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New Assignments for the Infrared Spectrum of H_3^+

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Calculations are presented for H_3^+ using two potential energy surfaces, one *ab initio,* the other spectroscopically determined, both of which include allowance for the adiabatic correction to the Born–Oppenheimer potential. Systematically labeled energy levels for H_3^+ are presented and the spectra calculated for a number of temperatures. Assignments are given for 105 or about 85% of the published unassigned H_3^+ infrared transitions. Forty previously assigned transitions are relabeled or reassigned. Calculations for higher J levels are discussed.

I. INTRODUCTION

The H_3^+ molecular ion, the electronically simplest polyatomic molecule, is a fundamental molecule in many areas of science. It is thought to be a key molecule in the chemical reactions of the interstellar medium, it is a major cation in hydrogen plasmas, and it plays an important role in ion–molecule reaction schemes involving hydrogen. Moreover, due to its simplicity, it can be considered a benchmark for *ab initio* molecular theory.

Because of its importance, H_3^+ has been the subject of extensive studies, both experimental and theoretical. Details on this can be found in a number of recent reviews (*1–5*).

Even if H_3^+ is a very simple and symmetric molecule, the task of assigning its vibration–rotation spectrum is not at all simple. In fact H_3^+ is a light molecule with large vibration–rotation interactions and conventional effective Hamiltonians give poor representations of its energy levels. Thus predictions of its spectrum are difficult to make and the assignment of lines, even from the first detection of its fundamental band (*6*), has only been possible with the help of extensive *ab initio* calculations.

Even with the improving quality of the analysis of the H_3^+ spectrum a number of lines were left unassigned; see Xu *et al.* (*7*) and Bawendi *et al.* (*8*).

Recently there has been a great effort in producing an effective potential energy surface for H_3^+ accurate enough to predict its spectrum with close to experimental precision. These efforts have used both *ab initio* electronic structure theory (*9, 10*) and potentials derived from detailed fits to spectroscopic data (*11–15*). In particular the most recent fit, by Dinelli *et al.* (*15*) is close to the intrinsic accuracy of the experimental data (*16*).

Of the 229 published unassigned lines (*7, 8*), 85 have already been assigned by Majewski *et al.* (*14*), using their effective potential. In this paper we make use of the greatly improved potential energy surfaces, both *ab initio* and spectroscopic, to attempt an assignment of all the published lines of H_3^+ that were left unassigned by previous work.

II. CALCULATIONS

In order to be able to assign H_3^+ transitions we need to calculate all the energy levels and to predict the whole spectrum. The energy levels have been calculated using two different program suites: TRIATOM (*17*) and DVR3D (*18*). In both cases scattering coordinates were used. Both methods also solve the rotation–vibration problem in two steps by first diagonalizing an effective vibrational problem and then using the lower solutions of this problem to solve the full problem (*19*).

The TRIATOM calculations closely paralleled calculations used for previous spectroscopic studies of H_3^+ (*10, 15*). In these calculations Morse oscillator-like functions were used to represent stretching motions in both radial coordinates. We selected the lowest 800 energy solutions from a 1200 dimension secular problem for the first step and used the lowest $600 \times (J + 1)$ solutions to solve the full rovibrational problem. For more details see Dinelli *et al.* (*15*).

Using TRIATOM, we calculated the energy levels of H_3^+ using two different potential energy surfaces: the effective spectroscopic surface obtained by a fit to the experimental data by Dinelli *et al.* (*15*) (henceforth called the DPT potential) and an *ab initio* Born–Oppenheimer surface due to Röhse *et al.* (*9*) augmented by the *ab initio* non-Born–Oppenheimer adiabatic corrections of Dinelli *et al.* (*10*) (henceforth called *ab initio*). Because the basis functions used for the TRIATOM calculations are not reliable for linear H_3^+ geometries, calculations

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using TRIATOM were restricted to energy levels up to 9000 cm^{-1} above the vibrational ground state and to rotationally excited states with $J \leqslant 9$.

The DVR3D calculations were explicitly designed to probe geometries above linearity (*20*). For this reason the discrete variable representation (DVR) grid in the radial coordinate that probes linear geometries was based on the less efficient spherical oscillator functions. In the first ''vibrational'' step the lowest 700 energy solutions were selected from a 3000 dimension secular problem, and the lowest 500 $\times (J + 1)$ solutions were used to solve the full rovibrational problem. These calculations are considerably more computationally expensive than the TRIATOM ones, and there is some evidence, discussed below, that the high lying rotational states were not fully converged with this basis set.

Calculations were performed for energies up to 15 000 cm^{-1} and J up to 20 (*20, 21*). DVR3D calculations were only attempted for the more accurate DPT potential. For more details of the DVR3D calculations see Neale *et al.* (*20*).

A list of the energy levels obtained with the three calculations is reported in Table 1.

III. ASSIGNMENTS

III.1. Energy Level Labeling

To assign the measured lines we need to assign quantum numbers to the calculated energy levels. This is by no means a trivial procedure. In particular, we rapidly found that if we relied only on observed transitions and propensity rules, it was easy both to label different energy states with the same quantum numbers and to omit some rovibrational labels altogether. We therefore attempted a systematic labeling of all the low-lying energy levels of H_3^+ in conjunction with analyzing the observed transitions.

This analysis led us to change some of the labels previously assigned to particular energy states. This of course has the effect of reassigning the quantum numbers associated to transitions involving these particular energy levels. We will refer to this as relabeling transitions to distinguish it from the altogether more fundamental process of reassigning a transition to different energy states. The labeling of the rovibrational states was made in accordance with the convention of Xu *et al.* (*7*).

The H_3^+ molecule has an equilateral triangle structure and has D_{3h} symmetry. Its vibrational modes are the symmetric ''breathing'' mode ν_1 and the degenerate bending ν_2. States which include v_2 quanta of the ν_2 mode have an additional vibrational angular momentum quantum number l_2, with values given by $|l_2| = v_2, (v_2 - 2), \ldots$. So for the levels with nonzero values of l_2, the rotational quantum numbers will be the total angular momentum J, the projection of J onto the symmetry axis $G = |K - l_2|$, and the $|U| = |l_2|$ quantum numbers. The sign of U is + or − for the upper and lower levels of the l-doublet, respectively, with the sign being taken as positive when there is only one level. For levels with $v_2 = 0$ or $l_2 = 0$ the rotational quantum numbers will be J, $G = K$, and $U = 0$. We note that the only rigorous rovibrational quantum numbers are J and symmetry labels determined by whether $G + v_2$ is even or odd and whether G is divisible by 3. For a full discussion of symmetry and quantum numbers in this system see Watson (*22*).

The labeling of all the calculated energy levels is not an easy task, since the program suites used give only rigorous quantum numbers. Indeed, because of our use of scattering coordinates, we even lose the distinction between *ortho* and *para* states which depends on whether G is divisible by 3. Our programs give no indication about the other vibrational or rotational quantum numbers. A further complication is that for high energies the vibrational states start to interact heavily and the eigenfunctions are a mixture of basis states with different values of the quantum numbers. In some cases this mixing is so complete that the usual approximate quantum numbers cease to have meaning. This behavior is particularly marked for vibrational states differing only in l_2.

In our attempt to label the energy levels we used as a guide the energy patterns of the level themselves, the previously assigned energy levels (*14*), and the selection rules for the dipole transitions. Further help came from comparing our energy levels with those calculated by Watson (*23*). His program calculates expectation values of the v_1, v_2, G, and U quantum numbers for each vibration–rotation eigenfunction. This comparison proved invaluable but also showed that for many levels belonging to high vibrational states the application of these quantum numbers must be treated with caution.

The result of our labeling is shown in Table 1. For reasons given above, the labels ascribed to many of the higher levels considered are not unique and alternative labeling schemes are possible. However, the labels we propose are consistent and satisfactory. It is worth adding, however, that the rotational quantum numbers G and U are not well determined for many of the higher levels listed with $J = 4$–8, and that there is probably little point in trying to assign further levels in this fashion.

III.2. Assignment of the Transitions

Neale *et al.* (*20*) used the energy levels and wavefunctions computed by the DVR3D calculation and the DPT potential and the *ab initio* dipole surfaces of Röhse *et al.* (*9*) to calculate transition frequencies and transition probabilities for H_3^+. Their dataset, which is available electronically,[2] contains some 3 million transitions.

We used this dataset to calculate absorption spectra at

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[2] The entire linelist is available via either our group World Wide Web page on http://jonny.phys.ucl.ac.uk/home.html or anonymous ftp from jonny.phys.ucl.ac.uk (128.40.6.12) by looking in directory pub/astrodata/h3+. See Neale *et al.* (*20*) for details of how to use this data.

TABLE 1

Calculated and Observed Energy Levels, in cm^{-1}, for H_3^+ Relative to Its $J = 0$ Ground State, where n Is the Number of Combination Differences Used to Generate the Tabulated Experimental Energy Level (the Error (1σ), in cm^{-1}, Is Given when $n > 1$)

