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A TABLE OF ASTRONOMICALLY IMPORTANT RO-VIBRATIONAL TRANSITIONS FOR THE H_3^+ MOLECULAR ION

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ABSTRACT

A table of transition frequencies and Einstein A_{ij} coefficients for the astronomically important molecular ion H_3^+ is presented. The table consists of calculated frequencies and A_{ij}-values, and frequencies measured in the laboratory, augmented by recent observations of the H_3^+ spectrum taken from the upper atmosphere of Jupiter. The frequencies given cover the L and K atmospheric windows.

Subject headings: line identifications — molecular processes — transition probabilities

For many years, the simplest polyatomic molecular ion H_3^+ has been proposed as an important agent in the chemistry of the interstellar medium (Herbst & Klemperer 1973; Watson 1973; Dalgarno & Black 1976; Suzuki 1979). Although its infrared spectrum has been known from laboratory experiments since 1980 (Oka 1980), to date attempts to detect H_3^+ spectroscopically in the interstellar medium have proved unsuccessful (Oka 1981; Oka & Geballe 1990; Black et al. 1990).

Recently, however, the emission spectrum of H_3^+ has been observed in the upper atmosphere of Jupiter, located on the northern and southern auroral hot spots (Drossart et al. 1989; Trafton, Lester, & Thompson 1989). The lines were initially detected not as part of a search for H_3^+, but during studies of the K-window 2 μm spectrum of the planet in which measurement of the quadrupole spectrum of H_2 was the principal aim.

Identification of the newly discovered lines proved possible as a result of accurate first principle calculations (Miller & Tennyson 1988a, 1989), which also led to the assignment of the laboratory emission spectrum of Majewski et al. (1989) and the absorption spectrum of hot bands (Bawendi, Rehfuss, & Oka 1990) and overtone band (Xu, Gabrys, & Oka 1990).

The Jovian H_3^+ lines turned out to be due to overtone transitions from the $2\nu_2(l = 2)$ state to the vibrational ground state, and indicated that the gas being probed by the observations was relatively hot ($T = 1100$ K). The results also indicated that it ought to be possible to measure transitions of the fundamental ν_2 to ground state band, as well as "hot band" transitions.

A number of recent studies of the Jovian atmosphere have indeed detected the ν_2 fundamental (Oka & Geballe 1990; Miller, Joseph, & Tennyson 1990; Maillard et al. 1990). So far, "hot band" transitions have not been identified.

In view of the great potential of H_3^+ as an astronomical probe, we present here a table of transition frequencies for states with up to a total of three quanta of asymmetric stretch/bend (ν_2) or symmetric stretch (ν_1), together with computed absolute energy levels and Einstein A_{ij} coefficients in the frequency range between 5750 and 1600 cm^{-1}. A small region between 6939.3 to 6862.9 cm^{-1} studied recently in the laboratory (Lee et al. 1991) is also added. As well as the fundamental and overtone bands of ν_2, "hot band" transitions between states of one and two quanta, and two and three quanta, are included. The authors consider that these transitions are the most likely to be of astronomical importance.

Experimental data has been collected from a number of studies, but in all cases frequency measurements were of an accuracy better than 0.01 cm^{-1}. The observed frequencies of fundamental $\nu_2 \leftarrow 0$ ("I" in table) are from Oka (1981), Watson et al. (1984), Majewski et al. (1987), and Bawendi et al. (1990). Observed frequencies of hot bands $2\nu_2(2) \leftarrow \nu_2(1)$ (I-1a), $2\nu_2(0) \leftarrow \nu_2(1)$ (I-1b) and $\nu_2 + \nu_2 \leftarrow \nu_1$ (I-1c) are from Bawendi et al. (1990). The observed frequencies of the first overtone $2\nu_2(2) \leftarrow 0$ are from Majewski et al. (1989) and Xu et al. (1990). The observed frequencies of the second overtone band $3\nu_2(1) \leftarrow 0$ are from Lee et al. (1991).

Details of the calculated frequencies and A_{ij}-values have been published elsewhere (Miller & Tennyson 1988b, 1989). All the computed quantities made use of the potential energy and dipole surfaces of Meyer, Botschwina, & Burton (1986). Comparison with experimental data shows that the accuracy of theoretically calculated frequencies of the fundamental transition have a standard deviation of 0.24 cm^{-1} and are scattered around the measured frequencies. The calculated overtone and one to two quanta "hot band" transitions are uniformly too low in frequency, with an average error of 0.6 cm^{-1}.

