

## Nonadiabatic rovibrational levels of hydrogenlike molecules formed in the process of muon-catalyzed fusion

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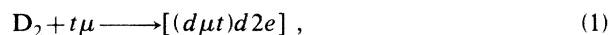
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The nonadiabatic rovibronic energy levels for all species of hydrogenlike molecules of the form  $[(x\mu y)z2e]$ , where  $x, y, z = p, d, t$ , have been calculated. Employing an isotopic scaling method for the nonadiabatic corrections, an accuracy of 0.05 meV was achieved.

### I. INTRODUCTION

In the process of formation of muonic molecular ions of hydrogen isotopes ( $d\mu d, d\mu t$ , etc.) these ions are imbedded in ordinary hydrogen molecules. In the case of resonant molecular formation (see, e.g., Ref. 1) such as



the resonance energies are the difference between the energies of the initial electronic hydrogen molecule  $D_2$  plus the noninteracting muonic hydrogen atom  $t\mu$  and the energy of the resulting hybrid complex of a hydrogen molecule with one hydrogen nucleus replaced by the muonic molecular ion  $td\mu$ . The details of the temperature behavior of the resonant formation rate are extremely sensitive to the exact location of the resonance energies. Since errors from fits to experimental data are smaller than 0.5 meV,<sup>2</sup> we wish to eliminate one source of uncertainty in comparison with theory by obtaining, with an accuracy of 0.1 meV or better, the energy levels of hydrogenlike molecules with one nuclear mass corresponding to one of the hydrogen isotopes  $p, d$ , or  $t$  and the other one equal to the mass of muonic molecular ions like  $d\mu t$ .

In extending the very accurate calculations for hydrogen molecules  $H_2, HD, D_2$  (Refs. 3–5) to the hybrid case the only problem arises in finding the nonadiabatic corrections. The best calculations accounting for these effects in hybrid molecules<sup>6</sup> were based on a method (method I in the following) that, for ordinary hydrogen molecules, claimed agreement of 0.5 meV with experimental data<sup>7–9</sup> and the sophisticated calculations of Ref. 4. Recently a simple and highly satisfactory phenomenological isotopic scaling procedure (method II) has been proposed,<sup>10</sup> that reduces differences with experimental data<sup>11</sup> to less than 0.5 meV.

In the present work both methods<sup>10,6</sup> have been applied to the hybrid molecule case using the new adiabatic potential.<sup>5</sup> The results agree to better than 0.2 meV, with disagreement clearly due to the neglect of angular motion effects in method I. The discrepancies of 0.05 meV for ordinary hydrogen molecules between the results obtained by method II in Ref. 10 and experimental results can be regarded as upper limits for the errors of the energy levels of the hybrid molecules, since the nonadiabatic effects decrease with increasing masses. Tables II and III

give the energy levels for all hybrid molecules computed by method II. The range of vibronic levels in Table II covers the energies relevant for muon catalyzed fusion.

### II. CALCULATION OF ISOTOPIC EFFECTS

The traditional approach to nonadiabatic corrections is based on the following formula for the radial wave function derived by Van Vleck:<sup>12</sup>

$$\begin{aligned} &\{ -[1 - \alpha(R)]/2M(d/dR)^2 + U(R) \\ &\quad + J(J+1)[1 - \alpha'(R)]/2MR^2 \} \chi(R) = E_{v,J} \chi(R), \end{aligned} \quad (2)$$

with  $1/M = 1/M_1 + 1/M_2$ , where  $M_1$  and  $M_2$  are the nuclear masses,  $U(R)$  the adiabatic potential, and

$$\begin{aligned} \alpha(R) &= c \, 1/2M \langle \Psi_0 | d^2 \Psi_0 / dR^2 \rangle, \\ \alpha'(R) &= c' \, 1/(2MR^2) \langle \Psi_0 | J_X^2 + J_Y^2 | \Psi_0 \rangle. \end{aligned} \quad (3)$$

