B. SUPPLEMENTARY MATERIAL — PART B

Li^+–H_2 COMPLEX

VIBRATIONAL ENERGY LEVELS

TABLE BI: Li^+–$H_2(I{=}0)$. Positions (E) and widths (Γ) of 'vibrational' levels $b\,k\,v_R$ J=k p associated with the v=0–1 j=0–4 thresholds ($b{\sim}j$). The positions are relative to the respective $v\,j$=0 threshold. The positions of the j>0 thresholds[a] are shown in lines marked with ε. All data are in cm^{-1}.

			v=0 (ε=0[b])				v=1 (ε=4158.571)			
			p=1		p=−1		p=1		p=−1	
b	k	v_R	E	Γ^c	$E-E(p{=}1)$	Γ^c	E	Γ^d	$E-E(p{=}1)$	Γ^e
0	0	0	−1674.606	0			−1780.080	2.37 (−2)		
		1	−1269.455	0			−1369.531	6.84 (−2)		
		2	−924.249	0			−1016.090	1.12 (−1)		
		3	−638.892	0			−719.617	1.46 (−1)		
		4	−412.415	0			−479.275	1.54 (−1)		
		5	−242.898	0			−293.678	1.42 (−1)		
		6	−126.201	0			−160.125	1.11 (−1)		
		7	−53.841	0			−72.835	7.46 (−2)		
		8	−16.453	0			−24.154	*3.86 (−2)		
		9	−1.463	0			* − 3.384	*1.23 (−2)		
2	2	0	−1410.848	0	0.000	0	−1531.768	2.88 (−2)	0.000	2.88 (−2)
		1	−1000.198	0	0.001	0	−1116.200	7.95 (−2)	−0.001	7.94 (−2)
		2	−649.119	0	0.001	0	−757.453	1.32 (−1)	0.003	1.32 (−1)
		3	−357.328	0	0.000	0	−455.339	1.70 (−1)	0.005	1.72 (−1)
		4	* − 123.714	0	0.001	0	−209.105	1.82 (−1)	0.000	1.82 (−1)
		5	54.279	1.72 (−4)	0.000	0	−16.570	1.73 (−1)	0.000	1.73 (−1)
		6	181.463	1.22 (−4)	0.000	0	125.573	1.42 (−1)	0.000	1.42 (−1)
		7	265.674	7.72 (−5)	0.000	0	223.459	1.03 (−1)	0.000	1.02 (−1)
		8	316.923	2.43 (−5)	0.001	0	285.233	6.48 (−2)	0.000	6.48 (−2)
		9	344.468	3.45 (−4)	0.186	0	319.911	3.40 (−2)	0.004	3.39 (−2)
		10					334.810	9.68 (−3)	0.019	9.77 (−3)
2	1	0	−982.522	0	0.266	0	−1086.260	2.21 (−2)	0.262	2.31 (−2)
		1	−621.269	0	0.333	0	−720.657	7.08 (−2)	0.340	8.78 (−2)
		2	−318.794	0	0.368	0	−409.786	1.16 (−1)	0.297	1.16 (−1)
		3	−76.129	0	0.351	0	−155.060	1.42 (−1)	0.283	1.48 (−1)
		4	106.755	4.98 (−3)	0.317	0	43.104	1.53 (−1)	0.269	1.49 (−1)
		5	232.093	3.35 (−3)	0.275	0	185.276	1.27 (−1)	0.241	1.24 (−1)
		6	306.427	1.96 (−3)	0.235	0	275.139	8.13 (−2)	0.210	7.92 (−2)
		7	342.400	1.26 (−3)	0.212	0	320.789	3.69 (−2)	0.190	3.56 (−2)
		8	354.251	1.37 (−3)	0.110	7.92 (−3)	336.101	1.42 (−2)	−0.042	5.85 (−3)
2	0	0	−606.428	0			−685.307	1.59 (−2)		
		1	−303.126	0			−380.288	3.34 (−2)		
		2	−57.127	0			−125.325	5.48 (−2)		
		3	130.541	1.64 (−1)			75.205	3.51 (−1)[f]		
		4	259.938	1.07 (−1)			218.930	2.92 (−1)		
		5	327.186	5.79 (−2)			303.584	1.60 (−1)		
		6	352.005	*1.41 (−2)			*334.790	*3.05 (−2)		
ε			354.300				336.285			

TABLE BI: continued

4	4	0	−658.879	0	0.000	0	−821.633	4.87 (−2)	0.001	4.87 (−2)
		1	−242.132	0	0.000	0	−400.014	1.28 (−1)	0.000	1.28 (−1)
		2	115.046	5.51 (−8)	0.000	0	−35.385	2.09 (−1)	0.000	2.09 (−1)
		3	413.152	6.70 (−4)	0.000	6.67 (−4)	272.661	2.60 (−1)	0.000	2.60 (−1)
		4	653.564	1.23 (−3)	0.000	1.20 (−3)	525.362	2.75 (−1)	0.000	2.75 (−1)
		5	837.255	2.88 (−3)	0.001	1.89 (−3)	723.049	2.60 (−1)	0.001	2.59 (−1)
		6	972.314	9.61 (−4)	0.002	1.07 (−4)	872.203	2.15 (−1)	0.003	2.17 (−1)
		7	1063.672	2.38 (−2)	0.000	1.16 (−5)	976.913	1.59 (−1)	0.000	1.59 (−1)
		8	1121.099	2.94 (−5)	0.000	1.03 (−5)	1045.170	1.05 (−1)	0.000	1.05 (−1)
		9	1167.498	2.11 (−5)	−0.013	3.05 (−3)	1085.525	5.91 (−2)	0.000	5.91 (−2)
		10					1105.121	2.28 (−2)	0.000	2.28 (−2)
4	3	0	−337.791	0	0.000	0	−484.916	4.22 (−2)	0.002	4.25 (−2)
		1	43.791	6.29 (−7)	0.000	0	−98.985	1.19 (−1)	−0.002	1.20 (−1)
		2	365.522	4.97 (−3)	0.000	4.50 (−3)	230.351	1.96 (−1)	−0.001	1.96 (−1)
		3	627.361	4.85 (−3)	0.000	4.65 (−3)	502.815	2.51 (−1)	0.000	2.51 (−1)
		4	830.325	4.29 (−3)	−0.010	6.97 (−2)	719.045	2.59 (−1)	0.000	2.59 (−1)
		5	977.745	1.39 (−2)	0.013	6.75 (−3)	881.759	2.19 (−1)	0.020	2.09 (−1)
		6	1073.003	1.44 (−2)	0.048	4.56 (−3)	990.978	1.81 (−1)	0.045	1.75 (−1)
		7	1130.221	1.57 (−2)	0.059	2.47 (−3)	1059.478	1.08 (−1)	0.009	1.07 (−1)
		8	1168.600	1.53 (−1)	0.202	2.21 (−1)	1108.666	7.36 (−3)	0.052	3.58 (−3)
4	2	0	−69.497	0	−0.581	0	−199.742	1.80 (−2)	−0.014	3.97 (−2)
		1	279.752	5.22 (−5)	0.009	0	153.177	6.30 (−2)	0.009	6.34 (−2)
		2	568.621	4.48 (−2)	0.015	3.67 (−2)	449.386	1.91 (−1)	0.010	1.85 (−1)
		3	796.505	4.52 (−2)	0.017	3.57 (−2)	688.204	2.27 (−1)	−0.012	2.15 (−1)
		4	964.206	4.07 (−2)	0.024	2.84 (−2)	869.610	2.10 (−1)	0.018	2.01 (−1)
		5	1075.070	3.76 (−2)	0.057	1.76 (−2)	995.318	1.63 (−1)	0.048	1.49 (−1)
		6	1137.590	6.60 (−2)	0.387	5.30 (−3)	1064.278	2.43 (−1)	1.500	1.29 (−1)
		7	1163.090	7.54 (−2)	0.286	4.35 (−3)	1102.416	3.87 (−2)	0.006	3.85 (−2)
4	1	0	129.644	3.94 (−2)	3.591	0	18.620	2.18 (−2)	1.861	2.17 (−2)
		1	455.260	2.83 (−1)	1.883	7.25 (−3)	345.520	3.65 (−1)[f]	1.455	2.00 (−1)[e]
		2	716.334	2.85 (−1)	1.598	8.13 (−3)	613.188	4.09 (−1)	1.217	2.56 (−1)
		3	914.312	2.54 (−1)	1.376	6.92 (−3)	821.537	3.82 (−1)	1.037	2.55 (−1)
		4	1050.477	2.06 (−1)	1.169	4.67 (−3)	970.774	2.99 (−1)	0.861	1.98 (−1)
		5	1129.508	1.48 (−1)	0.923	2.39 (−3)	1062.739	1.78 (−1)	0.683	1.21 (−1)
		6	1163.559	9.20 (−2)	0.559	7.68 (−4)	1104.043	5.98 (−2)	0.361	3.88 (−2)
4	0	0	243.658	1.08 (−2)			151.015	1.98 (−2)		
		1	559.743	*2.29 (−2)			466.586	*4.51 (−1)[f]		
		2	803.985	1.95			* 715.923	*2.98 (−1)		
		3	981.014	1.41			* 901.463	*1.95 (−1)		
		4	1094.319	8.33 (−1)			*1025.395	*1.21 (−1)		
		5	1151.769	3.48 (−1)			*1091.675	*5.33 (−2)		
ε			1168.550				1108.829			

[a]The thresholds obtained from the PES of the LiHH$^+$ system are used. In comparison with the accurate data for H_2[1], the values of $\varepsilon_{v,j}-\varepsilon_{0,0}$ are too low by 0.073, 0.247, 2.595, 2.982, and 3.979 cm^{-1} for (v,j)=(0,2), (0,4), (1,0), (1,2), and (1,4), respectively. These deviations become larger ($\sim$4−2 times) when the Born-Oppenheimer energies of H_2 are taken as reference, which is probably more appriopriate. See Fig. B1.

[b]Lies 4339.9 cm^{-1} above the minimum of the PES.

[c]All widths $\Gamma>0$ in the column are due to rotational predissociation.

[d]The widths in the column that pertain to states of negative energies (relative to $\varepsilon_{1\,0}$) are due to vibrational predissociation.

[e]The widths in this column are due to pure vibrational predissociation for states with E up to $\varepsilon_{1\,2}$; f-parity states cannot predissociate to v=1 j=0 channel.

[f]The substantial increase of the width, as compared to the preceding value in the column, is due to contribution of rotational predissociation to v=1 j=b−2 channel.

TABLE BII: Li^+–H_2(I=1). Positions (E) and widths (Γ) of 'vibrational' levels $b\,k\,v_R$ J=k p associated with the v=0–1 j=1–5 thresholds ($b\sim j$). The positions are relative to the respective $v\,j$=0 threshold. The positions of the j>0 thresholds are shown in lines marked with ε. All data are in cm^{-1}.

			v=0 (ε=0)				v=1 (ε=4158.571) -2.595[a]			
			p=1		p=−1		p=1		p=−1	
b	k	v_R	E	Γ^b	$E-E(p{=}1)$	Γ^b	E	Γ^c	$E-E(p{=}1)$	Γ^c
1	1	0	−1606.666	0	0.150	0	−1716.209	2.49 (−2)	0.152	2.49 (−2)
		1	−1199.367	0	0.138	0	−1303.813	6.97 (−2)	0.140	6.95 (−2)
		2	−851.638	0	0.125	0	−948.181	1.17 (−1)	0.127	1.17 (−1)
		3	−563.320	0	0.109	0	−649.210	1.51 (−1)	0.112	1.51 (−1)
		4	−333.412	0	0.092	0	−406.117	1.62 (−1)	0.096	1.62 (−1)
		5	* − 159.590	0	0.076	0	−217.337	1.50 (−1)	0.081	1.50 (−1)
		6	* − 36.978	0	0.058	0	−79.032	1.22 (−1)	0.062	1.22 (−1)
		7	42.312	0	0.047	0	14.268	8.58 (−2)	0.049	8.58 (−2)
		8	88.791	0	0.038	0	71.188	5.16 (−2)	0.037	5.16 (−2)
		9	112.056	0	0.036	0	101.337	2.52 (−2)	0.036	2.52 (−2)
		10					112.137	3.94 (−3)	0.055	4.02 (−3)
1	0	0	−1080.273	0			−1174.657	1.67 (−2)		
		1	−734.044	0			−822.709	6.37 (−2)		
		2	−445.659	0			−524.636	1.01 (−1)		
		3	−218.247	0			−287.689	7.32 (−2)		
		4	−50.548	0			−97.985	1.19 (−1)		
		5	55.281	*0			30.615	6.92 (−2)		
		6	106.443	*0			96.446	3.99 (−2)		
ε			118.462 -0.025[a]				112.448 -0.126[a]			
3	3	0	−1092.972	0	0.000	0	−1231.797	3.62 (−2)	0.000	3.62 (−2)
		1	−679.058	0	0.000	0	−812.993	9.86 (−2)	0.000	9.86 (−2)
		2	−324.724	0	0.000	0	−451.021	1.59 (−1)	0.000	1.59 (−1)
		3	−28.565	0	0.000	0	−146.515	2.05 (−1)	0.004	2.02 (−1)
		4	207.129	7.38 (−4)	0.011	9.72 (−4)	103.162	2.20 (−1)	0.004	2.20 (−1)
		5	388.822	4.80 (−5)	0.000	4.67 (−5)	298.959	2.06 (−1)	0.001	2.07 (−1)
		6	519.863	6.36 (−5)	0.000	6.26 (−5)	444.635	1.71 (−1)	0.000	1.71 (−1)
		7	607.866	4.52 (−5)	0.000	4.62 (−5)	546.103	1.25 (−1)	0.000	1.25 (−1)
		8	662.484	2.40 (−5)	0.000	2.53 (−5)	611.397	8.12 (−2)	0.000	8.13 (−2)
		9	692.736	1.99 (−5)	0.000	3.17 (−7)	649.272	4.46 (−2)	0.000	4.46 (−2)
		10					666.892	1.58 (−2)	0.004	1.58 (−2)
3	2	0	−727.971	0	0.007	0	−850.106	2.97 (−2)	0.002	2.97 (−2)
		1	−354.991	0	0.002	0	−472.902	8.43 (−2)	0.002	8.43 (−2)
		2	−41.538	0	−0.023	0	−151.641	1.39 (−1)	0.016	1.41 (−1)
		3	211.980	2.93 (−3)	0.014	7.21 (−4)	113.152	1.78 (−1)	0.030	1.78 (−1)
		4	406.939	1.21 (−2)	0.252	1.02 (−2)	319.591	2.40 (−1)	0.185	2.33 (−1)
		5	543.214	8.11 (−3)	0.015	7.51 (−3)	473.890	1.79 (−1)	−0.004	1.70 (−1)
		6	631.116	8.57 (−2)	−0.255	3.01 (−3)	576.210	1.28 (−1)	0.058	1.18 (−1)
		7	679.345	1.99 (−3)	0.036	1.48 (−3)	635.519	6.64 (−2)	0.017	6.56 (−2)
		8	701.382	1.21 (−3)	0.051	8.00 (−4)	663.158	2.95 (−2)	0.024	2.63 (−2)
3	1	0	−421.973	0	0.692	0	−523.992	2.07 (−2)	0.650	1.98 (−2)
		1	* − 88.692	0	0.590	0	−187.718	5.27 (−2)	0.463	5.30 (−2)
		2	184.644	9.17 (−2)	0.483	8.20 (−2)	92.970	8.36 (−2)	0.359	8.42 (−2)
		3	397.160	8.48 (−2)	0.378	7.93 (−2)	317.117	2.94 (−1)[d]	0.262	2.95 (−1)[d]
		4	549.184	6.26 (−2)	0.244	6.18 (−2)	483.772	2.60 (−1)	0.126	2.44 (−1)
		5	643.938	3.62 (−2)	0.028	3.74 (−2)	593.481	1.65 (−1)	0.252	1.74 (−1)
		6	691.025	2.13 (−2)	−0.393	1.59 (−2)	652.320	1.04 (−1)	−0.580	7.95 (−2)

TABLE BII: continued

3	0	0	−203.844	0			−276.520	5.54 (−2)		
		1	96.882	*0			18.241	3.90 (−2)		
		2	335.225	6.60 (−1)			263.967	1.77 (+0)[d]		
		3	510.348	5.31 (−1)			448.554	1.51 (+0)		
		4	624.462	3.27 (−1)			574.713	1.01 (+0)		
		5	684.050	1.41 (−1)			644.425	4.07 (−1)		
		6	*704.774	*2.91 (−2)			668.328	3.60 (−2)		
ε			705.372				669.425			
			-0.147[a]				*-0.800*[a]			
5	5	0	* − 114.529	0	0.000	0	−306.902	6.92 (−2)	0.000	6.92 (−2)
		1	304.730	3.82 (−9)	0.000	1.23 (−9)	117.223	1.74 (−1)	0.001	1.74 (−1)
		2	664.545	1.15 (−7)	0.000	0.71 (−9)	484.428	2.77 (−1)	0.000	2.77 (−1)
		3	965.451	6.74 (−4)	0.000	6.73 (−4)	795.096	3.40 (−1)	−0.021	3.35 (−1)
5	4	0	174.714	3.27 (−7)	0.000	1.69 (−7)	−3.112	6.65 (−2)	0.000	6.64 (−2)
		1	562.972	2.06 (−5)	0.000	1.84 (−5)	389.469	3.49 (−1)	0.148	1.81 (−1)
		2	891.314	4.65 (−3)	0.000	4.64 (−3)	725.420	2.97 (−1)	0.002	2.98 (−1)
		3	1159.911	5.24 (−3)	0.000	5.22 (−3)	1004.302	3.73 (−1)	0.000	3.73 (−1)
5	3	0	417.711	1.85 (−3)	0.084	2.56 (−3)	254.897	3.75 (−2)	−0.008	3.62 (−2)
		1	778.160	1.89 (−2)	0.002	1.83 (−2)	619.276	9.82 (−2)	0.013	1.03 (−1)
		2	1077.956	2.40 (−2)	−0.001	2.54 (−2)	926.338	2.14 (−1)	0.002	2.11 (−1)
5	2	0	608.285	1.63 (−4)	0.160	1.09 (−5)	459.550	3.74 (−2)	0.066	1.20 (−2)
		1	946.235	1.14 (−1)	0.136	7.84 (−2)	800.780	1.44 (−1)	0.084	1.15 (−1)
5	1	0	735.651	1.32	6.612	3.05 (−1)	602.791	4.52 (−2)	4.649	4.85 (−3)
		1	1059.582	2.02	5.378	5.22 (−1)	928.766	1.50	4.170	2.18 (−1)
5	0	0	* 799.754	* 7.58			* 679.742	* 1.26		
		1	*1120.386	*12.0			*1000.814	*12.0		
ε			1739.815				1650.598			
			-0.375[a]				*-2.158*[a]			

[a]Deviation of the threshold position from the accurate value for H_2[1].
[b]All $\Gamma>0$ widths in the column are due to rotational predissociation.
[c]Widths of levels below $v=1\,j=1$ are due to vibrational predissociation.
[d]Increased due to fast rotational predissociation to $v=1\,j=1$ channel.

COMMENTS

As indicated with the shaded strips in the captions of the above tables, the term 'vibrational' is used here (and also in Part C of this material) to name the $J=k$ levels. Purely vibrational energy is represented, of course, only by the $J=0$ ones.

A number of ro-vibrational states with low J-values (≤ 5) were determined from the same PES in Ref. 2. New results in Tables BI and BII are the energies and widths of all quasi-bound states assigned with $k>0$ and the energies and widths of bound and quasi-bound $k=0$ states marked with an asterisk. The symbol *0 in the width column means that the bound state was presented in Ref. 2 as a resonance, in some cases having even quite a large width. Generally, the widths of the $J=0$ resonances determined there agree very well with the present values. However, in some ($v_r\, b\, v_R$) cases, like (1 0 8), (0 2 6), (0 4 1), (1 4 1), they are substantially (at least 3 times) larger. Evidently, the stabilization method used in Ref. 2 has a difficulty with accounting for the impact of the higher $v\,j$ thresholds on stability of the states.

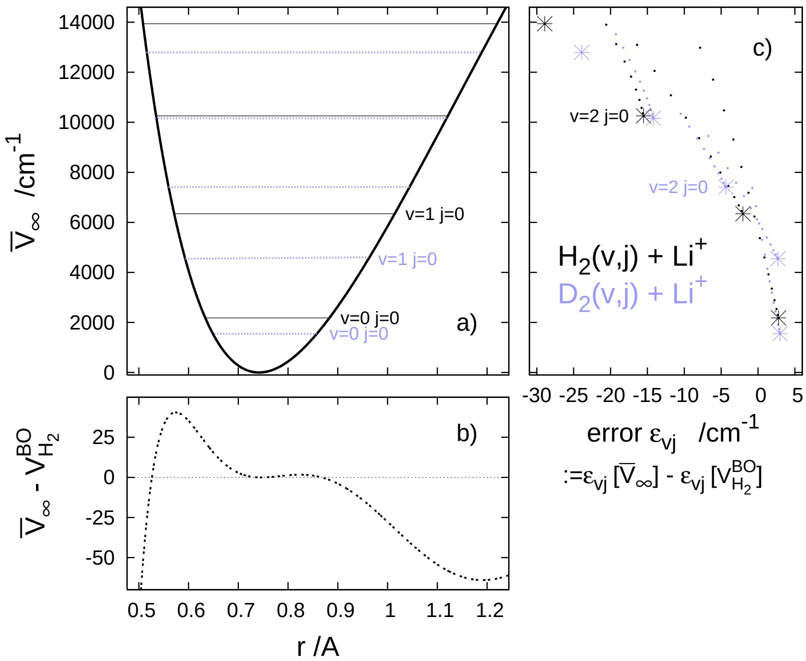


Fig. B1. Accuracy of the PES of the ground electronic state of the LiHH$^+$ system[2] in the H_2+Li^+ fragmentation region.
(a) 1D cut of the surface $\overline{V}(r,R,\theta)$ at $R{=}R_\infty{=}50$ Å. Several lowest vibrational energy levels of H_2 and D_2 (blue) in the potential $\overline{V}(r,R_\infty,\theta){:=}\overline{V}_\infty(r)$.
(b) Comparison of $\overline{V}_\infty$ with the Born-Oppenheimer potential of H_2 (taken from Ref. 3).
(c) Deviations of vibration-rotation energies of H_2(D_2) resulting from the two potentials. y-coordinates of the error points are the energies in the potential $\overline{V}_\infty$.

COMMENT

The errors of the threshold positions for fragmentation of the Li^+–H_2(D_2) complexes displayed in panel c) are believed to adequately reflect the accuracy of the asymptotic region of the used PES of LiHH$^+$. The lowest threshold, the zero-point energy of H_2 (D_2) taking the values of 2183.27 (1549.85) cm^{-1}, appear too high by 2.87 (2.97) cm^{-1} [by 4.0 (3.3) cm^{-1} if compared to the "experimental ZPEs" given in Ref. 4]. The positions of higher thresholds, $\varepsilon_{vj}-\varepsilon_{00}$, are too low by 0.093 (0.042), 0.278 (0.127), 0.921 (0.413), 4.832 (0.278), 5.402 (0.573), and 18.30 (4.45) cm^{-1} for $(v\,j){=}(0\,1)$, $(0\,2)$, $(0\,4)$, $(1\,0)$, $(1\,2)$, and $(2\,0)$, respectively. The errors of ε_{00} and of $\varepsilon_{10}-\varepsilon_{00}$ for H_2 are considerably larger than the deviations of the calculated $v_r{=}0{\to}1$ transition energies from the experimental data [all within the -1 to 1 cm^{-1} range, as shown in Fig. 4 of the paper]. Evidently, the PES is much more accurate in the well region than it is in the fragmentation region.

TABLE BIII: Li^+–H_2 versus Li^+–D_2. Positions of J=0 levels above the PES minimum in vibrational states $[v_r\,0\,0]$, $[0\,v_\theta\,0]$, and $[0\,0\,v_R]$ with v_r=0−2, $v_\theta(:=b-k)$=0−2 and v_R=0−2 represented by the diatomic-molecule formula: $G^m(v_m) = \omega_e^m\,(v_m+\frac{1}{2}) - \omega_e^m x_e^m\,(v_m+\frac{1}{2})^2$ for $m=r,\theta,R$. Comparison with results from other PESs.

				$(X(\text{Ref.}\,\ddagger)/X-1)\times 100\%$	
	m	ω_e^m	$\omega_e^m x_e^m$	$X=\omega_e^m$	$X=\omega_e^m x_e^m$
$Li^+{-}H_2$	r	4286.8	116.9	⌊ 2.8⌋ [0.5]	⌊−8.7⌋ [9]
	θ	714.8	60.2	⌊ 0.1⌋ [14.7] {−11.8}	⌊ 5.6⌋ [44] {−190}
	R	465.1	30.0	⌊−1.1⌋ [11.9] { −1.1}	⌊ 1.9⌋ [57] {−146}
$Li^+{-}D_2$	r	3036.1	60.3	⌊ 2.8⌋	⌊−8.9⌋
	θ	507.1	29.2	⌊−0.2⌋ {−11. }	⌊ 4.8⌋ {−163}
	R	370.1	18.5	⌊−0.2⌋ { −5.2}	⌊ 6.9⌋ {−118}
$\frac{Li^+-H_2}{Li^+-D_2}$ ♮	r	1.41	1.94		
	θ	1.41	2.06		
	R	1.26	1.62		

‡ Deviations within the symbols ⌊ ⌋ concerns the results from Ref. 5, in square brackets — from Ref. 6, in braces — from Refs. 7 and 8.

♮ The ratios of the constants for the two complexes. The ratios of ω_e^m and $\omega_e^m x_e^m$ for the $m=r,\theta$ modes compare well with the mass factors $\sqrt{\frac{m_{DD}}{m_{HH}}}$ and $\frac{m_{DD}}{m_{HH}}$=1.999, respectively, and in the case of the R-mode they are close to $\sqrt{\frac{\mu_{Li^+-DD}}{\mu_{Li^+-HH}}}$ and $\frac{\mu_{Li^+-DD}}{\mu_{Li^+-HH}}$=1.635, respectively.

COMMENTS

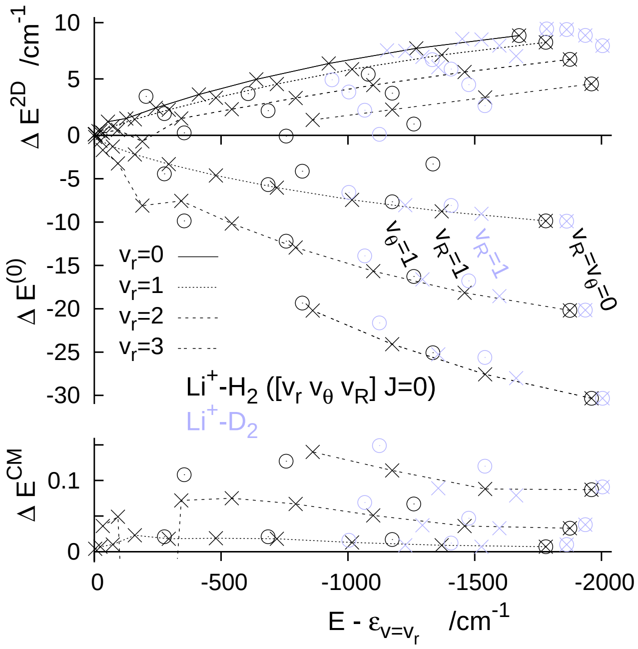
Table I of the paper is extended here with comparison of results from two more PESs, of Refs. 6 and 7, respectively. Not enough energies were generated from these PESs to make the comparison in terms of the same parameters as in Table I; hence the less adequate formula, neglecting mode's coupling, is exploited. Nevertheless, a context is provided to appreciate the consistency of the present PES and the PES of Ref. 5 in describing the two intermolecular modes; the deviations of the parameters ω_e^θ, ω_e^R, $\omega_e^\theta x_e^\theta$, and $\omega_e^R x_e^R$ resulting from these PESs are by far smaller (>10 or even ⋙10 times smaller) than the deviations with results from the other two PESs. This consistency is a positive sign, supporting our belief that results of the present calculations on the excited vibrational states of the complexes are reasonably accurate and may therefore be useful.

The sum $\sum_m G^m(0)$ should be a good approximation to the ZPE value of a given complex on a given PES. Indeed, the values 2681.6 and 1929.6 cm^{-1} obtained for $Li^+{-}H_2$ and $Li^+{-}D_2$, respectively, from the parameters listed in columns 'ω_e^m' and '$\omega_e^m x_e^m$', are only by 0.6 and 0.36% larger than the 'exact' values, see the caption of Fig. 1.

No energies have been calculated from the PES of Ref. 6 for the $Li^+{-}D_2$ complex. However, an estimation of the ZPE value for this complex on this PES can be obtained from the respective parameters ω_e^m and $\omega_e^m x_e^m$ for $Li^+{-}H_2$ (not listed explicitly) by scaling them with the mass factors described in footnote ♮. The result, 1982.9 cm^{-1}, is exploited in the description of the electronic structure input, in Sec. IIIB.

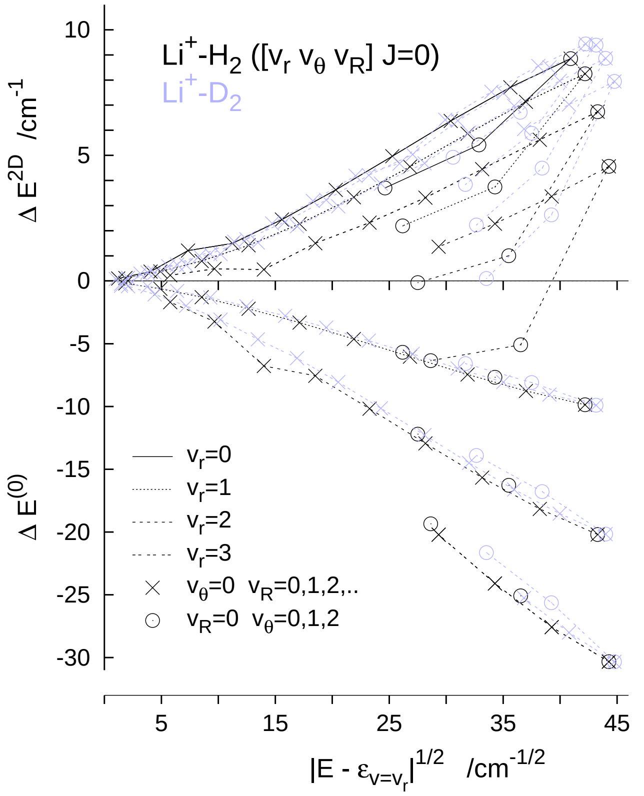
Fig. B2. Accuracy of 2D approximation in determination of vibrational energy levels

B2a. 2D versus 3D-CM approach



Shown are errors of energies obtained with the two approaches for J=0 levels in various vibrational states $[v_r\, v_\theta\, 0]$ and $[v_r\, 0\, v_R]$ of the Li$^+$–H$_2$ (D$_2$) complexes. The errors are defined as deviations from 3D 'exact' values (E), ΔE^{a}=$E^{\mathrm{a}}-E$ for a=2D,(0),CM. The upperscript '(0)' stands for 0-th order approximations to predissociating states (v_r>0) within the 3D-CM approach (bound states in appropriate Q-subspaces, chosen as described in Sec. III.A). In bound states cases (all v_r=0 states shown here), $E^{(0)}$=E and the error $\Delta E^{(0)}$ is strictly zero.

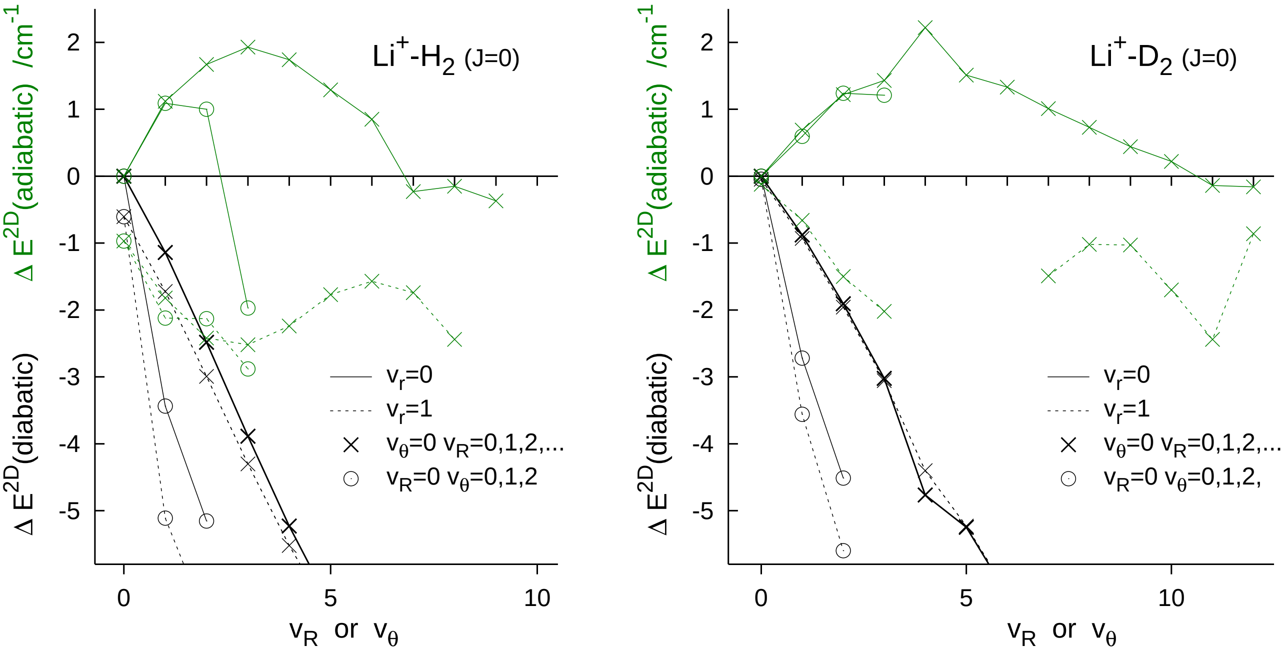
Obviously, the errors $\Delta E^{2\mathrm{D}}$ are, on average, much larger than ΔE^{CM}. Really disadvantageous is, however, the fact that they vary so strongly with the numbers v_θ and v_R. This variation translates into the substantial errors of the 2D transitions frequencies shown in Table II of the paper.