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TABLE 1

OBSERVED AND THEORETICAL FREQUENCIES OF H_3^+ WITH ABSOLUTE ENERGY LEVELS AND EINSTEIN'S A_{ij} COEFFICIENT

Band[a]	Transition						Lab	Space[b]	ab initio			
							ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	← J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
III	0	1		1	1				6939.349	7003.453	64.104	1.76 (+2)
III	4	1		4	1				6936.415	7769.726	833.311	1.45 (+2)
III	3	2		3	2				6931.058	7358.939	427.881	8.00 (+1)
III	4	2		4	2				6929.196	7697.421	768.225	1.20 (+2)
III	4	3		4	3		6891.792		6888.498	7547.001	658.503	6.50 (+1)
III	5	3		5	3				6879.669	7959.808	1080.139	1.09 (+2)
III	1	2		2	2		6877.512		6874.953	7044.199	169.246	1.75 (+2)
III	1	1		2	1		6865.708		6863.040	7100.319	237.279	8.40 (+1)
III	5	0		5	0		6866.338		6862.913	8133.775	1270.862	1.19 (+2)
II	5	0	+2	4	3				5732.177	6390.680	658.503	6.30 (+0)
II	4	0	-2	3	3				5580.356	5895.604	315.248	4.65 (+0)
II	5	2	-2	5	5				5438.967	6167.744	728.777	1.61 (+1)
II	4	1	-2	3	2				5417.541	5845.422	427.881	1.10 (+0)
II	3	1	+2	2	2				5403.596	5532.834	169.246	7.64 (+0)
II	4	2	+2	3	1				5392.792	5887.398	494.606	2.83 (+1)
II	4	1	-2	4	4				5343.547	5845.422	501.845	2.33 (+1)
II	5	2	+2	4	1				5334.433	6326.970	833.311	3.48 (+0)
II	5	0	+2	5	3				5311.388	6390.680	1080.139	2.69 (+1)
II	3	2	+2	2	1				5295.678	5532.956	237.279	2.27 (+1)
II	4	3	+2	3	0				5292.633	5810.346	516.713	7.94 (+1)
II	5	4	+2	4	1				5255.629	6088.940	833.311	4.69 (+1)
II	3	0	+2	3	3				5251.082	5566.330	315.248	3.22 (+1)
II	4	0	-2	4	3				5237.101	5895.604	658.503	4.54 (+1)
II	6	5	+2	5	2				5228.655	6414.529	1186.725	4.42 (+2)
II	7	6	+2	6	3				5206.158	6782.823	1576.335	6.22 (+1)
II	2	2	+2	1	1				5201.599	5265.703	64.104	1.67 (+1)
II	4	4	+2	3	1				5157.162	5651.768	494.606	5.72 (+1)
II	2	1	+2	2	2				5134.867	5304.112	169.246	4.76 (+1)
II	5	5	+2	4	2				5130.422	5898.647	768.225	7.01 (+1)
II	6	6	+2	5	3				5103.582	6183.321	1080.139	8.26 (+1)
II	2	3	+2	1	0		5094.218		5093.729	5180.662	86.933	9.10 (+1)
II	4	1	-2	4	2				5077.197	5845.422	768.235	3.35 (+0)
II	5	2	+2	5	1				5077.060	6326.970	1249.910	4.40 (+1)
II	7	7	+2	6	4				5073.988	6504.257	1430.258	8.96 (+1)
II	3	4	+2	2	1		5061.882		5061.407	5298.686	237.279	7.00 (+1)
II	3	1	-2	3	2				5057.270	5485.152	427.881	4.90 (-1)
II	4	2	+2	4	1		5054.742		5054.085	5887.398	833.311	5.80 (+1)
II	3	2	+2	3	1				5038.350	5532.956	494.606	6.38 (+1)
II	4	5	+2	3	2		5032.447		5032.028	5459.909	427.881	8.84 (+1)
II	2	2	+2	2	1		5029.071		5028.424	5265.703	237.279	7.22 (+1)
II	1	2	+2	1	1		5023.498		5022.899	5087.004	64.104	7.35 (+1)
II	5	6	+2	4	3		5000.499	5000.527	5000.138	5658.641	658.503	1.01 (+2)
II	6	4	-2	5	1				4999.111	6249.022	1249.910	2.19 (+0)
II	4	2	-2	5	5				4986.086	5714.864	728.777	1.06 (+2)
II	5	3	-2	6	6		4975.338		4973.813	5989.366	995.553	6.58 (+1)
II	2	0	-2	3	3		4971.561	4971.537	4970.645	5285.893	315.248	1.41 (+2)
II	2	4	+2	1	1		4968.272		4967.871	5031.976	64.104	9.30 (+1)
II	6	7	+2	5	4		4966.838	4966.859	4966.504	5895.176	928.672	1.11 (+2)
II	1	1	-2	2	2		4955.991		4955.262	5124.508	169.246	1.47 (+2)
II	6	4	-2	7	7				4947.300	6249.022	1301.722	1.52 (+1)
II	5	3	+2	5	0		4942.862		4941.722	6212.584	1270.862	1.25 (+2)
II	3	5	+2	2	2		4936.000	4935.946	4935.667	5104.913	169.246	1.14 (+2)
II	7	8	+2	6	5		4931.596	4931.561	4931.277	6169.328	1238.051	1.18 (+2)
II	5	2	-2	6	5		4930.981		4929.693	6167.744	1238.051	8.00 (+1)
II	4	1	-2	5	4				4916.750	5845.422	928.672	9.50 (+1)
II	3	3	+2	3	0		4914.248	4914.247	4913.634	5430.347	516.712	1.48 (+2)
II	3	0	-2	4	3		4908.672		4907.827	5566.330	658.503	1.00 (+2)
II	1	3	+2	1	0		4907.871	4907.859	4907.381	4994.314	86.933	1.55 (+2)
II	4	6	+2	3	3		4900.393	4900.377	4900.138	5215.387	315.248	1.27 (+2)
II	8	9	+2	7	6		4895.518	4895.498	4895.237	6481.318	1586.082	1.23 (+2)
II	2	1	-2	3	2		4876.938	4876.912	4876.231	5304.112	427.881	9.80 (+1)
II	5	7	+2	4	4		4861.790	4861.839	4861.606	5363.481	501.875	1.36 (+2)
II	9	10	+2	8	7		4859.212		4858.897	6831.068	1972.171	1.28 (+2)
II	1	2	+2	2	1		4850.264		4849.725	5087.004	237.279	7.51 (+1)
II	5	4	+2	5	1		4839.508		4839.030	6088.940	1249.910	7.50 (+1)
II	10	11	+2	9	8		4823.315		4823.076	7218.733	2395.657	1.31 (+2)
II	6	8	+2	5	5		4820.598	4820.542	4820.503	5549.281	728.777	1.44 (+2)
II	4	4	+2	4	1		4818.901		4818.456	5651.768	833.311	1.44 (+2)
II	4	0	-2	5	3		4816.353	4816.415	4815.465	5895.604	1080.139	8.90 (+1)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
II	5	0	-2		6	3		4814.521		4813.846	6390.680	1576.835	6.00 (+1)
II	3	1	+2		4	2		4805.287		4804.609	5572.834	768.225	7.80 (+1)
II	3	4	+2		3	1		4804.406	4804.463	4804.080	5298.686	494.606	7.00 (+1)
II	2	4	+2		2	1		4795.066	4795.018	4794.697	5031.976	237.279	5.60 (+1)
II	11	12	+2		10	9		4788.544		4788.666	7644.484	2855.818	1.32 (+2)
II	7	9	+2		6	6		4777.226	4777.215	4777.123	5772.677	995.553	1.51 (+2)
II	2	2	+2		3	1		4771.641		4771.097	5265.703	494.606	6.40 (+1)
II	12	13	+2		11	10		4756.345		4756.442	8108.318	3351.876	1.33 (+2)
II	4	1	+2		5	2		4744.797		4744.124	5930.849	1186.725	6.30 (+1)
II	6	5	+2		6	2		4735.941		4735.264	6414.529	1679.265	7.20 (+1)
II	8	10	+2		7	7		4732.060	4732.050	4732.158	6033.880	1301.722	1.58 (+2)
II	5	5	+2		5	2		4712.309	4712.334	4711.921	5898.647	1186.725	6.80 (+1)
II	3	2	+2		4	1		4700.139		4699.645	5532.956	833.311	5.60 (+1)
II	4	5	+2		4	2		4691.962		4691.684	5459.909	768.225	6.00 (+1)
II	9	11	+2		8	8		4685.564	4685.582	4685.694	6332.426	1646.732	1.64 (+2)
II	3	5	+2		3	2		4677.273	4677.268	4677.032	5104.913	427.881	4.30 (+1)
II	2	3	+2		3	0		4664.306	4664.274	4663.949	5180.662	516.713	6.50 (+1)
II	7	6	+2		7	3		4641.987		4641.550	6782.988	2141.437	6.40 (+1)
II	10	12	+2		9	9		4638.331	4638.361	4638.688	6668.656	2029.967	1.71 (+2)