$\Psi_0$  is the ground-state, clamped-nuclei electronic wave function,  $J_X^2$  and  $J_Y^2$  are the squared  $X$  and  $Y$  component of the  $R$ -angular momentum operator, and  $c$  and  $c'$  are constants (see also Ref. 13). Faifman *et al.*<sup>6</sup> arrive at a similar formula which neglects  $\alpha'(R)$  and replaces  $\alpha(R)$  by the constant

$$\alpha_0 = 2/M(\gamma + \kappa^2/4), \quad (4)$$

with  $\kappa = (M_1 - M_2)/(M_1 + M_2)$ . The parameter  $\gamma$  depends only on the clamped-nuclei wave functions, and therefore it can be derived from experimental data for any hydrogen isotopic molecule. Faifman *et al.*<sup>6</sup> derive a value of  $\gamma = 0.20$  from data on  $H_2$ . In view of the results below the major approximation made in Ref. 6 is the neglect of the correction for the angular kinetic energy of the nuclei (see Sec. III).

Wolniewicz<sup>4</sup> gave the following formula for the nonadiabatic corrections:

$$-\Delta E_J = \Sigma_g(\nu) + \Sigma_u(\nu) + J(J+1)[A_g(\nu) + A_u(\nu)] \quad (5)$$

and calculated the nonadiabatic correction parameters  $\Sigma_g, \Sigma_u, A_g, A_u$  for  $H_2, HD$ , and  $D_2$ . The authors of Ref. 10 start from the observation that these parameters as

calculated in<sup>4</sup> scale like  $1/M$  if viewed as functions of the reduced vibrational quantum number  $\eta = (\nu + 1/2)/\sqrt{M}$  instead of  $\nu$ . The dependence of the correction parameters on  $\eta$  resembles the dependence of the radial kinetic energy  $\langle -1/M(d/dR)^2 \rangle$  on the same parameter. Thus the correction parameters can be written as

$$x = \langle -1/2M(d/dR)^2 \rangle f_x(\eta), \quad x = \Sigma_g, \Sigma_u A_g, A_u, \quad (6)$$

with  $f_x(\eta)$  being weakly varying functions that can be fitted by polynomials from the values given in Ref. 4. By using radial functions with appropriate  $J$  for the expectation values  $\langle \nu, J | -(d/dR)^2 | \nu, J \rangle$  instead of  $J=0$  wave functions for all energies, an additional dependence on  $J$  not contained in Ref. 4 enters the nonadiabatic correction parameters. This dependence tends to dampen the overall variation of the energy levels with  $J$  (see Sec. 3 and Table I). Luckily this effect improves agreement with experimental data.<sup>10,11</sup>

TABLE I. Adiabatic energies in meV relative to separated atoms H and D and nonadiabatic corrections for HD.

$\nu$	$J$	Nonadiabatic corrections			
		Adiabatic energy	Method I <sup>a</sup>	Method II <sup>b</sup>	Ref. 3.
0	0	-4513.7322	-0.0380	-0.0443	-0.0461
0	1	-4502.6683	-0.0379	-0.0452	-0.0471
0	2	-4480.6167	-0.0378	-0.0472	-0.0491
0	3	-4447.7280	-0.0377	-0.0500	-0.0521
0	4	-4404.2236	-0.0376	-0.0538	-0.0561
0	5	-4350.3909	-0.0374	-0.0586	-0.0611
0	6	-4286.5764	-0.0371	-0.0644	-0.0671
0	7	-4213.1792	-0.0369	-0.0711	-0.0741
0	8	-4130.6426	-0.0366	-0.0787	-0.0822
0	9	-4309.4462	-0.0362	-0.0874	-0.0912
0	10	-3940.0978	-0.0359	-0.0969	-0.1012
0	11	-3833.1256	-0.0355	-0.1075	-0.1122
0	12	-3719.0708	-0.0350	-0.1190	-0.1243
6	0	-2134.6721	-0.3537	-0.4160	-0.4157
6	1	-2126.3858	-0.3532	-0.4163	-0.4166
6	2	-2109.8779	-0.3522	-0.4168	-0.4183
6	3	-2085.2761	-0.3508	-0.4177	-0.4209
6	4	-2052.7680	-0.3488	-0.4189	-0.4243
6	5	-2012.5970	-0.3464	-0.4203	-0.4286
6	6	-1965.0561	-0.3435	-0.4221	-0.4338
6	7	-1910.4825	-0.3402	-0.4242	-0.4398
6	8	-1849.2508	-0.3364	-0.4266	-0.4466
6	9	-1781.7661	-0.3322	-0.4294	-0.4544
6	10	-1708.4578	-0.3275	-0.4325	-0.4630
6	11	-1629.7736	-0.3225	-0.4359	-0.4724
6	12	-1546.1738	-0.3170	-0.4398	-0.4827
12	0	-540.7213	-0.3927	-0.5090	-0.5099
12	1	-535.5079	-0.3915	-0.5080	-0.5105
12	2	-525.1429	-0.3889	-0.5060	-0.5118
12	3	-509.7491	-0.3851	-0.5031	-0.5138
12	4	-489.5075	-0.3801	-0.4990	-0.5164
12	5	-464.6552	-0.3737	-0.4940	-0.5196
12	6	-435.4818	-0.3660	-0.4879	-0.5235
12	7	-402.3259	-0.3569	-0.4807	-0.5280
12	8	-365.5724	-0.3465	-0.4723	-0.5332
12	9	-325.6498	-0.3345	-0.4627	-0.5390
12	10	-283.0303	-0.3211	-0.4516	-0.5455
12	11	-238.2308	-0.3059	-0.4391	-0.5526
12	12	-191.8187	-0.2889	-0.4248	-0.5604