$\nu_1\nu_2^l$	J	G	U	E^D_{DPT}	E^T_{DPT}	$E_{abinitio}$	E_{exp}	$E_{exp}-E^D_{DPT}$	$Error$	n
01^1	0	1	1	2521.422	2521.422	2521.580	2521.430	0.008	0.011	4
02^2	0	2	2	4998.058	4998.058	4998.413	4997.965	−0.093	–	1
11^1	0	1	1	5554.275	5554.274	5554.614	–	–	–	
03^1	0	1	1	7006.189	7006.187	7006.620	–	–	–	
03^3	0	3	3	7493.113	7493.113	7493.712	7492.913	−0.200	–	1
12^2	0	2	2	7870.661	7870.664	7871.056	–	–	–	
00^0	1	1	0	64.126	64.126	64.125	64.126[a]	0.000	–	1
00^0	1	0	0	86.963	86.963	86.961	86.963[a]	0.000	–	1
01^1	1	2	1	2548.177	2548.176	2548.335	2548.169	−0.008	0.009	6
01^1	1	1	1	2609.552	2609.552	2609.709	2609.557	0.005	0.021	8
01^1	1	0	−1	2616.695	2616.694	2616.850	2616.648	−0.047	0.043	6
10^0	1	1	0	3240.746	3240.744	3240.843	3240.735	−0.011	0.001	3
10^0	1	0	0	3263.123	3263.122	3263.219	3263.006	−0.117	–	1
02^0	1	1	0	4842.568	4842.567	4842.792	4842.573	0.005	–	1
02^0	1	0	0	4870.313	4870.312	4870.536	4870.242	−0.071	0.046	4
02^2	1	3	2	4994.830	4994.829	4995.194	4994.832	0.002	0.002	4
02^2	1	2	2	5087.626	5087.626	5087.981	5087.622	−0.004	0.003	5
02^2	1	1	2	5125.302	5125.301	5125.644	5125.313	0.011	0.006	4
11^1	1	2	1	5584.237	5584.235	5584.588	5584.256	0.019	0.011	4
11^1	1	1	1	5640.503	5640.503	5640.845	5640.486	−0.017	0.002	3
11^1	1	0	−1	5644.746	5644.745	5645.077	–	–	–	
20^0	1	1	0	6323.290	6323.283	6323.219	–	–	–	
20^0	1	0	0	6345.290	6345.284	6345.218	–	–	–	
03^1	1	2	1	7046.855	7046.854	7047.293	7046.859	0.004	0.005	2
03^1	1	0	−1	7083.095	7083.095	7083.531	–	–	–	
03^1	1	1	1	7103.079	7103.078	7103.510	7103.090	0.011	–	1
03^3	1	4	3	7325.514	7325.514	7326.055	–	–	–	
03^3	1	3	3	7381.347	7381.347	7381.842	–	–	–	
03^3	1	2	3	7572.245	7572.244	7572.766	–	–	–	
12^0	1	1	0	7840.567	7840.562	7840.824	–	–	–	
12^0	1	0	0	7858.513	7858.509	7858.735	–	–	–	
12^2	1	3	2	7872.971	7872.971	7873.383	–	–	–	
12^2	1	2	2	7959.172	7959.172	7959.573	–	–	–	
12^2	1	1	2	7989.896	7989.897	7990.276	–	–	–	
21^1	1	2	1	8520.310	8520.304	8520.473	–	–	–	
21^1	1	1	1	8573.218	8573.222	8573.379	–	–	–	
21^1	1	0	1	8574.842	8574.839	8574.986	–	–	–	
00^0	2	2	0	169.302	169.302	169.299	169.311	0.009	0.007	9
00^0	2	1	0	237.359	237.359	237.356	237.356	−0.003	0.012	11
01^1	2	3	1	2614.284	2614.283	2614.442	2614.275	−0.009	0.004	6
01^1	2	2	1	2723.971	2723.971	2724.128	2723.970	−0.001	0.012	7
01^1	2	1	−1	2755.577	2755.577	2755.730	2755.559	−0.018	0.009	6
01^1	2	1	1	2790.353	2790.352	2790.509	2790.330	−0.023	0.022	10
01^1	2	0	1	2812.869	2812.869	2813.026	2812.843	−0.026	0.047	9
10^0	2	2	0	3343.148	3343.146	3343.242	3343.195	0.048	0.008	5
10^0	2	1	0	3409.833	3409.832	3409.926	3409.823	−0.010	0.001	4
02^0	2	2	0	4942.734	4942.733	4942.959	4942.719	−0.015	0.002	2
02^0	2	1	0	5023.471	5023.470	5023.696	5023.459	−0.012	0.019	3
02^2	2	4	2	5032.402	5032.399	5032.772	5032.400	−0.002	0.010	5
02^2	2	3	2	5181.190	5181.189	5181.555	5181.184	−0.006	0.005	7
02^2	2	2	2	5266.435	5266.435	5266.789	5266.427	−0.008	0.007	5
02^2	2	0	2	5286.921	5286.920	5287.246	5286.895	−0.026	0.004	5
02^2	2	1	2	5304.969	5304.969	5305.310	5304.966	−0.003	0.016	4
11^1	2	3	1	5654.012	5654.009	5654.380	5653.983	−0.029	0.003	7
11^1	2	2	1	5756.009	5756.008	5756.363	5756.063	0.054	0.032	4
11^1	2	1	−1	5779.011	5779.009	5779.338	5778.986	−0.025	0.003	3
11^1	2	1	1	5815.865	5815.862	5816.205	5815.857	−0.008	0.005	3
11^1	2	0	1	5835.346	5835.345	5835.681	5835.225	−0.120	0.001	4
20^0	2	2	0	6422.980	6422.972	6422.902	–	–	–	
20^0	2	1	0	6488.534	6488.531	6488.454	–	–	–	
03^1	2	3	1	7122.635	7122.635	7123.074	7122.638	0.003	0.002	2
03^1	2	1	−1	7208.350	7208.350	7208.784	7208.337	−0.013	0.001	2
03^1	2	2	1	7235.727	7235.725	7236.156	7235.761	0.034	0.003	2
03^1	2	1	1	7301.440	7301.438	7301.866	7301.424	−0.016	0.011	4
03^1	2	0	1	7328.246	7328.244	7328.649	7328.119	−0.127	0.056	4
03^3	2	5	3	7369.001	7368.995	7369.582	–	–	–	
03^3	2	4	3	7514.821	7514.820	7515.349	–	–	–	
00^3	2	1	3	7703.346	7703.345	7703.711	–	–	–	
03^3	2	2	3	7752.086	7752.085	7752.602	7751.836	−0.250	–	1
03^3	2	3	3	7759.018	7759.016	7759.618	7758.878	−0.140	–	1
12^2	2	4	2	7915.377	7915.369	7915.803	–	–	–	
12^0	2	2	0	7963.931	7963.926	7964.291	–	–	–	
12^0	2	1	0	8014.297	8014.294	8014.570	–	–	–	
12^2	2	3	2	8057.661	8057.661	8058.091	8057.335	−0.326	0.002	2
12^2	2	2	2	8136.060	8136.059	8136.462	–	–	–	
12^2	2	0	2	8142.466	8142.467	8142.827	–	–	–	
12^2	2	1	2	8168.537	8168.538	8168.918	–	–	–	
21^1	2	3	1	8590.748	8590.737	8590.924	–	–	–	
21^1	2	2	1	8688.749	8688.750	8688.917	–	–	–	
21^1	2	1	−1	8704.426	8704.420	8704.562	–	–	–	
21^1	2	1	1	8744.650	8744.640	8744.794	–	–	–	
21^1	2	0	1	8761.791	8761.792	8761.939	–	–	–	
00^0	3	3	0	315.351	315.351	315.347	315.342	−0.009	0.006	9
00^0	3	2	0	428.024	428.024	428.018	428.039	0.015	0.012	10
00^0	3	1	0	494.771	494.771	494.764	494.774	0.003	0.018	8
00^0	3	0	0	516.885	516.885	516.879	516.879	−0.006	0.034	7
01^1	3	4	1	2719.489	2719.488	2719.646	2719.466	−0.023	0.031	8
01^1	3	3	1	2876.849	2876.848	2877.004	2876.839	−0.010	0.005	7
01^1	3	2	−1	2931.380	2931.380	2931.530	2931.386	0.006	0.042	9
01^1	3	2	1	2992.444	2992.443	2992.599	2992.467	0.023	0.028	8
01^1	3	1	−1	3002.909	3002.909	3003.057	3002.897	−0.012	0.006	7
01^1	3	0	−1	3025.966	3025.965	3026.113	3025.940	−0.026	0.048	7
01^1	3	1	1	3063.481	3063.481	3063.638	3063.476	−0.005	0.011	10
10^0	3	3	0	3485.311	3485.308	3485.400	3485.280	−0.031	0.003	5
10^0	3	2	0	3595.745	3595.744	3595.832	3595.773	0.028	0.008	4
10^0	3	1	0	3661.091	3661.090	3661.176	3661.077	−0.014	0.001	4
10^0	3	0	0	3682.731	3682.730	3682.815	3682.610	−0.121	0.001	4
02^0	3	3	0	5078.934	5078.933	5079.159	5078.925	−0.009	0.005	4
02^2	3	5	2	5105.290	5105.284	5105.665	5105.311	0.021	0.004	4
02^0	3	2	0	5210.795	5210.794	5211.021	5210.797	0.002	0.012	4
02^0	3	1	0	5282.316	5282.315	5282.547	5282.299	−0.017	0.002	3
02^2	3	4	2	5299.236	5299.233	5299.606	5299.249	0.013	0.025	6
02^0	3	0	0	5305.584	5305.583	5305.815	5305.608	0.024	0.044	4
02^2	3	3	2	5431.119	5431.118	5431.480	5431.119	−0.001	0.008	6
02^2	3	1	−2	5486.459	5486.458	5486.755	5486.447	−0.012	0.010	5
02^2	3	2	2	5533.739	5533.738	5534.091	5533.747	0.008	0.009	6
02^2	3	0	2	5567.404	5567.403	5567.720	5567.370	−0.034	0.004	5
02^2	3	1	2	5573.768	5573.767	5574.106	5573.754	−0.014	0.010	5
11^1	3	4	1	5764.881	5764.873	5765.272	5764.849	−0.032	0.017	4
11^1	3	3	1	5910.108	5910.105	5910.478	5910.079	−0.029	0.003	5
11^1	3	2	−1	5949.457	5949.454	5949.780	5949.352	−0.105	0.002	2
11^1	3	2	1	6015.948	6015.945	6016.300	6015.990	0.042	0.008	4
11^1	3	1	−1	6023.774	6023.772	6024.104	6023.755	−0.019	0.001	4
11^1	3	0	−1	6047.545	6047.543	6047.877	6047.424	−0.121	0.001	2
11^1	3	1	1	6080.969	6080.969	6081.311	6080.965	−0.004	–	1
20^0	3	3	0	6561.305	6561.293	6561.214	–	–	–	
20^0	3	2	0	6669.894	6669.886	6669.797	–	–	–	
20^0	3	1	0	6734.054	6734.048	6733.952	–	–	–	
20^0	3	0	0	6755.287	6755.282	6755.184	–	–	–	
03^1	3	4	1	7229.814	7229.819	7230.265	–	–	–	
03^1	3	2	−1	7362.202	7362.213	7362.645	7362.221	0.019	0.005	2
03^1	3	3	1	7394.009	7394.007	7394.450	–	–	–	
03^3	3	6	3	7418.489	7418.485	7419.111	7418.421	−0.068	0.001	2
03^1	3	1	−1	7460.013	7460.014	7460.453	–	–	–	
03^1	3	2	1	7498.060	7498.056	7498.511	–	–	–	
03^1	3	0	−1	7525.657	7525.654	7526.073	–	–	–	
03^1	3	1	1	7597.116	7597.114	7597.558	–	–	–	
03^3	3	5	3	7659.583	7659.577	7660.118	–	–	–	
03^3	3	4	3	7796.717	7796.715	7797.231	7796.601	−0.116	–	1
03^3	3	3	3	7854.570	7854.569	7855.026	7854.413	−0.158	0.001	2
03^3	3	0	3	7866.781	7866.782	7866.992	7866.287	−0.494	0.003	3
03^3	3	1	3	7978.189	7978.186	7978.528	–	–	–	
03^3	3	2	3	7991.947	7991.928	7992.382	–	–	–	
12^0	3	5	0	8017.964	8017.963	8018.468	8017.719	−0.245	0.002	2
12^0	3	3	0	8139.349	8139.345	8139.828	8139.053	−0.296	0.003	2
12^2	3	4	2	8177.253	8177.246	8177.688	–	–	–	
12^0	3	2	0	8221.198	8221.193	8221.587	–	–	–	
12^0	3	1	0	8260.623	8260.620	8260.939	–	–	–	
12^0	3	0	0	8275.229	8275.225	8275.506	–	–	–	
12^2	3	3	2	8302.417	8302.413	8302.826	8302.090	−0.327	0.002	2
12^2	3	1	−2	8335.707	8335.708	8336.026	–	–	–	
12^2	3	2	2	8400.800	8400.798	8401.206	–	–	–	
12^2	3	0	2	8425.805	8425.804	8426.141	8425.297	−0.508	–	1
12^2	3	1	2	8435.779	8435.778	8436.157	–	–	–	
21^1	3	4	1	8700.775	8700.749	8700.961	–	–	–	
21^1	3	3	1	8841.675	8841.664	8841.846	–	–	–	
21^1	3	2	1	8869.043	8869.032	8869.169	–	–	–	
21^1	3	0	1	8942.580	8942.571	8942.732	–	–	–	
21^1	3	1	−1	8946.401	8946.396	8946.535	–	–	–	
21^1	3	1	1	9003.710	9003.711	9003.857	–	–	–	
00^0	4	4	0	502.038	502.038	502.032	502.035	−0.003	0.011	7
00^0	4	3	0	658.720	658.720	658.712	658.707	−0.013	0.007	10
00^0	4	2	0	768.478	768.478	768.468	768.513	0.035	0.019	7
00^0	4	1	0	833.585	833.585	833.574	833.583	−0.002	0.014	6
01^1	4	5	1	2863.940	2863.937	2864.095	2863.959	0.019	0.002	6
01^1	4	4	1	3069.324	3069.324	3069.479	3069.313	−0.011	0.031	7
01^1	4	3	−1	3145.285	3145.284	3145.431	3145.266	−0.019	0.006	9
01^1	4	3	1	3233.378	3233.378	3233.533	3233.368	−0.010	0.005	11
01^1	4	2	−1	3260.225	3260.224	3260.367	3260.258	0.033	0.019	10
01^1	4	1	−1	3326.123	3326.122	3326.263	3326.134	0.011	0.025	9
01^1	4	2	1	3351.389	3351.389	3351.546	3351.420	0.031	0.022	9
01^1	4	1	1	3423.128	3423.127	3423.286	3423.135	0.007	0.039	11
01^1	4	0	1	3447.056	3447.056	3447.215	3446.999	−0.057	0.057	7
10^0	4	4	0	3667.123	3667.119	3667.206	3667.096	−0.027	0.014	6
10^0	4	3	0	3820.803	3820.802	3820.884	3820.769	−0.034	0.002	4
10^0	4	2	0	3928.174	3928.173	3928.251	3928.255	0.081	0.005	3
10^0	4	1	0	3991.832	3991.831	3991.907	3991.802	−0.030	–	1
02^2	4	6	2	5215.740	5215.728	5216.116	5215.728	−0.012	0.003	8
02^0	4	4	0	5251.742	5251.740	5251.967	5251.731	−0.011	0.006	3
02^0	4	3	0	5434.332	5434.331	5434.558	5434.325	−0.007	–	1
02^2	4	5	2	5460.460	5460.459	5460.839	5460.480	0.020	0.004	4
02^0	4	2	0	5544.207	5544.206	5544.444	5544.236	0.029	0.014	3
02^0	4	1	0	5610.437	5610.436	5610.676	5610.474	0.037	0.009	2
02^2	4	4	2	5652.477	5652.474	5652.845	5652.445	−0.033	0.032	5
02^2	4	2	−2	5716.495	5716.493	5716.745	5716.525	0.030	0.015	6
02^2	4	3	2	5811.011	5811.011	5811.379	5810.997	−0.014	0.003	6
02^2	4	1	−2	5846.805	5846.804	5847.098	5846.810	0.005	0.010	4
02^2	4	2	2	5888.319	5888.318	5888.669	5888.354	0.035	0.037	7
02^2	4	0	−2	5896.853	5896.852	5897.177	5896.797	−0.056	0.058	6
11^1	4	5	1	5920.871	5920.857	5921.299	5920.926	0.055	0.034	6
02^2	4	1	2	5931.890	5931.889	5932.222	5931.894	0.004	0.011	5
11^1	4	4	1	6105.627	6105.625	6106.027	6105.619	−0.008	0.018	5
11^1	4	3	−1	6158.283	6158.278	6158.602	6158.238	−0.045	0.001	2
11^1	4	3	1	6254.695	6254.691	6255.063	6254.674	−0.021	0.004	5
11^1	4	2	−1	6276.387	6276.385	6276.716	6276.403	0.016	0.001	2
11^1	4	1	−1	6342.599	6342.596	6342.930	6342.577	−0.022	–	1
11^1	4	2	1	6363.408	6363.408	6363.758	6363.439	0.031	0.007	3
11^1	4	1	1	6430.939	6430.936	6431.279	6430.940	0.001	–	1
11^1	4	0	1	6453.656	6453.655	6453.995	6453.547	−0.109	0.003	3
20^0	4	4	0	6738.213	6738.192	6738.103	–	–	–	
20^0	4	3	0	6889.418	6889.412	6889.306	–	–	–	
20^0	4	2	0	6994.796	6994.789	6994.672	–	–	–	
20^0	4	1	0	7057.203	7057.200	7057.077	–	–	–	
00^1	4	5	1	7373.451	7373.464	7373.913	–	–	–	
03^3	4	7	3	7514.282	7514.265	7514.932	–	–	–	
03^1	4	3	−1	7550.328	7550.359	7550.782	7550.310	−0.018	0.010	4
03^1	4	4	1	7597.934	7597.935	7598.374	–	–	–	
03^1	4	2	−1	7700.837	7700.839	7701.270	–	–	–	
03^1	4	1	−1	7773.164	7773.162	7773.611	–	–	–	
03^3	4	6	−3	7786.796	7786.796	7787.423	7786.712	−0.084	0.003	3
03^1	4	3	1	7794.820	7794.816	7795.219	–	–	–	
03^1	4	2	1	7915.238	7915.236	7915.635	7915.176	−0.062	0.001	2
03^1	4	1	1	7966.167	7966.171	7966.621	–	–	–	
03^1	4	0	1	8031.022	8031.021	8031.419	8030.990	−0.032	0.011	3
03^3	4	5	3	8035.925	8035.919	8036.360	–	–	–	

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[a] Fixed at their *ab initio* values.

