C. SUPPLEMENTARY MATERIAL — PART C

Li^+–D_2 COMPLEX

VIBRATIONAL ENERGY LEVELS

TABLE CI: Li^{+}–$D_2(I{=}0,2)$. Positions (E) and widths (Γ) of 'vibrational' levels $v_r\,b\,k\,v_R$ J=k p associated with the v=0–1 j=0–6 thresholds ($v_r{\sim}v$, $b{\sim}j$). The positions are relative to the respective $v\,j$=0 threshold. Positions of $j{>}0$ thresholds[a] are shown in lines marked with ε. All data are in cm^{-1}.

			v=0 (ε=0)				v=1 (ε=2994.163[a])			
			p=1		p=−1		p=1		p=−1	
b	k	v_R	E^b	Γ^c	$E-E(p{=}1)^b$	Γ^c	E	Γ^{de}	$E-E(p{=}1)$	Γ^d
0	0	0	−1783.613	0			−1862.328	8.29 (−3)		
		1	−1450.470	0			−1526.430	2.52 (−2)		
		2	−1154.270	0			−1226.257	4.55 (−2)		
		3	−894.963	0			−961.733	6.41 (−2)		
		4	−673.039	0			−732.160	*6.91 (−2)		
		5	−485.932	0			−538.698	8.38 (−2)		
		6	−334.665	0			−378.773	8.20 (−2)		
		7	−216.860	0			−251.637	7.41 (−2)		
		8	−129.899	0			−155.264	5.95 (−2)		
		9	−69.732	0			−86.228	4.39 (−2)		
		10	−31.534	0			−40.829	2.85 (−2)		
		11	−10.109	0			−14.393	*1.55 (−2)		
		12	−1.009	0			−2.119	*1.45 (−2)		
2	2	0	−1654.734	0	0.000	0	−1738.591	9.31 (−3)	0.000	9.31 (−3)
		1	−1320.255	0	0.000	0	−1401.450	2.72 (−2)	0.000	2.73 (−2)
		2	−1022.590	0	0.000	0	−1099.928	4.92 (−2)	0.000	4.90 (−2)
		3	♭ −761.687	0	0.000	0	−833.994	6.95 (−2)	0.000	6.96 (−2)
		4	−537.248	0	0.000	0	−603.333	8.41 (−2)	0.000	8.41 (−2)
		5	* −348.676	0	0.000	0	−407.475	9.08 (−2)	0.000	9.08 (−2)
		6	* −194.570	0	0.000	0	−245.434	8.91 (−2)	−0.002	8.91 (−2)
		7	* −73.824	0	0.001	0	−115.764	8.05 (−2)	0.000	8.06 (−2)
		8	17.203	1.02 (−4)	0.000	0	−15.878	6.70 (−2)	0.000	6.70 (−2)
		9	82.886	5.84 (−5)	0.000	0	57.529	5.16 (−2)	0.000	5.15 (−2)
		10	127.662	8.46 (−6)	0.006	0	108.591	5.68 (−2)	0.170	3.98 (−2)
		11	156.318	3.20 (−5)	0.001	0	142.464	2.40 (−2)	0.000	2.39 (−2)
		12	172.572	2.85 (−5)	0.004	0	162.356	1.30 (−2)	0.000	1.30 (−2)
		13					171.455	4.11 (−3)	0.003	4.10 (−3)
2	1	0	−1292.413	0	0.134	0	−1368.873	1.26 (−2)	0.133	1.03 (−2)
		1	−988.448	0	0.130	0	−1062.189	3.27 (−2)	0.128	3.13 (−2)
		2	−720.830	0	0.125	0	−790.283	5.95 (−2)	0.124	5.85 (−2)
		3	♭ −489.941	0	0.130	0	−553.439	8.56 (−2)	0.121	8.41 (−2)
		4	−296.265	0	0.107	0	−352.467	1.01 (−1)	0.105	1.01 (−1)
		5	* −139.337	0	0.101	0	−186.586	1.06 (−1)	0.098	1.06 (−1)
		6	* −17.989	0	0.121	0	−55.657	9.80 (−2)	0.087	9.79 (−2)
		7	68.296	1.92 (−3)	0.079	0	41.246	8.22 (−2)	0.078	8.00 (−2)
		8	125.068	1.38 (−3)	0.069	0	106.412	6.05 (−2)	0.151	5.68 (−2)
		9	158.099	1.49 (−3)	0.042	0	146.724	1.41 (−2)	0.212	3.19 (−2)
		10	174.252	1.45 (−4)	0.228	0	166.434	1.38 (−2)	0.101	1.38 (−2)
2	0	0	−936.866	0			−1003.764	5.86 (−3)		
		1	−671.059	0			−735.811	3.15 (−2)		
		2	−441.179	0			* −499.746	4.14 (−2)		
		3	−246.547	0			* −297.861	5.74 (−2)		
		4	−87.136	0			* −129.744	5.81 (−2)		
		5	28.906	3.54 (−2)			* −2.933	5.58 (−2)		
		6	111.012	1.46 (−2)			* 90.133	1.08 (−1)		
		7	155.055	1.19 (−2)			* 144.950	6.23 (−2)		
		8	174.418	4.29 (−3)			* 168.263	1.96 (−2)		
ε			178.992				172.495			
4	4	0	−1279.949	0	0.000	0	−1378.606	1.21 (−2)	0.000	1.21 (−2)
		1	−942.932	0	0.000	0	−1038.999	3.41 (−2)	0.000	3.41 (−2)
		2	−642.700	0	0.000	0	−735.006	6.23 (−2)	0.000	6.23 (−2)

TABLE CI:

		3	♭ − 379.134	0	0.000	0	−466.528	8.64 (−2)	0.000	8.64 (−2)
		4	−151.822	0	0.000	0	−232.827	9.63 (−2)	−0.006	9.66 (−2)
		5	39.362	2.43 (−6)	0.001	0	−34.902	1.11 (−1)	0.005	1.09 (−1)
		6	196.466	4.85 (−5)	0.000	3.95 (−4)	129.969	1.14 (−1)	0.001	1.10 (−1)
		7	320.940	7.83 (−5)	0.000	7.84 (−4)	262.824	1.00 (−1)	0.000	1.00 (−1)
4	3	0	−994.024	0	0.000	0	−1084.579	1.40 (−2)	0.000	1.40 (−2)
		1	−681.444	0	0.000	0	−769.597	4.30 (−2)	0.000	4.30 (−2)
		2	−405.421	0	0.000	0	−489.689	7.90 (−2)	0.000	7.90 (−2)
		3	♭ − 166.162	0	0.000	0	−245.127	1.12 (−1)	0.000	1.12 (−1)
		4	36.409	2.82 (−5)	0.002	0	−35.812	1.34 (−1)	0.000	1.34 (−1)
		5	200.816	4.05 (−2)	0.023	3.07 (−2)	137.275	1.35 (−1)	0.017	1.38 (−1)
		6	333.396	8.94 (−3)	0.013	8.24 (−3)	277.847	1.60 (−1)	−0.351	2.13 (−1)
4	2	0	♭ − 734.601	0	0.001	0	−814.951	1.06 (−2)	0.012	1.05 (−2)
		1	−447.196	0	0.005	0	−525.708	3.25 (−2)	−0.002	3.24 (−2)
		2	∗ − 196.206	0	0.001	0	−270.718	6.07 (−2)	0.000	6.05 (−2)
		3	18.756	5.74 (−8)	0.005	0	−50.546	8.68 (−2)	0.011	8.70 (−2)
		4	196.161	2.82 (−2)	0.007	2.49 (−2)	134.122	1.05 (−1)	0.017	1.15 (−1)
		5	336.981	2.24 (−2)	0.014	1.83 (−2)	271.912	3.14 (−1)	0.686	3.04 (−1)
4	1	0	♭ − 508.614	0	0.471	0	−577.431	5.07 (−3)	0.406	5.30 (−3)
		1	−247.042	0	0.620	0	−314.631	2.31 (−2)	0.270	1.69 (−1)
		2	∗ − 21.618	0	0.329	0	−85.701	3.86 (−2)	0.302	3.85 (−2)
		3	167.729	1.93 (−6)	0.414	0	109.703	5.63 (−2)	0.294	5.40 (−2)
		4	320.418	9.16 (−2)	0.247	7.81 (−2)	269.031	2.99 (−1)	−0.238	3.05 (−1)
4	0	0	−334.240	0			∗ − 386.287	1.85 (−3)		
		1	−96.790	0			∗ − 150.236	1.52 (−2)		
		2	104.776	9.67 (−3)			∗ 52.894	1.88 (−2)		
		3	259.696	9.47 (−2)			∗ 201.400	1.57 (−1)		
ε			593.472				571.875			
6	6	0	∗ − 671.736	0	0.000	0	−794.012	1.84 (−2)	0.000	1.84 (−2)
		1	∗ − 332.303	0	−0.001	0	−452.008	5.07 (−2)	0.000	5.07 (−2)
		2	∗ − 29.595	0	0.000	0	−145.598	8.78 (−2)	0.000	8.78 (−2)
		3	236.539	3.85 (−6)	−0.001	2.33 (−6)	125.342	1.20 (−1)	0.000	1.20 (−1)
6	5	0	−432.701	0	−0.001	0	−547.406	2.34 (−2)	0.000	2.34 (−2)
		1	−113.193	0	0.000	0	−225.520	7.12 (−2)	0.000	7.13 (−2)
		2	169.541	1.3 (−11)	−0.003	0	61.031	1.34 (−1)	0.000	1.35 (−1)
6	4	0	♭ − 219.364	0	0.002	0	−325.148	1.91 (−2)	0.000	1.91 (−2)
		1	81.211	2.05 (−8)	0.000	0	−22.453	6.02 (−2)	0.000	6.01 (−2)
		2	344.908	6.52 (−4)	0.002	2.78 (−4)	244.750	1.01 (−1)	0.000	1.01 (−1)
6	3	0	♭ − 34.667	0	0.004	0	−132.060	1.13 (−2)	0.000	1.13 (−2)
		1	248.693	1.73 (−5)	-0.008	1.36 (−5)	153.044	9.52 (−2)	−0.042	4.83 (−2)
6	2	0	116.507	2.46 (−3)	−0.297	0	28.131	5.22 (−3)	0.052	4.84 (−3)
		1	385.374	7.26 (−4)	0.059	2.43 (−4)	298.670	2.45 (−2)	0.024	2.42 (−2)
6	1	0	223.914	1.41 (−2)	3.764	2.34 (−3)	146.724	1.41 (−2)	2.750	5.93 (−2)
6	0	0	295.806	6.91 (−1)			∗236.930	1.42 (+0)		
ε			1236.032				1190.874			

[a]The thresholds obtained from the PES of the LiHH$^+$ system are used. The threshold $\varepsilon_{0,0}$ lies 3707.4 cm^{-1} above the minimum of the PES. In comparison with the accurate data for D_2[1], the values of $\varepsilon_{v,j}-\varepsilon_{0,0}$ are too small by 0.075, 0.243, 0.490, −0.545, −0.297, 0.292, and 1.244 cm^{-1} for (v,j)=(0,2), (0,4), (0,6), (1,0), (1,2), (1,4), and (1,6), respectively. See Fig. B1 in Ref. 2 for a more detailed (and adequate) assessment of accuracy of the PES in the Li$^+$+HH fragmentation region.

[b]See the respective footnote in Table CII.

[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 ε_{10}) and to f-parity states in the $[\varepsilon_{1\,0},\,\varepsilon_{1\,2}]$ range are due to pure vibrational predissociation.

[e]J=0 resonances from the same PES were determined in Ref. 3. However, not all of them were assigned and for some resonances substantially larger widths were obtained (see the comments to Tables BI–BII in Part B). The cases with new information in the present table are marked with an asterisk.

TABLE CII: Li^+–D_2(I=1). Positions (E) and widths (Γ) of 'vibrational' levels $v_r\, b\, k\, v_R$ J=k p associated with the v=0–1 j=1–7 thresholds ($v_r{\sim}v$, $b{\sim}j$). The positions are relative to the respective $v\, j$=0 threshold. Positions of j>0 thresholds are shown in lines marked with ε. All data are in cm^{-1}.

			v=0 (ε=0)				v=1 (ε=2994.163) *0.545*[a]			
			p=1		p=−1		p=1		p=−1	
b	k	v_R	E^b	Γ^c	$E-E(p{=}1)^b$	Γ^c	E	Γ^d	$E-E(p{=}1)$	Γ^d
1	1	0	−1750.564	0	0.101	0	−1830.585	8.79 (−3)	0.103	8.40 (−3)
		1	−1417.064	0	0.095	0	−1494.364	2.55 (−2)	0.097	2.55 (−2)
		2	−1120.435	0	0.087	0	−1193.808	4.61 (−2)	0.089	4.61 (−2)
		3	♭ −860.603	0	0.079	0	−928.821	6.50 (−2)	0.081	6.50 (−2)
		4	♭ −637.420	0	0.070	0	−699.353	7.93 (−2)	0.074	8.01 (−2)
		5	∗ −450.175	0	0.060	0	−504.630	8.54 (−2)	0.063	8.54 (−2)
		6	∗ −297.870	0	0.050	0	−343.923	8.38 (−2)	0.053	8.38 (−2)
		7	∗ −178.706	0	0.041	0	−216.648	6.31 (−2)	0.236	7.25 (−2)
		8	∗ −89.621	0	0.037	0	−117.733	6.21 (−2)	0.042	6.20 (−2)
		9	∗ −26.538	0	0.026	0	−46.568	4.74 (−2)	0.033	4.73 (−2)
		10	15.750	0	0.015	0	2.343	3.24 (−2)	0.021	3.24 (−2)
		11	41.739	0	0.017	0	33.313	2.01 (−2)	0.017	2.01 (−2)
		12	55.598	0	0.019	0	50.606	1.00 (−2)	0.015	1.00 (−2)
1	0	0	−1332.321	0			−1406.703	9.00 (−3)		
		1	−1031.054	0			−1102.366	3.56 (−2)		
		2	−766.750	0			−833.388	5.55 (−2)		
		3	−539.672	0			−599.925	7.95 (−2)		
		4	−349.971	0			−402.052	9.25 (−2)		
		5	−198.973	0			−241.582	9.57 (−2)		
		6	−84.699	0			−115.754	8.73 (−2)		
		7	−7.309	0			−25.535	6.48 (−2)		
		8	37.696	∗0			29.418	3.87 (−2)		
		9	56.406	∗0			54.060	∗ 1.19 (−2)		
ε			59.755				57.583			
			-0.025[a]				*-0.087*[a]			
3	3	0	−1497.384	0	0.000	0	−1587.494	1.01 (−2)	0.000	1.01 (−2)
		1	−1161.650	0	0.000	0	−1249.109	3.01 (−2)	0.000	3.01 (−2)
		2	−862.859	0	0.004	0	−946.467	5.42 (−2)	0.000	5.42 (−2)
		3	♭ −600.547	0	−0.001	0	−679.270	7.63 (−2)	0.000	7.63 (−2)
		4	♭ −374.734	0	0.000	0	−447.359	9.19 (−2)	0.000	9.19 (−2)
		5	∗ −184.686	0	0.000	0	−250.169	9.90 (−2)	0.000	9.90 (−2)
		6	∗ −29.243	0	0.000	0	−86.743	9.75 (−2)	0.000	9.74 (−2)
		7	93.544	1.03 (−4)	0.000	1.03 (−4)	44.565	8.80 (−2)	0.000	8.80 (−2)
		8	186.639	7.81 (−5)	0.000	7.80 (−5)	146.145	7.38 (−2)	0.000	7.38 (−2)
		9	254.131	5.14 (−5)	0.000	5.23 (−5)	221.445	5.72 (−2)	0.000	5.72 (−2)
		10	300.827	2.81 (−5)	0.000	2.86 (−5)	274.638	4.13 (−2)	0.000	4.13 (−2)
		11	331.291	8.27 (−6)	0.000	8.33 (−6)	310.147	2.73 (−2)	0.000	2.73 (−2)
		12	349.133	4.57 (−6)	0.000	2.84 (−6)	331.813	1.59 (−2)	0.000	1.59 (−2)
3	2	0	−1178.105	0	0.000	0	−1260.178	1.14 (−2)	0.000	1.14 (−2)
		1	−869.749	0	0.005	0	−949.481	3.46 (−2)	0.019	3.49 (−2)
		2	−598.260	0	−0.185	0	−673.486	6.54 (−2)	0.010	6.52 (−2)
		3	♭ −362.739	0	−0.016	0	−432.759	9.45 (−2)	0.003	1.03 (−1)
		4	♭ −164.356	0	0.010	0	−227.391	1.13 (−1)	0.004	1.14 (−1)
		5	∗ −2.458	0	0.003	0	−57.204	1.20 (−1)	0.002	1.20 (−1)
		6	124.002	4.21 (−3)	0.002	4.09 (−3)	78.445	1.17 (−1)	0.001	1.17 (−1)
		7	217.280	3.15 (−3)	0.001	3.05 (−3)	181.249	9.78 (−2)	0.001	9.84 (−2)
		8	281.324	2.18 (−3)	0.002	2.11 (−3)	253.978	7.25 (−2)	0.001	7.24 (−2)
		9	321.879	1.42 (−3)	0.002	1.38 (−3)	301.201	4.72 (−2)	−0.001	4.73 (−2)
		10	355.856	1.14 (−3)	0.061	1.00 (−3)	328.548	2.96 (−2)	0.003	2.94 (−2)

TABLE CII: continued

3	1	0	♭ −880.887	0	0.212	0	−952.385	7.06 (−3)	0.199	7.08 (−3)
		1	♭ −603.130	0	−0.066	0	−672.917	2.73 (−2)	0.279	2.55 (−2)
		2	* −361.065	0	0.060	0	−425.505	2.76 (−2)	−0.844	4.33 (−2)
		3	* −155.168	0	0.095	0	−213.391	6.39 (−2)	−0.094	6.70 (−2)
		4	13.885	0	−0.155	0	−36.763	6.45 (−2)	−0.762	7.93 (−2)
		5	146.300	6.80 (−2)	−0.599	3.49 (−2)	102.587	3.14 (−1)	0.935	1.61 (−1)
		6	240.411	1.10 (−1)	0.955	2.56 (−2)	208.590	1.91 (−1)	0.607	1.33 (−1)
		7	302.944	5.29 (−2)	0.715	1.59 (−2)	280.475	1.19 (−1)	0.474	9.03 (−2)
		8	337.895	2.61 (−2)	0.611	8.25 (−3)	321.978	6.44 (−2)	0.449	4.87 (−2)
		9	353.712	1.19 (−2)	0.518	3.04 (−3)	340.432	2.57 (−2)	0.420	1.73 (−2)
3	0	0	−608.959	0			−666.235	5.04 (−3)		
		1	−372.362	0			−429.227	1.25 (−2)		
		2	−166.729	0			−218.723	2.45 (−2)		
		3	6.417	*0			−40.982	3.32 (−2)		
		4	141.103	3.74 (−1)			103.630	6.40 (−1)		
		5	242.103	2.88 (−1)			212.793	5.26 (−1)		
		6	305.985	1.79 (−1)			286.124	3.42 (−1)		
		7	340.659	8.60 (−2)			326.743	1.64 (−1)		
ε			357.166				344.183			
			-0.148[a]				*-0.503*[a]			
5	5	0	−1004.127	0	0.000	0	−1113.536	1.47 (−2)	0.000	1.47 (−2)
		1	−665.867	0	0.000	0	−772.700	3.91 (−2)	0.000	3.91 (−2)
		2	−364.375	0	0.000	0	−467.478	7.06 (−2)	0.000	7.06 (−2)
		3	−99.510	0	0.000	0	−197.753	1.06 (−1)	−0.008	1.01 (−1)
		4	129.080	5.52 (−8)	0.000	2.88 (−8)	36.774	1.20 (−1)	0.000	1.20 (−1)
		5	322.123	1.73 (−7)	0.000	2.10 (−7)	236.779	1.29 (−1)	0.000	1.29 (−1)
5	4	0	−744.331	0	0.000	0	−845.846	1.94 (−2)	0.000	1.94 (−2)
		1	−428.027	0	0.000	0	−527.146	5.62 (−2)	0.000	5.25 (−2)
		2	−148.399	0	0.008	0	−243.822	9.64 (−2)	0.000	9.64 (−2)
		3	94.371	3.63 (−6)	0.000	3.57 (−6)	4.241	1.35 (−1)	−0.001	1.36 (−1)
		4	300.522	6.69 (−7)	0.000	7.50 (−9)	216.834	1.62 (−1)	0.001	1.62 (−1)
5	3	0	♭ −511.426	0	0.000	0	−603.391	1.27 (−2)	0.000	1.25 (−2)
		1	♭ −216.598	0	0.000	0	−306.644	4.00 (−2)	0.000	4.00 (−2)
		2	41.616	0	0.000	0	−44.737	7.53 (−2)	0.001	7.53 (−2)
		3	262.827	1.53 (−5)	0.000	7.55 (−5)	181.678	1.07 (−1)	0.000	1.07 (−1)
5	2	0	♭ −310.174	0	0.006	0	−392.467	1.60 (−2)	−0.002	6.20 (−3)
		1	♭ −35.502	0	0.008	0	−116.487	2.49 (−2)	0.005	2.48 (−2)
		2	202.211	6.59 (−6)	0.007	7.45 (−8)	124.671	4.73 (−2)	−0.005	4.70 (−2)
5	1	0	* −150.432	0	0.767	0	−222.284	9.73 (−3)	1.917	7.52 (−3)
		1	107.568	8.62 (−4)	1.109	7.31 (−4)	37.715	1.08 (−2)	0.823	1.21 (−2)
		2	327.476	1.91 (−4)	0.846	1.28 (−3)	260.027	2.08 (−2)	0.733	2.31 (−2)
5	0	0	−48.984	0			−106.961	4.29 (−3)		
		1	205.236	1.78 (−4)			146.450	2.60 (−2)		
7	7	0	* −284.701	0	0.000	0	−421.892	4.71 (−4)	0.001	6.10 (−5)
		1	* 55.838	0	0.000	0	−78.789	6.25 (−2)	0.003	6.25 (−2)
		2	359.718	8.11 (−7)	0.000	9.87 (−7)	228.767	1.07 (−1)	0.005	1.07 (−1)
7	6	0	* −62.389	0	0.000	0	−192.352	3.34 (−2)	−0.002	3.34 (−2)
		1	259.863	3.41 (−8)	0.000	< 1 (−10)	132.353	9.20 (−2)	−0.002	9.20 (−2)
7	5	0	135.959	8.43 (−9)	0.000	6.80 (−9)	14.194	3.69 (−2)	−0.003	3.69 (−2)
		1	441.089	1.12 (−5)	0.000	1.10 (−5)	321.641	8.72 (−2)	−0.002	8.72 (−2)
7	4	0	308.693	2.84 (−5)	0.000	3.03 (−9)	194.692	1.98 (−2)	0.000	1.99 (−2)

[a]Deviation of the threshold position from the accurate value for D_2[1].

[b]Most of the bound state energies listed here and in Table CI (Γ=0 cases) were determined from the same PES in Ref. 3. However, the results presented in Tables 4 and 5 of that paper for cases marked here with the symbol ♭ disagree severly with the present results. Asterisks mark energies not determined in Ref. 3 or, when standing before the 0 width, bound states determined as resonances.

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

[d]Widths of levels below v=1 j=1 are due to vibrational predissociation.

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TABLE CIII: Li^+–D_2. Positions (E) and widths (Γ) of rotational levels (J) in thirty seven groups $(b\,k\,v_R)^a$ 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)^b.

				v_r=0		v_r=1			
b	k	v_R	J	$E(e)$	$E(f)-E(e)$	$E(e)$	$\Gamma(e)$	$E(f)-E(e)$	$\Gamma(f)$
0	0	0	0	−1783.613		1131.835	8.29 (−3)		
			1	−1780.534		1134.896	1.09 (−2)		
			2	−1774.381		1141.026	9.00 (−3)		
			3	−1765.158		1150.212	8.68 (−3)		
			4	−1752.875		1162.446	8.92 (−3)		
			5	−1737.544		1177.715	8.24 (−3)		
			6	−1719.179		1196.007	8.23 (−3)		
			7	−1697.800		1217.302	8.07 (−3)		
			8	−1673.427		1241.580	7.22 (−3)		
			9	−1646.085		1268.816	7.54 (−3)		
			10	−1615.800		1298.986	7.43 (−3)		
			11	−1582.603		1332.059	7.49 (−3)		
			12	−1546.527		1368.001	6.36 (−3)		
			13	−1507.609		1406.778	6.10 (−3)		
			14	−1465.888		1448.351	5.84 (−3)		
			15	−1421.406		1492.680	5.49 (−3)		
			16	−1374.210		1539.718	5.18 (−3)		
			17	−1324.348		1589.420	4.90 (−3)		
			18	−1271.873		1641.733	4.88 (−3)		
			19	−1216.840		1696.605	4.04 (−3)		
			20	−1159.307		1753.977	3.75 (−3)		
			21	−1099.339		1813.791	3.52 (−3)		
			22	−1037.001		1875.981	3.48 (−3)		
			23	−972.363		1940.483	3.64 (−3)		
			24	−905.500		2007.219	2.66 (−3)		
			25	−836.491		2076.120	2.85 (−3)		
			26	−765.420		2147.105	2.06 (−3)		
			27	−692.376		2220.087	1.83 (−3)		
			28	−617.454		2294.979	1.62 (−3)		
			29	−540.755		2371.684	1.42 (−3)		
			30	−462.389		2450.101	1.22 (−3)		
			31	−382.473		2530.121	1.04 (−3)		
			32	−301.135		2611.625	9.00 (−4)		
			33	−218.514		2694.487	7.84 (−4)		
			34	−134.765		2778.568	5.80 (−4)		
			35	−50.058		2863.712	4.79 (−4)		
1	1	0	1	−1750.564	0.101	1163.578	8.79 (−3)	0.103	8.40 (−3)
			2	−1744.520	0.302	1169.596	9.27 (−3)	0.308	8.34 (−3)
			3	−1735.461	0.604	1178.616	9.00 (−3)	0.615	8.26 (−3)
			4	−1723.394	1.004	1190.631	8.65 (−3)	1.022	8.16 (−3)
			5	−1708.331	1.502	1205.630	8.38 (−3)	1.529	8.03 (−3)
			6	−1690.285	2.096	1223.601	8.17 (−3)	2.133	7.87 (−3)
			7	−1669.271	2.784	1244.527	8.01 (−3)	2.833	7.71 (−3)
			8	−1645.310	3.563	1268.390	8.05 (−3)	3.627	7.53 (−3)
			9	−1618.421	4.431	1295.171	9.17 (−3)	4.510	7.64 (−3)
			10	−1588.629	5.385	1324.844	7.26 (−3)	5.481	7.20 (−3)

TABLE CIII: continued

			11	−1555.963	6.421	1357.382	6.77 (−3)	6.537	7.94 (−3)
			12	−1520.450	7.536	1392.758	6.49 (−3)	7.675	6.23 (−3)
			13	−1482.125	8.726	1430.940	6.66 (−3)	8.888	6.11 (−3)
			14	−1441.023	9.986	1471.893	5.88 (−3)	10.174	8.44 (−3)
			15	−1397.183	11.311	1515.577	5.78 (−3)	11.526	6.59 (−3)
			16	−1350.646	12.698	1561.957	5.03 (−3)	12.941	5.00 (−3)
			17	−1301.459	14.139	1610.982	4.72 (−3)	14.415	4.69 (−3)
			18	−1249.668	15.630	1662.612	5.18 (−3)	15.939	4.48 (−3)
			19	−1195.326	17.164	1716.794	5.48 (−3)	17.507	4.91 (−3)
			20	−1138.489	18.734	1773.473	3.91 (−3)	19.118	3.99 (−3)
			21	−1079.213	20.335	1832.596	3.73 (−3)	20.759	3.69 (−3)
			22	−1017.564	21.959	1894.101	4.12 (−3)	22.426	3.38 (−3)
			23	−953.607	23.597	1957.926	2.95 (−3)	24.110	3.00 (−3)
			24	−887.413	25.242	2024.000	2.68 (−3)	25.804	2.72 (−3)
			25	−819.058	26.886	2092.252	2.45 (−3)	27.499	2.42 (−3)
			36	47.447[c]		2960.470	4.18 (−4)	43.211	4.35 (−4)
2	2	0	2	−1654.734	0.000	1255.572	9.31 (−3)	0.000	9.31 (−3)
			3	−1645.564	−0.001	1264.709	9.18 (−3)	−0.001	9.18 (−3)
			4	−1633.349	−0.003	1276.880	9.02 (−3)	−0.003	9.01 (−3)
			5	−1618.100	−0.006	1292.075	8.83 (−3)	−0.007	8.83 (−3)
			6	−1599.829	−0.012	1310.282	8.62 (−3)	−0.014	8.62 (−3)
			7	−1578.553	−0.022	1331.484	8.39 (−3)	−0.025	8.39 (−3)
			8	−1554.291	−0.036	1355.665	8.18 (−3)	−0.042	8.14 (−3)
			9	−1527.062	−0.057	1382.803	7.99 (−3)	−0.064	7.87 (−3)
			10	−1496.892	−0.084	1412.877	7.61 (−3)	−0.095	7.58 (−3)
			11	−1463.807	−0.119	1445.858	7.32 (−3)	−0.136	7.29 (−3)
			12	−1427.837	−0.164	1481.719	7.04 (−3)	−0.187	6.99 (−3)
			13	−1389.016	−0.220	1520.428	7.52 (−3)	−0.251	6.80 (−3)
			14	−1347.379	−0.288	1561.951	6.31 (−3)	−0.328	1.05 (−2)
			15	−1302.966	−0.369	1606.247	5.85 (−3)	−0.422	5.81 (−3)
			16	−1255.820	−0.463	1653.276	5.51 (−3)	−0.531	5.48 (−3)
			17	−1205.987	−0.573	1702.995	5.20 (−3)	−0.657	5.16 (−3)
			18	−1153.517	−0.696	1755.353	5.17 (−3)	−0.800	4.99 (−3)
			19	−1098.464	−0.835	1810.301	4.32 (−3)	−0.962	4.68 (−3)
			20	−1040.885	−0.989	1867.781	4.05 (−3)	−1.140	4.00 (−3)
			21	−980.844	−1.157	1927.734	3.67 (−3)	−1.337	3.70 (−3)
			22	−918.407	−1.337	1990.096	3.33 (−3)	−1.549	3.26 (−3)
			23	−853.645	−1.529	2054.798	3.04 (−3)	−1.776	3.03 (−3)
			24	−786.634	−1.730	2121.767	2.87 (−3)	−2.017	3.09 (−3)
			25	−717.458	−1.937	2190.925	2.68 (−3)	−2.267	2.47 (−3)
3	3	0	3	−1497.384	0.000	1406.669	1.01 (−2)	0.000	1.01 (−2)
			4	−1485.257	0.000	1418.757	9.90 (−3)	0.000	9.90 (−3)
			5	−1470.118	0.000	1433.860	1.01 (−2)	0.001	1.00 (−2)
			6	−1451.983	0.000	1451.930	9.72 (−3)	0.000	9.57 (−3)
			7	−1430.866	0.000	1472.982	9.87 (−3)	0.000	9.30 (−3)
			8	−1406.788	0.000	1496.988	9.09 (−3)	0.000	8.86 (−3)
			9	−1379.770	0.001	1523.925	8.12 (−3)	−0.001	8.09 (−3)
			10	−1349.839	0.001	1553.772	8.14 (−3)	0.001	7.81 (−3)
			11	−1317.021	0.002	1586.497	8.78 (−3)	0.003	7.95 (−3)
			12	−1281.348	0.004	1622.084	9.85 (−3)	−0.007	7.21 (−3)
			13	−1242.855	0.006	1660.468	8.53 (−3)	0.004	7.55 (−3)
			14	−1201.578	0.009	1701.642	7.19 (−3)	0.007	7.21 (−3)
			15	−1157.559	0.015	1745.557	6.78 (−3)	0.012	6.79 (−3)