II	4	2	+2		5	1		4637.992		4637.488	5887.398	1249.910	5.50 (+1)
II	6	6	+2		6	3		4607.205		4606.887	6183.721	1576.835	5.80 (+1)
II	5	2	+2		6	1		4587.373		4586.619	6326.970	1740.351	4.50 (+1)
II	5	6	+2		5	3		4578.735		4578.502	5658.641	1080.139	5.20 (+1)
II	4	6	+2		4	3		4557.020	4557.057	4556.883	5215.387	658.503	3.50 (+1)
II	2	4	+2		3	1				4537.370	5031.976	494.606	1.03 (+1)
II	4	3	+2		5	0		4539.759		4539.484	5810.346	1270.862	7.20 (+1)
II	7	7	+2		7	4				4507.424	6504.257	2001.833	5.79 (+1)
II	3	4	+2		4	1				4465.375	5298.686	833.311	1.61 (+1)
II	6	7	+2		6	4				4464.918	5895.176	1430.258	4.58 (+1)
II	5	7	+2		5	4				4434.809	5363.481	928.672	3.02 (+1)
II	7	8	+2		7	5				4351.763	6169.328	1817.565	4.14 (+1)
II	5	4	+2		6	1				4348.590	6088.940	1740.251	2.00 (+1)
II	3	5	+2		4	2				4336.688	5104.913	768.225	5.84 (+0)
II	6	8	+2		6	5		4311.147		4311.229	5549.281	1238.051	2.69 (+1)
II	4	5	+2		5	2				4273.184	5459.909	1186.725	1.04 (+1)
II	8	9	+2		8	6				4239.822	6481.318	2241.496	3.79 (+1)
II	7	9	+2		7	6				4186.595	5772.677	1586.082	2.45 (+1)
II	6	5	+2		7	2				4173.226	6414.529	2241.303	7.85 (+0)
II	4	6	+2		5	3				4135.247	5215.387	1080.139	3.93 (+0)
II	5	6	+2		6	3				4081.806	5658.641	1576.835	7.59 (+0)
II	8	10	+2		8	7				4061.709	6033.880	1972.171	2.28 (+1)
II	6	6	+2		7	3				4042.284	6183.921	2141.437	1.09 (+1)
II	7	6	+2		8	3				4008.149	6782.988	2774.839	9.72 (+0)
II	5	7	+2		6	4				3933.223	5363.481	1430.258	2.90 (+0)
II	6	7	+2		7	4				3893.344	5895.176	2001.833	6.08 (+0)
II	6	8	+2		7	5				3731.715	5549.281	1817.565	2.31 (+0)
II	7	8	+2		8	5				3707.212	6169.228	2462.117	5.02 (+0)
II	7	9	+2		8	6				3531.180	5772.677	2241.496	1.95 (+0)
I	9	3	+1		8	3				3399.448	6174.287	2774.839	1.75 (+2)
I	9	4	+1		8	4				3392.458	6030.797	2638.339	1.81 (+2)
I	9	6	+1		8	6				3367.889	5609.386	2241.496	1.47 (+2)
I	9	7	+1		8	7				3355.205	5327.376	1972.171	1.10 (+2)
I	9	8	+1		8	8				3345.288	4992.020	1646.732	5.40 (+1)
I	8	3	+1		7	3				3320.969	5462.406	2141.437	1.60 (+2)
I-1a	8	9	+2		7	7	+1			3309.406	7185.815	3876.409	7.24 (+1)
I	8	1	+1		7	1				3305.722	5605.875	2300.153	1.69 (+2)
I	8	2	+1		7	2				3290.474	5531.717	2241.303	1.18 (+2)
I	8	5	+1		7	5				3288.887	5106.452	1817.565	1.36 (+2)
I	8	6	+1		7	6				3275.901	4861.983	1586.082	1.02 (+2)
I	8	7	+1		7	7				3264.749	4566.471	1301.722	4.95 (+1)
I	7	1	+1		6	1				3220.623	4960.974	1740.351	1.57 (+2)
I	7	3	+1		6	3				3216.207	4793.041	1576.835	1.39 (+2)
I-1a	7	6	+2		6	6	+1			3214.038	6782.988	3568.950	6.48 (+1)
I	7	2	+1		6	2		3212.380		3212.017	4891.282	1679.265	1.32 (+2)
I	7	4	+1		6	4				3205.066	4635.325	1430.258	1.24 (+2)
I	7	5	+1		6	5		3193.227		3197.952	4431.003	1238.051	9.47 (+1)
I	7	6	+1		6	6		3182.031		3181.687	4177.240	995.553	4.61 (+1)
I	10	9	-1		9	9		3167.598		3166.742	5196.710	2029.767	1.79 (+2)
I	6	1	+1		5	1				3127.874	4377.784	1249.910	1.46 (+2)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I	6	0	+1		5	0		3128.056		3127.431	4400.486	1270.862	1.42 (+2)
I	6	2	+1		5	2				3122.039	4308.765	1186.725	1.28 (+2)
I	6	3	+1		5	3		3121.806		3121.634	4201.773	1080.139	1.16 (+2)
I	9	8	-1		8	8		3120.310		3119.538	4766.270	1646.732	1.71 (+2)
I	9	7	+1		8	7		3113.529		3112.664	5084.834	1972.171	1.15 (+2)
I	8	4	+1		7	4				3107.128	5304.091	2001.833	1.20 (+2)
I	6	4	+1		5	4		3106.793		3106.543	4035.215	928.672	8.97 (+1)
I	9	6	-1		8	6				3099.000	5340.496	2241.496	7.14 (+1)
I	6	5	+1		5	5		3096.412		3096.095	3824.893	728.777	4.39 (+1)
I-1a	6	3	+2		5	3	-1			3086.109	6638.729	3552.620	1.41 (+2)
I	8	7	-1		7	7		3069.169		3068.482	4370.203	1301.722	1.61 (+2)
I-1a	5	3	+2		4	3	-1			3067.794	6212.584	3144.790	1.24 (+0)
I-1a	5	2	+2		4	2	-1			3067.306	6326.970	3259.663	2.73 (+1)
I	8	6	-1		7	6		3064.347		3063.586	4649.668	1586.082	1.05 (+2)
I	8	5	-1		7	5				3055.495	4873.060	1817.565	5.93 (+1)
I	9	4	-1		8	4		3053.500		3049.418	5687.757	2638.339	2.90 (+1)
I-1a	6	1	-2		5	1	-1			3045.178	6766.989	3721.811	1.54 (+2)
I	9	3	-1		8	3				3032.496	5807.335	2774.839	1.43 (+1)
I	5	1	+1		4	1		3029.822		3029.633	3862.944	833.311	1.26 (+2)
I	8	3	-1		7	3				3028.115	5169.552	2141.437	2.33 (+1)
I	8	4	-1		7	4				3025.046	5026.879	2001.833	3.65 (+1)
I	5	2	+1		4	2		3024.547		3024.343	3792.568	768.225	1.13 (+2)
I-1a	5	4	+2		4	4	+1			3019.937	6088.940	3069.003	5.91 (+1)
I	5	3	+1		4	3		3015.240		3014.994	3673.497	658.503	8.76 (+1)
I	8	2	-1		7	2				3014.312	5255.615	2241.303	8.87 (+0)
I	7	6	-1		6	6		3014.358		3013.750	4009.303	995.553	1.50 (+2)
I	8	1	-1		7	1				3011.114	5311.267	2300.153	2.27 (+0)
I	7	5	-1		6	5		3011.506		3010.840	4248.891	1238.051	9.36 (+1)
I	5	4	+1		4	4		3008.115		3007.828	3509.703	501.875	4.28 (+1)
I-1b	6	2			5	4	-1			2996.752	6392.663	3395.911	1.22 (+1)
I	7	4	-1		6	4		2989.480		2988.945	4419.204	1430.258	3.98 (+1)
I	7	3	-1		6	3				2986.672	4561.507	1576.835	2.69 (+1)
I	7	2	-1		6	2		2984.069		2983.272	4662.536	1679.264	1.22 (+1)
I-1a	5	3	+2		4	3	+1			2979.557	6212.584	3233.027	1.04 (+2)
I	7	1	-1		6	1				2978.657	4719.008	1740.351	2.98 (+0)
I-1a	5	2	+2		4	2	+2			2975.947	6326.970	3351.023	1.02 (+2)
I-1a	6	3	+2		5	3	+1			2965.232	6638.729	3673.497	3.93 (+1)
I-1a	6	3	-2		5	3	-1			2961.572	6514.192	3552.620	8.13 (+1)
I-1a	4	2	+2		3	2	-1			2956.400	5887.398	2930.998	8.79 (+0)
I	6	5	-1		5	5		2956.073		2955.548	3684.325	728.777	1.37 (+2)
I	6	4	-1		5	4		2955.154		2954.577	3883.248	928.672	8.01 (+1)
I	6	3	-1		5	3		2949.555		2948.932	4029.071	1080.139	4.29 (+1)
I-1a	5	0	-2		4	0	-1	2944.828		2943.996	6390.680	3446.685	2.28 (=2)
I	6	2	-1		5	2		2942.209		2941.547	4128.273	1186.725	1.74 (+1)
I	6	1	-1		5	1				2937.793	4187.703	1249.910	9.22 (+0)
I-1a	4	3	+2		3	3	+1	2934.155		2933.755	5810.346	2876.591	6.38 (+1)
I-1a	4	4	+2		3	4	+1	2932.988		2932.459	5651.768	2719.308	2.45 (+1)
