Letters to the Editor

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On the Value of the Electric Quadrupole Moment of the Deuteron

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The value of the electric quadrupole (E2) moment of the deuteron, as is well known, is one of the most fundamental properties of nuclei, and is connected with the existence of the D state or the character of the tensor force. Therefore we have evaluated this moment more exactly than before[1] assuming a nuclear quadrupole coupling based upon the electromagnetic interaction in response to recent precise experiments on the nuclear radiofrequency spectra.[2),3)]

The electronic wave function used is the James-Coolidge eleven-term function, although this is not fully optimised with respect to the non-linear term.[4] The reason why we did not use their thirteen-term function is that it is evaluated only at one point. Now a more accurate forty- or fifty-term function is available for this hydrogen system.[5] Since our purpose is, however, not to investigate the electronic structure, but to find the most probable value of the E2 moment of the deuteron in response to the present experimental accuracy, it does not seem inadequate to use this function, though it might not be the best, in so far as the electronic function is concerned.

Details of our calculations and evaluation of our nuclear quadrupole coupling integrals have already been published.[6] Final results in question are given in Table I, where R means the internuclear distance, and $q'(R) = \langle \partial^2 V/\partial z^2 \rangle$, the field gradient at the position of the deuteron.

Table I. Calculated values of $q'(R)$ in atomic units.

R	$q'(R)$	$q'(R)$ by reference[7]
1.2	0.338423	0.34936
1.3	0.239947	0.24906
1.4	0.171813	0.17816
1.5	0.124252	0.12769
1.6	(0.09071)	(0.09304)[1]

Next we evaluated the average of $q'(R)$ with respect to the nuclear motion on the following two assumptions:

(1) An extension of Ramsey's approximation for vibrational and rotational states: We assume the Morse function as an adiabatic potential and one of the parameters, aR_e is estimated from Kolos and Roothaan's forty-term function,[5] where R_e is the equilibrium internuclear spacing in the absence of zero-point vibration and rotation and a determines the asymmetry of the Morse potential.

(2) Newell used the following approximate expansion formula for $q'(R)$:

$$q'(R) = (R_e/R)^3 \sum_n a_n \xi^n,$$

where

$$\xi = (R - R_e)/R_e.$$

This expansion formula, however, is not unique, so we tried to take some other possible expansions, for example,

$$q'(R) = \sum_n \alpha_n e^{-n\xi}$$

in addition to the above one. The fluctua-

Table II. The mean deviation η_x of average values in percent.

$q(R'_e)$	${}_0\langle q'(R)\rangle_1{}^{HD}$	η_{HD}	${}_0\langle q'(R)\rangle_1{}^{DD}$	η_{DD}	references
0.1755	0.1768	+0.74	0.1763	+0.45	9)
0.1694	0.1729	+2.05	0.1723	+1.70	10)
0.17816	0.1757	−1.38	0.1761	−1.15	7)
	0.1745	−2.08	0.1749	−1.29	7)
0.171813	0.17086	−0.28	0.17116	−0.11	ours

tion of the values obtained by using these formulae is probably the largest source of error in these calculations; they yield at most 0.2 percent and we could estimate $q'(1.6)$ as 0.09071 a. u. instead of 0.09304 in Table I. This tendency seems to be reasonable from the empirical point of view.

The values averaged over these states are given in Table II, where the mean deviation of the average values ${}_0\langle q'(R)\rangle_1$ of the vibrational ($v=0$) and rotational ($J=1$) states is defined as

$$\eta_x = [{}_0\langle q'(R)\rangle_1^x - q'(R_e)]/q'(R_e)$$

with $R_e=1.4$ a. u.; a comparison with the former values are also given in Table II, (we could not compare our values with those obtained in a recent evaluation).[8]

Finally if we make use of the experimental results on nuclear quadrupole coupling obtained by Ramsey's group,[2),3)] the value of the E2 moment of the deuteron is given by

$$Q_d = 2.796_5 \pm 0.005 \text{ mb},$$

which is the mean value of 2.796 mb and 2.797 mb obtained from the HD and DD systems, respectively, and the largest source of the error is caused by the treatment of the nuclear motion mentioned above. However, we have reduced the former probable error of 0.9 percent,[7)] besides it is to be noted that the value of Q_d is 2 percent larger than the currently accepted value[*)] (3 percent in comparison with the first evaluation[9)]), because by using new values of the fundamental constants and new experimental results[2),3)] Newell's result should be rewritten as 2.736 mb, while Nordsieck's value should be 2.71 mb.

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*) In references 2) and 3) this value is given by 2.738 mb.