TABLE CIII: continued

			16	−1110.842	0.022	1792.171	6.36 (−3)	0.018	6.36 (−3)
			17	−1061.474	0.032	1841.438	6.08 (−3)	0.026	5.96 (−3)
			18	−1009.507	0.046	1893.308	5.98 (−3)	0.035	5.62 (−3)
			19	−954.997	0.066	1947.727	5.11 (−3)	0.053	6.00 (−3)
			20	−898.005	0.094	2004.639	4.70 (−3)	0.072	4.70 (−3)
			21	−838.596	0.134	2063.982	4.31 (−3)	0.099	4.29 (−3)
			22	−776.843	0.191	2125.689	3.99 (−3)	0.137	3.94 (−3)
			23	−712.826	0.274	2189.687	8.07 (−3)	0.191	4.18 (−3)
			24	−646.641	0.403	2255.903	3.17 (−3)	0.259	3.18 (−3)
			25	−578.405	0.610	2324.242	2.81 (−3)	0.361	2.78 (−3)
4	4	0	4	−1279.949	0.000	1615.557	1.21 (−2)	0.000	1.21 (−2)
			5	−1264.952	0.000	1630.521	1.18 (−2)	0.000	1.18 (−2)
			6	−1246.985	0.000	1648.452	1.15 (−2)	0.000	1.15 (−2)
			7	−1226.063	0.000	1669.331	1.11 (−2)	0.000	1.10 (−2)
			8	−1202.206	0.000	1693.141	1.06 (−2)	0.000	1.04 (−2)
			9	−1175.435	0.001	1719.863	1.51 (−2)	−0.002	1.31 (−2)
			10	−1145.776	0.002	1749.464	1.06 (−2)	0.001	1.27 (−2)
			11	−1113.258	0.005	1781.923	9.86 (−3)	0.000	9.89 (−3)
			12	−1077.916	0.014	1817.209	1.01 (−2)	0.000	9.94 (−3)
			13	−1039.794	0.040	1855.286	9.32 (−3)	0.002	8.32 (−3)
			14	−999.013	0.165	1896.122	8.81 (−3)	0.002	8.92 (−3)
			15	−954.915	−0.308	1939.673	7.88 (−3)	0.005	7.95 (−3)
			16	−908.735	−0.188	1985.896	7.40 (−3)	0.011	7.30 (−3)
			17	−859.821	−0.176	2034.744	7.76 (−3)	0.023	7.31 (−3)
			18	−808.304	−0.189	2086.166	6.43 (−3)	0.044	6.59 (−3)
			19	−754.251	−0.217	2140.097	6.40 (−3)	0.083	5.98 (−3)
			20	−697.723	−0.257	2196.463	6.21 (−3)	0.161	5.76 (−3)
			21	−638.782	−0.311	2255.131	5.21 (−3)	0.333	3.79 (−2)
			22	−577.493	−0.381	2315.797	4.53 (−3)	0.897	4.85 (−3)
			23	−513.927	−0.472	2381.751	4.05 (−3)	−1.565	4.36 (−3)
			24	−448.157	−0.592	2446.919	3.82 (−3)	−1.028	3.91 (−3)
			25	−380.262	−0.751	2514.592	3.56 (−3)	−0.860	3.48 (−3)
5	5	0	5	−1004.127	0.000	1880.627	1.47 (−2)	0.000	1.47 (−2)
			6	−986.367	−0.043	1898.352	1.42 (−2)	0.000	1.42 (−2)
			7	−965.689	0.000	1918.991	1.38 (−2)	0.000	1.37 (−2)
			8	−942.110	0.000	1942.526	1.32 (−2)	0.000	1.33 (−2)
			9	−915.653	0.000	1968.936	1.27 (−2)	0.000	1.27 (−2)
			10	−886.341	0.000	1998.197	1.24 (−2)	0.001	1.22 (−2)
			11	−854.203	0.000	2030.283	1.16 (−2)	−0.001	1.20 (−2)
			12	−819.268	0.000	2065.165	1.31 (−2)	0.003	1.54 (−2)
			13	−781.569	0.000	2102.806	1.10 (−2)	0.003	1.64 (−2)
			14	−741.144	0.000	2143.174	9.83 (−3)	0.004	1.90 (−2)
			15	−698.030	0.000	2186.231	1.15 (−2)	0.006	1.38 (−2)
			16	−652.271	0.000	2231.938	9.33 (−3)	0.001	9.77 (−3)
			17	−603.913	0.000	2280.246	8.69 (−3)	0.000	1.21 (−2)
			18	−553.004	0.000	2331.109	7.77 (−3)	0.001	8.01 (−3)
			19	−499.597	0.000	2384.476	7.01 (−3)	0.000	7.03 (−3)
			20	−443.748	0.000	2440.292	7.02 (−3)	0.000	7.31 (−3)

TABLE CIII: continued

0	0	1	0	−1450.470		1467.733	2.52 (−2)		
			1	−1447.596		1470.601	2.51 (−2)		
			2	−1441.852		1476.334	2.50 (−2)		
			3	−1433.243		1484.926	2.47 (−2)		
			4	−1421.779		1496.368	2.43 (−2)		
			5	−1407.473		1510.647	2.39 (−2)		
			6	−1390.341		1527.749	2.32 (−2)		
			7	−1370.400		1547.654	2.33 (−2)		
			8	−1347.674		1570.341	2.29 (−2)		
			9	−1322.188		1595.785	2.10 (−2)		
			10	−1293.971		1623.959	2.04 (−2)		
			11	−1263.053		1654.832	1.96 (−2)		
			12	−1229.471		1688.370	1.88 (−2)		
			13	−1193.262		1724.534	1.78 (−2)		
			14	−1154.469		1763.286	1.71 (−2)		
			15	−1113.137		1804.580	1.61 (−2)		
			16	−1069.316		1848.370	1.47 (−2)		
			17	−1023.057		1894.605	1.39 (−2)		
			18	−974.418		1943.230	1.28 (−2)		
			19	−923.459		1994.187	1.18 (−2)		
			20	−870.245		2047.415	1.13 (−2)		
			21	−814.845		2102.848	1.02 (−2)		
			22	−757.333		2160.414	9.08 (−3)		
			23	−697.790		2220.039	8.20 (−3)		
			24	−636.299		2281.644	7.37 (−3)		
			25	−572.953		2345.141	6.52 (−3)		
1	1	1	1	−1417.064	0.095	1499.799	2.55 (−2)	0.097	2.55 (−2)
			2	−1411.422	0.284	1505.429	2.49 (−2)	0.289	2.50 (−2)
			3	−1402.966	0.566	1513.866	2.46 (−2)	0.577	2.47 (−2)
			4	−1391.705	0.941	1525.103	2.44 (−2)	0.960	2.45 (−2)
			5	−1377.649	1.408	1539.129	2.41 (−2)	1.435	2.42 (−2)
			6	−1360.812	1.963	1555.932	2.37 (−2)	2.002	2.33 (−2)
			7	−1341.212	2.605	1575.492	2.27 (−2)	2.658	2.29 (−2)
			8	−1318.868	3.332	1597.792	2.22 (−2)	3.400	2.24 (−2)
			9	−1293.803	4.140	1622.811	2.26 (−2)	4.225	2.23 (−2)
			10	−1266.042	5.027	1650.522	2.09 (−2)	5.132	2.13 (−2)
			11	−1235.615	5.988	1680.899	2.03 (−2)	6.115	2.02 (−2)
			12	−1202.552	7.020	1713.911	1.94 (−2)	7.170	1.93 (−2)
			13	−1166.889	8.117	1749.524	1.87 (−2)	8.293	1.85 (−2)
			14	−1128.663	9.275	1787.701	1.73 (−2)	9.481	1.74 (−2)
			15	−1087.917	10.489	1828.403	1.64 (−2)	10.727	1.64 (−2)
			16	−1044.694	11.752	1871.586	1.54 (−2)	12.024	1.54 (−2)
			17	−999.042	13.058	1917.205	1.45 (−2)	13.369	1.44 (−2)
			18	−951.014	14.400	1965.209	1.41 (−2)	14.753	1.33 (−2)
			19	−900.663	15.770	2015.546	1.20 (−2)	16.168	1.23 (−2)
			20	−848.049	17.158	2068.158	1.11 (−2)	17.609	1.13 (−2)
			21	−793.232	18.555	2122.985	1.02 (−2)	19.064	1.03 (−2)
			22	−736.277	19.945	2179.965	9.36 (−3)	20.525	9.38 (−3)
			23	−677.249	21.312	2239.029	8.43 (−3)	21.978	9.97 (−3)
			24	−616.208	22.629	2300.107	8.69 (−3)	23.410	7.52 (−3)
			25	−553.205	23.852	2363.131	6.52 (−3)	24.799	6.77 (−3)

TABLE CIII: continued

2	2	1	2	−1320.255	0.000	1592.713	2.72 (−2)	0.000	2.73 (−2)
			3	−1311.694	−0.001	1601.260	2.69 (−2)	−0.001	2.70 (−2)
			4	−1300.292	−0.002	1612.641	2.65 (−2)	−0.002	2.66 (−2)
			5	−1286.062	−0.004	1626.844	2.60 (−2)	−0.005	2.61 (−2)
			6	−1269.019	−0.009	1643.855	2.54 (−2)	−0.010	2.55 (−2)
			7	−1249.178	−0.015	1663.658	2.48 (−2)	−0.018	2.48 (−2)
			8	−1226.562	−0.025	1686.234	2.42 (−2)	−0.030	2.41 (−2)
			9	−1201.193	−0.039	1711.563	2.41 (−2)	−0.046	2.33 (−2)
			10	−1173.097	−0.057	1739.618	2.22 (−2)	−0.068	2.29 (−2)
			11	−1142.305	−0.081	1770.371	2.13 (−2)	−0.096	2.14 (−2)
			12	−1108.850	−0.110	1803.792	2.04 (−2)	−0.131	2.04 (−2)
			13	−1072.766	−0.146	1839.845	1.95 (−2)	−0.175	1.94 (−2)
			14	−1034.094	−0.189	1878.493	1.89 (−2)	−0.227	1.85 (−2)
			15	−992.878	−0.240	1919.697	1.81 (−2)	−0.290	1.71 (−2)
			16	−949.164	−0.297	1963.406	1.63 (−2)	−0.361	1.63 (−2)
			17	−903.003	−0.362	2009.578	1.60 (−2)	−0.443	1.80 (−2)
			18	−854.452	−0.434	2058.154	1.40 (−2)	−0.533	1.39 (−2)
			19	−803.569	−0.512	2109.079	1.31 (−2)	−0.633	1.29 (−2)
			20	−750.420	−0.594	2162.292	1.20 (−2)	−0.740	1.22 (−2)
			21	−695.076	−0.679	2217.727	1.09 (−2)	−0.855	1.11 (−2)
			22	−637.611	−0.765	2275.310	1.02 (−2)	−0.973	9.97 (−3)
			23	−578.107	−0.849	2334.966	9.07 (−3)	−1.094	9.02 (−3)
			24	−516.655	−0.926	2396.609	8.12 (−3)	−1.213	8.66 (−3)
			25	−453.348	−0.993	2460.150	7.22 (−3)	−1.327	7.27 (−3)
3	3	1	3	−1161.650	0.000	1745.054	3.01 (−2)	0.000	3.01 (−2)
			4	−1150.310	0.000	1756.437	2.89 (−2)	0.000	2.89 (−2)
			5	−1136.155	0.000	1770.673	2.72 (−2)	0.000	2.71 (−2)
			6	−1119.197	0.000	1787.777	2.48 (−2)	−0.001	2.45 (−2)
			7	−1099.449	0.000	1807.774[g]	2.26 (−2)	−0.008	2.11 (−2)
			8	−1076.926	0.001	1828.447[g]	2.00 (−2)	−0.013	1.99 (−2)
			9	−1051.637	0.002	1853.758	2.15 (−2)	−0.015	2.32 (−2)
			10	−1023.587	0.003	1881.723	2.25 (−2)	−0.015	2.28 (−2)
			11	−992.757	0.005	1912.331	2.21 (−2)	−0.014	2.20 (−2)
			12	−959.106	0.004	1945.558	2.17 (−2)	−0.014	2.16 (−2)
			13	−922.586	−0.001	1981.376	2.18 (−2)	−0.011	2.14 (−2)
			14	−887.347	−0.023	2019.750	2.01 (−2)	−0.007	1.99 (−2)
			15	−846.273	−0.002	2060.638	1.91 (−2)	0.001	1.90 (−2)
			16	−802.830	0.031	2103.993	1.81 (−2)	0.014	1.80 (−2)
			17	−757.049	0.089	2149.762	1.70 (−2)	0.037	1.70 (−2)
			18	−708.997	0.197	2197.885	1.59 (−2)	0.075	1.58 (−2)
			19	−658.787	0.410	2248.296	1.48 (−2)	0.136	1.61 (−2)
			20	−606.644	0.884	2300.907	1.38 (−2)	0.243	1.34 (−2)
4	4	1	4	−942.932	0.000	1955.164	3.41 (−2)	0.000	3.41 (−2)
			5	−928.919	0.000	1969.159	3.32 (−2)	0.014	3.34 (−2)
			6	−912.134	0.000	1985.956	3.29 (−2)	−0.005	3.24 (−2)
			7	−892.594	0.000	2005.496	3.15 (−2)	−0.008	3.14 (−2)
			8	−870.319	0.000	2027.772	3.16 (−2)	−0.014	3.21 (−2)
			9	−845.331	0.000	2052.765	3.03 (−2)	−0.031	3.25 (−2)
			10	−817.655	0.001	2080.450	2.82 (−2)	−0.067	2.82 (−2)
			11	−787.322	0.001	2110.798	2.88 (−2)	−0.140	2.75 (−2)
			12	−754.361	0.002	2143.781	2.72 (−2)	−0.289	2.63 (−2)
			13	−718.808	0.004	2179.365	2.58 (−2)	−0.554	2.45 (−2)
			14	−680.701	0.007	2217.513	2.43 (−2)	0.515	2.28 (−2)
			15	−640.081	0.011	2258.188	2.28 (−2)	0.502	2.16 (−2)
			16	−596.993	0.017	2301.346	2.13 (−2)	0.517	2.02 (−2)
			17	−551.483	0.027	2346.944	1.98 (−2)	0.552	1.87 (−2)
			18	−503.603	0.040	2394.940	2.65 (−2)	0.595	1.76 (−2)
			19	−453.429	0.083	2445.269	1.67 (−2)	0.669	1.62 (−2)
			20	−400.945	0.084	2497.895	1.51 (−2)	0.742	1.65 (−2)

TABLE CIII: continued

0	0	2	0	−1154.270		1767.906	4.55 (−2)		
			1	−1151.608		1770.570	4.51 (−2)		
			2	−1146.287		1775.896	4.48 (−2)		
			3	−1138.313		1783.876	4.43 (−2)		
			4	−1127.697		1794.501	4.36 (−2)		
			5	−1114.452		1807.759	4.28 (−2)		
			6	−1098.594		1823.632	4.19 (−2)		
			7	−1080.145		1842.102	4.09 (−2)		
			8	−1059.126		1863.146	3.95 (−2)		
			9	−1035.566		1886.738	3.82 (−2)		
			10	−1009.494		1912.848	3.68 (−2)		
			11	−980.945		1941.444	3.49 (−2)		
			12	−949.957		1972.489	3.37 (−2)		
			13	−916.571		2005.943	3.20 (−2)		
			14	−880.833		2041.763	3.03 (−2)		
			15	−842.792		2079.901	2.82 (−2)		
			16	−802.502		2120.306	2.64 (−2)		
			17	−760.022		2162.923	2.46 (−2)		
			18	−715.413		2207.692	2.27 (−2)		
			19	−668.746		2254.549	2.09 (−2)		
			20	−620.092		2303.425	1.92 (−2)		
1	1	2	1	−1120.435	0.087	1800.355	4.61 (−2)	0.089	4.61 (−2)
			2	−1115.207	0.261	1805.585	4.51 (−2)	0.268	4.57 (−2)
			3	−1107.373	0.521	1813.423	4.52 (−2)	0.534	4.52 (−2)
			4	−1096.941	0.867	1823.861	4.45 (−2)	0.887	4.46 (−2)
			5	−1083.923	1.295	1836.886	4.39 (−2)	1.327	4.37 (−2)
			6	−1068.333	1.805	1852.487	4.48 (−2)	1.848	4.28 (−2)
			7	−1050.191	2.393	1870.643	4.22 (−2)	2.451	4.17 (−2)
			8	−1029.516	3.058	1891.335	4.07 (−2)	3.133	4.04 (−2)
			9	−1006.332	3.795	1914.540	3.93 (−2)	3.890	3.91 (−2)
			10	−980.666	4.601	1940.232	3.78 (−2)	4.719	3.76 (−2)
			11	−952.548	5.471	1968.382	3.62 (−2)	5.615	3.60 (−2)
			12	−922.011	6.399	1998.958	3.45 (−2)	6.574	3.44 (−2)
			13	−889.089	7.380	2031.925	3.31 (−2)	7.590	3.26 (−2)
			14	−853.819	8.403	2067.245	3.07 (−2)	8.656	3.09 (−2)
			15	−816.236	9.457	2104.878	2.89 (−2)	9.766	2.90 (−2)
			16	−776.373	10.522	2144.781	2.70 (−2)	10.909	2.72 (−2)
			17	−734.242	11.557	2186.913	2.51 (−2)	12.072	2.53 (−2)
			18	−689.782	12.448	2231.237	2.32 (−2)	13.234	2.34 (−2)
			19	−642.519	12.676	2277.736	2.13 (−2)	14.349	2.15 (−2)
			20	−596.587	16.363	2326.485	1.90 (−2)	15.280	1.96 (−2)
2	2	2	2	−1022.590	0.000	1894.235	4.92 (−2)	0.000	4.90 (−2)
			3	−1014.663	0.000	1902.165	4.87 (−2)	−0.001	4.85 (−2)
			4	−1004.108	−0.001	1912.727	4.77 (−2)	−0.002	4.78 (−2)
			5	−990.936	−0.002	1925.911	4.68 (−2)	−0.003	4.69 (−2)
			6	−975.164	−0.005	1941.700	4.59 (−2)	−0.006	4.59 (−2)
			7	−956.810	−0.008	1960.079	4.44 (−2)	−0.012	4.56 (−2)
			8	−935.897	−0.014	1981.024	4.32 (−2)	−0.018	4.31 (−2)
			9	−912.449	−0.021	2004.511	4.20 (−2)	−0.028	4.20 (−2)
			10	−886.497	−0.030	2030.513	4.00 (−2)	−0.041	4.15 (−2)
			11	−858.072	−0.042	2058.996	3.84 (−2)	−0.058	3.85 (−2)
			12	−827.213	−0.056	2089.927	3.66 (−2)	−0.078	3.73 (−2)
			13	−793.958	−0.072	2123.267	3.49 (−2)	−0.102	3.48 (−2)
			14	−758.353	−0.091	2158.973	3.30 (−2)	−0.130	3.31 (−2)
			15	−720.447	−0.111	2196.999	3.11 (−2)	−0.162	3.10 (−2)
			16	−680.292	−0.131	2237.295	2.91 (−2)	−0.197	2.91 (−2)
			17	−637.948	−0.151	2279.805	2.71 (−2)	−0.235	2.71 (−2)
			18	−593.477	−0.170	2324.470	2.51 (−2)	−0.274	2.51 (−2)
			19	−546.950	−0.184	2371.225	2.31 (−2)	−0.312	2.31 (−2)
			20	−498.440	−0.190	2420.000	2.14 (−2)	−0.347	2.11 (−2)

TABLE CIII: continued

0	0	3	0	−894.963		2032.430	6.41 (−2)		
			1	−892.521		2034.883	6.38 (−2)		
			2	−887.639		2039.787	6.34 (−2)		
			3	−880.325		2047.134	6.25 (−2)		
			4	−870.589		2056.914	6.16 (−2)		
			5	−858.447		2069.114	6.05 (−2)		
			6	−843.915		2083.715	5.91 (−2)		
			7	−827.016		2100.698	5.73 (−2)		
			8	−807.775		2120.039	5.56 (−2)		
			9	−786.221		2141.708	5.36 (−2)		
			10	−762.387		2165.676	5.15 (−2)		
			11	−736.309		2191.907	4.92 (−2)		
			12	−708.027		2220.364	4.67 (−2)		
			13	−677.570		2251.013	4.43 (−2)		
			14	−645.239		2283.877	3.96 (−2)		
			15	−610.538		2318.413	3.82 (−2)		
			16	−573.954		2355.360	3.65 (−2)		
			17	−535.456		2394.198	3.39 (−2)		
			18	−495.108		2434.918	3.13 (−2)		
			19	−452.963		2477.455	2.86 (−2)		
			20	−409.179		2521.733	2.60 (−2)		
1	1	3	1	−860.603	0.079	2065.342	6.50 (−2)	0.081	6.50 (−2)
			2	−855.799	0.236	2070.163	6.49 (−2)	0.243	6.51 (−2)
			3	−848.600	0.471	2077.386	6.40 (−2)	0.486	6.43 (−2)
			4	−839.012	0.782	2087.004	6.29 (−2)	0.806	6.33 (−2)
			5	−827.043	1.164	2099.005	6.17 (−2)	1.204	6.21 (−2)
			6	−812.696	1.610	2113.375	6.02 (−2)	1.677	6.08 (−2)
			7	−795.955	2.096	2130.099	5.85 (−2)	2.223	5.97 (−2)
			8	−776.700[e]	2.506	2149.160	5.66 (−2)	2.837	6.02 (−2)
			9	−756.757[e]	4.694	2170.544	5.45 (−2)	3.526	5.39 (−2)
			10	−732.351	5.157	2194.243[d]	5.25 (−2)	4.525[d]	3.77 (−2)[d]
			11	−708.675	5.192	2220.309[d]	4.93 (−2)	4.771[d]	4.97 (−2)[d]
			12	−680.202	6.230	2248.612	4.03 (−2)	5.581	4.72 (−2)
			13	−650.007	7.795	2280.020	3.30 (−2)	5.664	4.34 (−2)
			14	−617.853	6.569	2315.046	2.32 (−2)	4.820	3.73 (−2)
			15	−583.719	7.848	2353.315	1.83 (−2)	4.045	2.85 (−2)
			16	−547.635	8.978	2394.205	1.58 (−2)	3.928	2.30 (−2)
			17	−509.654	10.061	2437.486	1.42 (−2)	4.092	2.78 (−2)
			18	−469.839	11.127	2483.047	1.37 (−2)	4.393	1.81 (−2)
			19	−428.263	12.182	2530.807	1.19 (−2)	4.732	1.61 (−2)
			20	−385.008	13.224	2580.690	1.08 (−2)	5.102	1.46 (−2)
2	2	3	2	−761.687	0.000	2160.169	6.95 (−2)	0.000	6.96 (−2)
			3	−754.413	0.000	2167.478	6.87 (−2)	0.000	6.88 (−2)
			4	−744.729	0.000	2177.209	6.76 (−2)	−0.001	6.76 (−2)
			5	−732.650	0.000	2189.346	6.63 (−2)	−0.001	6.63 (−2)
			6	−718.194	−0.001	2203.876	6.48 (−2)	−0.002	6.48 (−2)
			7	−701.381	−0.001	2220.776	6.31 (−2)	−0.004	6.31 (−2)
			8	−682.236	−0.002	2240.025	6.11 (−2)	−0.007	6.11 (−2)
			9	−660.787	−0.002	2261.594	5.90 (−2)	−0.010	5.90 (−2)
			10	−637.068	−0.002	2285.454	5.66 (−2)	−0.013	5.66 (−2)
			11	−611.115	0.000	2311.568	5.41 (−2)	−0.017	5.42 (−2)
			12	−582.970	0.002	2339.899	5.15 (−2)	−0.022	5.16 (−2)
			13	−552.677	0.008	2370.403	4.88 (−2)	−0.025	4.89 (−2)
			14	−520.288	0.017	2403.033	4.61 (−2)	−0.028	4.61 (−2)
			15	−485.860	0.032	2437.735	4.33 (−2)	−0.027	4.32 (−2)
			16	−449.454	0.055	2474.454	4.03 (−2)	−0.023	4.03 (−2)
			17	−411.138	0.090	2513.125	3.74 (−2)	−0.012	3.74 (−2)
			18	−370.989	0.140	2553.679	3.44 (−2)	0.008	3.45 (−2)
			19	−329.091	0.213	2596.039	3.16 (−2)	0.042	3.16 (−2)
			20	−285.538	0.317	2640.122	2.87 (−2)	0.094	2.88 (−2)

TABLE CIII: continued

1	0	0	0	−1332.321		1587.460	9.00 (−3)		
			1	−1329.365		1590.397	9.36 (−3)		
			2	−1323.458		1596.271	1.46 (−2)		
			3	−1314.604		1605.075	1.00 (−2)		
			4	−1302.814		1616.797	8.81 (−3)		
			5	−1288.100		1631.427	9.15 (−3)		
			6	−1270.479		1648.946	8.87 (−3)		
			7	−1249.969		1669.341	9.56 (−3)		
			8	−1226.593		1692.586	9.25 (−3)		
			9	−1200.377		1718.657	8.96 (−3)		
			10	−1171.350		1747.526	8.64 (−3)		
			11	−1139.543		1779.163	8.47 (−3)		
			12	−1104.991		1813.533	7.93 (−3)		
			13	−1067.734		1850.598	7.27 (−3)		
			14	−1027.813		1890.318	6.88 (−3)		
			15	−985.273		1932.650	6.47 (−3)		
			16	−940.162		1977.547	6.06 (−3)		
			17	−892.533		2024.959	5.66 (−3)		
			18	−842.441		2074.833	5.30 (−3)		
			19	−789.944		2127.112	5.69 (−3)		
			20	−735.107		2181.737	4.38 (−3)		
			21	−677.996		2238.655	3.91 (−3)		
			22	−618.681		2297.761	3.53 (−3)		
			23	−557.239		2359.023	3.17 (−3)		
			24	−493.750		2422.351	3.17 (−3)		
			25	−428.300		2487.665	2.60 (−3)		
2	1	0	1	−1292.413	0.134	1625.290	1.26 (−2)	0.133	1.03 (−2)
			2	−1286.653	0.403	1631.016	1.38 (−2)	0.402	1.03 (−2)
			3	−1278.021	0.804	1639.603	1.07 (−2)	0.799	1.02 (−2)
			4	−1266.523	1.338	1651.040	9.93 (−3)	1.327	1.00 (−2)
			5	−1252.172	2.002	1665.316	9.57 (−3)	1.985	9.89 (−3)
			6	−1234.980	2.793	1682.418	1.00 (−2)	2.769	9.84 (−3)
			7	−1214.965	3.710	1702.332	9.71 (−3)	3.678	1.03 (−2)
			8	−1192.144	4.749	1725.036	8.77 (−3)	4.708	9.96 (−3)
			9	−1166.540	5.907	1750.511	8.33 (−3)	5.858	9.95 (−3)
			10	−1138.177	7.179	1778.732	8.07 (−3)	7.121	9.68 (−3)
			11	−1107.081	8.560	1809.673	1.09 (−2)	8.494	8.59 (−3)
			12	−1073.279	10.041	1843.305	7.72 (−3)	9.970	1.11 (−2)
			13	−1036.796	11.609	1879.595	7.09 (−3)	11.549	6.86 (−3)
			14	−997.582	13.170	1918.506	6.48 (−3)	13.223	6.51 (−3)
			15	−956.375	15.420	1960.004	7.78 (−3)	14.991	8.30 (−3)
			16	−912.030	17.162	2004.046	5.70 (−3)	16.836	2.98 (−2)
			17	−865.290	19.087	2050.591	5.31 (−3)	18.749	1.56 (−2)
			18	−816.123	21.108	2099.595	5.92 (−3)	20.728	4.88 (−3)
			19	−764.572	23.206	2151.014	5.31 (−3)	22.751	5.24 (−3)
			20	−710.690	25.370	2204.819	4.40 (−3)	24.790	4.40 (−3)
			21	−654.539	27.594	2261.016	4.17 (−3)	26.768	4.36 (−3)
			22	−596.184	29.872	2319.789	4.04 (−3)	28.431	3.86 (−3)
			23	−535.697	32.199	2381.751	4.05 (−3)	29.091	3.44 (−3)
			24	−473.155	34.573	2446.919	3.82 (−3)	28.649	3.04 (−3)
			25	−408.641	36.996	2514.592	3.56 (−3)	27.721	2.68 (−3)
3	2	0	2	−1178.105	0.000	1733.985	1.14 (−2)	0.000	1.14 (−2)
			3	−1169.340	0.000	1742.676	1.17 (−2)	−0.001	1.17 (−2)
			4	−1157.667	−0.001	1754.238	1.22 (−2)	−0.002	1.22 (−2)
			5	−1143.100	−0.002	1768.643	1.35 (−2)	−0.003	1.31 (−2)
			6	−1125.653	−0.005	1785.849	1.54 (−2)	−0.006	1.50 (−2)
			7	−1105.350	−0.008	1805.803[g]	1.99 (−2)	−0.012	1.75 (−2)
			8	−1082.215	−0.013	1830.668[g]	1.76 (−2)	−0.015	1.82 (−2)
			9	−1056.287	−0.020	1856.449	1.46 (−2)	−0.030	2.60 (−2)
			10	−1027.614	−0.028	1885.077	1.44 (−2)	−0.042	1.37 (−2)
			11	−996.275	−0.035	1916.502	1.09 (−2)	−0.060	1.15 (−2)
			12	−962.380	−0.039	1950.688	9.84 (−3)	−0.086	1.01 (−2)

TABLE CIII: continued

			13	−926.050	−0.036	1987.594	1.12 (−2)	−0.116	2.18 (−2)
			14	−883.222	−0.006	2027.169	8.19 (−3)	−0.148	8.40 (−3)
			15	−841.106	−0.003	2069.377	7.42 (−3)	−0.184	7.62 (−3)
			16	−796.351	0.019	2114.166	6.89 (−3)	−0.219	6.94 (−3)
			17	−749.068	0.085	2161.483	6.71 (−3)	−0.249	6.33 (−3)
			18	−699.421	0.282	2211.263	5.86 (−3)	−0.262	5.95 (−3)
			19	−647.953	1.065	2263.419	5.42 (−3)	−0.229	5.23 (−3)
			20	−590.506	−1.842	2317.762	5.44 (−3)	−0.023	7.02 (−3)
			21	−534.158	−1.638	2373.464	9.14 (−3)	1.097	4.37 (−3)
			22	−475.165	−3.234	2435.398	5.71 (−3)	−1.845	1.26 (−2)
			23	−413.935	0.839	2496.309	3.99 (−3)	−1.829	4.55 (−3)
			24	−350.625	0.664	2559.558	3.39 (−3)	−3.288	6.96 (−3)
			25	−285.356	0.762	2624.859	4.59 (−3)	0.388	4.05 (−3)
4	3	0	3	−994.024	0.000	1909.584	1.40 (−2)	0.000	1.40 (−2)
			4	−982.451	0.000	1921.120	1.39 (−2)	0.000	1.38 (−2)
			5	−968.008	0.001	1935.514	1.37 (−2)	0.000	1.36 (−2)
			6	−950.713	0.003	1952.752	1.36 (−2)	0.001	1.31 (−2)
			7	−930.588	0.009	1972.815	1.32 (−2)	0.002	1.31 (−2)
			8	−907.660	0.023	1995.680	1.28 (−2)	0.006	1.26 (−2)
			9	−881.967	0.056	2021.324	1.25 (−2)	0.011	1.16 (−2)
			10	−853.566	0.134	2049.716	1.05 (−2)	0.025	1.16 (−2)
			11	−822.565	0.329	2080.824	1.16 (−2)	0.047	1.14 (−2)
			12	-789.223^f	0.857	2114.603	1.14 (−2)	0.087	1.08 (−2)
			13	-749.232^f	−2.642	2151.005	1.07 (−2)	0.157	1.05 (−2)
			14	−710.677	−2.145	2189.959	1.03 (−2)	0.287	1.01 (−2)
			15	−669.130	−2.163	2231.362	1.01 (−2)	0.532	9.55 (−3)
			16	−624.889	−2.507	2275.031	1.01 (−2)	1.025	9.05 (−3)
			17	−578.101	−3.171	2320.623	1.09 (−2)	2.051	8.59 (−3)
			18	−528.860	−4.217	2375.992	1.18 (−2)	−4.315	8.10 (−3)
			19	−477.249	3.135	2426.433	1.04 (−2)	−3.425	7.66 (−3)
			20	−423.351	2.609	2479.659	8.40 (−3)	−3.092	1.18 (−2)
			21	−367.283	2.321	2535.336	7.52 (−3)	−3.095	6.92 (−3)
			22	−308.972	2.052	2593.250	6.89 (−3)	−3.345	6.56 (−3)
			23	−248.743	1.978	2653.242	6.40 (−3)	−3.862	6.26 (−3)
			24	−186.598	1.973	2715.534	8.45 (−3)	−5.094	5.99 (−3)
			25	−122.668	2.014	2779.047	5.76 (−3)	−6.201	5.70 (−3)
5	4	0	4	−744.331	0.000	2148.317	1.94 (−2)	0.000	1.94 (−2)
			5	−730.059	0.000	2162.549	1.80 (−2)	0.000	1.80 (−2)
			6	−712.964	0.000	2179.599	1.71 (−2)	0.000	1.71 (−2)
			7	−693.062	0.000	2199.450	1.65 (−2)	0.000	1.65 (−2)
			8	−670.372	0.000	2222.082	1.72 (−2)	0.000	1.58 (−2)
			9	−644.919	0.000	2247.475	1.56 (−2)	−0.001	1.52 (−2)
			10	−616.726	0.000	2275.602	1.47 (−2)	−0.001	1.47 (−2)
			11	−585.823	0.000	2306.434	1.62 (−2)	−0.007	2.83 (−2)
			12	−552.243	0.001	2339.942	1.37 (−2)	0.001	1.39 (−2)
			13	−516.020	0.002	2376.092	1.29 (−2)	0.001	1.29 (−2)
			14	−477.193	0.003	2414.844	1.26 (−2)	0.002	1.20 (−2)
			15	−435.804	0.006	2456.160	1.18 (−2)	0.005	1.27 (−2)
			16	−391.899	0.010	2499.993	1.04 (−2)	0.007	1.07 (−2)
			17	−345.529	0.016	2546.299	1.07 (−2)	0.010	1.03 (−2)
			18	−296.748	0.026	2595.019	9.63 (−3)	0.018	9.59 (−3)
			19	−245.612	0.037	2646.102	8.57 (−3)	0.031	1.09 (−2)
			20	−192.191	0.063	2699.485	8.10 (−3)	0.044	8.21 (−3)
			21	−136.551	0.094	2755.104	7.72 (−3)	0.064	7.63 (−3)
			22	−78.769	0.141	2812.885	7.58 (−3)	0.095	7.05 (−3)
			23	−18.935	0.212	2872.759	6.60 (−3)	0.131	6.40 (−3)