I	4	0	-1		3	0		2930.163		2929.972	3446.685	516.713	1.18 (+2)
I-1a	4	1	+2		3	1	-1			2928.363	5930.849	3002.486	1.51 (=1)
I	4	1	+1		3	1		2928.351		2928.152	3422.758	494.606	1.11 (+2)
I	4	2	+1		3	2		2923.361		2923.142	3351.023	427.881	8.71 (+1)
I	4	3	+1		3	3		2918.026		2917.779	3233.027	315.248	4.30 (+1)
I-1a	5	2	-2		4	2	-1			2908.081	6167.744	3259.663	1.50 (+2)
I-1a	6	1	-2		5	1	+1			2904.045	6766.989	3862.163	1.69 (+1)
I-1a	4	2	+2		3	2	+1	2895.874		2895.238	5887.298	2992.161	9.83 (+1)
I	5	3	-1		4	3		2894.610		2894.117	3552.620	658.503	6.29 (+1)
I	5	4	-1		4	4		2894.488		2894.037	3395.911	501.875	1.23 (+2)
I-1a	6	4	+2		5	4	+1			2893.454	6403.157	3509.703	3.77 (+1)
I	5	2	-1		4	2		2891.867		2891.338	3659.563	768.225	2.65 (+1)
I	5	1	-1		4	1		2889.052		2888.500	3721.811	833.311	6.23 (+0)
I-1a	4	0	-2		3	0	-1	2870.890		2870.076	5875.604	3025.528	1.65 (+2)
I-1a	4	1	+2		3	1	+1	2868.404		2867.657	5930.849	3063.103	1.46 (+20
I-1a	6	4	-2		5	4	-1	2854.191		2853.110	6249.022	3395.911	2.31 (+1)
I-1a	4	1	-2		3	1	-1			2842.936	5845.422	3002.486	1.59 (+2)
I-1a	6	3	-2		5	3	+1			2840.694	6514.192	3673.497	4.40 (+1)
I	4	2	-1		3	2		2832.197	2832.188	2831.782	3259.663	427.881	4.48 (+2)
I	4	1	-1		3	1		2831.340		2830.912	3325.518	494.606	1.07 (+1)
I	4	3	-1		3	3		2829.923	2829.924	2829.542	3144.790	315.248	1.06 (+2)
I	3	1	+1		2	1		2826.113	2826.117	2825.914	3063.193	237.279	9.19 (+1)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I-1a	5	3	-2		4	3	-1	2825.956		2824.576	5969.366	3144.790	1.19 (+2)
I	3	2	+1		2	2		2823.136	2823.152	2822.915	2992.161	169.246	4.77 (+2)
I-1a	3	1	+2		2	1	-1	2818.196		2817.543	5572.834	2755.291	1.16 (+1)
I-1a	5	2	-2		4	2	+1	2818.072		2816.721	6167.744	3351.023	5.19 (+1)
I-1a	3	3	+2		2	3	+1	2816.843		2816.212	5430.347	2614.135	2.86 (+1)
I-1a	3	2	+2		2	2	+1	2809.767		2809.191	5532.956	2723.765	7.41 (+1)
I-1b	8	7			7	7	+1			2797.093	6673.502	3876.409	7.21 (+1)
I-1b	7	4			6	4	-1			2788.114	6671.363	3883.248	5.11 (+1)
I-1a	4	2	-2		3	2	-1	2785.121		2783.866	5714.864	2930.998	1.81 (+2)
I-1a	3	1	+2		2	1	+1	2783.417		2782.707	5572.834	2790.127	1.17 (+2)
I-1a	4	1	-2		3	1	+1	2783.325		2782.229	5845.422	3063.193	4.70 (+1)
I-1a	7	6	+2		7	6	-1			2773.684	6782.988	4009.303	3.80 (+0)
I-1c	4	0	-1		3	0		2770.940		2770.112	6452.726	3682.614	1.13 (+2)
I-1b	8	8			7	8	+1			2769.010	6298.772	3529.762	8.99 (+1)
I-1c	4	3	+1		3	3		2769.393		2768.773	6254.046	3485.273	3.00 (+1)
I-1c	4	2	+1		3	2		2767.678		2766.901	6362.564	3595.663	7.52 (+1)
I	3	1	-1		2	1		2765.547	2765.531	2765.207	3002.486	237.279	2.10 (+1)
I-1b	7	5			6	5	-1			2764.567	6448.892	3684.325	6.19 (+1)
I-2b	2	3	+3		1	3	+2			2764.106	7758.420	4994.314	7.15 (+1)
I	3	2	-1		2	2		2762.068	2762.077	2761.752	2930.998	169.246	8.39 (+1)
I-1a	3	0	-2		2	0	-1	2754.535		2753.687	5566.330	2812.642	1.95 (+2)
I-1b	6	3			5	3	-1			2746.608	6299.228	3552.620	3.78 (+1)
I-1b	6	4			5	4	-1			2743.233	6139.144	3395.911	6.18 (+1)
I-1b	7	6			6	6	+1			2741.151	6310.101	3568.950	6.65 (+1)
I-1a	6	4	-2		5	4	+1	2740.568		2739.318	6249.022	3509.703	2.94 (+1)
I-1a	5	3	-2		4	3	+1	2737.851		2736.339	5969.366	3233.027	3.15 (+1)
I-1b	6	2			5	2	-1			2733.100	6392.663	3659.563	1.47 (+1)
I-1a	6	5	+2		6	5	-1			2730.204	6414.529	3684.325	4.02 (+0)
I-1a	3	1	-2		2	1	-1	2730.887		2729.861	5495.152	2755.291	1.86 (+2)
I	2	1	+1		1	1		2726.219	2726.309	2726.023	2790.627	64.104	6.04 (+1)
I	2	0	-1		1	0		2725.898	2725.894	2725.709	2812.642	86.933	9.88 (+1)
I-1a	4	2	-2		3	2	+1	2724.058		2722.703	5714.864	2992.161	3.54 (+1)
I-2b	2	2	-3		2	4	+2			2719.667	7751.643	5031.976	5.01 (+1)
I-1a	2	2	+2		1	2	+1	2718.262		2717.663	5265.703	2548.041	4.21 (+1)
I	9	3	+1		9	3				2714.245	6174.287	3460.042	4.00 (-3)
I	9	4	+1		9	4				2696.224	6030.797	3334.573	7.36 (-1)
I-1a	3	1	-2		2	1	+1	2696.110		2695.024	5485.152	2790.127	3.62 (+1)
I-1a	2	1	-2		1	1	+1	2695.420		2694.735	5304.112	2609.397	1.10 (+2)
I-1a	5	4	+2		5	4	-1			2693.029	6088.940	3395.911	5.89 (+0)
I	2	1	-1		1	1		2691.444	2691.448	2691.187	2755.291	64.104	5.16 (+1)
I	8	3	+1		8	3				2687.567	5462.406	2774.839	8.58 (-1)
I-1c	5	5	+1		5	5				2686.470	6346.032	3888.463	1.77 (+1)
I-1b	5	3			4	3	-1	2685.157		2683.731	5828.522	3144.790	3.02 (+1)
I-1b	6	5			5	5	+1	2683.755		2682.290	5982.015	3299.725	6.02 (+1)
I	8	1	+1		8	1				2681.051	5605.875	2924.537	2.65 (-1)
I-2d	2	3	+3		3	3				2680.930	7758.420	5077.489	1.12 (+0)
I-1c	4	2	-1		3	2		2680.631		2679.775	6275.437	3595.663	5.16 (+1)
I-1b	5	2			4	2	-1			2678.105	5937.769	3259.663	1.63 (+1)
I-1b	5	1			4	1	-1			2675.734	6001.251	3325.518	4.55 (+0)
I	9	5	+1		9	5				2675.514	5841.963	3166.389	1.83 (+0)
I-1c	4	3	-1		3	3		2672.958		2672.069	6157.342	3435.273	1.13 (+2)
I-1c	3	2	+1		2	2		2672.799		2672.138	6015.313	3343.175	3.65 (+1)
I-1c	3	1	+1		2	1		2671.142		2670.387	6080.220	3409.633	8.41 (+1)
I-1a	2	0	-2		1	0	-1	2670.234		2669.406	5285.893	2616.487	1.83 (+2)
I-1a	5	2	+2		5	2	-1			2667.604	6326.970	3659.563	1.22 (+1)
I	8	4	+1		8	4				2665.752	5304.091	2638.339	1.97 (+0)
I-1a	4	3	+2		4	3	-1	2665.729		2665.556	5810.346	3144.790	8.59 (+0)
I-2c	2	2	-3		1	2	+2			2664.639	7751.643	5087.004	1.18 (+2)
I	8	2	+1		8	2				2663.764	5531.777	2868.013	1.50 (+0)
I	7	1	+1		7	1				2660.821	4960.974	2300.153	3.16 (-1)
I-1a	5	3	+2		5	3	-1	2660.373		2659.964	6212.584	3552.620	1.36 (+1)
I-1b	6	6			5	6	+1	2657.652		2656.269	5703.358	3047.090	7.99 (+1)
I	9	6	+1		9	6				2652.981	5609.386	2956.405	3.86 (+0)
I-1a	8	9	+2		8	9	+1	2653.095		2652.907	6481.318	3828.412	3.96 (+1)
I	7	3	+1		7	3				2651.604	4793.041	2141.437	9.00 (-1)
I	7	2	+1		7	2				2649.979	4891.282	2241.303	1.65 (+0)
I-1a	5	0	-2		5	0	-1	2648.692		2648.335	6390.680	3742.346	2.71 (+1)
I	8	5	+1		8	5				2644.325	5106.452	2462.117	4.31 (+0)
I-1a	7	8	+2		7	8	+1	2639.806		2639.566	6169.328	3529.762	4.31 (+1)