Errors $\Delta E^{2\mathrm{D}}$ and $\Delta E^{(0)}$ as functions of square root of the binding energy in the Q-subspace.

The energies $E^{(0)}$ of states with a given v_r>0 represent convergent results in the respective Q-subspace, i.e. they account for all important interactions within and between the v=v_r and v>v_r vibrational channels. Actually, the inter-channel interactions are strongly dominated by the v=$v_r$$\leftrightarrow$$v$=$v_r$+1 ones. Some regularities are displayed by the errors $\Delta E^{(0)}$ of states in the sequences $[v_r\, 0\, v_R{=}0,1,\ldots]$ and $[v_r\, v_\theta{=}0,1,2\, v_R{=}0]$: the crosses and circles, black and blue, lie nearly on the same nearly straight lines with slopes nearly proportional to v_r. The energies $E^{2\mathrm{D}}$ disregard all, in particular the v=$v_r$$\leftrightarrow$$v$=$v_r$+1, vibrational couplings in the Q-subspace. In consequence, the errors $\Delta E^{2\mathrm{D}}$ show much less regularities in their dependencies on the quantum numbers, stronger variation with the number v_θ, and larger sensitivity to the H$_2$$\rightarrow$D$_2$ substitution.

B2b. 2D diabatic versus 2D adiabatic approach



The errors $\Delta E^{\rm 2D}$ of part a) of the figure are shown here relative to the error of [0 0 0] state and as functions of the vibrational numbers v_R or v_θ. The errors $\Delta E^{\rm 2D}$(adiabatic) concern results obtained in Ref. 2 by exploiting an adiabatic separation scheme of intra- and intermolecular vibrations in atom-diatom complexes.

The adiabatic separation scheme of Ref. 2 is capable of providing reasonably accurate energies of all vibrational states of the present complexes provided the energies do not come to close together. /Such situation occurs in the case of states [1 0 4–6] of the Li^+–D_2 complex. Their errors $\Delta E^{\rm 2D}$(adiabatic) are not shown in the figure because of 'wild' behavior caused by crossing with states [1 2 0–2] and [1 4 0], cf. Table CI (in Part C, Ref. 9)./

The diabatic decoupling is much simpler to implement but reasonable accuracy, $|\Delta E^{\rm 2D}|$ below 2 $\rm cm^{-1}$, may be expected only in determining transition energies of low Δv transitions.

ROTATIONAL ENERGY LEVELS

TABLE BIV: Li^+–H_2. Positions (E) and widths (Γ) of rotational levels (J) in thirty groups ($b\,k\,v_R$) below v=0 j=0 and v=1 j=0 thresholds. E=0 is at the lowest threshold. All data are in cm^{-1}. ($v_r \sim v$, $e \sim p$=1, and $f \sim p = -1$)[a].

				v_r=0				v_r=1			
b	k	v_R	J	$E(e)$	$\Gamma(e)$	$E(f)-E(e)$	$\Gamma(f)$	$E(e)$	$\Gamma(e)$[b]	$E(f)-E(e)$	$\Gamma(f)$
0	0	0	0	−1674.606				2378.491	2.37 (−2)		
			1	−1669.651				2383.418	2.33 (−2)		
			2	−1659.749				2393.270	2.98 (−2)		
			3	−1644.915				2408.018	2.26 (−2)		
			4	−1625.174				2427.653	2.31 (−2)		
			5	−1600.557				2452.139	2.42 (−2)		
			6	−1571.104				2481.439	2.33 (−2)		
			7	−1536.861				2515.506	2.24 (−2)		
			8	−1497.885				2554.287	2.13 (−2)		
			9	−1454.239				2597.720	2.02 (−2)		
			10	−1405.997				2645.735	1.91 (−2)		
			11	−1353.239				2698.256	1.78 (−2)		
			12	−1296.054				2755.196	1.65 (−2)		
			13	−1234.542				2816.461	1.52 (−2)		
			14	−1168.810				2881.947	1.39 (−2)		
			15	−1098.977				2951.542	1.27 (−2)		
			16	−1025.171				3025.126	1.13 (−2)		
			17	−947.531				3102.565	1.01 (−2)		
			18	−866.209				3183.718	8.96 (−3)		
			19	−781.367				3268.430	8.01 (−3)		
			20	−693.185				3356.540	6.61 (−3)		
			21	−601.856				3447.862	5.68 (−3)		
			22	−507.593				3542.204	4.81 (−3)		
			23	−410.629				3639.353	4.01 (−3)		
			24	−311.223				3739.078	3.27 (−3)		
			25	−209.665				3841.120	2.62 (−3)		
			26	−106.285				3945.193	2.07 (−3)		
1	1	0	1	−1606.666		0.150		2442.362	2.49 (−2)	0.152	2.49 (−2)
			2	−1596.937		0.449		2452.038	2.46 (−2)	0.455	2.46 (−2)
			3	−1582.361		0.897		2466.531	2.44 (−2)	0.910	2.41 (−2)
			4	−1562.961		1.489		2485.847	3.36 (−2)	1.489	2.35 (−2)
			5	−1538.764		2.224		2509.903	2.38 (−2)	2.242	2.29 (−2)
			6	−1509.809		3.097		2538.705	2.25 (−2)	3.125	2.23 (−2)
			7	−1476.140		4.105		2572.202	2.14 (−2)	4.134	2.52 (−2)
			8	−1437.807		5.241		2610.343	2.03 (−2)	5.325	2.99 (−2)
			9	−1394.871		6.499		2653.072	1.92 (−2)	6.584	2.05 (−2)
			10	−1347.400		7.873		2700.310	1.87 (−2)	7.985	1.84 (−2)
			11	−1295.468		9.355		2752.016	1.67 (−2)	9.481	1.69 (−2)
			12	−1239.159		10.936		2808.084	1.55 (−2)	11.087	1.57 (−2)
			13	−1178.568		12.607		2868.438	1.50 (−2)	12.779	1.43 (−2)
			14	−1113.794		14.359		2932.971	1.31 (−2)	14.559	1.32 (−2)
			15	−1044.950		16.180		3001.580	1.24 (−2)	16.420	1.18 (−2)
			16	−972.157		18.059		3074.158	1.06 (−2)	18.324	1.54 (−2)
			17	−895.546		19.983		3150.572	9.41 (−3)	20.298	9.43 (−3)
			18	−815.262		21.939		3230.688	8.48 (−3)	22.300	8.27 (−3)
			19	−731.459		23.912		3314.365	8.35 (−3)	24.321	7.55 (−3)
			20	−644.309		25.886		3401.439	7.17 (−3)	26.352	7.16 (−3)
			21	−553.994		27.845		3491.740	6.19 (−3)	28.373	6.04 (−3)
			22	−460.719		29.769		3585.083	5.24 (−3)	30.367	5.55 (−3)
			23	−364.705		31.638		3681.263	4.42 (−3)	32.316	4.66 (−3)
			24	−266.199		33.428		3780.058	3.98 (−3)	34.197	3.87 (−3)
			25	−165.475		35.113		3881.222	3.33 (−3)	35.988	3.17 (−3)
			26	−62.844		36.661		3984.483	2.71 (−3)	37.660	2.56 (−3)
			27	41.336[c]		38.031		4089.531	2.20 (−3)	39.181	2.03 (−3)

TABLE BIV: continued

2	2	0	2	−1410.848		0.000		2626.803	2.88 (−2)	0.000	2.88 (−2)
			3	−1396.149		0.000		2641.436	2.83 (−2)	0.000	2.83 (−2)
			4	−1376.585		0.000		2660.913	2.77 (−2)	−0.001	2.77 (−2)
			5	−1352.186		0.000		2685.205	2.69 (−2)	−0.002	2.69 (−2)
			6	−1322.991		0.000		2714.276	2.59 (−2)	−0.004	2.60 (−2)
			7	−1289.045		0.001		2748.083	2.49 (−2)	−0.007	2.49 (−2)
			8	−1250.400		0.003		2786.573	2.37 (−2)	−0.010	2.38 (−2)
			9	−1207.121		0.005		2829.687	2.25 (−2)	−0.015	2.25 (−2)
			10	−1159.275		0.010		2877.360	2.12 (−2)	−0.020	2.12 (−2)
			11	−1106.943		0.018		2929.514	1.98 (−2)	−0.025	1.98 (−2)
			12	−1050.211		0.031		2986.066	1.83 (−2)	−0.028	1.84 (−2)
			13	−989.178		0.050		3046.935	1.80 (−2)	−0.041	1.70 (−2)
			14	−923.949		0.079		3111.995	1.57 (−2)	−0.038	1.55 (−2)
			15	−854.644		0.120		3181.152	1.41 (−2)	−0.018	1.46 (−2)
			16	−781.390		0.180		3254.280	1.27 (−2)	−0.007	1.27 (−2)
			17	−704.329		0.263		3331.249	1.13 (−2)	0.022	1.14 (−2)
			18	−623.615		0.379		3411.908	1.05 (−2)	0.073	1.00 (−2)
			19	−539.422		0.540		3496.113	8.78 (−3)	0.147	8.88 (−3)
			20	−451.939		0.766		3583.677	7.58 (−3)	0.260	7.64 (−3)
			21	−361.387		1.086		3674.419	6.39 (−3)	0.422	6.53 (−3)
			22	−268.030		1.562		3768.121	5.49 (−3)	0.659	5.52 (−3)
			23	−172.226		2.327		3864.544	4.37 (−3)	1.005	4.59 (−3)
			24	−74.611		3.767		3963.398	3.86 (−3)	1.522	3.75 (−3)
			25	23.102	7.9 (−27)	7.322		4064.287	3.03 (−3)	2.359	3.11 (−3)
3	3	0	3	−1092.972		0.000		2926.774	3.62 (−2)	0.000	3.62 (−2)
			4	−1073.621		0.000		2946.060	3.93 (−2)	−0.003	3.50 (−2)
			5	−1049.488		0.000		2970.109	3.39 (−2)	−0.002	3.35 (−2)
			6	−1020.610		0.001		2998.893	3.38 (−2)	0.006	3.66 (−2)
			7	−987.033		0.002		3032.363	3.16 (−2)	0.003	3.19 (−2)
			8	−948.809		0.004		3070.471	3.11 (−2)	0.004	3.04 (−2)
			9	−906.001		0.007		3113.157	2.90 (−2)	0.006	2.88 (−2)
			10	−858.677		0.014		3160.353	2.60 (−2)	0.010	2.72 (−2)
			11	−806.917		0.025		3211.987	2.53 (−2)	0.014	2.54 (−2)
			12	−750.810		0.044		3267.973	2.44 (−2)	0.024	2.49 (−2)
			13	−690.454		0.076		3328.219	2.23 (−2)	0.038	2.27 (−2)
			14	−625.964		0.130		3392.624	2.08 (−2)	0.057	2.08 (−2)
			15	−557.470		0.224		3461.077	1.89 (−2)	0.085	1.89 (−2)
			16	−485.139		0.401		3533.456	1.71 (−2)	0.124	1.71 (−2)
			17	−409.227		0.785		3609.629	1.53 (−2)	0.179	1.53 (−2)
			18	−330.323		1.816		3689.449	1.35 (−2)	0.259	1.36 (−2)
			19	−242.940		−2.149		3772.756	1.19 (−2)	0.374	1.19 (−2)
			20	−157.113		−1.248		3859.368	1.03 (−2)	0.545	1.04 (−2)
			21	−67.685		−0.833		3949.070	8.80 (−3)	0.810	8.93 (−3)
			22	24.700		−0.483		4041.593	7.39 (−3)	1.248	7.58 (−3)
			23	117.382		2.093	<1 (−30)	4136.521	6.00 (−3)	2.064	6.35 (−3)
4	4	0	4	−658.879		0.000		3336.938	4.87 (−2)	0.001	4.87 (−2)
			5	−635.093		0.000		3360.669	4.71 (−2)	0.002	4.70 (−2)
			6	−606.631		0.000		3389.063	4.53 (−2)	0.008	4.46 (−2)
			7	−573.540		0.000		3422.022	1.16 (−1)	0.139	7.01 (−2)
			8	−535.875		0.000		3459.723	4.69 (−2)	−0.023	4.28 (−2)
			9	−493.709		0.002		3501.824	4.09 (−2)	−0.012	3.99 (−2)
			10	−447.010		−0.214		3548.381	3.76 (−2)	−0.007	3.71 (−2)
			11	−395.811		0.006		3599.310	3.28 (−2)	−0.056	4.25 (−2)
			12	−340.602		0.014		3654.537	3.28 (−2)	−0.003	3.20 (−2)
			13	−281.134		0.034		3713.950	2.99 (−2)	−0.002	3.01 (−2)
			14	−217.760		0.253		3777.432	2.72 (−2)	0.005	2.74 (−2)
			15	−149.794		−0.137		3844.541	2.89 (−2)	0.231	2.58 (−2)
			16	−78.385		−0.135		3917.750	3.15 (−2)	−0.070	2.99 (−2)
			17	−3.210		−0.535		3991.982	2.03 (−2)	0.079	2.04 (−2)
			18	75.563	1.22 (−5)	0.185		4070.606	1.74 (−2)	0.149	1.77 (−2)
			19	157.765	1.05 (−4)	0.114		4152.154	1.55 (−2)	0.841	1.71 (−2)
			20	243.213	1.49 (−3)	0.123		4238.690	2.20 (−2)	−0.130	1.90 (−2)

TABLE BIV: continued

0	0	1	0	−1269.455		2789.040	6.84 (−2)		
			1	−1264.932		2793.557	6.80 (−2)		
			2	−1255.894		2802.583	6.72 (−2)		
			3	−1242.358		2816.102	6.60 (−2)		
			4	−1224.349		2834.089	6.44 (−2)		
			5	−1201.903		2856.512	6.25 (−2)		
			6	−1175.060		2883.330	6.03 (−2)		
			7	−1143.873		2914.495	5.77 (−2)		
			8	−1108.402		2949.948	5.49 (−2)		
			9	−1068.717		2989.623	5.20 (−2)		
			10	−1024.898		3033.446	4.88 (−2)		
			11	−977.032		3081.332	4.55 (−2)		
			12	−925.220		3133.187	4.21 (−2)		
			13	−869.572		3188.908	3.86 (−2)		
			14	−810.209		3248.381	3.52 (−2)		
			15	−747.266		3311.480	3.17 (−2)		
			16	−680.887		3378.070	2.84 (−2)		
			17	−611.236		3448.000	2.52 (−2)		
			18	−538.489		3521.106	2.24 (−2)		
			19	−462.838		3597.217	1.89 (−2)		
			20	−384.496		3676.125	1.61 (−2)		
			21	−303.691		3757.624	1.36 (−2)		
			22	−220.657		3841.477	1.23 (−2)		
			23	−135.605		3927.433	9.18 (−3)		
			24	−48.554		4015.218	7.33 (−3)		
1	1	1	1	−1199.367	0.138	2854.758	6.97 (−2)	0.140	6.95 (−2)
			2	−1190.484	0.414	2863.631	7.20 (−2)	0.417	6.87 (−2)
			3	−1177.178	0.826	2876.910	6.77 (−2)	0.842	6.74 (−2)
			4	−1159.475	1.371	2894.592	6.60 (−2)	1.394	6.60 (−2)
			5	−1137.407	2.047	2916.634	6.37 (−2)	2.080	6.40 (−2)
			6	−1111.012	2.848	2942.999	6.12 (−2)	2.895	6.16 (−2)
			7	−1080.341	3.770	2973.636	7.18 (−2)	3.839	5.90 (−2)
			8	−1045.451	4.808	3008.511	5.62 (−2)	4.886	5.60 (−2)
			9	−1006.406	5.954	3047.538	5.28 (−2)	6.053	5.29 (−2)
			10	−963.283	7.201	3090.654	4.97 (−2)	7.286	9.70 (−2)
			11	−916.165	8.541	3137.785	4.60 (−2)	8.693	4.65 (−2)
			12	−865.147	9.965	3188.837	4.28 (−2)	10.145	4.35 (−2)
			13	−810.332	11.461	3243.712	4.07 (−2)	11.675	4.00 (−2)
			14	−751.838	13.020	3302.304	3.71 (−2)	13.271	3.70 (−2)
			15	−689.791	14.629	3364.493	3.36 (−2)	14.923	3.38 (−2)
			16	−624.332	16.274	3430.150	3.05 (−2)	16.616	3.04 (−2)
			17	−555.616	17.940	3499.130	2.70 (−2)	18.337	2.70 (−2)
			18	−483.815	19.613	3571.278	2.37 (−2)	20.072	2.33 (−2)
			19	−409.117	21.273	3646.422	2.06 (−2)	21.803	2.06 (−2)
			20	−331.735	22.900	3724.371	1.77 (−2)	23.512	1.77 (−2)
			21	−251.905	24.472	3804.916	1.50 (−2)	25.178	1.49 (−2)
			22	−169.894	25.962	3887.821	1.25 (−2)	26.778	1.25 (−2)
			23	−86.009	27.337	3972.824	1.03 (−2)	28.284	1.02 (−2)
			24	−0.612	28.556	4059.623	8.26 (−3)	29.664	8.21 (−3)
			25	85.867	29.565	4147.868	6.50 (−3)	30.875	6.46 (−3)

TABLE BIV: continued

2	2	1	2	−1000.198	0.001	3042.371	7.95 (−2)	−0.001	7.94 (−2)
			3	−986.790	0.003	3055.774	7.80 (−2)	0.001	7.80 (−2)
			4	−968.951	0.008	3073.610	7.80 (−2)	0.004	7.62 (−2)
			5	−946.715	0.019	3095.844	7.39 (−2)	0.010	7.40 (−2)
			6	−920.126	0.036	3122.438	7.13 (−2)	0.020	7.13 (−2)
			7	−889.232	0.064	3153.342	6.84 (−2)	0.036	6.84 (−2)
			8	−854.096	0.103	3188.499	6.51 (−2)	0.060	6.52 (−2)
			9	−814.787	0.158	3227.844	6.16 (−2)	0.093	6.17 (−2)
			10	−771.384	0.232	3271.301	5.79 (−2)	0.140	5.80 (−2)
			11	−723.978	0.329	3318.815	5.41 (−2)	0.173	5.41 (−2)
			12	−672.671	0.456	3370.209	5.02 (−2)	0.272	5.10 (−2)
			13	−617.579	0.622	3425.456	4.60 (−2)	0.391	4.64 (−2)
			14	−558.834	0.841	3484.415	4.19 (−2)	0.525	4.21 (−2)
			15	−496.592	1.139	3546.955	3.78 (−2)	0.701	3.80 (−2)
			16	−431.050	1.571	3612.929	3.42 (−2)	0.932	3.52 (−2)
			17	−362.497	2.268	3682.168	3.02 (−2)	1.234	3.04 (−2)
			18	−291.514	3.637	3754.477	2.64 (−2)	1.649	2.66 (−2)
			19	−219.661	7.046	3829.595	2.42 (−2)	2.262	2.31 (−2)
			20	−132.528	−2.125	3907.125	1.98 (−2)	3.276	1.98 (−2)
			21	−53.772	−0.457	3986.246	1.73 (−2)	5.298	1.68 (−2)
3	3	1	3	−679.058	0.000	3345.578	9.86 (−2)	0.000	9.86 (−2)
			4	−661.329	0.000	3363.350	9.60 (−2)	0.001	9.60 (−2)
			5	−639.226	0.000	3385.511	9.27 (−2)	0.002	9.27 (−2)
			6	−612.787	−0.001	3412.023	8.89 (−2)	0.009	8.89 (−2)
			7	−582.059	−0.002	3442.837	8.46 (−2)	0.026	8.46 (−2)
			8	−547.095	−0.003	3477.884	7.98 (−2)	0.075	7.97 (−2)
			9	−507.958	−0.006	3517.044	7.43 (−2)	0.221	7.45 (−2)
			10	−464.718	−0.008	3559.981	6.59 (−2)	0.738	6.88 (−2)
			11	−417.453	−0.008	3609.656	5.08 (−2)	−1.400	6.28 (−2)
			12	−366.253	−0.003	3660.830	5.01 (−2)	−1.024	5.65 (−2)
			13	−311.216	0.016	3716.218	4.57 (−2)	−0.924	5.00 (−2)
			14	−252.461	0.069	3775.524	4.02 (−2)	−0.879	4.34 (−2)
			15	−190.164	0.216	3838.582	3.47 (−2)	−0.803	3.68 (−2)
			16	−125.193	1.100	3905.240	2.92 (−2)	−0.628	3.05 (−2)
			17	−54.088	2.261	3975.322	2.39 (−2)	−0.281	2.45 (−2)
			18	18.102	1.546	4048.581	2.00 (−2)	0.357	2.17 (−2)
			19	93.462	2.548	4127.522	2.61 (−2)	−1.621	1.50 (−2)
0	0	2	0	−924.249		3142.481	1.12 (−1)		
			1	−920.179		3146.569	1.12 (−1)		
			2	−912.049		3154.737	1.10 (−1)		
			3	−899.876		3166.966	1.08 (−1)		
			4	−883.690		3183.232	1.05 (−1)		
			5	−863.527		3203.498	1.02 (−1)		
			6	−839.434		3227.720	9.82 (−2)		
			7	−811.469		3255.845	9.32 (−2)		
			8	−779.697		3287.808	8.92 (−2)		
			9	−744.195		3323.539	8.41 (−2)		
			10	−705.052		3362.953	7.87 (−2)		
			11	−662.363		3405.959	7.30 (−2)		
			12	−616.233		3452.453	6.68 (−2)		
			13	−566.768		3502.322	6.18 (−2)		
			14	−514.045		3555.441	5.59 (−2)		
			15	−457.868		3611.680	5.00 (−2)		
			16	−401.665		3670.927	4.43 (−2)		
			17	−339.605		3733.213	3.82 (−2)		
			18	−275.138		3795.315	2.31 (−2)		
			19	−219.661		3863.435	2.59 (−2)		
			20	−149.195		3933.004	2.47 (−2)		
			21	−79.554		4005.122	1.84 (−2)		
			22	−9.790		4081.287	1.44 (−2)		

TABLE BIV: continued

1	1	2	1	−851.638		0.125	3210.390	1.17 (−1)	0.127	1.17 (−1)
			2	−843.642		0.373	3218.420	1.16 (−1)	0.381	1.16 (−1)
			3	−831.671		0.743	3230.444	1.13 (−1)	0.759	1.14 (−1)
			4	−815.750		1.232	3246.437	1.11 (−1)	1.259	1.11 (−1)
			5	−795.917		1.837	3266.366	1.08 (−1)	1.877	1.08 (−1)
			6	−772.214		2.554	3290.188	1.04 (−1)	2.610	1.04 (−1)
			7	−744.698		3.376	3317.853	9.92 (−2)	3.452	9.93 (−2)
			8	−713.433		4.297	3349.300	9.42 (−2)	4.397	9.43 (−2)
			9	−678.492		5.311	3384.459	8.89 (−2)	5.437	8.90 (−2)
			10	−639.962		6.409	3423.252	8.32 (−2)	6.565	8.34 (−2)
			11	−597.940		7.582	3465.588	7.74 (−2)	7.773	7.75 (−2)
			12	−552.534		8.818	3511.366	7.13 (−2)	9.049	7.14 (−2)
			13	−503.868		10.108	3560.475	6.52 (−2)	10.383	6.53 (−2)
			14	−452.078		11.437	3612.790	5.91 (−2)	11.762	5.92 (−2)
			15	−397.319		12.791	3668.171	5.30 (−2)	13.173	5.31 (−2)
			16	−339.762		14.153	3726.463	4.71 (−2)	14.602	4.71 (−2)
			17	−279.601		15.505	3787.494	4.14 (−2)	16.030	4.13 (−2)
			18	−217.055		16.826	3851.072	3.59 (−2)	17.439	3.58 (−2)
			19	−152.374		18.088	3916.980	3.07 (−2)	18.806	3.05 (−2)
			20	−85.841		19.260	3984.972	2.59 (−2)	20.106	2.57 (−2)
			21	−17.784		20.291	4054.768	2.14 (−2)	21.307	2.12 (−2)
			22	51.470		21.065	4126.041	1.74 (−2)	22.367	1.71 (−2)
2	2	2	2	−649.119		0.001	3401.118	1.32 (−1)	0.003	1.32 (−1)
			3	−637.051		0.005	3413.249	1.30 (−1)	0.006	1.30 (−1)
			4	−621.007		0.017	3429.383	1.27 (−1)	0.011	1.27 (−1)
			5	−601.028		0.041	3449.483	1.23 (−1)	0.022	1.23 (−1)
			6	−577.169		0.090	3473.503	1.18 (−1)	0.043	1.18 (−1)
			7	−549.511		0.190	3501.389	1.13 (−1)	0.078	1.13 (−1)
			8	−518.204		0.432	3533.072	1.08 (−1)	0.133	1.08 (−1)
			9	−483.809		1.311	3568.481	1.02 (−1)	0.140	1.40 (−1)
			10	−442.669		−0.796	3607.509	9.53 (−2)	0.339	9.55 (−2)
			11	−401.044		−0.424	3650.047	8.86 (−2)	0.537	8.87 (−2)
			12	−355.359		−0.205	3695.926	8.17 (−2)	0.872	8.18 (−2)
			13	−306.407		−0.035	3744.842	7.53 (−2)	1.543	7.50 (−2)
			14	−254.311		0.132	3795.971	6.70 (−2)	3.267	6.77 (−2)
			15	−199.239		0.314	3857.450	5.93 (−2)	−2.116	6.00 (−2)
			16	−141.372		0.525	3913.640	4.41 (−2)	−0.965	4.68 (−2)
			17	−80.919		0.779	3975.490	4.94 (−2)	−0.433	4.69 (−2)
			18	−18.127		1.105	4039.274	4.08 (−2)	0.038	4.12 (−2)
0	0	3	0	−638.892			3438.954	1.46 (−1)		
			1	−635.309			3442.611	1.42 (−1)		
			2	−628.151			3449.919	1.40 (−1)		
			3	−617.437			3460.895	1.35 (−1)		
			4	−603.196			3475.668	1.20 (−1)		
			5	−585.466			3492.564	1.07 (−1)		
			6	−564.292			3514.313	1.17 (−1)		
			7	−539.716			3539.322	1.14 (−1)		
			8	−511.733			3567.645	1.09 (−1)		
			9	−479.940			3599.232	1.03 (−1)		
			10	−448.276			3634.010	9.60 (−2)		
			11	−410.795			3671.893	8.85 (−2)		
			12	−370.880			3712.825	8.12 (−2)		
			13	−328.396			3756.854	7.36 (−2)		
			14	−283.483			3804.542	6.62 (−2)		
			15	−236.344			3857.450	5.93 (−2)		
			16	−187.223			3913.640	4.41 (−2)		
			17	−136.414			3975.490	4.92 (−2)		
			18	−84.278			4039.274	4.08 (−2)		
			19	−31.263			4105.381	3.54 (−2)		
			20	22.034	1.1 (−14)		4173.532	2.98 (−2)		

TABLE BIV: continued

1	1	3	1	−563.320		0.109	3509.361	1.51 (−1)	0.112	1.51 (−1)
			2	−556.260		0.327	3516.511	1.49 (−1)	0.336	1.49 (−1)
			3	−545.696		0.650	3527.211	1.46 (−1)	0.670	1.46 (−1)
			4	−531.657		1.078	3541.436	1.42 (−1)	1.110	1.42 (−1)
			5	−514.186		1.604	3559.146	1.37 (−1)	1.653	1.37 (−1)
			6	−493.332		2.226	3580.294	1.32 (−1)	2.295	1.32 (−1)
			7	−469.159		2.936	3604.822	1.26 (−1)	3.029	1.26 (−1)
			8	−441.743		3.728	3632.663	1.19 (−1)	3.849	1.19 (−1)
			9	−411.169		4.593	3663.734	1.12 (−1)	4.747	1.12 (−1)
			10	−377.538		5.523	3697.947	1.04 (−1)	5.714	1.04 (−1)
			11	−340.966		6.506	3735.197	9.60 (−2)	6.740	9.61 (−2)
			12	−301.582		7.529	3775.364	8.78 (−2)	7.813	8.79 (−2)
			13	−259.533		8.578	3818.316	7.95 (−2)	8.921	7.95 (−2)
			14	−214.975		9.630	3863.903	7.13 (−2)	10.049	7.12 (−2)
			15	−168.045		10.633	3911.956	6.32 (−2)	11.178	6.34 (−2)
			16	−118.228		10.964	3962.288	5.52 (−2)	12.289	5.50 (−2)
			17	−69.354		17.528	4014.695	4.77 (−2)	13.348	4.73 (−2)
			18	−17.066		13.365	4069.019	4.05 (−2)	14.273	4.01 (−2)
			19	36.229		14.268	4122.338	2.33 (−2)	17.919	3.31 (−2)
			20	90.106		14.820	4179.096	2.61 (−2)	17.526	2.36 (−2)
1	0	0	0	−1080.273			2983.914	1.67 (−2)		
			1	−1075.617			2988.535	2.28 (−2)		
			2	−1066.314			2997.754	2.22 (−2)		
			3	−1052.379			3011.562	2.15 (−2)		
			4	−1033.839			3029.936	2.05 (−2)		
			5	−1010.726			3052.844	1.99 (−2)		
			6	−983.082			3080.246	1.76 (−2)		
			7	−950.958			3112.098	2.14 (−2)		
			8	−914.412			3148.334	1.52 (−2)		
			9	−873.514			3188.900	1.63 (−2)		
			10	−828.338			3233.718	1.81 (−2)		
			11	−778.971			3282.707	1.48 (−2)		
			12	−725.507			3335.782	1.63 (−2)		
			13	−668.049			3392.838	1.45 (−2)		
			14	−606.706			3453.768	1.31 (−2)		
			15	−541.592			3518.453	1.17 (−2)		
			16	−472.808			3586.766	1.04 (−2)		
			17	−400.389			3658.565	9.12 (−3)		
			18	−324.069			3733.702	7.90 (−3)		
			19	−249.689			3812.015	6.76 (−3)		
			20	−167.605			3893.331	5.70 (−3)		
			21	−83.423			3977.478	4.76 (−3)		
			22	2.932			4064.295	3.94 (−3)		
			23	91.234			4153.709	3.31 (−3)		
			24	180.973	4.5 (−12)		4245.960	3.01 (−3)		
			25	272.698	2.69 (−4)		4340.977	3.78 (−3)		
2	1	0	1	−982.522		0.266	3072.311	2.21 (−2)	0.262	2.31 (−2)
			2	−973.512		0.797	3081.277	2.32 (−2)	0.751	2.38 (−2)
			3	−960.014		1.589	3094.699	2.37 (−2)	1.483	2.38 (−2)
			4	−942.051		2.639	3112.551	2.33 (−2)	2.464	2.34 (−2)
			5	−919.653		3.940	3134.810	2.24 (−2)	3.683	2.29 (−2)
			6	−892.856		5.487	3161.443	2.14 (−2)	5.133	2.21 (−2)
			7	−861.705		7.273	3192.407	2.02 (−2)	6.808	2.12 (−2)
			8	−826.253		9.288	3227.652	1.88 (−2)	8.702	2.02 (−2)
			9	−786.563		11.526	3267.117	1.67 (−2)	10.808	1.92 (−2)
			10	−742.704		13.977	3310.753	1.95 (−2)	13.110	2.00 (−2)
			11	−694.758		16.635	3358.456	1.60 (−2)	15.464	1.76 (−2)
			12	−642.818		19.493	3410.162	1.42 (−2)	18.252	1.35 (−2)
			13	−586.999		22.558	3465.772	1.24 (−2)	21.108	1.26 (−2)
			14	−527.465		25.874	3525.177	9.90 (−3)	24.133	1.19 (−2)
			15	−464.670		29.763	3588.270	9.78 (−3)	27.310	1.03 (−2)