TABLE CIII: continued

6	5	0	5	−432.701	−0.001	2446.757	2.34 (−2)	0.000	2.34 (−2)
			6	−415.846	0.000	2463.587	2.28 (−2)	0.000	2.28 (−2)
			7	−396.223	0.000	2483.173	2.24 (−2)	0.000	2.23 (−2)
			8	−373.855	0.000	2505.528	2.26 (−2)	−0.001	2.26 (−2)
			9	−348.762	0.000	2530.587	2.15 (−2)	−0.001	2.15 (−2)
			10	−320.973	0.001	2558.344	2.07 (−2)	0.000	2.06 (−2)
			11	−290.507	−0.008	2588.772	2.00 (−2)	−0.002	1.97 (−2)
			12	−257.421	−0.005	2621.838	1.92 (−2)	−0.001	1.88 (−2)
			13	−221.735	0.005	2657.505	1.78 (−2)	−0.001	1.78 (−2)
			14	−183.500	−0.003	2695.737	1.68 (−2)	−0.001	1.70 (−2)
			15	−142.781	−0.004	2736.491	1.57 (−2)	0.003	2.98 (−2)
			16	−99.590	−0.021	2779.720	1.49 (−2)	0.004	1.47 (−2)
			17	−54.828	0.044	2825.370	1.39 (−2)	0.010	1.37 (−2)
			18	−7.164	0.071	2873.329	1.28 (−2)	0.068	1.32 (−2)
			19	46.455†	0.410	2923.679	1.27 (−2)	0.057	1.19 (−2)
			20	98.882†	−0.225	2975.710	1.70 (−2)	0.530	1.13 (−2)
1	0	1	0	−1031.054		1891.797	3.56 (−2)		
			1	−1028.311		1894.535	3.13 (−2)		
			2	−1022.827		1900.003	3.05 (−2)		
			3	−1014.609		1908.197	3.00 (−2)		
			4	−1003.667		1919.107	2.94 (−2)		
			5	−990.014		1932.721	2.87 (−2)		
			6	−973.668		1949.023	2.78 (−2)		
			7	−954.646		1967.995	2.77 (−2)		
			8	−932.974		1989.607	2.82 (−2)		
			9	−908.676		2013.844	2.62 (−2)		
			10	−881.784		2040.673	2.51 (−2)		
			11	−852.331		2070.061	2.42 (−2)		
			12	−820.353		2101.972	2.56 (−2)		
			13	−785.892		2136.371	2.08 (−2)		
			14	−748.992		2173.210	2.00 (−2)		
			15	−709.700		2212.444	1.84 (−2)		
			16	−668.069		2254.027	1.70 (−2)		
			17	−624.156		2297.903	1.58 (−2)		
			18	−578.021		2344.015	1.52 (−2)		
			19	−529.730		2392.303	1.60 (−2)		
			20	−479.352		2442.697	1.20 (−2)		
			21	−426.964		2495.130	1.40 (−2)		
			22	−372.647		2549.524	9.66 (−3)		
			23	−316.490		2605.797	8.49 (−3)		
			24	−258.588		2663.863	7.76 (−3)		
			25	−199.047		2723.626	6.88 (−3)		
2	1	1	1	−988.448	0.130	1931.974	3.27 (−2)	0.128	3.13 (−2)
			2	−983.104	0.389	1937.303	3.50 (−2)	0.386	3.10 (−2)
			3	−975.095	0.777	1945.292	3.17 (−2)	0.771	3.06 (−2)
			4	−964.428	1.292	1955.932	3.04 (−2)	1.280	3.00 (−2)
			5	−951.114	1.932	1969.225	3.09 (−2)	1.900	2.94 (−2)
			6	−935.165	2.694	1985.118	3.32 (−2)	2.669	2.88 (−2)
			7	−916.595	3.573	2003.634	2.83 (−2)	3.546	2.88 (−2)
			8	−895.417	4.561	2024.743	2.70 (−2)	4.547	2.72 (−2)
			9	−871.641	5.646	2048.426	2.67 (−2)	5.664	3.05 (−2)
			10	−845.265	6.796	2074.657	2.51 (−2)	6.901	2.56 (−2)
			11	−816.241	7.936	2103.413	2.38 (−2)	8.274	2.41 (−2)
			12	−784.376^{f}	8.847	2134.673	2.42 (−2)	9.807	2.53 (−2)
			13	−754.054^{f}	13.882	2168.416	2.22 (−2)	10.395	2.45 (−2)
			14	−717.270	15.017	2204.630	2.10 (−2)	11.941	2.27 (−2)
			15	−678.544	16.756	2243.336	1.94 (−2)	13.413	2.10 (−2)
			16	−637.675	18.905	2284.620	1.74 (−2)	14.694	1.95 (−2)
			17	−594.625	21.455	2328.722	1.48 (−2)	15.501	1.80 (−2)
			18	−549.415	24.465	2367.677	1.21 (−2)	23.755	1.67 (−2)
			19	−502.093	19.149	2416.067	1.34 (−2)	24.823	1.50 (−2)
			20	−452.721	21.782	2466.047	1.18 (−2)	26.494	1.36 (−2)

TABLE CIII: continued

			21	−401.369	24.282	2517.798	1.09 (−2)	28.548	1.23 (−2)
			22	−348.122	26.703	2571.372	1.00 (−2)	30.900	1.10 (−2)
			23	−293.081	29.092	2626.744	9.00 (−3)	33.572	9.81 (−3)
			24	−236.391	31.517	2683.843	8.04 (−3)	36.657	8.79 (−3)
			25	−178.372	34.201	2742.569	7.36 (−3)	40.282	7.60 (−3)
3	2	1	2	−869.749	0.005	2044.682	3.46 (−2)	0.019	3.49 (−2)
			3	−861.412	0.025	2052.713	3.30 (−2)	0.075	3.41 (−2)
			4	−850.400	0.083	2063.411	3.13 (−2)	0.176	3.34 (−2)
			5	−836.710	0.233	2076.766	2.97 (−2)	0.318	3.27 (−2)
			6	−820.357	0.588	2092.764	2.81 (−2)	0.499	3.21 (−2)
			7	−801.384[e]	1.332	2111.386	2.67 (−2)	0.715	3.13 (−2)
			8	−779.935[e]	−1.822	2132.611	2.57 (−2)	0.960	3.04 (−2)
			9	−754.181	−3.449	2156.400	2.52 (−2)	1.243	2.94 (−2)
			10	−727.759	−3.622	2182.726	2.31 (−2)	1.553	2.84 (−2)
			11	−698.383	−0.782	2211.509	2.32 (−2)	1.925	2.77 (−2)
			12	−666.384	−1.513	2242.580	2.32 (−2)	2.459	3.68 (−2)
			13	−631.855	−1.969	2275.425	2.93 (−2)	3.516	2.63 (−2)
			14	−594.852	−2.345	2315.047	2.24 (−2)	−0.269	2.84 (−2)
			15	−555.424	−2.704	2353.313	1.80 (−2)	−1.468	3.29 (−2)
			16	−513.624	−3.069	2394.205	2.85 (−2)	3.925	2.64 (−2)
			17	−469.507	−3.450	2437.486	1.43 (−2)	4.109	2.01 (−2)
			18	−423.130	−3.849	2483.046	1.30 (−2)	4.395	1.81 (−2)
			19	−374.560	−4.270	2530.807	1.20 (−2)	4.731	1.62 (−2)
			20	−323.863	−4.712	2580.690	1.09 (−2)	5.102	1.44 (−2)
			21	−271.119	−5.171	2632.617	1.00 (−2)	5.499	1.29 (−2)
			22	−216.414	−5.643	2686.506	9.43 (−3)	5.926	1.28 (−2)
			23	−159.848	−6.112	2742.265	8.27 (−3)	6.390	1.10 (−2)
			24	−101.547	−6.549	2799.791	7.66 (−3)	6.904	9.72 (−3)
			25	−41.689	−6.883	2858.965	6.83 (−3)	7.489	8.54 (−3)
4	3	1	3	−681.444	0.000	2224.566	4.30 (−2)	0.000	4.30 (−2)
			4	−670.666	0.000	2235.338	4.23 (−2)	0.001	4.23 (−2)
			5	−657.215	0.001	2248.784	4.17 (−2)	0.005	4.15 (−2)
			6	−641.106	0.003	2264.890	4.05 (−2)	0.012	4.06 (−2)
			7	−622.356	0.007	2283.639	3.94 (−2)	0.024	3.95 (−2)
			8	−600.990	0.014	2305.007	3.82 (−2)	0.041	3.83 (−2)
			9	−577.033	0.029	2328.970	3.68 (−2)	0.067	3.70 (−2)
			10	−550.506	0.041	2355.498	5.66 (−2)	0.098	3.55 (−2)
			11	−521.467	0.079	2384.554	3.43 (−2)	0.136	3.63 (−2)
			12	−489.943	0.133	2416.100	3.25 (−2)	0.196	3.23 (−2)
			13	−455.987	0.214	2450.090	3.08 (−2)	0.267	3.06 (−2)
			14	−419.655	0.334	2486.452	2.94 (−2)	0.375	3.04 (−2)
			15	−381.014	0.509	2525.231	2.76 (−2)	0.438	2.98 (−2)
			16	−340.141	0.758	2566.205	2.59 (−2)	0.593	2.65 (−2)
			17	−297.125	1.100	2609.380	2.48 (−2)	0.776	2.49 (−2)
			18	−252.062	1.559	2654.655	2.32 (−2)	1.006	2.33 (−2)
			19	−205.052	2.142	2701.934	2.18 (−2)	1.285	2.19 (−2)
			20	−156.199	2.838	2751.121	2.17 (−2)	1.617	2.06 (−2)
5	4	1	4	−428.027	0.000	2467.017	5.62 (−2)	0.000	5.25 (−2)
			5	−414.735	0.000	2480.313	5.23 (−2)	0.001	5.29 (−2)
			6	−398.817	0.000	2496.233	5.10 (−2)	0.001	5.13 (−2)
			7	−380.292	0.000	2514.766	5.11 (−2)	−0.001	4.93 (−2)
			8	−359.181	0.000	2535.885	4.77 (−2)	0.000	4.72 (−2)
			9	−335.509	0.000	2559.572	4.61 (−2)	−0.001	4.52 (−2)
			10	−309.305	0.001	2585.796	4.44 (−2)	0.002	4.87 (−2)
			11	−280.601	0.001	2614.525	4.41 (−2)	0.005	4.15 (−2)
			12	−249.435	0.002	2645.739	4.00 (−2)	0.002	4.06 (−2)
			13	−215.850	0.005	2679.385	3.81 (−2)	0.003	3.82 (−2)
			14	−179.901	0.011	2715.427	3.60 (−2)	0.005	3.59 (−2)
			15	−141.691	0.023	2753.818	3.36 (−2)	0.008	3.36 (−2)
			16	−100.476	0.069	2794.507	3.14 (−2)	0.015	3.14 (−2)
			17	−58.344	0.228	2837.431	2.90 (−2)	0.027	2.91 (−2)
			18	−13.404	−0.012	2882.515	2.66 (−2)	0.050	2.67 (−2)
			19	31.510	1.207	2929.333	2.77 (−2)	0.108	2.76 (−2)
			20	82.550	−1.759	2979.031	2.26 (−2)	0.085	2.26 (−2)

TABLE CIII: continued

6	5	1	5	−113.193	0.000	2768.643	7.12 (−2)	0.000	7.13 (−2)
			6	−97.476	0.000	2784.225	7.39 (−2)	0.002	7.19 (−2)
			7	−79.183	0.000	2803.280	7.74 (−2)	0.000	7.74 (−2)
			8	−58.337	0.000	2823.882	6.75 (−2)	−0.001	6.75 (−2)
			9	−34.959	0.000	2847.229	6.38 (−2)	−0.003	6.41 (−2)
			10	−9.078	0.000	2873.124	6.07 (−2)	0.006	6.75 (−2)
			11	19.276†	0.000	2901.513	5.79 (−2)	0.002	5.89 (−2)
			12	50.066†	0.004	2932.354	5.47 (−2)	0.002	5.48 (−2)
			13	83.265†	0.000	2965.628	5.15 (−2)	−0.024	5.17 (−2)
			14	118.822†	0.000	3001.256	4.99 (−2)	0.003	4.83 (−2)
			15	156.693†	0.001	3039.209	4.44 (−2)	0.009	4.64 (−2)
			16	196.830‡	0.003	3079.458	4.19 (−2)	0.008	4.09 (−2)
			17	239.177‡	0.005	3121.934	3.87 (−2)	0.010	3.93 (−2)
			18	283.672‡	0.010	3166.632	5.26 (−2)	−0.034	3.62 (−2)
2	0	0	0	−936.866		1990.399	5.86 (−3)		
			1	−934.015		1993.223	5.96 (−3)		
			2	−928.318		1998.870	1.05 (−2)		
			3	−919.780		2007.333	8.78 (−3)		
			4	−908.412		2018.600	7.58 (−3)		
			5	−894.228		2032.659	6.68 (−3)		
			6	−877.243		2049.493	5.73 (−3)		
			7	−857.480		2069.086	6.10 (−3)		
			8	−834.960		2091.411	6.59 (−3)		
			9	−809.712		2116.443	5.79 (−3)		
			10	−781.765		2144.154	7.33 (−3)		
			11	−751.154		2174.508	6.44 (−3)		
			12	−717.919		2207.471	6.19 (−3)		
			13	−682.115		2242.993	6.09 (−3)		
			14	−643.536		2280.961	7.89 (−3)		
			15	−602.779		2321.821	6.12 (−3)		
			16	−559.469		2364.731	4.75 (−3)		
			17	−513.755		2410.096	4.35 (−3)		
			18	−465.701		2457.804	4.15 (−3)		
			19	−415.368		2507.791	3.82 (−3)		
			20	−362.823		2559.991	3.31 (−3)		
			21	−308.134		2614.340	2.98 (−3)		
			22	−251.373		2670.768	2.65 (−3)		
			23	−192.619		2729.201	2.35 (−3)		
			24	−131.956		2789.563	2.08 (−3)		
			25	−69.472		2851.769	1.92 (−3)		
3	1	0	1	−880.887	0.212	2041.778	7.06 (−3)	0.199	7.08 (−3)
			2	−875.489	0.631	2047.290	8.02 (−3)	0.578	7.60 (−3)
			3	−867.398	1.242	2055.542	1.44 (−2)	1.122	7.85 (−3)
			4	−856.626	2.008	2066.547	2.22 (−2)	1.795	7.92 (−3)
			5	−843.184	2.803	2080.248	1.41 (−2)	2.638	7.78 (−3)
			6	−827.092	4.147	2096.649	1.34 (−2)	3.629	7.53 (−3)
			7	−808.372	4.807	2115.727	1.33 (−2)	4.771	7.24 (−3)
			8	−787.058	9.791	2137.462	1.34 (−2)	6.064	7.02 (−3)
			9	−763.202	11.732	2161.826	4.85 (−2)	7.494	7.24 (−3)
			10	−736.887	14.056	2188.783^{d}	1.24 (−2)	8.821^{d}	2.17 (−2)^{d}
			11	−705.122	13.748	2218.288^{d}	1.71 (−2)	11.050^{d}	7.08 (−3)^{d}
			12	−674.325	17.148	2250.528	1.65 (−2)	12.766	6.89 (−3)
			13	−640.550	20.259	2285.072	1.27 (−2)	14.863	9.78 (−2)
			14	−604.167	23.397	2322.124	1.12 (−2)	17.074	7.83 (−3)
			15	−565.322	26.653	2361.607	1.44 (−2)	19.406	7.26 (−3)
			16	−524.100	30.060	2403.471	1.07 (−2)	21.869	4.16 (−3)
			17	−480.574	33.628	2447.660	8.84 (−3)	24.464	3.65 (−3)
			18	−434.810	37.362	2494.126	9.28 (−3)	27.188	3.35 (−3)
			19	−386.880	41.264	2542.802	8.86 (−3)	30.030	1.19 (−2)
			20	−336.859	45.338	2593.631	9.22 (−3)	32.994	3.30 (−3)

4	2	0	2	−734.601	0.001	2179.212	1.06 (−2)	0.012	1.05 (−2)
			3	−726.260	0.007	2187.510	9.77 (−3)	0.013	1.02 (−2)
			4	−715.159	0.020	2198.559	9.52 (−3)	0.018	9.99 (−3)
			5	−701.313	0.048	2212.344	9.38 (−3)	0.032	9.83 (−3)
			6	−684.745	0.098	2228.847	9.23 (−3)	0.059	9.79 (−3)
			7	−665.487	0.183	2248.048	9.04 (−3)	0.114	1.43 (−2)
			8	−643.585	0.328	2269.924	8.88 (−3)	0.166	8.84 (−3)
			9	−619.132	0.594	2294.438	8.65 (−3)	0.267	8.67 (−3)
			10	−592.445	1.255	2321.559	8.44 (−3)	0.408	8.47 (−3)
			11	−560.662	−0.636	2351.238	8.30 (−2)	0.608	8.26 (−3)
			12	−528.785	−0.299	2383.402	9.82 (−3)	0.907	8.05 (−3)
			13	−494.127	−1.075	2417.832	1.25 (−2)	1.483	7.87 (−3)
			14	−456.968	2.770	2456.267	1.55 (−2)	0.545	7.79 (−3)
			15	−417.481	3.303	2495.441	9.14 (−3)	1.278	8.26 (−3)
			16	−375.528	3.953	2537.246	8.33 (−3)	1.506	1.17 (−2)
			17	−331.446	4.915	2581.350	7.09 (−3)	3.446	1.19 (−2)
			18	−285.213	6.071	2627.714	7.69 (−3)	3.841	1.49 (−2)
			19	−236.918	7.426	2676.151	6.43 (−3)	4.614	7.67 (−3)
			20	−186.652	8.978	2726.644	5.96 (−3)	5.512	8.27 (−3)
5	3	0	3	−511.426	0.000	2390.772	1.26 (−2)	0.000	1.25 (−2)
			4	−500.448	0.000	2401.704	1.26 (−2)	0.000	1.21 (−2)
			5	−486.748	0.001	2415.347	1.26 (−2)	0.000	1.32 (−2)
			6	−470.340	0.002	2431.689	1.39 (−2)	0.000	1.43 (−2)
			7	−451.243	0.005	2450.714	1.12 (−2)	0.000	1.14 (−2)
			8	−429.477	0.010	2472.399	1.14 (−2)	0.001	1.16 (−2)
			9	−405.069	0.021	2496.709	3.71 (−2)	0.021	1.59 (−2)
			10	−378.048	0.039	2523.657	1.02 (−2)	0.011	1.10 (−2)
			11	−348.446	0.069	2553.179	1.35 (−2)	0.017	1.06 (−2)
			12	−316.301	0.115	2585.297	1.76 (−2)	0.028	9.59 (−3)
			13	−281.657	0.185	2619.824	9.94 (−3)	0.057	9.63 (−3)
			14	−244.560	0.289	2656.871	9.42 (−3)	0.092	9.98 (−3)
			15	−205.065	0.437	2696.340	9.16 (−3)	0.143	9.62 (−3)
			16	−163.232	0.645	2738.173	9.00 (−3)	0.223	8.98 (−3)
			17	−119.130	0.932	2782.334	8.47 (−3)	0.319	8.52 (−3)
			18	−72.836	1.323	2828.731	8.03 (−3)	0.470	8.00 (−3)
			19	−24.439	1.847	2877.302	7.44 (−3)	0.680	7.65 (−3)
			20	25.950	2.549	2927.966	6.89 (−3)	0.970	7.13 (−3)
6	4	0	4	−219.364	0.002	2669.015	1.91 (−2)	0.000	1.91 (−2)
			5	−205.883	0.000	2682.456	1.87 (−2)	0.000	1.89 (−2)
			6	−189.741	0.000	2698.553	1.83 (−2)	0.002	1.95 (−2)
			7	−170.957	0.001	2717.290	1.79 (−2)	−0.003	4.86 (−2)
			8	−149.552	0.001	2738.642	1.74 (−2)	−0.004	1.76 (−2)
			9	−125.556	0.003	2762.587	1.70 (−2)	−0.001	1.66 (−2)
			10	−99.001	0.007	2789.096	1.65 (−2)	0.003	1.61 (−2)
			11	−69.927	0.017	2818.137	1.62 (−2)	0.011	1.62 (−2)
			12	−38.390	0.046	2849.669	1.35 (−2)	0.030	1.32 (−2)
			13	−4.478	0.131	2883.618	1.42 (−2)	0.093	1.39 (−2)
			14	31.834†	0.178	2920.169	2.22 (−2)	−0.016	1.73 (−2)
			15	71.546†	−0.828	2958.869	1.57 (−2)	0.080	1.28 (−2)
			16	113.772†	−2.191	2999.906	1.22 (−2)	0.159	1.22 (−2)
			17	154.293†	0.629	3043.148	1.13 (−2)	0.251	1.23 (−2)
			18	201.702‡	−2.164	3088.964	1.70 (−2)	−0.308	1.37 (−2)
			19	252.514‡	−6.212	3134.659	2.88 (−2)	0.904	2.03 (−2)
			20	301.723‡	−7.021	3186.036	1.58 (−2)	1.044	1.28 (−2)
7	5	0	5	135.959‡	0.000	3008.357	3.69 (−2)	−0.003	3.69 (−2)
			6	151.847‡	0.000	3024.623	4.22 (−2)	0.023	6.56 (−2)
			7	170.338‡	0.000	3042.951	2.10 (−2)	0.021	3.46 (−2)
			8	191.412‡	0.000	3063.968	2.77 (−2)	0.127	2.36 (−1)
			9	215.044‡	0.000	3087.546	2.55 (−2)	−0.032	3.20 (−2)
			10	241.206‡	0.001	3113.658	2.39 (−2)	−0.016	2.44 (−2)
			11	269.870‡	0.001	3142.310	2.49 (−2)	−0.011	2.48 (−2)
			12	300.998‡	0.003	3173.388	2.61 (−2)	−0.009	2.18 (−2)
			13	334.555‡	0.008	3206.918	2.07 (−2)	−0.003	2.04 (−2)
			14	370.496‡	0.017	3242.837	2.01 (−2)	0.003	1.94 (−2)
			15	408.775‡	0.032	3281.111	1.82 (−2)	0.009	1.81 (−2)

3	0	0	0	−608.959		2327.928	5.04 (−3)		
			1	−606.435		2330.766	5.34 (−3)		
			2	−601.428		2336.426	6.44 (−3)		
			3	−593.988		2344.875	9.11 (−3)		
			4	−577.644		2356.093	3.69 (−3)		
			5	−563.761		2370.042	3.72 (−3)		
			6	−547.106		2386.697	3.42 (−3)		
			7	−527.698		2406.030	2.50 (−3)		
			8	−505.569		2428.021	5.87 (−3)		
			9	−480.752		2452.632	3.77 (−3)		
			10	−453.282		2479.832	3.69 (−3)		
			11	−423.202		2509.587	4.29 (−3)		
			12	−390.554		2541.862	3.40 (−3)		
			13	−355.385		2576.609	2.99 (−3)		
			14	−317.747		2613.781	2.90 (−3)		
			15	−277.703		2653.314	2.68 (−3)		
			16	−235.260		2694.907	4.75 (−2)		
			17	−190.566		2739.482	2.30 (−3)		
			18	−143.643		2785.789	3.08 (−3)		
			19	−94.564		2834.258	2.64 (−3)		
			20	−43.415		2884.798	2.37 (−3)		
4	1	0	1	−508.614	0.471	2416.732	5.07 (−3)	0.406	5.30 (−3)
			2	−503.728	1.408	2421.658	9.33 (−3)	1.219	2.95 (−2)
			3	−496.397	2.799	2429.029	7.51 (−3)	2.419	1.87 (−2)
			4	−486.621	4.626	2438.856	7.05 (−3)	4.008	3.27 (−2)
			5	−474.399	6.862	2451.132	6.83 (−3)	5.894	2.55 (−2)
			6	−459.733	9.453	2465.851	6.73 (−3)	8.201	5.56 (−3)
			7	−442.629	12.199	2483.004	6.73 (−3)	10.777	7.10 (−3)
			8	−423.106	17.000	2502.577	6.94 (−3)	13.523	1.13 (−2)
			9	−401.248	20.390	2524.580	1.33 (−2)	15.861	2.93 (−2)
			10	−376.795	24.246	2548.878	7.72 (−3)	21.984	1.45 (−2)
			11	−350.547	29.025	2575.496	1.01 (−2)	25.451	8.01 (−3)
			12	−318.649	30.759	2604.023	2.22 (−2)	29.808	6.97 (−3)
			13	−287.571	35.818	2635.448	4.12 (−2)	33.761	7.13 (−3)
			14	−253.704	40.477	2672.580	1.73 (−2)	34.316	8.37 (−3)
			15	−217.363	44.887	2708.098	8.74 (−3)	38.596	9.62 (−3)
			16	−178.653	48.929	2746.287	6.12 (−3)	42.046	1.10 (−2)
			17	−137.635	52.355	2786.843	5.11 (−3)	44.768	1.34 (−2)
			18	−94.361	55.377	2829.646	4.60 (−3)	46.666	1.57 (−2)
			19	−48.882	48.882	2874.617	4.22 (−3)	47.673	1.80 (−2)
			20	−1.253	56.989	2921.689	4.13 (−3)	48.452	2.22 (−2)

[a] The lowest levels of the groups shown are marked with the yellow crosses in Fig. 3 of the paper.

[b] 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 represent thus 16 vibrational states: $[v_r\,0\,0]$, $[v_r\,0\,1]$, $[v_r\,0\,2]$, $[v_r\,0\,3]$, $[v_r\,1\,0]$, $[v_r\,1\,1]$, $[v_r\,2\,0]$, and $[v_r\,3\,0]$ with $v_r{=}0,1$.

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

† Level of e-parity pertains to a rotational resonance. ‡ Both e- and f-parity level have nonzero widths due to rotational predissociation and/or tunneling through centrifugal barriers.

[d] An example of crossing of sequences of J^p-levels from different $(v_r\, b\, k\, v_R)$ groups, here, of the f-parity levels from groups (1 1 1 3) and (1 3 1 0).

[e] A crossing between levels from groups (0 3 2 1) and (0 1 1 3).

[f] A crossing between levels from groups (0 4 3 0) and (0 2 1 1). The groups belong to vibrational states [0 1 0] and [0 1 1], repectively. Thus, this crossing as well as the one mentioned in footnote e may have a significant role in lowering the accuracy of the approximate formula for the integrated band intensity, Eq. (C21), in application to bands [0 1 0]→[0 1 1] and [0 1 0]→[1 1 0], see Fig. C6.

[g] A crossing between levels from groups (1 3 3 1) and (1 3 2 0). Its effects are the enhanced intensities of several P- and Q-lines in the K_a=3−3 subband of the [0 0 0]→[1 0 1] band, seen in Fig. C3 as the two peaks around $\nu_{\rm if}$=3200 cm^{-1}.

TABLE CIV: Positions (E) and widths (Γ, in 10^{-2} cm^{-1}) of lowest rotational levels in four groups ($b\,k{=}b\,v_R{=}0$) below $v{=}2\,j{=}0$ threshold[a], i.e. in the $[v_r{=}2\,0\,0]$ vibrational state.

	k=0		k=1				k=2				k=3			
J	E	Γ	$E(e)$	$\Gamma(e)$	$E(f-e)$[b]	$\Gamma(f)$	$E(e)$	$\Gamma(e)$	$E(f-e)$	$\Gamma(f)$	$E(e)$	$\Gamma(e)$	$E(f-e)$	$\Gamma(f)$
0	3926.60	3.2												
1	3929.66	3.2	3957.13	3.2	0.10	3.2								
2	3935.76	3.2	3963.12	3.1	0.31	3.1	4045.52	3.1	0.00	3.1				
3	3944.91	3.2	3972.10	3.1	0.62	3.1	4054.62	3.0	−0.00	3.0	4190.72	3.5	−0.00	3.5
4	3957.10	3.2	3984.07	3.0	1.04	3.0	4066.75	3.1	−0.00	3.0	4202.77	3.4	−0.00	3.4
5	3972.31	2.6	3998.90	3.0	1.56	3.0	4081.89	3.1	−0.01	2.9	4217.81	3.4	0.00	3.4
6	3990.53	2.8	4016.86	2.9	2.17	2.9	4100.04	2.9	−0.01	2.9	4235.84	3.4	−0.00	3.3
7	4011.75	2.9	4037.75	2.9	2.88	2.9	4121.17	2.6	−0.03	3.1	4256.83	3.4	−0.00	3.3
8	4035.93	2.9	4061.51	2.8	3.69	2.8	4145.27	4.1	−0.07	3.2	4280.78	5.4	−0.01	9.1
9	4063.07	2.4	4088.19	2.7	4.59	2.7	4172.33	2.8	−0.07	2.6	4307.63	3.0	0.00	2.9
10	4093.12	2.8	4117.75	2.7	5.58	2.6	4202.31	2.7	−0.11	3.1	4337.39	2.8	0.00	2.7
11	4126.08	2.4	4150.16	2.6	6.66	2.6	4235.19	2.8	−0.16	3.7	4370.03	4.4	0.00	3.8
12	4161.89	2.5	4185.40	2.8	7.82	3.0	4270.94	2.6	−0.21	2.6	4405.52	2.9	−0.01	2.7
13	4200.53	2.6	4223.45	2.1	9.05	2.2	4309.54	2.5	−0.28	2.5	4443.81	2.7	0.01	2.6
14	4241.96	2.1	4264.26	2.1	10.36	2.2	4350.95	2.4	−0.37	2.3	4484.88	2.7	0.01	2.4
15	4286.14	2.1	4307.79	2.1	11.75	2.0	4395.14	2.3	−0.48	2.3	4528.69	2.6	0.01	2.0
16	4333.02	2.2	4354.01	1.9	13.19	1.8	4442.05	2.2	−0.60	2.1	4575.20	2.0	0.02	2.2
17	4382.57	1.7	4402.88	1.8	14.70	1.8	4491.66	2.1	−0.75	2.0	4624.37	2.2	0.02	2.5
18	4434.72	1.6	4454.35	3.4	16.24	1.7	4543.91	1.9	−0.91	1.9	4676.14	2.1	0.03	2.1
19	4489.43	1.1	4508.37	1.7	17.86	1.6	4598.75	2.4	−1.10	1.9	4730.46	2.0	0.04	1.9
20	4546.64	1.4	4564.89	1.4	19.51	1.9	4656.13	1.6	−1.30	1.6	4787.28	2.0	0.06	1.9
21	4606.29	1.4	4623.86	1.3	21.19	1.3	4715.99	1.5	−1.53	1.7	4846.55	1.6	0.08	1.6
22	4668.33	1.2	4685.21	1.3	22.90	1.2	4778.27	1.6	−1.77	1.4	4908.19	1.5	0.11	1.5
23	4732.68	1.1	4748.89	1.1	24.63	1.1	4842.91	1.1	−2.03	1.1	4972.14	1.4	0.15	1.9
24	4799.28	1.0	4814.84	1.0	26.37	1.0	4909.83	1.0	−2.31	1.0	5038.33	1.3	0.20	1.2
25	4868.06	0.9	4882.97	0.9	28.12	0.9	4978.95	0.8	−2.61	1.0	5106.67	1.0	0.26	1.1

[a]As obtained from the asymptotic part of the PES for $LiHH^+$ of Ref. 3, the threshold lies 5862.36 cm^{-1} above the $v{=}0\,j{=}0$ threshold. This is too low by 5.76 cm^{-1} in comparison with the exact value of $\varepsilon_{20}-\varepsilon_{00}$ for D_2[1] (and by 7.33 cm^{-1} in comparison with the value determined in the Born-Oppenheimer approximation, see Fig. B1 in Part B).