TABLE 1—*Continued*

Band[a]	Transition						Lab	Space[b]	ab initio			
							ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	← J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I	6	1	+1	6	1				2637.433	4377.784	1740.351	5,20 (-1)
I	6	2	+1	6	2				2629.500	4308.765	1679.265	2.31 (+0)
I-1a	7	7	+2	7	7	+1	2628.119		2627.848	6504.257	3876.409	6.25 (+1)
I-1a	4	2	+2	4	2	-1	2628.097		2627.735	5887.398	3259.663	1.77 (+1)
I	9	7	+1	9	7				2626.132	5327.376	2301.244	7.27 (+0)
I-1a	6	7	+2	6	7	+1	2626.220		2625.969	5895.176	3269.207	4.78 (+1)
I	6	3	+1	6	3		2624.967		2624.939	4201.773	1576.835	4.66 (+0)
I	8	6	+1	8	6				2620.487	4861.983	2241.496	8.31 (+0)
I-1b	5	4		4	4	+1	2621.514		2620.109	5689.112	3069.003	5.27 (+1)
I-1a	6	6	+2	6	6	+1	2615.068		2614.771	6183.721	3568.950	7.06 (+1)
I	7	5	+1	7	5		2613.540		2613.438	4431.004	1817.565	9.25 (+0)
I-1c	3	1	-1	2	1		2613.932		2613.148	6022.981	3409.633	2.54 (+1)
I	5	1	+1	5	1				2613.034	3862.944	1249.910	9.82 (-1)
I-1a	5	6	+2	5	6	+1	2611.838		2611.551	5658.641	3047.090	5.40 (+1)
I-1b	4	2		3	2	-1	2612.842		2611.506	5542.504	2930.998	1.15 (+1)
I-1a	6	3	+2	6	3	-1			2609.658	6638.729	4029.071	6.51 (+0)
I-1b	4	1		3	1	-1			2606.196	5608.682	3002.486	4.15 (+0)
I	5	2	+1	5	2		2605.921		2605.843	3792.568	1186.725	4.26 (+0)
I-1a	7	6	+2	7	6	+1	2606.154		2605.747	6782.988	4177.240	6.28 (+1)
I-1c	3	2	-1	2	2		2606.296		2605.441	5948.615	3343.175	9.08 (+1)
I-1a	4	1	+2	4	1	-1	2605.763		2605.331	5930.849	3325.518	2.91 (+1)
I	6	4	+1	6	4		2605.062		2604.957	4035.215	1430.258	1.00 (+1)
I-1a	1	1	-2	0	1	+1	2603.883		2603.226	5124.508	2521.282	1.01 (+2)
I-1a	3	2	+2	3	2	-1	2602.367		2601.958	5532.956	2930.998	1.08 (+1)
I-1a	5	5	+2	5	5	+1	2599.268		2598.922	5898.647	3299.725	1.55 (+1)
I-2c	2	1	-3	3	5	+2			2598.522	7703.435	5104.913	8.86 (+1)
I-1b	5	3		4	3	+1	2597.058		2596.495	5828.522	3233.207	1.20 (+1)
I-1a	4	5	+2	4	5	+1	2596.520		2596.198	5459.909	2863.711	6.26 (+1)
I	9	8	+1	9	8				2595.363	4992.020	2395.657	1.24 (+1)
I-1b	5	5		4	5	+1			2595.142	5458.853	2863.711	7.35 (+1)
I	8	7	+1	8	7		2594.477		2594.300	4566.471	1972.171	1.41 (+1)
I	5	3	+1	5	3		2593.460		2593.358	3673.497	1080.179	9.82 (+0)
I	7	6	+1	7	6		2591.323		2591.159	4177.240	1586.082	1.59 (+1)
I-1a	6	5	+2	6	5	+1	2590.315		2589.656	6414.529	3824.873	6.30 (+1)
I	4	1	+1	4	1		2589.541		2589.446	3422.758	833.311	2.29 (+1)
I	6	5	+1	6	5		2586.985		2586.822	3824.873	1238.051	1.79 (+1)
I-1b	5	2		4	2	+1			2586.746	5937.769	3351.023	3.88 (+0)
I	4	2	+1	4	2		2582.909		2582.798	3351.023	768.225	9.74 (+0)
I-1a	4	4	+2	4	4	+1	2583.155		2582.764	5651.768	3069.003	9.24 (+1)
I	5	4	+1	5	4		2581.184		2581.031	3509.703	928.672	2.01 (+1)
I-1a	6	1	-2	6	1	-1			2579.286	6766.989	4187.707	5.60 (-2)
I-1a	3	4	+2	3	4	+1	2579.748		2579.378	5298.686	2719.308	7.54 (+1)
I-1a	5	4	+2	5	4	+1	2579.672		2579.237	6088.940	3509.703	8.19 (+1)
I-2c	2	1	-3	1	1	-2			2578.927	7703.435	5124.508	1.79 (+2)
I-2c	2	3	+3	2	3	+2			2577.758	7758.420	5180.662	2.51 (+2)
I-1a	4	3	+2	4	3	+1	2577.629		2577.319	5810.346	3233.027	1.01 (+2)
I	8	8	+1	8	8		2575.312		2575.077	4221.809	1646.732	1.58 (+1)
I	9	9	+1	9	9		2575.112		2574.834	4604.801	2029.967	1.43 (+1)
I	7	7	+1	7	7		2574.893		2574.687	3876.409	1301.722	1.77 (+1)
I	4	3	+1	4	3		2574.660	2574.647	2574.524	3233.027	658.503	2.29 (+1)
I-2c	1	2	-3	0	2	+2			2574.518	7571.941	4997.423	1.09 (+2)
I-1c	2	1	+1	1	1				2574.369	5815.188	3240.819	5.04 (+1)
I-2d	3	5	+3	2	1				2573.756	7595.812	5022.056	8.57 (+1)
I	6	6	+1	6	6		2573.582	2573.581	2573.397	3568.950	995.553	2.01 (+1)
I-2d	2	4	+3	2	2				2573.237	7514.590	4941.353	3.37 (-1)
I-1c	2	0	-1	1	0		2572.220		2571.455	5834.642	3263.187	9.66 (+1)
I	5	5	+1	5	5		2571.111	2571.076	2570.947	3299.725	728.777	2.24 (+1)
I-1a	3	1	+2	3	1	-1	2570.858		2570.348	5572.834	3002.486	2.72 (+1)
I	3	1	+1	3	1		2568.703		2568.587	3063.193	494.606	6.46 (+0)
I	4	4	+1	4	4		2567,285	2567.263	2567.129	3069.003	501.875	3.78 (+1)
I-1a	2	3	+2	2	3	+1	2566.904		2566.527	5180.662	2614.135	9.84 (+1)
I	3	2	+1	3	2		2564.408	2564.373	2564.279	2992.161	427.881	2.44 (+1)
I	3	3	+1	3	3		2561.493	2561.503	2561.343	2876.591	315.248	3.41 (+1)
I-1b	4	3		3	3	+1	2557.484		2556.144	5432.735	2876.591	4.48 (+1)
I	2	2	+1	2	2		2554.664	2554.656	2554.519	2723.765	169.246	4.50 (+1)
I-1a	3	3	+2	3	3	+1	2554.276		2553.756	5430.347	2876.590	1.06 (+2)
I	2	1	+1	2	1		2552.987	2552.947	2552.849	2790.127	237.279	2.26 (+1)
I-1b	4	2		3	2	+1			2550.343	5542.504	2992.161	1.40 (+1)
I-1a	2	1	-2	2	1	-1			2548.821	5304.112	2755,291	1.60 (+1)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I-1b	4	1			3	1	+1			2545.489	5608.682	3063.193	4.95 (+0)
I	1	1	+1		1	1		2545.418	2545.413	2545.273	2609.377	64.104	6.63 (+1)
I-1a	2	2	+2		2	2	=1	2542.467		2541.908	5265.703	2723.765	1.29 (+2)
I-1a	3	0	-2		3	0	-1	2541.433		2540.802	5566.330	3025.528	5.64 (+1)
I-1a	3	2	+2		3	2	+1	2541.293		2540.796	5532.956	2992.161	1.04 (+2)
I-2c	1	2	-3		2	4	+2			2539.965	7571.941	5031.976	1.44 (+2)
I-1a	5	3	+2		5	3	+1	2539.744		2539.087	6212.584	3673.497	6.23 (+1)
I-1a	1	2	+2		1	2	+1	2539.451		2538.963	5087.004	2548.041	1.38 (+2)
I-1c	2	1	-1		1	1		2538.253		2537.444	5778.263	3240.819	5.88 (+1)
I-1a	4	2	+2		4	2	+1	2536.931		2536.375	5887.398	3351.023	7.94 (+1)
I-1a	5	2	+2		5	2	+1	2534.922		2534.401	6326.970	3792.568	5.83 (+1)
I-1b	4	4			3	4	+1	2532.253		2530.911	5250.219	2719.308	6.60 (+1)
I-2f	2	1	-2		1	1	+1			2530.370	8170.369	5639.999	1.09 (+2)
I	1	0	-1		1	0		2529.724	2529.721	2529.554	2616.487	86.933	1.29 (+2)
I-2d	2	5	+3		1	1				2527.795	7369.035	4841.240	1.63 (+0)
I-1b	3	1			2	1	-1			2525.508	5280.799	2755.291	1.99 (+0)
I-1a	6	4	+2		6	4	-1			2519.909	6403.157	3883.248	6.12 (+0)
I-1a	4	1	-2		4	1	-1	2520.677		2519.904	5845.422	3325.518	8.32 (+0)
I	2	1	-1		2	1		2518.207	2518.226	2518.012	2755.291	237.279	8.38 (+1)
I-1a	1	1	-2		1	1	+1	2515.755		2515.130	5124.508	2609.377	1.25 (+2)
I-1a	2	1	-2		2	1	+1	2514.619		2513.985	5304.112	2790.127	9.98 (+1)
I-1a	3	1	+2		3	1	+1	2510.291		2509.642	5572.834	3063.193	7.28 (+1)
I	3	0	-1		3	0		2509.075	2509.074	2508.815	3025.528	516.713	1.23 (+2)
I-1a	5	2	-2		5	2	-1			2508.181	6167.744	3659.563	1.71 (+0)
I-1a	4	1	+2		4	1	+1	2508.757		2508.092	5930.849	3422.758	4.62 (+1)
I	3	1	-1		3	1		2508.131	2508.145	2507.880	3002.486	494.606	1.07 (+2)
I	3	2	-1		3	2		2503.347	2503.354	2503.117	2930.998	427.881	5.97 (+1)
I-2c	0	3	+3		1	3	+2			2498.346	7492.660	4994.314	4.71 (+2)
I	4	1	-1		4	1		2492.541	2492.540	2492.207	3325.518	833.311	1.11 (+2)
I	4	2	-1		4	2		2491.749	2491.741	2491.438	3259.663	768.225	8.71 (+1)
I-1b	3	0			2	0	-1	2492.728		2491.394	5304.036	2812.642	6.32 (+0)
I-2c	3	5	+3		3	5	+2			2490.899	7595.812	5104.913	2.04 (+1)
I-1b	3	1			2	1	+1	2491.976		2490.672	5280.799	2790.127	1.18 (+1)
I	4	3	-1		4	3		2486.559	2486.567	2486.287	3144.790	658.503	4.58 (+1)
I-2c	2	2	-3		2	2	+2			2485.940	7751.643	5265.703	1.39 (+2)
I-1b	3	2			2	2	+1	2486.844		2485.543	5209.308	2723.765	3.29 (+1)
I-1a	6	3	-2		6	3	-1			2485.121	6514.192	4029.071	5.90 (-1)
I-2c	1	2	-3		1	2	+2			2484.937	7571.941	5087.004	1.41 (+2)
I-1a	3	1	-2		3	1	-1	2483.553		2482.665	5485.152	3002.486	1.75 (+1)
I-2c	2	4	+3		2	4	+2			2482.614	7514.590	5031.976	9.98 (+1)
I-1a	2	0	-2		2	0	-1	2474.054		2473.251	5285.893	2812.642	7.86 (+1)
I	5	2	-1		5	2		2473.238	2473.268	2472.838	3659.563	1186.725	9.55 (+1)
I	5	3	-1		5	3		2472.846	2472.829	2472.481	3552.620	1080.139	7.24 (+1)
I	5	1	-1		5	1		2472.325	2472.370	2471.901	3721.811	1249.910	1.09 (+2)
I	5	0	-1		5	0		2471.923	2471.921	2471.483	3742.346	1270.862	1.14 (+2)
I	5	4	-1		5	4		2467.553	2467.552	2467.239	3395.911	928.672	3.70 (+1)
I-1b	3	3			2	3	+1	2464.652		2463.355	5077.489	2614.135	5.65 (+10
I-2a	2	1	+1		1	1				2458.294	7299.534	4841.240	6.21 (+1)
I-2a	2	0	-1		1	0				2457.877	7326.850	4868.973	1.13 (+2)
I	0	1	+1		1	1		2457.290	2457.248	2457.178	2521.282	64.104	1.19 (+2)
I-1a	4	2	-2		4	2	-1	2456.273		2455.200	5714.864	3259.663	5.71 (+0)
I	6	4	-1		6	4		2453.408	2453.394	2452.990	3883.248	1430.258	6.07 (+1)
I-2c	2	2	-3		3	4	+2			2452.957	7751,643	5298.686	8.54 (+1)
I	6	3	-1		6	3		2452.718	2452.706	2452.236	4029.071	1576.835	8.11 (+1)
I-1a	0	2	+2		1	2	+1	2449.885		2449.382	4997.423	2548.041	2.48 (+2)
I	6	2	-1		6	2		2449.533	2449.541	2449.008	4128.273	1679.265	9.64 (+1)
I-1a	4	0	-2		4	0	-1	2449.800		2448.920	5895.604	3446.685	1.01 (+2)
I	6	1	-1		6	1		2447.903	2447.915	2447.353	4187.703	1740.351	1.05 (+2)
I	6	5	-1		6	5		2446.632	2446.637	2446.274	3684.325	1238.051	3.01 (+1)
I-2a	3	1	-1		2	1				2438.640	7460.696	5022.056	2.18 (+1)
I-1c	4	4	+1		4	4		2438.509		2438.252	6106.255	3667.003	2.89 (+1)
I-2f	1	1	-2		0	1	+1			2437.969	7991.681	5553.712	9.37 (+1)
I-1a	6	3	+2		6	3	+1			2436.956	6638.729	4201.773	2.80 (+1)
I-1c	4	2	+1		4	2				2434.610	6362.564	3927.953	1.47 (+1)
I-1c	4	3	+1		4	3		2433.901		2432.420	6254.046	3820.625	3.03 (+1)
I	7	5	-1		7	5		2431.821		2431.325	4248.891	1817.565	5.18 (+1)
I-2c	2	4	+3		1	2	+2			2427.587	7514.590	5097.003	!.53 (+1)
I-1c	3	3	+1		3	3		2424.797		2424.376	5909.649	3485.273	3.48 (+1)
I	7	6	-1		7	6		2423.646	2423.684	2423.221	4009.303	1586.082	2.58 (+1)