			16	−395.450		30.915		3654.875	9.07 (−3)	30.683	9.10 (−3)
			17	−325.854		35.224		3724.661	8.10 (−3)	34.437	7.89 (−3)
			18	−252.428		39.060		3800.555	1.96 (−2)	35.487	6.97 (−3)
			19	−175.809		42.871		3876.013	8.47 (−3)	40.199	5.60 (−3)
			20	−96.258		46.707		3955.381	6.62 (−3)	44.041	5.18 (−3)
			21	−14.007		50.568		4037.662	4.39 (−3)	47.798	4.05 (−3)
			22	70.692	6.8 (−10)	54.444		4122.555	7.68 (−3)	51.544	3.86 (−3)
			23	157.469	1.86 (−2)	58.410		4209.802	4.16 (−3)	55.273	3.08 (−3)
			24	246.512	2.86 (−1)	61.936		4299.111	3.38 (−3)	58.993	2.34 (−3)
			25	336.889	2.50 (−1)	65.552	1.4 (−18)	4390.276	5.71 (−1)	62.577	1.78 (−3)
			26	428.389	2.19 (−1)	68.968	2.13 (−7)	4482.914	2.45 (−1)	66.018	2.00 (−3)
3	2	0	2	−727.971		0.007		3308.465	2.97 (−2)	0.002	2.97 (−2)
			3	−714.296		0.043		3322.059	2.95 (−2)	0.009	2.95 (−2)
			4	−696.172		0.166		3340.140	2.92 (−2)	0.026	2.92 (−2)
			5	−673.836[d]		0.583[d]		3362.672	2.89 (−2)	0.063	2.89 (−2)
			6	−644.629[d]		−1.403[d]		3389.602	2.85 (−2)	0.129	2.85 (−2)
			7	−613.409		−0.980		3420.871	2.81 (−2)	0.238	2.81 (−2)
			8	−577.577		−0.799		3456.403	2.77 (−2)	0.411	2.78 (−2)
			9	−537.395		−0.664		3496.104	2.73 (−2)	0.675	2.74 (−2)
			10	−493.005		−0.505		3539.858	2.68 (−2)	1.071	2.71 (−2)
			11	−444.525		−0.287		3587.512	2.62 (−2)	1.665	2.68 (−2)
			12	−392.077		0.015		3638.847	2.56 (−2)	2.572	2.66 (−2)
			13	−335.793		0.424		3693.535	2.48 (−2)	4.006	2.66 (−2)
			14	−275.819		0.954		3751.094	2.37 (−2)	6.317	2.66 (−2)
			15	−212.314		1.614		3824.431	3.19 (−2)	9.832	2.66 (−2)
			16	−145.457		2.398		3889.461	2.93 (−2)	−3.555	2.64 (−2)
			17	−75.480		3.307		3958.247	2.70 (−2)	−1.693	2.60 (−2)
			18	−2.383		4.199		4030.376	2.57 (−2)	0.702	2.52 (−2)
			19	73.340		4.992		4105.429	2.30 (−2)	1.647	2.40 (−2)
4	3	0	3	−337.791		0.000		3673.655	4.22 (−2)	0.002	4.25 (−2)
			4	−319.793		0.001		3691.567	4.11 (−2)	0.003	4.17 (−2)
			5	−297.358		0.003		3713.902	3.98 (−2)	0.003	4.05 (−2)
			6	−270.531		0.009		3740.618	3.87 (−2)	0.005	3.98 (−2)
			7	−239.372		0.029		3771.669	3.72 (−2)	0.009	3.80 (−2)
			8	−204.001		0.117		3806.996	3.54 (−2)	0.018	3.65 (−2)
			9	−163.358		−0.889		3846.515	3.43 (−2)	0.031	3.47 (−2)
			10	−120.078		−0.688		3890.327	3.40 (−2)	0.077	3.35 (−2)
			11	−72.245		0.992		3938.021	3.24 (−2)	0.121	3.12 (−2)
			12	−20.463		0.725		3989.662	2.91 (−2)	0.251	2.60 (−2)
			13	35.065	1.42 (−3)	0.995		4045.056	4.63 (−2)	0.504	2.69 (−2)
			14	93.876	3.55 (−3)	1.849		4103.031	3.08 (−2)	1.921	2.51 (−2)
			15	161.294	1.30 (−2)	−2.195		4168.656	2.63 (−2)	−0.812	3.03 (−2)
			16	226.035	5.16 (−3)	0.005		4234.194	1.35 (−1)	−1.099	2.55 (−2)
			17	295.320	2.00 (−3)	1.125		4304.245	2.47 (−2)	2.622	2.62 (−2)
			18	367.587	1.44 (−2)	2.464	5.3 (−14)	4376.894	2.19 (−2)	2.835	2.19 (−2)
5	4	0	4	174.714	3.27 (−7)	0.000	1.69 (−7)	4155.459	6.65 (−2)	0.000	6.64 (−2)
			5	196.769	2.85 (−6)	0.000	1.23 (−6)	4177.467	6.50 (−2)	−0.001	6.50 (−2)
			6	223.150	1.53 (−5)	0.000	5.74 (−6)	4203.781	6.30 (−2)	0.013	6.32 (−2)
			7	253.807	6.68 (−5)	0.001	2.38 (−5)	4234.380	6.35 (−2)	0.015	6.10 (−2)
			8	288.678	2.63 (−4)	0.002	1.19 (−4)	4269.220	5.80 (−2)	−0.006	5.93 (−2)
			9	327.776	5.17 (−3)	−0.050	6.37 (−4)	4308.203	5.50 (−2)	0.010	5.47 (−2)
			10	370.779	1.04 (−2)	0.265	8.10 (−3)	4351.277	5.18 (−2)	0.015	5.16 (−2)
			11	418.745	1.10 (−1)	−0.769	7.24 (−4)	4398.362	4.78 (−2)	0.040	4.76 (−2)
			12	469.332	5.03 (−3)	0.284	1.11 (−4)	4449.369	4.82 (−2)	−0.002	4.54 (−2)
			13	524.162	5.82 (−4)	0.120	2.78 (−5)	4504.191	4.37 (−2)	0.039	4.21 (−2)
			14	582.720	2.65 (−4)	0.170	1.24 (−4)	4562.677	5.88 (−2)	0.094	3.94 (−2)
			15	644.895	5.15 (−3)	0.383	1.11 (−2)	4624.400	2.44 (−1)	−0.379	1.04 (−1)
			16	710.283	4.32 (−2)	0.199	1.05 (−2)	4691.232	1.53 (−1)	−0.170	3.59 (−2)
			17	779.512	3.18 (−1)	0.567	1.91 (−1)	4759.775	3.74 (−2)	0.163	2.83 (−2)
			18	851.382	5.15 (−1)	1.163	4.37 (−1)	4830.668	5.50 (−2)	1.524	5.87 (−1)

TABLE BIV: continued

1	0	1	0	−734.044			3335.862	6.37 (−2)		
			1	−729.840			3340.052	6.32 (−2)		
			2	−721.436			3348.424	6.24 (−2)		
			3	−708.831			3360.964	6.11 (−2)		
			4	−691.999			3377.648	5.95 (−2)		
			5	-670.774^d			3398.449	5.74 (−2)		
			6	-647.906^d			3423.331	5.50 (−2)		
			7	−618.650			3452.260	5.24 (−2)		
			8	−585.733			3485.206	4.95 (−2)		
			9	−549.047			3522.183	4.66 (−2)		
			10	−508.626			3563.416	4.62 (−2)		
			11	−464.548			3605.841	5.21 (−2)		
			12	−416.917			3654.627	4.35 (−2)		
			13	−365.854			3707.068	3.86 (−2)		
			14	−311.497			3763.586	3.50 (−2)		
			15	−254.002			3811.044	2.23 (−2)		
			16	−193.548			3873.240	2.04 (−2)		
			17	−130.338			3937.779	1.82 (−2)		
			18	−64.606			4004.704	1.57 (−2)		
			19	3.367			4073.937	1.47 (−2)		
			20	73.220			4145.264	1.12 (−2)		
2	1	1	1	−621.269		0.333	3437.914	7.08 (−2)	0.340	8.78 (−2)
			2	−613.263		0.987	3445.937	6.90 (−2)	0.801	6.24 (−2)
			3	−601.255		1.944	3457.922	6.92 (−2)	1.806	6.32 (−2)
			4	−585.251		3.183	3473.689	7.83 (−2)	3.223	6.34 (−2)
			5	−565.268		4.681	3494.846	8.35 (−2)	3.468	6.18 (−2)
			6	−541.336		6.417	3518.584	7.15 (−2)	5.314	6.00 (−2)
			7	−513.492		8.373	3546.385	6.02 (−2)	7.219	5.72 (−2)
			8	−481.792		10.532	3578.085	5.48 (−2)	9.288	5.40 (−2)
			9	−446.298		12.878	3613.590	4.92 (−2)	11.538	5.06 (−2)
			10	−407.088		15.399	3652.844	6.34 (−2)	13.943	4.67 (−2)
			11	−364.248		18.077	3695.715	4.61 (−2)	16.539	4.32 (−2)
			12	−317.877		20.898	3742.147	4.06 (−2)	19.276	3.89 (−2)
			13	−268.077		23.834	3792.027	3.53 (−2)	22.141	3.29 (−2)
			14	−214.789		26.686	3845.218	7.07 (−2)	25.176	3.22 (−2)
			15	−158.962		30.247	3901.679	2.97 (−2)	28.239	3.02 (−2)
			16	−99.737		33.500	3961.180	2.67 (−2)	31.407	2.65 (−2)
			17	−37.765		37.239	4023.606	3.23 (−2)	34.623	2.19 (−2)
			18	26.605	2.5 (−10)	40.082	4088.802	2.16 (−2)	37.847	1.87 (−2)
			19	94.062	1.27 (−1)	43.008	4157.133	1.75 (−2)	40.489	1.77 (−2)
3	2	1	2	−354.991		0.002	3685.669	8.43 (−2)	0.002	8.43 (−2)
			3	−342.563		0.009	3697.998	8.51 (−2)	0.009	8.51 (−2)
			4	−326.043		0.028	3714.382	8.62 (−2)	0.028	8.61 (−2)
			5	−305.477		0.068	3734.769	8.77 (−2)	0.068	8.75 (−2)
			6	−280.933		0.146	3759.095	8.83 (−2)	0.142	8.78 (−2)
			7	−251.985		−0.350	3787.289	9.10 (−2)	0.270	9.08 (−2)
			8	−220.043		0.467	3819.260	9.23 (−2)	0.469	9.22 (−2)
			9	−184.020		0.740	3854.921	9.27 (−2)	0.768	9.26 (−2)
			10	−144.383		1.150	3894.172	9.19 (−2)	1.213	9.14 (−2)
			11	−101.285		1.726	3936.861	9.28 (−2)	1.915	8.79 (−2)
			12	−54.880		2.529	3983.502	8.40 (−2)	1.622	8.60 (−2)
			13	−5.329		3.687	4032.677	8.11 (−2)	5.084	6.49 (−2)
			14	47.191		19.571	4085.291	7.57 (−2)	7.606	5.24 (−2)
			15	102.669		24.097	4140.966	6.94 (−2)	10.747	4.27 (−2)
4	3	1	3	43.791	6.29 (−7)	0.000	4059.586	1.19 (−1)	−0.002	1.20 (−1)
			4	60.158	6.97 (−6)	0.000	4075.978	1.17 (−1)	−0.002	1.17 (−1)
			5	80.521	1.18 (−4)	0.002	4096.409	1.13 (−1)	−0.006	1.14 (−1)
			6	105.015	3.44 (−5)	0.006	4120.840	1.10 (−1)	−0.011	1.10 (−1)
			7	133.299	9.99 (−6)	0.015	4149.216	1.06 (−1)	−0.014	1.06 (−1)
			8	165.459	1.47 (−4)	0.039	4181.483	1.01 (−1)	−0.019	1.01 (−1)
			9	201.333	1.68 (−3)	0.129	4217.562	9.66 (−2)	−0.015	9.63 (−2)
			10	241.446	5.28 (−3)	−0.532	4257.366	9.18 (−2)	0.003	9.11 (−2)
			11	284.455	1.81 (−4)	0.491	4301.305	1.45 (−1)	0.127	9.42 (−2)

			12	330.956	7.17 (−4)	0.750		4347.770	8.05 (−2)	0.146	8.01 (−2)
			13	382.340	1.65 (−1)	−0.562	2.57 (−2)	4398.016	7.62 (−2)	0.353	7.42 (−2)
			14	434.852	7.19 (−1)	0.837	4.08 (−1)	4453.481	1.21 (−1)	−1.471	6.79 (−2)
			15	491.325	1.26 (+0)	1.235	4.79 (−1)	4508.605	6.44 (−2)	1.722	6.23 (−2)
5	4	1	4	562.972	2.06 (−5)	0.000	1.84 (−5)	4548.040	3.49 (−1)	0.148	1.81 (−1)
			5	583.028	2.32 (−3)	0.027	1.01 (−4)	4568.340	1.77 (−1)	−0.039	1.71 (−1)
			6	607.074	1.35 (−5)	0.001	2.45 (−5)	4592.420	1.68 (−1)	0.099	1.98 (−1)
			7	634.945	4.71 (−5)	0.001	4.43 (−5)	4620.393	1.59 (−1)	0.031	1.65 (−1)
			8	666.649	2.67 (−4)	0.006	9.53 (−5)	4652.196	1.49 (−1)	0.020	1.51 (−1)
			9	702.176	3.71 (−3)	−0.034	2.08 (−6)	4687.900	2.64 (−1)	−0.092	1.32 (−1)
			10	741.221	1.42 (−1)	0.038	1.06 (−1)	4726.999	1.35 (−1)	0.044	1.37 (−1)
			11	783.881	2.01 (−1)	0.096	1.49 (−1)	4769.492	3.12 (−1)	0.685	1.25 (−1)
			12	830.062	2.87 (−1)	0.126	2.02 (−1)	4816.402	1.13 (−1)	0.002	1.12 (−1)
			13	879.534	4.44 (−1)	0.249	2.67 (−1)	4865.956	3.01 (−1)	0.413	3.23 (−1)
			14	932.186	6.78 (−1)	0.463	3.32 (−1)	4919.290	5.98 (−1)	0.196	4.52 (−1)
			15	987.868	9.80 (−1)	0.790	4.30 (−1)	4975.443	8.14 (−1)	0.412	5.62 (−1)
1	0	2	0	−445.659				3633.935	1.01 (−1)		
			1	−441.960				3637.728	9.90 (−2)		
			2	−434.573				3645.316	9.51 (−2)		
			3	−423.514				3656.713	8.80 (−2)		
			4	−408.813				3671.962	7.54 (−2)		
			5	−390.506				3691.154^e	5.79 (−2)		
			6	−368.645				3710.765^e	6.13 (−2)		
			7	−343.293				3736.614	6.65 (−2)		
			8	−314.528				3765.836	6.70 (−2)		
			9	−282.441				3798.382	6.49 (−2)		
			10	−247.141				3834.174	6.12 (−2)		
			11	−208.754				3873.113	5.67 (−2)		
			12	−167.427				3915.082	5.18 (−2)		
2	0	0	0	−606.428				3473.264	1.59 (−2)		
			1	−601.889				3477.690	2.39 (−2)		
			2	−592.831				3486.465	8.02 (−3)		
			3	−579.289				3499.672	9.93 (−3)		
			4	−561.307				3517.227	1.02 (−2)		
			5	−538.938				3539.105	9.94 (−3)		
			6	−512.240				3565.246	9.18 (−3)		
			7	−481.276				3595.588	7.92 (−2)		
			8	−446.116				3630.123	1.09 (−2)		
			9	−406.836				3668.719	9.84 (−3)		
			10	−363.522				3711.320	9.26 (−3)		
			11	−316.268				3757.832	9.28 (−3)		
			12	−265.180				3808.094	4.28 (−3)		
			13	−210.375				3862.185	5.16 (−3)		
			14	−151.985				3919.844	6.45 (−3)		
			15	−90.160				3980.857	4.23 (−3)		
			16	−25.019				4045.259	5.91 (−3)		
			17	43.188	1.16 (−6)			4113.123	1.17 (−2)		
			18	114.307	6.06 (−3)			4183.346	3.21 (−3)		
			19	188.100	4.94 (−3)			4256.639	1.93 (−2)		
			20	264.310	4.09 (−3)			4332.505	1.13 (−2)		
			21	342.652	3.53 (−3)			4410.676	8.54 (−3)		
			22	422.082	6.88 (−3)			4490.871	2.71 (−2)		
			23	503.851	1.29 (−2)			4572.738	7.62 (−3)		
3	1	0	1	−421.973		0.692		3634.579	2.07 (−2)	0.650	1.98 (−2)
			2	−414.064		2.070		3642.356	2.28 (−2)	1.954	1.97 (−2)
			3	−402.207		4.117		3653.974	2.74 (−2)	3.935	1.94 (−2)
			4	−386.412		6.812		3669.344	3.65 (−2)	6.645	1.92 (−2)
			5	−366.688		10.124		3688.322^e	4.99 (−2)^e	10.190^e	1.89 (−2)
			6	−343.052		14.013		3714.358^e	4.18 (−2)^e	11.057^e	1.87 (−2)
			7	−315.522		18.431		3741.550	3.12 (−2)	15.076	1.86 (−2)
			8	−284.121		23.313		3772.661	2.51 (−2)	19.387	1.89 (−2)
			9	−248.880		28.576		3807.617	2.10 (−2)	23.932	1.97 (−2)
			10	−209.834		33.980		3846.362	1.82 (−2)	28.586	2.16 (−2)

			11	−167.038		40.080		3888.832	1.60 (−2)	33.138	2.53 (−2)
			12	−120.619		45.808		3934.958	1.40 (−2)	37.233	3.22 (−2)
			13	−69.975		50.574		3984.690	1.36 (−2)	53.070	5.89 (−2)
			14	−16.370		54.873		4037.903	1.42 (−2)	54.994	5.40 (−2)
			15	40.876		57.067		4093.562	2.86 (−2)	58.151	5.88 (−2)
			16	101.532		56.961		4154.863	1.17 (−2)	58.779	3.61 (−2)
4	2	0	2	−69.497		−0.581		3958.829	1.80 (−2)	−0.014	3.97 (−2)
			3	−57.155		0.280		3971.330	2.03 (−2)	0.064	1.62 (−2)
			4	−40.461		0.372		3987.958	2.01 (−2)	0.171	1.87 (−2)
			5	−20.013		0.977		4008.634	2.34 (−2)	0.404	1.97 (−2)
			6	4.280	3.77 (−3)	1.950		4033.294	2.04 (−2)	0.807	1.82 (−2)
			7	31.948	1.66 (−2)	3.740		4061.841	3.10 (−2)	1.446	1.94 (−2)
			8	62.327	3.28 (−2)	6.985		4094.164	2.28 (−2)	2.402	2.14 (−2)
			9	107.213	2.94 (−2)	−0.141		4130.119	2.13 (−2)	3.756	2.20 (−2)
			10	145.625	1.38 (−2)	3.302		4169.696	2.57 (−2)	5.286	2.41 (−2)
			11	187.879	5.63 (−3)	6.935		4212.431	2.81 (−2)	8.850	2.98 (−2)
			12	233.747	2.07 (−2)	11.010		4258.352	2.99 (−2)	11.905	2.29 (−2)
			13	282.491	2.02 (−3)	16.033		4307.146	3.43 (−2)	16.160	2.15 (−2)
			14	334.301	2.48 (−3)	21.288	1.7 (−18)	4358.435	4.28 (−2)	21.675	2.09 (−2)
			15	389.011	1.20 (−2)	28.586	1.25 (−1)	4411.576	6.27 (−2)	29.147	1.96 (−2)
			16	445.333	2.65 (−1)	37.258	1.39 (−1)	4465.612	5.50 (−2)	39.140	1.86 (−2)
5	3	0	3	417.711	1.85 (−3)	0.084	2.56 (−3)	4413.468	3.75 (−2)	-0.008	3.62 (−2)
			4	434.162	4.91 (−4)	0.025	3.06 (−4)	4429.862	3.41 (−2)	0.042	3.58 (−2)
			5	454.703	2.43 (−4)	0.037	1.64 (−4)	4450.365	3.37 (−2)	0.037	3.53 (−2)
			6	479.245	1.03 (−4)	0.088	1.29 (−4)	4474.841	3.34 (−2)	0.074	3.47 (−2)
			7	507.709	1.63 (−4)	0.208	1.18 (−4)	4503.234	3.35 (−2)	0.164	3.44 (−2)
			8	539.997	8.28 (−4)	0.453	1.15 (−4)	4535.627	1.51 (−1)	0.424	4.70 (−2)
			9	575.979	3.22 (−3)	0.907	1.08 (−4)	4571.524	3.09 (−2)	0.772	4.63 (−2)
			10	615.503	1.18 (−2)	1.699	4.10 (−4)	4611.032	3.23 (−2)	1.082	2.93 (−2)
			11	658.319	3.13 (−2)	2.815	4.09 (−3)	4653.982	4.37 (−2)	2.018	2.95 (−2)
			12	705.115	1.11 (−2)	3.966	6.11 (−5)	4699.509	3.74 (−2)	3.540	3.50 (−2)
			13	753.377	1.72 (−1)	7.674	3.77 (−1)	4755.860	1.28 (−1)	0.989	9.38 (−2)
			14	806.232	2.33 (+0)	10.204	5.79 (−1)	4805.721	1.24 (−1)	5.164	2.54 (−2)
			15	860.972	2.79 (+0)	14.536	6.50 (−1)	4859.345	3.62 (−1)	9.868	4.25 (−2)
3	0	0	0	−203.844				3882.051	5.54 (−2)		
			1	−199.243				3885.966	4.92 (−2)		
			2	−190.026				3893.960	3.82 (−2)		
			3	−176.189				3906.287	2.65 (−2)		
			4	−157.769				3923.121	1.79 (−2)		
			5	−134.835				3944.444	1.38 (−2)		
			6	−107.439				3970.192	1.20 (−2)		
			7	−75.805				4000.094	1.11 (−2)		
			8	−39.999				4034.255	1.49 (−2)		
			9	−0.235				4071.937	1.14 (−2)		
			10	43.207				4113.304	1.20 (−2)		
			11	89.738				4157.943	1.30 (−2)		
			12	141.195	3.05 (−2)			4205.437	1.43 (−2)		
			13	192.989	9.45 (−1)			4255.462	1.55 (−2)		
			14	247.272	9.93 (−1)			4305.990	7.33 (−2)		

[a]The conversion of the label $(v_r\, b\, k\, v_R\, J\, p)$ to the labels $[v_r\, v_\theta\, v_R]$ and J_{K_a,K_c} of the vibrational state and the rotational level, respectively, is: $v_\theta{=}b{-}k$, $K_a{=}k$, and $K_c{=}J{-}k{+}\frac{1-p_k p}{2}$ with $p_k{=}(-1)^k$. The levels shown in the table represent 18 vibrational states: $[v_r\, 0\, 0]$, $[v_r\, 0\, 1]$, $[v_r\, 0\, 2]$, $[v_r\, 0\, 3]$, $[v_r\, 1\, 0]$, $[v_r\, 1\, 1]$, $[v_r\, 1\, 2]$, $[v_r\, 2\, 0]$, and $[v_r\, 3\, 0]$ with $v_r{=}0, 1$.

[b]$\Gamma{>}0$ in this column is due to decay of the corresponding state by rotational predissociation and/or tunneling.

[c] Bound state level of the highest J-value in the complex.

[d]A crossing between $J^e{=}5$ and $J^e{=}6$ levels from groups $(v_r\, b\, k\, v_R){=}(0\,3\,2\,0)$ and $(0\,1\,0\,1)$. It affects line intensities, in particular, in $[0\,0\,0]{\rightarrow}[0\,1\,0]$ band, eee Table BXI.C.

[e]There is a crossing between $J^e{=}5$ and $J^e{=}6$ levels from groups $(v_r\, b\, k\, v_R){=}(1\,1\,0\,2)$ and $(1\,3\,1\,0)$. Coriolis interactions between the close levels from these groups cause the disturbance in the $K{=}1$ doubling function for state $[1\,2\,0]$ of Li^+–H_2 which is seen in Fig. 7 of the paper. Effects on the line intensities are seen in Table BX.C and in Fig. C4a of Part C (the panel for $[0\,0\,0]{\rightarrow}[1\,2\,0]$ band).

TABLE BV: Positions (E) and widths (Γ) of lowest rotational levels in three groups ($b\,k$=$b\,v_R$=0) below v=2 j=0 threshold[a]. v_r=2. All data are in cm^{-1}.

	k=0		k=1				k=2			
J	E	Γ	$E(e)$	$\Gamma(e)$	$\Delta E(f-e)^b$	$\Gamma(f)$	$E(e)$	$\Gamma(e)$	$\Delta E(f-e)$	$\Gamma(f)$
0	6197.85	1.1 (−1)								
1	6202.75	1.2 (−1)	6258.05	1.1 (−1)	0.15	1.1 (−1)				
2	6212.57	1.1 (−1)	6267.68	1.1 (−1)	0.46	1.1 (−1)	6432.01	1.2 (−1)	−0.01	1.2 (−1)
3	6227.24	1.0 (−1)	6282.07	1.2 (−1)	0.94	1.1 (−1)	6446.58	1.2 (−1)	0.00	1.2 (−1)
4	6246.77	9.8 (−2)	6301.28	1.1 (−1)	1.54	1.1 (−1)	6465.98	1.3 (−1)	0.00	1.2 (−1)
5	6271.13	9.6 (−2)	6325.23	1.0 (−1)	2.29	1.0 (−1)	6490.17	1.2 (−1)	0.00	1.2 (−1)
6	6300.29	9.4 (−2)	6353.89	1.0 (−1)	3.20	9.9 (−2)	6519.12	1.2 (−1)	−0.01	1.2 (−1)
7	6334.20	1.2 (−1)	6387.19	2.0 (−1)	4.25	9.7 (−2)	6552.79	1.1 (−1)	−0.01	1.1 (−1)
8	6372.79	8.5 (−2)	6425.19	9.1 (−2)	5.39	9.0 (−2)	6591.14	1.1 (−1)	−0.02	1.1 (−1)
9	6416.02	8.0 (−2)	6467.71	8.6 (−2)	6.73	8.6 (−2)	6634.09	1.0 (−1)	−0.03	1.0 (−1)
10	6463.82	8.3 (−2)	6514.75	8.1 (−2)	8.09	8.2 (−2)	6681.60	9.7 (−2)	−0.05	9.7 (−2)
11	6516.12	9.0 (−2)	6566.22	7.6 (−2)	9.63	7.6 (−2)	6733.58	9.1 (−2)	−0.06	8.8 (−2)
12	6572.82	7.2 (−2)	6622.05	7.2 (−2)	11.26	7.1 (−2)	6789.96	8.5 (−2)	−0.08	8.5 (−2)
13	6633.84	6.7 (−2)	6682.16	6.6 (−2)	13.00	6.6 (−2)	6850.65	7.8 (−2)	−0.11	7.8 (−2)
14	6699.08	6.0 (−2)	6746.47	9.1 (−2)	14.79	6.2 (−2)	6915.54	7.2 (−2)	−0.13	7.2 (−2)
15	6768.44	5.6 (−2)	6814.83	5.5 (−2)	16.70	5.4 (−2)	6984.54	6.5 (−2)	−0.15	6.5 (−2)
16	6841.79	5.1 (−2)	6887.18	4.9 (−2)	18.66	4.9 (−2)	7057.53	5.9 (−2)	−0.17	5.9 (−2)
17	6919.01	4.6 (−2)	6963.39	5.0 (−2)	20.66	4.4 (−2)	7134.40	7.1 (−2)	−0.21	5.3 (−2)
18	6999.96	4.1 (−2)	7043.30	3.9 (−2)	22.72	3.9 (−2)	7214.96	4.7 (−2)	−0.19	4.7 (−2)
19	7084.51	3.6 (−2)	7126.83	6.4 (−2)	24.79	3.5 (−2)	7299.11	4.2 (−2)	−0.18	4.2 (−2)
20	7172.50	3.0 (−2)	7213.77	3.3 (−2)	26.88	3.2 (−2)	7386.68	3.6 (−2)	−0.14	3.6 (−2)

[a]As obtained from the asymptotic part of the PES for $LiHH^+$ of Ref. 2, the threshold lies 8072.85 cm^{-1} above the v=0 j=0 threshold. This is too low by 14.15 cm^{-1} in comparison with the exact value of $\varepsilon_{20}-\varepsilon_{00}$ for H_2[1].

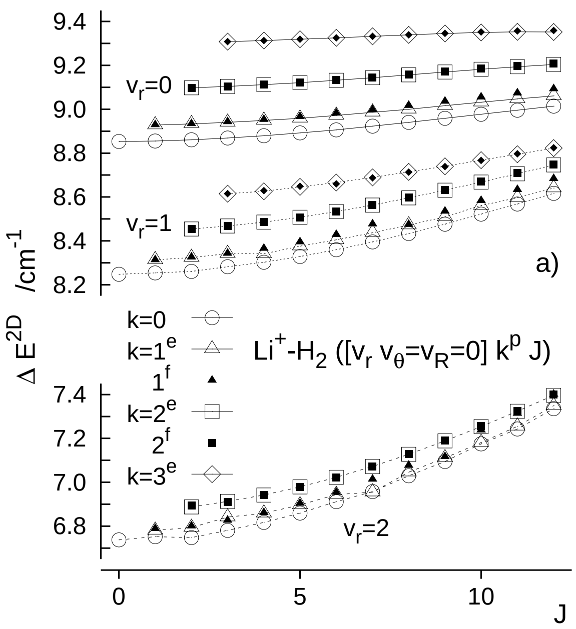
[b]Denotes $E(f)-E(e)$, i.e. the K-type doubling.

COMMENTS

(i). The groups $v_r\,b\,k\,v_R$ included into Tables BIV and BV are the ones whose lowest levels (J=k) are marked with the yellow crosses in Fig. 2 of the paper. The rotational states shown in the two tables were used in the simulations of the infrared absorption spectrum of the complex, of the bands which are presented in Tables BVIII–BXI and in Figs. 13–15, B5a–e, and/or in the calculations of the integrated band intensities listed in Table XIII.

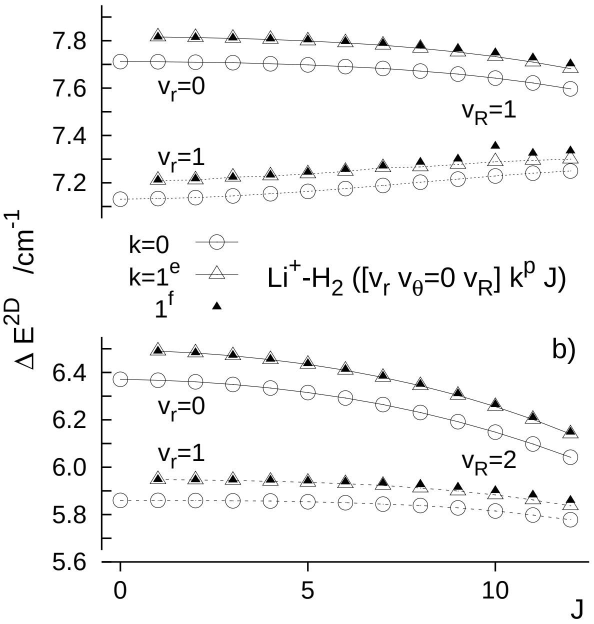
(ii). As it follows from Fig. B1 (and footnotes to Tables BI and BV), the thresholds $\varepsilon_{vj=0}$ that result from the PES of the $LiHH^+$ system depart from the true positions in H_2 the more the higher they lie. This testifies on some inaccuray of the asymptotic region of the PES. Actually, the higher energy parts of the PES may be less accurate not only at large R's but also at close Li relative to H_2 separations. Therefore the transitions energies predicted for the v_r=0→2 band, and listed in Table BX.B, should be taken with some reservation. The relative positions of lines should be more reliable. For this reason the prediction is believed to be useful.

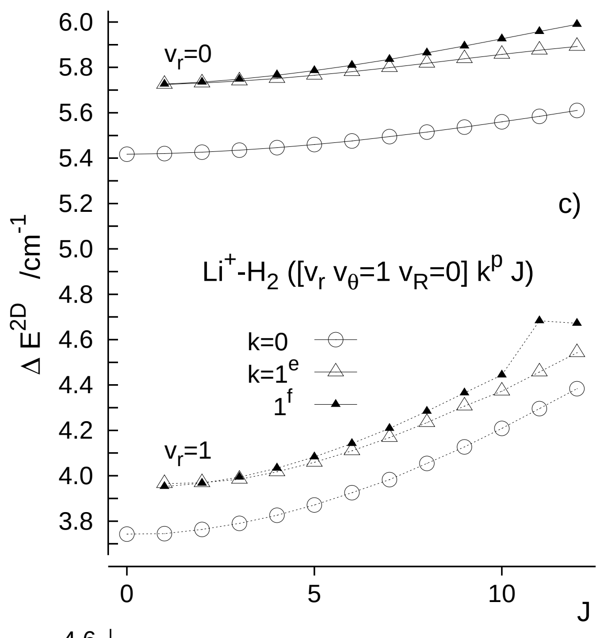
Fig. B3. Accuracy of 2D approximation in description of rotational energy levels



Plotted are the deviations $E^{2D} - E^{3D} := \Delta E^{2D}$ in the positions of the levels relative to the $v{=}0\, j{=}0$ threshold.

In the ground vibrational state [0 0 0], the deviations ΔE^{2D} clearly enlarge with increasing number k but are almost independent of J. In states with excited monomer vibrations, the deviations ΔE^{2D} become visibly dependent on J; the accuracy of 2D approximation in describing the rotational structure in [2 0 0] state is lower than in [0 0 0]. Obviously, the fact is reflected by the rotational constants in Table BVI. In [0 0 0] state, the percentage deviations of 2D and 3D values of the constants B and C are very small, about 10 times smaller than the deviations of the 3D values from the experimental data. In [2 0 0] state, the 2D relative to 3D deviations of the constants become about three times larger.





Deviations ΔE^{2D} of rotational energy levels in states with excited intermolecular vibrations.

The curves in panel b) compared to those in panel a) indicate that the rotational constants for states [0 0 1] and [1 0 1] should be even less impaired by the 2D approximation than the constants for states [0 0 0] and [1 0 0], respectively. In turn, a comparison of panels c)–d) with a) suggests that inaccuracy of 2D values of the constants for states with excited θ-mode may be larger. These indications are partly confirmed in Table BVI.