<sup>a</sup>Results obtained in the present work with method of Ref. 6. The discrepancies between a and Ref. 4 for the  $J=0$  states are significantly smaller than in the results of the original computation (Ref. 6, Fig. 2), see paragraph 3.

<sup>b</sup>Results obtained with the method of Ref. 10.

### III. RESULTS AND DISCUSSION

For all adiabatic calculations the code, algorithm, and potential of Ref. 5 were used. For masses the values  $M_p = 1836.1515$ ,  $M_d = 3670.4807$ ,  $M_t = 5496.920$ , and  $M_\mu = 206.7686$  were adopted (atomic units). The integration step was  $0.005a_0$  for the adiabatic energies and  $0.01a_0$  for radial kinetic energy expectation values.

Surprisingly in our present calculations by method I we got better agreement with Refs. 4 and 5 than indicated in Ref. 6 (see Ref. 6, Fig. 2). Discrepancies to the nonadiabatic calculations<sup>4</sup> are below 0.15 meV. For example, for the  $v = 12$ ,  $J = 0$  state of HD (cf. Table I) our result differs from the accurate result of Ref. 4 by 0.15 meV, whereas Fig. 2 of Ref. 6 shows a discrepancy of about 0.45 meV for this state. This discrepancy cannot be attributed to the slight improvement of the newest Born-Oppenheimer potential over the one of Ref. 4 used in Ref. 6, since these changes are below 0.02 meV (see Ref. 5, Table II). Since all other parameters employed are the same in both calculations, the reason for this disagreement remains unclear.

The parameters  $A_g, A_u$  determining the variation of the nonadiabatic correction with  $J$  [see formula (5)] are

about 0.0003 meV. A glance at Table I shows that method I does not at all reflect such an angular dependence, which is not surprising, since in Ref. 6 the angular motion contribution to the nonadiabatic corrections was neglected.

On the other hand, the good agreement of results of Ref. 10 with the experimental data<sup>11</sup> and the fact that the absolute size of nonadiabatic corrections decreases with increasing masses gives confidence that the errors of the rovibronic levels for the various molecules given in Tables II and III are accurate to better than 0.05 meV. The somewhat larger corrections of Ref. 4 (up to 0.14 meV for highly excited states of HD, Table I) compare less favorably with experiment.<sup>5</sup> From Table I it can also be concluded that the approach of Ref. 6 is correct to about 0.15 meV with the discrepancies being mainly due to the neglect of the  $J$  dependence of the nonadiabatic corrections.