TABLE 1—*Continued*

$\nu_1\nu_2^l$	J	G	U	E^D_{DPT}	E^T_{DPT}	$E_{abinitio}$	E_{exp}	$E_{exp}-E^D_{DPT}$	$Error$	n
03^3	4	1	−3	8074.133	8074.131	8074.305	–	–	–	
12^2	4	6	2	8105.507	8105.462	8105.940	8105.827	0.320	–	1
03^3	4	4	3	8167.631	8167.631	8168.133	–	–	–	
03^3	4	0	−3	8248.193	8248.191	8248.348	–	–	–	
03^3	4	1	3	8332.286	8332.285	8332.586	–	–	–	
12^2	4	5	2	8340.316	8340.313	8340.779	–	–	–	
12^0	4	4	0	8364.906	8364.907	8365.480	–	–	–	
03^3	4	3	3	8365.676	8365.672	8366.278	8365.475	−0.201	–	1
03^3	4	2	3	8366.381	8366.380	8366.860	8366.198	−0.183	0.010	3
12^0	4	3	0	8483.503	8483.501	8484.031	–	–	–	
12^2	4	4	−2	8522.865	8522.855	8523.302	–	–	–	
12^2	4	4	2	8532.782	8532.779	8533.191	–	–	–	
12^0	4	4	0	8573.147	8573.145	8573.469	–	–	–	
12^0	4	1	0	8579.374	8579.371	8579.743	–	–	–	
12^2	4	3	2	8679.799	8679.799	8680.254	–	–	–	
12^2	4	1	−2	8696.738	8696.737	8697.057	8696.617	−0.121	–	1
12^2	4	0	2	8748.469	8748.470	8748.842	–	–	–	
12^2	4	2	2	8751.784	8751.782	8752.189	8751.510	−0.274	0.003	2
12^2	4	1	2	8790.807	8790.808	8791.174	–	–	–	
21^1	4	5	1	8852.636	–	–	–	–	–	
21^1	4	3	−1	9071.260	–	–	–	–	–	
00^0	5	5	0	729.014	729.012	729.004	729.035	0.021	0.007	6
00^0	5	4	0	928.975	928.974	928.963	928.972	−0.003	0.011	8
00^0	5	3	0	1080.490	1080.489	1080.476	1080.473	−0.017	0.032	10
00^0	5	2	0	1187.108	1187.108	1187.094	1187.148	0.040	0.047	9
00^0	5	1	0	1250.311	1250.311	1250.296	1250.300	−0.011	0.008	5
00^0	5	0	0	1271.269	1271.269	1271.254	1271.234	−0.035	0.012	5
01^1	5	6	1	3047.387	3047.378	3047.537	3047.378	−0.009	0.004	6
01^1	5	5	1	3300.131	3300.127	3300.281	3300.155	0.024	0.007	8
01^1	5	4	−1	3396.538	3396.536	3396.678	3396.537	−0.001	0.013	7
01^1	5	4	1	3510.150	3510.148	3510.302	3510.141	−0.009	0.027	9
01^1	5	3	−1	3553.340	3553.340	3553.477	3553.326	−0.014	0.007	8
01^1	5	2	−1	3660.349	3660.349	3660.483	3660.392	0.043	0.016	9
01^1	5	3	1	3673.964	3673.963	3674.120	3673.953	−0.011	0.007	10
01^1	5	1	−1	3722.638	3722.638	3722.771	3722.608	−0.030	0.033	6
01^1	5	0	−1	3743.187	3743.186	3743.319	3743.151	−0.036	0.011	5
01^1	5	2	1	3793.033	3793.032	3793.192	3793.077	0.044	0.058	8
01^1	5	1	1	3863.413	3863.412	3863.574	3863.404	−0.009	0.008	5
10^0	5	5	0	3888.684	3888.674	3888.755	3888.732	0.048	0.016	6
10^0	5	4	0	4084.721	4084.717	4084.791	4084.712	−0.009	0.004	4
10^0	5	3	0	4232.699	4232.696	4232.765	4232.654	−0.045	0.007	6
10^0	5	2	0	4337.030	4337.028	4337.094	–	–	–	
10^0	5	1	0	4398.704	4398.703	4398.766	–	–	–	
10^0	5	0	0	4419.147	4419.146	4419.209	–	–	–	
02^2	5	7	2	5363.836	5363.811	5364.206	5363.823	−0.013	0.002	4
02^0	5	5	0	5460.465	5460.461	5460.688	5460.477	0.012	0.001	2
02^2	5	6	2	5659.225	5659.211	5659.598	5659.212	−0.013	0.006	6
02^0	5	4	0	5690.840	5690.837	5691.065	5690.840	0.000	0.003	2
02^0	5	3	0	5830.419	5830.418	5830.661	5830.426	0.007	0.003	5
02^2	5	5	2	5899.400	5899.392	5899.769	5899.413	0.013	0.008	5
02^0	5	2	0	5939.691	5939.690	5939.936	5939.740	0.049	0.002	2
02^2	5	3	−2	5971.239	5971.225	5971.429	5971.218	−0.021	0.003	5
02^0	5	1	0	6003.163	6003.162	6003.412	6003.066	−0.097	0.085	3
02^0	5	0	0	6023.076	6023.074	6023.325	6023.059	−0.017	0.002	2
02^2	5	4	2	6089.819	6089.814	6090.182	6089.820	0.001	0.005	5
11^1	5	6	1	6129.561	6129.537	6130.024	6129.513	−0.048	0.017	5
02^2	5	2	−2	6169.466	6169.463	6169.711	6169.490	0.024	0.003	3
02^2	5	3	2	6213.702	6213.699	6214.051	6213.699	−0.003	0.001	4
02^2	5	1	−2	6276.731	6276.729	6277.030	6276.715	−0.016	0.029	5
02^2	5	2	2	6327.961	6327.958	6328.298	6327.978	0.017	0.009	4
11^1	5	5	1	6346.289	6346.275	6346.731	6346.337	0.048	0.013	6
02^2	5	1	2	6376.537	6376.535	6376.859	6376.482	−0.055	0.073	7
02^2	5	0	2	6391.893	6391.892	6392.202	6391.837	−0.056	0.003	4
11^1	5	4	−1	6410.568	6410.556	6410.883	6410.503	−0.065	0.007	3
11^1	5	4	1	6529.265	6529.256	6529.651	6529.235	−0.030	0.007	3
11^1	5	3	−1	6568.277	6568.272	6568.610	6568.224	−0.053	0.006	4
11^1	5	2	−1	6672.774	6672.770	6673.104	6672.827	0.053	–	1
11^1	5	3	1	6679.233	6679.229	6679.581	–	–	–	
11^1	5	1	−1	6733.247	6733.245	6733.577	–	–	–	
11^1	5	0	1	6753.128	6753.125	6753.455	–	–	–	
11^1	5	2	1	6792.501	6792.497	6792.840	6792.622	0.122	0.006	2
11^1	5	1	1	6859.851	6859.850	6860.188	6859.842	−0.009	–	1
20^0	5	5	0	6953.812	6953.763	6953.661	–	–	–	
20^0	5	4	0	7146.931	7146.912	7146.787	–	–	–	
20^0	5	3	0	7292.111	7292.099	7291.957	–	–	–	
20^0	5	2	0	7394.378	7394.369	7394.216	–	–	–	
20^0	5	1	0	7454.731	7454.723	7454.563	–	–	–	
20^0	5	0	0	7474.726	7474.719	7474.557	–	–	–	
03^1	5	6	1	7552.148	7552.197	7552.643	–	–	–	
03^3	5	8	3	7638.501	7638.479	7639.162	–	–	–	
03^1	5	4	−1	7767.965	7768.065	7768.473	7767.915	−0.050	0.001	3
03^1	5	5	1	7830.292	7830.294	7830.735	–	–	–	
03^1	5	3	−1	7963.536	7963.554	7963.994	7963.575	0.039	0.002	2
03^3	5	7	3	7963.769	7963.756	7964.408	–	–	–	
03^1	5	4	1	8053.102	8053.113	8053.552	–	–	–	
03^1	5	2	−1	8090.127	8090.145	8090.564	–	–	–	
03^1	5	0	−1	8137.599	8137.611	8138.114	8137.588	−0.011	0.002	2
03^1	5	1	−1	8152.309	8152.323	8152.790	–	–	–	
03^1	5	3	1	8229.624	8229.620	8230.024	8229.538	−0.086	–	1
12^2	5	7	2	8256.630	8256.524	8257.027	–	–	–	
03^1	5	2	1	8269.095	8269.095	8269.180	–	–	–	
03^3	5	6	3	8277.121	8277.102	8277.688	8277.017	−0.104	0.002	3
03^3	5	2	−3	8396.945	8396.941	8397.273	8396.868	−0.077	0.005	2
03^1	5	1	1	8404.998	8404.992	8405.405	8404.715	−0.283	0.002	2
03^3	5	5	3	8485.553	8485.544	8485.982	–	–	–	
12^2	5	6	2	8539.900	8539.855	8540.344	–	–	–	
03^3	5	1	−3	8557.124	8557.118	8557.286	–	–	–	
03^3	5	4	3	8620.290	–	–	–	–	–	
12^0	5	5	0	8634.809	–	–	8634.696	−0.113	0.003	3
03^3	5	0	3	8651.706	–	–	–	–	–	
03^3	5	3	3	8683.163	8683.162	8683.543	8682.934	−0.229	–	1
03^3	5	1	3	8759.116	8759.117	8759.363	–	–	–	
12^2	5	5	2	8774.309	–	–	–	–	–	
03^3	5	2	3	8793.047	–	–	–	–	–	
12^0	5	4	0	8793.787	8793.786	8794.382	–	–	–	
12^2	5	3	−2	8808.113	–	–	–	–	–	
12^0	5	3	0	8886.702	–	–	8887.025	0.323	0.003	2
12^0	5	2	0	8938.016	8938.011	8938.545	–	–	–	
00^0	6	6	0	995.875	995.871	995.860	995.871	−0.004	0.004	7
00^0	6	5	0	1238.450	1238.449	1238.435	1238.465	0.015	0.008	7
00^0	6	4	0	1430.716	1430.715	1430.698	1430.705	−0.011	0.020	8
00^0	6	3	0	1577.333	1577.333	1577.315	1577.325	−0.008	0.070	8
00^0	6	2	0	1679.792	1679.792	1679.774	1679.832	0.040	0.056	7
00^0	6	1	0	1740.895	1740.895	1740.877	1740.871	−0.024	0.052	5
01^1	6	7	1	3269.591	3269.576	3269.733	3269.584	−0.007	0.001	5
01^1	6	6	1	3569.452	3569.450	3569.602	3569.450	−0.002	0.003	7
01^1	6	5	−1	3685.102	3685.098	3685.235	3685.103	0.001	0.004	5
01^1	6	5	1	3825.423	3825.419	3825.573	3825.455	0.032	0.008	7
01^1	6	4	−1	3884.134	3884.133	3884.265	3884.122	−0.012	0.005	6
01^1	6	3	−1	4030.044	4030.042	4030.170	4030.049	0.005	0.012	8
01^1	6	4	1	4035.774	4035.773	4035.931	4035.774	0.000	0.007	8
01^1	6	2	−1	4129.322	4129.322	4129.447	4129.342	0.020	0.006	6
10^0	6	6	0	4147.059	4147.039	4147.117	4147.014	−0.045	0.032	7
01^1	6	1	−1	4188.794	4188.793	4188.916	4188.794	0.000	0.008	5
01^1	6	3	1	4202.298	4202.296	4202.454	4202.295	−0.003	0.013	9
01^1	6	2	1	4309.351	4309.350	4309.514	4309.367	0.016	0.007	4
01^1	6	1	1	4378.369	4378.368	4378.536	4378.351	−0.018	0.004	3
10^0	6	5	0	4389.280	4389.276	4389.342	4389.403	0.123	0.093	5
01^1	6	0	1	4401.070	4401.070	4401.239	4401.034	−0.036	0.008	7
10^0	6	4	0	4575.975	4575.969	4576.027	–	–	–	
10^0	6	3	0	4719.288	4719.287	4719.339	–	–	–	
10^0	6	2	0	4818.399	4818.397	4818.447	–	–	–	
10^0	6	1	0	4877.835	4877.834	4877.882	–	–	–	
02^2	6	8	2	5549.663	5549.618	5550.018	5549.620	−0.043	0.019	5
02^0	6	6	0	5705.062	5705.062	5705.287	5705.030	−0.032	0.001	2
02^2	6	7	2	5895.799	5895.794	5896.186	5895.802	0.003	0.002	6
02^0	6	5	0	5983.883	5983.887	5984.115	5983.907	0.024	0.004	3
02^0	6	4	0	6141.253	6141.242	6141.475	6141.263	0.010	0.002	2
02^2	6	6	2	6184.529	6184.515	6184.899	6184.518	−0.011	–	1
02^2	6	4	−2	6250.761	6250.711	6250.915	6250.728	−0.033	0.009	4
02^0	6	3	0	6301.421	6301.423	6301.666	6301.448	0.027	0.015	3
02^0	6	2	0	6394.856	6394.853	6395.124	6394.898	0.042	0.012	4
11^1	6	7	1	6403.553	6403.535	6404.011	6403.528	−0.025	0.010	3
02^2	6	5	2	6415.726	6415.725	6416.088	6415.757	0.031	0.005	4
02^0	6	1	0	6461.094	6461.093	6461.361	–	–	–	
02^2	6	3	−2	6516.158	6516.151	6516.341	6516.147	−0.011	0.001	4
02^2	6	4	2	6608.131	6608.125	6608.489	6608.134	0.003	0.004	3
11^1	6	6	1	6638.948	6638.941	6639.439	6638.933	−0.015	0.017	6
11^1	6	5	−1	6650.963	6650.943	6651.225	6651.004	0.041	0.020	4
02^2	6	2	−2	6724.739	6724.725	6725.025	6724.759	0.020	0.016	3
02^2	6	1	−2	6768.681	6768.681	6768.989	6768.642	−0.039	0.017	3
02^2	6	3	2	6775.358	6775.357	6775.742	6775.352	−0.006	0.009	7
02^2	6	0	−2	6803.698	6803.696	6804.026	6803.651	−0.047	0.003	5
11^1	6	5	1	6842.622	6842.606	6842.977	6842.985	0.363	–	1
02^2	6	2	2	6858.605	6858.601	6859.013	6858.719	0.114	0.076	4
02^2	6	1	2	6885.842	6885.837	6886.151	6885.821	−0.021	0.003	3
11^1	6	4	−1	6929.198	6929.195	6929.557	6929.371	0.173	0.136	2
11^1	6	4	1	7034.272	7034.268	7034.635	–	–	–	
11^1	6	3	−1	7043.316	7043.306	7043.641	7043.252	−0.064	0.010	2
11^1	6	2	−1	7136.912	7136.909	7137.244	–	–	–	
11^1	6	3	1	7184.161	7184.134	7184.392	7184.092	−0.069	0.010	2
11^1	6	1	−1	7192.479	7192.474	7192.801	–	–	–	
20^0	6	6	0	7214.030	7213.952	7213.932	–	–	–	
11^1	6	2	1	7295.745	7295.744	7296.072	–	–	–	
11^1	6	1	1	7361.886	7361.884	7362.213	–	–	–	
11^1	6	0	1	7383.828	7383.827	7384.155	–	–	–	
20^0	6	5	0	7443.884	7443.859	7443.715	–	–	–	
20^0	6	4	0	7627.681	7627.656	7627.487	–	–	–	
03^1	6	7	1	7766.287	7766.465	7766.904	–	–	–	
20^0	6	3	0	7768.154	7768.146	7767.959	–	–	–	
03^3	6	9	3	7797.323	7797.285	7797.973	–	–	–	
20^0	6	2	0	7864.856	7864.845	7864.647	–	–	–	
20^0	6	1	0	7922.880	7922.876	7922.672	–	–	–	
03^1	6	5	−1	8019.092	8019.358	8019.741	–	–	–	
03^1	6	6	1	8097.710	8097.770	8098.209	–	–	–	
03^3	6	8	3	8180.188	8180.196	8180.869	8180.118	−0.070	0.005	2
03^1	6	4	−1	8274.552	8274.621	8275.037	–	–	–	
03^1	6	5	1	8375.919	8375.895	8376.307	–	–	–	
03^1	6	3	−1	8412.419	8412.507	8412.850	–	–	–	
12^2	6	8	2	8446.541	8446.326	8446.858	–	–	–	
03^3	6	7	3	8481.110	8481.102	8481.710	–	–	–	
03^1	6	2	−1	8515.847	8515.867	8516.321	–	–	–	
12^0	6	6	0	8549.321	8549.269	8549.332	–	–	–	
03^1	6	1	−1	8604.645	8604.629	8605.129	8604.581	−0.064	0.001	2
03^1	6	4	1	8623.336	8623.335	8623.717	–	–	–	
03^3	6	6	3	8756.603	8756.604	8757.190	–	–	–	
12^2	6	7	2	8777.254	8777.218	8777.734	–	–	–	
03^3	6	4	3	8794.869	8794.866	8794.983	–	–	–	
03^1	6	3	1	8833.809	8833.818	8834.207	8833.678	−0.131	0.001	2
03^3	6	5	3	8897.504	8897.532	8897.855	–	–	–	
03^1	6	2	1	8946.148	8946.149	8946.427	–	–	–	
03^3	6	3	−3	8947.057	8947.148	8947.734	8946.868	−0.189	0.003	2
03^1	6	0	1	8972.477	8972.480	8972.886	–	–	–	
03^1	6	1	1	8984.203	8984.157	8984.513	–	–	–	
03^3	6	1	−3	9038.356	9038.284	9038.685	–	–	–	
12^2	6	6	2	9061.717	9061.679	9062.202	–	–	–	
12^0	6	4	0	9130.050	9129.964	9130.063	–	–	–	
03^3	6	2	−3	9142.343	9142.346	9142.876	9141.890	−0.453	0.002	2
03^3	6	2	3	9158.670	9158.675	9159.238	–	–	–	
12^0	6	3	0	9189.171	9189.165	9189.344	–	–	–	
12^0	6	2	0	9246.105	9246.109	9246.342	–	–	–	
12^2	6	4	−2	9281.639	–	–	–	–	–	
12^0	6	5	0	9284.200	9284.195	9284.562	–	–	–	
03^3	6	3	3	9290.095	–	–	–	–	–	
12^2	6	5	2	9296.952	9296.950	9297.437	9296.939	−0.013	0.002	2
12^2	6	4	2	9313.412	–	–	–	–	–	
12^2	6	3	−2	9376.019	9375.998	9376.158	–	–	–	
03^3	6	0	3	9409.633	9409.635	9410.260	–	–	–	
03^3	6	1	3	9428.762	0.000	0.000	9428.588	−0.174	0.003	2
12^0	6	1	0	9440.524	9440.519	9441.076	–	–	–	
12^2	6	4	−2	9472.583	–	–	–	–	–	
12^2	6	2	−2	9510.754	–	–	–	–	–	
21^1	6	6	1	9548.477	9548.430	9548.744	–	–	–	
21^1	6	7	1	9607.785	–	–	–	–	–	
12^2	6	1	−2	9612.812	9612.812	9613.150	–	–	–	
12^2	6	3	2	9625.362	–	–	–	–	–	
00^0	7	7	0	1302.141	1302.134	1302.120	1302.133	−0.008	0.007	7
00^0	7	6	0	1586.589	1586.586	1586.568	1586.577	−0.012	0.002	7
00^0	7	5	0	1818.140	1818.138	1818.117	1818.197	0.057	0.085	6