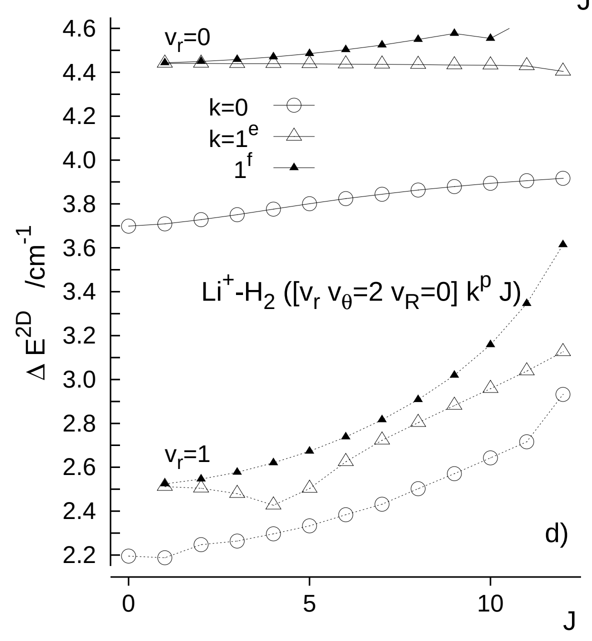


TABLE BVI: Li^+-H_2. Parameters of Watson A-reduced Hamiltonian from fitting to sets of lowest rotational energies in $k{=}0,1$ groups of eight vibrational states $[v_r\, v_\theta\, v_R]$ calculated 'exactly' (3D) and in the 2D approximation. For each parameter, deviation 2D−3D is shown in lower line. Deviations 3D−Exp /and (3D/Exp−1)×100%)/ from the experimental data of Ref. 10 for states [0 0 0] and [1 0 0] are shown in third lines. Except for the percentage deviations, all data are in cm^{-1}

	[0 0 0]	[0 0 1]	[0 1 0]	[1 0 0]	[2 0 0]	[1 0 1]	[1 1 0]	[0 2 0]
E_0 [a]	−1674.606	−1269.455	−1080.273	2378.491	6197.852	2789.040	2983.914	−606.428
	8.853	7.712	5.417	8.247	6.739	7.131	3.743	3.699
$N_{\rm fit}$ [b]	45	45	39	45	45	45	39	24
A	65.537(4) [c]	67.896(7)	95.573(5)	61.487(3)	57.822(3)	63.536(6)	86.244(8)	182.682
	0.074	0.105	0.309 ∗	0.062	0.042	0.079	0.199 ∗	0.735 ∗
B	2.5538(1)	2.3330(2)	2.4618(2)	2.5410(1)	2.5295(1)	2.3306(2)	2.4320(4)	2.6072(31)
	0.0016	− 0.0001	0.0022	0.0031	0.0046	0.0016	0.0053	0.0050
	− 0.0162 /−0.6/			− 0.0170 /−0.7/				
C	2.4037(1)	2.1945(2)	2.1972(2)	2.3891(1)	2.3753(1)	2.1902(2)	2.1843(4)	1.9130(34)
	0.0011	− 0.0005	0.0010	0.0024	0.0038	0.0009	0.0036	0.0019
	− 0.0146 /−0.6/			− 0.0161 /−0.7/				
$\Delta_J{\times}10^4$	3.251(3)	3.593(6)	3.345(7)	3.118(3)	3.011(3)	3.401(5)	3.170(11)	3.73(26)
	0.022	0.024	0.022	0.026	0.025	0.031	0.020	0.13
	0.071 /2.2/			0.068 /2.2/				
$\delta_J{\times}10^5$	1.59(3)	1.73(6)	2.32(7)	1.57(3)	1.56(3)	1.67(5)	2.20(1)	16.1(26)
	0.01	0.01	0.00	0.01	0.01	0.04	−0.01	0
	− 0.11 /−6.5/			0.07 /4.7/				
$\Delta_{JK}{\times}10^3$	5.59(4)	4.66(7)	7.61(7)	5.04(4)	4.61(4)	4.63(6)	5.1610	100.6(10)
	0.07	0.06	− 0.14 ∗	0.10	0.07	0.06	−0.20 ∗	1.7 ∗
	0.09 /1.3/			0.04 /0.8/				
$\sigma{\times}10^3$ [d]	10	19	13	10	10	17	20	56
	0	0	2	− 2	0	0	−12	8

[a]Energy of $J{=}0$ level relative to $Li^+{+}H_2(v{=}0, j{=}0)$ threshold.
[b]Total number of rotational energies used in the fit: for $k{=}0$–1, $p{=}\pm1$, and $J{=}1$–$J_{\rm max}{=}N_{\rm fit}/3$.
[c]The numbers in parentheses are the calculated uncertainties of the constants in their last figures shown.
[d]Root mean square error of the fit; below — the difference between fitting errors of 2D and 3D results.

COMMENTS

(i). The fits of the experimental transition energies and of the calculated energies of the initial and final states to energies of the A-reduced Hamiltonian truncated to three quartic terms show here practically the same consistency as the fits presented in Table II of the paper using only two quartic terms.

(ii). The deviations 2D−3D of the parameters A and Δ_{JK} for states [0 1 0] and [1 1 0], marked with an asterisk in the table, change most significantly in comparison with the deviations for states [0 0 0] and [1 0 0], respectively. Generally, these increased deviations reflect a lower rigidity of the complex in the θ-excited states. The changes in the deviations of Δ_{JK} are connected with the significantly increased separations between the error curves $k{=}0$ and $k{=}1^{e,f}$ in panel c) of Fig. B3 as compared to the separations seen in panel a).

(iii). The set of parameters in the table allows for checking if the dependence on the quantum numbers $v_r(:=v_1)$, $v_\theta(:=v_2)$, and $v_R(:=v_3)$ is linear, as it is in semirigid asymmetric top molecules[11] or equivalently, if the parameters of states with $\sum_i v_i{>}1$ satisfy the relation: $X([v_1\, v_2\, v_3]){\approx}X([0\,0\,0])(1-\sum_i v_i)+\sum_i X([\delta_{i,1}\, \delta_{i,2}\, \delta_{i,3}])v_i$. The rotational constants $X{=}A, B, C$ for states [2 0 0] and [1 0 1] and the constants B and C for state [1 1 0] satisfy this relation with deviations smaller than 1%. However, a dramatic departure from the linear behavior occurs in state [0 2 0]. The fitted values of A, B, and $B{-}C$ are larger than the values obtained from the above formula by 45, 10, and 83%, respectively. This fact is exhibited in Fig. 6 of the paper and interpreted as indicator of inapplicability of the semirigid rotor model to the Li^+–H_2 complex excited in the bending mode above $v_\theta{=}1$.

TABLE BVII: Total internal partition sum[a] (Z) of the Li^+–H_2 ion at selected temperature values below 400 K. Contribution of resonances ($Z_{\rm res}$).

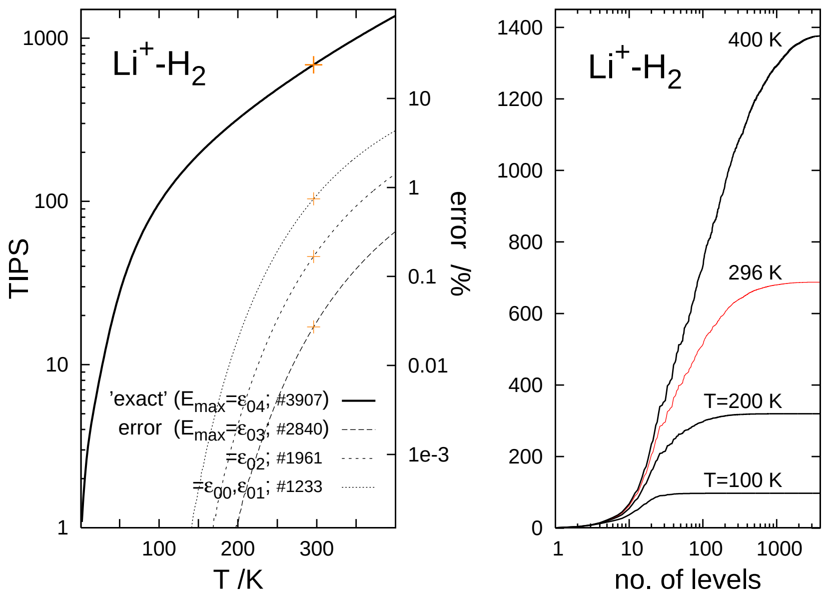
T	Z	T	Z	T	Z	$Z_{\rm res}$	T	Z	$Z_{\rm res}$
1	1.002	34	13.613	105	105.86	0.00	260	525.81	1.24
2	1.085	38	16.568	110	114.63	0.00	270	567.52	1.84
3	1.283	40	18.186	115	123.63	0.00	273.15	581.15	2.08
4	1.529	44	21.691	120	132.88	0.00	280	611.66	2.67
5	1.792	48	25.533	130	152.13	0.00	290	658.36	3.77
6	2.062	50	27.573	140	172.41	0.00	296	687.65	4.59
7	2.335	54	31.876	150	193.79	0.00	300	707.73	5.21
8	2.611	58	36.457	160	216.32	0.00	310	759.92	7.06
10	3.167	60	38.845	170	240.10	0.00	320	815.03	9.39
12	3.731	65	45.081	180	265.21	0.01	330	873.21	12.29
14	4.312	70	51.668	190	291.73	0.03	340	934.56	15.85
16	4.921	75	58.581	200	319.77	0.05	350	999.21	20.16
18	5.574	80	65.794	210	349.43	0.10	360	1067.3	25.3
20	6.283	85	73.289	220	380.81	0.18	370	1138.9	31.4
24	7.922	90	81.054	230	414.02	0.31	380	1214.1	38.6
28	9.909	95	89.075	240	449.18	0.51	390	1293.0	49.9
30	11.046	100	97.347	250	486.40	0.81	400	1375.8	56.4

[a]Evaluated according to Eq. (8) of the paper. Actually listed are the values of $Z(T)/Z^{\rm ref}(T)$ where $Z_{\rm ref}{=}\exp(-E_0/k_BT)$ and $E_0{=}{-}1674.606$ cm^{-1} is the energy of the lowest state of the complex relative to the ε_{00} threshold. States of energies up to $E_{\max}{=}\varepsilon_{04}$ (the $H_2(v{=}0,j{=}4)$ + Li^+ dissociation threshold) are included into the sum. About two-thirds of them are resonances of lifetimes no shorter than 1 ps ($\Gamma{<}5$ cm^{-1}). See Fig. B4 below for some details on convergence of the TIPS with the number of included energy levels.

Fig. B4. Total internal partition sum

The error curves in the left panel show effects of shifting the upper bound $E_{\max}$ of the included levels to lower dissociation thresholds. $E_{\max}{=}\varepsilon_{00},\varepsilon_{01}$ means that only bound state levels are included.

In full rigour, the TIPS function should account for all states of the system that exist in the energy range up to the assumed/necessary $E_{\max}$, bound and continuum. All the continuum states, irrespective of the value of the collision-time delay characterizing them (large positive, small positive, or negative), should be included.



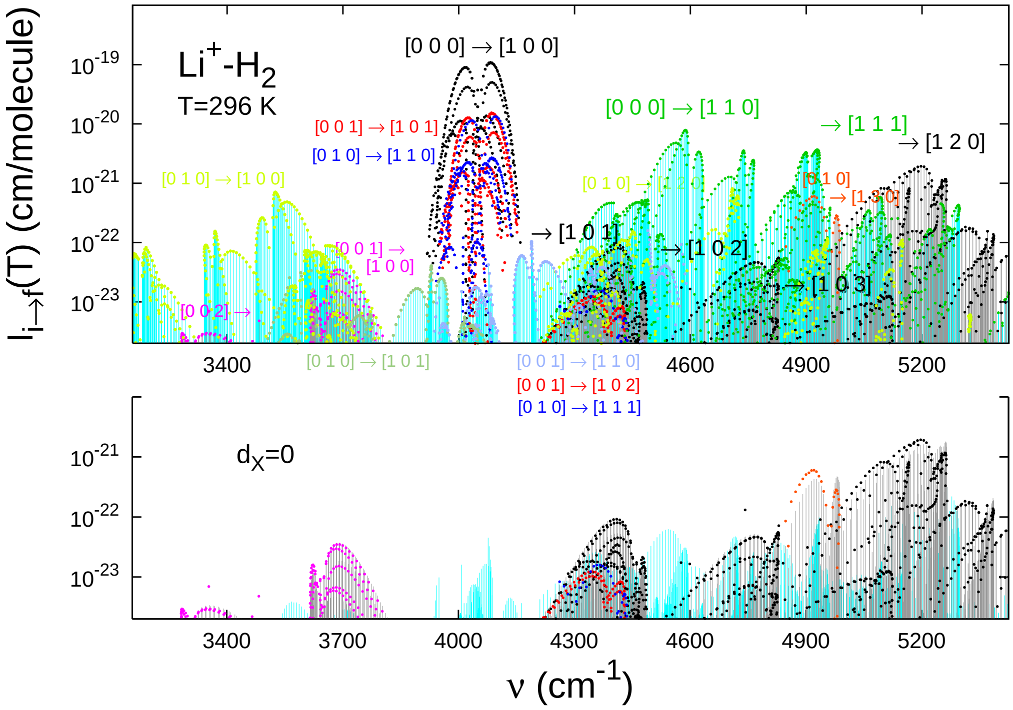
For this purpose, the following term, not shown in Eq. (8),

$$(2\pi\hbar)^{-1}\sum_{I=0,1}\int_{\varepsilon_{0\,j=I}}^{E_{\max}}\sum_{J,p}(2J{+}1)\,g_I\,\mathrm{Tr}\,\mathbf{Q}^{IJp}(E)\,\exp(-E/kT)\,dE$$

needs to be evaluated. The present 'exact' TIPS includes the contribution of the overwhelming majority of the resonance peaks in the integrands $\mathrm{Tr}\mathbf{Q}^{IJp}(E)$ but omits their backgrounds stemming from 'flat' continuum states. Quite likely, however, this omission has negligible impact on the TIPS value at T=296 K, i.e. at the temperature used in the calculation of the line intensities in this work. The highest lying red cross on the error curves shows that all the included resonances contribute merely 0.7% to the value. The continuum state contribution should be rather smaller (in absolute value, it may be negative), at this relatively low temperature.

INFRARED ABSORPTION SPECTRUM

Fig. B5. Absolute intensities of lines at T=296 K.
The role of d_X dipole component



Upper: Extended version of the upper panel of Fig. 13 of the paper. Added are intensities of about 560 lines in four hot bands (listed below the bottom axis). The two b-type bands, [0 1 0]→[1 0 1] and [0 0 1]→[1 1 0], surround and partly overlap with the [0 0 0]→[1 0 0], and the two bands with the net excitations in the θ- and R-modes Δv_θ=0 and Δ_R=1, respectively, occur in the region of the combination band [0 0 0]→[1 0 1]. Altogether, about 4680 lines are shown in the panel.
Bottom: Line intensities from calculations with the d_X dipole component set to zero. The intensities are represented by the heights of the gray and green sticks. The dots are at the same positions as in the upper panel. For clarity, the lines from the v_r=0→1 fundamental and the two hot a-type bands overlapping with it are omitted.

COMMENTS

(i). The intensities in the bands added here are generally smaller than the intensities in the hot bands of the same type shown in Fig. 13 of the paper. This is an indication that no important information is missing there as to the most intense bands in the NIR range other than the v_r=0→1 fundamental.

(ii). The displacements of the dots from the tops of the corresponding lines in the bottom panel show the contributions of the d_X component to the intensities. In the majority of the a-type bands, these contributions are small, barely noticeable on the scale of the figure.

(iii). Since the d_X connects λ-components of the initial and final states differing by ±1, see Eqs. (20)–(24), it is the primary driver of $\Delta K_a(:=k_\mathrm{f}-k_\mathrm{i})=\pm1$ transitions of which the bands with the labels $[.\,v_\theta\,.]\to[.\,v_\theta\pm1\,.]$ are formed. Therefore, the omission of this dipole component lowers dramatically the line intensities in the b-type bands. The green sticks in the bottom panel are lower than their counterparts in the upper panel by more than one, even two, orders of magnitude. They represent actually intensities of $\Delta\lambda=0$ transitions between the small(er) components of the i- and/or f-states, $\lambda\neq k_\mathrm{i}$ and/or $\lambda\neq k_\mathrm{f}$, which arise due to Coriolis interactions in these states.

(iv). The effect of the d_X component on the integrated intensities of the bands (cf. Table XII), described by the deviation $\left(\frac{I_{[\mathrm{v}]\to[\mathrm{v}]'}(d_X=0)}{I_{[\mathrm{v}]\to[\mathrm{v}]'}}-1\right)\times100\,\%$, is <1, 2, and 6 % for [0 0 0]→[1 0 0], [0 1 0]→[1 1 0], and [0 0 0]→[1 2 0], respectively, but −99 % for [0 0 0]→[1 1 0].

Absorption cross-section $\sigma(\nu; T{=}296\,\mathrm{K})$

NEAR-INFRARED

Fig. B6a. Fundamental $v_r{=}0{\rightarrow}1$ band and two hot bands: $v_r{=}0{\rightarrow}1 + v_\theta{=}1{\rightarrow}1$ and $v_r{=}0{\rightarrow}1 + v_R{=}1{\rightarrow}1$ in R-branch region

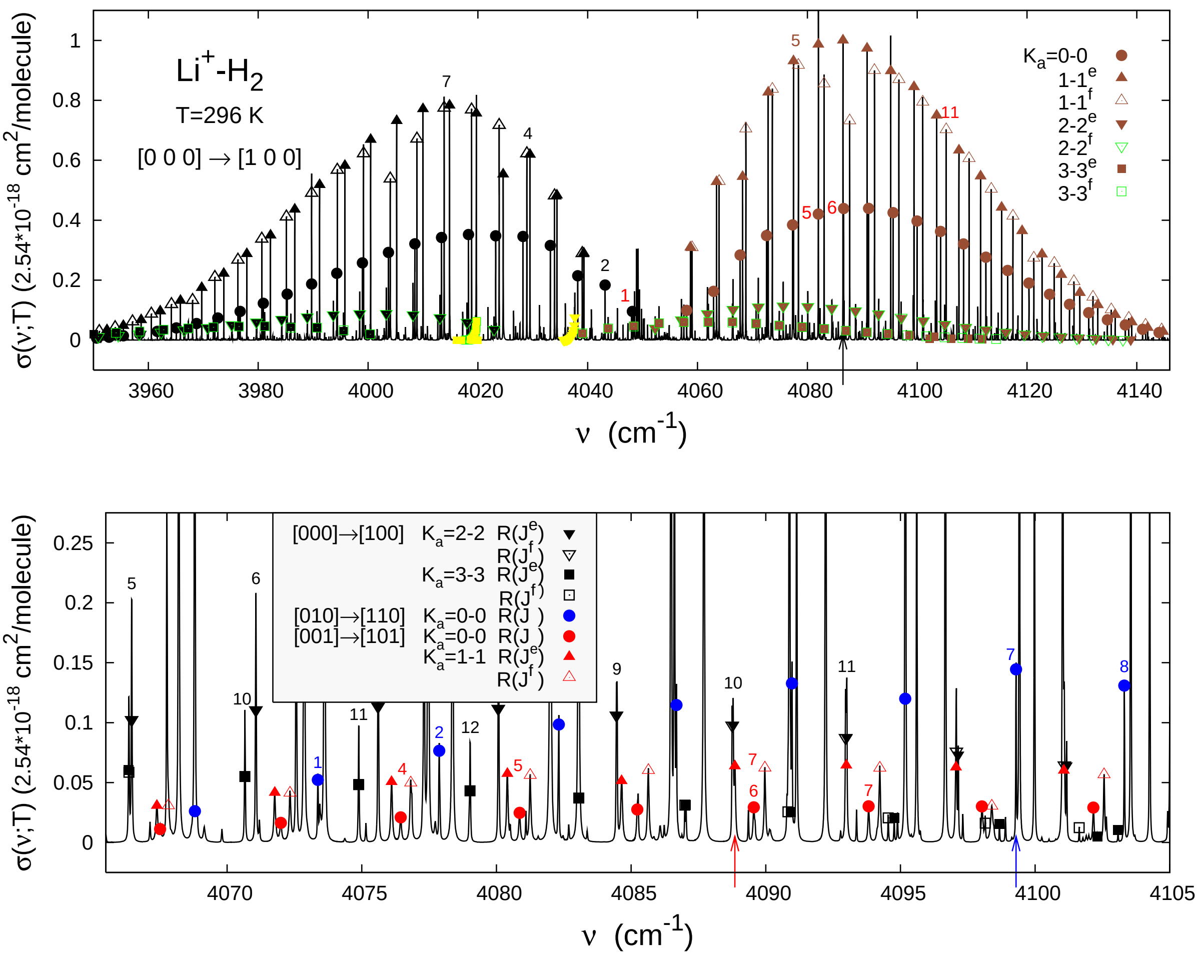


Fig. B6b. Overtone $v_r{=}0{\rightarrow}2$ band

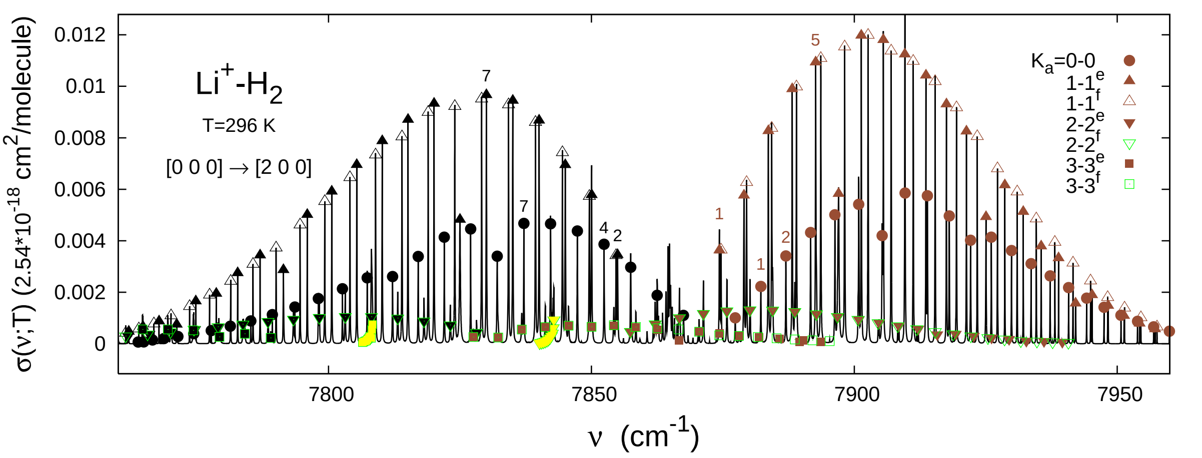
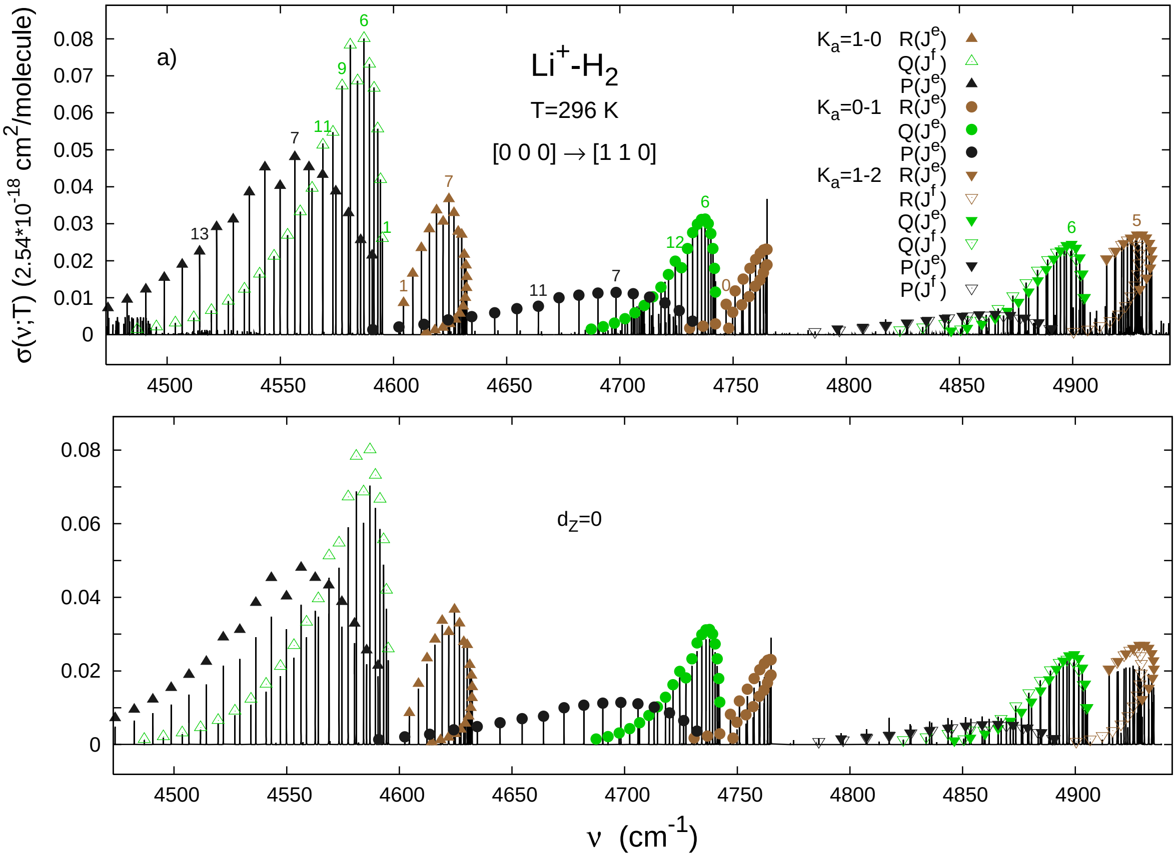
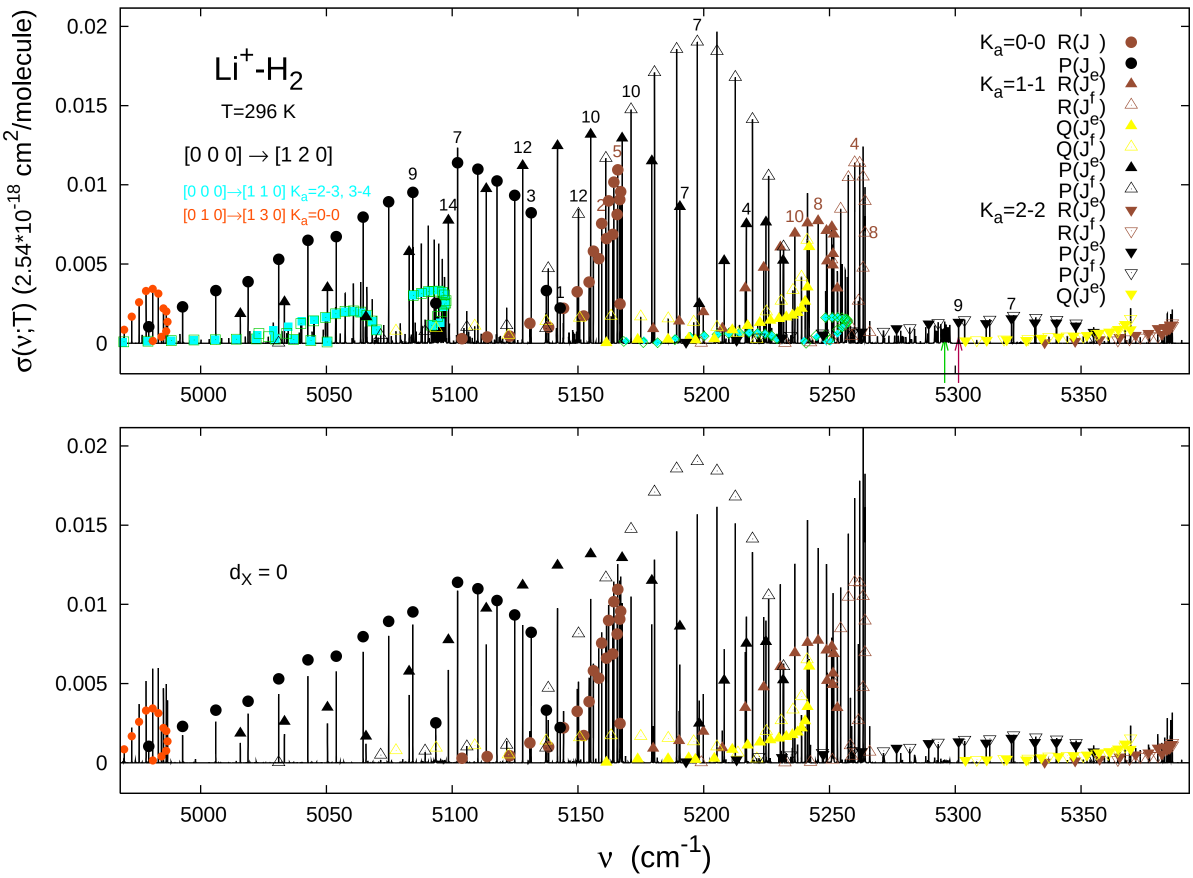


Fig. B6c. Two most intense combination bands, the role of d_X dipole component

v_r=0→1 + v_θ=0→1



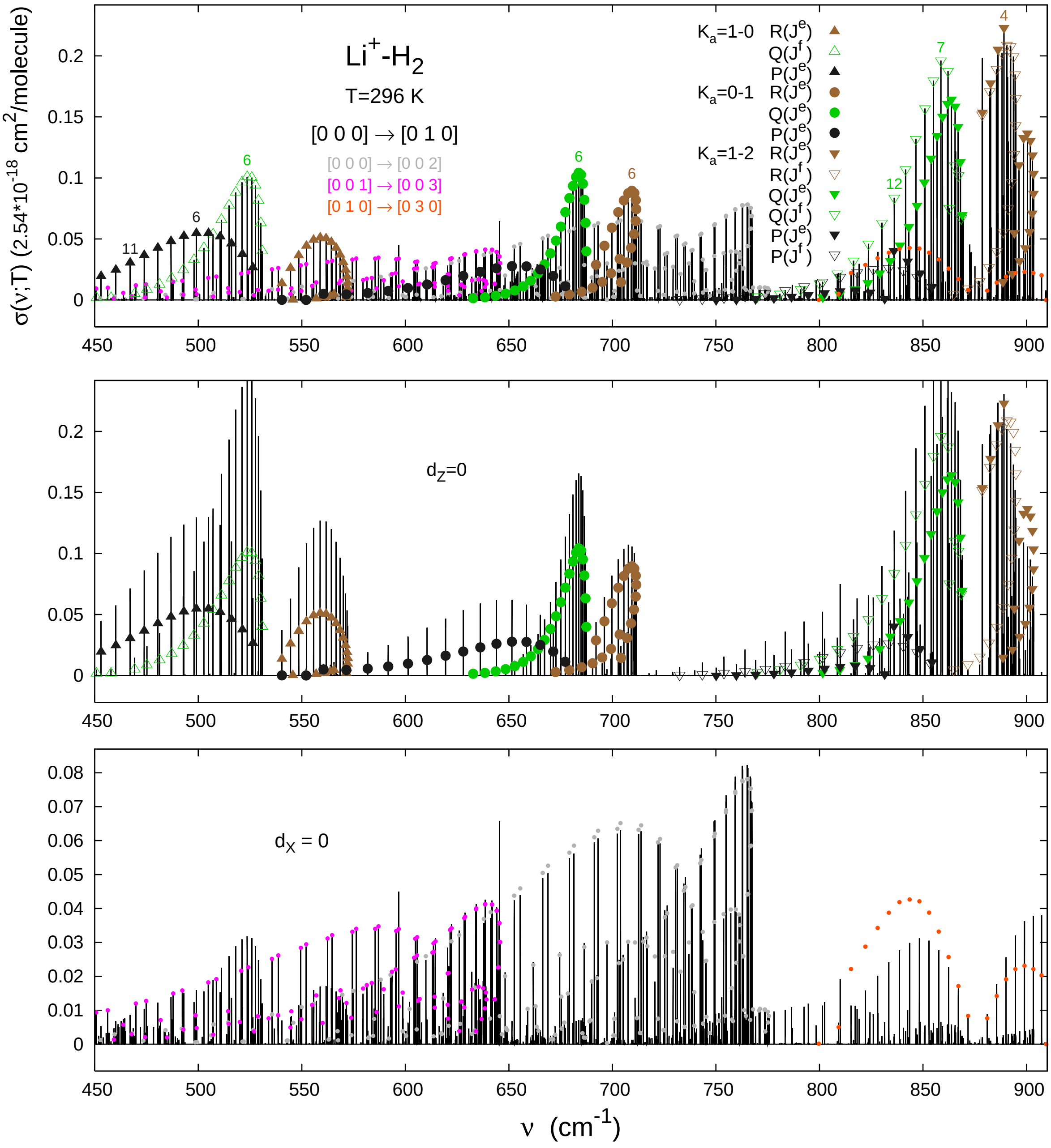
v_r=0→1 + v_θ=0→2



FAR-INFRARED

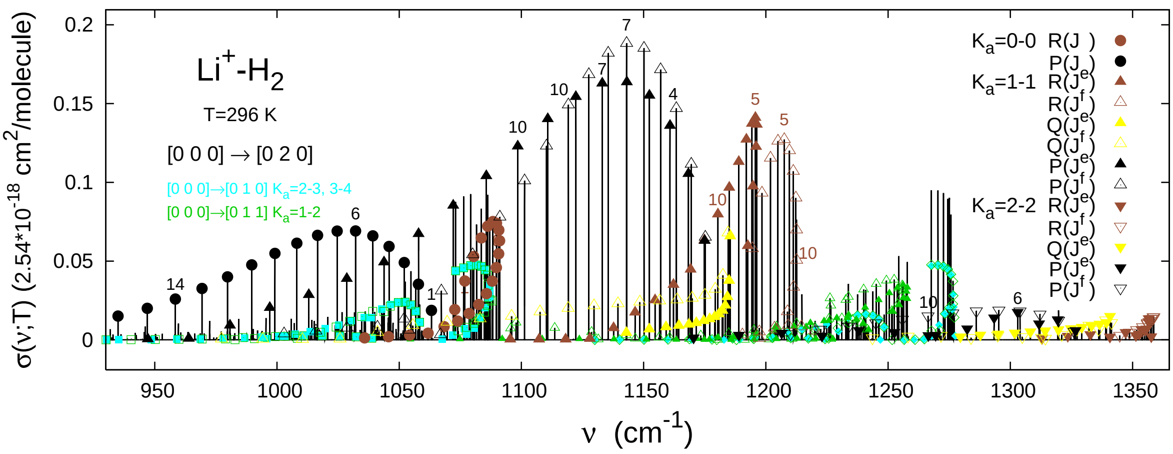
Fig. B6d. Fundamental v_θ=0→1 band

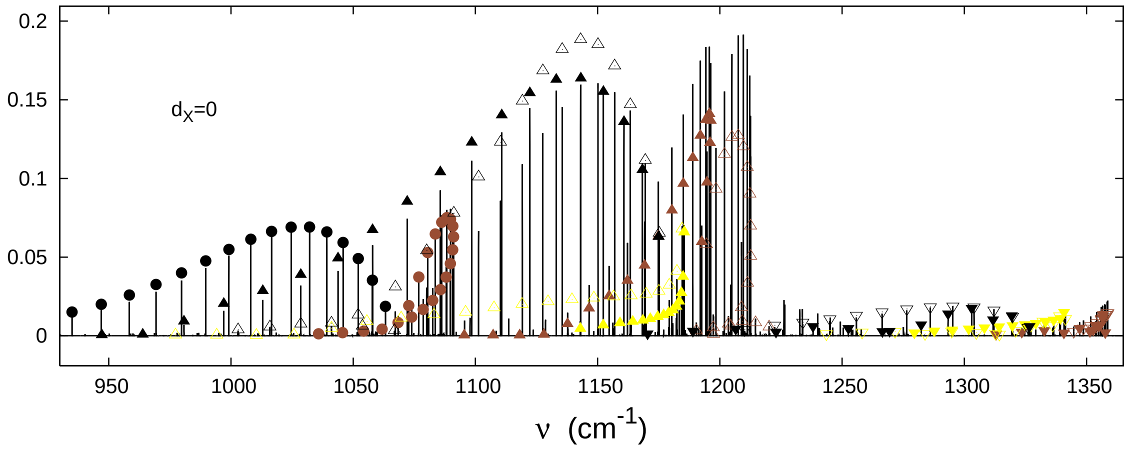
The role of d_X dipole component



MID-INFRARED

Fig. B6e. Overtone v_θ=0→2 band





COMMENTS

(i). As described in the paper, Secs. IIB and IV, the absorption cross-section $\sigma(\nu;T)$ presented in the figures of this work is the sum of the individual absorption lines with the intensity distribution described by the Voigt profile,

$$\sigma_{\mathrm{i}\to\mathrm{f}}(\nu;T) = I_{\mathrm{i}\to\mathrm{f}}(T)\times V(\nu-\nu_{\mathrm{if}};\gamma,\alpha)\,. \tag{B1}$$

Some information on the parameters of the Voigt profiles involved in the construction of the function $\sigma(\nu;T)$ in the region of several vibrational bands in the NIR is provided in Fig. B7.