[b]Denotes $E(f)-E(e)$, i.e. the K-type doubling. See Figs. C1 and C2.

TABLE CV: Total internal partition sum (Z) of the Li^+–D_2 ion at selected temperatures below 400 K. Bound states levels only (3503) are included into the sum. See Table BVII and Fig. B4 in Part B.

T	Z	T	Z	T	Z	T	Z
0.5	6.003	20	62.130	85	430.76	250	2821.2
1	6.215	22	69.605	90	469.40	260	3069.8
1.5	6.944	24	77.369	95	509.54	270	3334.2
2	8.005	26	85.408	100	551.22	273.15	3420.9
2.5	9.210	28	93.712	110	639.32	280	3615.0
3	10.477	30	102.27	120	734.08	290	3912.6
3.5	11.774	34	120.13	130	835.92	296	4099.5
4	13.088	38	138.96	140	945.35	300	4227.7
5	15.746	42	158.74	150	1062.9	310	4560.6
6	18.429	46	179.48	160	1189.1	320	4911.7
7	21.139	50	201.16	170	1324.7	330	5281.3
8	23.882	54	223.79	180	1470.1	340	5669.8
9	26.669	58	247.36	190	1626.1	350	6077.4
10	29.512	62	271.86	200	1793.3	360	6504.1
12	35.396	66	297.29	210	1972.4	370	6950.3
14	41.588	70	323.65	220	2164.1	380	7415.8
16	48.109	75	357.90	230	2369.0	390	7900.7
18	54.960	80	393.60	240	2587.9	400	8404.9

TABLE CVI: Li^+–D_2. Least-squares fits of rotational energies in vibrational states $[v_r\, v_\theta\, v_R]$=[0 0 0] and [1 0 0] to eigenvalues of A-reduced Hamiltonian of Watson (Ref. 5) with four and five quartic terms. Comparison of the parameters obtained from energies calculated in this work and in Ref. 4 with the parameters obtained in Ref. 7 from transitions energies measured in the v_r=0→1 band[a]. All entries are in cm^{-1}.

	[0 0 0]				[1 0 0]			
	This work	Cal (Ref. 4)	Cal↔Exp[b]	This work	This work	Cal (Ref. 4)	Cal↔Exp[b]	This work
E_0[c]	0.000	0.00		0.000	2915.447	2917.6	0.827 {3.0}	2915.447
$N_{\rm fit}$[d]	51[e]	48[g]		61[f]	51[e]	42[h]		61[f]
A	31.5960(7)	31.111(1)		31.5954(14)	30.2929(9)	29.616(7)		30.2929(12)
ΔA					−1.303(2)	−1.495(7)	3.6 { 18.8}	−1.302(3)
B	1.58998(4)	1.5857(1)	−0.5 { − 0.8}	1.59610(40)	1.58453(5)	1.5914(5)	−0.6 {−0.1}	1.5904(3)
C	1.48902(4)	1.4902(1)	−0.7 { − 0.7}	1.48274(41)	1.48187(4)	1.4955(5)	−0.8 { 0.1}	1.4759(3)
$\Delta_J\times10^4$	1.168(1)	1.046(5)	0.4 {−10.1}	1.188(2)	1.134(1)	− 0.09(2)	0.8	1.155(1)
$\delta_J\times10^6$	6.9(1)	5.5(6)		6.8(3)	6.8(2)			6.7(2)
$\Delta_{JK}\times10^3$	2.279(7)	2.20(9)	0.4 { − 3.1}[j]	2.173(11)	2.101(8)	− 1.84(7)	0.0	2.018(9)
$\Delta_K\times10^2$	3.28(2)	2.04(3)		3.32(4)	2.79(2)	− 6.4(2)		2.83(3)
$\delta_K\times10^3$	-	-		3.12(20)	-	-		2.96(16)
$\sigma\times10^3$[i]	1.8	4		3.8	2.1	15		3.2

[a]Fit to 103 transition energies in the three K_a=0–0, 1–1, 2-2 subbands.

[b]Shown are absolute deviations Cal−Exp for E_0 and percentage deviations for the other quantities: $(X^{\rm Cal}/X^{\rm Exp}-1)\times100\%$. These in braces concern the calculations of Ref. 4.

[c]Energy of J=0 level relative to the ground state of the complex.

[d]Total number of rotational energies used in the fit.

[e]Levels from k=0, k=1, and k=2 groups included in the fit: J=1–15, $J^{e,f}$=1–12, and $J^{e,f}$=2–7, respectively.

[f]$J^{e,f}$=8–12 levels of k=2 group added to the set specified in e.

[g]Included all levels available from $k=0,1,2$ groups, for Js up to $J_{\rm max}$=10

[h]Levels included: $J^{e,f}$=1–10 from $k=0,1$ groups and $J^{e,f}$=2–7 from k=2.

[i]Root mean square deviation between fitted and calculated energies.

[j]The '−' sign of the experimental value listed in Table II of Ref. 7 is most likely a misprint. The value of Δ_{JK} should be close to the difference between the values of $(B+C)/2$ from the fits to $K_a=0,1,2$ and to K_a=1 manifolds. See comment (ii) and Table CVIIa below.

TABLE CVIa. Comparison of the parameters $A, B, C, \ldots := X^a$ from the fits to the full Watson's Hamiltonian (H of Eq. 26) with parameters ${}_{(i)}X$ from fits to truncated versions (${}_{(i)}H$) with $2\leq i<5$ quartic terms [b].

	[0 0 0]						[1 0 0]					
	${}_{(i)}X$			$({}_{(i)}X/{}_{(i)}X^{\times}-1)\times10^5$ [c]			${}_{(i)}X$			$({}_{(i)}X/{}_{(i)}X^{\times}-1)\times10^5$ [c]		
	i=2	i=3	i=4	i=2	i=3	i=4	i=2	i=3	i=4	i=2	i=3	i=4
${}_{(i)}A$	31.562	31.563	31.5960	6	3	2	30.263	30.265	31.5954	1	1	0
${}_{(i)}B$	1.5877	1.5900	1.58998	0.4	8	7	1.5824	1.5846	1.59610	−4	8	3
${}_{(i)}C$	1.4867	1.4890	1.48902	−7	2	3	1.4797	1.4819	1.48274	−7	5	3
				$({}_{(i)}X/X-1)\times10^2$						$({}_{(i)}X/X-1)\times10^2$		
${}_{(i)}\Delta_J\times10^4$	1.165	1.170	1.168	−2	−1.5	−2	1.132	1.137	1.134	2	−2	−2
${}_{(i)}\delta_J\times10^6$	7.0	6.9	6.9	3	1.5	1	6.9	6.9	6.8	3	3	1.5
${}_{(i)}\Delta_{JK}\times10^3$		2.29	2.279		5	5		2.12	2.101		5	4
${}_{(i)}\Delta_K\times10^2$			3.28			−1			2.79			−1

[a] X — the parameters listed in 5-th and 9-th columns of Table CVI.

[b] ${}_{(i)}X$ — from fits to k=1, k=0−1, and k=0−2 groups for i=2, 3, and 4, respectively, rewritten from Tables III, CIX, and CVI.

[c] ${}_{(i)}X^{\times}$ — functions of the parameters X, the right-hand sides of the relations listed in Table CVIIa, e.g. ${}_{(2)}A^{\times}=A-\Delta_{JK}-\Delta_K$, ${}_{(3)}A^{\times}=A-\Delta_K$, ${}_{(4)}A^{\times}=A$.

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 four quartic terms show the same consistency as the fits presented in Table III of the paper, using two quartic terms.

(ii) The relations tested in Table CVIIa, between the parameters of Watson's Hamiltonian H (in the 'full' quartic approximation, Eq. 26) and the parameters of its truncated versions ${}_{(i)}H$, come from inspection of the matrix elements of these Hamiltonians in the basis of symmetric top wavefunctions[6]. Let us denote them as: $\langle JKM|H|JK'M\rangle{:=}H_{K,K'}(X;J)$ and $\langle JKM|{}_{(i)}H|JK'M\rangle{:=}H_{K,K'}({}_{(i)}X;J)$ where X and ${}_{(i)}X$ are the sets of $3{+}i$ parameters: $X{:=}(A,B,C,\Delta_J,\delta_J,\Delta_{JK},\Delta_K,\delta_K)$ for $i{=}5$, ${}_{(2)}X{:=}({}_{(2)}A,{}_{(2)}B,{}_{(2)}C,{}_{(2)}\Delta_J,{}_{(2)}\delta_J)$, ...

The use of the Hamiltonian H for parametrization of sets including $k{=}0{-}2$ groups of levels consists in fitting to the following five eigenvalues of the matrix $\{H_{K,K'}(X;J)\}$ for $K,K'{=}-2,\ldots,2$,

$$E(X;k{=}0\;,J) \approx H_{0,0}(X;J) - \frac{2H^2_{0,2}(X;J)}{H_{2,2}(X;J)-H_{0,0}(X;J)}\,, \tag{C1}$$

$$E(X;k{=}1^p,J) = H_{1,1}(X;J) - p\,H_{-1,1}(X;J)\,, \tag{C2}$$

$$E(X;k{=}2^p,J) \approx H_{2,2}(X;J) + \delta_{p,1}\frac{2H^2_{0,2}(X;J)}{H_{2,2}(X;J)-H_{0,0}(X;J)} \quad \text{for} \quad p{=}1,-1\,(e,f)\,. \tag{C3}$$

The two matrix elements in the two eigenvalue functions for representing levels in $k{=}1$ group are:

$$H_{1,1}(X;J) = A{-}\tfrac{1}{2}(B{+}C){-}\Delta_K + \big(\tfrac{1}{2}(B{+}C){-}\Delta_{JK}\big)[J] - \Delta_J[J]^2\,,$$
$$H_{-1,1}(X;J) = \big(\tfrac{1}{4}(B{-}C){-}\delta_K\big)[J] - \delta_J[J]^2\,.$$

Comparing them to the elements of ${}_{(2)}H$,

$$H_{1,1}({}_{(2)}X;J) = {}_{(2)}A{-}\tfrac{1}{2}({}_{(2)}B{+}{}_{(2)}C) + \tfrac{1}{2}({}_{(2)}B{+}{}_{(2)}C)[J] - {}_{(2)}\Delta_J[J]^2\,,$$
$$H_{-1,1}({}_{(2)}X;J) = \tfrac{1}{4}({}_{(2)}B{-}{}_{(2)}C)[J] - {}_{(2)}\delta_J[J]^2\,,$$

one notices that

$$H_{K,K'}(X;J){=}H_{K,K'}({}_{(2)}X;J) \qquad \text{for} \quad (K,K'){=}(1,1),(-1,1) \tag{C4}$$

when

${}_{(2)}A{=}A{-}\Delta_{JK}{-}\Delta_K$, ${}_{(2)}B{=}B{-}\Delta_{JK}{-}2\delta_K$, ${}_{(2)}C{=}C{-}\Delta_{JK}{+}2\delta_K$, ${}_{(2)}\Delta_J{=}\Delta_J$, and ${}_{(2)}\delta_J{=}\delta_J$.

The elements $H_{0,0}(X;J)$ and $H_{2,2}(X;J)$ are also second-order polynomials of $[J]$,

$$H_{0,0}(X;J) = \tfrac{1}{2}(B{+}C)[J] - \Delta_J[J]^2\,, \tag{C5}$$

$$H_{2,2}(X;J) = 4A{-}2(B{+}C) - 16\Delta_K - 4\Delta_{JK}[J] + H_{0,0}(X;J)\,. \tag{C6}$$

Thus, the following equalities

$$H_{K,K'}(X;J){=}H_{K,K'}({}_{(3)}X;J) \qquad \text{for} \quad (K,K'){=}(0,0),(1,1),(-1,1) \tag{C7}$$

and $$H_{K,K'}(X;J){=}H_{K,K'}({}_{(4)}X;J) \qquad \text{for} \quad (K,K'){=}(0,0),(1,1),(-1,1),(2,2) \tag{C8}$$

give two systems of linear equations for determining the parameters ${}_{(3)}X$ and ${}_{(4)}X$ in terms of the parameters X. The solutions should be treated as approximate relations between the parameters obtained from actual fits to $k{=}0{-}1$ and $k{=}0{-}2$ sets of levels, in part, because of $H_{0,2}({}_{(i)}X,J){\neq}H_{0,2}(X;J)$,

$$H_{0,2}(X;J) = \big\{\tfrac{1}{4}(B{-}C) - 2\delta_K - \delta_J[J]\big\}\big\{([J]{-}2)[J]\big\}^{1/2}\,. \tag{C9}$$

All the relations established, in the described way, between the parameters ${}_{(i<5)}X$ and ${}_{(5)}X{:=}X$ are collected in Table CVIIa.

(iii) Using Eqs. (C1)–(C6) one can derive approximate formulas which connect the parameters ${}_{(i)}X$ for i=2, 3, 4 to the parameters X^{kp}=($E_{\rm o}^{kp}$, B^{kp}, D^{kp}) defined in Sec. IVB of the paper. These formulas are listed in part b) of Table CVII.
Overall usefulness of the relations is tested in Table CVIII, on the parameters ${}_{(4)}X$ for five vibrational states with $\sum_{\rm m} v_{\rm m}$=1, 2 of the Li^+–D_2 complex, and in Table CIX — on the parameters ${}_{(3)}X$ for the four $\sum_{\rm m} v_{\rm m}\leq 1$ states of both complexes. The conclusion is that the relations allow for predicting values of the rotational constants ${}_{(i)}A$, ${}_{(i)}B$, and ${}_{(i)}C$ obtainable from actual fits to the truncated Hamiltonians ${}_{(i)}H$ with accuracy better than 0.1%.

(iv) Defining: $\overline{E}(X;k,J)=\frac{1}{2-\delta_{k,0}}\sum_{p} E(X;k^p,J)$
and expanding these quantities in powers of $[J]$,

$$\overline{E}(X;k,J) \approx \overline{E}_{\rm o}(X;k) + \overline{B}(X;k)[J] - \overline{D}(X;k)[J]^2 + \ldots$$

one can derive the following relations between coefficients of these expansions for k=0−2:

$$-3\,\overline{E}_{\rm o}(X;k{=}0) + 4\,\overline{E}_{\rm o}(X;k{=}1) - \overline{E}_{\rm o}(X;k{=}2) \;=\; 12\,\Delta_K\,, \tag{C10}$$

$$\overline{B}(X;k{=}0) - 3\,\overline{B}(X;k{=}1) + 2\,\overline{B}(X;k{=}2) \;\approx\; -6\,\Delta_{JK}\,, \tag{C11}$$

$$\overline{D}(X;k{=}0) - 3\,\overline{D}(X;k{=}1) + 2\,\overline{D}(X;k{=}2) \;\approx\; 0\,. \tag{C12}$$

These relations should be approximately satisfied by the respective averages of the parameters X^{kp}, $\overline{X}(k)=\frac{1}{2-\delta_{k,0}}\sum_{p} X^{kp}$ for X=$E_{\rm o}$, B, D,
and the parameters ${}_{(4)}\Delta_K$ and ${}_{(4)}\Delta_{JK}$ or ${}_{(3)}\Delta_{JK}$.
For the seven states $[v_r\,v_\theta\,v_R]$ for which the ${}_{(4)}\Delta_K$'s and ${}_{(4)}\Delta_{JK}$'s are available in Tables CVI and CVIII and the X^{kp}'s — in Table VII, relation (C10) is satisfied with deviations |lhs/rhs−1|×100% $\lesssim$ 5 % and relation (C11) — with deviations $\lesssim$ 18 %.

The relations described in comment (iii) can also be used to analyze the $f-e$ energy splitting (K-type doubling) which is shown for K=1 in Fig. 7 of the paper, namely, to indicate the 'asymmetry splitting' contribution[8]. This is done in Fig. C1.

In some vibrational states of the Li^+–D_2 complex, the $f-e$ splitting of rotational levels in k=2 groups, i.e. the K=2 doubling, appears also describable with the near-rigid rotor model in the quartic approximation. This is demonstrated in the right panel of Fig. C1.

TABLE CVII: a) Relations of parameters ${}_{(i)}X$ of A-reduced Hamiltonian truncated to include $2\leq i<5$ quartic centrifugal distortion terms to parameters $X{=}A, B, C, \Delta_J, \delta_J, \Delta_{JK}, \Delta_K, \delta_K$ of the Hamiltonian with all five these terms$^{\diamondsuit}$. b) Relations of parameters ${}_{(i)}X$ to parameters $E_{\rm o}^{k^p}$, B^{k^p}, and D^{k^p} representing levels in single subgroups k^p for $p{=}e, f$, see Table VII in the paper.

a)	${}_{(2)}A \approx A - \Delta_{JK} - \Delta_K$	${}_{(3)}A \approx A - \Delta_K$	${}_{(4)}A \approx A$	
	${}_{(2)}B \approx B - \Delta_{JK} - 2\delta_K$	${}_{(3)}B \approx B - 2\delta_K$	${}_{(4)}B \approx B - 2\delta_K$	
	${}_{(2)}C \approx C - \Delta_{JK} + 2\delta_K$	${}_{(3)}C \approx C + 2\delta_K$	${}_{(4)}C \approx C + 2\delta_K$	.........(+)
b)	${}_{(2)}A \approx \frac{1}{2}\sum_p (E_{\rm o}^{1^p}+B^{1^p}) - E_{\rm o}^0$	${}_{(3)}A \approx \frac{1}{2}(E_{\rm o}^{1^e}+E_{\rm o}^{1^f}) + B^0 - E_{\rm o}^0$	${}_{(4)}A \approx \frac{1}{2}(E_{\rm o}^{1^e}+E_{\rm o}^{1^f}) + B^0 - E_{\rm o}^0 + {}_{(4)}\Delta_K$	
	${}_{(2)}B \approx \frac{1}{2}(3B^{1^f}-B^{1^e})$	${}_{(3)}B \approx B^0+B^{1^f}-B^{1^e}$	${}_{(4)}B \approx {}_{(3)}B$	
	${}_{(2)}C \approx \frac{1}{2}(3B^{1^e}-B^{1^f})$	${}_{(3)}C \approx B^0+B^{1^e}-B^{1^f}$	${}_{(4)}C \approx {}_{(3)}C$	
	${}_{(2)}\Delta_J \approx \frac{1}{2}(D^{1^f}+D^{1^e})$	${}_{(3)}\Delta_J \approx {}_{(2)}\Delta_J$	${}_{(4)}\Delta_J \approx \frac{1}{4}(D^{1^f}+D^{1^e}) + \frac{1}{2}D^{2^f}$	(∗)
	${}_{(2)}\delta_J \approx \frac{1}{2}(D^{1^f}-D^{1^e})$	${}_{(3)}\delta_J \approx {}_{(2)}\delta_J$	${}_{(4)}\delta_J \approx {}_{(2)}\delta_J$	
		${}_{(3)}\Delta_{JK} \approx B^0 - \frac{1}{2}(B^{1^f}+B^{1^e})$	${}_{(4)}\Delta_{JK} \approx \frac{1}{8}(5B^0-B^{2^f}) - \frac{1}{4}(B^{1^f}+B^{1^e})$	(∗)
			${}_{(4)}\Delta_K \approx \sum_p(\frac{1}{6}E^{1^p}-\frac{1}{24}E^{2^p}) - \frac{1}{4}E_{\rm o}^0$	

$^{\diamondsuit}$ obtained by analyzing fits to $k{=}1$, $k{=}0$–1, and $k{=}0$–2 groups of J levels for $i{=}2$, $i{=}3$, and $i{=}4, 5$, respectively. See, Eqs. (C1)–(C6). (+) the relations for the centrifugal distortion parameters are: ${}_{(i)}\Delta_J{\approx}\Delta_J$ and ${}_{(i)}\delta_J{\approx}\delta_J$ for $i{=}2{-}4$, ${}_{(i)}\Delta_{JK}{\approx}\Delta_{JK}$ for $i{=}3{-}4$, and ${}_{(4)}\Delta_K{\approx}\Delta_K$.
(∗) the expression for ${}_{(3)}\Delta_J$ and for ${}_{(3)}\Delta_{JK}$ should be used when values of the parameters D^{2^f} and B^{2^f} are evidently disturbed, as eg. in the case of state [1 1 0] in Table VII.

TABLE CVIII: Parameters of A-reduced Hamiltonian, truncated to four quartic terms, for rotational energies in several low-excited vibrational states of the Li^+–D_2 complex obtained from fits to $N_{\rm fit}$ levels belonging to $k{=}0{-}2$ groups, denoted as ${}_{(4)}X$ for $X{=}A, B, C, \ldots$, and from the expressions of Table CVIIb, denoted here as ${}_{(4)}\widetilde{X}$.

	${}_{(4)}X$					$({}_{(4)}\widetilde{X}/{}_{(4)}X - 1)\times 100\%$				
	[0 1 0]	[0 0 1]	[2 0 0]	[1 1 0]	[1 0 1]	[0 1 0]	[0 0 1]	[2 0 0]	[1 1 0]	[1 0 1]
E_0	451.292	333.143	5710.215	3371.072	3251.345					
$N_{\rm fit}$	45	59	51	45	57					
A	38.694(6)	32.082(2)	29.077(1)	36.619(8)	30.741(3)	0.09	−0.01	−0.00	−0.05	−0.03
B	1.5457(2)	1.4846(1)	1.57950(4)	1.5361(3)	1.4827(1)	−0.01	0.01	−0.01	0.00	−0.00
C	1.4109(2)	1.3899(1)	1.47508(3)	1.4028(3)	1.3861(1)	−0.01	0.00	−0.01	−0.01	0.00
$\Delta_J\times 10^4$	1.210(6)	1.238(2)	1.107(1)	1.15(1)	1.20(2)	8.0	1.4	1.1	3.6	1.4
$\delta_J\times 10^6$	9.8(7)	7.5(2)	6.6(1)	8.7(9)	7.4(2)	−3.1	2.0	0.8	1.1	0.7
$\Delta_{JK}\times 10^3$	3.36(6)	2.03(2)	1.977(6)	3.18(8)	1.95(2)	9.0	2.2	−2.6	0.6	3.8
$\Delta_K\times 10^2$	21.5(1)	5.90(6)	2.48(2)	17.8(2)	5.08(7)	3.5	−2.6	0.5	−4.2	−6.3
$\sigma\times 10^3$	11	4	1.6	16	8					

TABLE CVIIIb. Test of linear dependence of the rotational constants and their inverses (∼moments of inertia) on the vibrational quantum numbers $v_r(:=v_1)$, $v_\theta(:=v_2)$, and $v_R(:=v_3)$ in low-excited states.

The symbol ${}_{(4)}\widehat{X}$ for states with $\sum_i v_i{>}1$ denotes value extrapolated from the values ${}_{(4)}X$ for states with $\sum_i v_i{\leq}1$ according to the formula

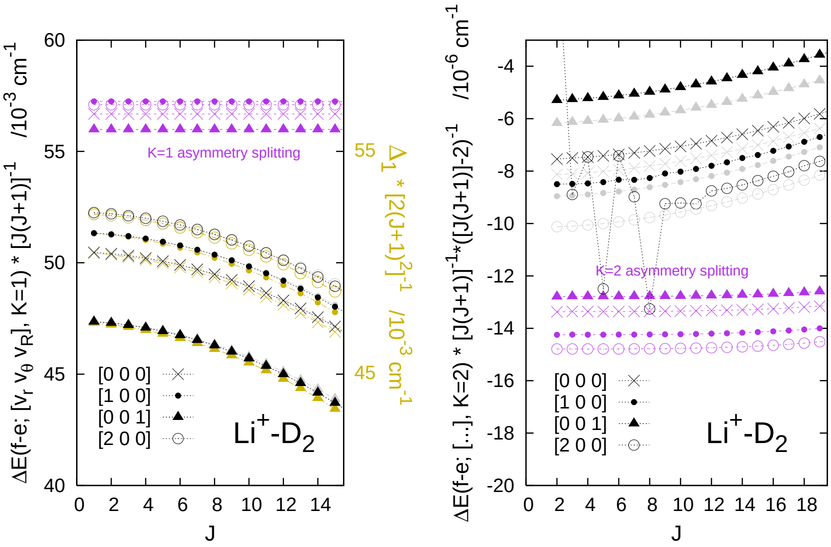
$$\widehat{X}([v_1\, v_2\, v_3]){=}X([0\,0\,0])\times(1-\sum_{i=1}^{3} v_i) + \sum_{i=1}^{3} X([\delta_{i,1}\, \delta_{i,2}\, \delta_{i,3}])\times v_i\,. \quad \text{(C13)}$$

The values of ${}_{(4)}X([0\,0\,0])$ and ${}_{(4)}X([1\,0\,0])$ for $X{=}A, B, C$ are listed in Table CVI, in 2-nd and 6-th column, respectively. $\sim\Delta{:=}1/C{-}1/A{-}1/B$.

	$({}_{(4)}\widehat{X}/{}_{(4)}X - 1)\times 100\%$		
	[2 0 0]	[1 1 0]	[1 0 1]
A	−0.3	2.1	0.12
B	−0.03	0.27	−0.24
C	−0.02	0.07	−0.24
$1/A$	−0.05	−0.38	0.01
$1/B$	0.02	−0.29	0.19
$1/C$	0.02	−0.12	0.18
$\sim\Delta$	−0.01	3.27	−0.24

Li^+–D_2

Fig. C1. K-type doubling



Left: K=1 doubling, from 'exact' close-coupling calculations (black symbols), from approximate expressions (gray symbols, indistinguishable from the black ones):

$$\Delta(J) := (B^{1^f} - B^{1^e})[J] - (D^{1^f} - D^{1^e})[J]^2 \approx \tfrac{1}{2}(B-C)[J] - 2(\delta_K + \delta_J[J])[J] \tag{C14}$$

with $[J]$:=$J(J+1)$, and the 'K=1 asymmetry splitting' part[8] — the first term of the second expression. $\Delta_1(J)$:=$\Delta(J)+\Delta(J+1)$ is the quantity which, for states [0 0 0] and [1 0 0], is confronted with experiment in Table IV of the paper. Since

$$\Delta_1(J) \approx \left\{\tfrac{1}{2}(B-C) - 2(\delta_K + \delta_J[J]) - 2\delta_J(J+2)\right\} \times 2(J+1)^2\,,$$

the pure asymmetry part of this quantity, $(B-C)\times(J+1)^2$, is also represented by the violet symbols.

Right: K=2 doubling, 'exact' (black), approximated (gray) by the expression:

$$\tfrac{1}{2}(H_{2,2} - H_{0,0})\left\{1 - \left(1 + 8\frac{H_{0,2}^2}{(H_{2,2} - H_{0,0})^2}\right)^{1/2}\right\} \tag{C15}$$

with $H_{0,0}$, $H_{2,2}$, and $H_{0,2}$ given in Eqs. (C5)–(C6) and (C9), respectively,

and the 'K=2 asymmetry splitting' part[8] — obtained by setting the Δs and δs to zero.

The constants A, B, C, Δ_{JK}, δ_J, and δ_K come from fitting sets of 'exact' energies in k=0−2 groups to eingenvalues of Watson A-reduced Hamiltonian with all quartic terms included; the values for states [0 0 0] and [1 0 0] are listed in Table CVI, in 5-th and 9-th column, respectively. The values from analogous fit for [2 0 0] are: A=29.077(1), B=1.5843(4), C=1.4701(4), $\Delta_J\times10^4$=1.124(2), $\delta_J\times10^6$=6.5(3), $\Delta_{JK}\times10^3$=1.91(1), $\Delta_K\times10^2$=2.53(4), and $\delta_K\times10^3$=2.46(20) cm^{-1}. [Error: $\sigma\times10^3$=4.0].

The values for [0 0 1]: A=32.084(4), B=1.4933(7), C=1.3814(8), $\Delta_J\times10^4$=1.271(3), $\delta_J\times10^6$=7.3(6), $\Delta_{JK}\times10^3$=2.01(3), $\Delta_K\times10^2$=5.93(7), and $\delta_K\times10^3$=4.3(4) cm^{-1}. [Error: $\sigma\times10^3$=7.6].

It should be noted that the K=2 doubling, Eq. (C15), unlike the K=1 doubling, Eq. (C14), is not adequately described by polynomial which would result from the fits in Table VII of the paper, i.e. by the polynomial $(B^{2^f} - B^{2^e})[J] - (D^{2^f} - D^{2^e})[J]^2$. Apart from a practical difficulty with obtaining the coefficient of the linear term (as it is about 10^5 times smaller than the Bs themselves) the order of the polynomial is too low to account properly for J dependence of this subtle effect.

The $f-e$ splitting of J levels in the shown vibrational states would be clearly larger if it were induced solely by the asymmetry $B-C$ of the effective rotational constants in these states. The centrifugal distortion term associated with the parameter δ_K is primarily responsible for the decrease of the splitting.

According to simulations presented in Fig. C4a below, the K=2 doubling may be a noticeable effect in the spectrum of Li^+–D_2, most likely in the R-branch of the v_r=0→1 band.

TABLE CIX: **Li^+–D_2 and Li^+–H_2**

as near-rigid asymmetric tops

Inertia defects[8]

A. Rotational constants (A, B, C) and centrifugal distortion parameters of A-reduced Watson Hamiltonian representing rotational energies in the ground and three lowest-excited vibrational states of the complexes.
B. Moments of inertia $I_X{=}\hbar^2/(2X)$ for $X{=}A,B,C$ and inertia defect $\Delta{=}I_C{-}I_A{-}I_B$.
Dependence on vibrational quantum numbers $v_r(:=v_1)$, $v_\theta(:=v_2)$, and $v_R(:=v_3)$, see also Table CVIII,

$$I_X([v_1\,v_2\,v_3]) = I_X^{\rm e} - \textstyle\sum_{k=1}^{3}(v_k{+}\frac{1}{2})\eta_{X,k}\ , \qquad \Delta([v_1\,v_2\,v_3]) = \Delta^{\rm e} + \textstyle\sum_{k=1}^{3}(v_k{+}\frac{1}{2})\Delta_k\ .$$

	Li^+-D_2				Li^+-H_2			
A.	[0 0 0]	[1 0 0]	[0 1 0]	[0 0 1]	[0 0 0]	[1 0 0]	[0 1 0]	[0 0 1]
$E_0{}^a$	−1783.613	1131.835	−1332.321	−1450.470	−1674.606	2378.491	−1080.273	−1269.455
$N_{\rm fit}{}^b$	45	45	39	45	45	45	39	45
A^c	31.563(1)	30.265(1)	38.503(1)	32.016(1)	65.537(4)	61.487(3)	95.573(5)	67.896(7)
B^c	1.5900	1.5846	1.5454(1)	1.4847	2.5538(1)	2.5410(1)	2.4618(2)	2.3330(2)
C^c	1.4890	1.4819	1.4106	1.3899	2.4037(1)	2.3891(1)	2.1972(2)	2.1945(2)
$\Delta_J{\times}10^{4\,c}$	1.170(1)	1.137(1)	1.191(1)	1.243(1)	3.251(3)	3.118(3)	3.345(7)	3.593(6)
$\Delta_{JK}{\times}10^{3\,c}$	2.29(1)	2.12(1)	3.53(2)	1.92(1)	5.59(4)	5.04(4)	7.61(7)	4.66(7)
$\delta_J{\times}10^{5\,c}$	0.69(1)	0.69(1)	0.97(2)	0.76(1)	1.59(3)	1.57(3)	2.32(7)	1.73(6)
$\sigma{\times}10^{3\,d}$	2	2.5	2.7	3	10	10	13	19
B.								
$I_A{}^i$	0.5341	0.5570	0.4378	0.5265	0.2572	0.2742	0.1764	0.2483
$I_B{}^i$	10.6023	10.6384	10.9083	11.3542	6.6010	6.6343	6.8477	7.2257
Δ^{fi}	0.1851	0.1803	0.6046	0.2479	0.1550	0.1476	0.6482	0.2077

	$I_A^{\rm e}$	$I_B^{\rm e}$	$r_{\rm e}{}^g$	$R_{\rm e}{}^g$	$\Delta^{{\rm e}\,h}$	Δ_1	Δ_2	Δ_3
Li^+–D_2	0.5746	10.0553	0.7554	1.9825	−0.0537	−0.0048	0.4195	0.0628
Li^+–H_2	0.2936	6.1487	0.7636	1.9821	−0.1144	−0.0073	0.4933	0.0528

[a] Energy of $J{=}0$ level relative to the $Li^+{+}a_2(v{=}0,j{=}0)$ threshold for a=H, D; given in cm^{-1}.
[b] Total number of rotational energies used in the fit: for $k{=}0,1$, $p{=}\pm1$, and $J{=}1,\ldots,J_{\rm max}{=}N_{\rm fit}/3$.
[c] All in cm^{-1}. Obtained from fitting to Watson's Hamiltonian truncated to three quartic terms. In the notation used in Tables CVIa–CVII, they are the parameters ${}_{(3)}X$. Their values ${}_{(3)}\widetilde{X}$ obtained from the parameters X^{k^p} according to the expressions of Table CVIIb show deviations $|{}_{(3)}\widetilde{X}/{}_{(3)}X{-}1|{\times}100\,\%$ smaller than 0.06 % for $X{=}A,B,C$. In cases of the three centrifugal distortion parameters, $X{=}\Delta_J\,\delta_J,\Delta_{JK}$, the deviations are much larger, of the size of several or even a dozen of percent.
[d] Root mean square error of the fit. [i] Given in amu$\AA^2$.
[f] The inertia defect in a given vibrational state $\Delta{=}I_C{-}I_A{-}I_B$.
[g] Obtained as $r_{\rm e}{=}\sqrt{I_A^{\rm e}/\mu_{\rm aa}}$ and $R_{\rm e}{=}\sqrt{I_B^{\rm e}/\mu_{{\rm Li}^+-aa}}$ for a=D,H. [h] $\Delta^{\rm e}{=}I_C^{\rm e}{-}I_A^{\rm e}{-}I_B^{\rm e}$.

