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Corrigendum

Erratum to “A critical compilation of experimental data on spectral lines and energy levels of hydrogen, deuterium, and tritium” [At. Data Nucl. Data Tables 96 (2010) 586–644]



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ABSTRACT

In the critical compilation of experimental and theoretical data on the H, D, and T spectra (Kramida, 2010), there were errors in some of the hyperfine structure parameters for deuterium. These errors are corrected here.

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It was recently brought to my attention by Dr. Thomas Udem of Max-Planck-Institut für Quantenoptik, Germany, that there is an error in the description of deuterium quadrupole hyperfine structure (hfs) shifts in my article [1]. In Section 3.1.3 of that article, I have incorrectly stated that those shifts are non-zero for the $2P_{1/2}$ levels of deuterium (in fact, for all $nP_{1/2}$ levels). In my derivation, I used Eq. (27.45) from Chapter 7 of Sobel'man [2] describing the hyperfine splittings of atomic energy levels, corresponding to Eq. (19) of Ref. [1]. However, I overlooked the fact that Sobel'man [2] gave in Chapter 6 equations (23.10) through (23.15) for the quadrupole hfs-induced shifts of energy levels. According to these equations, an additional shift Δ (independent of F) must be added to the right side of Eq. (20) of Ref. [1]:

$$\Delta E_{nlf}^{\text{quad}} = B_{nlj}C(C+1) + \Delta, \quad (1)$$

where $C = F(F+1) - j(j+1) - I(I+1)$, F , j , and I are the total, orbital, and nuclear angular momentum quantum numbers, respectively, and B_{nlj} is the magnetic dipole hfs constant correctly described by Eq. (19) of Ref. [1]. Neglecting the fact that Sobel'man's Eqs. (23.14) and (23.15) both contain $(2j-1)^{1/2}$ in the denominator (which is zero for $j = 1/2$), the additional term Δ can be obtained from these equations in the following form:

$$\Delta = -\frac{4}{3}B_{nlj}I(I+1)j(j+1), \quad (2)$$

where the above-mentioned term $(2j-1)^{1/2}$ cancels out.

It can easily be shown that Eqs. (1) and (2) lead to a zero quadrupole shift for $j = 1/2$ levels with any value of I .

Although Sobel'man's equations leading to this result are mathematically inapplicable in the case $j = 1/2$, the result is correct:

it was already well known as early as in 1940 [3] that quadrupole hyperfine shift is zero for $j = 0$ and $j = 1/2$ levels because their wavefunctions are spherically symmetric. Thus, Eqs. (1) and (2) are valid for all $j \neq 0$, which is probably the reason for Sobel'man's not mentioning the exception for $j = 1/2$ in his book [2].

The omission of the independent of F term Δ in Ref. [1] resulted in incorrect values for hfs-induced shifts of centers of gravity of all fine-structure levels of deuterium (except $nS_{1/2}$) in Table 2 of Ref. [1]. The corrected values are given here in Table 1.

All data derived from experiments reported in Ref. [1] were not affected by this error, because the hfs-induced shifts were much smaller than experimental uncertainties. However, the hfs-induced shifts given in columns " ΔE_{hfs} " of Tables 6 and 7 of Ref. [1] are incorrect for the non-S levels, as well as the theoretical energies E_{th} to which those shifts were added. The correct values of ΔE_{hfs} and E_{th} are easy to obtain by adding the differences of the shift values given here in Table 1 from those given in Table 2 of Ref. [1].

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- [1] A.E. Kramida, *At. Data Nucl. Data Tables* 96 (2010) 586.
- [2] I.I. Sobel'man, *Introduction to the Theory of Atomic Spectra*, Pergamon Press, NY, 1972.
- [3] H. Kopfermann, *Kernmomente*, Edwards Brothers, Michigan, 1940.

Explanation of Tables**Table 1**

Corrected hfs-induced shifts $\Delta E_{c.g.}$ in nL_j ($n > 1, L > 0$) levels of deuterium (Hz)
 n Principal quantum number

Table 1
Corrected hfs-induced shifts $\Delta E_{c.g.}$ in nL_j ($n > 1, L > 0$) levels of deuterium (Hz).

n	$nP_{1/2}$	$nP_{3/2}$	$nD_{3/2}$	$nD_{5/2}$	$nF_{5/2}$	$nF_{7/2}$
2	(−470.1)(25)	(235.1)(12)				
3	(−139.3)(7)	(69.6)(4)	(−376.1)(20)	(250.7)(13)		
4	(−58.8)(3)	(29.38)(15)	(−158.7)(8)	(105.8)(6)	(−302.2)(16)	(226.7)(12)
5	(−30.09)(16)	(15.04)(8)	(−81.2)(4)	(54.2)(3)	(−154.7)(8)	(116.1)(6)
6	(−17.41)(9)	(8.71)(5)	(−47.01)(25)	(31.34)(16)	(−89.5)(5)	(67.2)(4)
7	(−10.96)(6)	(5.48)(3)	(−29.60)(16)	(19.74)(10)	(−56.4)(3)	(42.29)(22)
8	(−7.35)(4)	(3.673)(19)	(−19.83)(10)	(13.22)(7)	(−37.78)(20)	(28.33)(15)
9	(−5.16)(3)	(2.580)(14)	(−13.93)(7)	(9.29)(5)	(−26.53)(14)	(19.90)(10)
10	(−3.761)(20)	(1.880)(10)	(−10.15)(5)	(6.77)(4)	(−19.34)(10)	(14.51)(8)
11	(−2.826)(15)	(1.413)(7)	(−7.63)(4)	(5.09)(3)	(−14.53)(8)	(10.90)(6)
12	(−2.177)(11)	(1.088)(6)	(−5.88)(3)	(3.918)(21)	(−11.19)(6)	(8.39)(4)

All purely theoretical values are given in parentheses. Uncertainty in the units of the last decimal place is given in parentheses next to the value. For example, (−470.1)(25) means a purely theoretical value -470.1 ± 2.5 .