TABLE 1—*Continued*

$\nu_1\nu_2^l$	J	G	U	E^D_{DPT}	E^T_{DPT}	$E_{abinitio}$	E_{exp}	$E_{exp}-E^D_{DPT}$	*Error*	n
00^0	7	4	0	2002.457	2002.455	2002.434	2002.454	−0.003	0.017	7
00^0	7	3	0	2142.099	2142.098	2142.077	2142.106	0.007	0.057	7
00^0	7	2	0	2241.988	2241.987	2241.966	2241.990	0.002	0.011	4
00^0	7	1	0	2300.853	2300.852	2300.831	2300.850	−0.003	0.004	5
00^0	7	0	0	2320.389	2320.389	2320.368	2320.367	−0.022	0.027	4
01^1	7	8	1	3530.264	3530.233	3530.387	3530.227	−0.037	0.026	6
01^1	7	7	1	3877.035	3877.024	3877.173	3877.034	−0.001	0.007	6
01^1	7	6	−1	4010.255	4010.248	4010.378	4010.227	−0.028	0.004	3
01^1	7	6	1	4177.910	4177.901	4178.054	4177.903	−0.007	0.003	9
01^1	7	5	−1	4249.967	4249.963	4250.087	4249.981	0.014	0.010	4
01^1	7	4	−1	4420.240	4420.220	4420.325	4420.205	−0.035	0.005	5
01^1	7	5	1	4431.677	4431.672	4431.831	4431.680	0.003	0.045	7
10^0	7	7	0	4456.901	4456.869	4456.949	4456.864	−0.037	0.002	4
01^1	7	3	−1	4562.818	4562.815	4562.931	4562.873	0.055	0.068	5
01^1	7	4	1	4636.014	4636.011	4636.174	4635.974	−0.040	0.032	4
01^1	7	2	−1	4663.865	4663.863	4663.979	4663.888	0.023	0.007	4
01^1	7	1	−1	4720.394	4720.392	4720.506	4720.405	0.011	0.006	4
10^0	7	6	0	4721.798	4721.782	4721.849	4721.692	−0.106	0.054	5
01^1	7	0	−1	4739.272	4739.270	4739.384	4739.282	0.010	0.024	4
01^1	7	3	1	4793.689	4793.686	4793.843	4793.676	−0.013	0.004	5
01^1	7	2	1	4892.026	4892.023	4892.189	4892.057	0.031	0.010	5
01^1	7	1	1	4961.695	4961.694	4961.872	4961.655	−0.040	0.066	4
10^0	7	5	0	4962.119	4962.108	4962.164	4962.125	0.006	0.001	2
10^0	7	4	0	5136.668	5136.661	5136.701	–	–	–	
10^0	7	3	0	5269.939	5269.934	5269.970	–	–	–	
10^0	7	2	0	5368.016	5368.013	5368.046	–	–	–	
10^0	7	1	0	5424.982	5424.980	5425.011	–	–	–	
10^0	7	0	0	5443.894	5443.891	5443.922	–	–	–	
02^2	7	9	2	5773.233	5773.139	5773.535	5773.095	−0.138	0.004	3
02^0	7	7	0	5985.213	5985.259	5985.471	5985.143	−0.070	–	1
02^2	7	8	2	6170.071	6170.042	6170.436	6170.045	−0.026	0.019	4
02^0	7	6	0	6312.171	6312.176	6312.399	6312.145	−0.026	0.001	4
11^1	7	8	1	6451.252	6451.157	6451.373	6451.133	−0.119	–	1
02^2	7	7	2	6505.169	6505.143	6505.531	6505.152	−0.017	0.003	4
02^0	7	5	0	6571.788	6571.716	6571.966	–	–	–	
02^0	7	4	0	6673.862	6673.864	6674.104	6673.860	−0.002	0.002	2
02^2	7	5	−2	6736.544	6736.548	6737.000	6736.506	−0.038	–	1
02^2	7	6	2	6784.067	6784.053	6784.435	6784.053	−0.014	0.002	4
02^0	7	3	0	6801.616	6801.616	6801.875	6801.641	0.025	0.008	2
02^2	7	4	−2	6863.496	6863.446	6863.661	6863.449	−0.047	0.002	2
02^0	7	2	0	6910.239	6910.238	6910.495	–	–	–	
02^0	7	1	0	6961.138	6961.137	6961.407	–	–	–	
11^1	7	6	−1	6985.211	6985.129	6985.414	6985.039	−0.172	0.005	2
02^0	7	0	0	6989.781	6989.777	6990.038	6989.820	0.039	0.009	2
11^1	7	7	1	7002.660	7002.651	7003.130	7002.638	−0.023	0.006	3
02^2	7	5	2	7027.095	7027.083	7027.449	7027.114	0.019	0.003	2
02^2	7	3	−2	7126.730	7126.706	7126.931	7126.730	0.000	0.028	5
02^2	7	2	−2	7193.270	7193.252	7193.558	7193.261	−0.009	0.003	2
11^1	7	6	1	7209.170	7209.145	7209.624	7209.164	−0.006	0.008	2
02^2	7	4	2	7215.781	7215.771	7216.112	7215.767	−0.014	0.006	3
11^1	7	5	−1	7317.772	7317.760	7318.103	7317.901	0.129	0.003	2
02^2	7	1	−2	7318.332	7318.319	7318.629	7318.308	−0.024	0.003	2
02^2	7	3	2	7340.103	7340.100	7340.448	7340.109	0.006	–	1
11^1	7	5	1	7422.572	7422.553	7422.950	7422.745	0.173	0.007	2
11^1	7	4	−1	7436.699	7436.653	7436.928	7436.682	−0.017	0.003	2
02^2	7	2	2	7462.307	7462.304	7462.660	7462.312	0.005	–	1
20^0	7	7	0	7499.698	7499.496	7499.429	–	–	–	
02^2	7	0	2	7504.964	7504.956	7505.230	7504.899	−0.065	0.001	2
02^2	7	1	2	7529.120	7529.106	7529.502	–	–	–	
11^1	7	3	−1	7595.889	7595.880	7596.305	7595.823	−0.066	0.001	2
11^1	7	4	1	7618.558	7618.539	7618.838	–	–	–	
11^1	7	2	−1	7667.411	7667.400	7667.740	–	–	–	
11^1	7	1	−1	7716.672	7716.666	7716.987	–	–	–	
11^1	7	2	1	7733.609	7733.602	7733.918	–	–	–	
11^1	7	3	1	7743.136	7743.096	7743.218	–	–	–	
20^0	7	6	0	7797.011	7796.961	7796.957	–	–	–	
11^1	7	0	1	7865.957	7865.949	7866.249	–	–	–	
11^1	7	1	1	7931.167	7931.163	7931.475	–	–	–	
03^3	7	10	3	7991.974	7991.871	7992.542	–	–	–	
20^0	7	5	0	8003.376	8003.327	8003.150	–	–	–	
03^1	7	8	1	8015.872	8016.491	8016.876	–	–	–	
20^0	7	4	0	8176.386	8176.357	8176.136	–	–	–	
03^1	7	6	1	8301.217	8302.012	8302.359	–	–	–	
20^0	7	3	0	8306.220	8306.197	8305.957	–	–	–	
03^1	7	7	1	8398.904	8399.085	8399.507	–	–	–	
20^0	7	2	0	8402.136	8402.122	8401.872	–	–	–	
03^3	7	9	3	8430.577	8430.576	8431.251	–	–	–	
20^0	7	1	0	8457.583	8457.572	8457.315	–	–	–	
20^0	7	0	0	8475.985	8475.974	8475.715	–	–	–	
03^1	7	5	−1	8610.282	8610.540	8610.931	–	–	–	
12^1	7	9	1	8670.659	8670.182	8670.661	–	–	–	
03^1	7	4	−1	8721.794	8722.076	8722.278	–	–	–	
03^3	7	6	3	8727.492	8727.513	8727.964	–	–	–	
03^3	7	8	3	8790.711	8790.710	8791.357	8790.635	−0.076	0.004	2
03^1	7	4	1	8866.842	8866.802	8866.967	–	–	–	
03^1	7	3	−1	8884.158	8884.299	8884.758	–	–	–	
03^1	7	5	1	8986.075	8986.135	8986.563	8986.260	0.185	0.002	2
03^1	7	2	−1	9019.308	9019.379	9019.844	–	–	–	
03^3	7	5	3	9045.023	9044.998	9045.453	–	–	–	
03^3	7	7	3	9059.096	9059.010	9059.570	–	–	–	
03^1	7	0	1	9074.638	9074.683	9075.144	–	–	–	
03^1	7	3	1	9139.687	9139.630	9139.680	9139.422	−0.265	0.001	2
03^1	7	1	−1	9158.549	9158.520	9159.106	9158.443	−0.106	0.001	2
03^3	7	3	−3	9364.745	9364.760	9365.131	–	–	–	
03^1	7	1	1	9438.718	9438.674	9438.919	–	–	–	
03^3	7	3	3	9558.278	9558.297	9558.810	–	–	–	
03^3	7	1	−3	9560.900	9560.899	9561.208	–	–	–	
03^3	7	1	3	9618.427	–	–	–	–	–	
12^0	7	6	0	9661.051	–	–	9661.269	0.218	0.003	2
12^2	7	8	2	9743.576	–	–	–	–	–	
12^0	7	4	0	9787.580	–	–	–	–	–	
12^2	7	6	2	9794.386	–	–	–	–	–	
12^2	7	4	−2	9846.213	–	–	–	–	–	
12^2	7	4	2	9912.230	–	–	–	–	–	
12^0	7	0	0	9979.117	–	–	9981.081	1.964	0.003	2
12^0	7	2	0	10008.072	–	–	–	–	–	
00^0	8	8	0	1647.264	1647.251	1647.232	1647.263	−0.001	0.019	6
00^0	8	7	0	1972.795	1972.792	1972.769	1972.794	−0.001	0.010	7
00^0	8	6	0	2242.196	2242.192	2242.168	2242.192	−0.004	0.013	6
00^0	8	5	0	2462.871	2462.870	2462.846	2462.895	0.024	0.007	6