Formally, $r_{\rm e}$ and $R_{\rm e}$ are the equilibrium distances, i.e., their values, no matter whether inferred from the rotational constants of the four states of the Li^+–D_2 or the Li^+–H_2 complex, should equal the values at the PES minimum, $r_*{=}0.7503$ and $R_*{=}1.9870$ Å, respectively, see Fig. 1. Thus, the values of $r_{\rm e}$ and $R_{\rm e}$ obtained from the constants of Li^+–D_2, the more accurate ones, are in error by 0.0051 and −0.0045 Å, respectively. For comparison, if one attempted to extract the same quantities from the rotational constants for the ground state only, i.e. from $I_A([0\,0\,0])$ and $I_B([0\,0\,0])$ for Li^+–D_2, one would get values deviating from r_* and R_* by −0.0220 and 0.0487 Å, respectively.

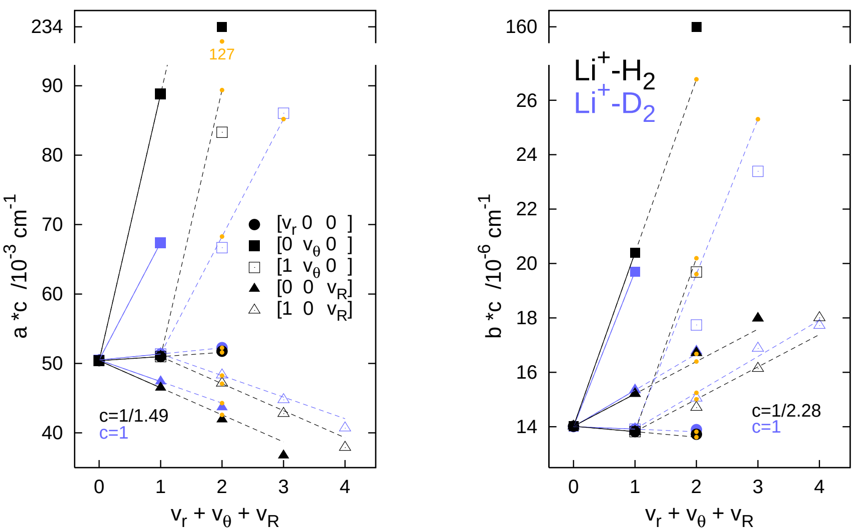
Strictly, the defects $\Delta^{\rm e}$ should be zero. The nonzero values actually obtained may stem from: i) uncertain adequacy of the near-rigidity assumption, especially in describing the Li^+–H_2 complex in its excited bending states, ii) approximate character of the functions $I_X([v_1\,v_2\,v_3])$, and iii) inaccuracies of the fits (some disturbances of the energies used).

$\mathbf{Li^+–D_2}$ and $\mathbf{Li^+–H_2}$

in several low-excited vibrational states

Fig. C2. K=1 doubling

$$\Delta E(f\!-\!e;[v_r\,v_\theta\,v_R]\,k\!=\!1,J) \approx a([\ldots])[J] - b([\ldots])[J]^2$$



The symbols in the plots represent parameters obtained from least-squares fits of the polynomial $a[J]-b[J]^2$ to sets of the calculated doubling values $\{\Delta E(f\!-\!e;[v_r\,v_\theta\,v_R]\,k\!=\!1,J)\,,J\!=\!J_{\rm min}\,\ldots,$ $J_{\rm min}\!+\!N_{\rm fit}\}$ for 11 different states $[v_r\,v_\theta\,v_R]$ of the complexes, see Tables CIII–CIV and BIV–BV. [Formally, $a\!=\!B^{1^f}\!-\!B^{1^e}$ and $b\!=\!D^{1^f}\!-\!D^{1^e}$, where B^{1^p} and D^{1^p} for $p\!=\!e,f$ are the parameters representing the energies $E(f,\ldots)$ and $E(e,\ldots)$, cf. Tables VII-VIII. Direct fitting to the differences $\Delta E(f\!-\!e,\ldots)$ obviously assures better accuracy, especially of the parameters b.] $J_{\rm min}$=1 in all sets except for the set chosen for state [1 2 0] of the $Li^+–D_2$ complex in which $J_{\rm min}$=6. (*) The number of items in the sets: $N_{\rm fit}$=15 for the states with v_θ=0 and v_R<2, $N_{\rm fit}$=13 — for v_θ=1 states, $N_{\rm fit}$=10 — for v_R=2, 3, and $N_{\rm fit}$=8 — for v_θ=2. The dashed lines join the values of the parameters obtained from the fits for states [0 0 0], [1 0 0], [0 1 0], and [0 0 1] of a given complex with values extrapolated linearly to its higher excited states using Eq. (C13) for $X\!=\!a,b$. Perfectly linear dependence of the parameters on the vibrational quantum numbers would give all the symbols lying on the lines.
The yellow dots indicate the values of the parameters a and b used for plotting the 'extrpl' lines in Fig. 7 of the paper.

(*) The ΔEs for lower Js are evidently disturbed in this state, as seen in Fig. 7 of the paper. Occurrence of even bigger disturbances is the reason for which the fitting could not be made for [0 2 0] state of $Li^+–D_2$ and [1 2 0] state of $Li^+–H_2$.

In the range of the numbers $v_{\rm m}$ (m=r,θ,R) shown here, the departure from linearity, especially of the parameter a, is small except for the case of [0 2 0] state of $Li^+–H_2$. A consequence of this fact is the near-coincidence of the 'fit' and 'extrpl' lines seen in Fig. 7 of the paper for states [2 0 0] and [0 0 2] of both complexes and for states [1 1 0] and [1 2 0] of $Li^+–D_2$ and the contrastingly different separation between these lines for [0 2 0] state of $Li^+–H_2$. The factors c are chosen to place at the same point the symbols of $a([0\,0\,0])$ for the two complexes, in the left panel, and the symbols of $b([0\,0\,0]))$— in the right panel. Their values listed in the black labels give also a semi-quantitative estimation of the effect of the $D_2 \to H_2$ substitution on the parameters for the 10 excited states considered. The parameters $a([v_r\,0\,v_R])$ for v_r=0–2 and v_R=0–3, i.e. for states un-excited in the bending mode, become increased by factors close to 1.5 (the ratio of the reduced masses of the complexes is 1.635). Substantially bigger is the increase of the parameters $a([0\,1\,0])$ and $a([1\,1\,0])$. In states excited above v_θ=1, the complexes, especially $Li^+–H_2$, become too floppy to be modeled by near-rigid tops.

INFRARED ABSORPTION SPECTRUM

Fig. C3. Absolute intensities of lines at T=296 K

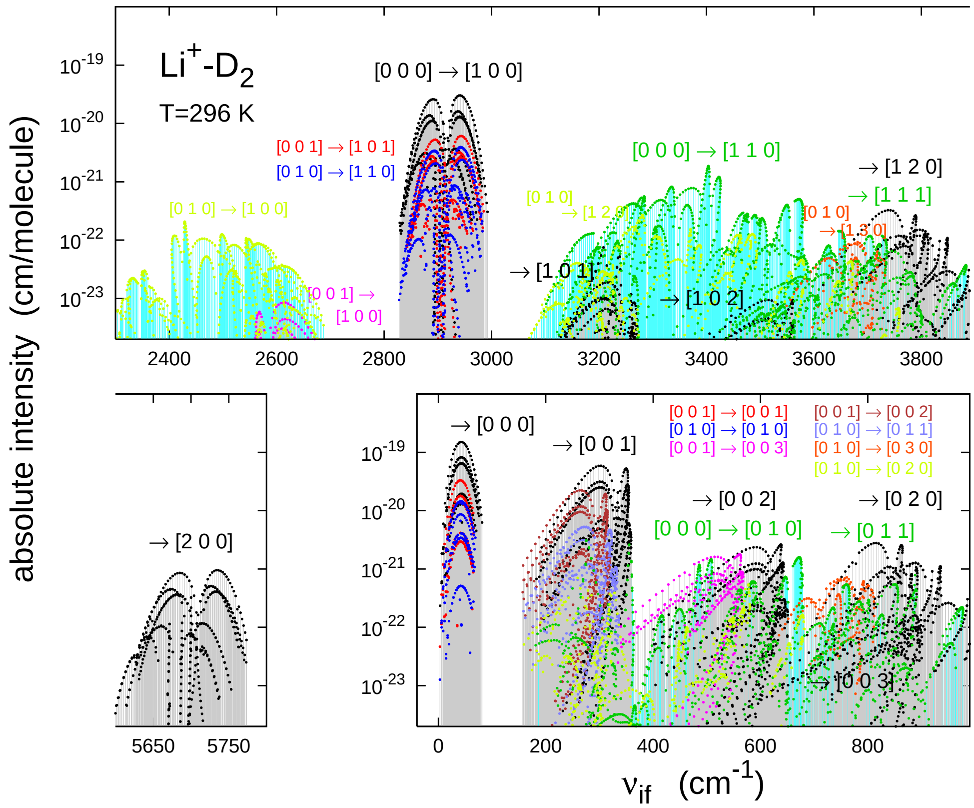
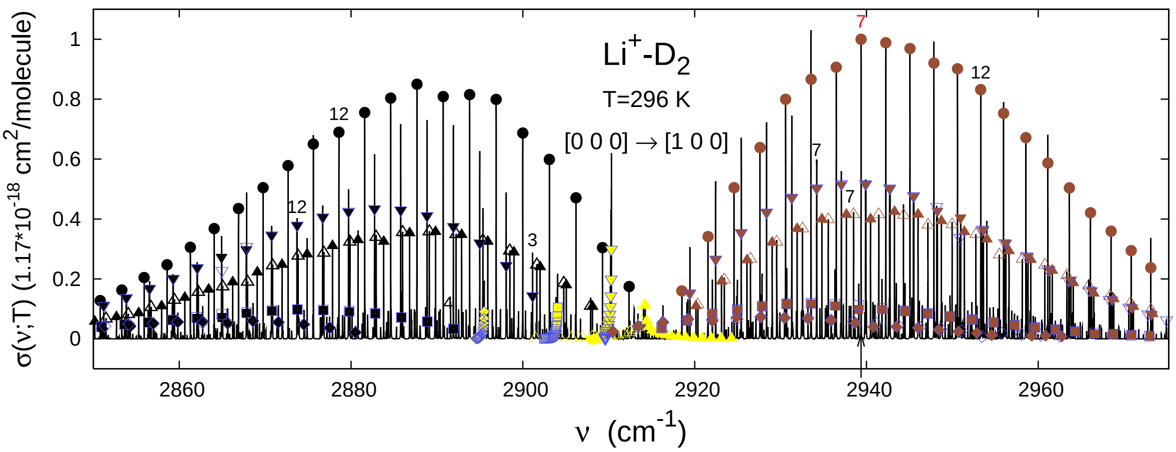
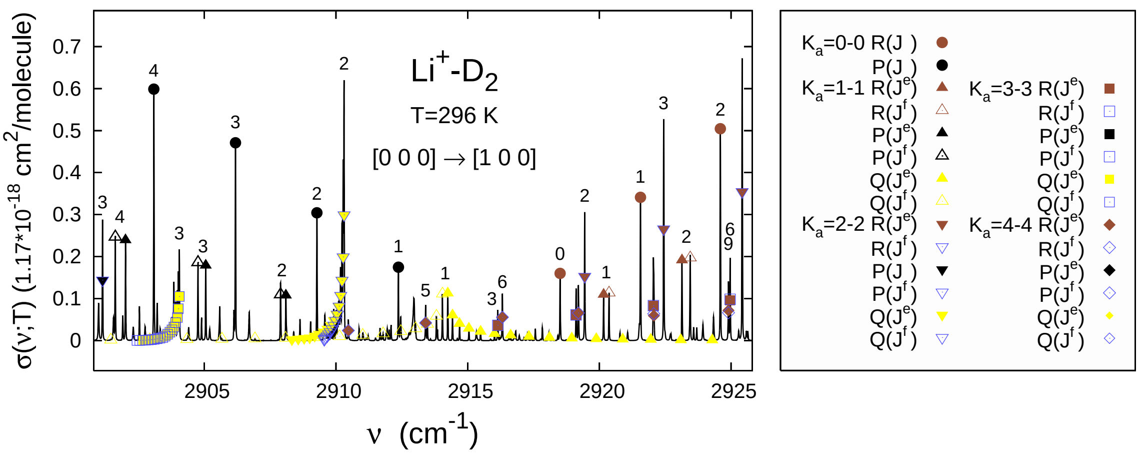
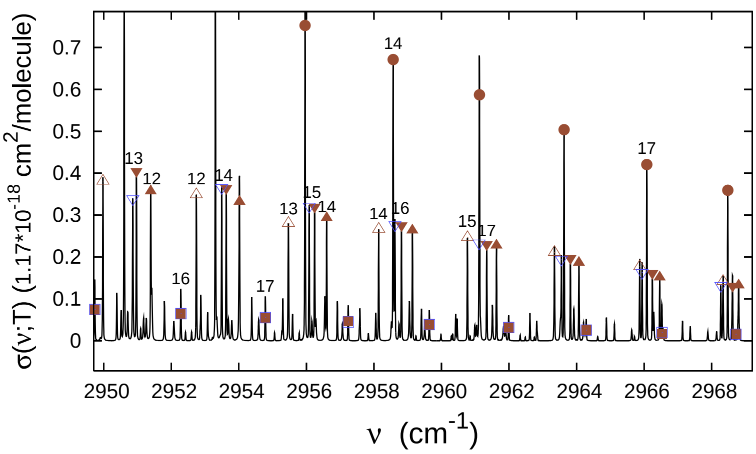


Fig. 14 of the paper is supplied here with the panels showing one more band in the near-infrared range, namely the overtone v_r=0→2 band, and fourteen bands in the mid- and far-infrared (counterparts of the bands of Li^+–H_2 shown in the lower panels of Fig. 13). The intensities shown with the green sticks are due to *b*-type transitions, $\Delta K_a = \pm 1$. Altogether above 12100 lines are shown in the three panels of the present figure. Nearly 39 % of the lines belong to the seven *b*-type bands shown.

Fig. C4a. Fundamental v_r=0→1 band and ...

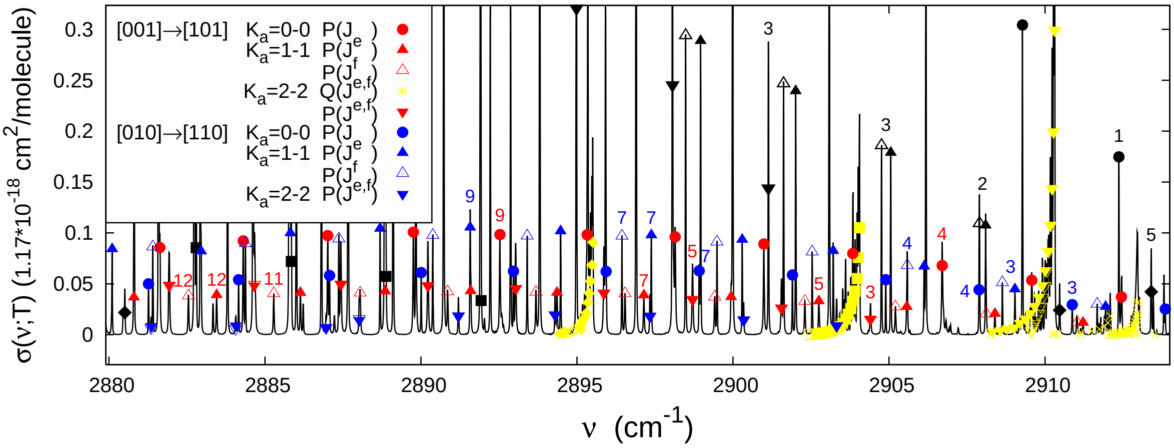






The splitting $\nu[R(J^f)]-\nu[R(J^e)]$ caused by K=2 doubling and its relation to the splitting caused by K=1 doubling manifested here most clearly in the simulated spectrum

... two hot bands overlapping with v_r=0→1



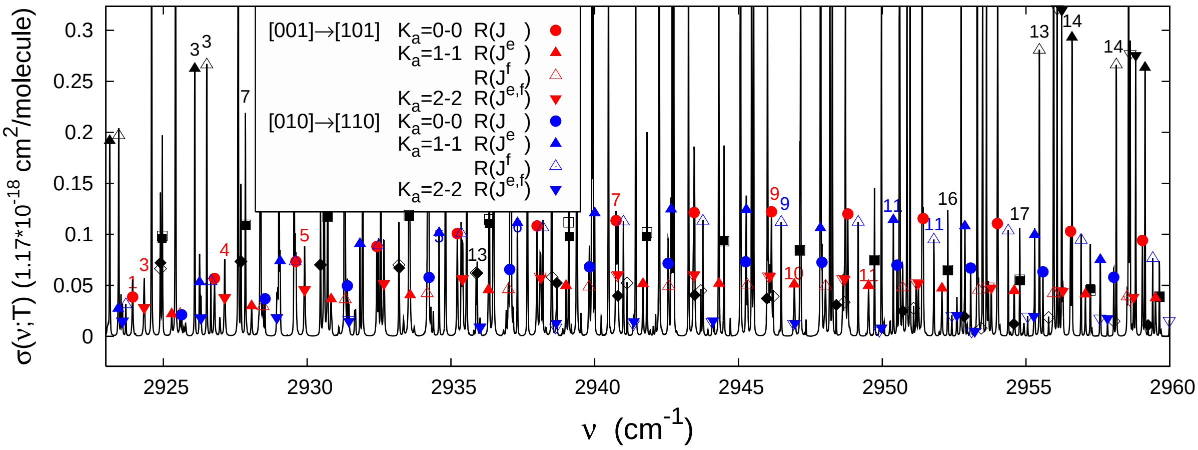
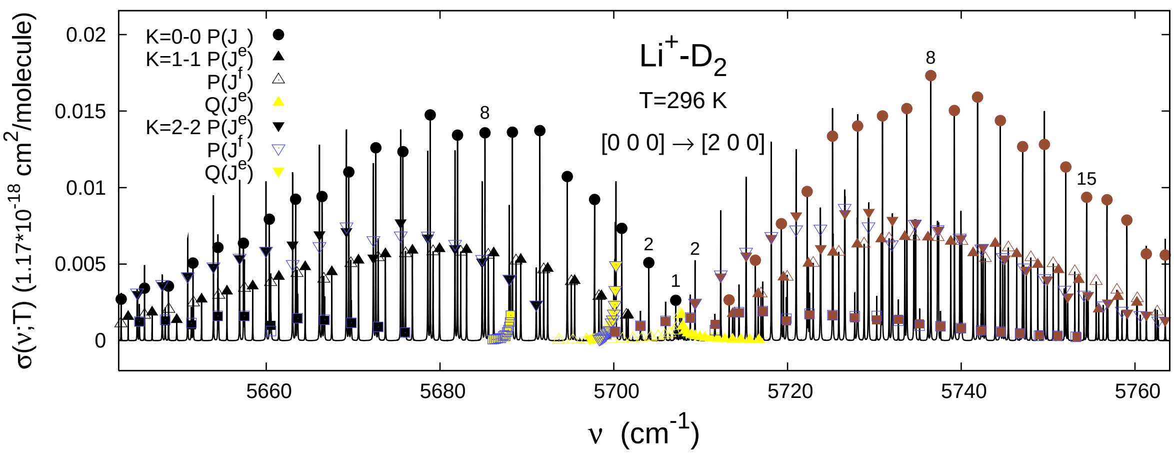


Fig. C4b. Overtone v_r=0→2 band



Splitting in level position due to K doubling: K=2 versus K=1

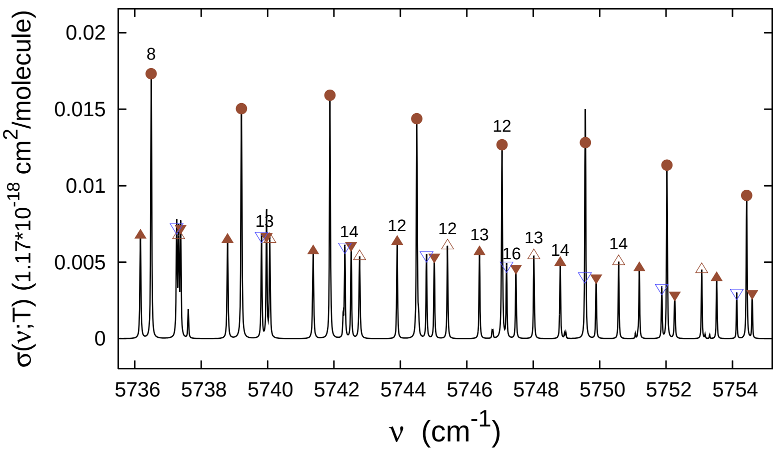
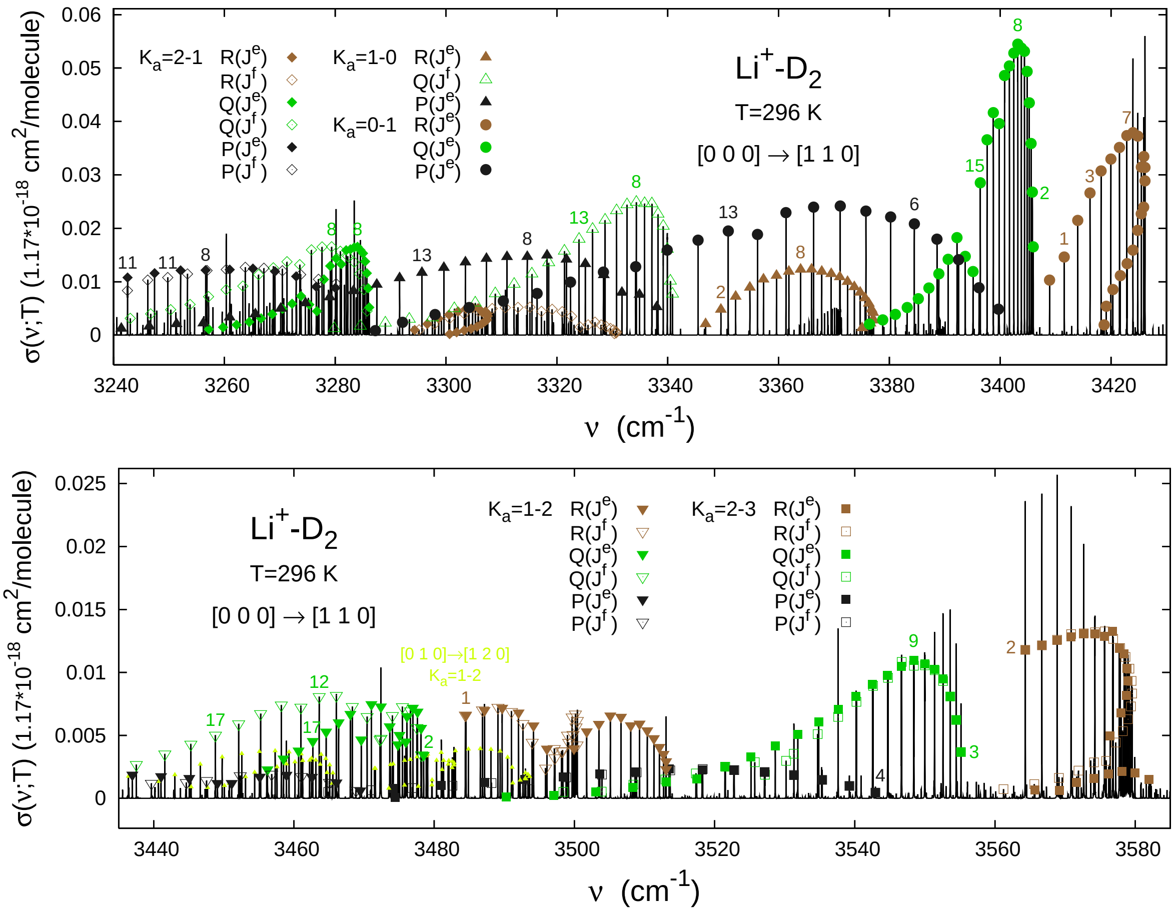


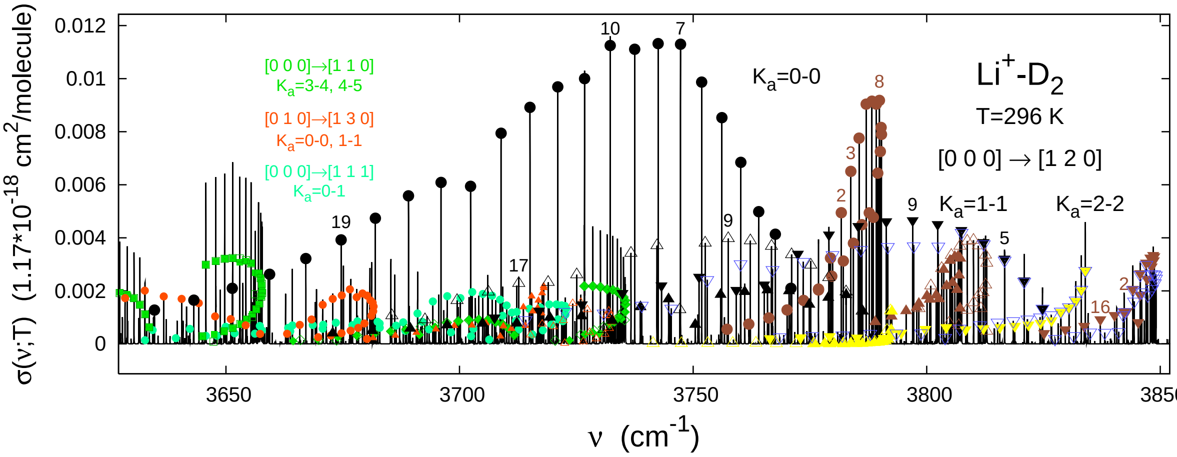
Fig. C4c. Two most intense combination bands:

v_r=0→1 + v_θ=0→1



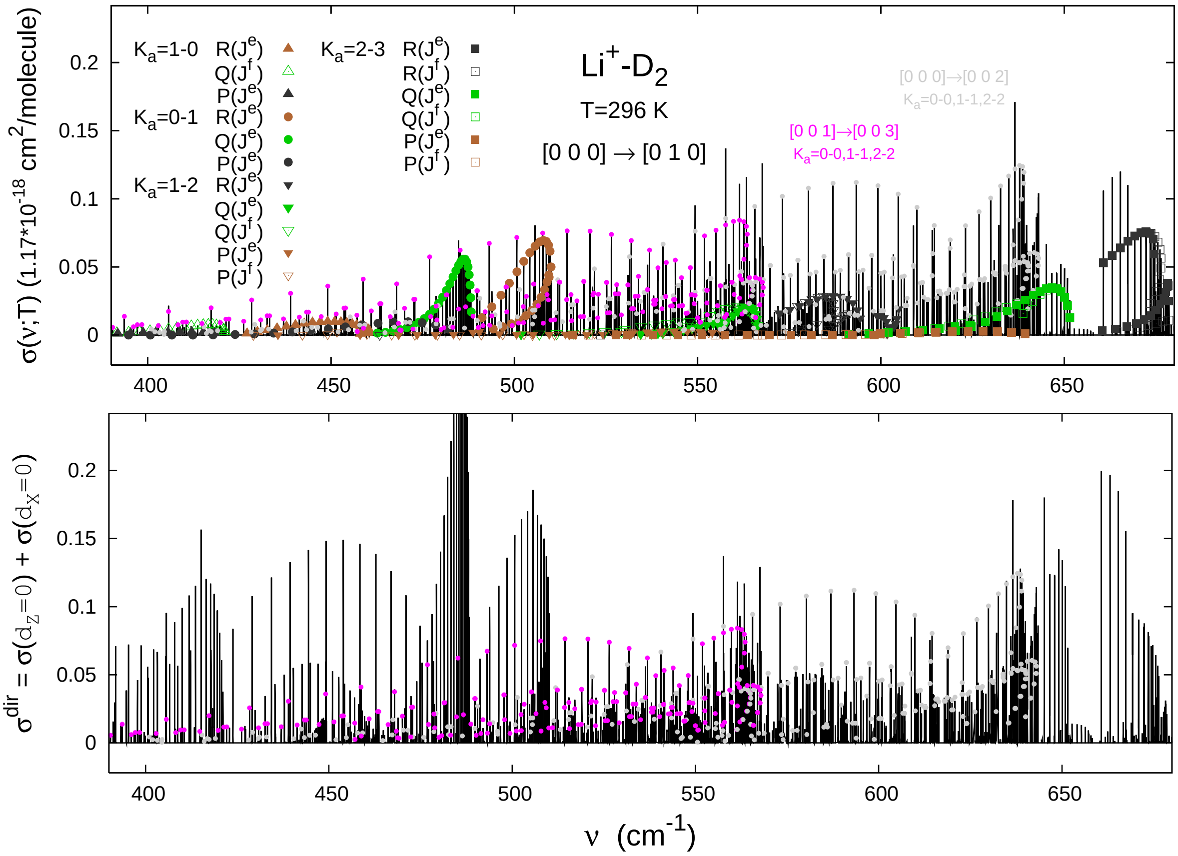
Enlarged version of Fig. 17b of the paper

v_r=0→1 + v_θ=0→2



Like in the plots of the absorption cross-section presented in Part B (Fig. B6), the symbols are placed at the tops of profiles pertaining to individual i→f transitions, i.e. at the positions $(\nu_{\rm if},\ \sigma_{\rm i\to f}(\nu_{\rm if};T))$. Most frequently in the subbands K_a=k−k' with k>1 and k'>1, the symbols appear near the middle (or much below the tops) of the peaks in the $\sigma(\nu;T)$. This is because the peaks in these subbands are enlarged by merging of lines $B(J^p)$ for p=e and p=f in the branches B=R,P,Q, especially for low Js.

Fig. C4d. Fundamental v_θ=0→1 band
and two a-type bands overlapping with it,
'direct' contribution♠ to the cross-section $\sigma(\nu; T)$



♠ obtained by using the parts $S^{\mathrm{dir}}_{\mathrm{i}\to\mathrm{f}}$ of line strengths, see Eq. (C19).