However, one major point has not been addressed in this treatment: the  $d\mu t$  ( $J=1, v=1$ ) molecule forming one of the nuclei in the hybrid molecule is by no means pointlike, the expectation value of the distance of  $d$  and  $t$  being  $9.0a_\mu$  ( $a_\mu$  is the muonic Bohr radius).<sup>14</sup> The effects of the finite size of the muonic molecule on the surround-

TABLE II. Rovibronic quanta of hydrogenlike molecules with one nuclear mass equal to the mass of  $d\mu d$  and  $d\mu t$  and each of the hydrogenic isotopes as the second nucleus.  $E_{00}$  is the dissociation energy of the ground state into two hydrogenlike atoms with nuclear masses as in the molecule. All energies are in meV.

$J$	$v$	5	6	7	8
[( $d\mu d$ ) $p2e$ ] $E_{00} = 4534.526$					
0		1879.114	2202.015	2507.423	2795.179
1		1886.547	2209.104	2514.166	2801.571
2		1901.367	2223.238	2527.609	2814.313
3		1923.483	2244.327	2547.663	2833.317
4		1952.760	2272.239	2574.200	2858.459
5		1989.022	2306.803	2607.053	2889.573
6		2032.058	2347.811	2646.017	2926.459
7		2081.621	2395.024	2690.857	2968.887
8		2137.435	2448.171	2741.310	3016.596
9		2199.201	2506.959	2797.088	3069.304
10		2266.599	2571.075	2857.883	3126.708
11		2339.291	2640.190	2923.371	3188.488
12		2416.928	2713.961	2993.217	3254.311
[( $d\mu d$ ) $d2e$ ] $E_{00} = 4582.442$					
0		1500.226	1768.343	2026.007	2273.231
1		1504.931	1772.888	2030.393	2277.459
2		1514.324	1781.962	2039.150	2285.897
3		1528.370	1795.532	2052.244	2298.515
4		1547.020	1813.548	2069.628	2315.264
5		1570.208	1835.946	2091.236	2336.083
6		1597.851	1862.645	2116.992	2360.893
7		1629.856	1893.552	2146.803	2389.606
8		1666.113	1928.561	2180.566	2422.118
9		1706.503	1967.555	2218.163	2458.315
10		1750.894	2010.404	2259.471	2498.075
11		1799.147	2056.971	2304.352	2541.264
12		1851.112	2107.110	2352.665	2587.741

TABLE II. (Continued).

$J$	$v$	5	6	7	8
			[( $d\mu d$ ) $t2e$ ] $E_{00} = 4601.937$		
0		1338.868	1581.726	1816.442	2043.044
1		1342.603	1585.352	1819.959	2046.452
2		1350.063	1592.593	1826.982	2053.258
3		1361.226	1603.429	1837.492	2063.442
4		1376.062	1617.830	1851.458	2076.975
5		1394.531	1635.755	1868.842	2093.818
6		1416.582	1657.155	1889.595	2113.924
7		1442.156	1681.973	1913.660	2137.236
8		1471.185	1710.142	1940.971	2163.690
9		1503.594	1741.587	1971.455	2193.214
10		1539.299	1776.227	2005.033	2225.730
11		1578.213	1813.975	2041.618	2261.152
12		1620.239	1854.736	2081.118	2299.390
$J$	$v$	1	2	3	4
			[( $d\mu t$ ) $p2e$ ] $E_{00} = 4538.586$		
0		404.229	790.857	1160.209	1512.531
1		412.729	799.022	1168.044	1520.040
2		429.682	815.307	1183.670	1535.015
3		454.994	839.620	1206.998	1557.369
4		488.528	871.826	1237.897	1586.973
5		530.101	911.749	1276.194	1623.660
6		579.496	959.177	1321.683	1667.229
7		636.459	1013.862	1374.122	1717.444
8		700.703	1075.527	1433.242	1774.041
9		771.919	1143.868	1498.747	1836.735
10		849.773	1218.563	1570.323	1905.216
11		933.915	1299.270	1647.637	1979.163
12		1023.980	1385.636	1730.316	2058.239
			[( $d\mu t$ ) $d2e$ ] $E_{00} = 4587.754$		
0		311.692	613.058	904.258	1185.427
1		316.714	617.930	908.982	1190.004
2		326.741	627.657	918.413	1199.143
3		341.741	642.208	932.521	1212.813
4		361.666	661.536	951.260	1230.969
5		386.453	685.579	974.569	1253.552
6		416.025	714.262	1002.374	1280.488
7		450.290	747.494	1034.587	1311.692
8		489.144	785.175	1071.108	1347.066
9		532.473	827.190	1111.827	1386.502
10		580.149	873.417	1156.622	1429.880
11		632.037	923.722	1205.364	1477.073
12		687.993	977.966	1257.915	1527.947
			[( $d\mu t$ ) $t2e$ ] $E_{00} = 4608.007$		
0		273.123	538.359	795.819	1045.599
1		276.968	542.104	799.465	1049.148
2		284.650	549.586	806.749	1056.236
3		296.148	560.785	817.653	1066.846
4		311.436	575.674	832.148	1080.952
5		330.476	594.217	850.200	1098.518
6		353.222	616.369	871.764	1119.501
7		379.621	642.077	896.789	1143.849
8		409.611	671.280	925.214	1171.505
9		443.123	703.910	956.974	1202.403
10		480.081	739.894	991.995	1236.470
11		520.402	779.149	1030.197	1273.629
12		563.998	821.590	1071.496	1313.796