00^0	8	4	0	2639.137	2639.136	2639.112	2639.114	−0.023	0.021	7
00^0	8	3	0	2775.665	2775.664	2775.641	2775.650	−0.015	0.004	6
00^0	8	2	0	2868.865	2868.864	2868.841	2868.898	0.033	0.007	5
00^0	8	1	0	2925.402	2925.402	2925.380	2925.439	0.037	0.004	2
01^1	8	9	1	3829.080	3829.006	3829.152	3829.001	−0.079	0.005	5
01^1	8	8	1	4222.571	4222.555	4222.700	4222.586	0.015	0.004	6
01^1	8	7	−1	4371.350	4371.340	4371.460	4371.304	−0.046	0.007	3
01^1	8	7	1	4567.275	4567.258	4567.409	4567.269	−0.006	0.008	6
01^1	8	6	−1	4650.944	4650.943	4651.059	4650.923	−0.021	0.002	5
10^0	8	8	0	4775.075	4774.970	4775.030	–	–	–	
01^1	8	6	1	4862.775	4862.770	4862.931	4862.767	−0.008	0.009	6
01^1	8	5	−1	4874.398	4874.389	4874.494	4874.423	0.025	0.007	3
01^1	8	4	−1	5028.380	5028.375	5028.478	5028.382	0.002	0.002	3
01^1	8	5	1	5107.243	5107.236	5107.405	5107.499	0.256	0.015	2
10^0	8	7	0	5109.762	5109.742	5109.791	5109.727	−0.035	0.003	2
01^1	8	3	−1	5171.152	5171.148	5171.254	5171.147	−0.005	0.004	4
01^1	8	2	−1	5257.293	5257.293	5257.398	5257.355	0.062	0.006	2
01^1	8	4	1	5304.865	5304.864	5305.037	5304.862	−0.003	0.006	3
01^1	8	1	−1	5312.984	5312.981	5313.085	5313.275	0.291	0.002	2
10^0	8	6	0	5361.230	5361.207	5361.258	5361.190	−0.041	0.003	3
01^1	8	3	1	5463.104	5463.100	5463.265	5463.084	−0.020	0.001	3
01^1	8	2	1	5532.724	5532.722	5532.877	5532.724	0.000	0.016	3
10^0	8	5	0	5604.262	5604.256	5604.316	–	–	–	
01^1	8	1	1	5606.759	5606.757	5606.949	5606.770	0.011	0.001	3
01^1	8	0	1	5629.053	5629.052	5629.248	5629.023	−0.030	0.002	3
10^0	8	4	0	5762.527	5762.517	5762.540	–	–	–	
10^0	8	3	0	5895.161	5895.158	5895.173	–	–	–	
10^0	8	2	0	5981.418	5981.413	5981.427	–	–	–	
02^2	8	10	2	6034.596	6034.350	6034.720	6034.183	−0.413	0.008	3
10^0	8	1	0	6035.660	6035.658	6035.671	–	–	–	
02^0	8	8	0	6300.623	6300.777	6300.942	6300.415	−0.208	0.011	2
02^2	8	9	2	6482.167	6482.121	6482.508	6482.096	−0.071	0.002	4
02^0	8	7	0	6675.684	6675.743	6675.948	6675.659	−0.025	0.002	3
02^0	8	6	0	6766.861	6766.490	6766.699	–	–	–	
02^2	8	8	2	6862.815	6862.752	6863.142	6862.761	−0.053	0.001	2
02^2	8	6	−2	6942.281	6942.273	6942.537	–	–	–	
02^0	8	5	0	7072.724	7072.735	7072.955	7072.706	−0.018	0.001	2
11^1	8	9	1	7119.176	7119.224	7119.621	7119.090	−0.086	–	1
02^2	8	7	2	7186.959	7186.941	7187.330	–	–	–	
02^2	8	5	−2	7237.520	7237.450	7237.712	–	–	–	
02^0	8	4	0	7245.067	7245.040	7245.287	7244.958	−0.109	–	1
11^1	8	7	1	7352.729	7352.558	7352.825	–	–	–	
02^0	8	3	0	7401.097	7401.109	7401.354	–	–	–	
11^1	8	8	1	7425.172	7425.174	7425.605	7425.153	−0.019	0.001	2
02^2	8	6	2	7463.685	7463.661	7464.049	7463.668	−0.017	–	1
02^0	8	2	0	7477.832	7477.834	7478.089	–	–	–	
02^0	8	1	0	7533.781	7533.778	7534.038	–	–	–	
11^1	8	7	−1	7550.602	7550.516	7550.763	7550.526	−0.076	0.001	2
11^1	8	6	−1	7620.468	7620.428	7620.695	7620.300	−0.168	0.019	2
02^2	8	4	−2	7656.528	7656.523	7656.976	7656.468	−0.060	0.001	2
02^2	8	5	2	7697.683	7697.678	7698.063	7697.612	−0.071	0.060	3
02^2	8	2	−2	7785.030	7784.756	7784.880	–	–	–	
02^2	8	3	−2	7822.671	7822.663	7822.908	7822.801	0.130	0.024	3
20^0	8	8	0	7837.454	7837.157	7837.173	–	–	–	
11^1	8	6	1	7851.264	7851.249	7851.730	7851.345	0.081	0.063	2
02^2	8	4	2	7883.923	7883.901	7884.269	7883.837	−0.086	–	1
02^2	8	1	−2	7921.815	7921.813	7922.119	–	–	–	
11^1	8	5	−1	7956.430	7956.411	7956.777	7956.398	−0.032	–	1
02^2	8	0	−2	7959.486	7959.478	7959.814	7959.475	−0.011	0.004	3
02^2	8	3	2	8043.466	8043.464	8043.890	8043.463	−0.003	0.001	2
11^1	8	4	1	8044.941	8044.907	8045.186	–	–	–	
02^2	8	2	2	8070.965	8070.936	8071.334	8071.158	0.193	0.003	2
11^1	8	5	1	8139.733	8139.726	8140.054	8139.736	0.003	0.002	2
20^0	8	7	0	8143.469	8143.360	8143.235	–	–	–	
11^1	8	3	−1	8182.810	8182.785	8183.114	–	–	–	
02^2	8	1	2	8182.904	8182.904	8183.347	8182.802	−0.102	0.011	3
03^3	8	11	3	8223.613	8223.184	8223.775	–	–	–	
11^1	8	2	−1	8253.330	8253.320	8253.639	–	–	–	
11^1	8	4	1	8288.495	8288.486	8288.755	–	–	–	
11^1	8	1	−1	8300.920	8302.399	8302.629	–	–	–	
03^1	8	9	1	8302.639	8302.622	8302.942	–	–	–	
11^1	8	3	1	8370.267	8370.193	8370.253	–	–	–	
20^0	8	6	0	8447.649	8447.590	8447.625	–	–	–	
11^1	8	2	1	8496.338	8496.331	8496.581	–	–	–	
11^1	8	1	1	8561.768	8561.763	8562.050	–	–	–	
11^1	8	0	1	8582.859	8582.857	8583.151	–	–	–	
03^1	8	7	−1	8613.966	8615.764	8615.978	–	–	–	
20^0	8	5	0	8628.830	8628.796	8628.576	–	–	–	
03^3	8	11	3	8717.479	8717.474	8718.124	–	–	–	
03^1	8	7	1	8735.931	8736.487	8736.832	–	–	–	
20^0	8	4	0	8788.825	8788.783	8788.506	–	–	–	
20^0	8	3	0	8918.808	8918.795	8918.497	–	–	–	
12^2	8	10	2	8939.320	8938.323	8938.729	–	–	–	
03^1	8	6	−1	8978.497	8979.207	8979.517	8978.285	−0.212	0.001	2
20^0	8	2	0	9001.935	9001.915	9001.604	–	–	–	
20^0	8	1	0	9054.513	9054.506	9054.189	–	–	–	
03^1	8	4	−1	9309.504	9309.798	9310.141	–	–	–	
12^2	8	9	2	9361.302	9361.014	9361.478	–	–	–	
03^1	8	6	1	9446.362	9446.385	9446.809	–	–	–	
00^0	9	9	0	2030.640	2030.604	2030.581	2030.597	−0.043	0.005	6
00^0	9	8	0	2396.415	2396.403	2396.377	2396.426	0.011	0.001	6
00^0	9	7	0	2702.080	2702.071	2702.044	2702.058	−0.022	0.013	6
00^0	9	6	0	2957.299	2957.295	2957.268	2957.266	−0.033	0.019	6
00^0	9	5	0	3167.331	3167.328	3167.302	3167.386	0.055	0.083	5
00^0	9	4	0	3335.552	3335.550	3335.526	3335.537	−0.015	0.003	4
00^0	9	3	0	3461.056	3461.054	3461.031	3461.039	−0.017	0.003	5
00^0	9	2	0	3555.426	3555.425	3555.403	3555.389	−0.037	0.014	4
00^0	9	1	0	3609.584	3609.583	3609.562	3609.597	0.013	0.002	3
00^0	9	0	0	3627.576	3627.575	3627.553	3627.526	−0.050	0.034	4
01^1	9	10	1	4165.740	4165.519	4165.650	4165.488	−0.252	0.006	3
01^1	9	9	1	4605.765	4605.702	4605.839	4605.705	−0.060	0.002	4
01^1	9	8	−1	4767.673	4767.647	4767.745	4767.580	−0.093	–	1
01^1	9	8	1	4992.989	4992.946	4993.095	4992.974	−0.015	0.001	2
01^1	9	7	−1	5086.349	5086.339	5086.442	5086.315	−0.034	0.005	4
10^0	9	9	0	5149.365	5149.097	5149.142	–	–	–	
01^1	9	7	1	5328.308	5328.290	5328.453	5328.320	0.012	0.016	4
01^1	9	6	−1	5342.114	5342.103	5342.199	5342.079	−0.035	0.010	4
10^0	9	8	0	5487.361	5487.295	5487.353	5487.331	−0.030	0.007	2