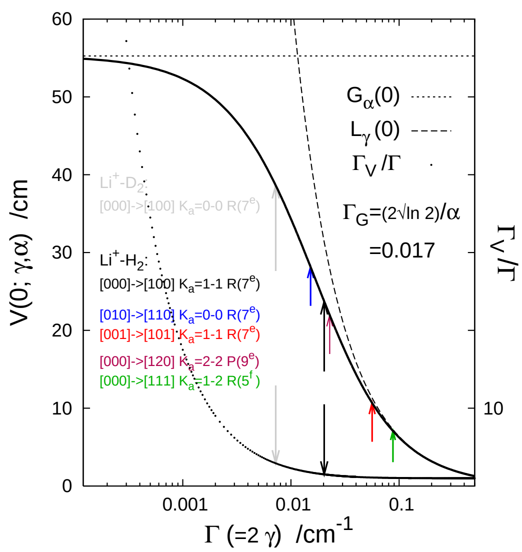


Fig. B7. Voigt profile $(L_\gamma{\star}G_\alpha)(\nu){:=}V(\nu;\gamma,\alpha)$ used to describe the shape of individual absorption line, Eq. (B1). Plotted are: the maximum of the profile, $V(0;\gamma,\alpha)$, and its full-width-at half-maximum (FWHM), Γ_V, as functions of Γ — the FWHM of the Lorentzian component, i.e. the predissociation width of the f-state. The arrows indicate the heights and widths of the profiles which describe the lines $\sigma_{\mathrm{i}\to\mathrm{f}}(\nu;T)$ due to transitions i$\to$f specified in the labels. The lines are selected from those which are included into the sums $\sum_{\mathrm{i,f}}\sigma_{\mathrm{i}\to\mathrm{f}}$ plotted in Figs. B6a,c and C4a (in Ref. 9). The centers ν_{if} of the selected lines are marked by the arrows on ν-axes of these figures. The black (grey) arrows indicate the parameters of the profile which describes the reference line in the plots of $\sigma(\nu;T)$ for Li^+–H_2 (Li^+–D_2). The pairs of lines specified in the colored labels represent the subbands referred to in comment (v).

(ii). The highest peaks in the cross-section $\sigma(\nu;T{=}296\,\mathrm{K})$ plotted in Figs. B6a–e are given symbols to fully specify the underlying transition i$(:=[v_r\,v_\theta\,v_R]\,k\,J\,p)\to$f$(:=[v_r'\,v_\theta'\,v_R']\,k'\,J'\,p')$, strictly, the rotational transition within the vibrational band specified in the (black) label or, equivalently, the subband $K_a{=}k{\to}k'$, the branch ΔJ, and the subbranch (i.e. the parity p) if $k{>}0$ and $k'{>}0$. The symbols are placed at the positions $(\nu_{\mathrm{if}},\sigma_{\mathrm{i}\to\mathrm{f}}(\nu_{\mathrm{if}};T))$. So, they may lie far below the tops of the peaks which result from accumulation of intensities (addition of the $\sigma_{\mathrm{i}\to\mathrm{f}}$s) from several transitions with very close frequencies ν_{if}. In particular, such accumulation occurs as an effect of very small K-doubling of J and J' levels in the R- and P-branches of the subbands with $k{>}1$ and $k'{>}1$. Examples: the $K_a{=}2{-}2$ subbands of the bands $[0\,0\,0]{\to}[1,2\,0\,0]$ in Fig. B6a,b and $K_a{=}2{-}3$ of $[0\,0\,0]{\to}[1\,1\,0]$ in Fig. B6c.

(iii). In Fig. B6c, devoted to the two important combination bands in the NIR, additional panels are enclosed which show the cross-section functions obtained for the same frequency intervals when one of the dipole-moment components is set to zero. In order to better see the role of the neglected component, the symbols labelling the peaks are left at the same positions as in the panels with the 'complete' cross-section.
The band [0 0 0]→[1 1 0] is almost entirely determined by the component d_X (see also Fig. B5). The d_Z enhances the intensity (and the heights by the same) of lines in the most intense subband K_a=1−0 by about 30%, at most. In turn, the band [0 0 0]→[1 2 0], as an a-type band, is determined by the component d_Z. The impact of the d_X is non-negligible, however. Easily noticeable is the alteration of the relative heights of R- and P-lines in the K_a=1−1 subband caused by this component.

(iv). Figs. B6d and B6e demonstrate the cross-section $\sigma(\nu; T{=}296\,\mathrm{K})$ in the frequency regions of the bands [0 0 0]→[0 1 0] and [0 0 0]→[0 2 0]. Viewed together with Fig. B6c, they inform on how the lack of excitation in the r-mode modifies the roles of the d_X and d_Z dipole components in producing line intensities in the b- and a-type bands. Substantial changes in this respect are expected upon looking at the matrix elements of the dipole strength functions $\langle v|D_{L|\Lambda|}(r,R)|v'\rangle_r$ in Fig. 1b of the paper. While the elements $\langle 0|..|1\rangle$ for D_{L0} and D_{L1} are of comparable size, the $\langle 0|D_{00}|0\rangle$ clearly dominates among the (larger in overall) elements $\langle 0|..|0\rangle$. The obvious consequences are: 1) the v_r=0→0 bands are generally more intense as their counterparts combined with the v_r=0→1 excitation and 2) the band [0 0 0]→[0 1 0] dominates much less over the a-type bands in the same range than the [0 0 0]→[1 1 0] does. A less obvious fact, revealed by the comparison of the upper and middle panels of Fig. B6d, is that the heights of lines in the [0 0 0]→[0 1 0] band and their dominance over lines in the three bands specified in the colored labels is additionally reduced, even more than two times in the K_a=1−0 subband, by a destructive interference of the d_X with the (much larger) d_Z dipole component. More extensively the interference is discussed in Part C of the material, in comments to Fig. C4 and C5.
The impact of the component d_X on the heights of lines in the band [0 2 0] (the lower panel of Fig. B6d) and in the other three a-type bands (the bottom panel of Fig. B6d) is qualitatively the same as that observed in the [0 0 0]→[1 2 0]; it is the intensity increase of P- and decrease of R-lines mentioned in comment (iii). Here, one may add that this impact is much smaller in the bands [0 0 0]→[0 0 2] and [0 0 1]→[0 0 3] than it is in the bands [0 0 0]→[0 2 0] and [0 1 0]→[0 3 0]. This should be attributed to the fact that excitations in the R-mode are primarily determined by the large isotropic ($\sim D_{00}$) part of the $d_Z(r,R)$ dipole component function while the anisotropic part of d_Z, of magnitude comparable to d_X, is more important in promoting excitations in the θ-mode.
The Q-lines in the a-type bands are affected by the presence of the d_X even more than the R- and P-lines. Though not quite well-visible in the plots of the cross-section, this fact becomes evident in the analysis of the line strengths which is presented in Part C.

(v). The heights of lines $\sigma_{\mathrm{i}\to\mathrm{f}}$ in the NIR region, where the f-states decay by vibrational predissociation and the predissociation widths vary from a few hundredths to a few dozens of cm^{-1} (see Table BIV), do not simply mirror the relations between the line intensities $I_{\mathrm{i}\to\mathrm{f}}$ seen in Fig. B5. Indeed, numerous cases of changeover of the relation 'greater' between the $I_{\mathrm{i}\to\mathrm{f}}$s to the relation 'smaller' or 'nearly equal' between the $\sigma_{\mathrm{i}\to\mathrm{f}}(\nu_{\mathrm{if}})$s are exhibited in the comparison of lines from the bands [0 0 1]→[1 0 1] and [0 1 0]→[1 1 0] in Fig. 16 of the paper. Further examples of the same effect emerge from comparison of lines belonging to the bands [0 0 0]→[1 1 1] and [0 0 0]→[1 2 0], strictly, to their subbands K_a=1−2 and K_a=2−2, respectively, in the frequency interval 5250–5300 cm^{-1}. The intensities of lines from the former band are clearly seen in Fig. B5 as outgrowing the intensities of lines from the latter band. In the plot of the cross-section in turn, the third panel of Fig. B6c, the profiles of lines from the latter band appear higher.

TABLE BVIII: Infrared absorption spectrum of Li^+–H_2. Line positions (ν, in cm^{-1}), deviations from observed values ($\Delta=\nu-\nu^{obs}$), vibrational factors of line strengths (S_{vib}, in 10^{-3} D^2), and line intensities (I, in cm/molecule) at T=296 K in four subbands of v_r=0→1 band, ($b\,k$=$b\,v_R$=0)→($k\,k\,0$) for k=0–3 [a]. (Extended version of Table XIII of the paper).

	R(J)					P(J)					Q(J)			
J	ν	Δ	Δ (Ref. 8)	S_{vib} [b]	I	ν	Δ	Δ (Ref. 8)	S_{vib} [b]	I	ν	Δ	S_{vib} [b]	I [c]
						$k=0$ $p=1$								
0	4058.02	−0.31	5.64	4.73	1.16 (−20)									
1	4062.92	−0.34	5.84	4.74	2.28 (−20)	4048.14			4.74	1.13 (−20)				
2	4067.77	−0.38	6.11	4.74	3.26 (−20)	4043.17	−0.20	5.50	4.73	2.15 (−20)				
3	4072.57	−0.42	6.46	4.76	4.07 (−20)	4038.18	−0.18	5.58	4.73	3.00 (−20)				
4	4077.31	−0.47	6.88	4.77	4.63 (−20)	4033.19	−0.15	5.75	4.72	3.63 (−20)				
5	4082.00			4.77	4.93 (−20)	4028.21	−0.14	5.96	4.74	4.03 (−20)				
6	4086.61			4.79	5.01 (−20)	4023.24	−0.12		4.74	4.19 (−20)				
7	4091.15	−0.61		4.79	4.85 (−20)	4018.30	−0.10		4.73	4.13 (−20)				
8	4095.60	−0.65		4.80	4.54 (−20)	4013.39	−0.08		4.75	3.91 (−20)				
9	4099.97	−0.72		4.81	4.09 (−20)	4008.53	−0.06		4.74	3.55 (−20)				
10	4104.25	−0.77		4.84	3.58 (−20)	4003.72	−0.05		4.75	3.12 (−20)				
11	4108.43			4.84	3.03 (−20)	3998.97	−0.03		4.76	2.66 (−20)				
12	4112.51			4.85	2.50 (−20)	3994.31			4.77	2.20 (−20)				
13	4116.49			4.87	2.00 (−20)	3989.74			4.78	1.77 (−20)				
14	4120.35			4.88	1.56 (−20)	3985.27			4.78	1.38 (−20)				
15	4124.10			4.89	1.19 (−20)	3980.92			4.79	1.05 (−20)				
16	4127.74			4.91	8.87 (−21)	3976.71			4.80	7.87 (−21)				
17	4131.25			4.92	6.46 (−21)	3972.66			4.80	5.73 (−21)				
18	4134.64			4.93	4.61 (−21)	3968.77			4.81	4.09 (−21)				
19	4137.91			4.93	3.22 (−21)	3965.08			4.82	2.86 (−21)				
20	4141.05			4.94	2.21 (−21)	3961.61			4.82	1.96 (−21)				
						$k=1$ p=1 /p=−1 [c]								
1	4058.70	−0.37	5.48	4.74	3.76 (−20)						4049.18	−0.31	4.68	3.71 (−20)
	4059.01	−0.37	5.44	4.72	3.75 (−20)						4048.88	−0.31	4.70	3.72 (−20)
2	4063.47	−0.41	5.76	4.73	6.39 (−20)	4039.30	−0.24	5.10	4.71	3.55 (−20)	4049.43	−0.33	4.62	1.94 (−20)
	4063.93	−0.41	5.71	4.72	6.35 (−20)	4039.00	−0.24	5.12	4.72	3.55 (−20)	4048.52	−0.30	4.66	1.95 (−20)
3	4068.21	−0.43	6.12	4.73	8.37 (−20)	4034.40	−0.22	5.18	4.71	5.88 (−20)	4049.80	−0.32	4.52	1.24 (−20)
	4068.80	−0.46	6.05	4.72	8.31 (−20)	4033.96	−0.20	5.22	4.72	5.87 (−20)	4048.00	−0.34	4.58	1.25 (−20)
4	4072.86	−0.50	6.56	4.77	9.84 (−20)	4029.49	−0.19	5.35	4.70	7.49 (−20)	4050.30	−0.32	4.39	8.46 (−21)
	4073.62	−0.50	6.48	4.73	9.70 (−20)	4028.91	−0.19	5.37	4.71	7.47 (−20)	4047.32	−0.28	4.48	8.56 (−21)
5	4077.47	−0.53		4.78	1.07 (−19)	4024.61	−0.16	5.57	4.68	8.49 (−20)	4050.91		4.25	5.93 (−21)
	4078.37	−0.55		4.73	1.04 (−19)	4023.88	−0.15	5.62	4.71	8.45 (−20)	4046.44		4.40	6.06 (−21)
6	4082.01	−0.58		4.79	1.09 (−19) [d]	4019.71	−0.14		4.71	9.00 (−20)	4051.64		4.06	4.15 (−21)
	4083.05	−0.61		4.71	1.06 (−19)	4018.86	−0.13		4.73	8.91 (−20)	4045.42		4.28	4.30 (−21)
7	4086.48	−0.66		4.81	1.07 (−19)	4014.84	−0.12		4.71	8.97 (−20)	4052.48		3.84	2.89 (−21)
	4087.70	−0.62		4.70	1.03 (−19)	4013.86	−0.10		4.72	8.82 (−20)	4044.24		4.13	3.04 (−21)
8	4090.88	−0.68		4.81	1.01 (−19)	4010.01	−0.11		4.71	8.54 (−20)	4053.48		3.61	1.99 (−21)
	4092.22	−0.69		4.76	9.70 (−20)	4008.90	−0.12		4.70	8.31 (−20)	4042.91		3.98	2.13 (−21)
9	4095.18	−0.74		4.83	9.13 (−20)	4005.21	−0.08		4.72	7.83 (−20)	4054.53		3.41	1.36 (−21)
	4096.67	−0.75		4.78	8.76 (−20)	4004.04	−0.05		4.69	7.55 (−20)	4041.44		3.79	1.46 (−21)
10	4099.42	−0.79		4.85	8.03 (−20)	4000.47	−0.06		4.71	6.91 (−20)	4055.69		3.16	9.07 (−22)
	4101.02	−0.82		4.77	7.61 (−20)	3999.18	−0.05		4.75	6.70 (−20)	4039.84		3.60	9.91 (−22)
11	4103.54	−0.86		4.86	6.84 (−20)	3995.78	−0.06		4.72	5.92 (−20)	4056.96		2.89	5.87 (−22)
	4105.28			4.80	6.45 (−20)	3994.41	−0.05		4.77	5.71 (−20)	4038.13		3.40	6.58 (−22)
12	4107.60	−0.90		4.88	5.67 (−20)	3991.18			4.73	4.92 (−20)	4058.33		2.62	3.73 (−22)
	4109.44			4.81	5.30 (−20)	3989.72			4.76	4.70 (−20)	4036.30		3.18	4.27 (−22)

TABLE BVIII: continued

13	4111.54			4.90	4.57 (−20)	3986.64			4.73	3.97 (−20)	4059.79		2.34	2.29 (−22)
	4113.49			4.81	4.23 (−20)	3985.13			4.79	3.78 (−20)	4034.40		2.96	2.71 (−22)
14	4115.37			4.91	3.59 (−20)	3982.23			4.75	3.13 (−20)	4061.32		2.05	1.37 (−22)
	4117.43			4.83	3.29 (−20)	3980.65			4.79	2.95 (−20)	4032.41		2.72	1.68 (−22)
15	4119.11			4.93	2.76 (−20)	3977.92			4.75	2.40 (−20)	4062.95		1.78	7.94 (−23)
	4121.27			4.81	2.48 (−20)	3976.30			4.79	2.24 (−20)	4030.35		2.48	1.01 (−22)
16	4122.73			4.95	2.07 (−20)	3973.74			4.76	1.80 (−20)	4064.64		1.49	4.40 (−23)
	4124.97			4.85	1.85 (−20)	3972.10			4.81	1.67 (−20)	4028.26		2.23	5.97 (−23)
17	4126.23			4.96	1.51 (−20)	3969.70			4.77	1.32 (−20)	4066.42		1.24	2.38 (−23)
	4128.55			4.86	1.34 (−20)	3968.06			4.79	1.20 (−20)	4026.13		1.99	3.42 (−23)
18	4129.63			4.98	1.09 (−20)	3965.83			4.78	9.48 (−21)	4068.25		1.00	1.22 (−23)
	4132.01			4.87	9.54 (−21)	3964.19			4.82	8.59 (−21)	4024.01		1.74	1.90 (−23)
19	4132.90			5.00	7.64 (−21)	3962.15			4.78	6.65 (−21)	4070.14		0.77	5.97 (−24)
	4135.34			4.87	6.64 (−21)	3960.53			4.83	5.98 (−21)	4021.91		1.50	1.02 (−23)
20	4136.05			5.01	5.27 (−21)	3958.67			4.79	4.60 (−21)	4072.10		0.56	2.72 (−24)
	4138.53			4.88	4.53 (−21)	3957.11			4.83	4.08 (−21)	4019.86		1.26	5.28 (−24)
21	4139.08			5.02	3.57 (−21)	3955.43			4.80	3.11 (−21)	4074.11		0.38	1.14 (−24)
	4141.60			4.88	3.03 (−21)	3953.94			4.83	2.74 (−21)	4017.89		1.03	2.63 (−24)
22	4141.98			5.02	2.38 (−21)	3952.46			4.80	2.07 (−21)	4076.17		0.24	4.25 (−25)
	4144.53			4.88	2.00 (−21)	3951.06			4.83	1.80 (−21)	4016.03		0.81	1.25 (−24)
						$k=2$ $p{=}1\,/p{=}{-1}^{d}$								
2	4052.28	−0.51	5.16	4.69	5.32 (−21)						4037.65	−0.38	4.60	1.04 (−20)
	4052.28	−0.51	5.15	4.69	5.32 (−21)						4037.65		4.60	1.04 (−20)
3	4057.06	−0.54	5.60	4.71	8.96 (−21)	4022.95	−0.29	4.59	4.67	4.90 (−21)	4037.58		4.52	6.66 (−21)
	4057.06	−0.54	5.60	4.71	8.96 (−21)	4022.95	−0.29	4.59	4.67	4.90 (−21)	4037.58		4.52	6.66 (−21)
4	4061.79	−0.59	6.13	4.72	1.14 (−20)	4018.02	−0.23	4.84	4.67	8.00 (−21)	4037.50		4.42	4.57 (−21)
	4061.79	−0.60	6.12	4.72	1.14 (−20)	4018.02	−0.23	4.84	4.67	8.00 (−21)	4037.50		4.42	4.57 (−21)
5	4066.46	−0.64		4.72	1.29 (−20)	4013.10	−0.25	5.11	4.68	9.96 (−21)	4037.39		4.29	3.21 (−21)
	4066.46	−0.65		4.73	1.30 (−20)	4013.10	−0.25	5.11	4.68	9.96 (−21)	4037.39		4.29	3.21 (−21)
6	4071.07	−0.71		4.74	1.36 (−20)	4008.20			4.68	1.10 (−20)	4037.26		4.14	2.27 (−21)
	4071.07	−0.72		4.73	1.36 (−20)	4008.19			4.68	1.10 (−20)	4037.27		4.13	2.26 (−21)
7	4075.62			4.75	1.35 (−20)	4003.32			4.67	1.12 (−20)	4037.12		3.96	1.59 (−21)
	4075.61			4.75	1.35 (−20)	4003.32			4.69	1.12 (−20)	4037.13		3.96	1.59 (−21)
8	4080.09			4.76	1.28 (−20)	3998.48			4.69	1.08 (−20)	4036.96		3.77	1.11 (−21)
	4080.07			4.76	1.28 (−20)	3998.47			4.68	1.08 (−20)	4036.97		3.77	1.11 (−21)
9	4084.48			4.78	1.17 (−20)	3993.69			4.69	1.00 (−20)	4036.79		3.56	7.57 (−22)
	4084.45			4.78	1.17 (−20)	3993.68			4.69	1.00 (−20)	4036.80		3.55	7.56 (−22)
10	4088.79			4.80	1.03 (−20)	3988.96			4.70	8.91 (−21)	4036.61		3.33	5.07 (−22)
	4088.75			4.80	1.03 (−20)	3988.94			4.70	8.90 (−21)	4036.62		3.32	5.07 (−22)
11	4093.01			4.81	8.82 (−21)	3984.30			4.71	7.66 (−21)	4036.43		3.08	3.32 (−22)
	4092.96			4.81	8.81 (−21)	3984.26			4.71	7.65 (−21)	4036.44		3.08	3.32 (−22)
12	4097.15			4.83	7.30 (−21)	3979.72			4.72	6.38 (−21)	4036.25		2.82	2.12 (−22)
	4097.07			4.83	7.31 (−21)	3979.67			4.72	6.38 (−21)	4036.25		2.82	2.12 (−22)
13	4101.17			4.85	5.90 (−21)	3975.24			4.73	5.17 (−21)	4036.07		2.55	1.32 (−22)
	4101.08			4.85	5.90 (−21)	3975.17			4.73	5.16 (−21)	4036.06		2.54	1.32 (−22)
14	4105.10			4.87	4.64 (−21)	3970.88			4.74	4.07 (−21)	4035.91		2.28	8.00 (−23)
	4105.00			4.86	4.63 (−21)	3970.76			4.74	4.07 (−21)	4035.86		2.27	7.99 (−23)
15	4108.92			4.89	3.56 (−21)	3966.64			4.76	3.13 (−21)	4035.78		2.00	4.68 (−23)
	4108.80			4.86	3.54 (−21)	3966.48			4.75	3.12 (−21)	4035.67		1.99	4.66 (−23)
16	4112.64			4.91	2.67 (−21)	3962.54			4.78	2.35 (−21)	4035.66		1.71	2.64 (−23)
	4112.48			4.90	2.66 (−21)	3962.34			4.76	2.34 (−21)	4035.49		1.71	2.63 (−23)
17	4116.24			4.93	1.95 (−21)	3958.61			4.79	1.72 (−21)	4035.60		1.44	1.44 (−23)
	4116.05			4.92	1.95 (−21)	3958.34			4.76	1.71 (−21)	4035.31		1.43	1.43 (−23)
18	4119.73			4.95	1.40 (−21)	3954.86			4.80	1.24 (−21)	4035.60		1.17	7.49 (−24)
	4119.49			4.94	1.40 (−21)	3954.51			4.79	1.23 (−21)	4035.14		1.16	7.41 (−24)
19	4123.10			4.97	9.86 (−22)	3951.33			4.81	8.69 (−22)	4035.68		0.92	3.69 (−24)
	4122.82			4.95	9.80 (−22)	3950.86			4.80	8.64 (−22)	4034.99		0.91	3.65 (−24)
20	4126.36			4.99	6.80 (−22)	3948.05			4.83	6.00 (−22)	4035.88		0.68	1.69 (−24)
	4126.01			4.97	6.75 (−22)	3947.43			4.81	5.96 (−22)	4034.85		0.67	1.68 (−24)

TABLE BVIII: continued

					$k=3$ $p{=}1/p{=}{-1}$[c]						
3	4039.03	−0.69	4.69	3.56 (−21)				4019.75	−0.46	4.50	1.02 (−20)
	4039.03	−0.69	4.69	3.56 (−21)				4019.75		4.50	1.02 (−20)
4	4043.73	−0.71	4.70	5.95 (−21)	4000.39	4.65	3.18 (−21)	4019.68		4.40	7.01 (−21)
	4043.73	−0.72	4.70	5.95 (−21)	4000.39	4.65	3.18 (−21)	4019.68		4.40	7.01 (−21)
5	4048.38		4.71	7.46 (−21)	3995.55	4.65	5.17 (−21)	4019.59		4.28	4.94 (−21)
	4048.39		4.70	7.45 (−21)	3995.54	4.65	5.17 (−21)	4019.60		4.28	4.94 (−21)
6	4052.97	−0.83	4.73	8.29 (−21)	3990.72	4.66	6.32 (−21)	4019.51		4.12	3.48 (−21)
	4052.98	−0.83	4.73	8.29 (−21)	3990.72	4.66	6.32 (−21)	4019.50		4.12	3.49 (−21)
7	4057.50		4.74	8.50 (−21)	3985.93	4.65	6.81 (−21)	4019.40		3.96	2.47 (−21)
	4057.51		4.75	8.51 (−21)	3985.93	4.65	6.80 (−21)	4019.39		3.96	2.47 (−21)
8	4061.97		4.75	8.24 (−21)	3981.17	4.67	6.82 (−21)	4019.28		3.77	1.72 (−21)
	4061.97		4.76	8.25 (−21)	3981.17	4.67	6.82 (−21)	4019.28		3.77	1.72 (−21)
9	4066.35		4.78	7.66 (−21)	3976.47	4.68	6.44 (−21)	4019.16		3.56	1.18 (−21)
	4066.36		4.78	7.67 (−21)	3976.47	4.68	6.45 (−21)	4019.15		3.56	1.18 (−21)
10	4070.66		4.80	6.85 (−21)	3971.83	4.68	5.82 (−21)	4019.04		3.34	7.93 (−22)
	4070.66		4.80	6.85 (−21)	3971.82	4.69	5.83 (−21)	4019.02		3.34	7.93 (−22)
11	4074.89		4.83	5.92 (−21)	3967.27	4.69	5.08 (−21)	4018.92		3.10	5.23 (−22)
	4074.89		4.82	5.92 (−21)	3967.25	4.70	5.08 (−21)	4018.88		3.10	5.23 (−22)
12	4079.03		4.76	4.87 (−21)	3962.78	4.71	4.28 (−21)	4018.81		2.85	3.36 (−22)
	4079.02		4.85	4.96 (−21)	3962.77	4.71	4.28 (−21)	4018.74		2.85	3.37 (−22)
13	4083.08		4.87	4.04 (−21)	3958.43	4.72	3.50 (−21)	4018.71		2.58	2.10 (−22)
	4083.06		4.87	4.04 (−21)	3958.37	4.73	3.50 (−21)	4018.60		2.55	2.07 (−22)
14	4087.04		4.89	3.20 (−21)	3954.18	4.65	2.73 (−21)	4018.64		2.31	1.28 (−22)
	4086.99		4.90	3.20 (−21)	3954.09	4.75	2.78 (−21)	4018.46		2.32	1.29 (−22)
15	4090.93		4.91	2.47 (−21)	3950.09	4.73	2.14 (−21)	4018.63		2.02	7.53 (−23)
	4090.82		4.92	2.47 (−21)	3949.93	4.76	2.15 (−21)	4018.32		2.05	7.63 (−23)
16	4094.77		4.90	1.85 (−21)	3946.21	4.70	1.60 (−21)	4018.72		1.72	4.24 (−23)
	4094.54		4.95	1.86 (−21)	3945.90	4.78	1.63 (−21)	4018.19		1.78	4.37 (−23)
17	4098.68		4.78	1.33 (−21)	3942.68	4.53	1.14 (−21)	4019.03		1.38	2.21 (−23)
	4098.15		4.97	1.38 (−21)	3942.02	4.80	1.20 (−21)	4018.07		1.51	2.42 (−23)
18	4103.08		4.08	8.19 (−22)	3939.95	3.76	6.84 (−22)	4020.03		0.89	9.16 (−24)
	4101.64		5.00	9.94 (−22)	3938.31	4.82	8.69 (−22)	4017.96		1.25	1.28 (−23)
19	4102.31		2.68	3.70 (−22)	3932.39	2.84	3.57 (−22)	4016.07		0.69	4.43 (−24)
	4105.00		5.02	7.03 (−22)	3934.80	4.84	6.16 (−22)	4017.84		1.00	6.49 (−24)
20	4106.18		3.66	3.52 (−22)	3929.87	3.83	3.35 (−22)	4017.03		0.68	2.74 (−24)
	4108.24		5.05	4.88 (−22)	3931.49	4.86	4.28 (−22)	4017.73		0.77	3.10 (−24)

[a]The labeling of vibration-rotation states by the set of quantum numbers $(v_r\, b\, k\; v_R\; J\, p)$ exposes similarity of Li^+–H_2 to van der Waals complexes of intermediate anisotropy strength of atom-diatom interaction. In the labeling referring to asymmetric top model, the symbols $J_{K_a\, K_c}$ and $[v_r\; v_\theta\; v_R]$ are used to denote rotation and vibration state, respectively. The relation between the two labels is: $v_\theta{=}b{-}k$, $K_a{=}k$, and $K_c{=}J{-}k+\frac{1-(-1)^k p}{2}$.

[b]$S_{\rm vib}{=}S/S_{\rm rot}$ where $S_{\rm rot}$ is the Hönl-London factor for $\Delta k{=}0$ symmetric top transitions[12], $S_{\rm rot}(J{\to}J';k) = J{+}1{-}\frac{k^2}{J+1}$, $J{-}\frac{k^2}{J}$, and $k^2\frac{2J+1}{J^2+J}$ for $J'{=}J{+}1$, $J{-}1$, and J , respectively.

[c]The entries in the lower lines concern $(J\,p){\to}(J{\pm}1\,p)$, $(J\,{-p})$ transitions from the initial $p{=}{-1}$ parity state.

[d]Underlined, here as well in Tables BIX–BXI and CXIII–CXVI (in Part C of the Material), is the largest line intensity in the band shown.