TABLE 1—*Continued*

Band[a]	Transition						Lab	Space[b]	ab initio			
							ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	← J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I-1a	4	1	-2	4	1	+1	2423.675		2422.664	5845.422	3422.758	5.35 (+1)
I-1a	3	1	-2	3	1	+1	2422.983		2421.959	5485.152	3063.193	2.52 (+1)
I	7	2	-1	7	2		2421.877	2421.940	2421.233	4662.536	2241.303	9.15 (+1)
I	7	3	-1	7	3		2420.724	2420.696	2420.070	4561.507	2141.437	8.27 (+1)
I-1c	3	2	+1	3	2		2420.207		2419.240	6015.313	3595.663	9.95 (+0)
I	7	1	-1	7	1		2419.551		2418.855	4719.008	2300.153	9.94 (+1)
I	7	0	-1	7	0		2418.891	2418.923	2418.188	4737.873	2319.685	1.01 (+2)
I	7	4	-1	7	4		2417.764	2417.863	2417.371	4419.204	2001.833	4.60 (+1)
I-1a	5	3	-2	5	3	-1			2416.746	5969.366	3552.620	2.00 (-3)
I-1b	2	1		1	1	+1	2413.922		2412.679	5022.056	2609.377	1.88 (+1)
I-1c	2	2	+1	2	2		2412.859		2412.316	5755.490	3343.175	4.52 (+1)
I	8	5	-1	8	5		2411.518		2410.943	4873.060	2462.117	5.93 (+1)
I	8	6	-1	8	6		2408.730		2408.171	4649.668	2241.496	4.46 (+1)
I-1c	3	1	+1	2	1				2405.355	5815.188	3409.833	2.98 (+1)
I-2f	2	3	+2	2	3	+1			2404.531	8058.213	5653.682	9.05 (+1)
I-2c	2	1	-3	2	1	-2			2399.322	7703.435	5304.112	6.99 (=1)
I-1c	1	1	+1	1	1		2399.749		2399.179	5639.999	3240.819	6.58 (+1)
I	8	7	-1	8	7		2398.519		2398.033	4370.203	1972.171	2.20 (+1)
I	9	5	-1	9	5				2397.470	5563.859	3166.389	4.71 (+1)
I	8	3	-1	8	3		2395.493		2394.713	5169.552	2774.839	8.14 (+1)
I-1b	2	2		1	2	+1	2394.556		2393.313	4941.353	2548.041	4.42 (+1)
I-1a	6	1	-2	6	1	+1			2389.205	6766.989	4377.784	7.65 (+1)
I	8	2	-1	8	2				2387.602	5255.615	2868.013	8.71 (+1)
I-2c	1	3	+3	1	3	+2			2387.255	7381.569	4994.314	1.35 (+2)
I	9	6	-1	9	6				2384.094	5340.496	2956.405	5.30 (+1)
I	9	7	-1	9	7				2383.590	5327.376	2701.244	3.86 (+1)
I-1c	1	0	-1	1	0				2380.927	5644.114	3263.187	1.27 (+2)
I-1a	1	3	+2	2	3	+1			2380.179	4994.314	2614.135	2.30 (+2)
I-2f	1	2	+2	1	2	+1			2380.029	7963.841	5583.811	1.29 (+2)
I	1	2	+1	2	2		2378.869		2378.795	2548.041	169.246	1.09 (+2)
I-1a	5	2	-2	5	2	+1			2375.176	6167.744	3792.568	3.99 (+1)
I-2e	2	1		1	1	+1			2374.245	8014.243	5639.999	1.83 (+1)
I	1	1	+1	2	1		2372.185		2371.099	2609.377	64.104	5.40 (+1)
I	9	8	-1	9	8				2370.613	4766.270	2395.657	1.88 (+1)
I-1a	1	1	-2	2	1	-1			2369.217	5124.508	2755.291	5.07 (+0)
I-1c	2	1	-1	2	1				2368.430	5778.263	3409.833	7.56 (+1)
I-1a	6	4	+2	6	4	-1			2367.942	6403.157	3883.248	1.19 (+1)
I-1a	6	4	-2	6	4	-1			2365.773	6249.022	3883.248	1.11 (+1)
I-2a	2	1	-1	1	1				2365.621	7206.861	4841.240	5.44 (+1)
I-1c	3	0	-1	3	0				2364.118	6046.732	3682.614	1.23 (+2)
I-1a	4	2	-2	4	2	+1			2363.841	5714.864	3351.023	1.87 (+1)
I-1a	1	2	+2	2	2	+1			2363.239	5087.003	2723.765	1.11 (+2)
I-1c	3	1	-1	3	1				2361.998	6022.981	3660.983	1.03 (+2)
I-2b	3	1	-1	3	5	+2			2355.784	7460.696	5104.913	6.45 (-1)
I-2f	2	1	-2	2	1	+1			2355.181	8170.369	5815.188	9.14 (+1)
I	9	4	-1	9	4				2353.184	5687.757	3334.573	6.48 (+1)
I-1c	3	2	-1	3	2				2352.952	5948.615	3595.663	5.27 (+1)
I	9	2	-1	9	2				2352.220	5906.619	3554.399	8.22 (+1)
I-2f	1	1	-2	1	1	+1			2351.683	7991.681	5639.999	1.17 (+2)
I-1c	4	1	-1	4	1				2350.019	6341.605	3991.586	1.10 (+2)
I-1c	4	2	-1	4	2				2347.485	6275.437	3927.953	8.28 (+1)
I	9	3	-1	9	3				2347.293	5807.335	3460.042	7.58 (+1)
I-2d	2	5	+3	2	1				2346.979	7369.035	5022.056	3.04 (+0)
I-1c	4	3	-1	4	3				2336.717	6157.342	3820.625	3.95 (+1)
I-1a	2	2	+2	3	2	-1			2334.705	5265.703	2930.998	8.11 (+0)
I-1a	1	1	-2	2	1	+1			2334.380	5124.508	2790.127	3.13 (+1)
I-2c	1	4	+3	0	2	+2			2328.510	7325.932	4997.423	1.39 (+1)
I-2c	2	3	+3	3	3	+2			2328.073	7758.420	5430.347	1.53 (+2)
I-1b	1	1		0	1	+1			2319.958	4841.240	2521.282	2.24 (+1)
I-2a	3	3	+1	3	3				2315.492	7392.981	5077.489	4.76 (+1)
I-2d	3	5	+3	3	1				2315.013	7595.812	5280.799	5.85 (+0)
I-1c	0	1	+1	1	1				2312.893	5553.712	3240.819	1.18 (+2)
I-1a	2	4	+2	3	4	+1			2312.668	5031.976	2719.308	2.15 (+2)
I-1a	6	3	-2	6	3	+1			2312.418	6514.192	4201.773	1.83 (+1)
I-2c	1	2	-3	2	2	+2			2306.238	7571.941	5265.703	3.52 (+1)
I-2d	2	4	+3	3	2				2305.283	7514.590	5209.308	9.27 (-1)
I-1a	2	3	+2	3	3	+1			2304.071	5180.662	2876.591	1.41 (+20
I-1a	2	1	-2	3	1	-1			2301.626	5304.112	3002.486	1.07 (+1)
I	2	3	+1	3	3		2298.930		2298.887	2614.135	315.248	9.92 (+1)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I-1b	6	5			6	5	-1			2297.690	5982.015	3684.325	2.52 (+1)
I	2	0	-1		3	0		2295.980		2295.930	2812.642	516.713	3.96 (+1)
I-1a	5	3	-2		5	3	+1			2295.869	5969.366	3673.497	1.53 (+1)
I	2	2	+1		3	2		2295.947		2295.884	2723.765	427.881	6.56 (+1)
I	2	1	+1		3	1		2295.577		2295.521	2790.127	494.606	4.60 (+1)
I-2c	1	4	+3		2	4	+2			2293.956	7325.932	5031.976	2.19 (+2)
I-1b	5	4			5	4	-1			2293.201	5689.112	3395.911	2.86 (+1)
I-2a	2	2	+1		2	2				2292.548	7233.902	4941.353	5.67 (+1)
I-1b	4	3			4	3	-1			2287.944	5432.735	3144.790	3.29 (+1)
I-2e	1	1			0	1	+1			2287.817	7841.529	5553.712	2.75 (+1)
I-1a	3	3	+2		4	3	-1			2285.556	5430.347	3144.790	7.76 (+0)
I-2f	0	2	+2		1	2	+1			2284.960	7868.771	5583.811	2.27 (+2)
I-1b	4	1			4	1	-1			2283.164	5608.682	3325.518	1.11 (+2)
I-1b	4	2			4	2	-1			2282.840	5542.504	3259.663	8.16 (+1)
I-1b	5	1			5	1	-1			2279.441	6001.251	3721.811	1.24 (+2)
I-1b	5	0			5	0	-1			2278.743	6021.089	3742.346	1.30 (+2)
I-1b	3	0			3	0	-1			2278.508	5304.036	3025.528	1.05 (+2)
I-1b	3	1			3	1	-1			2278.313	5280.799	3002.486	8.77 (+1)
I-1b	3	2			3	2	-1			2278.309	5209.308	2930.998	4.01 (+1)
I-1b	5	2			5	2	-1			2278.205	5037.769	3659.563	1.05 (+2)
I-2a	2	1	+1		2	1				2277.478	7299.534	5022.056	3.12 (+1)
I-1b	5	3			5	3	-1			2275.902	5828.522	3552.820	7.32 (+1)
I-1a	2	2	+2		3	2	+1			2273.543	5265.703	2992.161	7.47 (+1)
I-1a	3	2	+2		4	2	-1			2273.293	5532.956	3259.663	1.36 (+1)
I-1b	6	3			6	3	-1			2270.157	6299.228	4029.071	9.70 (+1)
I-1b	2	1			2	1	-1			2266.765	5022.056	2755.291	5.13 (+1)
I-1b	6	3			6	2	-1			2264.391	6392.663	4128.273	1.08 (+2)
I-2c	2	5	+2		3	5	+2			2264.122	7369.035	5104.913	2.57 (+2)
I-2a	1	1	+1		1	1				2262.378	7103.618	4841.240	7.48 (+1)
I	2	1	+1		3	1				2260.685	2755.291	494.606	4.00 (-2)
I-1a	2	0	-2		3	0	-1			2260.365	5285.893	3025.528	1.74 (+1)
I-1a	4	3	+2		5	3	-1			2257.726	5810.346	3552.620	1.65 (+1)
I-1b	6	4			6	4	-1			2255.896	6139.144	3883.248	5.29 (+1)
I-1a	4	4	+2		5	4	-1			2255.856	5651.768	3395.911	8.21 (+0)
I-1b	1	0			1	0	-1			2252.986	4868.973	2616.487	6.90 (+1)
I-2c	2	4	+3		2	2	+2			2248.887	7514.590	5265.703	1.11 (+1)
I-1a	3	1	+2		4	1	-1			2247.317	5572.834	3325.518	1.19 (+1)
I-2c	2	5	+3		1	1	-2			2244.527	7369.035	5124.508	7.56 (+0)
I-1a	3	5	+2		4	5	+1	2241.347		2241.202	5104.913	2863.711	1.98 (+2)
I-1a	2	1	-2		3	1	+1			2240.920	5304.112	3063.193	3.18 (+1)
I-1c	1	2	+1		2	2		2241.077		2240.637	5583.811	3343.175	1.09 (+2)
I-2c	1	4	+3		1	2	+2			2238.929	7325.932	5087.004	1.62 (+1)
I-2e	2	1			2	1	-1			2235.980	8014.243	5778.263	6.11 (+1)
I-1b	2	1			2	1	+1			2231.929	5022.056	2790.127	1.59 (+1)
I-1b	1	1			1	1	+1			2231.863	4841.240	2609.377	3.60 (+1)
I-1c	1	1	+1		2	1				2230.166	5639.999	3409.833	5.31 (+1)
I	3	1	+1		4	1		2229.895		2229.881	3063.193	833.311	4.26 (+1)
I-1a	3	4	+2		4	4	+1			2229.683	5298.686	3069.003	1.44 (+2)
I-1a	4	2	+2		5	2	-1			2227.835	5887.398	3659.563	1.48 (+1)
I	3	2	+1		4	2		2223.965		2223.936	2992.161	768.225	5.13 (+1)
I-2f	1	3	+2		2	3	+1			2220.720	7874.402	5653.682	2.10 (+2)
I-2c	2	2	-3		3	2	+2			2218.686	7751.643	5532.956	3.89 (+1)
I	3	3	+1		4	3		2218.129		2218.088	2876.591	658.503	6.70 (+1)
I-1b	3	1			3	1	+1			2217.607	5280.799	3063.193	5.36 (+0)
I-1b	2	2			2	2	+1			2217.588	4941.353	2723.765	2.63 (+1)
I	3	4	+1		4	4		2217.451		2217.434	2719.308	501.875	8.97 (+1)
I-1b	3	2			3	2	+1			2217.147	5209.308	2992.161	1.96 (+1)
I-2c	2	4	+2		3	4	+2			2215.904	7514.590	5298.686	1.31 (+2)
I-2e	1	0			1	0	-1			2215.211	7859.324	5644.114	8.78 (+1)
I-1a	5	5	+2		6	5	-1			2214.322	5898.647	3684.325	7.78 (+0)
I-1a	6	4	-2		6	4	+1			2213.806	6249.022	4035.215	1.12 (+1)
I-2a	1	0	-1		1	0				2213.270	7082.243	4868.973	1.27 (+2)
I-2b	3	3	+1		2	3	+2			2212.320	7392.981	5180.662	1.33 (+1)
I-1a	4	1	+2		5	1	-1			2209.038	5930.849	3721.811	9.29 (+0)
I-2f	1	2	+2		2	2	+1			2208.350	7963.841	5755.490	1.03 (+2)
I-1a	5	4	+2		6	4	-1			2203.692	6088.940	3883.248	1.37 (+1)
I-2b	2	2	+1		2	4	+2			2201.926	7233.902	5031.976	2.85 (+1)
I-2e	1	1			1	1	+1			2201.530	7841.529	5639.999	4.40 (+1)