TABLE 1—*Continued*

$\nu_1\nu_2^l$	J	G	U	E^D_{DPT}	E^T_{DPT}	$E_{abinitio}$	E_{exp}	$E_{exp}-E^D_{DPT}$	*Error*	n
01^1	9	5	−1	5565.263	5565.240	5565.310	5565.265	0.002	0.008	3
01^1	9	6	1	5610.306	5610.293	5610.467	5610.320	0.014	0.024	4
01^1	9	4	−1	5689.674	5689.662	5689.756	5689.663	−0.011	0.003	3
01^1	9	3	−1	5809.386	5809.382	5809.478	5809.395	0.010	0.002	2
10^0	9	7	0	5819.804	5819.751	5819.780	–	–	–	
01^1	9	5	1	5842.874	5842.866	5843.049	5842.906	0.032	0.006	4
01^1	9	2	−1	5908.658	5908.654	5908.750	5908.627	−0.031	0.010	3
01^1	9	1	−1	5962.163	5962.162	5962.258	–	–	–	
01^1	9	0	−1	5979.190	5979.187	5979.282	5979.132	−0.058	0.038	3
01^1	9	4	1	6031.674	6031.667	6031.854	6031.665	−0.009	0.003	3
10^0	9	6	0	6053.118	6053.093	6053.140	6053.061	−0.057	0.003	3
01^1	9	3	1	6175.172	6175.164	6175.332	6175.163	−0.009	0.004	3
01^1	9	2	1	6225.602	6225.591	6225.730	6225.646	0.044	0.005	2
01^1	9	1	1	6306.772	6306.767	6306.975	6306.839	0.067	0.007	3
10^0	9	5	0	6310.318	6310.304	6310.381	6310.310	−0.008	0.006	2
02^2	9	11	2	6334.021	6333.248	6333.555	6332.834	−1.187	–	1
10^0	9	4	0	6449.191	6449.180	6449.189	–	–	–	
10^0	9	3	0	6559.034	6559.025	6559.025	–	–	–	
02^0	9	9	0	6651.032	6651.360	6651.407	6650.520	−0.512	–	1
10^0	9	2	0	6654.097	6654.091	6654.085	–	–	–	
10^0	9	1	0	6705.285	6705.282	6705.275	–	–	–	
10^0	9	0	0	6722.358	6722.353	6722.345	–	–	–	
02^2	9	10	2	6832.300	6832.081	6832.449	6831.996	−0.304	0.007	3
02^0	9	8	0	7074.147	7074.251	7074.410	7074.106	−0.041	0.002	2
11^1	9	10	1	7106.334	7105.215	7105.421	–	–	–	
02^2	9	9	2	7256.885	7256.687	7257.072	7256.658	−0.227	0.001	2
02^0	9	7	0	7349.125	7349.299	7349.508	–	–	–	
02^0	9	6	0	7487.624	7487.495	7487.688	–	–	–	
02^2	9	7	−2	7543.501	7543.596	7543.933	7543.354	−0.147	–	1
02^2	9	8	2	7622.514	7622.438	7622.829	–	–	–	
11^1	9	9	1	7651.260	7651.138	7651.412	7651.028	−0.232	0.002	2
02^0	9	5	0	7677.050	7676.750	7676.980	–	–	–	
11^1	9	8	−1	7778.014	7777.851	7778.082	–	–	–	
02^0	9	4	0	7875.517	7875.558	7875.792	–	–	–	
02^2	9	6	−2	7891.377	7891.375	7891.770	7891.306	−0.071	0.001	3
02^2	9	7	2	7935.877	7935.821	7936.214	–	–	–	
11^1	9	8	1	7980.286	7980.082	7980.367	–	–	–	
02^0	9	1	0	7983.936	7983.962	7984.216	–	–	–	
11^1	9	7	−1	8055.709	8055.573	8055.832	–	–	–	
02^0	9	2	0	8104.314	8104.325	8104.572	–	–	–	
02^0	9	5	0	8135.763	8135.771	8136.109	–	–	–	
02^0	9	0	0	8145.793	8145.796	8146.082	–	–	–	
20^0	9	9	0	8170.468	8169.255	8169.135	–	–	–	
02^2	9	5	−2	8176.105	8176.134	8176.456	–	–	–	
02^2	9	6	2	8237.773	8237.746	8238.119	8237.678	−0.095	–	1
11^1	9	6	−1	8294.224	8294.065	8294.260	–	–	–	
11^1	9	7	1	8295.873	8295.784	8296.085	–	–	–	
02^2	9	4	−2	8359.807	8359.801	8360.210	–	–	–	
02^2	9	5	2	8438.814	8438.795	8439.199	8438.783	−0.031	–	1
11^1	9	5	−1	8444.465	8444.317	8444.502	–	–	–	
03^3	9	12	3	8492.859	8491.157	8491.592	–	–	–	
02^2	9	3	−2	8500.074	8500.022	8500.391	–	–	–	
20^0	9	8	0	8548.195	8547.915	8547.833	–	–	–	
11^1	9	6	1	8564.792	8564.713	8565.057	8564.706	−0.086	0.001	2
02^2	9	1	−2	8575.423	8575.373	8575.669	–	–	–	
02^2	9	4	2	8618.660	8618.638	8618.981	–	–	–	
03^1	9	10	1	8622.296	8625.045	8624.902	–	–	–	
02^2	9	2	−2	8645.539	8645.506	8645.894	–	–	–	
11^1	9	4	−1	8707.130	8707.082	8707.362	–	–	–	
02^2	9	3	2	8762.094	8762.085	8762.428	–	–	–	
11^1	9	3	−1	8765.365	8765.332	8765.543	–	–	–	
11^1	9	5	1	8780.047	8780.011	8780.407	–	–	–	
20^0	9	7	0	8835.228	8834.993	8834.843	–	–	–	
02^2	9	1	2	8872.138	8872.109	8872.463	–	–	–	
02^2	9	2	2	8873.361	8873.347	8873.628	–	–	–	
11^1	9	2	−1	8924.623	8924.597	8925.019	–	–	–	
02^2	9	0	2	8940.060	8940.057	8940.619	–	–	–	
11^1	9	1	−1	8951.557	8951.552	8951.904	–	–	–	
02^1	9	10	1	8956.632	8958.739	8959.048	–	–	–	
11^1	9	0	1	8958.758	8959.768	8959.791	–	–	–	
11^1	9	4	1	9014.703	9014.665	9014.881	–	–	–	
03^3	9	11	3	9042.197	9041.773	9042.355	9041.265	−0.932	0.001	2
20^0	9	6	0	9051.018	9050.921	9050.826	–	–	–	
03^1	9	9	1	9108.377	9109.461	9109.632	–	–	–	
11^1	9	3	1	9164.891	9164.839	9164.827	–	–	–	
11^1	9	2	1	9180.995	9180.961	9181.137	–	–	–	
11^1	9	1	1	9247.952	9247.934	9248.185	–	–	–	
03^1	9	7	1	9376.144	9377.668	9377.782	9376.233	0.089	0.001	2
20^0	9	4	0	9460.589	9460.543	9460.208	–	–	–	
12^2	9	11	2	9714.709	9713.852	9714.259	–	–	–	
00^0	10	10	0	2451.609	–	–	–	–	–	
00^0	10	9	0	2856.729	–	–	2856.698	−0.032	0.001	5
00^0	10	8	0	3196.903	–	–	3196.912	0.009	–	1
00^0	10	7	0	3484.774	–	–	3484.755	−0.019	0.004	4
00^0	10	6	0	3726.563	–	–	3726.549	−0.014	0.009	5
00^0	10	5	0	3926.171	–	–	3926.188	0.017	0.001	3
00^0	10	4	0	4086.428	–	–	4086.412	−0.016	0.005	3
00^0	10	3	0	4215.239	–	–	4215.210	−0.029	0.004	4
00^0	10	2	0	4296.621	–	–	–	–	–	
00^0	10	1	0	4348.363	–	–	4348.423	0.060	0.004	2
01^1	10	11	1	4539.952	–	–	4539.256	−0.696	–	1
01^1	10	10	1	5026.286	–	–	–	–	–	
01^1	10	9	−1	5198.463	–	–	5198.195	−0.268	0.001	3
01^1	10	9	1	5454.531	–	–	5454.402	−0.129	0.002	3
01^1	10	8	−1	5555.503	–	–	5555.435	−0.068	–	1
10^0	10	10	0	5559.156	–	–	–	–	–	
01^1	10	8	1	5827.729	–	–	5827.725	−0.004	0.001	3
01^1	10	7	−1	5842.782	–	–	5842.700	−0.082	0.005	3
10^0	10	9	0	5944.843	–	–	–	–	–	
01^1	10	6	−1	6087.546	–	–	6087.491	−0.055	0.013	3
01^1	10	7	1	6145.235	–	–	6145.206	−0.029	0.003	2
01^1	10	5	−1	6226.789	–	–	6226.730	−0.059	0.011	2
01^1	10	1	−1	6326.432	–	–	–	–	–	
01^1	10	4	−1	6401.110	–	–	6401.093	−0.017	0.005	2
01^1	10	6	1	6412.298	–	–	6412.266	−0.032	0.002	3
01^1	10	3	−1	6539.917	–	–	6539.914	−0.003	0.004	3
10^0	10	7	0	6579.774	–	–	–	–	–	
01^1	10	2	−1	6612.443	–	–	–	–	–	
01^1	10	5	1	6628.627	–	–	6628.605	−0.022	0.011	2
01^1	10	1	−1	6666.069	–	–	–	–	–	
02^2	10	12	2	6671.817	–	–	6668.926	−2.891	0.001	2
10^0	10	6	0	6804.443	–	–	–	–	–	
01^1	10	4	1	6811.731	–	–	6811.713	−0.019	0.002	3
01^1	10	3	1	6959.027	–	–	6959.003	−0.024	0.002	2
10^0	10	5	0	6967.289	–	–	6967.239	−0.050	0.005	2
02^0	10	10	0	7036.309	–	–	7035.025	−1.284	–	1
01^1	10	1	1	7055.249	–	–	7055.291	0.042	0.002	2
01^1	10	2	1	7072.408	–	–	–	–	–	
01^1	10	0	1	7080.385	–	–	7080.398	0.013	0.003	3
10^0	10	4	0	7191.838	–	–	–	–	–	
02^2	10	11	2	7220.652	–	–	7219.741	−0.911	–	1
10^0	10	3	0	7316.346	–	–	–	–	–	
10^0	10	2	0	7381.697	–	–	–	–	–	
10^0	10	1	0	7429.303	–	–	–	–	–	
11^1	10	11	1	7477.810	–	–	–	–	–	
02^2	10	10	2	7687.224	–	–	–	–	–	
02^0	10	8	0	7787.014	–	–	–	–	–	
02^2	10	8	−2	8006.515	–	–	8006.238	−0.277	0.001	2
02^0	10	7	0	8109.399	–	–	8110.218	0.819	0.001	2
02^2	10	6	−2	8109.734	–	–	–	–	–	
02^0	10	6	0	8259.969	–	–	–	–	–	
11^1	10	8	−1	8380.666	–	–	8380.427	−0.239	–	1
02^2	10	8	2	8443.842	–	–	–	–	–	
02^2	10	6	2	8445.703	–	–	–	–	–	
11^1	10	6	−1	9057.019	–	–	–	–	–	
11^1	10	6	1	9347.039	–	–	9346.842	−0.197	0.001	2
12^2	10	12	2	9598.235	–	–	9593.440	−4.795	–	1
00^0	11	11	0	2909.483	–	–	–	–	–	
00^0	11	10	0	3352.986	–	–	–	–	–	
00^0	11	9	0	3725.675	–	–	3725.591	−0.084	–	1
00^0	11	8	0	4044.174	–	–	4044.302	0.128	–	1
00^0	11	7	0	4315.583	–	–	–	–	–	
00^0	11	6	0	4544.400	–	–	4544.412	0.012	0.085	4
00^0	11	5	0	4734.082	–	–	–	–	–	
00^0	11	4	0	4886.475	–	–	4886.458	−0.017	–	1
01^1	11	12	1	4951.561	–	–	–	–	–	
00^0	11	3	0	4994.960	–	–	–	–	–	
00^0	11	2	0	5087.451	–	–	–	–	–	
00^0	11	1	0	5136.726	–	–	–	–	–	
00^0	11	0	0	5153.130	–	–	5153.108	−0.022	0.004	4
01^1	11	11	1	5483.887	–	–	–	–	–	
01^1	11	10	−1	5662.999	–	–	–	–	–	
01^1	11	10	1	5951.292	–	–	–	–	–	
10^0	11	11	0	6004.840	–	–	–	–	–	
01^1	11	9	−1	6057.667	–	–	6057.414	−0.253	–	1
01^1	11	9	1	6360.146	–	–	6360.037	−0.109	–	1
01^1	11	8	−1	6374.288	–	–	6374.378	0.090	0.001	2
10^0	11	10	0	6430.135	–	–	–	–	–	
01^1	11	7	−1	6645.114	–	–	–	–	–	
01^1	11	8	1	6710.509	–	–	6710.444	−0.065	–	1
10^0	11	9	0	6765.863	–	–	6765.462	−0.401	–	1
01^1	11	6	−1	6889.164	–	–	–	–	–	
01^1	11	5	−1	6999.329	–	–	–	–	–	
01^1	11	7	1	7008.796	–	–	7008.724	−0.072	0.001	2
02^2	11	13	2	7048.763	–	–	–	–	–	
10^0	11	8	0	7143.501	–	–	–	–	–	
01^1	11	4	−1	7157.950	–	–	–	–	–	
01^1	11	3	−1	7255.416	–	–	–	–	–	
01^1	11	6	1	7257.846	–	–	7257.825	−0.021	–	1
01^1	11	2	−1	7357.805	–	–	–	–	–	
10^0	11	7	0	7391.168	–	–	–	–	–	
01^1	11	1	−1	7405.690	–	–	–	–	–	
01^1	11	0	−1	7427.360	–	–	7427.368	0.008	0.004	2
02^0	11	11	0	7456.833	–	–	7455.154	−1.679	0.001	2
01^1	11	5	1	7472.728	–	–	7472.757	0.029	0.001	2
10^0	11	6	0	7592.384	–	–	–	–	–	
01^1	11	4	1	7638.739	–	–	–	–	–	
02^2	11	12	2	7647.643	–	–	–	–	–	
10^0	11	5	0	7754.428	–	–	–	–	–	
01^1	11	3	1	7766.818	–	–	7766.773	−0.045	0.001	2
01^1	11	1	1	7846.677	–	–	–	–	–	
01^1	11	2	1	7882.816	–	–	–	–	–	
11^1	11	10	1	8565.017	–	–	–	–	–	
11^1	11	9	−1	8895.546	–	–	–	–	–	
00^0	12	12	0	3403.539	–	–	–	–	–	
00^0	12	11	0	3884.331	–	–	–	–	–	
00^0	12	10	0	4287.296	–	–	–	–	–	
00^0	12	9	0	4634.287	–	–	–	–	–	
00^0	12	8	0	4933.239	–	–	–	–	–	
00^0	12	7	0	5189.271	–	–	–	–	–	
01^1	12	13	1	5400.537	–	–	–	–	–	
00^0	12	6	0	5406.244	–	–	–	–	–	
00^0	12	5	0	5585.814	–	–	–	–	–	
00^0	12	4	0	5730.425	–	–	–	–	–	
00^0	12	3	0	5856.883	–	–	–	–	–	
00^0	12	2	0	5923.072	–	–	–	–	–	
00^0	12	1	0	5969.777	–	–	–	–	–	
01^1	12	12	1	5978.159	–	–	–	–	–	
01^1	12	11	−1	6160.605	–	–	–	–	–	
01^1	12	11	1	6482.549	–	–	–	–	–	
10^0	12	12	0	6486.032	–	–	–	–	–	
01^1	12	10	−1	6592.111	–	–	–	–	–	
01^1	12	10	1	6924.534	–	–	–	–	–	
01^1	12	9	−1	6935.404	–	–	6934.662	−0.742	–	1
10^0	12	11	0	6947.951	–	–	–	–	–	
01^1	12	8	−1	7231.943	–	–	–	–	–	
01^1	12	9	1	7305.212	–	–	7304.882	−0.331	–	1
01^1	12	6	−1	7607.610	–	–	7607.571	−0.039	0.092	3
01^1	12	8	1	7632.617	–	–	–	–	–	
10^0	12	9	0	7749.316	–	–	–	–	–	
01^1	12	4	−1	7955.112	–	–	–	–	–	
02^2	12	14	2	8113.476	–	–	–	–	–	
01^1	12	6	1	8149.590	–	–	–	–	–	
01^1	12	2	−1	8151.448	–	–	–	–	–	
10^0	12	7	0	8238.008	–	–	–	–	–	
02^0	12	10	0	8478.893	–	–	–	–	–	
01^1	12	4	1	8506.777	–	–	–	–	–	