The comparison of line heights in the two panels of Fig. C4d illustrates the role of the d_Z–d_X interference. In the b-type band, especially in its K_a=1−0 and K_a=0−1 subbands, the lines become substantially lowered, by factors exceeding 10 in numerous cases (i.e. the effect is much bigger than that observed in the analogous band of the spectrum of Li^+–H_2, in Fig. B6d in Part B). In contrast to this, the heights of lines in the two a-type bands, precisely, in the R- and P- branches of their K_a=0−0, 1−1, 2−2 subbands are affected very little (the grey and pink dots in the lower panel, placed at the same positions as in the upper panel, are almost invisibly shifted relative to the tops of the lines). No doubts, of significance to the bigness/smallness of these d_Z–d_X interference effects is the size of the d_Z dipole component for Li^+–D_2, more precisely, the size of its isotropic part $D_{0,0}(r, R)$, see Fig. 1b in the paper.

TABLE CX: Infrared spectrum of Li^{+}–D_2. Line positions (ν, in cm^{-1}), vibrational factors of line strengths[a] ($S_{\rm vib}$ in 10^{-3} D^2), and relative line intensities ($I_{\rm rel}$) at T=296 K in five sub-bands $(b\,k{=}b\,v_R{=}0)\rightarrow(k\,k\,0)$ of v_r=0→1 band, for k=0–4. Deviations ($\Delta=\nu^{\rm Cal}-\nu^{\rm Exp}$) of transition frequencies calculated in this work and in Ref. 4 from the values measured in Ref. 7. The asymmetric top labels of initial and final rotational levels $J_{K_aK_c}$ and $J'_{K'_aK'_c}$ are: $K_a=K'_a=k$, $K_c=J-k+\frac{1-(-1)^kp}{2}$, $K'_c=K_c+\Delta K_c$ with $\Delta K_c=\pm1$ and $\Delta K_c=(-1)^kp$ for $J'=J\pm1$ and J, respectively.

	$R(J)$					$P(J)$					$Q(J)$				
J	ν	Δ	Δ Ref. 4	$S_{\rm vib}$	I	ν	Δ	Δ Ref. 4	$S_{\rm vib}$	I	ν	Δ	Δ Ref. 4	$S_{\rm vib}$	I
								k=0 p=1							
0	2918.51	0.80	2.9	3.17	5.63 (−21)										
1	2921.56	0.78	2.9	3.17	1.11 (−20)	2912.37	0.86	3.0	3.16	5.52 (−21)					
2	2924.59	0.75	3.1	3.17	1.62 (−20)	2909.28	0.85	3.0	3.16	1.07 (−20)					
3	2927.60	0.72	3.1	3.18	2.07 (−20)	2906.18	0.88	3.1	3.16	1.53 (−20)					
4	2930.59	0.71	3.3	3.28	2.52 (−20)	2903.09	0.90	3.2	3.16	1.92 (−20)					
5	2933.55	0.68	3.5	3.19	2.73 (−20)	2899.99	0.91	3.3	3.16	2.23 (−20)					
6	2936.48	0.66	3.9	3.19	2.92 (−20)	2896.89	0.94	3.5	3.26	2.52 (−20)					
7	2939.38	0.62	4.2	3.19	3.02 (−20)	2893.81	0.94	3.7	3.16	2.56 (−20)					
8	2942.24	0.60	4.8	3.20	3.02 (−20)	2890.73	0.96	4.1	3.16	2.60 (−20)					
9	2945.07	0.58	5.4	3.21	2.95 (−20)	2887.66	0.96	4.6	3.16	2.56 (−20)					
10	2947.86	0.54		3.21	2.81 (−20)	2884.62	0.97	5.1	3.16	2.45 (−20)					
11	2950.60	0.50		3.22	2.61 (−20)	2881.59	0.99		3.16	2.29 (−20)					
12	2953.30	0.48		3.23	2.38 (−20)	2878.59	0.99		3.16	2.10 (−20)					
13	2955.96	0.45		3.23	2.13 (−20)	2875.61	0.98		3.17	1.88 (−20)					
14	2958.57	0.41		3.24	1.87 (−20)	2872.67	1.01		3.17	1.65 (−20)					
15	2961.12	0.38		3.25	1.61 (−20)	2869.76			3.17	1.43 (−20)					
16	2963.63			3.26	1.37 (−20)	2866.89			3.17	1.21 (−20)					
17	2966.08			3.27	1.14 (−20)	2864.07			3.18	1.01 (−20)					
18	2968.48			3.27	9.35 (−21)	2861.29			3.18	8.29 (−21)					
19	2970.82			3.28	7.55 (−21)	2858.57			3.18	6.70 (−21)					
20	2973.10			3.29	6.01 (−21)	2855.91			3.18	5.33 (−21)					
21	2975.32			3.29	4.72 (−21)	2853.32			3.19	4.18 (−21)					
22	2977.48			3.28	3.63 (−21)	2850.79			3.19	3.23 (−21)					
23	2979.58			3.31	2.79 (−21)	2848.34			3.19	2.47 (−21)					
24	2981.62			3.31	2.11 (−21)	2845.98			3.18	1.85 (−21)					
25	2983.60			3.32	1.57 (−21)	2843.71			3.20	1.38 (−21)					
								k=1 p=1 /p=−1[b]							
1	2920.16	0.76	2.9	3.17	3.60 (−21)						2914.24	0.79	2.8	3.15	3.57 (−21)
	2920.37	0.75	2.9	3.16	3.59 (−21)						2914.04	0.79	2.8	3.15	3.57 (−21)
2	2923.14	0.72	3.0	3.17	6.23 (−21)	2908.10	0.82	2.9	3.16	3.47 (−21)	2914.42	0.78	2.9	3.12	1.91 (−21)
	2923.45	0.73	3.0	3.16	6.21 (−21)	2907.90	0.84	3.2	3.16	3.47 (−21)	2913.81	0.78	3.0	3.14	1.92 (−21)
3	2926.09	0.71	3.1	3.18	8.41 (−21)	2905.06	0.84	3.0	3.15	5.89 (−21)	2914.69	0.78	3.0	3.08	1.26 (−21)
	2926.51	0.70	3.1	3.17	8.36 (−21)	2904.76	0.85	3.0	3.16	5.89 (−21)	2913.47	0.78	3.1	3.11	1.27 (−21)
4	2929.02	0.67	3.2	3.18	1.01 (−20)	2902.01	0.85	3.1	3.15	7.80 (−21)	2915.05	0.79	3.1	3.02	9.01 (−22)
	2929.55	0.68	3.2	3.17	1.00 (−20)	2901.62	0.87	3.1	3.16	7.79 (−21)	2913.02			3.08	9.13 (−22)
5	2931.93	0.65	3.5	3.19	1.15 (−20)	2898.96	0.88	3.3	3.15	9.26 (−21)	2915.49			2.95	6.67 (−22)
	2932.56	0.66	3.5	3.17	1.13 (−20)	2898.48	0.88	3.3	3.16	9.23 (−21)	2912.46			3.04	6.80 (−22)
6	2934.81	0.62	3.9	3.20	1.24 (−20)	2895.91	0.89	3.5	3.15	1.03 (−20)	2916.02			2.87	5.01 (−22)
	2935.55	0.62	3.9	3.17	1.22 (−20)	2895.35	0.88	3.5	3.17	1.02 (−20)	2911.79			2.99	5.16 (−22)
7	2937.66	0.60	4.3	3.20	1.29 (−20)	2892.87	0.91	3.8	3.15	1.09 (−20)	2916.63			2.78	3.79 (−22)
	2938.50	0.61	4.3	3.18	1.26 (−20)	2892.22	0.92	3.8	3.17	1.08 (−20)	2911.01			2.93	3.94 (−22)
8	2940.48	0.58	4.9	3.22	1.30 (−20)	2889.84	0.91	4.2	3.15	1.11 (−20)	2917.33			2.67	2.86 (−22)
	2941.43	0.57	4.9	3.18	1.27 (−20)	2889.11	0.92	4.2	3.17	1.10 (−20)	2910.14			2.87	3.01 (−22)
9	2943.26	0.55	5.6	3.22	1.28 (−20)	2886.81	0.93	4.6	3.15	1.10 (−20)	2918.10			2.56	2.15 (−22)
	2944.31	0.55	5.6	3.19	1.24 (−20)	2886.01	0.94	4.7	3.17	1.09 (−20)	2909.16			2.80	2.30 (−22)
10	2946.01	0.52		3.23	1.22 (−20)	2883.80	0.94	5.2	3.15	1.06 (−20)	2918.95			2.44	1.60 (−22)
	2947.16	0.51		3.19	1.18 (−20)	2882.92			3.17	1.04 (−20)	2908.09			2.72	1.74 (−22)
11	2948.72			3.23	1.14 (−20)	2880.81			3.15	9.97 (−21)	2919.88			2.31	1.18 (−22)
	2949.97	0.47		3.20	1.09 (−20)	2879.87			3.18	9.75 (−21)	2906.92			2.64	1.31 (−22)
12	2951.39			3.24	1.05 (−20)	2877.83			3.15	9.16 (−21)	2920.88			2.17	8.63 (−23)
	2952.74			3.20	1.00 (−20)	2876.83			3.18	8.91 (−21)	2905.67			2.55	9.72 (−23)
13	2954.02			3.25	9.42 (−21)	2874.88			3.15	8.24 (−21)	2921.95			2.03	6.21 (−23)
	2955.47			3.21	8.92 (−21)	2873.83			3.18	7.98 (−21)	2904.34			2.46	7.15 (−23)

14	2956.60			3.25	8.27 (−21)	2871.96			3.15	7.27 (−21)	2923.09		1.89	4.40 (−23)
	2958.14			3.21	7.80 (−21)	2870.86			3.19	7.00 (−21)	2902.93		2.36	5.20 (−23)
15	2959.14			3.27	7.18 (−21)	2869.08			3.16	6.29 (−21)	2924.29		1.74	3.07 (−23)
	2960.77			3.22	6.70 (−21)	2867.94			3.19	6.03 (−21)	2901.45		2.25	3.72 (−23)
16	2961.63			3.28	6.11 (−21)	2866.22			3.15	5.34 (−21)	2925.54		1.60	2.11 (−23)
	2963.35			3.23	5.66 (−21)	2865.05			3.19	5.10 (−21)	2899.90		2.16	2.65 (−23)
17	2964.07			3.29	5.12 (−21)	2863.41			3.16	4.48 (−21)	2926.86		1.45	1.42 (−23)
	2965.87			3.23	4.70 (−21)	2862.22			3.20	4.24 (−21)	2898.30		2.05	1.86 (−23)
18	2966.46			3.30	4.21 (−21)	2860.65			3.16	3.69 (−21)	2928.22		1.30	9.40 (−24)
	2968.34			3.24	3.84 (−21)	2859.43			3.21	3.47 (−21)	2896.65		1.94	1.28 (−23)
19	2968.80			3.31	3.42 (−21)	2857.94			3.17	2.99 (−21)	2929.63		1.16	6.10 (−24)
	2970.75			3.25	3.09 (−21)	2856.71			3.21	2.79 (−21)	2894.96		1.83	8.73 (−24)
20	2971.08			3.32	2.73 (−21)	2855.28			3.17	2.39 (−21)	2931.08		1.02	3.88 (−24)
	2973.11			3.25	2.45 (−21)	2854.05			3.22	2.21 (−21)	2893.23		1.72	5.87 (−24)
21	2973.31			3.32	2.15 (−21)	2852.69			3.17	1.88 (−21)	2932.57		8.89	2.41 (−24)
	2975.41			3.26	1.91 (−21)	2851.47			3.22	1.73 (−21)	2891.47		1.60	3.88 (−24)
22	2975.49			3.33	1.67 (−21)				3.18	1.46 (−21)	2934.09		7.61	1.46 (−24)
	2977.64			3.26	1.47 (−21)				3.22	1.33 (−21)	2889.71		1.49	2.53 (−24)
23	2977.61			3.34	1.28 (−21)				3.18	1.12 (−21)	2935.64		6.40	8.62 (−25)
	2979.81			3.27	1.12 (−21)				3.23	1.01 (−21)	2887.93		1.37	1.62 (−24)
24	2979.66			3.35	9.74 (−22)				3.18	8.48 (−22)	2937.22		5.27	4.94 (−25)
	2981.92			3.27	8.42 (−22)				3.23	7.61 (−22)	2886.17		1.26	1.03 (−24)

k=2 p=1 / p=−1

2	2919.44	0.66	3.6	3.17	5.02 (−21)						2910.30		3.13	9.88 (−21)
	2919.44	0.66	3.6	3.17	5.02 (−21)						2910.31	0.73	3.13	9.88 (−21)
3	2922.44	0.64	3.8	3.17	8.67 (−21)	2901.13	0.79	3.6	3.16	4.75 (−21)	2910.27		3.09	6.54 (−21)
	2922.44	0.64	3.8	3.17	8.67 (−21)	2901.14	0.79	3.6	3.16	4.75 (−21)	2910.27		3.09	6.54 (−21)
4	2925.42	0.62	4.1	3.18	1.15 (−20)	2898.06	0.80	3.7	3.16	8.05 (−21)	2910.23		3.05	4.69 (−21)
	2925.42	0.62	4.1	3.18	1.15 (−20)	2898.06	0.80	3.7	3.16	8.05 (−21)	2910.23		3.05	4.69 (−21)
5	2928.38	0.58	4.5	3.18	1.35 (−20)	2894.98	0.83	4.0	3.16	1.05 (−20)	2910.17		2.99	3.48 (−21)
	2928.37	0.57	4.5	3.18	1.36 (−20)	2894.98	0.83	4.0	3.16	1.05 (−20)	2910.18		2.99	3.48 (−21)
6	2931.31	0.56	5.0	3.19	1.50 (−20)	2891.90	0.82	4.3	3.16	1.21 (−20)	2910.10		2.93	2.63 (−21)
	2931.30	0.55	5.0	3.19	1.50 (−20)	2891.91	0.83	4.3	3.16	1.21 (−20)	2910.12		2.93	2.63 (−21)
7	2934.22	0.54	5.7	3.20	1.58 (−20)	2888.83	0.83	4.8	3.16	1.32 (−20)	2910.01		2.85	2.00 (−21)
	2934.20	0.52	5.7	3.20	1.58 (−20)	2888.84	0.84	4.8	3.16	1.32 (−20)	2910.06		2.85	2.00 (−21)
8	2937.09	0.51	6.5	3.20	1.61 (−20)	2885.77	0.84	5.4	3.16	1.37 (−20)	2909.91		2.76	1.52 (−21)
	2937.07	0.48	6.6	3.20	1.61 (−20)	2885.79	0.85	5.4	3.16	1.37 (−20)	2909.99		2.76	1.52 (−21)
9	2939.94	0.49	7.6	3.21	1.59 (−20)	2882.73			3.16	1.36 (−20)	2909.80		2.67	1.15 (−21)
	2939.90	0.45	7.6	3.21	1.59 (−20)	2882.74			3.16	1.36 (−20)	2909.92		2.66	1.15 (−21)
10	2942.75			3.22	1.52 (−20)	2879.69			3.16	1.32 (−20)	2909.67		2.56	8.62 (−22)
	2942.70			3.22	1.52 (−20)	2879.71			3.16	1.32 (−20)	2909.85		2.56	8.60 (−22)
11	2945.53			3.22	1.43 (−20)	2876.68			3.17	1.25 (−20)	2909.53		2.45	6.40 (−22)
	2945.46			3.22	1.43 (−20)	2876.71			3.16	1.25 (−20)	2909.78		2.44	6.38 (−22)
12	2948.26			3.23	1.31 (−20)	2873.70			3.17	1.15 (−20)	2909.37		2.33	4.70 (−22)
	2948.18			3.23	1.31 (−20)	2873.72			3.17	1.15 (−20)	2909.72		2.32	4.68 (−22)
13	2950.97			3.24	1.17 (−20)	2870.73			3.17	1.03 (−20)	2909.19		2.21	3.41 (−22)
	2950.86			3.24	1.17 (−20)	2870.77			3.17	1.03 (−20)	2909.66		2.19	3.39 (−22)
14	2953.63			3.25	1.03 (−20)	2867.81			3.18	9.14 (−21)	2909.00		2.07	2.44 (−22)
	2953.49			3.25	1.03 (−20)	2867.84			3.17	9.14 (−21)	2909.62		2.05	2.42 (−22)
15	2956.24			3.25	8.92 (−21)	2864.92			3.18	7.91 (−21)	2908.79		1.93	1.71 (−22)
	2956.08			3.26	8.95 (−21)	2864.96			3.18	7.92 (−21)	2909.58		1.91	1.69 (−22)
16	2958.81			3.26	7.58 (−21)	2862.07			3.19	6.73 (−21)	2908.57		1.79	1.18 (−22)
	2958.62			3.27	7.60 (−21)	2862.11			3.18	6.74 (−21)	2909.56		1.76	1.17 (−22)
17	2961.34			3.27	6.33 (−21)	2859.26			3.19	5.63 (−21)	2908.32		1.65	8.06 (−23)
	2961.11			3.27	6.34 (−21)	2859.30			3.19	5.63 (−21)	2909.55		1.61	7.91 (−23)
18	2963.82			3.28	5.20 (−21)	2856.51			3.20	4.63 (−21)	2908.07		1.50	5.37 (−23)
	2963.55			3.28	5.22 (−21)	2856.55			3.19	4.63 (−21)	2909.57		1.46	5.25 (−23)
19	2966.24			3.29	4.21 (−21)	2853.82			3.21	3.75 (−21)	2907.80		1.35	3.51 (−23)
	2965.94			3.29	4.23 (−21)	2853.85			3.20	3.75 (−21)	2909.60		1.30	3.41 (−23)
20	2968.62			3.29	3.35 (−21)	2851.19			3.21	2.99 (−21)	2907.53		1.20	2.25 (−23)
	2968.27			3.30	3.38 (−21)	2851.21			3.20	2.99 (−21)	2909.65		1.15	2.17 (−23)
21	2970.94			3.30	2.63 (−21)	2848.62			3.22	2.35 (−21)	2907.24		1.05	1.41 (−23)
	2970.55			3.31	2.65 (−21)	2848.64			3.21	2.35 (−21)	2909.73		1.00	1.34 (−23)
22	2973.20			3.31	2.04 (−21)	2846.14			3.23	1.82 (−21)	2906.95		0.91	8.56 (−24)
	2972.77			3.32	2.06 (−21)	2846.14			3.21	1.82 (−21)	2909.84		0.85	8.07 (−24)

					k=3 p=1 /p=−1					
3	2916.14	3.18	1.23 (−21)				2904.05		3.10	3.58 (−21)
	2916.14	3.18	1.23 (−21)				2904.05	0.60	3.10	3.58 (−21)
4	2919.12	3.13	2.09 (−21)	2891.93	3.16	1.14 (−21)	2904.01		3.05	2.56 (−21)
	2919.12	3.12	2.08 (−21)	2891.93	3.16	1.14 (−21)	2904.01		3.05	2.56 (−21)
5	2922.05	3.19	2.78 (−21)	2888.87	3.16	1.94 (−21)	2903.98		2.94	1.87 (−21)
	2922.05	3.18	2.78 (−21)	2888.88	3.16	1.94 (−21)	2903.98		2.95	1.88 (−21)
6	2924.96	3.20	3.25 (−21)	2885.84	3.11	2.45 (−21)	2903.91		2.93	1.44 (−21)
	2924.96	3.20	3.25 (−21)	2885.84	3.10	2.45 (−21)	2903.91		2.93	1.44 (−21)
7	2927.85	3.20	3.54 (−21)	2882.80	3.16	2.85 (−21)	2903.85		2.86	1.10 (−21)
	2927.85	3.20	3.54 (−21)	2882.80	3.15	2.85 (−21)	2903.85		2.86	1.10 (−21)
8	2930.71	3.21	3.67 (−21)	2879.77	3.16	3.05 (−21)	2903.78		2.77	8.35 (−22)
	2930.71	3.21	3.67 (−21)	2879.77	3.16	3.05 (−21)	2903.77		2.77	8.35 (−22)
9	2933.54	3.22	3.68 (−21)	2876.76	3.16	3.12 (−21)	2903.70		2.68	6.32 (−22)
	2933.54	3.22	3.68 (−21)	2876.76	3.16	3.12 (−21)	2903.69		2.68	6.32 (−22)
10	2936.33	3.23	3.57 (−21)	2873.76	3.17	3.06 (−21)	2903.61		2.57	4.75 (−22)
	2936.34	3.23	3.57 (−21)	2873.76	3.17	3.06 (−21)	2903.61		2.57	4.75 (−22)
11	2939.10	3.16	3.30 (−21)	2870.79	3.17	2.92 (−21)	2903.52		2.46	3.54 (−22)
	2939.09	3.23	3.37 (−21)	2870.79	3.17	2.92 (−21)	2903.51		2.46	3.54 (−22)
12	2941.82	3.25	3.12 (−21)	2867.84	3.17	2.72 (−21)	2903.42		2.34	2.60 (−22)
	2941.82	3.24	3.11 (−21)	2867.84	3.18	2.72 (−21)	2903.43		2.29	2.54 (−22)
13	2944.50	3.25	2.81 (−21)	2864.94	3.11	2.41 (−21)	2903.33		2.22	1.89 (−22)
	2944.50	3.25	2.81 (−21)	2864.92	3.18	2.46 (−21)	2903.32		2.22	1.89 (−22)
14	2947.13	3.26	2.49 (−21)	2862.05	3.19	2.19 (−21)	2903.23		2.08	1.35 (−22)
	2947.14	3.26	2.49 (−21)	2862.04	3.18	2.19 (−21)	2903.21		2.08	1.35 (−22)
15	2949.73	3.27	2.17 (−21)	2859.20	3.19	1.91 (−21)	2903.13		1.94	9.54 (−23)
	2949.73	3.27	2.17 (−21)	2859.19	3.19	1.91 (−21)	2903.10		1.95	9.54 (−23)
16	2952.28	3.29	1.85 (−21)	2856.40	3.20	1.63 (−21)	2903.03		1.80	6.61 (−23)
	2952.28	3.28	1.85 (−21)	2856.39	3.20	1.63 (−21)	2902.99		1.80	6.62 (−23)
17	2954.78	3.30	1.55 (−21)	2853.64	3.20	1.37 (−21)	2902.94		1.65	4.50 (−23)
	2954.78	3.30	1.55 (−21)	2853.63	3.20	1.37 (−21)	2902.88		1.66	4.51 (−23)
18	2957.23	3.31	1.28 (−21)	2850.94	3.21	1.13 (−21)	2902.85		1.51	3.01 (−23)
	2957.24	3.31	1.28 (−21)	2850.92	3.21	1.13 (−21)	2902.77		1.51	3.02 (−23)
19	2959.64	3.32	1.04 (−21)	2848.31	3.22	9.22 (−22)	2902.78		1.36	1.97 (−23)
	2959.64	3.32	1.04 (−21)	2848.27	3.22	9.22 (−22)	2902.66		1.36	1.98 (−23)
20	2961.99	3.33	8.36 (−22)	2845.73	3.23	7.38 (−22)	2902.72		1.20	1.26 (−23)
	2961.99	3.33	8.35 (−22)	2845.69	3.23	7.38 (−22)	2902.55		1.21	1.27 (−23)
					k=4 p=1 /p=−1					
4	2910.47	3.19	8.80 (−22)				2895.51		3.06	3.36 (−21)
	2910.47	3.19	8.80 (−22)				2895.51		3.06	3.36 (−21)
5	2913.40	3.19	1.52 (−21)	2880.51	3.17	8.04 (−22)	2895.47		3.00	2.50 (−21)
	2913.40	3.19	1.52 (−21)	2880.51	3.17	8.04 (−22)	2895.47		3.00	2.50 (−21)
6	2916.32	3.20	1.97 (−21)	2877.51	3.16	1.36 (−21)	2895.44		2.93	1.89 (−21)
	2916.32	3.20	1.97 (−21)	2877.51	3.16	1.36 (−21)	2895.44		2.93	1.89 (−21)
7	2919.20	3.20	2.27 (−21)	2874.51	3.16	1.74 (−21)	2895.39		2.86	1.44 (−21)
	2919.20	3.20	2.27 (−21)	2874.51	3.16	1.74 (−21)	2895.39		2.86	1.44 (−21)
8	2922.07	3.21	2.45 (−21)	2871.54	3.16	1.97 (−21)	2895.35		2.77	1.09 (−21)
	2922.07	3.21	2.45 (−21)	2871.54	3.16	1.97 (−21)	2895.35		2.77	1.09 (−21)
9	2924.90	3.22	2.51 (−21)	2868.58	3.16	2.08 (−21)	2895.30		2.68	8.30 (−22)
	2924.90	3.22	2.51 (−21)	2868.58	3.16	2.08 (−21)	2895.30		2.68	8.31 (−22)
10	2927.70	3.23	2.48 (−21)	2865.64	3.17	2.09 (−21)	2895.24		2.58	6.25 (−22)
	2927.70	3.23	2.48 (−21)	2865.63	3.17	2.09 (−21)	2895.24		2.58	6.26 (−22)
11	2930.47	3.24	2.38 (−21)	2862.72	3.17	2.03 (−21)	2895.18		2.47	4.67 (−22)
	2930.46	3.24	2.37 (−21)	2862.72	3.17	2.03 (−21)	2895.18		2.47	4.67 (−22)
12	2933.20	3.25	2.21 (−21)	2859.84	3.17	1.91 (−21)	2895.12		2.35	3.43 (−22)
	2933.19	3.26	2.22 (−21)	2859.83	3.18	1.91 (−21)	2895.11		2.36	3.45 (−22)
13	2935.92	3.24	2.00 (−21)	2857.00	3.15	1.73 (−21)	2895.08		2.19	2.47 (−22)
	2935.88	3.27	2.02 (−21)	2856.96	3.18	1.75 (−21)	2895.04		2.23	2.51 (−22)
14	2938.68	2.95	1.62 (−21)	2854.30	2.83	1.39 (−21)	2895.14		1.83	1.58 (−22)
	2938.52	3.28	1.80 (−21)	2854.14	3.19	1.57 (−21)	2894.97		2.11	1.81 (−22)
15	2940.81	2.52	1.20 (−21)	2851.04	2.51	1.08 (−21)	2894.59		1.60	1.04 (−22)
	2941.13	3.29	1.58 (−21)	2851.35	3.20	1.38 (−21)	2894.90		1.97	1.28 (−22)

[a]Obtained from the calculated total strength as S_{vib}=S/S_{rot} using the S_{rot}s listed in Eq. (C17).
[b]Entries in the lower line for each J value concern $J \to J\pm1, J$ transitions from the p=−1 parity state.

TABLE CXI: Near-infrared absorption spectrum of Li^{+}–D_2. Line positions (ν, in cm^{-1}), vibrational factors of line strengths (S_{vib} in 10^{-3} D^2), and line intensities (I, in 10^{-21} cm/molecule) at T=296 in two hot bands overlapping with the fundamental v_r=0→1 band.

	$[v_r\, v_\theta\, v_R]$=[0 1 0] → [1 1 0] K_a=0–0 $(b\,k)$=(1 0) → (1 0)									K_a=0–0 of [0 0 1] → [1 0 1] K_a=0–0 $(b\,k)$=(0 0) → (0 0)								
	$R(J)$			$P(J)$			$Q(J)$			$R(J)$			$P(J)$			$Q(J)$		
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	2922.72	4.39	0.44							2921.07	3.12	1.10						
1	2925.64	4.39	0.86	2916.83	4.39	0.43				2923.93	3.13	2.18	2915.33	3.12	1.08			
2	2928.53	4.39	1.25	2913.85	4.39	0.83				2926.78	3.13	3.18	2912.45	3.12	2.10			
3	2931.40	4.39	1.60	2910.87	4.39	1.20				2929.61	3.13	4.07	2909.58	3.12	3.02			
4	2934.24	4.39	1.90	2907.89	4.39	1.50				2932.43	3.13	4.82	2906.71	3.11	3.80			
5	2937.05	4.39	2.12	2904.90	4.39	1.75				2935.22	3.14	5.41	2903.84	3.11	4.43			
6	2939.82	4.39	2.27	2901.91	4.39	1.92				2937.99	3.14	5.82	2900.99	3.11	4.88			
7	2942.55	4.40	2.36	2898.92	4.40	2.03				2940.74	3.14	6.04	2898.15	3.11	5.16			
8	2945.25	4.41	2.38	2895.93	4.40	2.07				2943.46	3.15	6.10	2895.33	3.11	5.28			
9	2947.90	4.42	2.33	2892.96	4.40	2.05				2946.15	3.16	6.01	2892.53	3.11	5.23			
10	2950.51	4.41	2.22	2890.01	4.42	1.98				2948.80	3.15	5.77	2889.76	3.11	5.06			
11	2953.08	4.41	2.08	2887.07	4.42	1.87				2951.42	3.16	5.42	2887.01	3.11	4.80			
12	2955.59	4.42	1.91	2884.15	4.42	1.72				2954.01	3.16	5.00	2884.30	3.11	4.43			
13	2958.05	4.43	1.72	2881.27	4.42	1.55				2956.55	3.16	4.52	2881.63	3.10	4.02			
14	2960.46	4.43	1.52	2878.41	4.42	1.38				2959.05	3.16	4.02	2879.00	3.10	3.58			
15	2962.82	4.44	1.32	2875.59	4.43	1.20				2961.51	3.17	3.51	2876.42	3.10	3.13			
16	2965.12	4.44	1.13	2872.81	4.43	1.03				2963.92	3.17	3.02	2873.90	3.10	2.70			
17	2967.37	4.45	0.95	2870.08	4.44	0.87				2966.29	3.17	2.56	2871.43	3.10	2.28			
18	2969.55	4.45	0.79	2867.40	4.44	0.72				2968.61	3.17	2.13	2869.02	3.09	1.91			
19	2971.68	4.46	0.64	2864.78	4.45	0.59				2970.87	3.17	1.75	2866.69	3.09	1.57			
20	2973.75	3.72	0.43	2862.22	4.45	0.48				2973.09	3.17	1.42	2864.43	3.09	1.27			
21	2975.76	4.47	0.41	2859.73	4.46	0.38				2975.26	3.17	1.14	2862.26	3.08	1.02			
22	2977.70	4.47	0.32	2857.32	3.72	0.25				2977.37	3.17	0.90	2860.18	3.08	0.80			
23	2979.59	4.47	0.25	2855.00	4.46	0.23				2979.43	3.16	0.70	2858.20	3.07	0.63			
24	2981.41	4.48	0.19	2852.77	4.46	0.18				2981.44	3.16	0.54	2856.34	3.06	0.48			
25	2983.18	4.36	0.14	2850.65	4.46	0.13				2983.39	3.15	0.41	2854.60	3.05	0.37			
	K_a=1–1 $(b\,k)$=(2 1) → (2 1)									K_a=1–1 $(b\,k)$=(1 1) → (1 1)								
	$R(J^e)$ / $R(J^f)$			$P(J^e)$ / $P(J^f)$			$Q(J^e)$ / $Q(J^f)$			$R(J^e)$ / $R(J^f)$			$P(J^e)$ / $P(J^f)$			$Q(J^e)$ / $Q(J^f)$		
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	2923.43	4.35	1.07				2917.84	4.33	1.06	2922.49	3.12	0.70				2916.96	3.10	0.70
	2923.70	4.35	1.07				2917.57	4.34	1.06	2922.69	3.12	0.70				2916.77	3.11	0.70
2	2926.26	4.35	1.85	2911.94	4.35	1.03	2918.07	4.31	0.57	2925.29	3.13	1.22	2911.22	3.11	0.68	2917.14	3.07	0.37
	2926.65	4.35	1.84	2911.67	4.35	1.03	2917.27	4.32	0.57	2925.58	3.12	1.21	2911.03	3.11	0.68	2916.57	3.09	0.37
3	2929.06	4.36	2.50	2909.04	4.35	1.76	2918.42	4.27	0.38	2928.07	3.13	1.65	2908.40	3.11	1.15	2917.41	3.03	0.25
	2929.58	4.35	2.48	2908.63	4.35	1.75	2916.82	4.29	0.38	2928.46	3.12	1.64	2908.12	3.11	1.15	2916.27	3.06	0.25
4	2931.84	4.36	3.03	2906.13	4.35	2.34	2918.89	4.22	0.27	2930.83	3.14	2.00	2905.57	3.10	1.53	2917.77	2.98	0.18
	2932.49	4.35	3.00	2905.59	4.35	2.32	2916.23	4.25	0.27	2931.33	3.12	1.98	2905.21	3.11	1.53	2915.87	3.03	0.18
5	2934.59	4.37	3.44	2903.21	4.35	2.79	2919.47	4.16	0.20	2933.58	3.03	2.20	2902.75	3.10	1.83	2918.21	2.91	0.13
	2935.36	4.35	3.39	2902.54	4.35	2.76	2915.49	4.21	0.21	2934.17	3.13	2.25	2902.30	3.11	1.82	2915.37	2.99	0.13
6	2937.31	4.37	3.72	2900.30	4.35	3.11	2920.17	4.08	0.16	2936.30	3.05	2.40	2899.94	3.10	2.05	2918.75	2.84	0.10
	2938.20	4.35	3.66	2899.49	4.36	3.08	2914.60	4.16	0.16	2937.00	3.12	2.43	2899.41	3.11	2.04	2914.78	2.84	0.10
7	2940.00	4.37	3.89	2897.38	4.36	3.32	2920.97	4.00	0.12	2939.00	3.15	2.58	2897.14	2.99	2.11	2919.36	2.74	0.08
	2941.00	4.35	3.80	2896.44	4.36	3.27	2913.59	4.10	0.12	2939.80	3.13	2.54	2896.54	3.12	2.17	2914.10	2.80	0.08
8	2942.65	4.38	3.94	2894.48	4.36	3.41	2921.89	3.91	0.09	2941.68	3.26	2.71	2894.36	3.00	2.18	2920.06	2.64	0.06
	2943.76	4.35	3.83	2893.40	4.36	3.34	2912.43	4.03	0.09	2942.57	3.13	2.56	2893.69	3.12	2.22	2913.33	2.81	0.06
9	2945.27	4.39	3.88	2891.58	4.36	3.40	2922.91	3.81	0.07	2944.32	3.15	2.59	2891.59	3.09	2.24	2920.84	2.52	0.04
	2946.49	4.36	3.75	2890.38	4.37	3.31	2911.14	3.96	0.07	2945.32	3.16	2.55	2890.85	3.12	2.21	2912.47	2.83	0.05
10	2947.85	4.39	3.74	2888.69	4.36	3.30	2924.03	3.70	0.05	2946.94	3.16	2.50	2888.85	3.19	2.25	2921.70	2.43	0.03
	2949.16	4.36	3.58	2887.37	4.37	3.19	2909.73	3.88	0.06	2948.03	3.13	2.42	2888.05	3.11	2.14	2911.54	2.66	0.04