I-2c	1	3	+3		2	3	+2			2200.907	7381.569	5180.662	1.02 (+2)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I-1b	3	3			3	3	+1			2200.898	5077.489	2876.591	2.11 (+1)
I-1b	4	3			4	3	+1			2199.708	5432.735	3233.027	1.89 (+1)
I-2e	2	1			2	1	+1			2199.055	8014.243	5815.188	2.92 (+1)
I-1a	5	2	+2		6	2	-1			2198.697	6326.970	4128.273	1.44 (+1)
I-1a	3	3	+2		4	3	+1			2197.320	5430.347	3233.027	9.22 (+1)
I-2b	2	1	+1		3	5	+2			2194.621	7299.534	5104.913	8.74 (+0)
I-1b	4	2			4	2	+1			2191.481	5542.504	3351.023	7.69 (+0)
I-2a	2	1	-1		2	1				2184.805	7206.861	5022.056	7.87 (+1)
I-1a	5	3	+2		6	3	-1			2183.513	6212.584	4029.071	1.02 (+1)
I-1a	3	2	+2		4	2	+1			2181.933	5532.956	3351.023	5.72 (+1)
I-1b	4	4			4	4	-1			2181.216	5250.219	3069.003	1.71 (+1)
I-2a	3	1	-1		3	1				2179.897	7460.696	5280.799	1.16 (+2)
I-1b	5	4			5	4	+1			2179.409	5089.112	3509.703	1.81 (+1)
I-2f	1	1	-2		2	1	+1			2176.493	7991.681	5815.188	3.05 (+1)
I	4	0	+1		5	0		2175.780		2175.822	3446.685	1270.862	3.97 (+1)
I-2b	2	1	+1		1	1	-2			2175.026	7299.534	5124.508	1.02 (+0)
I	4	1	+1		5	1		2172.815		2172.847	3422.758	1249.910	4.07 (+1)
I	3	1	-1		4	1				2169.175	3002.486	833.311	3.56 (-1)
I-1c	2	3	+1		3	3		2168.698		2168.409	5653.682	3485.273	9.96 (+1)
I-1a	4	6	+2		5	6	+1	2168.349		2168.297	5215.387	3047.090	1.81 (+2)
I-1a	6	5	+2		7	5	-1			2165.628	6414.529	4248.891	1.13 (+1)
I	4	2	+1		5	2		2164.278		2164.298	3351.023	1186.725	4.44 (+1)
I	3	2	-1		4	2				2162.773	2930.998	768.225	5.47 (-1)
I-2a	0	1	+1		1	1				2162.212	7003.453	4841.240	1.19 (+2)
I-1a	4	5	+2		5	5	+1			2160.185	5459.909	3299.725	1.42 (+2)
I-1c	2	2	+1		3	2				2159.827	5755.490	3595.663	6.51 (+1)
I-1a	3	1	-2		4	1	-1			2159.634	5485.152	3325.518	5. 96 (+0)
I-1b	5	5			5	5	+1			2159.129	5458.853	3299.725	1.44 (+1)
I-1c	2	1	+1		3	1				2154.205	5815.188	3660.983	4.50 (+1)
I-1a	4	0	-2		5	0	-1			2153.258	5895.604	3742.346	2.28 (+1)
I	4	3	+1		5	3		2152.887		2152.888	3233.027	1080.139	5.24 (+1)
I-1c	2	0	-1		3	0				2152.028	5834.642	3682.614	3.84 (+1)
I-2f	2	4	+2		3	4	+1			2151.684	7916.363	5764.679	1.90 (+2)
I-1a	3	1	+2		4	1	+1			2150.077	5572.834	3422.758	3.41 (+1)
I-2f	2	3	+2		3	3	+1			2148.563	8058.213	5909.649	1.30 (+2)
I-2b	2	2	+1		1	2	+2			2146.898	7233.902	5087.004	8.10 (+0)
I-1a	4	4	+2		5	4	+1			2142.064	5651.768	3509.703	1.02 (+2)
I	4	4	+1		5	4		2140.348		2140.331	3069.003	928.672	6.48 (+1)
I-1a	4	3	+2		5	3	+1			2136.849	5810.346	3673.497	7.39 (+1)
I-2c	3	5	+3		4	5	+2			2135.903	7595.812	5459.909	3.40 (+1)
I	4	5	+1		5	5		2134.922		2134.934	2863.711	728.777	8.08 (+1)
I-1b	6	6			6	6	+1			2134.408	5703.358	3568.950	1.23 (+1)
I-1a	7	7	+2		8	7	-1			2134.054	6504.257	4370.203	7.10 (+0)
I-2c	2	1	-3		3	1	+2			2130.600	7703.435	5572.834	1.09 (+1)
I-2b	2	3	+1		1	3	+2			2127.381	7121.694	4994.314	2.17 (+1)
I-1a	4	1	-2		5	1	-1			2122.611	5845.422	3721.811	1.30 (+1)
I	5	1	+1		6	1		2122.513		2122.593	3862.944	1740.351	3.96 (+1)
I-1a	3	0	+2		4	0	+1			2119.645	5566.330	3446.685	3.16 (+1)
I-1c	2	1	-1		3	1				2117.280	5778.263	3660.983	8.90 (-2)
I	5	2	+1		6	2		2113.241		2113.304	3792.568	1679.265	4.10 (+1)
I-2c	3	5	+2		3	1	-2			2110.660	7595.812	5485.152	5.11 (+0)
I-2a	1	2	+1		2	2				2104.682	7046.035	4941.353	1.13 (+2)
I-2c	2	1	-1		3	5	+2			2101.948	7206.861	5104.913	4.44 (-1)
I-1c	3	4	+1		4	4		2097.745		2097.676	5764.679	3667.003	8.95 (+1)
I	5	3	+1		6	3		2096.629		2096.663	3673.497	1576.835	4.40 (+1)
I-1a	4	2	+2		5	2	+1			2094.830	5887.398	3792.568	4.97 (+1)
I-1a	5	7	+2		6	7	+1			2094.274	5363.481	3269.207	1.65 (+2)
I-2f	2	1	-2		3	1	+1			2090.149	8170.369	6080.220	3.62 (+1)
I-1a	5	6	+2		6	6	+1	2089.764		2089.691	5658.641	3568.950	1.35 (+2)
I-1c	3	2	+1		4	3		2089.305		2089.024	5909.649	3820.625	6.65 (+1)
I-1c	3	1	+1		4	1				2088.674	6080.220	3991.586	4.13 (+1)
I-2d	2	5	+3		3	1				2088.236	7369.035	5280.799	1.31 (+0)
I-1c	3	2	+1		4	2				2087.360	6015.313	3927.953	5.07 (+1)
I-1b	1	1			2	1	-1			2085.949	4841.240	2755.291	3.17 (+1)
I-2a	1	1	+1		2	1				2081.562	7103.618	5022.056	4.91 (+1)
1	6	0	+1		7	0				2080.801	4400.486	2319.685	3.89 (+1)
I	5	4	+1		6	4		2079.433		2079.445	3509.703	1430.258	5.10 (+1)
I	6	1	+1		7	1		2077.500		2077.631	4201.773	2300.153	3.90 (+1)
I-1a	6	3	+2		7	3	-1			2077.222	6638.729	4561.507	1.30 (+1)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I	4	1	-1		5	1				2075.608	3325.518	1249.910	4.10 (-1)
I-1a	5	5	+2		6	5	+1			2073.774	5898.647	3824.873	1.02 (+2)
I	4	2	-1		5	2				2072.938	3259.663	1186.725	1.19 (+0)
I-1a	4	1	+2		5	1	+1			2067.905	5930.849	3862.944	3.99 (+1)
I	6	2	+1		7	2		2067.366		2067.462	4308.765	2241.303	3.84 (+1)
I	4	3	-1		5	3				2064.651	3144.790	1080.139	1.01 (+0)
I-2e	1	1			2	1	-1			2063.266	7841.529	5778.263	4.69 (+1)
I-1a	3	1	-2		4	1	+1			2062.294	5485.152	3422.758	3.47 (+0)
I	5	5	+1		6	5		2061.680		2061.673	3299.725	1238.051	6.07 (+1)
I	6	3	+1		7	3		2060.200		2060.336	4201.773	2141.437	4.01 (+1)
I-2c	3	4	+3		2	2	+2			2060.229	7325.932	5265.703	5.66 (+0)
I-1b	1	0			2	0	-1			2056.331	4868.973	2812.642	5.21 (+1)
I-1a	4	2	-2		5	2	-1			2055.301	5714.864	3659.563	5.56 (+0)
I-1a	5	4	+2		6	4	+1			2053.725	6088.940	4035.215	7.63 (+1)
I	5	6	+1		6	6		2051.510		2051.536	3047.090	995.553	7.23 (+1)
I-1b	1	1			2	1	+1			2051.113	4841.240	2790.127	3.01 (+1)
I-2b	1	2	+1		0	2	+2			2048.613	7046.035	4997.423	1.05 (+1)
I-1a	6	1	-2		7	1	-1			2047.981	6766.989	4719.008	2.08 (+1)
I-2a	2	3	+1		3	3				2044.205	7121.694	5077.489	1.07 (+2)
I-2b	2	0	-1		2	0	-2			2040.957	7326.850	5285.893	1.19 (+1)
I-1a	5	2	-2		6	2	-1			2039.471	6167.744	4128.273	1.10 (+1)
I	7	1	+1		8	1				2036.437	4960.974	2924.537	3.83 (+1)
I	6	4	+1		7	4		2033.318		2033.382	4035.215	2001.833	4.34 (+1)
I-1c	4	5	+1		5	5				2032.371	5920.834	3888.463	7.52 (+1)
I-1c	3	1	-1		4	1				2031.390	6022.981	3991.586	6.60 (-2)
I-2e	1	1			2	1	+1			2026.341	7841.529	5815.188	3.18 (+1)
I-2e	1	0			2	0	-1			2024.682	7859.324	5834.642	6.61 (+1)
I-2a	2	2	+1		3	2				2024.594	7233.902	5209.308	6.24 (+1)
I	7	2	-1		8	4				2024.197	4662.536	2638.339	1.06 (+0)
I	7	2	+1		8	2				2023.269	4891.282	2868.013	3.44 (+1)
I-2c	3	5	+3		3	1	-2			2022.978	7595.812	5485.152	1.51 (+1)
I-2a	2	0	-1		3	0				2022.814	7326.850	5304.036	2.24 (+1)
I-1c	4	3	+1		5	3				2021.657	6254.046	4232.349	5.22 (+1)
I-1c	3	2	-1		4	2				2020.662	5948.615	3927.953	4.10 (-2)
I-1b	2	1			3	1	-1			2019.570	5022.056	3002.486	1.05 (+1)
I-1a	6	8	+2		7	8	+1			2019.518	5549.281	3529.762	1.50 (+2)
I-1a	6	7	+2		7	7	+1			2018.767	5895.176	3876.409	1.26 (+2)
I-2a	2	1	+1		3	1				2018.735	7299.534	5280.799	3.19 (+1)
I	7	3	+1		8	3				2018.202	4793.041	2774.839	3.51 (+1)
I-1a	5	3	+2		6	3	+1			2010.910	6212.584	4201.773	5.64 (+1)
I-1b	2	2			3	2	-1			2010.355	4941.353	2930.998	3.77 (+1)
I	6	5	+1		7	5		2007.290		2007.307	3824.873	1817.565	4.85 (+1)
I-1a	6	6	+2		7	6	+1			2006.481	6183.721	4177.240	1.00 (+2)
I	8	3	+1		9	3				2002.364	5462.406	3460.042	3.69 (+1)
I-1a	6	4	+2		7	4	-1			1983.953	6403.157	4419.204	2.76 (+1)
I-1a	6	5	+2		7	5	+1			1983.525	6414.529	4431.004	6.83 (+1)
I	6	6	+1		7	6		1982.874		1982.868	3568.950	1586.082	5.60 (+1)
I-1a	4	1	-2		5	1	+1			1982.478	5845.422	3862.944	3.72 (+1)
I	5	1	-1		6	1				1981.460	3721.811	1740.351	3.44 (-1)
I	5	2	-1		6	2				1980.299	3659.563	1679.265	1.19 (+0)
I	5	3	-1		6	3				1975.785	3552.620	1576.835	2.06 (+0)
I	7	5	+1		8	5		1968.800		1968.887	4431.004	2462.117	4.16 (+1)
I	6	7	+1		7	7		1967.456		1967.485	3269.207	1301.922	6.43 (+1)
I	5	4	-1		6	4				1965.653	3395.911	1430.258	1.40 (+0)
I-1a	6	3	-2		7	3	-1			1952.685	6514.192	4561.507	6.44 (+0)
I-1a	5	3	-2		6	3	-1			1940.295	5989.366	4029.071	4.81 (+0)
I	7	6	+1		8	6				1935.705	4177.240	2241.496	4.54 (+1)
I-1c	4	3	-1		5	3				1924.990	6157.342	4232.349	1.58 (-1)
I-1a	4	2	-2		5	2	+1			1922.295	5714.864	3792.568	1.84 (+0)
I	6	1	-1		7	1				1887.555	4187.703	2300.153	2.52 (-1)
I	6	3	-1		7	3				1887.534	4029.071	2141.437	1.63 (+0)
I	6	2	-1		7	2				1886.970	4128.273	2241.303	9.40 (-1)
I	6	4	-1		7	4				1881.416	3883.248	2001.833	2.40 (+0)
I	6	5	-1		7	5				1866.760	3684.325	1817.565	1.55 (+0)
I	8	7	+1		9	7				1865.227	4566.471	2701.244	4.20 (+1)
I-1a	6	4	-2		7	4	-1			1829.811	6249.022	4419.204	1.67 (-1)
I	8	8	+1		9	8		1826.160		1826.152	4221.809	2395.657	4.58 (+1)
I	8	9	+1		9	9		1798.396		1798.444	3828.412	2029.967	5.00 (+1)
I	7	5	-1		8	5				1786.774	4248.891	2462.117	2.64 (+0)