TABLE 1—*Continued*

$\nu_1\nu_2^l$	J	G	U	E_{DPT}^D	E_{DPT}^T	$E_{abinitio}$	E_{exp}	$E_{exp}-E_{DPT}^D$	*Error*	n
02^2	7	2	2	7462.307	7462.304	7462.660	7462.312	0.005	–	1
20^0	7	7	0	7499.698	7499.496	7499.429	–	–	–	
02^2	7	0	2	7504.964	7504.956	7505.230	7504.899	−0.065	0.001	2
02^2	7	1	2	7529.120	7529.106	7529.502	–	–	–	
11^1	7	3	−1	7595.889	7595.880	7596.305	7595.823	−0.066	0.001	2
11^1	7	4	1	7618.558	7618.539	7618.838	–	–	–	
11^1	7	2	−1	7667.411	7667.400	7667.740	–	–	–	
11^1	7	1	−1	7716.672	7716.666	7716.987	–	–	–	
11^1	7	2	1	7733.609	7733.602	7733.918	–	–	–	
11^1	7	3	1	7743.136	7743.096	7743.218	–	–	–	
20^0	7	6	0	7797.011	7796.961	7796.957	–	–	–	
11^1	7	0	1	7865.957	7865.949	7866.249	–	–	–	
11^1	7	1	1	7931.167	7931.163	7931.475	–	–	–	
03^3	7	10	3	7991.974	7991.871	7992.542	–	–	–	
20^0	7	5	0	8003.376	8003.327	8003.150	–	–	–	
03^1	7	8	1	8015.872	8016.491	8016.876	–	–	–	
20^0	7	4	0	8176.386	8176.357	8176.136	–	–	–	
03^1	7	6	1	8301.217	8302.012	8302.359	–	–	–	
20^0	7	3	0	8306.220	8306.197	8305.957	–	–	–	
03^1	7	7	1	8398.904	8399.085	8399.507	–	–	–	
20^0	7	2	0	8402.136	8402.122	8401.872	–	–	–	
03^3	7	9	3	8430.577	8430.576	8431.251	–	–	–	
20^0	7	1	0	8457.583	8457.572	8457.315	–	–	–	
20^0	7	0	0	8475.985	8475.974	8475.715	–	–	–	
03^1	7	5	−1	8610.282	8610.540	8610.931	–	–	–	
12^1	7	9	1	8670.659	8670.182	8670.661	–	–	–	
03^1	7	4	−1	8721.794	8722.076	8722.278	–	–	–	
03^3	7	6	3	8727.492	8727.513	8727.964	–	–	–	
03^3	7	8	3	8790.711	8790.710	8791.357	8790.635	−0.076	0.004	2
03^1	7	4	1	8866.842	8866.802	8866.967	–	–	–	
03^1	7	3	−1	8884.158	8884.299	8884.758	–	–	–	
03^1	7	5	1	8986.075	8986.135	8986.563	8986.260	0.185	0.002	2
03^1	7	2	−1	9019.308	9019.379	9019.844	–	–	–	
03^3	7	5	3	9045.023	9044.998	9045.453	–	–	–	
03^3	7	7	3	9059.096	9059.010	9059.570	–	–	–	
03^1	7	0	1	9074.638	9074.683	9075.144	–	–	–	
03^1	7	3	1	9139.687	9139.630	9139.680	9139.422	−0.265	0.001	2
03^1	7	1	−1	9158.549	9158.520	9159.106	9158.443	−0.106	0.001	2
03^3	7	3	−3	9364.745	9364.760	9365.131	–	–	–	
03^1	7	1	1	9438.718	9438.674	9438.919	–	–	–	
03^3	7	3	3	9558.278	9558.297	9558.810	–	–	–	
03^3	7	1	−3	9560.900	9560.899	9561.208	–	–	–	
03^3	7	1	3	9618.427	–	–	–	–	–	
12^0	7	6	0	9661.051	–	–	9661.269	0.218	0.003	2
12^2	7	8	2	9743.576	–	–	–	–	–	
12^0	7	4	0	9787.580	–	–	–	–	–	
12^2	7	6	2	9794.386	–	–	–	–	–	
12^2	7	4	−2	9846.213	–	–	–	–	–	
12^2	7	4	2	9912.230	–	–	–	–	–	
12^0	7	0	0	9979.117	–	–	9981.081	1.964	0.003	2
12^0	7	2	0	10008.072	–	–	–	–	–	
00^0	8	8	0	1647.264	1647.251	1647.232	1647.263	−0.001	0.019	6
00^0	8	7	0	1972.795	1972.792	1972.769	1972.794	−0.001	0.010	7
00^0	8	6	0	2242.196	2242.192	2242.168	2242.192	−0.004	0.013	6

several temperatures appropriate to the conditions under which the various experiments recorded H_3^+ spectra. A first attempt to assign the H_3^+ transitions was made by simply taking the measured line frequency and checking if, in a 1 cm^{-1} frequency interval around the line, a strong enough predicted transition was present. Although in nearly all cases our predictions lay very close to the observed transitions, this procedure is questionable and can lead to ambiguities. In particular, on occasion there is more than a single choice for a single line, several experimental lines are close in frequency or several predicted lines are close in intensity. This procedure could thus easily generate misassignments.

A further assignment criterion was clearly needed to reduce the chance of errors. From previous work (*10*, *24*) we knew that, using the *ab initio* potential including adiabatic corrections, it was possible to predict the H_3^+ energy levels with $\nu_{obs} - \nu_{calc}$ residuals almost constant within each vibrational band. We therefore analyzed the behavior of the $\nu_{obs} - \nu_{calc}$ obtained using the TRIATOM calculations and the *ab initio* potential. First we checked the behavior of $\nu_{obs} - \nu_{calc}$ for the transitions which had already been assigned; this allowed us to determine a typical trend for each vibrational band. During this procedure a number of deviations from the average trend were noted, and in most cases a reassignment was possible. The list of these reassignments appears in Table 2.

Having established a typical trend for each observed vibrational band, we rechecked all the new assignments with this method. An important further check was then made by calculating the combination differences of all the assigned transitions and checking any that did not match. This procedure eliminated a great number of ambiguities. The new assignments appear in Table 3.

In both Table 2 and Table 3 intensities of the transitions are given for absorption at 1000 K. This figure is given simply as a guide. The experiments and our calculations cover a wide range of temperatures and the transitions observed involve levels spanning a wide range of energies. This leads to spectra which are strongly temperature dependent but it is not possible or useful to try and represent all temperatures here. Furthermore, because the experimental work on H_3^+ is performed under discharge conditions, it is unlikely that any of the observations are recorded in conditions that really correspond to thermodynamic equilibrium.

TABLE 2

Relabeled and Reassigned Transitions for H_3^+, where Intensity, *I*, Is Given for Absorption at 1000 K in Units $cm^{-1}/mol\ cm^{-2}$

Obs/cm^{-1}	Calc/cm^{-1}	$\nu_1\nu_2^l$	J'	G'	U'	$\nu_1\nu_2^l$	J''	G''	U''	I
2028.198	2028.461	03^1	5	1	1	02^2	5	1	2	.644E-23
2134.241	2134.260	02^0	7	6	0	01^1	7	6	1	.620E-21
2134.607	2134.268	12^2	4	−6	2	02^2	5	3	−2	.107E-21
2324.698	2324.678	01^1	10	−3	−1	00^0	10	−3	0	.347E-20
2341.498	2341.734	01^1	10	−9	−1	00^0	10	−9	0	.531E-20
2766.032	2766.150	11^1	7	8	1	01^1	6	5	−1	.319E-20
2844.521	2844.476	11^1	6	4	−1	10^0	5	4	0	.946E-21
2851.518	2851.575	02^0	9	8	0	01^1	8	8	1	.220E-20
2864.369	2864.326	11^1	5	2	1	10^0	4	2	0	.256E-20
2941.187	2941.266	11^1	8	−9	1	01^1	7	6	1	.183E-20
2979.786	2979.672	02^2	7	3	−2	10^0	6	−6	0	.105E-20
2984.258	2984.276	11^1	5	6	1	01^1	4	−3	−1	.107E-19
2990.280	2989.849	12^0	5	3	0	02^2	4	0	−2	.290E-21
3000.105	3000.316	11^1	9	9	1	01^1	8	−6	−1	.326E-21
3002.355	3002.192	03^1	7	5	1	02^0	6	5	0	.913E-22
3003.250	3002.938	11^1	9	8	−1	10^0	8	8	0	.873E-21
3005.898	3005.861	11^1	11	10	1	10^0	10	10	0	.679E-21
3023.904	3023.050	02^0	10	7	0	01^1	9	7	−1	.439E-21
3023.674	3023.847	11^1	7	3	1	10^0	6	−3	0	.645E-21
3065.574	3065.571	02^2	6	2	2	01^1	5	2	1	.664E-20
3065.767	3065.785	11^1	6	4	−1	01^1	5	1	1	.507E-20
3078.881	3078.861	01^1	10	−3	−1	00^0	9	3	0	.125E-20
3093.664	3093.701	11^1	8	7	−1	10^0	7	7	0	.638E-21
3096.662	3096.687	02^2	7	3	−2	01^1	6	−3	−1	.219E-20
3103.868	3103.893	02^2	7	0	2	01^1	6	0	1	.231E-20
3167.598	3167.823	01^1	10	−9	−1	00^0	9	9	0	.108E-18
3179.109	3179.127	11^1	7	6	1	01^1	6	−3	−1	.311E-20
3194.792	3194.819	11^1	7	3	−1	01^1	6	0	1	.215E-20
3201.662	3201.672	02^2	7	5	2	01^1	6	5	1	.312E-20
3241.009	3241.048	03^3	7	8	3	02^2	6	8	2	.813E-22
3247.685	3247.707	11^1	8	5	1	01^1	7	2	1	.147E-20
3247.890	3247.905	11^1	7	4	−1	01^1	6	1	−1	.978E-21
3249.699	3249.646	11^1	5	2	−1	01^1	4	1	1	.215E-25
3249.788	3249.777	02^2	8	−3	2	01^1	7	3	1	.223E-20
3266.011	3266.006	02^2	8	5	2	01^1	7	5	1	.245E-20
3269.492	3269.521	01^1	9	2	−1	00^0	8	4	0	.253E-21
3292.512	3292.565	11^1	8	5	−1	01^1	7	2	−1	.148E-20
3423.809	3423.891	01^1	10	−9	1	00^0	9	9	0	.308E-19
4553.340	4553.418	03^3	4	6	−3	01^1	4	−3	1	.293E-20
4557.731	4557.752	02^2	6	2	2	00^0	7	1	0	.380E-20

