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Abstract

The vibrational eigenvalues belonging to the ground electronic state of the HD^+ and HT^+ ions have been calculated. These calculations have been done for the $J = 0$ rotational state and neglecting the dynamic corrections to the potential. For the HD^+ ion we find twenty-two bound states, and for the HT^+ ion twenty-three bound states.

Introduction and Quantitative Discussion

The previous calculations[1] for the vibrational levels of the H_2^+ ion have been extended to determine the vibrational eigenvalues for the HD^+ and HT^+ ions. The vibrational levels are the eigenvalues, W_v, of the radial differential equation,

$$\frac{d^2\phi_v}{dr_n^2} + \left\{ \frac{M_n}{M_e} \left[W_v - W_o(r_n) - \frac{2}{r_n} \right] - \frac{J(J+1)}{r_n^2} \right\} \phi_v = 0 \quad , \qquad (1)$$

where

$$M_n = m_p m_1 / (m_p + m_1) \quad ,$$

$$M_e = m(m_p + m_1) / (m + m_p + m_1) \quad ,$$

m = electronic mass, m_p = proton mass, and m_1 is either the deuteron or triton mass. The potential function, $W_o(r_n)$, is tabulated in Reference 2. For HD^+ and HT^+ we have taken $M_n/M_e = 1224.10$, and 1376.62, respectively.

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[1] Stanley Cohen, John R. Hiskes, and Robert J. Riddell, Jr., Phys. Rev. 119, 1025 (1960).

[2] Stanley Cohen, David L. Judd, and Robert J. Riddell, Jr., Tabulation of Potential Functions and Dynamic Correction Terms for the Hydrogen Molecular Ion, UCRL-8802, June 1959.

The dynamic corrections[3] to the nuclear potential have been neglected. As a consequence of neglecting these dynamic coupling terms, the potential function in Eq. (1) tends to the limiting value

$$W_o(\infty) = -\frac{m}{1+\frac{m}{m_p+m_1}} \frac{e^4}{2\hbar^2} ,$$

which differs from the correct limiting value,

$$R = -\frac{m}{1+\frac{m}{m_1}} \frac{e^4}{2\hbar^2} .$$

To lowest order in m/m_p, these differences are $1/6\ (m/m_p)\ R$, and $1/12\ (m/m_p)\ R$, respectively, for the HD^+ and HT^+ ions. Since the lowest-order potential, $W_o(r_n)$, is known to have systematic errors several times as large as these differences, we have felt justified in neglecting the dynamic corrections in these calculations.

Equation (1) has been integrated numerically over the range $0 \leq r_n \leq 20$ (in units of the Bohr radius a_0), the integration proceeding in steps $\Delta r_n = 0.05$, and for the $J = 0$ rotational state. For the HD^+ ion we find twenty-two bound states and for the HT^+ ion twenty-three bound states. The eigenvalues are given in Table I.

The potential $W_o(r_n)$ is known to be systematically high by 4 to 5 millivolts (mv); hence we would suspect the correct eigenvalues (whose binding energies cover the range from 2.67 to 0.0013 electron volts) to be lower by 4 to 5 mv than those shown in Table I. Upon examining the differences of the eigenvalues of the uppermost levels we conclude that because of this systematic error in the potential there may exist an additional bound state for either of these ions with a binding energy on the order of 1 mv.

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[3] Stanley Cohen, David L. Judd, and Robert J. Riddell, Jr., Mu-Mesonic Molecules: I. The Three-Body Problem, Phys. Rev. 119, 384 (1960).

Table I.

Vibrational eigenvalues for the HD^+ and HT^+ ions

V	HD^+	HT^+
0	-1.1958037	-1.1963171
1	-1.1783752	-1.1798348
2	-1.1618234	-1.1641346
3	-1.1461231	-1.1491957
4	-1.1312519	-1.1349986
5	-1.1171900	-1.1215261
6	-1.1039202	-1.1087623
7	-1.0914283	-1.0966944
8	-1.0797030	-1.0853109
9	-1.0687371	-1.0746040
10	-1.0585270	-1.0645688
11	-1.0490734	-1.0552037
12	-1.0403816	-1.0465109
13	-1.0324619	-1.0384967
14	-1.0253301	-1.0311711
15	-1.0190081	-1.0245493
16	-1.0135246	-1.0186506
17	-1.0089152	-1.0135004
18	-1.0052240	-1.0091300
19	-1.0025007	-1.0055752
20	-1.0007944	-1.0028782
21	-1.0000948	-1.0010814
22		-1.0001982

Dissociation limit = $W_o(\infty) = -1.0000000$

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