	2.860(15)	D_2	[48]
	New	2.85783(30)	HD, D_2	[20]
S-33	Old	−67.8(13)	S^- $(^2P_{3/2})$	[1]
	New	−69.4(4)	CS, SiS	[53]
S-35	Old	47.1(9)	S^- $(^2P_{3/2})$	[1]
	New	48.3(3)	CS, SiS	[53]
Cl-35	Old	−81.65(80)	Cl ground state.	[55]
	New	−81.12	Cl ground state.	[23]
Cl-37	Old	−64.35(64)	Cl $3p^5$ $^2P_{3/2}$	[55]
	New	−63.93	a+BrCl	[23]
Ar-37	New	76(3)	a	[59]
Ar-39	New	−116(2)	a	[59]
K-39	Old	60.1(15)	K $4p^1$ $^2P_{3/2}$, K$3p^5 3d4s$ $^4F_{9/2}$	[55]
	New	60.3(6)	KF, KCl, KBr	[62]
K-40	Old	−73	See text	[3]
	New	−75.0(8)	See text	
K- 41	Old	71.1	See text	[3]
	New	73.4(7)	See text	
Zn-67	Old	150(15)	Zn $4s4p$ $^2P_1$	[76]
	New	122(10)	Zn $4s4p$ $^2P_{1,2}$	[74]
As-75	Old	314(6)	μ	[135]
	New	311(2)	AsP	[79]
Br-79	Old	313(3)	a+m	[2]
	New	308.7 (2)	Br+HBr	[80]
Br-81	Old	262(3)	a+m	[3]
	New	257.9(2)	Ratio	[80]
Cd-109	New	604(1)(25)	Cd^+	[88]
Cd-111, $I = \frac{5}{2}$	New	641(25)	Cd(s), Cd(CH$_3$)$_2$	[75]
Cd-111m, $I = \frac{11}{2}$	New	−745	Cd, Cd^+	[88]
In-113	Old	759(8)	In-115 + ratio.	[3]
	New	761(5)	In-115 + ratio.	[78]
In-115	Old	770(8)	InX, X=F-I.	[90]
	New	772(5)	In $5p$ $^2P_{3/2}$	[78]
<u>Sn-119</u>	Old	−128(7)	Ten tin compounds	[136]
	New	−132(1)	Thirty-four tin compounds	[94]
Sb-121	Old	−360(40)	Sb atom	[137]
	New	−543(11)	SbN,SbP,SbF,SbCl	[138]
Sb-123	Old	−490(50)	Sb atom	[137]
	New	−692(14)	See text	[138]
I-127	Old	−696(12)	HI	[21]
	New	−688.22	$I\,^2P_{3/2}$	[23]
<u>I-127</u>	Old	−624(11)	See text	[3]
	New	−617	See text	
<u>I-129</u>	Old	−604(10)	See text	[3]
	New	−598	See text	
Xe-131	Old	114(1)	XeD^+	[102]
	New	114.6(1.1)	Six molecules	[101]
Ba-135	Old	160(3)	See text	[3]
	New	153(2)	Ba^+ $5d$ state	[103]
Ba-137	Old	245(4)	See text	[3]
	New	236(3)	Ba^+ $5d$ state	[103]
La-139	Old	200(6)	LaX; X=F-I	[106]
	New	206(4)	La $^1D_2$	[107]
Hg-201	Old	386(49)	Muonic	[139]
	New	387(6)	Hg($^3P_1$)	[30]
Fr-211	Old	−190(30)	Fr	[9]
	New	−210(20)	Fr $7p$ $^2P_{3/2}$	[128]
Fr-223	Old	1170(10)	a	[3,9]
Th-229	Old	4300(900)	a	[130]
	New	3110(60)	a	[129]
Am-241	Old	4200(1300)	a	[9,140]
Es-253	Old	6900(800)	a	[9,133]

Iridium. The current Q(Ir) is a muonic one. Measurements on IrN [111], IrP [112] and on the monohydrides [113] would also exist.