11	2950.39	4.40	3.51	2885.81	4.36	3.12	2925.25	3.59	0.04	2949.53	3.17	2.37	2886.14	3.08	2.06	2922.63	2.28	0.02
	2951.80	4.37	3.35	2884.37	4.37	3.00	2908.19	3.80	0.04	2950.71	3.12	2.27	2885.28	3.15	2.04	2910.53	2.58	0.03
12	2952.88	4.40	3.24	2882.95	4.36	2.89	2926.56	3.48	0.03	2952.08	3.17	2.19	2883.45	3.08	1.91	2923.63	2.14	0.02
	2954.38	4.37	3.07	2881.41	4.38	2.76	2906.54	3.71	0.03	2953.35	3.15	2.10	2882.55	3.11	1.87	2909.44	2.50	0.02
13	2955.30	4.36	2.90	2880.10	4.31	2.59	2927.94	3.34	0.02	2954.59	3.18	1.99	2880.80	3.09	1.75	2924.71	2.02	0.01
	2956.92	4.38	2.75	2878.46	4.39	2.49	2904.78	3.62	0.02	2955.95	3.13	1.89	2879.85	3.11	1.69	2908.30	2.40	0.02
14	2957.59	3.93	2.32	2877.18	3.86	2.07	2929.31	2.96	0.02	2957.07	3.18	1.77	2878.19	3.09	1.56	2925.85	1.87	0.01
	2959.41	4.36	2.41	2875.56	4.39	2.20	2902.92	3.53	0.02	2958.52	3.13	1.67	2877.21	3.13	1.52	2907.09	2.31	0.01
15	2960.42	3.45	1.78	2874.88	3.49	1.64	2931.37	2.30	0.01	2959.50	3.19	1.56	2875.62	3.08	1.37	2927.05	1.73	0.01
	2961.84	4.44	2.13	2872.68	4.39	1.91	2900.96	3.44	0.01	2961.04	3.14	1.46	2874.61	3.11	1.31	2905.83	2.20	0.01
16	2962.62	4.13	1.83	2872.03	4.15	1.67	2932.91	2.75	0.01	2961.90	3.19	1.34	2873.10	3.08	1.18	2928.30	1.59	0.00
	2964.21	4.42	1.80	2869.86	4.38	1.62	2898.91	3.35	0.01	2963.52	3.13	1.25	2872.07	3.11	1.13	2904.53	2.10	0.01
17	2964.88	4.23	1.58	2869.34	4.25	1.45	2934.63	2.70	0.01	2964.25	3.19	1.14	2870.63	3.08	1.01	2929.62	1.44	0.00
	2966.52	4.39	1.49	2867.08	4.46	1.39	2896.79	3.27	0.01	2965.95	3.13	1.05	2869.60	3.11	0.95	2903.19	1.99	0.00
18	2967.14	4.24	1.32	2866.71	4.28	1.22	2936.45	2.59	0.00	2966.56	3.20	0.96	2868.22	3.08	0.84	2930.98	1.31	0.00
	2968.78	4.39	1.23	2864.35	4.43	1.14	2894.61	3.20	0.00	2968.33	3.13	0.87	2867.19	3.11	0.79	2901.82	1.88	0.00
19	2969.39	4.16	1.06	2864.17	4.28	1.00	2938.34	2.48	0.00	2968.82	3.20	0.79	2865.87	3.08	0.70	2932.38	1.17	0.00
	2970.97	4.39	1.00	2861.69	4.40	0.92	2892.38	3.14	0.00	2970.66	3.13	0.72	2864.85	3.10	0.65	2900.44	1.77	0.00
20	2971.71	3.91	0.81	2861.70	4.25	0.80	2940.30	2.36	0.00	2971.03	3.20	0.64	2863.59	3.07	0.57	2933.82	1.04	0.00
	2973.10	4.39	0.80	2859.09	4.40	0.73	2890.14	3.12	0.00	2972.94	3.13	0.58	2862.60	3.10	0.53	2899.05	1.66	0.00
	K_a=2−2 (b k)=(3 2) → (3 2)									K_a=2−2 (b k)=(2 2) → (2 2)								
2	2920.78	4.25	0.33				2912.09	4.23	0.66	2921.52	3.11	0.97				2912.97	3.07	1.91
	2920.78	4.25	0.33				2912.09	4.23	0.66	2921.51	3.11	0.97				2912.97	3.07	1.91
3	2923.58	4.16	0.56	2903.32	4.28	0.32	2912.01	4.13	0.43	2924.33	3.11	1.68	2904.41	3.10	0.92	2912.95	3.04	1.27
	2923.58	4.16	0.56	2903.32	4.28	0.32	2912.02	4.13	0.43	2924.33	3.11	1.68	2904.41	3.10	0.92	2912.95	3.04	1.27
4	2926.31	3.97	0.71	2900.34	4.24	0.54	2911.90	3.96	0.30	2927.14	3.11	2.22	2901.55	3.10	1.57	2912.93	2.99	0.91
	2926.31	3.93	0.70	2900.34	4.23	0.54	2911.91	3.96	0.30	2927.13	3.11	2.22	2901.55	3.10	1.57	2912.94	2.99	0.91
5	2928.95	3.64	0.77	2897.34	4.14	0.68	2911.74	3.67	0.21	2929.92	3.11	2.64	2898.70	3.10	2.04	2912.90	2.93	0.68
	2928.94	3.64	0.77	2897.34	4.14	0.68	2911.74	3.70	0.21	2929.91	3.11	2.64	2898.70	3.10	2.04	2912.91	2.93	0.68
6	2931.46	3.09	0.72	2894.30	3.97	0.76	2911.50	3.31	0.15	2932.68	3.11	2.93	2895.86	3.09	2.38	2912.86	2.86	0.51
	2931.45	3.15	0.74	2894.30	3.93	0.76	2911.51	3.30	0.15	2932.67	3.11	2.93	2895.86	3.09	2.38	2912.88	2.86	0.51
7	2936.02	1.69	0.42	2891.20	3.67	0.77	2911.14	2.80	0.10	2935.41	3.12	3.11	2893.03	3.09	2.60	2912.82	2.78	0.39
	2936.01	1.68	0.42	2891.20	3.67	0.77	2911.16	2.74	0.10	2935.40	3.12	3.11	2893.04	3.09	2.60	2912.85	2.78	0.39
8	2938.66	2.11	0.53	2888.02	3.18	0.69	2912.87	1.35	0.04	2938.12	3.09	3.16	2890.22	3.09	2.72	2912.77	2.69	0.30
	2938.65	2.06	0.52	2888.02	3.24	0.70	2912.90	1.36	0.04	2938.10	3.11	3.18	2890.23	3.08	2.72	2912.82	2.69	0.30
9	2941.36	2.36	0.59	2886.95	1.47	0.32	2912.70	1.49	0.03	2940.81	3.13	3.17	2887.43	3.09	2.74	2912.71	2.59	0.23
	2941.34	1.88	0.47	2886.96	1.46	0.32	2912.75	1.52	0.03	2940.78	3.15	3.19	2887.44	3.09	2.74	2912.79	2.57	0.23
10	2944.12	2.25	0.54	2884.06	1.71	0.37	2912.65	1.15	0.02	2943.47	3.13	3.07	2884.66	3.06	2.65	2912.65	2.50	0.17
	2944.08	2.16	0.52	2884.06	1.67	0.36	2912.72	1.46	0.02	2943.43	3.12	3.06	2884.67	3.08	2.67	2912.77	2.48	0.17
11	2946.96	1.93	0.44	2881.35	1.67	0.34	2912.72	1.01	0.01	2946.10	3.14	2.91	2881.92	3.09	2.55	2912.58	2.36	0.13
	2946.91	1.92	0.44	2881.34	1.33	0.27	2912.81	1.07	0.01	2946.05	3.14	2.91	2881.93	3.11	2.57	2912.76	2.37	0.13
12	2949.97	1.44	0.30	2878.88	1.24	0.24	2912.98	0.55	0.01	2948.69	3.14	2.69	2879.22	3.09	2.38	2912.51	2.25	0.10
	2949.90	1.44	0.30	2878.86	1.21	0.23	2913.11	0.59	0.01	2948.63	3.14	2.70	2879.23	3.07	2.37	2912.75	2.24	0.10
13	2953.22	0.84	0.16	2876.74	0.75	0.13	2913.53	0.17	0.00	2951.26	3.15	2.45	2876.56	3.09	2.17	2912.44	2.12	0.07
	2953.11	0.85	0.16	2876.69	0.76	0.13	2913.68	0.20	0.00	2951.18	3.15	2.45	2876.57	3.09	2.17	2912.76	2.10	0.07
14	2952.60	3.82	0.64	2870.81	3.75	0.57	2910.24	3.92	0.02	2953.79	3.15	2.18	2873.94	3.09	1.94	2912.36	1.98	0.05
	2952.42	3.80	0.63	2870.71	3.75	0.57	2910.39	3.88	0.02	2953.69	3.15	2.19	2873.95	3.09	1.94	2912.78	1.96	0.05
15	2955.27	4.07	0.59	2868.28	3.98	0.53	2910.30	3.69	0.02	2956.28	3.16	1.92	2871.37	3.09	1.71	2912.28	1.84	0.04
	2955.05	4.04	0.59	2868.13	3.96	0.52	2910.49	3.68	0.02	2956.16	3.16	1.92	2871.38	3.09	1.71	2912.81	1.82	0.04
16	2957.83	4.19	0.52	2865.73	4.10	0.46	2910.30	3.40	0.01	2958.74	3.16	1.65	2868.86	3.09	1.47	2912.21	1.69	0.03
	2957.57	4.17	0.52	2865.53	4.08	0.46	2910.50	3.41	0.01	2958.60	3.17	1.66	2868.87	3.09	1.47	2912.87	1.67	0.02
17	2960.33	4.25	0.45	2863.23	4.15	0.40	2910.30	3.07	0.01	2961.16	3.16	1.40	2866.41	3.09	1.25	2912.14	1.54	0.02
	2959.98	4.24	0.44	2862.93	4.15	0.40	2910.47	3.13	0.01	2960.99	3.17	1.41	2866.41	3.09	1.25	2912.94	1.51	0.02
18	2962.84	4.24	0.37	2860.90	4.10	0.33	2910.42	2.64	0.01	2963.53	3.17	1.17	2864.03	3.09	1.05	2912.07	1.39	0.01
	2962.33	4.28	0.37	2860.37	4.20	0.33	2910.40	2.84	0.01	2963.33	3.17	1.18	2864.02	3.10	1.05	2913.04	1.36	0.01
19	2965.71	3.88	0.28	2859.22	3.46	0.23	2911.14	1.69	0.00	2965.86	3.17	0.97	2861.72	3.11	0.87	2912.01	1.23	0.01
	2964.63	4.29	0.31	2857.89	4.21	0.27	2910.31	2.50	0.00	2965.63	3.17	0.97	2861.70	3.09	0.87	2913.16	1.20	0.01

TABLE CXII: Near-infrared absorption spectrum of Li^+–D_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 the 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 (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_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0										3408.90	1.87	3.87						
1	3346.83	1.93	0.84	3338.02	1.97	1.71	3340.86	1.95	2.54	3411.55	1.87	5.76				3405.96	1.86	5.69
2	3349.60	1.92	1.62	3334.92	1.98	2.50	3340.49	1.95	4.10	3413.98	1.88	7.49	3399.67	1.85	1.83	3405.80	1.85	9.19
3	3352.26	1.92	2.32	3331.73	2.00	3.22	3339.93	1.94	5.46	3416.20	1.89	9.01	3396.17	1.85	3.49	3405.56	1.85	12.26
4	3354.82	1.91	2.91	3328.47	2.02	3.82	3339.19	1.94	6.58	3418.19	1.91	10.25	3392.48	1.84	4.92	3405.24	1.84	14.79
5	3357.28	1.90	3.38	3325.13	2.04	4.30	3338.26	1.93	7.42	3419.96	1.92	11.20	3388.58	1.84	6.08	3404.84	1.83	16.69
6	3359.63	1.90	3.71	3321.71	2.06	4.63	3337.14	1.92	7.96	3421.51	1.93	11.79	3384.50	1.84	6.95	3404.37	1.82	17.92
7	3361.86	1.90	3.91	3318.22	2.08	4.83	3335.83	1.90	8.21	3422.84	1.95	12.05	3380.22	1.85	7.52	3403.81	1.81	18.50
8	3363.97	1.91	3.99	3314.65	2.11	4.88	3334.33	1.89	8.18	3423.94	1.97	12.00	3375.76	1.85	7.79	3403.17	1.79	18.47
9	3365.95	1.91	3.94	3311.01	2.13	4.81	3332.65	1.88	7.94	3424.82	1.98	11.66	3371.12	1.85	7.80	3402.45	1.77	17.90
10	3367.79	1.90	3.78	3307.29	2.16	4.64	3330.77	1.86	7.47	3425.47	2.00	11.09	3366.31	1.86	7.58	3401.65	1.75	16.89
11	3369.50	1.91	3.56	3303.49	2.19	4.37	3328.70	1.83	6.86	3425.91	2.02	10.31	3361.34	1.86	7.18	3400.77	1.73	15.56
12	3371.05	1.91	3.28	3299.61	2.21	4.01	3326.45	1.81	6.16	3426.12	2.04	9.41	3356.20	1.87	6.65	3399.80	1.72	14.03
13	3372.44	1.92	2.96	3295.66	2.23	3.63	3324.00	1.79	5.42	3426.12	2.06	8.42	3350.91	1.88	6.01	3398.75	1.69	12.36
14	3373.67	1.92	2.62	3291.62	2.26	3.22	3321.36	1.77	4.67	3425.89	2.08	7.41	3345.48	1.89	5.33	3397.62	1.67	10.68
15	3374.73	1.93	2.28	3287.50	2.29	2.80	3318.52	1.74	3.95	3425.45	2.10	6.39	3339.91	1.89	4.64	3396.40	1.63	9.02
16	3375.61	1.94	1.94	3283.30	2.32	2.40	3315.50	1.72	3.28	3424.80	2.11	5.42	3334.21	1.90	3.96	3395.09	1.64	7.63
17	3376.29	1.95	1.63	3279.01	2.35	2.02	3312.28	1.69	2.67	3423.94	2.13	4.52	3328.39	1.91	3.32	3393.69	1.60	6.20
18	3376.78	1.95	1.35	3274.63	2.37	1.68	3308.87	1.66	2.14	3422.89	2.13	3.70	3322.46	1.91	2.74	3392.20	1.56	4.94
19	3377.06	1.96	1.10	3270.16	2.40	1.37	3305.27	1.63	1.69	3421.66	2.12	2.95	3316.43	1.92	2.22	3390.61	1.53	3.91
20	3377.13	1.64	0.74	3265.60	2.42	1.10	3301.49	1.60	1.31	3420.32	2.02	2.23	3310.32	1.91	1.76	3388.92	1.49	3.04
21	3376.97	1.98	0.70	3260.95	2.45	0.87	3297.52	1.31	0.84	3419.13	1.63	1.40	3304.16	1.89	1.37	3387.12	1.46	2.33
22	3376.59	1.98	0.54	3256.21	2.06	0.57	3293.37	1.54	0.76	3418.75	0.75	0.50	3298.02	1.80	1.01	3385.22	1.43	1.76
23	3375.96	1.99	0.42	3251.37	2.49	0.52	3289.03	1.51	0.56	3419.28	0.28	0.14	3292.15	1.45	0.62	3383.21	1.39	1.31
24	3375.08	1.99	0.32	3246.44	2.51	0.40	3284.52	1.48	0.41	3420.09	0.13	0.05	3287.25	0.67	0.22	3381.07	1.36	0.96

	K_a=2−1 (b k)=(2 2) → (2 1)									K_a=1−2 (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										3484.55	1.75	2.37						
										3484.45	1.75	2.38						
2	3294.34	1.88	0.34	3280.02	2.07	3.31	3286.15	2.00	1.79	3487.20	1.74	2.54				3478.50	1.70	1.24
	3295.14	1.89	0.34	3280.16	2.07	3.32	3285.75	1.99	1.78	3486.89	1.75	2.55				3478.20	1.70	1.24
3	3296.60	1.83	0.70	3276.58	2.10	3.57	3285.97	2.01	3.00	3489.70	1.69	2.67	3469.45	1.60	0.22	3478.14	1.66	2.03
	3297.93	1.86	0.72	3276.98	2.11	3.59	3285.17	1.99	2.97	3489.09	1.71	2.68	3468.84	1.62	0.22	3477.53	1.67	2.04
4	3298.66	1.78	1.04	3272.95	2.13	3.84	3285.72	2.02	3.94	3492.04	1.59	2.65	3466.07	1.53	0.45	3477.63	1.59	2.55
	3300.65	1.82	1.06	3273.75	2.15	3.87	3284.39	1.99	3.88	3491.03	1.60	2.65	3465.07	1.56	0.46	3476.63	1.62	2.58
5	3300.52	1.73	1.30	3269.14	2.16	4.04	3285.40	2.03	4.66	3494.18	1.40	2.41	3462.57	1.44	0.63	3476.97	1.46	2.76
	3303.29	1.79	1.34	3270.47	2.19	4.09	3283.42	1.98	4.56	3492.67	1.43	2.45	3461.07	1.48	0.64	3475.47	1.51	2.83
6	3302.16	1.68	1.48	3265.15	2.18	4.15	3285.02	2.04	5.17	3496.09	1.10	1.92	3458.93	1.30	0.73	3476.13	1.29	2.68
	3305.85	1.76	1.55	3267.14	2.23	4.23	3282.26	1.98	5.02	3493.98	1.16	2.00	3456.83	1.34	0.74	3474.04	1.33	2.74
7	3303.59	1.63	1.59	3260.97	2.21	4.16	3284.56	2.05	5.48	3499.94	1.04	1.78	3455.12	1.10	0.71	3475.06	1.03	2.25
	3308.32	1.73	1.69	3263.76	2.27	4.28	3280.91	1.97	5.27	3497.14	1.07	1.82	3452.33	1.16	0.74	3472.29	1.05	2.27
8	3304.80	1.58	1.62	3256.62	2.23	4.08	3284.04	2.07	5.61	3501.76	1.30	2.16	3451.11	0.84	0.59	3475.96	0.93	2.07
	3310.70	1.70	1.75	3260.34	2.31	4.23	3279.36	1.97	5.33	3498.17	1.33	2.18	3447.54	0.91	0.63	3472.42	0.98	2.14
9	3305.79	1.52	1.58	3252.10	2.25	3.91	3283.43	2.08	5.57	3503.50	1.51	2.38	3449.09	0.75	0.55	3474.84	1.13	2.49
	3312.97	1.66	1.74	3256.86	2.35	4.09	3277.63	1.96	5.23	3499.02	1.28	1.97	3444.64	0.81	0.58	3470.44	1.22	2.63
10	3306.56	1.46	1.49	3247.40	2.26	3.67	3282.75	2.10	5.38	3505.13	1.58	2.32	3445.08	0.89	0.65	3473.66	1.06	2.24
	3315.14	1.63	1.68	3253.34	2.39	3.88	3275.71	1.95	4.99	3499.69	1.63	2.32	3439.66	0.97	0.69	3468.32	1.43	2.94
11	3307.11	1.40	1.37	3242.54	2.28	3.37	3281.97	2.12	5.08	3506.65	1.63	2.18	3441.04	0.99	0.70	3472.40	1.32	2.62
	3317.20	1.61	1.57	3249.78	2.43	3.61	3273.60	1.95	4.65	3500.14	1.76	2.28	3434.58	0.90	0.62	3466.04	1.50	2.88
12	3307.43	1.34	1.21	3237.51	2.29	3.04	3281.11	2.15	4.71	3508.04	1.72	2.07	3436.95	0.99	0.66	3471.05	1.40	2.55
	3319.15	1.58	1.44	3246.17	2.47	3.29	3271.31	1.94	4.23	3500.39	1.89	2.18	3429.36	1.11	0.71	3463.60	1.56	2.73

13	3307.52	1.27	1.05	3232.32	2.30	2.68	3280.16	2.17	4.26	3509.29	1.76	1.87	3432.81	0.97	0.60	3469.60	1.47	2.40
	3320.97	1.55	1.28	3242.51	2.52	2.96	3268.83	1.93	3.77	3500.42	1.94	1.96	3424.00	1.16	0.68	3460.99	1.66	2.59
14	3307.38	1.20	0.88	3226.97	2.30	2.33	3279.11	2.20	3.79	3510.40	1.79	1.64	3428.62	0.97	0.54	3468.04	1.48	2.13
	3322.66	1.51	1.11	3238.81	2.56	2.60	3266.17	1.92	3.30	3500.23	2.00	1.74	3418.52	1.20	0.63	3458.21	1.71	2.33
15	3307.01	1.13	0.72	3221.47	2.31	1.98	3277.96	2.22	3.29	3511.35	1.81	1.42	3424.35	0.94	0.45	3466.38	1.49	1.85
	3324.22	1.50	0.97	3235.06	2.60	2.25	3263.34	1.92	2.84	3499.82	2.05	1.51	3412.89	1.19	0.54	3455.25	1.75	2.05
16	3306.41	1.06	0.58	3215.82	2.31	1.66	3276.70	2.29	2.87	3512.13	1.83	1.20	3420.02	0.90	0.37	3464.59	1.50	1.58
	3325.62	1.46	0.81	3231.28	2.63	1.91	3260.33	1.91	2.39	3499.18	2.10	1.29	3407.14	1.18	0.46	3452.11	1.78	1.76
17	3305.58	0.97	0.45	3210.03	2.30	1.37	3275.33	2.30	2.41	3512.72	1.84	1.00	3415.62	0.85	0.30	3462.69	1.50	1.32
	3326.88	1.42	0.66	3227.44	2.72	1.63	3257.15	1.91	1.99	3498.32	2.14	1.08	3401.27	1.17	0.38	3448.80	1.81	1.48
18	3304.53	0.88	0.33	3204.11	2.29	1.10	3273.84	2.31	1.98	3513.09	1.85	0.82	3411.15	0.79	0.23	3460.67	1.49	1.08
	3327.98	1.39	0.53	3223.55	2.74	1.33	3253.81	1.90	1.63	3497.23	2.18	0.89	3395.27	1.15	0.31	3445.30	1.83	1.22
19	3303.28	0.76	0.23	3198.06	2.27	0.88	3272.23	2.34	1.62	3513.09	1.82	0.64	3406.59	0.73	0.17	3458.52	1.48	0.87
	3328.91	1.35	0.42	3219.62	2.76	1.08	3250.31	1.91	1.32	3495.90	2.21	0.72	3389.16	1.13	0.25	3441.58	1.83	0.98
20	3301.90	0.58	0.14	3191.90	2.24	0.68	3270.49	2.37	1.31				3401.91	0.65	0.13	3456.23	1.47	0.69
	3329.66	1.31	0.33	3215.64	2.80	0.86	3246.69	1.91	1.05				3382.94	1.10	0.19	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										3564.32	1.61	4.67						
										3564.32	1.61	4.67						
3	3251.62	1.48	0.05	3231.37	2.16	1.32	3240.06	1.86	0.40	3566.68	1.64	4.79				3555.15	1.51	1.46
	3251.62	1.49	0.05	3231.37	2.16	1.32	3240.06	1.86	0.40	3566.68	1.64	4.79				3555.15	1.51	1.46
4	3253.90	1.30	0.09	3227.93	2.22	1.34	3239.49	1.78	0.65	3568.86	1.68	4.92	3542.93	1.38	0.18	3554.47	1.50	2.46
	3253.90	1.29	0.09	3227.93	2.22	1.34	3239.49	1.78	0.65	3568.87	1.68	4.92	3542.94	1.38	0.18	3554.47	1.50	2.46
5	3255.97	1.06	0.12	3224.36	2.24	1.34	3238.76	1.63	0.77	3570.85	1.71	5.01	3539.22	1.34	0.39	3553.61	1.49	3.17
	3255.96	1.07	0.12	3224.35	2.24	1.34	3238.76	1.64	0.78	3570.86	1.71	5.00	3539.23	1.34	0.39	3553.62	1.49	3.17
6	3257.79	0.77	0.11	3220.63	2.21	1.30	3237.83	1.42	0.78	3572.64	1.75	5.02	3535.34	1.30	0.57	3552.58	1.48	3.64
	3257.77	0.79	0.11	3220.62	2.19	1.29	3237.83	1.42	0.78	3572.66	1.75	5.02	3535.36	1.30	0.57	3552.59	1.48	3.64
7	3261.53	1.03	0.17	3216.72	2.08	1.18	3236.66	1.12	0.67	3574.23	1.79	4.96	3531.31	1.26	0.71	3551.37	1.47	3.92
	3261.52	1.03	0.17	3216.71	2.08	1.18	3236.67	1.10	0.65	3574.26	1.79	4.95	3531.33	1.26	0.71	3551.39	1.46	3.91
8	3263.24	1.15	0.21	3212.59	1.79	0.96	3237.44	1.19	0.73	3575.61	1.84	4.81	3527.11	1.22	0.80	3549.98	1.45	4.02
	3263.21	1.14	0.21	3212.58	1.82	0.98	3237.46	1.19	0.73	3575.66	1.83	4.80	3527.14	1.21	0.80	3550.01	1.45	4.01
9	3264.85	1.24	0.24	3210.44	1.09	0.55	3236.19	1.42	0.87	3576.78	1.88	4.59	3522.74	1.18	0.85	3548.40	1.44	3.96
	3264.80	0.99	0.19	3210.42	1.08	0.54	3236.22	1.44	0.88	3576.86	1.87	4.58	3522.80	1.17	0.84	3548.44	1.43	3.94
10	3266.34	1.21	0.24	3206.29	1.46	0.68	3234.87	1.31	0.78	3577.72	1.93	4.31	3518.22	1.14	0.85	3546.63	1.42	3.79
	3266.28	1.17	0.23	3206.26	1.43	0.66	3234.91	1.64	0.97	3577.85	1.92	4.29	3518.31	1.13	0.84	3546.69	1.41	3.75
11	3267.71	1.17	0.23	3202.10	1.80	0.75	3233.46	1.64	0.92	3578.41	2.05	4.12	3513.52	1.10	0.81	3544.68	1.40	3.51
	3267.62	1.17	0.23	3202.05	1.44	0.60	3233.52	1.70	0.95	3578.62	1.96	3.95	3513.67	1.09	0.80	3544.75	1.38	3.46
12	3268.94	1.17	0.21	3197.85	1.98	0.73	3231.95	1.73	0.89	3578.84	2.02	3.60	3508.66	1.06	0.75	3542.53	1.38	3.18
	3268.82	1.17	0.21	3197.79	1.90	0.70	3232.03	1.73	0.89	3579.16	2.00	3.57	3508.87	1.04	0.74	3542.61	1.39	3.21
13	3270.02	1.13	0.19	3193.54	2.12	0.69	3230.33	1.82	0.84	3578.98	2.06	3.21	3503.62	1.06	0.70	3540.18	1.35	2.80
	3269.87	1.12	0.19	3193.45	2.11	0.68	3230.44	1.82	0.84	3579.48	2.04	3.17	3503.93	1.00	0.66	3540.24	1.29	2.68
14	3270.95	1.09	0.17	3189.17	2.32	0.65	3228.60	1.84	0.75	3578.74	2.09	2.79	3498.38	0.99	0.60	3537.62	1.32	2.41
	3270.76	1.08	0.16	3189.05	2.31	0.64	3228.74	1.85	0.76	3579.56	2.08	2.77	3498.83	0.96	0.58	3537.63	1.22	2.22
15	3271.72	1.04	0.14	3184.73	2.45	0.58	3226.75	1.86	0.66	3578.00	2.06	2.32	3492.93	0.96	0.51	3534.86	1.29	2.02
	3271.49	1.03	0.14	3184.57	2.42	0.57	3226.92	1.87	0.66	3579.39	2.11	2.38	3493.58	0.91	0.49	3534.70	1.10	1.73
16	3272.32	0.99	0.12	3180.22	2.56	0.50	3224.79	1.87	0.56	3576.44	1.87	1.75	3487.18	0.93	0.43	3531.88	1.24	1.66
	3272.05	0.98	0.11	3180.01	2.54	0.50	3224.99	1.89	0.57	3578.96	2.14	2.01	3488.18	0.87	0.41	3531.31	0.90	1.21
17	3272.74	0.94	0.09	3175.64	2.67	0.43	3222.71	1.88	0.47	3581.98	0.71	0.54	3481.02	0.90	0.35	3528.66	1.19	1.33
	3272.44	0.93	0.09	3175.39	2.64	0.43	3222.93	1.90	0.48	3578.24	2.17	1.67	3482.61	0.83	0.33	3527.18	0.59	0.66
18	3272.93	0.88	0.07	3170.99	2.77	0.36	3220.51	1.89	0.39	3579.95	1.13	0.70	3474.14	0.82	0.27	3525.20	1.13	1.03
	3272.65	0.88	0.07	3170.69	2.74	0.36	3220.72	1.90	0.39	3577.22	2.19	1.36	3476.89	0.79	0.26	3530.20	1.19	1.09
19	3272.76	0.80	0.05	3166.26	2.86	0.30	3218.19	1.89	0.32	3578.12	1.39	0.68	3474.46	0.12	0.03	3521.47	1.06	0.78
	3272.67	0.82	0.06	3165.93	2.83	0.30	3218.35	1.89	0.32	3575.87	2.19	1.09	3470.98	0.74	0.20	3525.73	1.33	0.99
20										3576.22	1.52	0.59	3467.32	0.23	0.05	3517.45	0.96	0.56
										3574.11	2.19	0.85	3464.88	0.70	0.15	3521.53	1.35	0.80

[a]The calculated values of the strengths S divided by the rotational factors of Eq. (C18) are the S_{vib}s which are listed for the bands due to b-type transitions (Δv_θ=±1).