TABLE BIX: Near-infrared absorption spectrum of Li^{+}–H_2. Line positions (ν, in cm^{-1}), vibrational factors of line strengths ($S_{vib}{}^{a}$, in 10^{-3} D^2), and line intensities (I, in 10^{-21} cm/molecule) at T=296 K in two hot bands overlapping with fundamental v_r=0→1 band.

K_a=0–0 of $[v_r\, v_\theta\, v_R]$=[0 1 0] → [1 1 0], $(b\,k)$=(1 0) → (1 0)

	$R(J)$			$P(J)$			$Q(J)$		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0	4068.81	7.36	3.03						
1	4073.37	7.36	5.93	4059.53	7.37	2.95			
2	4077.88	7.36	8.51	4054.85	7.37	5.64			
3	4082.31	7.36	10.61	4050.13	7.38	7.91			
4	4086.68	7.36	12.13	4045.40	7.38	9.64			
5	4090.97	7.36	13.03	4040.66	7.39	10.76			
6	4095.18	7.37	13.31	4035.93	7.39	11.28			
7	4099.29	7.37	13.03	4031.20	7.40	11.25			
8	4103.31	7.38	12.30	4026.51	7.41	10.77			
9	4107.23	7.40	11.24	4021.85	7.41	9.93			
10	4111.04	7.39	9.93	4017.24	7.42	8.86			
11	4114.75	7.41	8.54	4012.69	7.45	7.68			
12	4118.34	7.41	7.15	4008.21	7.44	6.45			
13	4121.82	7.41	5.83	4003.83	7.45	5.29			
14	4125.16	7.40	4.63	3999.54	7.44	4.22			
15	4128.36	7.38	3.59	3995.36	7.41	3.27			
16	4131.37	7.29	2.70	3991.26	7.32	2.46			
17	4134.09	7.00	1.93	3987.15	6.98	1.76			
18	4136.08	5.78	1.16	3982.63	5.65	1.04			
19	4143.02	4.24	0.63	3983.39	4.60	0.62			
20	4145.08	5.64	0.59	3979.62	6.07	0.58			

K_a=0–0 of [0 0 1] → [1 0 1], $(b\,k)$=(0 0) → (0 0)

	$R(J)$			$P(J)$			$Q(J)$		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0	4063.01	4.66	1.60						
1	4067.51	4.66	3.13	4053.97	4.65	1.56			
2	4071.99	4.66	4.51	4049.45	4.65	2.98			
3	4076.45	4.67	5.64	4044.94	4.65	4.18			
4	4080.86	4.67	6.47	4040.45	4.65	5.10			
5	4085.23	4.67	6.97	4035.99	4.64	5.70			
6	4089.55	4.68	7.15	4031.57	4.64	6.00			
7	4093.82	4.68	7.03	4027.20	4.64	6.00			
8	4098.03	4.68	6.67	4022.90	4.64	5.76			
9	4102.16	4.68	6.12	4018.66	4.63	5.34			
10	4106.23	4.68	5.44	4014.52	4.63	4.78			
11	4110.22	4.68	4.71	4010.48	4.62	4.16			
12	4114.13	4.68	3.97	4006.55	4.62	3.52			
13	4117.95	4.68	3.26	4002.76	4.61	2.90			
14	4121.69	4.67	2.62	3999.12	4.60	2.33			
15	4125.33	4.66	2.05	3995.65	4.59	1.83			
16	4128.89	4.65	1.58	3992.37	4.57	1.41			
17	4132.34	4.63	1.19	3989.31	4.55	1.06			
18	4135.71	4.61	0.88	3986.49	4.53	0.79			
19	4138.96	4.59	0.64	3983.94	4.49	0.57			
20	4142.12	4.55	0.45	3981.71	4.45	0.41			

K_a=1–1, $(b\,k)$=(2 1) → (2 1)

	$R(J^e)$ / $R(J^f)$			P			Q		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
1	4063.80	7.04	0.90				4055.09	7.02	0.89
	4064.28	7.04	0.90				4054.57	7.03	0.89
2	4068.21	7.05	1.53	4045.82	7.03	0.86	4055.54	6.99	0.47
	4068.90	7.04	1.53	4045.29	7.04	0.85	4053.99	7.00	0.47
3	4072.56	7.06	2.02	4041.29	7.02	1.42	4056.20	6.94	0.31
	4073.44	7.04	2.00	4040.45	7.04	1.41	4053.12	6.98	0.31
4	4076.86	7.06	2.38	4036.75	7.03	1.83	4057.07	6.87	0.22
	4077.91	7.04	2.34	4035.59	7.04	1.81	4051.96	6.93	0.21
5	4081.10	7.08	2.60	4032.20	7.03	2.10	4058.15	6.79	0.16
	4082.29	7.04	2.54	4030.73	7.04	2.06	4050.52	6.87	0.15
6	4085.26	7.09	2.69	4027.67	7.02	2.24	4059.43	6.70	0.11
	4086.58	7.05	2.60	4025.86	7.05	2.18	4048.81	6.81	0.11
7	4089.36	7.10	2.66	4023.15	7.04	2.26	4060.92	6.58	0.08
	4090.79	7.05	2.55	4021.01	7.05	2.19	4046.84	6.73	0.08
8	4093.37	7.12	2.54	4018.66	7.05	2.19	4062.61	6.45	0.06
	4094.89	7.05	2.40	4016.18	7.06	2.09	4044.62	6.63	0.06
9	4097.32	7.13	2.34	4014.21	7.05	2.03	4064.49	6.30	0.04
	4098.90	7.03	2.18	4011.39	7.06	1.92	4042.15	6.51	0.04
10	4101.16	7.14	2.09	4009.82	7.06	1.83	4066.57	6.12	0.03
	4102.65	6.05	1.65	4006.65	7.06	1.71	4039.48	6.38	0.03
11	4104.92	7.15	1.81	4005.51	7.06	1.60	4068.68	5.09	0.02
	4106.54	7.05	1.64	4001.98	7.06	1.47	4036.58	6.24	0.02
12	4108.59	7.16	1.53	4001.27	7.07	1.35	4071.23	5.73	0.01
	4110.20	7.06	1.37	3997.24	6.07	1.06	4033.49	6.09	0.01

K_a=1–1, $(b\,k)$=(1 1) → (1 1)

	R			P			Q		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
1	4063.00	4.60	5.06				4054.26	4.56	5.00
	4063.28	4.60	5.05				4053.99	4.58	5.01
2	4067.39	4.61	8.64	4045.24	4.59	4.81	4054.53	4.50	2.62
	4067.82	4.60	8.60	4044.97	4.59	4.80	4053.70	4.52	2.63
3	4071.77	4.62	11.42	4040.81	4.58	7.99	4054.93	4.41	1.68
	4072.34	4.60	11.33	4040.40	4.60	7.98	4053.26	4.46	1.70
4	4076.11	4.63	13.45	4036.39	4.58	10.29	4055.46	4.28	1.16
	4076.82	4.60	13.28	4035.86	4.59	10.26	4052.70	4.37	1.17
5	4080.41	4.63	14.72	4032.00	4.57	11.81	4056.12	4.13	0.81
	4081.25	4.60	14.47	4031.35	4.59	11.74	4051.99	4.26	0.83
6	4084.65	4.64	15.26	4027.65	4.57	12.60	4056.91	3.95	0.58
	4085.64	4.60	14.92	4026.88	4.59	12.49	4051.16	4.12	0.59
7	4088.85	4.65	15.13	4023.34	4.57	12.74	4057.82	3.74	0.41
	4089.97	4.60	14.71	4022.46	4.59	12.57	4050.21	3.97	0.42
8	4092.99	4.65	14.45	4019.09	4.57	12.33	4058.85	3.52	0.28
	4094.23	4.60	13.96	4018.12	4.59	12.11	4049.15	3.80	0.30
9	4097.06	4.66	13.34	4014.92	4.56	11.49	4060.00	3.28	0.19
	4098.39	4.31	11.98	4013.85	4.59	11.22	4047.99	3.61	0.21
10	4101.07	4.67	11.95	4010.82	4.56	10.35	4061.22	2.83	0.12
	4102.56	4.59	11.36	4009.67	4.58	10.05	4046.74	3.41	0.14
11	4105.00	4.67	10.40	4006.82	4.55	9.05	4062.64	2.75	0.08
	4106.61	4.59	9.82	4005.56	4.29	8.18	4045.41	3.19	0.09
12	4108.86	4.67	8.82	4002.93	4.55	7.71	4064.13	2.47	0.05
	4110.57	4.59	8.25	4001.66	4.57	7.37	4044.02	2.96	0.06

13	4112.18	7.15	1.25	3997.16	7.06	1.12	4073.88	5.47	0.01	4112.64	4.68	7.29	3999.17	4.54	6.39	4065.73	2.19	0.03
	4113.75	7.06	1.11	3992.85	7.08	1.00	4030.21	5.91	0.01	4114.45	4.59	6.76	3997.85	4.56	6.07	4042.58	2.72	0.04
14	4115.76	7.12	1.00	3993.24	6.98	0.89	4076.77	5.05	0.01	4116.33	4.68	5.89	3995.55	4.54	5.17	4067.41	1.91	0.02
	4117.17	7.06	0.88	3988.47	7.09	0.80	4026.77	5.71	0.01	4118.23	4.58	5.41	3994.20	4.56	4.87	4041.12	2.48	0.02
15	4119.54	6.66	0.74	3989.85	6.33	0.64	4080.25	3.86	0.00	4119.94	4.67	4.65	3992.09	4.53	4.09	4069.216	1.64	0.01
	4120.47	7.06	0.68	3984.22	7.09	0.62	4023.18	5.50	0.00	4121.93	4.57	4.23	3990.74	4.54	3.82	4039.655	2.23	0.01
16	4120.11	4.05	0.34	3983.72	5.20	0.40	4081.01	5.09	0.00	4123.46	4.67	3.59	3988.82	4.52	3.16	4071.10	1.37	0.00
	4123.63	7.05	0.51	3980.11	7.09	0.47	4019.41	5.20	0.00	4125.52	4.55	3.24	3987.47	4.53	2.93	4038.21	1.97	0.00
17	4126.41	5.65	0.36	3980.73	6.46	0.37	4084.95	5.28	0.00	4126.89	4.66	2.72	3985.77	4.50	2.40	4073.08	1.12	0.00
	4126.67	7.05	0.38	3976.19	7.09	0.35	4015.29	4.49	0.00	4129.03	4.47	2.39	3984.44	4.51	2.20	4036.81	1.72	0.00
18	4128.44	7.04	0.33	3977.09	6.16	0.26	4088.47	5.05	0.00	4130.24	4.65	2.02	3982.94	4.48	1.78	4075.16	0.87	0.00
	4129.58	7.03	0.27	3972.47	7.08	0.25	4013.92	4.26	0.00	4132.43	4.51	1.79	3981.67	4.48	1.62	4035.48	1.47	0.00
19	4131.19	7.15	0.24	3976.36	5.14	0.16	4092.02	4.81	0.00	4133.49	4.63	1.48	3980.40	4.46	1.30	4077.34	0.66	0.00
	4132.36	7.02	0.19	3968.98	7.07	0.18	4008.95	5.13	0.00	4135.73	4.48	1.29	3979.19	4.39	1.15	4034.27	1.23	0.00
20	4133.92	7.18	0.18	3972.27	6.92	0.15	4095.68	4.59	0.00	4136.65	4.61	1.06	3978.16	4.43	0.93	4079.62	0.47	0.00
	4135.01	6.99	0.14	3965.76	7.05	0.13	4004.93	4.98	0.00	4138.93	4.45	0.92	3977.06	4.42	0.83	4033.21	1.00	0.00
	K_a=2−2									K_a=2−2								
	$(b\,k)$=(3 2) → (3 2)									$(b\,k)$=(2 2) → (2 2)								
2	4050.03	6.74	0.83				4036.44	6.61	1.62	4055.97	4.55	0.70				4042.57	4.44	1.37
	4050.03	6.74	0.83				4036.43	6.62	1.62	4055.97	4.55	0.70				4042.57	4.44	1.37
3	4054.44	6.72	1.39	4022.76	6.69	0.77	4036.36	6.45	1.04	4060.40	4.67	1.22	4029.16	4.53	0.65	4042.56	4.35	0.88
	4054.42	6.74	1.40	4022.72	6.73	0.77	4036.31	6.50	1.04	4060.40	4.56	1.19	4029.16	4.53	0.65	4042.56	4.35	0.88
4	4058.84	6.59	1.75	4018.23	6.52	1.23	4036.34	6.10	0.69	4064.79	4.57	1.53	4024.72	4.53	1.07	4042.56	4.22	0.60
	4058.74	6.74	1.79	4018.07	6.73	1.27	4036.15	6.34	0.72	4064.80	4.57	1.53	4024.72	4.53	1.07	4042.55	4.32	0.62
5	4063.44	5.84	1.77	4013.98	5.65	1.33	4036.57	5.02	0.42	4069.15	4.58	1.75	4020.32	4.64	1.38	4042.57	4.07	0.42
	4062.98	6.73	2.04	4013.42	6.73	1.58	4035.92	6.13	0.51	4069.15	4.57	1.75	4020.31	4.53	1.34	4042.54	4.07	0.42
6	4065.50	3.14	1.00	4007.30	3.44	0.89	4034.36	3.30	0.20	4073.47	4.59	1.86	4015.97	4.53	1.50	4042.58	3.89	0.30
	4067.14	6.73	2.15	4008.77	6.72	1.76	4035.63	5.90	0.36	4073.47	4.58	1.86	4015.94	4.53	1.50	4042.53	3.90	0.30
7	4069.81	4.64	1.48	4003.01	4.98	1.34	4034.52	4.49	0.20	4077.73	4.59	1.87	4011.67	4.53	1.55	4042.61	3.69	0.21
	4071.20	6.72	2.15	4004.12	6.72	1.81	4035.26	5.61	0.25	4077.73	4.59	1.87	4011.63	4.53	1.55	4042.51	3.70	0.21
8	4073.68	5.12	1.57	3998.45	5.51	1.45	4034.39	4.71	0.16	4081.94	4.61	1.80	4007.44	4.53	1.53	4042.65	3.46	0.15
	4075.16	6.70	2.06	3999.49	6.71	1.77	4034.78	5.29	0.18	4081.93	4.59	1.80	4007.37	4.53	1.53	4042.49	3.48	0.15
9	4077.25	5.18	1.46	3993.80	5.67	1.40	4034.17	4.60	0.11	4086.09	4.62	1.68	4003.29	4.53	1.44	4042.72	3.22	0.10
	4078.99	6.67	1.89	3994.87	6.70	1.66	4034.16	4.91	0.12	4086.07	4.60	1.67	4003.19	4.53	1.44	4042.47	3.24	0.10
10	4080.52	5.02	1.27	3989.11	5.68	1.26	4033.93	4.35	0.08	4090.20	4.63	1.51	3999.23	4.54	1.31	4042.82	2.96	0.07
	4082.69	6.62	1.68	3990.29	6.68	1.49	4033.37	4.47	0.08	4090.14	4.60	1.50	3999.09	4.53	1.30	4042.45	2.98	0.07
11	4083.37	4.60	1.01	3984.38	5.57	1.08	4033.70	4.01	0.05	4094.19	4.64	1.32	3995.28	4.54	1.15	4042.97	2.69	0.05
	4086.23	6.56	1.44	3985.74	6.65	1.30	4032.32	3.97	0.05	4094.13	4.60	1.31	3995.09	4.53	1.14	4042.46	2.72	0.05
12	4085.61	3.86	0.71	3979.59	5.33	0.88	4033.50	3.63	0.03	4098.13	4.65	1.12	3991.49	4.55	0.98	4043.15	2.40	0.03
	4089.60	6.47	1.20	3981.24	6.61	1.09	4030.91	3.38	0.03	4098.06	4.62	1.11	3991.20	4.53	0.98	4042.42	2.44	0.03
13	4086.89	2.74	0.42	3974.64	4.89	0.67	4033.33	3.21	0.02	4101.99	4.65	0.93	3987.79	4.54	0.82	4043.43	2.13	0.02
	4092.78	6.35	0.96	3976.79	6.55	0.89	4028.90	2.65	0.02	4101.90	4.61	0.92	3987.44	4.52	0.81	4042.41	2.16	0.02
14	4100.25	4.32	0.53	3969.35	4.14	0.46	4033.23	2.76	0.01	4105.79	4.67	0.75	3984.29	4.54	0.66	4043.77	1.83	0.01
	4095.74	6.20	0.75	3972.41	6.47	0.71	4025.96	1.79	0.01	4105.65	4.61	0.74	3983.84	4.53	0.66	4042.41	1.88	0.01
15	4101.77	5.00	0.48	3963.41	3.01	0.26	4033.19	2.30	0.01	4109.52	4.67	0.60	3981.01	4.53	0.52	4044.25	1.54	0.01
	4098.47	6.02	0.57	3968.11	6.37	0.55	4035.13	1.32	0.00	4109.31	4.61	0.58	3980.39	4.51	0.52	4042.41	1.60	0.01
16	4103.70	5.31	0.39	3969.89	4.18	0.28	4033.22	1.84	0.00	4113.22	4.67	0.46	3978.00	4.51	0.41	4044.91	1.26	0.00
	4100.96	5.83	0.43	3963.93	6.24	0.41	4032.52	1.42	0.00	4112.88	4.60	0.45	3977.13	4.50	0.40	4042.41	1.33	0.00
17	4105.86	5.44	0.30	3964.94	4.88	0.25	4033.38	1.41	0.00	4116.97	4.63	0.35	3975.43	4.43	0.30	4045.90	0.97	0.00
	4103.25	5.64	0.31	3959.94	6.08	0.30	4030.42	1.32	0.00	4116.36	4.60	0.34	3974.09	4.49	0.30	4042.40	1.06	0.00
18	4107.81	5.25	0.22	3960.63	5.21	0.20	4033.46	1.03	0.00	4121.11	4.47	0.25	3973.68	4.15	0.21	4047.64	0.65	0.00
	4105.26	5.24	0.21	3956.08	5.75	0.21	4028.56	1.03	0.00	4119.73	4.58	0.25	3971.28	4.47	0.23	4042.35	0.82	0.00

TABLE BX: Near-infrared absorption spectrum of Li^+–H_2. Line positions (ν, in cm^{-1}), vibrational factors of line strengths (S_{vib}), and line intensities (I) at T=296 K in four vibrational bands non-overlapping with fundamental v_r=0→1 band.

A. Combination v_r=0→1 v_θ=0→1 band ($S_{vib}{}^a$ in 10^{-4} D^2, I in 10^{-22} cm/molecule).

	$[v_r\, v_\theta\, v_R]$=[0 0 0] → [1 1 0]																	
	K_a=1−0									K_a=0−1								
	$(b\,k)$=(1 1) → (1 0)									$(b\,k)$=(0 0) → (2 1)								
	$R(J^e)$			$P(J^e)$			$Q(J^f)$			$R(J^e)$			$P(J^e)$			$Q(J^e)$		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0										4746.92	3.25	9.33						
1	4604.42	3.24	9.75	4590.58	3.40	20.37	4595.05	3.34	30.06	4750.93	3.29	13.84				4742.22	3.20	13.46
2	4608.50	3.19	18.33	4585.47	3.45	29.58	4594.24	3.34	47.63	4754.45	3.33	17.85	4732.06	3.12	4.15	4741.78	3.19	21.33
3	4612.30	3.14	25.24	4580.11	3.51	37.29	4593.03	3.33	61.82	4757.47	3.38	21.04	4726.19	3.07	7.61	4741.10	3.19	27.70
4	4615.80	3.09	30.16	4574.52	3.57	43.06	4591.41	3.32	71.84	4759.98	3.41	23.20	4719.87	3.03	10.22	4740.19	3.17	32.21
5	4619.01	3.05	33.02	4568.70	3.62	46.61	4589.38	3.30	77.35	4762.00	3.46	24.38	4713.11	2.99	11.90	4739.05	3.16	34.76
6	4621.91	3.00	33.92	4562.65	3.68	47.90	4586.96	3.28	78.62	4763.51	3.51	24.46	4705.91	2.94	12.66	4737.68	3.14	35.38
7	4624.47	2.95	33.09	4556.39	3.74	47.16	4584.13	3.26	76.16	4764.51	3.55	23.59	4698.30	2.90	12.68	4736.08	3.12	34.32
8	4626.71	2.91	30.92	4549.90	3.80	44.67	4580.90	3.24	70.69	4765.00	3.59	21.94	4690.29	2.86	12.03	4734.24	3.09	31.91
9	4628.59	2.87	27.84	4543.21	3.86	40.84	4577.27	3.22	63.23	4764.99	3.63	19.75	4681.89	2.81	10.92	4732.16	3.06	28.58
10	4630.11	2.82	24.13	4536.30	3.92	36.18	4573.24	3.20	54.72	4764.45	3.68	17.24	4673.11	2.76	9.53	4729.86	3.03	24.68
11	4631.25	2.77	20.28	4529.19	3.98	31.13	4568.82	3.17	45.73	4763.40	3.72	14.62	4663.99	2.71	8.03	4727.16	2.57	17.75
12	4632.00	2.72	16.52	4521.87	4.04	25.96	4564.01	3.14	37.15	4761.83	3.76	12.05	4654.51	2.66	6.55	4724.47	2.97	16.84
13	4632.34	2.66	13.06	4514.35	4.10	21.10	4558.80	3.11	29.32	4759.72	3.79	9.65	4644.70	2.60	5.18	4721.42	2.93	13.33
14	4632.25	2.60	10.03	4506.63	4.15	16.69	4553.20	3.08	22.52	4757.08	3.83	7.56	4634.58	2.54	3.97	4718.12	2.89	10.26
15	4631.72	2.54	7.50	4498.72	4.20	12.88	4547.22	3.04	16.86	4753.85	3.87	5.76	4624.15	2.47	2.95	4714.56	2.85	7.70
16	4630.72	2.46	5.45	4490.61	4.25	9.70	4540.86	3.01	12.34	4749.83	3.76	4.14	4613.44	2.22	1.98	4710.73	2.81	5.63
17	4629.25	2.38	3.85	4482.31	4.30	7.14	4534.13	2.97	8.81	4748.09	2.29	1.82	4602.41	2.29	1.49	4706.63	2.77	4.02
18	4627.28	2.27	2.64	4473.83	4.33	5.13	4527.03	2.93	6.16	4742.22	3.60	2.03	4590.87	2.02	0.94	4702.25	2.72	2.81
19	4624.79	2.15	1.75	4465.16	4.36	3.61	4519.56	2.90	4.22	4736.75	3.80	1.49	4581.92	1.76	0.57	4697.58	2.67	1.92
20	4621.79	1.99	1.11	4456.32	4.36	2.48	4511.75	2.86	2.83	4730.85	3.87	1.03	4569.20	2.19	0.49	4692.61	2.61	1.29

	K_a=2−1									K_a=1−2								
	$(b\,k)$=(2 2) → (2 1)									$(b\,k)$=(1 1) → (3 2)								
	$R(J^e)$ /$R(J^f)$			$P(J^e)$/$P(J^f)$			$Q(J^e)$/$Q(J^f)$			$R(J^e)$ /$R(J^f)$			$P(J^e)$/$P(J^f)$			$Q(J^e)$/$Q(J^f)$		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
1										4915.13	2.99	28.76						
										4914.98	2.98	28.70						
2	4505.55	3.05	0.38	4483.16	3.67	4.14	4492.88	3.43	2.16	4919.00	3.09	31.52				4905.40	2.78	14.15
	4507.03	3.07	0.39	4483.42	3.67	4.15	4492.12	3.42	2.15	4918.56	3.07	31.29				4904.95	2.77	14.05
3	4508.70	2.91	0.77	4477.43	3.78	4.41	4492.33	3.44	3.52	4922.50	3.19	34.13	4890.83	2.50	2.37	4904.43	2.77	22.95
	4511.16	2.95	0.78	4478.18	3.80	4.43	4490.85	3.42	3.50	4921.63	3.16	33.63	4889.93	2.48	2.34	4903.52	2.74	22.63
4	4511.39	2.77	1.07	4471.28	3.90	4.65	4491.60	3.44	4.45	4925.63	3.29	35.90	4885.02	2.40	4.65	4903.13	2.75	28.79
	4515.08	2.83	1.09	4472.77	3.92	4.67	4489.14	3.41	4.41	4924.21	3.23	35.03	4883.54	2.37	4.55	4901.61	2.70	28.10
5	4513.63	2.64	1.25	4464.74	4.01	4.75	4490.68	3.45	5.02	4928.37	3.40	36.68	4878.90	2.31	6.34	4901.50	2.72	32.14
	4518.76	2.71	1.29	4467.20	4.04	4.79	4487.00	3.39	4.94	4926.27	3.30	35.23	4876.71	2.26	6.14	4899.21	2.65	30.89
6	4515.40	2.50	1.32	4457.80	4.11	4.69	4489.57	3.46	5.26	4930.68	3.51	36.29	4872.48	2.21	7.30	4899.54	2.69	33.28
	4522.21	2.60	1.38	4461.48	4.17	4.75	4484.43	3.39	5.16	4927.82	3.36	34.19	4869.45	2.15	6.99	4896.31	2.58	31.41
7	4516.70	2.35	1.30	4450.49	4.23	4.50	4488.26	3.46	5.22	4932.54	3.63	34.86	4865.74	2.11	7.62	4897.25	2.65	32.52
	4525.40	2.48	1.37	4455.62	4.29	4.57	4481.45	3.37	5.08	4928.85	3.41	32.03	4861.77	2.03	7.17	4892.91	2.49	29.92
8	4517.52	2.21	1.19	4442.81	4.34	4.17	4486.75	3.47	4.96	4933.91	3.76	32.54	4858.68	2.02	7.39	4894.62	2.61	30.28
	4528.32	2.37	1.28	4449.61	4.42	4.26	4478.05	3.36	4.78	4929.35	3.43	28.97	4853.68	1.91	6.81	4888.97	2.38	26.90
9	4517.87	2.06	1.04	4434.77	4.44	3.76	4485.05	3.48	4.53	4934.73	3.90	29.60	4851.27	1.92	6.77	4891.65	2.55	27.00
	4530.98	2.25	1.14	4443.47	4.55	3.85	4474.23	3.34	4.33	4929.30	3.44	25.30	4845.19	1.79	6.08	4884.48	2.23	22.83
10	4517.73	1.91	0.87	4426.39	4.55	3.29	4483.14	3.48	3.98	4934.91	4.05	26.27	4843.50	1.84	5.94	4888.33	2.48	23.11
	4533.19	1.84	0.84	4437.19	4.67	3.38	4470.02	3.32	3.78	4928.70	3.42	21.32	4836.31	1.66	5.15	4879.39	2.03	18.20

TABLE BX: A. continued

11	4517.10	1.75	0.70	4417.70	4.66	2.80	4480.86	2.99	2.91	4934.31	4.22	22.71	4835.33	1.76	5.02	4884.64	2.39	19.02
	4535.34	2.03	0.81	4430.79	4.79	2.89	4465.38	3.29	3.19	4927.53	3.37	17.31	4827.04	1.53	4.15	4873.62	1.77	13.43
12	4515.98	1.60	0.53	4408.67	4.76	2.32	4478.62	3.51	2.82	4932.69	4.34	18.90	4826.67	1.71	4.13	4880.58	2.28	15.04
	4537.06	1.93	0.65	4424.10	4.23	2.06	4460.34	3.27	2.62	4925.77	3.27	13.50	4817.40	1.39	3.19	4867.07	1.42	8.84
13	4514.35	1.44	0.39	4399.34	4.87	1.87	4476.06	3.52	2.28	4929.66	4.26	14.67	4817.41	1.67	3.33	4876.11	2.15	11.42
	4538.44	1.82	0.50	4417.54	5.06	1.95	4454.90	3.23	2.08	4923.37	3.12	10.09	4807.38	1.25	2.35	4859.50	0.97	4.80
14	4512.22	1.29	0.28	4389.72	4.98	1.48	4473.26	3.53	1.79	4938.23	0.34	0.90	4807.33	1.65	2.63	4871.20	1.99	8.30
	4539.45	1.72	0.37	4410.75	5.20	1.55	4449.05	3.20	1.61	4920.31	2.91	7.19	4796.98	1.11	1.64	4850.53	0.47	1.81
15	4509.52	1.13	0.19	4379.82	5.09	1.14	4470.22	3.55	1.37	4934.41	0.73	1.46	4796.04	1.61	1.99	4865.83	1.81	5.75
	4540.08	1.62	0.27	4403.83	5.34	1.20	4442.79	3.16	1.21	4916.54	2.63	4.86	4786.18	0.96	1.10	4853.20	1.99	5.83
16	4506.05	0.94	0.12	4369.66	5.21	0.86	4466.95	3.55	1.02	4930.40	1.02	1.51	4796.59	0.00	0.00	4859.92	1.59	3.78
	4540.31	1.52	0.19	4396.79	5.47	0.91	4436.08	3.11	0.89	4912.00	2.30	3.11	4774.97	0.81	0.69	4843.56	1.94	4.20
17	4504.88	0.49	0.05	4359.20	5.32	0.63	4463.43	3.56	0.75	4925.92	1.17	1.25	4785.01	0.02	0.01	4853.45	1.35	2.35
	4540.09	1.57	0.15	4389.62	5.61	0.67	4428.73	2.92	0.61	4906.64	1.94	1.87	4763.33	0.66	0.41	4833.81	1.75	2.74
18	4499.63	0.62	0.04	4348.28	5.21	0.44	4459.64	3.95	0.59	4920.69	1.19	0.90	4773.51	0.04	0.02	4846.34	1.11	1.38
	4539.45	1.32	0.09	4382.33	5.74	0.48	4423.79	1.89	0.28	4900.40	1.56	1.06	4751.22	0.52	0.23	4823.70	1.52	1.68
19	4494.80	0.52	0.02	4339.98	3.42	0.20	4455.63	3.57	0.37				4761.84	0.05	0.02	4838.53	0.88	0.76
	4538.30	1.22	0.06	4374.91	6.49	0.38	4414.89	2.79	0.29				4738.63	0.39	0.12	4812.98	1.26	0.97
20	4489.60	0.40	0.01	4327.95	5.33	0.21	4451.36	3.57	0.26				4749.74	0.04	0.01	3456.23	1.46	0.69
	4536.63	1.12	0.04	4367.39	5.99	0.24	4406.55	2.85	0.20				4725.50	0.28	0.06	3437.52	1.76	0.75
	K_a=3−2 (b k)=(3 3) → (3 2)									K_a=2−3 (b k)=(2 2) → (4 3)								
2										5084.50	2.63	5.62						
										5084.50	2.63	5.62						
3	4433.11	2.62	0.16	4401.44	3.92	4.63	4415.04	3.30	1.37	5087.72	2.75	5.75				5069.81	2.25	1.56
	4433.14	2.62	0.16	4401.44	3.92	4.64	4415.03	3.30	1.37	5087.72	2.75	5.75				5069.80	2.25	1.56
4	4436.29	2.45	0.32	4395.68	4.12	4.65	4413.79	3.27	2.23	5090.49	2.86	5.79	5050.24	1.78	0.16	5068.15	2.24	2.55
	4436.36	2.46	0.32	4395.69	4.12	4.65	4413.76	3.27	2.23	5090.49	2.87	5.83	5050.24	1.78	0.16	5068.15	2.24	2.54
5	4439.09	2.30	0.44	4389.63	4.33	4.63	4412.22	3.24	2.74	5092.80	2.97	5.74	5043.75	1.66	0.32	5066.09	2.23	3.13
	4439.22	2.30	0.44	4389.65	4.33	4.63	4412.16	3.24	2.73	5092.81	2.99	5.78	5043.76	1.66	0.32	5066.09	2.21	3.11
6	4441.48	2.14	0.51	4383.28	4.53	4.51	4410.34	3.20	2.98	5094.66	3.09	5.55	5036.89	1.53	0.42	5063.61	2.21	3.41
	4441.72	2.15	0.52	4383.34	4.54	4.52	4410.21	3.20	2.97	5094.67	3.11	5.59	5036.90	1.54	0.43	5063.61	2.19	3.39
7	4443.44	1.99	0.53	4376.64	4.75	4.29	4408.14	3.15	2.99	5096.04	3.21	5.22	5029.66	1.41	0.47	5060.72	2.18	3.44
	4443.85	2.00	0.54	4376.76	4.76	4.30	4407.90	3.14	2.98	5096.06	3.23	5.26	5029.67	1.42	0.48	5060.71	2.17	3.41
8	4444.91	1.84	0.51	4369.68	4.95	3.97	4405.62	3.09	2.83	5096.92	3.32	4.78	5022.07	1.29	0.47	5057.41	2.15	3.27
	4445.59	1.86	0.51	4369.92	4.97	3.98	4405.21	3.07	2.81	5096.94	3.34	4.81	5022.08	1.30	0.47	5057.39	2.13	3.24
9	4445.86	1.69	0.46	4362.40	5.14	3.56	4402.78	3.01	2.55	5097.45	3.35	4.15	5014.12	1.17	0.43	5053.67	2.10	2.94
	4446.92	1.72	0.46	4362.81	5.18	3.59	4402.10	2.98	2.52	5097.52	3.32	4.12	5014.13	1.18	0.43	5053.63	2.08	2.91
10	4446.19	1.53	0.38	4354.78	5.31	3.10	4399.61	2.92	2.19	5097.30	3.53	3.68	5005.79	1.02	0.36	5049.68	2.05	2.54
	4447.84	1.59	0.40	4355.44	5.38	3.15	4398.52	2.87	2.15	5097.41	3.54	3.69	5005.81	1.03	0.36	5049.59	2.04	2.53
11	4445.76	1.35	0.30	4346.78	5.43	2.61	4396.09	2.80	1.81	5096.60	3.69	3.16	4997.27	1.01	0.32	5045.08	2.04	2.17
	4448.31	1.46	0.33	4347.82	5.57	2.68	4394.40	2.71	1.75	5096.84	3.66	3.13	4997.33	1.01	0.32	5044.95	2.00	2.12
12	4444.34	1.12	0.21	4338.32	5.47	2.11	4392.23	2.65	1.42	5095.27	3.77	2.58	4988.23	0.87	0.24	5040.12	1.99	1.75
	4448.31	1.34	0.26	4339.94	5.74	2.22	4389.61	2.48	1.33	5095.74	3.78	2.58	4988.32	0.88	0.24	5039.84	1.94	1.71
13	4441.55	0.82	0.13	4329.30	5.33	1.62	4388.00	2.46	1.07	5092.21	3.24	1.73	4978.84	0.77	0.18	5034.74	1.93	1.37
	4447.79	1.23	0.20	4331.80	5.87	1.78	4383.91	2.14	0.93	5094.08	3.88	2.08	4979.04	0.77	0.18	5034.18	1.79	1.27
14	4450.40	0.70	0.09	4319.50	4.87	1.14	4383.37	2.23	0.76	5092.61	3.41	1.40	4969.01	0.67	0.12	5028.90	1.84	1.03
	4446.71	1.12	0.14	4323.38	5.95	1.39	4376.93	1.65	0.56	5091.71	3.96	1.62	4969.43	0.67	0.12	5026.90	1.07	0.59
15	4446.93	0.91	0.09	4308.56	3.91	0.68	4378.35	1.94	0.51				4957.68	0.57	0.08	5022.49	1.69	0.72
	4445.01	1.02	0.10	4314.66	5.95	1.04	4381.68	0.93	0.25				4959.48	0.58	0.08	5023.18	1.87	0.80
16	4443.39	1.08	0.08	4309.57	3.11	0.40	4372.91	1.58	0.31									
	4442.64	0.93	0.07	4305.61	5.86	0.75	4374.20	1.15	0.23									

[a]For bands with Δv_θ=±1, the $S_{\rm vib}$s are obtained using the Hönl-London factors for perpendicular transitions[11,12]. Strictly, in the subbands K_a=k→k±1 with both k and k±1 greater than 0, the standard factors divided by 2 are used, see Part C, Eqs. (C16) and (C18).