TABLE 1—*Continued*

Band[a]	Transition							Lab	Space[b]	ab initio			
								ω_{ij}	ω_{ij}	ω_{ij}	E'	E"	A_{ij}
	J'	G'	U'	←	J"	K"	U"	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(s^{-1})
I	7	3	-1		8	3				1786.668	4561.507	2774.839	1.55 (+0)
I	7	4	-1		8	4				1780.865	4419.204	2638.339	1.14 (+0)
I	7	6	-1		8	6				1767.806	4009.303	2241.496	1.59 (+0)
I-1a	5	3	-2		6	3	+1			1767.593	5969.366	4201.773	3.24 (+0)
I-1a	6	3	-2		7	3	+1			1721.151	6514.192	4793.041	5.34 (+0)
I	8	5	-1		9	5				1706.671	4873.060	3166.389	2.78 (+0)
I	8	6	-1		9	6				1693.263	4649.668	2956.405	2.70 (+0)
I	8	7	-1		9	7				1668.960	4370.203	2701.244	1.55 (+0)
I-1a	6	4	-2		7	4	+1			1613.697	6249.022	4635.325	2.24 (+0)

[a] The notation for the bands are as follows:
I: $\nu_2(1) \leftarrow 0$, I-1a: $2\nu_2(2) \leftarrow \nu_2(1)$,
I-1b: $2\nu_2(0) \leftarrow \nu_2(1)$, I-1c: $\nu_2 + \nu_1 \leftarrow \nu_1$,
I-2a: $3\nu_2(1) \leftarrow 2\nu_2(0)$, I-2b: $3\nu_2(1) \leftarrow 2\nu_2(2)$,
I-2c: $3\nu_2(3) \leftarrow 2\nu_2(2)$, I-2d: $3\nu_2(3) \leftarrow 2\nu_2(0)$,
I-2e: $2\nu_2(0) + \nu_1 \leftarrow \nu_2 + \nu_1$, I-2f: $2\nu_2(2) + \nu_1 \leftarrow \nu_2 + \nu_1$,
II: $2\nu_2(2) \leftarrow 0$, III: $3\nu_2(1) \leftarrow 0$.

[b] The data from 5000.527–4557.057 wave-number are from Drossart et al. 1989, and the data from 2832.188–2417.863 wave-number are from Maillard et al. 1990.