Gold. Reiterating the year-2008 discussion, the muonic $Q(^{197}$Au) is 547(16) mb. Both atomic and molecular data suggest that the true value may be slightly lower. Yakobi *et al.* [114] obtain 521(7) mb using atomic data for the $5d^9 6s^2$ $^2D_{3/2,\,5/2}$ states. Four-component CCSD(T) calculations were performed. The results for the two J-states agreed within 0.1 %. Previous, relatively small

Table 2. '2017' Quadrupole moments. New values are indicated by '•'. Unless otherwise mentioned, see [1] for $Z \leq 20$ and [2,9] 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	2.85783(30)•	m	Ga-69	171(2)	m	Eu-151	903(10)	μ
Li-6	−0.808	m	Ga-71	107(1)	m	Eu-153	2412(21)	μ
Li-7	−40.1	m	Ge-73	−196	m	Gd-155	1270(30)	μ
Be-9	52.88(38)	a	As-75	311(2)•	m	Gd-157	1350(30)	μ
			<u>Se-77</u>	760	s	Tb-159	1432(8)	μ
B-10	84.59(24)	a	Br-79	308.7(2)•	a+m	Dy-161	2507	μa
B-11	40.59(10)	a	Br-81	257.9(2)•	a+m	Dy-163	2648(21)	μ
C-11	33.27(24)	a	Kr-83	+259(1)	m	Ho-165	3580(20)	π
N-14	20.44(3)	a	Rb-85	276(1)	m	Er-167	3565(29)	μ
O-17	−25.58(22)	a	Rb-87	133.5(5)	m	Yb-173	2800(40)	μ
F-19*	−94.2(9)	m+s	Sr-87	305(2)	a	Lu-175	3490(20)	μ
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	−69.4(4)•	m	Mo-97	255(13)	a	Re-185	2180(20)	π
S-35	48.3(3)•	m	Tc-99	−129(6)	a	Re-187	2070(20)	π
Cl-35	−81.12•	a	Ru-99	79(4)	a	Os-189	856(28)	μ
Cl-37	−63.93•	am	Ru-101	457(23)	a	Ir-191	816(9)	μ
			Rh-100*	153	s			
K-39	60.3(6)•	m	Pd-105	660(11)	μ	Ir-193	751(9)	μ
K-40	−75.0(8)•	m	In-113	761(5)•	a,m	Au-197	547(16)	μ
K-41	73.4(7)•	m	In-115	772(5)•	a	Hg-201	387(6)	a
			<u>Sn-119</u>	−132(1)	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	−688.22•	m	Rn-209	311(31)	a
Ti-47	302(10)	a	Xe-131	−114.6(1.1)•	m	Fr-211	−210(20)•	a
Ti-49	247(11)	a	Cs-133	−3.43(10)	m	Ac-227	1700(200)	a
V-50	210(40)	a	Ba-135	153(2)•	a	Th-229	3110(60)•	a
V-51	−52(10)	a	Ba-137	236(3)•	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	206(4)•	a	U-235	4936(6)	μ
<u>Fe-57</u>	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-241	4200(1300)	a
			Pm-147	+740(200)	a	Am-243	4200(1300)	a
Cu-65	−204(14)	μs	Sm-147	−259(26)	μ	Es-253	6700(800)	a
Zn-67	122(10)•	a	Sm-149	+75(7)	μa			

MCDF atomic calculations by Itano [115] 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.* [116]. A comparison of these two systems improved the accuracy and gave a Q value of 510(15) mb for $Q(^{197}Au)$. The AuH molecule had to be omitted from the data-set. The same idea was also tested at DFT level [117]. At four-component DFT level, Thierfelder *et al.* [71] obtain a Q of 526 mb.

Solid-state calculations using WIEN97 and their new measurements on gold-aluminium intermetallic compounds by Palade *et al.* [118] would yield for the nuclear ground state 560(30) mb. Since 2008, Santiago and Haiduke [119] obtain 515(15) mb from molecules of the type NgAuX, OCAuX, X = F-I, $Ng =$ Ar-Xe. The molecules AuH and AuX had more scatter and were

omitted. In all, the situation for $Q(^{197}Au)$ must still be considered somewhat unsettled.