TABLE III. The first six rotational and vibrational quanta of all hybrid hydrogenlike molecules (except for those given in Table II).  $E_{00}$  is the dissociation energy of the ground state into two hydrogenlike atoms with nuclear masses as in the molecule. All energies are in meV.

$J \setminus \nu$	0	1	2	3	4	5
$[(p\mu p)p2e]E_{00}=4515.858$						
0	0.000	446.478	871.346	1275.024	1657.813	2019.885
1	10.867	456.880	881.291	1284.520	1666.865	2028.493
2	32.527	477.612	901.113	1303.446	1684.903	2045.647
3	64.836	508.533	930.674	1331.667	1711.797	2071.218
4	107.579	549.435	969.772	1368.987	1747.356	2105.022
5	160.479	600.050	1018.146	1415.154	1791.335	2146.818
$[(p\mu p)d2e]E_{00}=4558.817$						
0	0.000	366.341	718.306	1056.145	1380.056	1690.185
1	7.214	373.304	725.023	1062.618	1386.289	1696.178
2	21.611	387.200	738.425	1075.534	1398.724	1708.137
3	43.126	407.964	758.452	1094.834	1417.305	1726.003
4	71.665	435.506	785.013	1120.429	1441.944	1749.693
5	107.103	469.703	817.990	1152.203	1472.528	1779.095
$[(p\mu p)t2e]E_{00}=4575.550$						
0	0.000	334.806	657.658	968.753	1268.250	1556.274
1	5.993	340.609	663.275	974.185	1273.500	1561.343
2	17.958	352.194	674.486	985.028	1283.978	1571.460
3	35.850	369.517	691.250	1001.240	1299.645	1586.586
4	59.603	392.515	713.504	1022.761	1320.441	1606.662
5	89.131	421.102	741.166	1049.509	1346.285	1631.610
$[(p\mu d)p2e]E_{00}=4528.005$						
0	0.000	423.940	828.464	1213.938	1580.636	1928.728
1	9.758	433.303	837.438	1222.530	1588.850	1936.565
2	29.216	451.971	855.331	1239.661	1605.225	1952.189
3	58.256	479.830	882.032	1265.220	1629.655	1975.495
4	96.706	516.712	917.377	1299.051	1661.986	2006.333
5	144.340	562.399	961.154	1340.945	1702.016	2044.506
$[(p\mu d)d2e]E_{00}=4574.051$						
0	0.000	337.637	663.113	976.628	1278.345	1568.391
1	6.098	343.540	668.824	982.149	1283.680	1573.540
2	18.271	355.324	680.224	993.172	1294.328	1583.818
3	36.474	372.943	697.270	1009.651	1310.248	1599.182
4	60.638	396.332	719.896	1031.525	1331.377	1619.573
5	90.675	425.403	748.017	1058.709	1357.634	1644.910
$[(p\mu d)t2e]E_{00}=4592.463$						
0	0.000	302.748	595.766	879.202	1153.181	1417.805
1	4.874	307.483	600.364	883.664	1157.509	1422.000
2	14.607	316.937	609.544	892.574	1166.152	1430.377
3	29.170	331.084	623.280	905.905	1179.081	1442.909
4	48.519	349.879	641.529	923.615	1196.258	1459.557
5	72.598	373.267	664.237	945.651	1217.629	1480.269
$[(p\mu t)p2e]E_{00}=4534.505$						
0	0.000	411.841	805.391	1180.991	1538.898	1879.279
1	9.190	420.669	813.864	1189.115	1546.677	1886.714
2	27.517	438.275	830.762	1205.315	1562.186	1901.536
3	54.877	464.556	855.984	1229.494	1585.333	1923.656
4	91.118	499.364	889.386	1261.511	1615.979	1952.938
5	136.039	542.504	930.779	1301.182	1653.944	1989.207