TABLE BX: B. Overtone v_r=0→2 band ($S_{\rm vib}$ in 10^{-4} D^2, I in 10^{-22} cm/molecule).

	$[v_r\, v_\theta\, v_R]$=[0 0 0] → [2 0 0]														
	K_a=0−0						K_a=1−1								
	$(b\,k)$=(0 0) → (0 0)						$(b\,k)$=(1 1) → (1 1)								
	$R(J^e)$			$P(J^e)$			$R(J^e)/R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$		
J	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0	7877.36	1.05	5.00												
1	7882.22	1.05	9.75	7867.50	1.05	4.89	7874.34	1.05	16.17				7864.86	1.05	16.21
							7874.65	1.05	16.21				7864.57	1.05	16.16
2	7886.99	1.05	13.94	7862.50	1.05	9.33	7879.01	1.04	27.28	7854.99	1.06	15.52	7865.07	1.05	8.60
							7879.50	1.05	27.45	7854.68	1.05	15.42	7864.16	1.04	8.49
3	7891.69	1.04	17.29	7857.48	1.05	13.01	7883.65	1.04	35.81	7850.04	1.06	25.74	7865.38	1.05	5.61
							7884.29	1.05	35.88	7849.60	1.05	25.51	7863.54	1.03	5.46
4	7896.31	1.04	19.61	7852.41	1.06	15.79	7888.19	1.04	41.64	7845.04	1.06	32.88	7865.78	1.05	3.94
							7888.99	1.05	41.67	7844.49	1.06	32.54	7862.76	1.02	3.78
5	7900.85	1.04	20.86	7847.33	1.06	17.53	7892.65	1.04	45.00	7840.05	1.06	37.59	7866.29	1.05	2.85
							7893.63	1.05	44.72	7839.36	1.06	36.88	7861.77	1.00	2.69
6	7905.30	1.05	21.19	7842.24	1.06	18.24	7897.00	1.05	46.19	7835.04	1.07	39.74	7866.89	1.05	2.09
							7898.15	1.05	45.56	7834.23	1.06	38.76	7860.60	0.99	1.93
7	7909.65	1.04	20.35	7837.15	1.06	18.02	7901.33	1.03	44.46	7830.03	1.07	39.78	7867.58	1.05	1.54
							7902.62	1.05	44.14	7829.12	1.05	38.36	7859.23	0.97	1.39
8	7913.91	1.03	18.90	7832.08	1.07	17.14	7905.52	1.03	41.62	7825.00	1.08	38.22	7868.39	1.05	1.12
							7907.01	1.02	39.99	7824.01	1.06	36.43	7857.76	0.94	0.97
9	7918.06	1.03	16.98	7827.03	1.06	15.50	7909.62	1.03	37.55	7820.06	1.07	34.66	7869.32	1.02	0.79
							7911.21	1.04	36.90	7818.96	1.05	33.11	7856.09	0.91	0.68
10	7922.12	1.03	14.72	7822.02	1.06	13.61	7913.62	1.03	32.77	7815.11	1.07	30.70	7870.24	1.05	0.58
							7915.37	1.04	32.07	7813.97	1.03	28.26	7854.27	0.88	0.47
11	7926.06	1.03	12.41	7817.06	1.06	11.60	7917.52	1.02	27.78	7810.22	1.07	26.29	7871.32	1.05	0.41
							7919.43	1.04	27.00	7808.95	1.05	24.67	7852.33	0.85	0.32
12	7929.89	1.03	10.16	7812.18	1.06	9.56	7921.32	1.02	22.81	7805.38	1.07	21.84	7872.48	1.05	0.29
							7923.38	1.04	22.06	7804.07	1.05	20.33	7850.28	0.82	0.21
13	7933.62	0.99	7.86	7807.36	1.06	7.68	7925.04	1.01	18.23	7800.62	1.08	17.66	7873.73	1.04	0.20
							7927.23	1.04	17.53	7799.28	1.05	16.26	7848.12	0.78	0.14
14	7937.25	1.02	6.28	7802.65	1.06	6.00	7928.63	1.01	14.24	7795.95	1.07	13.86	7875.06	1.04	0.13
							7930.97	1.03	13.57	7794.59	1.05	12.65	7845.91	0.74	0.09
15	7940.76	1.01	4.75	7798.06	1.03	4.44	7932.13	1.01	10.83	7791.42	1.07	10.60	7876.49	1.03	0.09
							7934.61	1.03	10.24	7790.04	1.05	9.59	7843.60	0.71	0.06
16	7944.18	1.01	3.51	7793.61	1.06	3.39	7935.54	1.00	8.03	7786.99	1.07	7.94	7878.00	1.02	0.06
							7938.15	1.03	7.55	7785.64	1.05	7.10	7841.28	0.67	0.03
17	7947.50	1.00	2.54	7789.32	1.05	2.46	7938.85	0.99	5.78	7782.72	1.07	5.80	7879.60	1.02	0.04
							7941.59	1.02	5.43	7781.40	1.04	5.13	7838.95	0.63	0.02
18	7950.72	1.00	1.79	7785.22	1.05	1.75	7942.09	0.99	4.16	7778.65	1.06	4.14	7881.29	1.01	0.02
							7944.94	1.02	3.83	7777.37	1.04	3.63	7836.63	0.58	0.01
19	7953.87	0.99	1.24	7781.33	1.05	1.22	7945.23	0.98	2.89	7774.76	1.05	2.87	7883.07	0.99	0.01
							7948.20	1.01	2.64	7773.57	1.03	2.51	7834.38	0.55	0.01
20	7956.93	0.98	0.84	7777.70	1.04	0.83	7948.29	0.97	1.97	7771.14	1.06	1.99	7884.96	0.98	0.01
							7951.39	1.00	1.78	7770.04	1.02	1.70	7832.19	0.51	0.00
							K_a=2−2								
							$(b\,k)$=(2 2) → (2 2)								
2							7857.43	1.05	2.32				7842.85	1.05	4.62
							7857.43	1.05	2.32				7842.86	1.05	4.63
3							7862.13	1.05	3.89	7828.16	1.06	2.17	7842.73	1.05	3.00
							7862.12	1.05	3.89	7828.15	1.06	2.16	7842.73	1.05	3.00
4							7866.75	1.05	4.95	7823.17	1.06	3.55	7842.56	1.04	2.09
							7866.75	1.05	4.95	7823.17	1.06	3.55	7842.56	1.04	2.09
5							7871.31	1.05	5.58	7818.16	1.07	4.43	7842.35	1.03	1.50
							7871.30	1.05	5.57	7818.16	1.07	4.43	7842.35	1.03	1.50

TABLE BX: B. continued

6	7875.79	1.05	5.83	7813.16	1.07	4.88	7842.10	1.02	1.09
	7875.77	1.05	5.83	7813.15	1.07	4.88	7842.11	1.02	1.09
7	7880.18	1.05	5.76	7808.17	1.07	4.99	7841.82	1.01	0.79
	7880.16	1.05	5.76	7808.16	1.07	4.99	7841.84	1.01	0.79
8	7884.49	1.05	5.44	7803.19	1.07	4.82	7841.51	1.00	0.57
	7884.46	1.05	5.44	7803.18	1.07	4.82	7841.53	1.00	0.57
9	7888.72	1.04	4.94	7798.26	1.07	4.46	7841.18	0.98	0.41
	7888.67	1.05	4.95	7798.23	1.07	4.46	7841.21	0.98	0.41
10	7892.85	1.04	4.33	7793.37	1.07	3.96	7840.82	0.97	0.29
	7892.78	1.01	4.18	7793.32	1.07	3.97	7840.86	0.97	0.29
11	7896.90	1.04	3.68	7788.54	1.07	3.40	7840.46	0.91	0.19
	7896.80	1.04	3.68	7788.47	1.07	3.41	7840.50	0.95	0.20
12	7900.86	1.04	3.03	7783.79	1.07	2.83	7840.08	0.92	0.14
	7900.72	1.04	3.03	7783.70	1.04	2.74	7840.14	0.93	0.14
13	7904.72	1.04	2.43	7779.13	1.07	2.29	7839.72	0.90	0.09
	7904.54	1.04	2.43	7779.00	1.07	2.29	7839.77	0.90	0.09
14	7908.49	1.03	1.90	7774.60	1.07	1.80	7839.36	0.88	0.06
	7908.26	1.03	1.89	7774.41	1.07	1.80	7839.41	0.88	0.06
15	7912.17	1.03	1.44	7770.18	1.07	1.38	7839.03	0.85	0.04
	7911.88	1.03	1.44	7769.93	1.07	1.38	7839.06	0.85	0.04
16	7915.79	1.02	1.06	7765.93	1.07	1.03	7838.75	0.82	0.02
	7915.40	1.03	1.07	7765.60	1.07	1.03	7838.74	0.83	0.02
17	7919.29	1.02	0.78	7761.86	1.06	0.75	7838.52	0.79	0.02
	7918.83	1.02	0.78	7761.42	1.07	0.75	7838.47	0.79	0.02
18	7922.73	1.01	0.55	7758.02	1.05	0.53	7838.38	0.76	0.01
	7922.17	1.02	0.55	7757.43	1.06	0.54	7838.19	0.77	0.01
19	7926.10	1.01	0.38	7754.38	1.05	0.37	7838.35	0.72	0.01
	7925.42	1.01	0.38	7753.65	1.06	0.37	7837.99	0.73	0.01
20	7929.43	1.00	0.26	7751.05	1.05	0.25	7838.48	0.68	0.00
	7928.59	1.00	0.26	7750.11	1.05	0.26	7837.85	0.70	0.00

TABLE BX: C. Combination v_r=0→1 v_θ=0→2 band ($S_{\rm vib}$ in 10^{-5} D^2, I in 10^{-22} cm/molecule).

	$[v_r\, v_\theta\, v_R]$=[0 0 0] → [1 2 0]														
	K_a=0−0 (b k)=(0 0) → (2 0)						K_a=1−1 (b k)=(1 1) → (3 1)								
	$R(J^e)$			$P(J^e)$			$R(J^e)/R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$		
J	$E_{\rm trn}$	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0	5152.30	6.57	2.05												
1	5156.11	6.50	3.96	5142.91	6.78	2.07	5249.02	5.81	5.98				5241.89	6.25	6.41
							5250.83	5.38	5.53				5241.09	6.89	7.06
2	5159.42	6.39	5.58	5137.44	6.85	3.97	5250.91	5.53	9.64	5231.52	5.80	5.67	5241.25	6.82	3.71
							5254.40	5.07	8.82	5231.72	6.57	6.41	5238.84	8.90	4.83
3	5162.14	6.19	6.70	5131.38	6.95	5.61	5251.70	4.94	11.28	5224.72	5.46	8.82	5240.27	7.72	2.74
							5257.45	4.75	10.81	5225.77	6.89	11.08	5235.44	12.43	4.39
4	5164.27	6.11	7.51	5124.85	7.06	6.90	5251.28	3.95	10.51	5216.93	4.79	9.89	5238.95	9.05	2.25
							5259.98	4.41	11.66	5219.38	7.18	14.73	5230.82	17.74	4.38
5	5165.80	5.98	7.83	5117.78	7.06	7.64	5253.12	2.21	6.36	5208.11	3.63	8.52	5237.28	10.92	1.97
							5261.95	4.05	11.56	5212.53	7.46	17.34	5224.86	23.89[a]	4.25[a]

TABLE BX: C. continued

6	5166.69	6.12	8.10	5110.20	7.23	8.11	5251.36	2.78	8.17	5198.13	2.14	5.30	5235.22	13.53	1.79
							5263.34	3.68	10.66	5205.22	7.73	18.86	5221.07	3.54[a]	0.46[a]
7	5166.98	5.73	7.34	5102.10	7.36	8.16	5248.80	3.06	8.75	5190.50	6.41	15.80	5232.77	17.14	1.66
							5264.08	3.26	9.17	5197.45	7.99	19.33	5213.58	9.56	0.91
8	5166.60	5.59	6.67	5093.47	7.86	8.23	5245.42	3.15	8.44	5179.36	7.11	16.66	5229.85	22.17	1.57
							5264.12	2.79	7.31	5189.19	8.23	18.83	5205.23	18.14	1.25
9	5165.55	5.44	5.83	5084.36	7.70	7.31	5241.23	3.13	7.58	5167.53	7.44	15.95	5226.42	29.21	1.50
							5263.32	2.25	5.29	5180.42	8.41	17.50	5195.99	29.44	1.46
10	5163.83	5.29	4.93	5074.71	7.88	6.58	5236.23	3.05	6.44	5155.02	7.62	14.40	5222.35	39.02	1.44
							5261.50	1.62	3.31	5171.08	8.49	15.50	5185.89	44.02	1.55
11	5161.33	4.82	3.79	5064.55	8.08	5.72	5230.42	2.92	5.23	5141.83	7.72	12.46	5217.44	52.22	1.36
							5258.30	0.94	1.61	5161.06	8.40	13.00	5174.94	62.64	1.55
12	5158.24	4.96	3.20	5053.89	8.29	4.84	5223.85	2.75	4.07	5127.99	7.78	10.41	5211.35	67.61	1.23
							5265.98	1.30	1.85	5150.19	7.95	10.13	5163.18	86.22	1.48
13	5154.39	4.77	2.45	5042.64	7.98	3.73	5216.47	2.55	3.02	5113.52	7.82	8.42	5204.20	52.25	0.66
							5258.86	0.85	0.95	5138.15	6.89	7.01	5150.65	116.00	1.36
14	5149.67	4.65	1.86	5030.99	8.70	3.18	5207.36	1.36	1.26	5098.48	7.82	6.61	5194.01	77.59	0.66
							5251.15	0.38	0.33	5137.20	3.21	2.55	5137.34	152.90	1.20
15	5144.24	4.51	1.37	5018.82	8.88	2.47	5199.81	2.21	1.56	5082.85	7.77	5.02	5196.66	64.39	0.37
							5242.41	0.10	0.06	5121.67	4.15	2.50	5122.33	132.90	0.69
16	55138.29	3.55	0.80	5006.03	9.21	1.91	5190.18	1.98	1.04	5065.72	4.68	2.26	5185.80	100.20	0.38
							5232.29	0.00	0.00	5105.81	4.24	1.89	5108.96	253.30	0.86
17	55130.88	4.19	0.68	4992.79	9.51	1.44	5179.87	1.73	0.66	5050.41	7.85	2.77	5173.74	130.40	0.32
							5198.98	0.05	0.02	5089.20	3.75	1.21	5093.59	324.70	0.71
							K_a=2−2 $(b\,k)$=(2 2) → (4 2)								
2							5382.18	4.15	0.63				5369.66	5.16	1.55
							5382.24	4.14	0.62				5369.68	5.17	1.55
3							5384.11	3.62	0.91	5354.98	5.07	0.71	5367.54	5.77	1.13
							5384.28	3.97	1.00	5354.96	5.06	0.71	5367.48	5.79	1.13
4							5385.22	3.41	1.10	5347.91	5.23	1.19	5364.71	6.61	0.90
							5385.62	3.79	1.22	5347.98	5.23	1.19	5364.54	6.03	0.82
5							5385.48	3.45	1.25	5340.14	4.88	1.38	5361.22	7.74	0.76
							5386.29	3.56	1.29	5340.31	5.38	1.52	5360.82	7.00	0.69
6							5384.83	3.62	1.37	5331.62	4.92	1.53	5357.09	9.09	0.66
							5386.28	3.07	1.16	5332.03	5.50	1.71	5356.28	8.91	0.64
7							5383.21	3.15	1.18	5322.34	5.32	1.69	5352.33	9.99	0.53
							5385.61	3.23	1.21	5323.14	5.55	1.76	5350.88	11.97	0.63
8							5380.52	2.96	1.05	5312.24	5.96	1.83	5346.97	13.57	0.52
							5384.27	3.05	1.08	5313.68	5.14	1.58	5344.56	13.55	0.52
9							5376.82	2.52	0.81	5301.28	5.53	1.57	5340.99	16.71	0.47
							5382.10	2.80	0.90	5303.68	5.81	1.65	5337.23	16.80	0.47
10							5371.71	2.49	0.70	5289.39	5.49	1.38	5334.26	20.59	0.41
							5380.55	2.20	0.62	5293.14	5.85	1.47	5328.96	18.31	0.36
11							5365.29	2.27	0.54	5276.64	5.50	1.18	5328.22	19.69	0.28
							5377.18	2.29	0.55	5281.91	5.45	1.17	5319.36	24.81	0.35
12							5357.36	2.00	0.40	5262.64	5.48	0.98	5320.47	27.94	0.27
							5373.49	2.13	0.42	5271.46	5.90	1.06	5308.53	30.60	0.30
13							5347.61	1.69	0.27	5247.53	5.30	0.76	5312.48	34.81	0.23
							5369.24	1.91	0.30	5259.38	6.25	0.90	5296.27	36.83	0.25
14							5335.53	1.30	0.16	5231.10	4.99	0.56	5304.06	42.34	0.19
							5364.59	1.75	0.22	5247.17	6.32	0.72	5282.30	42.82	0.19

[a]Affected by the crossing between levels of the groups $(v_r\,b\,k\,v_R)$=(1 3 1 0) and (1 1 0 2) noted in Table BIV.

TABLE BX: D. Difference v_r=0→1 v_θ=1→0 band ($S_{\rm vib}$ in 10^{-4} D^2, I in 10^{-22} cm/molecule).

	$[v_r\, v_\theta\, v_R]$=[0 1 0] → [1 0 0]																	
	K_a=1−0 $(b\,k)$=(2 1) → (0 0)									K_a=0−1 $(b\,k)$=(1 0) → (1 1)								
	$R(J^e)$			$P(J^e)$			$Q(J^f)$			$R(J^e)$			$P(J^e)$			$Q(J^e)$		
J	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0										3522.64	5.10	1.81						
1	3375.79	5.46	0.19	3361.01	5.59	0.39	3365.67	5.53	0.58	3527.66	5.15	2.69				3518.13	5.03	2.63
2	3381.53	5.41	0.37	3356.93	5.61	0.57	3365.98	5.51	0.93	3532.85	5.20	3.47	3508.68	4.93	0.82	3518.81	5.03	4.17
3	3387.67	5.37	0.51	3353.28	5.64	0.71	3366.44	5.48	1.20	3538.23	5.20	4.06	3504.42	4.88	1.51	3519.82	5.00	5.43
4	3394.19	5.31	0.62	3350.07	5.66	0.82	3367.07	5.47	1.41	3543.74	5.30	4.54	3500.37	4.81	2.04	3521.17	4.97	6.35
5	3401.09	5.24	0.69	3347.31	5.70	0.88	3367.85	5.43	1.52	3549.43	5.34	4.78	3496.57	4.74	2.39	3522.87	4.95	6.91
6	3408.36	5.19	0.72	3344.99	5.71	0.91	3368.81	5.37	1.55	3555.28	5.39	4.83	3492.98	4.70	2.59	3524.91	4.90	7.08
7	3415.99	5.11	0.71	3343.14	5.73	0.89	3369.94	5.33	1.51	3561.30	5.44	4.70	3489.66	4.63	2.61	3527.29	4.84	6.90
8	3423.97	5.04	0.68	3341.76	5.75	0.85	3371.25	5.26	1.41	3567.48	5.47	4.40	3486.61	4.56	2.51	3530.08	4.75	6.44
9	3432.30	4.95	0.62	3340.85	5.75	0.78	3372.76	5.20	1.27	3573.82	5.50	4.00	3483.86	4.49	2.31	3533.17	4.77	5.92
10	3440.96	4.87	0.55	3340.42	5.76	0.69	3374.46	5.13	1.11	3580.35	5.54	3.53	3481.41	4.39	2.04	3536.63	4.73	5.21
11	3449.95	4.77	0.47	3340.49	5.77	0.60	3376.38	5.06	0.94	3587.06	5.56	3.03	3479.28	4.33	1.76	3540.47	4.65	4.43
12	3459.28	4.65	0.39	3341.07	5.79	0.51	3378.52	4.97	0.77	3593.95	5.57	2.52	3477.52	4.22	1.45	3544.68	4.61	3.68
13	3468.95	4.49	0.31	3342.20	5.79	0.42	3380.90	4.88	0.61	3601.02	5.56	2.05	3476.13	4.09	1.16	3549.27	4.55	2.97
14	3479.01	4.24	0.24	3343.93	5.78	0.33	3383.54	4.79	0.48	3608.29	5.53	1.61	3475.14	3.95	0.90	3554.24	4.49	2.34
15	3489.80	3.43	0.15	3346.62	5.44	0.25	3386.45	4.69	0.36	3615.75	5.45	1.23	3474.56	3.76	0.67	3559.59	4.44	1.81
16	3498.01	3.91	0.13	3346.99	3.78	0.13	3389.66	4.59	0.27	3623.38	5.26	0.90	3474.39	3.47	0.48	3565.29	4.36	1.35
17	3509.57	4.27	0.11	3350.98	5.05	0.13	3393.20	4.48	0.19	3631.08	4.77	0.61	3474.55	2.94	0.30	3571.26	4.28	0.99
18	3520.86	4.16	0.08	3354.99	5.25	0.10	3397.09	4.36	0.14	3638.43	3.35	0.31	3474.64	1.78	0.13	3577.06	3.76	0.64
19	3532.35	4.01	0.06	3359.53	5.30	0.07	3401.37	4.24	0.09	3651.13	4.72	0.32	3480.38	3.53	0.20	3588.37	1.82	0.23
20	3544.12	3.85	0.04	3364.69	5.30	0.05	3406.09	4.11	0.06	3659.34	5.59	0.27	3481.97	3.80	0.15	3595.39	2.69	0.24

TABLE BXI: Far- and mid-infrared absorption spectrum of Li^+–H_2. Line positions (ν, in cm^{-1}), vibrational factors of line strengths (S_{vib}), and line intensities (I) at T=296 K in one rotational and in four vibrational bands.

A. Rotational band (S_{vib} in D^2, I in 10^{-20} cm/molecule).

$[v_r\, v_\theta\, v_R]$=[0 0 0] → [0 0 0]

	K_a=0−0, $(b\,k)$=(0 0) → (0 0), $R(J^e)$			K_a=1−1, $(b\,k)$=(1 1) → (1 1), $R(J^e)/R(J^f)$			K_a=2−2, $(b\,k)$=(2 2) → (2 2), $R(J^e)/R(J^f)$			K_a=3−3, $(b\,k)$=(3 3) → (3 3), $R(J^e)/R(J^f)$		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0	4.955	2.326	0.02									
1	9.902	2.329	0.13	9.729	2.323	0.20						
				10.028	2.323	0.22						
2	14.834	2.334	0.41	14.576	2.328	0.77	14.699	2.314	0.07			
				15.023	2.328	0.82	14.699	2.314	0.07			
3	19.741	2.342	0.89	19.400	2.335	1.77	24.399	2.331	0.38	19.351	2.301	0.08
				19.994	2.336	1.87	24.399	2.331	0.38	19.351	2.301	0.08
4	24.617	2.352	1.55	24.197	2.345	3.19	29.195	2.342	0.61	24.133	2.310	0.19
				24.931	2.346	3.36	29.195	2.342	0.61	24.133	2.310	0.19
5	29.453	2.364	2.35	28.955	2.356	4.90	33.946	2.356	0.86	28.878	2.322	0.34
				29.828	2.358	5.14	33.948	2.356	0.86	28.878	2.322	0.34
6	34.243	2.378	3.20	33.669	2.370	6.74	38.645	2.373	1.09	33.577	2.335	0.51
				34.677	2.373	7.03	38.645	2.373	1.09	33.578	2.335	0.51
7	38.976	2.395	3.99	38.333	2.387	8.48	43.279	2.392	1.29	38.224	2.351	0.67
				39.468	2.390	8.80	43.283	2.392	1.29	38.226	2.351	0.67
8	43.646	2.414	4.65	42.936	2.405	9.94	47.846	2.413	1.44	42.808	2.370	0.81
				44.195	2.410	10.25	47.850	2.413	1.44	42.812	2.369	0.81
9	48.242	2.437	5.10	47.471	2.427	10.96	52.332	2.438	1.51	47.324	2.390	0.92
				48.845	2.433	11.23	52.340	2.437	1.51	47.330	2.390	0.92
10	52.758	2.462	5.30	51.932	2.451	11.47	56.732	2.465	1.51	51.760	2.414	0.97
				53.414	2.458	11.67	56.745	2.464	1.51	51.771	2.414	0.97
11	57.185	2.490	5.26	56.309	2.478	11.45	61.033	2.495	1.44	56.107	2.440	0.98
				57.889	2.487	11.57	61.052	2.495	1.44	56.126	2.440	0.98
12	61.512	2.521	5.01	60.591	2.508	10.96	65.229	2.529	1.33	60.356	2.470	0.95
				62.263	2.519	10.98	65.257	2.528	1.33	60.387	2.470	0.95
13	65.732	2.556	4.59	64.774	2.542	10.09	69.305	2.567	1.18	64.490	2.502	0.88
				66.526	2.554	10.02	69.348	2.565	1.18	64.544	2.502	0.88
14	69.833	2.594	4.05	68.844	2.579	8.97	73.254	2.608	1.01	68.494	2.538	0.79
				70.665	2.594	8.83	73.313	2.607	1.01	68.588	2.539	0.79
15	73.806	2.637	3.46	72.793	2.620	7.71	77.061	2.654	0.84	72.331	2.576	0.68
				74.672	2.637	7.52	77.145	2.652	0.84	72.509	2.578	0.68
16	77.640	2.684	2.87	76.611	2.665	6.43	80.714	2.705	0.68	75.912	2.605	0.56
				78.535	2.685	6.20	80.829	2.702	0.68	76.295	2.622	0.57
17	81.322	2.736	2.31	80.284	2.715	5.20	84.193	2.762	0.54	78.904	2.552	0.43
				82.240	2.738	4.98	84.355	2.758	0.54	79.936	2.671	0.46
18	84.842	2.793	1.81	83.803	2.770	4.10	87.483	2.826	0.41	87.383	0.357	0.05
				85.776	2.797	3.88	87.707	2.819	0.41	83.418	2.725	0.37
19	88.182	2.857	1.38	87.150	2.831	3.15	90.552	2.897	0.31	85.827	2.734	0.27
				89.125	2.862	2.95	90.873	2.887	0.31	86.727	2.784	0.28
20	91.329	2.927	1.03	90.315	2.899	2.37	93.357	2.978	0.23	89.428	2.873	0.21
				92.273	2.934	2.20	93.833	2.962	0.23	89.844	2.850	0.21
21	94.263	3.006	0.75	93.275	2.974	1.74	95.804	3.071	0.16	92.385	2.951	0.16
				95.199	3.015	1.60	96.569	3.046	0.16	92.734	2.925	0.16
22	96.964	3.094	0.54	96.014	3.059	1.25	97.615	3.175	0.11	92.682	2.096	0.07
				97.883	3.105	1.14	99.055	3.140	0.11	95.259	3.004	0.11
23	99.406	3.192	0.38	98.506	3.153	0.88	97.713	3.234	0.08	101.105	1.166	0.03
				100.297	3.207	0.80	101.268	3.246	0.08	100.087	2.029	0.05
24	101.558	3.304	0.26	100.724	3.259	0.61	93.777	3.477	0.05			
				102.409	3.321	0.55	103.169	3.366	0.05			

TABLE BXI: B. Fundamental v_R=0→1 band (S_{vib} in 10^{-2} D^2, I in 10^{-21} cm/molecule).