Mercury. Improved atomic calculations by Bieroń *et al.* [30] on the $^3P_1$ state of neutral mercury yield a $Q(^{201}Hg)$ of 387(6) mb. The value is close to the previous value of 386(49) mb, but has much smaller error limits. The ^{201}Hg, $I = 3/2$ is stable and has a natural abundancy of 13.18(9) %. Fornal *et al.* [120] used the $Q(^{201}Hg)$ to discuss the excited, quadrupolar nuclear states of of ^{206}Hg.

Arcisauskaite *et al.* [121] suggest for the $I = 5/2$, 158 keV excited nuclear state of ^{199}Hg a Q of 675(12) mb from a number of mercury compounds, using the Bieroń value as primary reference. Alternatively, if they use a measurement on $Hg(CH_3)_2$ and their own DC-CCSD-T calculation of q, they obtain 650 mb. Further tests on their methods of calculation were published by Arcisauskaite

[122] using 4-c and 2-c ZORA methods on HgL_2, L = Cl, Br, I, CH_3 and $[HgCl_3]^-$ compounds.

Lead. Mao *et al.* [123] performed Electric Field Gradient (EFG) calculations on solid $PbTiO_3$ and deduced a $Q(^{204m}Pb)$ of 0.62(1) b. The LDA functional and an LAPW plus local orbital method were used.

Itkin *et al.* [107] used atomic data to calculate $Q(^{191,\,193,\,195,\,197}Pb)$ obtaining 78(11), 179(9), 281(12) and 347(15) mb, respectively. The $B(^1D_2)$ experimental data were more accurate than the $^3P_1$ ones.

Bismuth is an interesting contradictory example. We have previously used the atomic value of $-516(15)$ mb by Bieroń and Pyykkö [124] but the recent molecular calculation by Teodoro [125] gives $-420(8)$ mb. The two molecules BiN and BiP gave the same result and approaches up to CCSD-T were used. Basis-set convergence was studied up to g and h functions. The Dirac–Coulomb–Gaunt Hamiltonian was used. Both the atomic and molecular experimental B have excellent accuracy and there is no reason to suspect either q calculation. Time will show, how to resolve the discrepancy. We so far keep the atomic value but take the molecular value seriously.

Moreover, in ref. [2] we quoted a 'pionic' value of $-500(80)$ mb. In addition, there is an overlapping value of $-500(210)$ mb by Batty *et al.* [126]. A further possibility would be to use the $2p_{3/2}$ states of highly-ionised, Li-like or B-like bismuth atoms. The theory was considered by Koshelev *et al.* [127], but the experiments are so far missing.

Francium. Sahoo [128] redetermined the $Q(^{211}Fr)$ from the $7p\ ^2P_{3/2}$ state as $-210(20)$ mb using CCSD calculations with a triple correction. The previous values were $-190(30)$ or -240 mb; see ref. [128].

Thorium. Safronova *et al.* [129] determined the $Q(^{229}Th)$ as 3.11(6) b. The previous value of 4.3(9) b goes back to Raghavan [9], who cites for it [130]. We accept the new value. Note that it agrees well with the value from the Coulomb excitation of the nucleus, 3.15(3) b [131].

Plutonium. Raghavan [9] gives the muonic Q for some excited states of ^{239}Pu. There are values for the 8, 57, 76 and 285 keV states [132].

Americium. Here, the q values were estimated from the semi-empirical Goudsmit–Fermi–Segrè formula. The atomic hyperfine structure was measured using optical spectroscopy.

Einsteinium is the heaviest element with a reported Q value, 6900(800) mb for ^{253}Es [133]. The hyperfine structure was measured using radiofrequency spectroscopy. The q was deduced from the magnetic hyperfine structure. The B was very precise, $-4316.254(76)$ MHz.

For elements not mentioned here, see the 1992, 2001 and 2008 reviews. The final values are given in Table 2.

4. Conclusion

The study of nuclear quadrupole moments of the elements is in a sense a tiny science, having about hundred objects, each characterised 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 a number of elements. The present Table 2 is offered as the new standard set. It will have applications both in atomic and nuclear physics and in chemical and solid-state spectroscopy.

Acknowledgments

Disclosure statement

No potential conflict of interest was reported by the author.

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