TABLE 3

Newly Assigned Transitions for H_3^+, Where the Observed Data Are Taken from Bawendi *et al.* (*8*) and Xu *et al.* (*7*)

Obs/cm^{-1}	Calc/cm^{-1}	$\nu_1\nu_2^l$	J'	G'	U'	$\nu_1\nu_2^l$	J"	G"	U"	I	Obs/cm^{-1}	Calc/cm^{-1}	$\nu_1\nu_2^l$	J'	G'	U'	$\nu_1\nu_2^l$	J"	G"	U"	I
2395.500	2395.488	01^1	8	−3	−1	00^0	8	−3	0	.233E-19	2713.789	2713.903	03^3	4	2	3	02^2	4	4	2	.756E-22
2403.350	2403.649	12^2	2	3	2	11^1	2	−3	1	.119E-21	2713.789	2713.938	12^0	5	5	0	11^1	4	5	1	.186E-21
2405.031	2404.932	02^2	7	3	−2	10^0	7	6	0	.946E-22	2719.437	2719.684	03^3	2	2	3	02^2	2	4	2	.128E-21
2413.314	2413.318	02^2	5	1	−2	01^1	5	1	1	.277E-20	2725.341	2725.438	03^1	4	0	1	02^0	3	0	0	.433E-21
2416.289	2416.502	21^1	2	0	1	20^0	1	0	0	.451E-22	2733.639	2733.246	02^2	13	14	2	01^1	13	14	1	.123E-21
2419.558	2419.541	01^1	7	1	−1	00^0	7	1	0	.487E-19	2734.526	2734.507	02^0	6	2	0	01^1	5	2	−1	.683E-21
2421.888	2421.877	01^1	7	2	−1	00^0	7	2	0	.487E-19	2735.515	2735.836	12^2	4	2	2	11^1	3	2	1	.122E-21
2457.614	2457.605	11^1	5	5	1	10^0	5	5	0	.790E-21	2742.697	2742.719	02^0	7	6	0	01^1	6	−6	1	.415E-20
2457.912	2457.933	03^1	2	0	1	02^0	1	0	0	.443E-21	2745.307	2745.314	02^2	6	−3	2	01^1	6	−3	−1	.548E-21
2458.850	2458.872	03^1	2	1	1	02^0	1	1	0	.245E-21	2747.457	2747.474	11^1	5	3	−1	10^0	4	−3	0	.221E-20
2469.235	2469.324	02^2	6	2	2	10^0	6	5	0	.739E-22	2771.586	2771.572	02^0	7	3	0	01^1	6	−3	−1	.841E-21
2470.605	2470.625	10^0	8	7	0	00^0	8	4	0	.420E-20	2795.213	2795.292	03^1	5	3	1	02^0	4	−3	0	.318E-21
2471.384	2471.394	03^1	4	−3	−1	02^0	3	3	0	.526E-21	2817.349	2817.496	03^3	6	3	−3	11^1	5	6	1	.241E-21
2477.797	2478.062	03^3	4	2	3	02^2	4	2	2	.194E-21	2821.518	2821.951	02^0	9	9	0	01^1	8	−9	1	.481E-20
2483.977	2484.225	12^0	3	5	0	02^2	3	2	2	.199E-23	2822.730	2822.758	02^0	8	5	0	01^1	7	5	−1	.149E-20
2491.905	2491.890	11^1	6	−6	1	10^0	6	−6	0	.302E-21	2824.754	2824.827	02^0	8	4	0	01^1	7	4	−1	.111E-20
2497.349	2497.480	03^3	3	4	3	02^2	3	4	2	.352E-21	2842.191	2842.194	02^2	6	−3	−2	01^1	5	3	1	.190E-20
2498.079	2498.284	03^3	0	3	3	02^2	1	3	2	.298E-21	2852.155	2852.428	12^0	3	3	0	02^2	2	0	2	.481E-21
2509.726	2509.954	21^1	4	3	−1	20^0	3	3	0	.663E-22	2853.598	2853.603	02^2	5	1	−2	01^1	4	1	1	.158E-20
2554.474	2554.664	03^3	4	3	3	02^2	4	−3	2	.355E-21	2869.535	2869.920	02^2	8	1	2	01^1	8	1	−1	.602E-22
2570.987	2570.999	02^2	6	0	−2	10^0	5	3	0	.509E-22	2869.535	2870.569	02^0	10	10	0	01^1	9	10	1	.327E-20
2570.987	2571.056	03^3	4	6	−3	02^2	4	−6	2	.348E-21	2893.103	2893.305	11^1	10	8	−1	10^0	9	8	0	.297E-21
2577.694	2577.829	03^3	2	3	3	02^2	2	−3	2	.573E-21	2895.600	2895.659	02^2	9	6	2	01^1	9	6	−1	.460E-22
2579.828	2579.747	02^2	3	4	2	01^1	3	4	1	.834E-20	2898.614	2898.670	11^1	8	−6	−1	10^0	7	6	0	.113E-20
2579.828	2579.767	02^2	7	4	2	01^1	7	4	1	.385E-21	2934.357	2934.556	03^3	4	3	3	02^2	3	3	2	.365E-21
2579.828	2580.035	02^0	5	1	0	01^1	4	1	1	.941E-22	2941.187	2941.266	11^1	8	−9	1	01^1	7	6	1	.183E-20
2590.071	2590.440	02^2	8	5	2	01^1	8	5	1	.302E-21	2950.605	2950.608	02^2	5	1	−2	01^1	4	1	−1	.877E-20
2590.071	2590.459	12^2	3	0	2	11^1	2	0	1	.238E-21	2950.605	2950.663	12^2	6	5	2	11^1	5	5	1	.931E-22
2595.880	2595.940	02^2	9	5	2	01^1	9	5	1	.617E-22	2950.605	2950.703	11^1	11	9	−1	10^0	10	9	0	.201E-21
2597.702	2597.802	01^1	10	−9	1	00^0	10	−9	0	.294E-20	2958.899	2958.715	11^1	6	2	1	10^0	5	2	0	.185E-20
2605.062	2605.058	01^1	6	4	1	00^0	6	4	0	.129E-19	2965.791	2965.656	11^1	2	2	1	01^1	2	1	1	.481E-21
2617.809	2617.897	03^3	5	6	3	02^2	5	6	2	.249E-21	2976.080	2976.226	02^2	9	7	−2	01^1	8	7	1	.134E-20
2621.514	2621.515	02^0	5	4	0	01^1	4	4	1	.539E-20	2977.488	2977.624	03^1	7	1	1	02^0	6	1	0	.844E-22
2623.274	2623.529	03^1	7	3	1	02^2	6	−3	−2	.553E-22	2979.325	2979.362	02^2	7	4	−2	01^1	6	4	−1	.478E-21
2626.289	2626.228	01^1	9	7	1	00^0	9	7	0	.217E-20	2979.507	2979.499	01^1	7	1	−1	00^0	6	1	0	.220E-20
2630.492	2630.525	03^3	6	8	3	02^2	6	8	2	.254E-21	2984.082	2984.073	01^1	7	2	−1	00^0	6	2	0	.976E-20
2630.814	2630.825	01^1	10	8	1	00^0	10	8	0	.100E-20	2993.467	2993.495	11^1	8	8	1	01^1	7	5	1	.141E-20
2640.172	2640.243	02^2	8	8	2	01^1	8	8	1	.164E-20	2998.339	2998.318	02^0	6	2	0	01^1	5	4	−1	.104E-20
2648.105	2648.405	12^2	3	3	2	11^1	2	−3	1	.507E-22	3022.332	3022.103	12^0	7	6	0	11^1	6	−6	1	.115E-21
2650.561	2651.041	03^3	3	0	3	02^2	4	−6	2	.177E-21	3022.416	3022.430	02^2	6	1	2	01^1	5	1	1	.192E-20
2650.954	2651.120	02^2	9	9	2	01^1	9	9	1	.941E-21	3028.539	3028.603	02^2	9	6	−2	01^1	8	−6	1	.945E-21
2653.290	2653.380	03^1	7	1	−1	02^2	7	7	2	.785E-22	3052.071	3052.225	03^3	6	1	3	02^2	5	1	2	.175E-21
2653.692	2653.899	02^2	5	1	2	01^1	5	1	−1	.775E-21	3052.071	3052.524	03^3	6	2	−3	02^2	5	4	2	.901E-22
2653.885	2653.973	21^1	6	7	1	20^0	5	5	0	.514E-22	3059.381	3059.458	01^1	10	5	−1	00^0	9	5	0	.371E-20
2660.638	2660.646	11^1	4	5	1	01^1	4	2	−1	.674E-21	3061.287	3061.184	01^1	11	2	−1	00^0	10	2	0	.107E-21
2664.213	2664.460	03^3	2	2	3	02^2	1	2	2	.286E-21	3061.287	3061.381	03^3	5	6	3	02^2	4	−6	2	.799E-22
2666.142	2666.326	03^1	8	6	−1	02^0	7	6	0	.119E-21	3063.273	3063.210	01^1	12	−6	−1	00^0	11	6	0	.570E-21
2666.142	2666.335	01^1	11	8	1	00^0	11	8	0	.141E-21	3063.273	3063.277	11^1	4	2	1	01^1	5	5	1	.528E-22
2666.499	2666.560	02^2	9	10	2	01^1	9	10	1	.129E-20	3067.730	3067.736	02^2	5	2	2	01^1	4	2	−1	.157E-20
2672.862	2672.964	12^2	4	1	−2	11^1	3	1	−1	.170E-21	3101.391	3101.394	02^2	6	−3	2	01^1	5	3	1	.540E-20
2673.229	2673.381	03^3	3	3	3	02^2	2	−3	2	.225E-21	3120.826	3120.699	11^1	6	5	−1	01^1	7	8	1	.198E-21
2680.330	2680.450	03^3	5	2	−3	02^2	4	2	−2	.530E-22	3182.593	3182.272	11^1	6	5	1	01^1	5	2	−1	.169E-20
2680.485	2680.699	02^2	10	11	2	01^1	10	11	1	.779E-21	3203.095	3203.142	11^1	5	4	1	01^1	4	1	−1	.792E-21
2699.334	2699.413	00^0	11	0	0	02^0	10	10	0	.462E-22	3206.893	3206.560	11^1	6	4	−1	01^1	5	1	−1	.164E-21
2700.573	2700.460	03^1	9	7	1	02^0	8	7	0	.759E-22	3206.893	3206.952	01^1	14	8	1	00^0	13	8	0	.562E-22
2704.382	2704.443	03^1	4	2	1	02^0	3	2	0	.359E-21	3209.071	3209.729	01^1	12	−9	−1	00^0	11	9	0	.779E-23
2708.432	2708.175	03^3	9	11	3	02^2	9	11	2	.972E-22	3240.382	3240.434	02^2	9	6	−2	01^1	8	−6	−1	.324E-20
2708.778	2708.846	03^1	6	1	−1	02^2	6	7	2	.553E-22	3269.492	3269.521	01^1	9	2	−1	00^0	8	4	0	.253E-21
2709.405	2709.414	02^2	5	1	2	10^0	4	4	0	.393E-21	3293.783	3293.920	11^1	10	−6	1	10^0	9	6	0	.290E-21

In particular, the effective vibrational and rotational temperatures differ in most cases.

III.3. High J Transitions

Although the majority of experimental data is for *J* values less than 10, there is data extending as far *J* = 15. Transitions with these higher *J* values are harder to treat for a number of reasons.

The DPT potential is the result of a fit of observed transitions with *J* values up to 9 and belonging to vibrational states up to $3\nu_2$, and its extrapolation properties are not known. On the other hand, it is thought that the *ab initio* potential, which is expressed using the same functional form of the DPT potential, shows systematic deviations from the experimental energy levels with increasing values of J due to nonadiabatic effects not included in the effective potential (*24*). It is possible that the fit used to construct the DPT effective potential energy surface in some way compensates for these nonadiabatic effects, although these should not be fully reproducible with a simple potential.

Furthermore, the influence of linear geometries for the higher rotational levels cannot be neglected. Our DVR3D calculations are designed to account for this, but these calculations proved difficult and the convergence is uncertain (*20*). Indeed, comparisons with the calculations of Watson (*11*) show a number of cases where our DVR3D calculations predict energy levels systematically higher than Watson's. These calculations, which generally agree well for $J \leqslant 9$, were performed using different potentials and different rovibrational procedures, but one explanation for this behavior is that our DVR3D calculations are not well converged.

For the above reasons, we do not attempt to give definite assignments or reassignments to the transitions with high J.

IV. SUMMARY AND CONCLUSION

We have undertaken a systematic reanalysis of the observed transitions of H_3^+ using first principles nuclear motion calculations and two potential energy surfaces, both of which allow for adiabatic correction to the Born–Oppenheimer approximation. By combining results obtained using a high quality *ab initio* potential, less accurate but showing systematic errors, with those from a spectroscopically determined potential, we have been able to assign about 85% of the previously unassigned H_3^+ transitions. At the same time we have found it necessary to reassign a few transitions.

This reanalysis is less complete for higher rotational levels of the system. Nonadiabatic corrections to Born–Oppenheimer plus adiabatic potentials become increasingly important for these states. We are currently working on methods of including these corrections in our calculations.

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