	$[v_r\,v_\theta\,v_R]$=[0 0 0] → [0 0 1]															
	K_a=0−0 (b k)=(0 0) → (0 0)						K_a=1−1 (b k)=(1 1) → (1 1)									
	$R(J^e)$			$P(J^e)$			$R(J^e)/R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$			
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	
0	409.67	3.83	8.20													
1	413.76	3.73	15.78	400.20	5.85	8.23	416.18	3.74	26.45				407.44	3.96	27.20	
							416.45	3.74	26.43				407.15	3.96	27.18	
2	417.39	3.63	22.22	394.82	6.12	15.89	419.76	3.64	44.19	397.57	4.19	26.61	406.87	3.96	14.42	
							420.14	3.64	44.10	397.26	4.19	26.55	406.00	3.98	14.39	
3	420.57	3.54	27.14	389.02	6.41	22.45	422.89	3.55	57.01	391.88	4.32	44.59	406.01	3.98	9.41	
							423.36	3.55	56.77	391.40	4.33	44.40	404.29	4.00	9.37	
4	423.27	3.45	30.31	382.82	6.73	27.50	425.55	3.47	65.35	385.78	4.46	57.71	404.86	4.00	6.61	
							426.11	3.46	64.89	385.12	4.47	57.30	402.00	4.04	6.57	
5	425.50	3.37	31.72	376.21	7.08	30.83	427.75	3.39	69.43	379.29	4.61	66.37	403.40	4.02	4.80	
							428.38	3.38	68.70	378.44	4.63	65.67	399.13	4.08	4.75	
6	427.23	3.29	31.49	369.20	7.47	32.39	429.47	3.31	69.67	372.40	4.78	70.77	401.64	4.05	3.52	
							430.14	3.31	68.64	371.35	4.80	69.73	395.70	4.13	3.47	
7	428.46	3.21	29.90	361.80	7.90	32.29	430.69	3.24	66.69	365.13	4.95	71.28	399.57	4.08	2.59	
							431.39	3.23	65.38	363.87	4.98	69.91	391.69	4.20	2.55	
8	429.17	3.14	27.28	354.01	8.37	30.80	431.40	3.17	61.28	357.47	5.14	68.52	397.16	4.12	1.90	
							432.12	3.16	59.73	356.00	5.17	66.84	387.12	4.28	1.86	
9	429.34	3.08	24.01	345.84	8.90	28.24	431.59	3.10	54.27	349.42	5.34	63.25	394.42	4.15	1.38	
							432.29	3.10	52.57	347.73	5.38	61.33	381.97	4.37	1.34	
10	428.97	3.01	20.43	337.28	9.50	24.98	431.24	3.04	46.46	340.99	5.57	56.30	391.32	4.20	0.99	
							431.90	3.03	44.69	339.08	5.61	54.23	376.24	4.47	0.96	
11	428.02	2.95	16.84	328.34	10.16	21.38	430.32	2.98	38.53	332.19	5.80	48.46	387.84	4.24	0.70	
							430.93	2.97	36.78	330.03	5.86	46.36	369.95	4.59	0.68	
12	426.48	2.89	13.47	319.02	10.90	17.74	428.83	2.92	31.01	322.99	6.06	40.44	383.98	4.28	0.49	
							429.35	2.91	29.35	320.60	6.14	38.39	363.08	4.73	0.47	
13	424.33	2.83	10.46	309.32	10.36	14.29	426.73	2.86	24.24	313.42	6.35	32.77	379.70	4.33	0.33	
							427.14	2.85	22.75	310.78	6.43	30.86	355.63	4.89	0.33	
14	421.54	2.77	7.90	299.24	10.73	11.19	424.00	2.80	18.43	303.46	6.66	25.82	374.98	4.37	0.23	
							424.27	2.79	17.13	300.56	6.76	24.11	347.60	5.06	0.22	
15	418.09	2.71	5.81	288.77	11.12	8.53	420.62	2.75	13.64	293.11	7.00	19.80	369.79	4.42	0.15	
							420.71	2.73	12.55	289.95	7.12	18.33	338.98	5.26	0.15	
16	413.94	2.65	4.16	277.91	11.53	6.34	416.54	2.69	9.84	282.37	7.38	14.81	364.10	4.46	0.10	
							416.42	2.67	8.95	278.94	7.52	13.58	329.77	5.49	0.10	
17	409.04	2.58	2.90	266.64	11.98	4.59	411.73	2.63	6.91	271.21	7.79	10.80	357.87	4.49	0.06	
							411.36	2.61	6.22	267.51	7.96	9.81	319.95	5.74	0.06	
18	403.37	2.51	1.97	254.97	12.45	3.25	406.14	2.56	4.73	259.65	8.26	7.69	351.06	4.52	0.04	
							405.48	2.54	4.21	255.65	8.46	6.92	309.51	6.03	0.04	
19	396.87	2.43	1.30	242.88	12.96	2.24	399.72	2.49	3.16	247.64	8.78	5.35	343.61	4.53	0.02	
							398.71	2.47	2.77	243.35	9.02	4.76	298.43	6.35	0.02	
20	389.49	2.34	0.83	230.35	13.50	1.51	392.40	2.42	2.06	235.19	9.37	3.64	335.47	4.53	0.01	
							390.99	2.39	1.78	230.58	9.66	3.21	286.69	6.72	0.02	
21	381.20	2.22	0.52	217.36	12.96	1.00	384.10	2.33	1.30	222.26	10.05	2.42	326.56	4.52	0.01	
							382.22	2.29	1.11	217.31	10.39	2.11	274.24	7.14	0.01	
22	371.99	2.07	0.31	203.90	13.50	0.64	374.71	2.24	0.80	208.81	10.82	1.57	316.79	4.48	0.00	
							372.28	2.18	0.67	203.52	11.23	1.36	261.06	7.61	0.01	

TABLE BXI: B. continued

	$[v_r\, v_\theta\, v_R]$=[0 0 0] → [0 0 1]																	
	K_a=2−2 (b k)=(2 2) → (2 2)									K_a=3−3 (b k)=(3 3) → (3 3)								
	$R(J^e)$ / $R(J^f)$			P			Q			R			P			Q		
J	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
2	424.06	3.65	3.78				410.65	3.97	7.89									
	424.06	3.65	3.78				410.65	3.97	7.89									
3	427.20	3.56	6.24	395.95	4.29	3.78	409.36	4.00	5.16	431.64	3.53	2.51				413.91	3.93	7.96
	427.21	3.56	6.24	395.95	4.29	3.78	409.36	4.00	5.16	431.64	3.53	2.51				413.91	3.93	7.96
4	429.87	3.48	7.82	389.80	4.42	6.24	407.64	4.03	3.63	434.40	3.43	4.10	394.56	4.45	2.57	412.29	3.93	5.56
	429.89	3.48	7.83	389.80	4.42	6.24	407.63	4.04	3.63	434.40	3.43	4.11	394.56	4.45	2.57	412.29	3.93	5.56
5	432.06	3.40	8.68	383.23	4.56	7.82	405.49	4.08	2.64	436.70	3.35	5.04	388.16	4.60	4.22	410.26	3.93	4.00
	432.10	3.40	8.68	383.24	4.56	7.83	405.47	4.08	2.64	436.70	3.35	5.04	388.16	4.60	4.22	410.26	3.93	4.00
6	433.76	3.32	8.92	376.28	4.71	8.69	402.90	4.13	1.94	438.55	3.26	5.44	381.38	4.76	5.21	407.82	3.92	2.90
	433.82	3.32	8.93	376.29	4.71	8.70	402.87	4.14	1.94	438.55	3.26	5.44	381.38	4.76	5.21	407.82	3.92	2.90
7	434.95	3.25	8.65	368.92	4.87	8.94	399.88	4.19	1.43	439.94	3.17	5.44	374.25	4.92	5.66	404.97	3.91	2.11
	435.05	3.25	8.67	368.95	4.88	8.97	399.81	4.21	1.43	439.93	3.18	5.44	374.24	4.92	5.66	404.97	3.91	2.11
8	435.61	3.17	8.02	361.17	5.04	8.69	396.41	4.25	1.05	440.85	3.09	5.13	366.75	5.10	5.70	401.71	3.89	1.52
	435.77	3.18	8.05	361.23	5.06	8.74	396.30	4.28	1.05	440.84	3.09	5.14	366.75	5.10	5.70	401.71	3.89	1.52
9	435.74	3.10	7.13	353.03	5.22	8.08	392.49	4.32	0.76	441.28	3.00	4.61	358.91	5.28	5.42	398.04	3.87	1.09
	435.96	3.12	7.17	353.12	5.26	8.13	392.33	4.36	0.77	441.27	3.01	4.62	358.90	5.28	5.42	398.04	3.87	1.09
10	435.30	3.04	6.11	344.49	5.43	7.21	388.12	4.40	0.55	441.22	2.91	3.98	350.72	5.46	4.91	393.95	3.85	0.76
	435.62	3.06	6.16	344.64	5.47	7.28	387.88	4.44	0.55	441.20	2.92	3.99	350.70	5.47	4.92	393.94	3.84	0.76
11	434.27	2.97	5.07	335.56	5.65	6.22	383.29	4.48	0.39	440.66	2.82	3.30	342.20	5.66	4.27	389.46	3.81	0.53
	434.71	3.00	5.12	335.77	5.71	6.29	382.95	4.53	0.39	440.64	2.83	3.31	342.17	5.67	4.28	389.44	3.81	0.53
12	432.63	2.90	4.07	326.23	5.89	5.18	378.00	4.56	0.27	439.59	2.71	2.64	333.36	5.85	3.58	384.55	3.75	0.36
	433.22	2.94	4.13	326.53	5.96	5.26	377.51	4.61	0.27	439.57	2.72	2.65	333.30	5.87	3.60	384.51	3.76	0.36
13	430.34	2.83	3.17	316.51	6.15	4.20	372.22	4.64	0.19	437.99	2.59	2.03	324.20	6.02	2.90	379.25	3.68	0.24
	431.13	2.88	3.23	316.91	6.24	4.27	371.55	4.70	0.19	437.99	2.60	2.04	324.12	6.07	2.92	379.16	3.69	0.24
14	427.36	2.76	2.39	306.37	6.44	3.30	365.96	4.73	0.13	435.80	2.43	1.49	314.75	6.17	2.26	373.57	3.57	0.15
	428.42	2.82	2.46	306.91	6.55	3.37	365.04	4.78	0.13	435.89	2.45	1.50	314.63	6.25	2.28	373.37	3.60	0.16
15	423.59	2.67	1.75	295.81	6.75	2.53	359.19	4.83	0.08	432.28	1.88	0.88	305.01	6.26	1.69	367.52	3.39	0.10
	425.04	2.76	1.82	296.53	6.89	2.58	357.93	4.84	0.08	433.15	2.22	1.04	304.85	6.40	1.73	367.08	3.48	0.10
16	418.89	2.55	1.23	284.80	7.10	1.88	351.91	4.92	0.05	431.05	2.02	0.70	294.98	6.18	1.20	361.05	3.09	0.06
	420.98	2.70	1.31	285.76	7.27	1.93	350.16	4.86	0.05	432.91	1.40	0.49	294.79	6.47	1.25	359.54	2.80	0.05

TABLE BXI: C. Fundamental v_θ=0→1 band ($S_{\rm vib}$ in 10^{-3} D^2), I in 10^{-22} cm/molecule

	$[v_r\, v_\theta\, v_R]$=[0 0 0] → [0 1 0]																	
	K_a=1−0 (b k)=(1 1) → (1 0)									K_a=0−1 (b k)=(0 0) → (2 1)								
	$R(J^e)$			$P(J^e)$			$Q(J^f)$			$R(J^e)$			$P(J^e)$			$Q(J^e)$		
J	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0										692.08	3.28	13.26						
1	540.35	1.90	6.23	526.39	1.92	12.18	530.90	1.91	18.37	696.14	3.43	20.42				687.40	3.12	18.36
2	544.56	1.90	11.94	521.32	1.92	17.26	530.17	1.91	28.99	699.74	3.57	27.20	677.23	2.82	5.18	687.03	3.12	29.07
3	548.52	1.88	16.74	516.05	1.93	21.21	529.09	1.89	37.42	702.86	3.71	33.04	671.40	2.67	9.03	686.49	3.10	37.71
4	552.24	1.87	20.33	510.58	1.93	23.84	527.63	1.88	43.18	705.52	3.84	37.48	665.16	2.52	11.50	685.76	3.09	43.79
5	555.68	1.86	22.58	504.92	1.93	25.11	525.81	1.86	46.11	707.70	3.97	40.22	658.51	2.37	12.66	684.84	3.07	47.16
6	558.85	1.84	23.47	499.08	1.93	25.11	523.63	1.84	46.36	709.40	4.09	41.13	651.45	2.23	12.72	683.74	3.05	47.90
7	561.73	1.82	23.11	493.06	1.93	24.01	521.08	1.82	44.32	710.61	4.20	40.28	644.01	2.09	11.95	682.43	3.03	46.34
8	564.29	1.79	21.73	486.85	1.94	22.07	518.15	1.79	40.54	711.32	4.26	37.63	636.18	1.95	10.63	680.92	3.01	42.98
9	566.53	1.76	19.59	480.46	1.94	19.58	514.86	1.76	35.64	711.54	4.35	34.21	627.99	1.82	9.03	679.20	2.98	38.37
10	568.43	1.72	16.97	473.89	1.94	16.81	511.19	1.72	30.21	711.24	4.39	29.75	619.43	1.72	7.47	677.27	2.94	33.09

TABLE BXI: C. continued

11	569.96	1.68	14.16	467.13	1.94	13.99	507.14	1.69	24.74	710.42	4.37	24.82	610.54	1.59	5.84	675.12	2.91	27.61
12	571.11	1.62	11.37	460.19	1.94	11.31	502.72	1.65	19.62	709.06	4.25	19.64	601.30	1.49	4.50	672.73	2.87	22.35
13	571.86	1.54	8.76	453.06	1.94	8.90	497.91	1.61	15.09	707.08	3.86	14.13	591.72	1.43	3.41	670.10	2.83	17.57
14	572.20	1.44	6.44	445.75	1.94	6.82	492.73	1.57	11.27	704.14	2.36	6.67	581.81	1.41	2.60	667.22	2.79	13.44
15	572.14	1.29	4.42	438.24	1.94	5.09	487.18	1.52	8.19	703.53	7.24	15.46	571.51	1.53	2.12	664.07	2.74	10.01
16	571.77	1.03	2.63	430.57	1.94	3.71	481.29	1.47	5.78	699.32	6.39	10.02	560.50	2.27	2.30	660.64	2.69	7.26
17	571.48	0.52	0.97	422.74	1.92	2.63	475.17	1.40	3.92	695.10	6.02	6.78	552.08	0.01	0.01	656.90	2.64	5.15
18	565.57	1.60	2.12	414.87	1.87	1.78	469.25	1.19	2.32	690.40	5.83	4.62	540.36	0.15	0.08	652.84	2.59	3.56

	K_a=1−2 $(b\,k)$=(1 1) → (3 2)									K_a=2−3 $(b\,k)$=(2 2) → (4 3)								
	$R(J^e)$ / $R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$			$R(J^e)$ / $R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$		
J	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
1	878.69	4.16	70.64															
	878.55	4.12	69.79															
2	882.64	4.52	81.67				868.97	3.61	32.07	1073.06	4.49	20.15						
	882.24	4.36	78.55				868.52	3.47	30.78	1073.06	4.49	20.15						
3	886.19	4.96	94.37	854.39	3.11	5.05	868.11	3.59	52.02	1076.36	4.78	21.03				1058.36	3.56	5.13
	885.46	4.60	86.95	853.50	2.89	4.67	867.17	3.26	46.93	1076.36	4.78	21.03				1058.36	3.56	5.13
4	889.13	5.27	102.56	848.66	3.05	10.08	866.96	3.58	65.28	1079.23	5.07	21.68	1038.79	2.52	0.46	1056.79	3.54	8.33
	888.22	4.83	93.10	847.22	2.65	8.67	865.30	2.80	50.64	1079.23	5.07	21.67	1038.79	2.52	0.46	1056.79	3.54	8.33
5	894.13	1.31	25.29[a]	842.59	3.12	14.56	865.51	3.55	72.92	1081.66	5.36	21.85	1032.39	2.29	0.89	1054.83	3.50	10.21
	890.51	5.05	96.09	840.53	2.41	11.11	862.70	1.71	34.62[a]	1081.66	5.35	21.83	1032.39	2.29	0.89	1054.83	3.50	10.20
6	896.40	2.74	50.85[a]	835.97	3.33	18.57	863.78	3.52	75.57	1083.62	5.65	21.45	1025.63	2.06	1.15	1052.47	3.45	11.03
	892.32	5.26	95.59	833.46	2.19	11.98	862.08	4.09	86.22	1083.65	5.64	21.42	1025.64	2.06	1.15	1052.46	3.44	11.00
7	898.56	3.53	61.04	831.51	0.09	0.55[a]	861.75	3.48	73.98	1085.04	5.90	20.36	1018.51	1.85	1.24	1049.70	3.39	10.99
	893.66	5.45	91.72	826.00	1.97	11.59	858.63	4.35	90.16	1085.16	5.92	20.42	1018.52	1.84	1.23	1049.67	3.36	10.89
8	900.41	4.02	62.80	824.40	0.47	2.88	859.43	3.44	69.08	1087.04	4.14	12.65	1011.03	1.64	1.19	1046.52	3.29	10.28
	894.51	5.62	84.97	818.18	1.75	10.35	854.99	4.24	82.65	1086.15	6.18	18.87	1011.05	1.63	1.18	1046.40	3.15	9.83
9	901.87	4.38	60.01	817.29	0.63	3.65	856.81	3.39	61.87	1087.04	6.16	16.21	1003.12	1.48	1.07	1042.87	3.14	9.00
	894.86	5.77	76.04	810.00	1.55	8.65	850.98	4.11	72.14	1086.35	6.07	15.97	1003.23	1.43	1.03	1043.76	2.88	8.26
10	902.88	4.66	54.56	810.01	0.64	3.37	853.89	3.33	53.34	1087.03	6.54	14.47	995.92	0.58	0.39	1038.51	2.59	6.56
	894.72	5.89	65.76	801.47	1.36	6.83	846.52	3.96	60.64	1088.01	5.12	11.34	995.02	1.25	0.85	1039.19	3.27	8.28
11	903.39	4.89	47.63	802.46	0.58	2.68	850.66	3.25	44.35	1086.48	6.82	12.37	986.87	0.88	0.54	1035.69	3.00	6.49
	894.05	5.97	54.94	792.60	1.17	5.11	841.59	3.82	49.18	1087.19	6.46	11.73	986.16	1.09	0.67	1034.68	3.15	6.81
12	903.37	5.09	40.10	794.63	0.49	1.93	847.10	3.16	35.59	1085.28	7.01	10.16	977.97	0.75	0.40	1030.47	3.13	5.60
	892.85	6.00	44.32	783.41	1.00	3.64	836.15	3.66	38.49	1086.24	6.87	9.98	978.93	0.49	0.26	1029.72	3.01	5.38
13	902.75	5.24	32.62	786.49	0.40	1.26	843.20	3.06	27.58	1083.05	6.73	7.63	968.72	0.60	0.26	1025.24	3.02	4.35
	891.10	5.96	34.44	773.90	0.84	2.46	830.17	3.48	29.06	1084.85	7.15	8.11	969.39	0.55	0.24	1024.19	2.81	4.03
14	901.48	5.35	25.66	778.00	0.30	0.76	838.93	2.92	20.59	1077.76	3.59	3.09	959.01	0.45	0.16	1019.67	2.90	3.26
	888.74	5.83	25.69	764.07	0.69	1.58	823.62	3.28	21.15	1082.97	7.38	6.39	959.93	0.45	0.16	1017.75	2.38	2.66
15	899.49	5.41	19.56	769.13	0.21	0.41	834.25	2.75	14.76	1080.68	6.77	4.37	948.52	0.30	0.08	1013.74	2.78	2.38
	885.71	5.56	18.28	753.91	0.55	0.96	816.46	3.06	14.80	1080.56	7.56	4.88	950.25	0.34	0.09	1008.34	0.95	0.81
16	896.68	5.54	14.72	759.84	0.13	0.19	829.10	2.53	10.09	1076.71	7.58	3.58	935.20	0.97	0.02	1007.43	2.65	1.68
	881.92	5.15	12.33	743.40	0.42	0.55	808.64	2.80	9.93	1077.66	7.79	3.67	940.31	0.25	0.05	1007.25	2.38	1.51
17	893.16	5.12	9.82	750.09	0.07	0.07	823.37	2.23	6.46	1071.92	7.73	2.60	930.36	0.13	0.02	1000.78	2.49	1.15
	877.38	4.15	7.07	732.50	0.31	0.29	800.08	2.45	6.22	1074.12	7.89	2.66	930.11	0.16	0.03	999.39	2.30	1.06

[a] The dips in the intensities as functions of J are effects of the crossing between the levels from groups $(v_r\,b\,k\,v_R)$=(0 3 1 0) and (0 1 0 1) noted in Table BIV.

TABLE BXI: D. Overtone v_R=0→2 band ($S_{\rm vib}$ in 10^{-3} D^2, I in 10^{-22} cm/molecule).

	$[v_r\, v_\theta\, v_R]$=[0 0 0] → [0 0 2]															
	K_a=0−0						K_a=1−1									
	$(b\,k)$=(0 0) → (0 0)						$(b\,k)$=(1 1) → (1 1)									
	$R(J^e)$			$P(J^e)$			$R(J^e)/R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$			
J	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0	754.43	0.87	3.86												
1	757.60	0.87	7.61	745.40	0.87	3.71	763.02	0.82	11.89				755.15	0.83	11.98
							763.25	0.82	11.92				754.88	0.83	11.94
2	759.87	0.88	11.03	739.57	0.87	7.05	765.27	0.82	20.28	745.30	0.83	11.31	753.67	0.86	6.52
							765.56	0.82	20.36	744.98	0.83	11.25	752.85	0.85	6.44
3	761.22	0.89	13.92	732.87	0.88	9.83	766.61	0.82	26.80	738.72	0.85	18.82	751.43	0.89	4.42
							766.95	0.83	26.90	738.20	0.84	18.66	749.79	0.88	4.31
4	761.65	0.91	16.12	725.30	0.89	11.92	767.04	0.83	31.57	731.29	0.86	24.24	748.44	0.94	3.26
							767.39	0.84	31.67	730.54	0.86	23.94	745.72	0.92	3.13
5	761.12	0.93	17.57	716.87	0.90	13.27	766.55	0.84	34.58	723.01	0.88	27.81	744.68	1.00	2.50
							766.88	0.85	34.65	722.02	0.88	27.36	740.62	0.96	2.36
6	759.63	0.96	18.26	707.58	0.92	13.87	765.11	0.86	35.91	713.89	0.90	29.65	740.15	1.08	1.96
							765.39	0.87	35.92	712.63	0.90	29.04	734.50	1.02	1.81
7	757.16	1.00	18.24	697.43	0.94	13.79	762.71	0.88	35.70	703.93	0.93	29.94	734.82	1.16	1.54
							762.90	0.90	35.62	702.37	0.92	29.18	727.34	1.09	1.40
8	753.69	1.04	17.62	686.42	0.97	13.15	759.32	0.90	34.20	693.11	0.96	28.92	728.67	1.26	1.21
							759.39	0.92	34.02	691.25	0.95	28.04	719.13	1.16	1.07
9	749.19	1.09	16.56	674.54	1.00	12.09	754.91	0.93	31.70	681.44	0.99	26.90	721.69	1.38	0.95
							754.82	0.95	31.42	679.24	0.99	25.94	709.88	1.25	0.82
10	743.63	1.17	15.22	661.80	1.03	10.73	749.46	0.97	28.53	668.91	1.03	24.19	713.85	1.50	0.73
							749.17	0.99	28.15	666.35	1.03	23.20	699.57	1.35	0.62
11	737.01	1.26	13.79	648.19	1.06	9.22	742.93	1.01	24.97	655.51	1.07	21.10	705.11	1.64	0.56
							742.40	1.04	24.51	652.56	1.07	20.12	688.17	1.45	0.46
12	729.29	1.41	12.52	633.69	1.10	7.68	735.29	1.05	21.30	641.22	1.12	17.89	695.44	1.78	0.42
							734.46	1.09	20.80	637.87	1.13	16.97	675.69	1.57	0.34
13	720.50	1.70	11.89	618.31	1.14	6.19	726.49	1.11	17.73	626.03	1.18	14.78	684.81	1.94	0.31
							725.32	1.15	17.21	622.25	1.19	13.93	662.09	1.71	0.25
14	710.94	2.58	13.78	602.04	1.16	4.78	716.48	1.17	14.43	609.93	1.24	11.92	673.15	2.10	0.22
							714.91	1.21	13.91	605.67	1.26	11.17	647.36	1.85	0.18
15	697.31	0.04	0.15	584.93	1.12	3.42	705.19	1.24	11.49	592.87	1.32	9.39	660.42	2.27	0.16
							703.16	1.29	10.99	588.13	1.34	8.74	631.45	2.01	0.12
16	685.57	0.51	1.48	567.30	0.81	1.77	692.56	1.32	8.96	574.84	1.41	7.24	646.55	2.44	0.11
							690.00	1.38	8.50	569.57	1.44	6.70	614.34	2.19	0.08
17	672.39	0.62	1.28	545.87	1.91	2.91	678.49	1.42	6.85	555.78	1.51	5.47	631.45	2.61	0.07
							675.33	1.48	6.44	549.95	1.55	5.03	595.96	2.39	0.06
18	646.55	0.97	1.36	526.60	1.86	1.94	662.89	1.53	5.14	535.66	1.63	4.05	615.03	2.77	0.05
							659.04	1.59	4.78	529.23	1.69	3.71	576.27	2.60	0.04
19	632.17	1.46	1.39	506.23	1.71	1.19	645.62	1.66	3.80	514.40	1.77	2.95	597.17	2.91	0.03
							640.97	1.72	3.48	507.32	1.85	2.68	555.17	2.83	0.02
20	613.63	1.71	1.07	473.52	1.08	0.47	626.52	1.82	2.76	491.93	1.95	2.11	577.73	3.00	0.02
							620.93	1.88	2.49	484.14	2.04	1.91	532.58	3.04	0.02

TABLE BXI: E. Overtone v_θ=0→2 band ($S_{\rm vib}$ in 10^{-3} D^2, I in 10^{-22} cm/molecule).

	$[v_r\,v_\theta\,v_R]$=[0 0 0] → [0 2 0]														
	K_a=0−0						K_a=1−1								
	$(b\,k)$=(0 0) → (2 0)						$(b\,k)$=(1 1) → (3 1)								
	$R(J^e)$			$P(J^e)$			$R(J^e)/R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$		
J	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0	1072.72	1.37	8.83												
1	1076.82	1.36	17.18	1063.22	1.37	8.58	1192.60	1.18	27.41				1185.39	1.31	30.24
							1194.52	1.14	26.60				1184.54	1.35	31.20
2	1080.46	1.34	24.32	1057.86	1.37	16.24	1194.73	1.13	44.80	1174.96	1.32	28.90	1184.94	1.41	17.24
							1198.40	1.08	42.84	1175.21	1.37	29.95	1182.42	1.55	18.87
3	1083.61	1.32	29.75	1052.08	1.37	22.55	1195.95	1.09	56.35	1168.30	1.35	48.45	1184.27	1.56	12.50
							1201.87	1.02	53.03	1169.47	1.43	51.25	1179.26	1.87	14.80
4	1086.24	1.29	33.16	1045.89	1.38	27.27	1196.27	1.04	62.84	1160.75	1.36	62.45	1183.36	1.79	10.03
							1204.91	0.96	58.02	1163.38	1.48	67.52	1175.06	2.36	13.02
5	1088.32	1.26	34.54	1039.25	1.39	30.33	1195.71	0.99	64.83	1152.35	1.38	71.29	1182.20	2.10	8.52
							1207.50	0.90	58.48	1156.94	1.53	78.84	1169.85	3.06	12.16
6	1089.83	1.23	34.05	1032.17	1.41	31.78	1194.29	0.95	63.08	1143.12	1.39	75.23	1180.77	2.52	7.47
							1209.62	0.83	55.21	1150.15	1.59	85.10	1163.66	4.06	11.69
7	1090.75	1.19	32.03	1024.62	1.44	31.76	1192.02	0.90	58.48	1133.09	1.40	74.83	1179.05	3.07	6.68
							1211.23	0.76	49.18	1143.00	1.63	86.53	1156.51	5.43	11.37
8	1091.05	1.15	28.91	1016.61	1.47	30.48	1188.93	0.86	51.96	1122.29	1.40	70.92	1177.00	3.79	6.04
							1212.26	0.69	41.40	1135.48	1.68	83.68	1148.45	7.28	11.02
9	1090.72	1.12	25.13	1008.12	1.51	28.20	1185.04	0.81	44.41	1110.75	1.41	64.46	1174.57	4.76	5.49
							1212.52	0.59	32.07	1127.56	1.72	77.39	1139.49	9.76	10.57
10	1089.73	1.08	21.09	999.16	1.55	25.23	1180.36	0.77	36.61	1098.52	1.41	56.46	1171.55	5.93	4.90
							1212.57	0.49	23.23	1119.22	1.75	68.61	1129.69	13.01	9.96
11	1088.06	1.04	17.13	989.72	1.59	21.87	1174.85	0.72	29.05	1085.63	1.41	47.79	1168.51	7.65	4.46
							1211.30	0.39	15.37	1110.26	1.71	56.60	1119.08	17.21	9.18
12	1085.68	1.00	13.49	979.79	1.64	18.38	1169.18	0.62	20.51	1072.12	1.41	39.18	1164.35	10.15	4.13
							1208.82	0.25	8.21	1101.27	1.71	46.45	1107.61	22.32	8.18
13	1082.56	0.96	10.31	969.36	1.69	15.01	1162.20	0.61	16.09	1057.95	1.40	30.90	1159.17	13.27	3.70
							1204.46	0.11	2.89	1091.15	1.67	35.85	1095.99	27.78	6.89
14	1078.65	0.92	7.69	958.43	1.73	11.91	1154.67	0.57	11.56	1043.82	1.32	22.64	1152.30	16.17	3.05
							1197.38	0.02	0.41	1080.03	1.50	24.85	1083.07	37.30	6.16
15	1073.96	0.86	5.45	946.99	1.77	9.21	1146.48	0.51	7.98	1028.58	1.37	17.83	1142.89	16.28	2.04
							1220.09	0.70	10.71	1067.27	1.15	14.29	1069.65	47.72	5.16
16	1068.36	0.83	3.85	935.01	1.82	6.94	1137.70	0.45	5.21	1013.03	1.37	13.09			
							1214.55	0.72	8.14	1052.04	0.67	6.07			
							K_a=2−2								
							$(b\,k)$=(2 2) → (4 2)								
2							1353.69	0.83	3.14				1340.77	0.93	6.94
							1353.97	0.75	2.83				1341.35	0.67	5.01
3							1355.69	0.51	3.24	1326.65	0.81	2.81	1339.27	1.05	5.12
							1356.06	0.79	5.01	1326.07	0.71	2.46	1338.99	1.19	5.79
4							1356.57	0.78	6.28	1319.43	1.06	5.96	1336.50	1.37	4.67
							1357.55	0.77	6.23	1319.71	1.01	5.69	1336.12	0.89	3.06
5							1356.47	0.72	6.56	1311.72	0.68	4.75	1333.15	1.68	4.15
							1358.42	0.74	6.75	1312.10	1.08	7.52	1332.17	1.74	4.28
6							1354.94	0.63	5.97	1302.98	1.06	8.09	1329.22	2.07	3.73
							1358.68	0.70	6.71	1303.95	1.11	8.42	1327.27	2.10	3.78
7							1351.37	0.47	4.39	1293.32	1.03	7.91	1324.73	2.56	3.38
							1358.35	0.66	6.26	1295.27	1.12	8.68	1320.99	2.44	3.21
8							1357.61	0.33	2.97	1282.35	0.92	6.79	1319.71	3.18	3.05
							1357.47	0.62	5.55	1286.09	1.14	8.44	1312.73	2.50	2.38
9							1352.75	0.40	3.27	1269.45	0.69	4.67	1314.19	3.95	2.73
							1356.04	0.58	4.70	1276.43	1.15	7.83	1314.33	2.09	1.45
10							1347.15	0.42	2.96	1266.49	0.66	3.98	1308.20	4.89	2.41
							1354.08	0.54	3.81	1266.34	1.16	6.97	1304.89	3.54	1.74
11							1340.69	0.37	2.20	1252.57	0.82	4.19	1301.76	6.02	2.09
							1351.68	0.49	2.96	1255.85	1.17	5.98	1294.80	5.08	1.76

TABLE BXI: F. Hot v_R=1→3 band (S_{vib} in 10^{-3} D^2, I in 10^{-22} cm/molecule).

	$[v_r\, v_\theta\, v_R]$=[0 0 1] → [0 0 3]														
	K_a=0−0						K_a=1−1								
	$(b\,k)$=(0 0) → (0 0)						$(b\,k)$=(1 1) → (1 1)								
	$R(J^e)$			$P(J^e)$			$R(J^e)/R(J^f)$			$P(J^e)/P(J^f)$			$Q(J^e)/Q(J^f)$		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0	634.15	3.44	1.76												
1	636.78	3.39	3.40	626.04	3.61	1.78	643.11	3.65	6.07				642.87	3.69	1.72
							643.30	3.66	6.09				642.87	3.69	1.72
2	638.46	3.36	4.86	620.59	3.71	3.47	644.79	3.66	10.40	627.16	3.74	5.78	640.12	3.74	1.14
							645.02	3.68	10.43	626.86	3.73	5.76	640.12	3.74	1.14
3	639.16	3.36	6.07	614.21	3.82	4.95	645.52	3.68	13.81	620.92	3.79	9.66	636.46	3.82	0.82
							645.77	3.71	13.85	620.42	3.78	9.60	636.44	3.83	0.82
4	638.88	3.38	7.00	606.91	3.94	6.14	645.29	3.72	16.37	613.78	3.86	12.53	631.86	3.94	0.61
							645.52	3.75	16.41	613.06	3.85	12.40	631.83	3.96	0.62
5	637.61	3.41	7.59	598.71	4.05	6.98	644.07	3.77	18.07	605.75	3.94	14.49	626.33	4.08	0.47
							644.25	3.81	18.09	604.78	3.94	14.30	626.27	4.12	0.47
6	635.34	3.44	7.79	589.59	4.18	7.45	641.85	3.83	18.93	596.83	4.04	15.61	619.85	4.25	0.36
							641.94	3.88	18.91	595.58	4.04	15.34	619.75	4.32	0.36
7	632.14	3.34	7.40	579.58	4.31	7.55	638.60	3.91	19.01	587.01	4.16	15.96	612.41	4.44	0.27
							638.56	3.97	18.94	585.46	4.16	15.62	612.24	4.55	0.28
8	628.46	2.39	4.98	568.69	4.43	7.30	634.28	4.01	18.40	576.29	4.30	15.64	603.98	4.66	0.21
							634.07	4.08	18.28	574.42	4.30	15.24	603.72	4.83	0.22
9	620.43	2.84	5.34	556.98	4.43	6.61	628.87	4.12	17.26	564.66	4.46	14.78	594.56	4.90	0.16
							628.44	4.20	17.08	562.44	4.47	14.33	594.16	5.14	0.16
10	614.10	3.90	6.44	544.96	3.42	4.46	622.32	4.25	15.72	552.11	4.64	13.53	584.10	5.17	0.12
							621.62	4.34	15.48	549.51	4.67	13.06	583.52	5.48	0.12
11	606.15	4.18	5.87	528.74	3.46	3.79	614.58	4.40	13.93	538.63	4.86	12.04	572.59	5.46	0.09
							613.57	4.50	13.65	535.61	4.89	11.55	571.77	5.86	0.09
12	596.82	4.41	5.13	514.42	4.98	4.47	605.61	4.57	12.04	524.18	5.10	10.43	559.98	5.77	0.06
							604.23	4.69	11.73	520.72	5.15	9.96	558.80	6.22	0.07
13	586.09	4.64	4.34	498.69	5.47	3.91	595.36	4.76	10.14	508.75	5.38	8.81	546.25	6.09	0.05
							593.53	4.89	9.82	504.82	5.45	8.37	543.89	5.25	0.04
14	573.87	4.89	3.58	481.81	5.91	3.26	583.79	4.94	8.30	492.30	5.70	7.28	531.35	6.42	0.03
							581.40	5.10	8.00	487.86	5.80	6.87	529.66	7.20	0.04
15	560.04	5.16	2.88	463.78	6.37	2.65	571.56	4.32	5.59	474.82	6.07	5.87			
							567.90	5.23	6.26	469.82	6.20	5.51			
16	544.47	5.44	2.26	444.54	6.89	2.10	554.98	5.50	5.31	456.29	6.44	4.60			
							549.81	3.84	3.39	450.64	6.65	4.32			
17	526.96	5.74	1.73	424.01	7.50	1.63	538.55	5.55	3.92	437.39	5.73	2.95			
							533.98	5.46	3.50	430.41	7.02	3.24			
18	507.23	6.02	1.29	402.08	8.21	1.23	520.04	5.94	3.00	414.46	7.24	2.60			
							514.70	6.09	2.76	405.95	5.57	1.77			

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