TABLE III. (Continued).

$J \backslash v$	0	1	2	3	4	5
$[(p\mu t)d2e]E_{00}=4582.414$						
0	0.000	321.817	632.611	932.557	1221.800	1500.455
1	5.525	327.174	637.803	937.585	1226.666	1505.162
2	16.556	337.870	648.167	947.623	1236.382	1514.557
3	33.056	353.867	663.669	962.636	1250.912	1528.608
4	54.969	375.111	684.255	982.572	1270.205	1547.264
5	82.222	401.530	709.854	1007.362	1294.194	1570.458
$[(p\mu t)t2e]E_{00}=4601.905$						
0	0.000	284.771	560.954	828.674	1088.038	1339.136
1	4.299	288.955	565.024	832.632	1091.885	1342.872
2	12.886	297.311	573.153	840.536	1099.568	1350.335
3	25.738	309.817	585.319	852.367	1111.065	1361.503
4	42.821	326.441	601.490	868.090	1126.346	1376.345
5	64.090	347.138	621.623	887.665	1145.369	1394.821
$[(t\mu t)p2e]E_{00}=4541.369$						
0	0.000	399.033	780.929	1146.000	1494.487	1826.552
1	8.607	407.313	788.887	1153.641	1501.815	1833.568
2	25.777	423.828	804.760	1168.882	1516.429	1847.561
3	51.416	448.490	828.461	1191.637	1538.248	1868.449
4	85.392	481.166	859.862	1221.781	1567.149	1896.113
5	127.527	521.686	898.797	1259.153	1602.974	1930.399
$[(t\mu t)d2e]E_{00}=4591.438$						
0	0.000	304.696	599.534	884.665	1160.215	1426.287
1	4.938	309.493	604.191	889.183	1164.596	1430.533
2	14.800	319.070	613.489	898.205	1173.345	1439.012
3	29.555	333.400	627.400	911.703	1186.435	1451.696
4	49.158	352.439	645.882	929.635	1203.823	1468.544
5	73.552	376.128	668.877	951.945	1225.455	1489.504
$[(t\mu t)t2e]E_{00}=4612.254$						
0	0.000	265.002	522.587	772.858	1015.902	1251.795
1	3.711	268.620	526.114	776.294	1019.249	1255.054
2	11.123	275.848	533.160	783.160	1025.936	1261.565
3	22.221	286.669	543.707	793.438	1035.947	1271.311
4	36.979	301.058	557.733	807.104	1049.258	1284.269
5	55.363	318.983	575.205	824.128	1065.839	1300.410

ing electrons were estimated to be negligible,<sup>15</sup> but the distortions of  $d\mu t$  by the electrons cause an energy shift of about 8 meV.<sup>15</sup> These uncertainties exceed the nonadiabatic corrections considered here by at least one order of magnitude. The energies given here must be considered as the zeroth approximation for a treatment including the finite-size effects.

#### IV. CONCLUSIONS

In the pointlike approximation for the muonic hydrogen molecular ion the rovibronic energy levels have been calculated for all relevant hybrid molecules by the isotropic scaling method of Ref. 10. The accuracy of better

than 0.05 meV can be regarded as final for the purpose of muonic molecular formation. However, the accuracy of the method employed in the earlier calculation of Ref. 6 can be regarded as sufficient, since the relatively large discrepancies indicated in Ref. 6 were not reproduced in the present calculation.

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