TABLE CXII: B. Overtone v_r=0→2 band (S_{vib} in 10^{-5} 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_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0	5713.27	5.24	1.82												
1	5716.30	5.23	3.59	5707.14	5.25	3.49	5713.68	5.23	1.16				5707.79	5.25	1.17
							5713.90	5.24	1.17				5707.59	5.24	1.16
2	5719.29	5.22	5.22	5704.04	5.26	5.01	5716.62	5.22	2.00	5701.65	5.27	1.14	5707.95	5.26	0.63
							5716.95	5.24	2.01	5701.45	5.26	1.13	5707.34	5.21	0.62
3	5722.26	5.24	6.68	5700.92	5.26	6.30	5719.53	5.21	2.69	5698.58	5.28	1.93	5708.19	5.27	0.42
							5719.97	5.24	2.70	5698.29	5.26	1.92	5706.96	5.18	0.41
4	5725.19	5.21	7.82	5697.79	5.27	7.34	5722.40	5.18	3.24	5695.50	5.29	2.57	5708.50	5.28	0.31
							5722.95	5.23	3.25	5695.12	5.26	2.54	5706.46	5.13	0.30
5	5728.08	5.20	8.71	5694.64	5.30	8.03	5725.24	5.17	3.65	5692.40	5.30	3.06	5708.89	5.29	0.23
							5725.90	5.23	3.66	5691.94	5.26	3.02	5705.84	5.06	0.22
6	5730.93	5.17	9.23	5691.49	5.28	8.45	5728.03	5.16	3.92	5689.29	5.29	3.40	5709.36	5.31	0.18
							5728.82	5.23	3.93	5688.75	5.26	3.35	5705.09	4.99	0.17
7	5733.73	5.19	9.55	5688.33	5.29	8.54	5730.79	5.15	4.06	5686.18	5.31	3.62	5709.90	5.33	0.14
							5731.69	5.22	4.06	5685.56	5.27	3.54	5704.23	4.91	0.13
8	5736.50	5.18	9.53	5685.17	5.26	8.46	5733.50	5.15	4.08	5683.06	5.31	3.70	5710.52	5.35	0.11
							5734.53	5.22	4.07	5682.38	5.27	3.60	5703.26	4.82	0.10
9	5739.21	5.16	9.24	5682.02	5.30	8.12	5736.17	5.14	3.99	5679.94	5.32	3.67	5711.20	5.38	0.09
							5737.32	5.21	3.96	5679.20	5.27	3.55	5702.18	4.73	0.08
10	5741.88	5.16	8.79	5678.87	5.30	7.58	5738.79	5.13	3.79	5676.82	5.34	3.54	5711.96	5.40	0.07
							5740.07	5.21	3.75	5676.03	5.27	3.41	5700.99	4.63	0.06
11	5744.49	5.15	8.14	5675.73	5.30	6.96	5741.37	5.12	3.53	5673.71	5.35	3.34	5712.78	5.43	0.05
							5742.77	5.14	3.43	5672.87	5.27	3.19	5699.71	4.52	0.04
12	5747.06	5.14	7.39	5672.61	5.32	6.24	5743.90	5.12	3.22	5670.61	5.36	3.07	5713.68	5.39	0.04
							5745.42	5.20	3.15	5669.74	5.27	2.91	5698.32	4.40	0.03
13	5749.57	5.13	6.58	5669.50	5.32	5.49	5746.38	5.10	2.87	5667.53	5.37	2.77	5714.63	5.49	0.03
							5748.02	5.19	2.80	5666.63	5.20	2.57	5696.85	4.28	0.02
14	5752.03	5.12	5.74	5666.42	5.32	4.74	5748.81	5.08	2.52	5664.47	5.39	2.45	5715.64	5.52	0.03
							5750.57	5.18	2.44	5663.54	5.27	2.28	5695.29	4.13	0.02
15	5754.43	5.08	4.90	5663.37	5.32	4.02	5751.19	5.07	2.16	5661.44	5.38	2.12	5716.72	5.56	0.02
							5753.07	5.17	2.09	5660.49	5.27	1.96	5693.66	3.99	0.01
16	5756.78	5.09	4.15	5660.35	5.32	3.33	5753.53	5.06	1.83	5658.44	5.38	1.80	5717.85	5.59	0.01
							5755.52	5.16	1.76	5657.48	5.26	1.66	5691.96	3.84	0.01
17	5759.077	5.08	3.44	5657.37	5.30	2.74	5755.82	4.76	1.44	5655.47	5.38	1.51	5719.03	5.63	0.01
							5757.92	5.15	1.45	5654.52	5.26	1.37	5690.20	3.69	0.01
18	5761.300	3.68	2.04	5654.44	5.32	2.21	5758.04	5.03	1.25	5652.55	5.39	1.24	5720.27	5.66	0.01
							5760.27	5.14	1.18	5651.61	5.25	1.12	5688.40	3.34	0.00
19	5763.488	5.04	2.25	5651.56	5.32	5.90	5760.22	5.00	1.00	5649.69	5.08	0.95	5721.55	5.70	0.01
							5762.56	5.12	0.95	5648.76	5.24	0.90	5686.53	3.39	0.00

TABLE CXII: B. continued

	K_a=2−2								
	$(b\,k)$=(2 2) → (2 2)								
2	5709.35	5.25	1.63				5700.25	5.25	3.25
	5709.35	5.25	1.63				5700.25	5.25	3.25
3	5712.31	5.24	2.80	5691.08	5.29	1.56	5700.18	5.24	2.17
	5712.31	5.24	2.80	5691.08	5.29	1.56	5700.19	5.24	2.17
4	5715.24	5.22	3.68	5687.97	5.29	2.65	5700.09	5.22	1.57
	5715.23	5.23	3.69	5687.97	5.29	2.65	5700.10	5.22	1.57
5	5718.14	5.14	4.27	5684.85	5.30	3.45	5699.98	5.20	1.18
	5718.13	5.22	4.34	5684.85	5.30	3.45	5700.00	5.19	1.18
6	5721.00	5.22	4.78	5681.72	5.29	4.00	5699.85	5.16	0.91
	5720.98	5.21	4.78	5681.72	5.30	4.01	5699.88	5.09	0.90
7	5723.82	5.22	5.04	5678.59	5.22	4.29	5699.69	5.13	0.70
	5723.78	5.11	4.93	5678.60	5.30	4.35	5699.75	5.14	0.71
8	5726.62	5.20	5.09	5675.46	5.31	4.52	5699.50	4.99	0.54
	5726.58	5.20	5.10	5675.47	5.31	4.52	5699.60	5.11	0.55
9	5729.37	5.19	5.00	5672.33	5.33	4.53	5699.31	5.05	0.43
	5729.31	5.13	4.95	5672.32	5.22	4.43	5699.44	5.06	0.43
10	5732.08	5.19	4.79	5669.22	5.32	4.38	5699.08	4.94	0.33
	5732.00	5.19	4.78	5669.23	5.32	4.38	5699.28	5.01	0.33
11	5734.75	5.19	4.47	5666.11	5.32	4.13	5698.84	4.94	0.25
	5734.66	5.18	4.46	5666.12	5.27	4.09	5699.11	4.97	0.25
12	5737.38	5.18	4.08	5663.02	5.33	3.81	5698.57	4.88	0.19
	5737.26	5.17	4.08	5663.03	5.33	3.81	5698.95	4.91	0.19
13	5739.97	5.17	3.64	5659.96	5.33	3.43	5698.28	4.82	0.15
	5739.82	5.17	3.64	5659.97	5.34	3.43	5698.78	4.86	0.15
14	5742.52	5.16	3.19	5656.92	5.33	3.02	5697.96	4.75	0.11
	5742.33	5.15	3.19	5656.93	5.34	3.03	5698.62	4.79	0.11
15	5745.02	5.09	2.71	5653.92	5.33	2.62	5697.63	4.66	0.08
	5744.79	5.15	2.75	5653.92	5.34	2.63	5698.47	4.72	0.08
16	5747.48	5.07	2.29	5650.96	5.33	2.22	5697.27	4.58	0.06
	5747.20	5.13	2.32	5650.94	5.34	2.23	5698.34	4.59	0.06
17	5749.89	5.06	1.90	5648.04	5.26	1.83	5696.90	4.49	0.04
	5749.56	5.12	1.93	5648.01	5.34	1.86	5698.22	4.51	0.04
18	5752.26	5.07	1.56	5645.18	5.24	1.50	5696.51	4.39	0.03
	5751.87	5.11	1.58	5645.13	5.34	1.53	5698.12	4.43	0.03
19	5754.59	5.02	1.25	5642.37	5.24	1.21	5696.12	4.28	0.02
	5754.13	5.10	1.27	5642.30	5.34	1.24	5698.05	4.36	0.02

TABLE CXII: 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	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	3776.84	2.52	0.58												
1	3779.40	2.47	1.12	3770.93	2.63	0.59	3797.85	2.88	0.43				3792.54	2.48	0.37
							3798.33	2.76	0.41				3792.24	2.52	0.37
2	3781.71	2.41	1.60	3767.60	2.68	1.18	3800.06	2.83	0.72	3786.30	2.55	0.37	3792.39	2.02	0.16
							3800.88	2.66	0.68	3786.19	2.59	0.37	3791.51	2.00	0.16
3	3783.76	2.36	1.99	3764.03	2.74	1.72	3802.01	2.76	0.95	3782.75	2.37	0.58	3792.12	1.60	0.09
							3803.20	2.58	0.88	3782.73	2.48	0.60	3790.40	1.39	0.07
4	3785.53	2.30	2.28	3760.21	2.80	2.21	3803.64	2.68	1.11	3778.94	2.18	0.70	3791.74	1.30	0.05
							3805.28	2.50	1.03	3779.05	2.42	0.78	3788.94	0.83	0.03
5	3787.04	2.30	2.55	3756.14	2.86	2.61	3804.98	2.59	1.22	3774.88	2.00	0.77	3791.22	1.09	0.03
							3807.11	2.42	1.13	3775.17	2.43	0.92	3787.08	0.39	0.01
6	3788.27	2.22	2.62	3751.84	2.90	2.91	3806.01	2.51	1.27	3770.53	1.86	0.79	3790.56	0.96	0.02
							3808.69	2.34	1.17	3771.07	2.47	1.04	3784.84	0.12	0.00
7	3789.21	2.18	2.65	3747.29	3.02	3.18	3806.73	2.44	1.28	3765.92	1.74	0.78	3789.77	0.87	0.02
							3810.01	2.26	1.17	3766.77	2.52	1.12	3782.22	0.00	0.00
8	3789.87	2.13	2.59	3742.51	3.04	3.24	3807.14	2.42	1.28	3761.04	1.65	0.76	3788.83	0.81	0.01
							3811.07	2.15	1.12	3762.25	2.59	1.17	3779.21	0.04	0.00
9	3790.24	2.09	2.47	3737.50	3.10	3.26	3807.20	2.34	1.20	3755.88	1.58	0.72	3787.74	0.74	0.01
							3811.59	1.35[a]	0.68	3757.52	2.66	1.19	3775.82	0.19	0.00
10	3790.31	2.05	2.30	3732.24	3.16	3.18	3806.92	2.33	1.14	3750.46	1.57	0.69	3786.23	0.16[a]	0.00
							3812.58	2.10[a]	1.00	3752.56	2.68	1.15	3772.03	0.39	0.00
11	3790.07	2.00	2.09	3726.76	3.22	3.03	3806.49	1.93	0.88	3744.75	1.53	0.63	3785.30	1.14[a]	0.01
							3812.83	2.04	0.90	3747.14	1.66[a]	0.66	3767.83	0.34	0.00
12	3789.52	1.95	1.84	3721.04	3.28	2.82	3805.52	2.08	0.87	3738.74	1.63	0.61	3783.74	1.13	0.01
							3812.85	2.17	0.87	3742.25	3.04[a]	1.11	3763.44	2.27	0.01
13	3788.57	1.75	1.48	3715.08	3.34	2.57	3804.25	2.08	0.78	3732.65	1.11	0.38	3782.06	1.32	0.01
							3812.60	1.92	0.69	3736.69	3.12	1.01	3758.47	2.05	0.01
14	3787.71	1.92	1.42	3708.88	3.37	2.28	3802.63	2.07	0.68	3726.10	1.32	0.39	3780.22	1.31	0.00
							3812.05	1.87	0.58	3730.97	3.51	1.00	3753.16	2.24	0.01
15	3786.14	1.91	1.21	3702.37	3.17	1.84	3800.65	2.06	0.58	3719.31	1.37	0.35	3778.20	1.45	0.00
							3811.21	1.81	0.48	3725.07	3.29	0.81	3747.48	2.39	0.01
16	3784.31	1.87	1.00	3696.03	3.55	1.75	3798.31	2.05	0.49	3712.25	1.41	0.31			
							3810.07	1.76	0.40	3718.96	3.38	0.70			
17	3782.15	1.84	0.82	3689.08	3.67	1.50	3795.58	2.05	0.41	3704.93	1.45	0.27			
							3808.63	1.71	0.32	3712.66	3.47	0.60			
18	3779.66	1.80	0.66	3681.97	3.73	1.25	3792.47	2.05	0.33	3697.33	1.50	0.23			
							3806.87	1.66	0.25	3706.16	3.56	0.50			
19	3776.83	1.77	0.52	3674.64	3.79	1.03	3788.96	2.05	0.27	3689.45	1.56	0.19			
							3804.79	1.61	0.20	3699.48	3.65	0.41			
							K_a=2−2 (b k)=(2 2) → (4 2)								
2							3842.24	1.98	0.41				3833.96	2.31	0.96
							3842.26	1.98	0.41				3833.95	2.31	0.96
3							3844.12	1.92	0.69	3824.78	2.33	0.46	3833.09	2.48	0.69
							3844.14	1.92	0.69	3824.79	2.33	0.46	3833.07	2.48	0.69
4							3845.69	1.86	0.88	3820.86	2.39	0.80	3831.93	2.70	0.55
							3845.73	1.86	0.88	3820.87	2.39	0.80	3831.91	2.70	0.55
5							3846.95	1.80	1.01	3816.66	2.45	1.07	3830.48	3.00	0.46
							3847.01	1.80	1.01	3816.68	2.45	1.07	3830.45	3.01	0.46
6							3847.88	1.72	1.06	3812.17	2.50	1.27	3828.74	3.40	0.40
							3848.00	1.72	1.06	3812.22	2.50	1.27	3828.69	3.41	0.40
7							3848.48	1.67	1.09	3807.40	2.56	1.41	3826.72	3.84	0.35
							3848.67	1.31	0.85	3807.48	2.57	1.41	3826.62	3.86	0.36
8							3848.73	1.61	1.06	3802.34	2.58	1.47	3824.38	3.53	0.25
							3849.03	1.26	0.83	3802.49	2.59	1.48	3824.25	4.51	0.33
9							3848.62	1.55	1.00	3796.99	2.65	1.51	3821.77	4.13	0.23
							3849.09	1.22	0.79	3797.21	2.10	1.19	3821.56	5.29	0.30

J									
10	3848.13	1.49	0.92	3791.33	2.69	1.48	3818.86	4.87	0.21
	3848.82	1.17	0.72	3791.68	2.14	1.18	3818.53	6.26	0.28
11	3847.21	1.43	0.83	3785.37	2.73	1.41	3815.65	5.80	0.20
	3848.24	1.12	0.65	3785.89	2.18	1.13	3815.16	7.48	0.26
12	3845.67	1.32	0.69	3779.08	2.73	1.30	3812.15	6.94	0.18
	3847.32	1.08	0.57	3779.85	2.22	1.06	3811.40	9.05	0.24
13	3845.28	0.73	0.34	3772.42	2.67	1.14	3808.33	8.39	0.17
	3846.05	1.28	0.60	3773.55	2.26	0.97	3807.07	10.84	0.22
14	3842.82	0.98	0.40	3765.21	2.22	0.84	3804.19	12.62	0.19
	3844.39	1.22	0.51	3766.98	2.29	0.87	3803.93	6.33	0.10
15	3840.21	0.97	0.34	3759.23	2.61	0.85	3799.69	15.31	0.18
	3842.09	1.11	0.40	3760.15	2.85	0.93	3798.78	11.58	0.13
16	3837.17	0.92	0.28	3751.26	2.99	0.83	3794.57	17.54	0.15
	3841.08	0.55	0.17	3753.00	2.75	0.76	3793.53	14.85	0.13
17	3833.70	0.83	0.21	3743.23	3.02	0.70	3790.78	12.69	0.08
	3838.11	0.70	0.18	3745.31	2.10	0.49	3787.91	18.22	0.12
18	3829.67	0.77	0.16	3734.87	3.04	0.57	3785.07	20.81	0.10
	3834.98	0.66	0.14	3739.01	2.80	0.53	3781.93	21.49	0.10
19	3825.11	0.70	0.12	3726.18	3.00	0.46	3779.23	26.43	0.09
	3831.45	0.57	0.09	3730.85	3.08	0.47	3775.45	25.83	0.09

[a]Affected by the crossing of levels from the groups $(v_r\, b\, k\, v_R)$=(1 3 1 0) and (1 1 1 3) marked in Table CIII. The effect on the strength of $Q(J^e)$ lines is also seen in Fig. C7.

TABLE CXII: 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										2495.90	3.05	0.26						
1	2433.44	3.12	0.21	2424.25	3.12	0.42	2427.17	3.12	0.63	2498.96	3.07	0.39				2493.05	3.03	0.38
2	2436.86	3.12	0.41	2421.55	3.13	0.62	2427.28	3.11	1.02	2502.07	3.09	0.50	2487.04	3.01	0.12	2493.36	3.02	0.61
3	2440.47	3.12	0.60	2419.05	3.14	0.79	2427.43	3.10	1.37	2505.23	3.11	0.61	2484.20	3.00	0.23	2493.83	3.01	0.82
4	2444.24	3.21	0.78	2416.74	3.15	0.94	2427.63	3.08	1.65	2508.44	3.13	0.69	2481.43	2.99	0.33	2494.47	3.00	0.99
5	2448.18	3.12	0.88	2414.62	3.16	1.05	2427.89	3.16	1.92	2511.70	3.15	0.76	2478.73	2.98	0.40	2495.26	2.98	1.12
6	2452.28	3.13	0.97	2412.70	3.27	1.17	2428.19	3.04	2.00	2515.01	3.17	0.80	2476.11	2.97	0.46	2496.21	2.96	1.21
7	2456.54	3.13	1.03	2410.97	3.18	1.18	2428.56	3.01	2.07	2518.36	3.20	0.83	2473.57	2.97	0.50	2497.33	2.93	1.25
8	2460.96	3.14	1.06	2409.45	3.19	1.19	2428.97	2.98	2.07	2521.76	3.23	0.83	2471.12	2.96	0.52	2498.61	2.91	1.25
9	2465.53	3.14	1.06	2408.12	3.20	1.17	2429.45	2.95	2.01	2525.22	3.25	0.81	2468.77	2.96	0.52	2500.06	2.88	1.22
10	2470.24	3.15	1.03	2406.99	3.22	1.13	2429.98	2.91	1.90	2528.73	3.28	0.77	2466.52	2.97	0.51	2501.67	2.84	1.16
11	2475.08	3.15	0.98	2406.07	3.23	1.06	2430.58	2.87	1.75	2532.30	3.30	0.72	2464.39	2.96	0.49	2503.46	2.81	1.08
12	2480.06	3.15	0.90	2405.34	3.23	0.97	2431.24	2.83	1.58	2535.93	3.33	0.67	2462.37	2.96	0.45	2505.42	2.77	0.98
13	2485.15	3.12	0.81	2404.80	3.20	0.87	2431.97	2.78	1.39	2539.63	3.36	0.60	2460.49	2.96	0.41	2507.56	2.73	0.87
14	2490.26	2.76	0.64	2404.36	2.85	0.68	2432.76	2.73	1.21	2543.39	3.37	0.53	2458.75	2.96	0.37	2509.88	2.68	0.75
15	2496.09	2.59	0.53	2404.73	2.68	0.56	2433.63	2.68	1.02	2547.23	3.41	0.46	2457.17	2.96	0.32	2512.38	2.64	0.65
16	2501.45	3.06	0.54	2404.71	3.17	0.57	2434.59	2.62	0.85	2551.14	3.43	0.40	2455.74	2.95	0.27	2515.06	2.59	0.54
17	2507.02	3.14	0.47	2405.01	3.25	0.49	2435.62	2.56	0.70	2555.14	3.46	0.34	2454.49	2.96	0.23	2517.93	2.54	0.45
18	2512.73	3.16	0.40	2405.54	3.29	0.42	2436.75	2.50	0.56	2559.23	3.48	0.28	2453.42	2.96	0.19	2520.99	2.49	0.36
19	2518.55	3.18	0.33	2406.30	3.32	0.34	2437.97	2.43	0.44	2563.42	3.50	0.23	2452.56	2.96	0.16	2524.25	2.44	0.29
20	2524.48	3.18	0.27	2407.29	3.33	0.28	2439.30	2.36	0.34	2567.70	3.52	0.19	2451.90	2.95	0.13	2527.70	2.38	0.23

TABLE CXIII: Far- and mid-infrared absorption spectrum of Li^{+}–D_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 in four vibrational bands.

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

	$[v_r\, v_\theta\, v_R]=[0\,0\,0] \rightarrow [0\,0\,0]$											
	K_a=0−0 $(b\,k)=(0\,0) \rightarrow (0\,0)$			K_a=1−1 $(b\,k)=(1\,1) \rightarrow (1\,1)$			K_a=2−2 $(b\,k)=(2\,2) \rightarrow (2\,2)$			K_a=3−3 $(b\,k)=(3\,3) \rightarrow (3\,3)$		
	$R(J^e)$			$R(J^e)/R(J^f)$			$R(J^e)/R(J^f)$			$R(J^e)/R(J^f)$		
J	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I	ν	S_{vib}	I
0	3.078	8.436	0.02									
1	6.154	8.442	0.18	6.044	8.435	0.06						
				6.245	8.436	0.06						
2	9.223	8.451	0.60	9.059	8.444	0.22	9.170	8.428	0.18			
				9.361	8.445	0.24	9.169	8.428	0.18			
3	12.283	8.464	1.34	12.066	8.457	0.53	12.215	8.440	0.56	12.127	8.415	0.08
				12.467	8.458	0.56	12.213	8.440	0.56	12.127	8.415	0.08
4	15.331	8.480	2.45	15.063	8.473	0.98	15.249	8.457	1.14	15.138	8.431	0.21
				15.561	8.475	1.04	15.246	8.457	1.14	15.138	8.431	0.21
5	18.364	8.500	3.90	18.046	8.492	1.59	18.270	8.477	1.91	18.136	8.451	0.39
				18.640	8.496	1.68	18.264	8.477	1.91	18.136	8.451	0.39
6	21.379	8.524	5.61	21.014	8.515	2.31	21.276	8.501	2.85	21.117	8.475	0.61
				21.701	8.521	2.43	21.266	8.500	2.85	21.117	8.475	0.61
7	24.373	8.552	7.48	23.962	8.542	3.10	24.263	8.528	3.88	24.078	8.502	0.85
				24.741	8.549	3.25	24.248	8.528	3.88	24.078	8.502	0.85
8	27.342	8.583	9.37	26.889	8.573	3.90	27.228	8.560	4.94	27.018	8.533	1.11
				27.757	8.582	4.09	27.208	8.560	4.93	27.018	8.533	1.11
9	30.285	8.619	11.16	29.791	8.608	4.67	30.170	8.596	5.95	29.932	8.568	1.35
				30.745	8.619	4.86	30.143	8.595	5.94	29.932	8.568	1.35
10	33.197	8.659	12.70	32.667	8.647	5.34	33.085	8.636	6.83	32.818	8.608	1.57
				33.703	8.660	5.53	33.049	8.635	6.81	32.819	8.608	1.57
11	36.076	8.703	13.90	35.512	8.690	5.87	35.970	8.680	7.52	35.673	8.651	1.74
				36.627	8.706	6.05	35.925	8.679	7.51	35.674	8.651	1.74
12	38.918	8.752	14.69	38.325	8.737	6.23	38.821	8.729	7.99	38.493	8.699	1.86
				39.515	8.756	6.39	38.765	8.728	7.98	38.496	8.699	1.87
13	41.721	8.805	15.04	41.102	8.789	6.41	41.637	8.783	8.22	41.277	8.752	1.93
				42.362	8.812	6.53	41.569	8.781	8.21	41.280	8.752	1.93
14	44.482	8.863	14.95	43.840	8.846	6.40	44.413	8.841	8.21	44.019	8.810	1.94
				45.166	8.872	6.47	44.332	8.839	8.19	44.024	8.810	1.94
15	47.196	8.926	14.48	46.536	8.907	6.23	47.146	8.905	7.98	46.717	8.872	1.89
				47.923	8.937	6.25	47.052	8.902	7.96	46.725	8.872	1.89
16	49.862	8.995	13.67	49.188	8.974	5.91	49.833	8.974	7.55	49.368	8.940	1.80
				50.629	9.008	5.88	49.724	8.970	7.54	49.378	8.940	1.80
17	52.475	9.068	12.60	51.791	9.046	5.47	52.470	9.049	6.99	51.967	9.014	1.67
				53.281	9.085	5.41	52.346	9.044	6.97	51.981	9.013	1.67
18	55.033	9.148	11.37	54.342	9.124	4.96	55.053	9.130	6.32	54.510	9.094	1.51
				55.876	9.168	4.86	54.914	9.124	6.30	54.530	9.093	1.51
19	57.532	9.234	10.05	56.838	9.208	4.40	57.578	9.217	5.59	56.992	9.180	1.34
				58.409	9.258	4.28	57.425	9.210	5.58	57.020	9.179	1.34
20	59.968	9.326	8.70	59.275	9.298	3.83	60.041	9.312	4.85	59.409	9.274	1.17
				60.876	9.354	3.69	59.873	9.302	4.85	59.449	9.271	1.17
21	62.338	9.425	7.40	61.650	9.395	3.27	62.437	9.414	4.13	61.753	9.375	1.00
				63.273	9.458	3.13	62.257	9.402	4.13	61.810	9.371	1.00
22	64.638	9.532	6.18	63.957	9.500	2.74	64.762	9.524	3.45	64.017	9.485	0.84
				65.596	9.570	2.60	64.570	9.510	3.45	64.100	9.479	0.84
23	66.863	9.647	5.07	66.194	9.612	2.26	67.010	9.642	2.84	66.185	9.605	0.69
				67.839	9.690	2.13	66.810	9.625	2.84	66.313	9.595	0.69
24	69.009	9.771	4.10	68.355	9.733	1.83	69.177	9.770	2.30	68.236	9.737	0.56
				69.998	9.820	1.71	68.969	9.750	2.30	68.443	9.722	0.56
25	71.071	9.904	3.26	70.435	9.864	1.47	71.255	9.907	1.83	70.116	9.878	0.45
				72.068	9.960	1.35	71.045	9.884	1.83	70.482	9.859	0.45

TABLE CXIII: B. Fundamental v_R=0→1 band ($S_{\rm vib}$ 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	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0	336.02	6.83	11.25												
1	338.68	6.65	21.83	330.06	7.20	11.40	339.14	6.66	7.10				333.59	7.01	7.30
							339.32	6.65	7.09				333.40	7.02	7.31
2	341.14	6.48	31.29	326.78	7.40	22.43	341.55	6.49	12.07	327.46	7.39	7.28	333.38	7.01	3.93
							341.82	6.47	12.03	327.25	7.41	7.28	332.79	7.05	3.94
3	343.38	6.32	39.24	323.31	7.61	32.58	343.76	6.33	15.98	324.04	7.60	12.55	333.06	7.00	2.63
							344.09	6.31	15.89	323.72	7.62	12.53	331.89	7.09	2.64
4	345.40	6.16	45.43	319.63	7.83	41.42	345.75	6.18	18.97	320.43	7.81	16.84	332.63	7.00	1.91
							346.15	6.15	18.82	319.99	7.84	16.80	330.69	7.14	1.92
5	347.20	6.01	49.71	315.76	8.06	48.61	347.52	6.03	21.06	316.63	8.03	20.25	332.09	6.99	1.44
							347.98	6.00	20.83	316.07	8.08	20.17	329.18	7.21	1.46
6	348.78	5.86	52.07	311.71	8.30	53.93	349.07	5.89	22.27	312.64	8.26	22.79	331.44	6.98	1.11
							349.58	5.85	21.95	311.95	8.32	22.64	327.38	7.30	1.13
7	350.13	5.72	52.62	307.46	8.55	57.29	350.40	5.75	22.67	308.46	8.51	24.43	330.66	6.97	0.86
							350.95	5.70	22.24	307.64	8.58	24.20	325.28	7.40	0.88
8	351.24	5.59	51.54	303.03	8.81	<u>58.72</u>	351.51	5.61	22.33	304.10	8.77	25.20	329.77	6.96	0.67
							352.08	5.56	21.81	303.14	8.85	24.89	322.88	7.51	0.69
9	352.11	5.45	49.11	298.41	9.09	58.35	352.38	5.48	21.38	299.55	9.04	25.18	328.76	6.94	0.52
							352.97	5.43	20.78	298.45	9.13	24.78	320.19	7.65	0.54
10	352.75	5.32	45.62	293.61	9.38	56.43	353.01	5.35	19.96	294.83	9.32	24.46	327.61	6.93	0.41
							353.62	5.30	19.29	293.58	9.44	23.98	317.20	7.81	0.43
11	353.13	5.19	41.41	288.63	9.69	53.22	353.41	5.23	18.19	289.92	9.62	23.16	326.34	6.91	0.31
							354.01	5.17	17.48	288.53	9.76	22.61	313.93	7.99	0.33
12	353.27	5.07	36.76	283.47	10.02	49.05	353.56	5.10	16.22	284.84	9.94	21.43	324.92	6.89	0.24
							354.14	5.04	15.48	283.29	10.09	20.82	310.36	8.19	0.26
13	353.14	4.95	31.96	278.14	10.36	44.25	353.46	4.98	14.16	279.57	10.27	19.41	323.35	6.86	0.18
							354.01	4.92	13.43	277.87	10.45	18.75	306.51	8.42	0.20
14	352.75	4.83	27.24	272.63	10.73	39.11	353.11	4.86	12.12	274.13	10.63	17.22	321.63	6.84	0.14
							353.61	4.79	11.41	272.27	10.83	16.54	302.37	8.69	0.15
15	352.09	4.71	22.78	266.94	11.12	33.90	352.49	4.75	10.18	268.52	11.01	14.98	319.75	6.81	0.10
							352.93	4.67	9.50	266.48	11.23	14.31	297.95	8.99	0.12
16	351.15	4.59	18.70	261.07	11.53	28.85	351.60	4.63	8.39	262.73	11.41	12.79	317.70	6.78	0.08
							351.96	4.55	7.77	260.52	11.67	12.14	293.25	9.32	0.09
17	349.93	4.48	15.07	255.03	11.98	24.11	350.44	4.51	6.79	256.76	11.84	10.73	315.47	6.75	0.06
							350.71	4.43	6.23	254.38	12.13	10.12	288.28	9.71	0.07
18	348.41	4.36	11.94	248.82	12.45	19.81	349.00	4.39	5.39	250.63	12.29	8.85	313.05	6.71	0.04
							349.15	4.31	4.91	248.05	12.62	8.29	283.02	10.15	0.05
19	346.59	4.25	9.29	242.42	12.96	16.01	347.28	4.27	4.21	244.31	12.78	7.18	310.43	6.67	0.03
							347.27	4.19	3.80	241.55	13.15	6.68	277.50	10.64	0.04
20	344.46	4.13	7.11	235.85	13.50	12.73	345.26	4.15	3.23	237.83	13.30	5.72	307.60	6.63	0.02
							345.08	4.07	2.89	234.86	13.71	5.29	271.71	11.22	0.03
21	342.01	4.01	5.36	229.09	14.09	9.96	342.94	4.02	2.44	231.16	13.85	4.49	304.54	6.58	0.01
							342.55	3.94	2.16	227.99	14.33	4.12	265.65	11.89	0.02
22	339.21	3.89	3.97	222.16	14.72	7.68	340.32	3.88	1.81	224.33	14.44	3.47	301.23	6.54	0.01
							339.67	3.81	1.59	220.93	14.99	3.16	259.33	12.67	0.01
23	336.06	3.77	2.89	215.03	15.41	5.84	337.40	3.73	1.31	217.33	15.07	2.64	297.67	6.49	0.01
							336.43	3.68	1.15	213.68	15.70	2.39	252.76	13.60	0.01
24	332.55	3.64	2.07	207.71	16.16	4.37	334.21	3.55	0.93	210.16	15.72	1.98	293.83	6.44	0.00
							332.82	3.53	0.81	206.23	16.48	1.78	245.96	14.74	0.01
25	328.64	3.51	1.46	200.19	16.97	3.22	330.81	3.30	0.63	202.85	16.37	1.46	289.70	6.40	0.00
							328.81	3.38	0.57	198.59	17.32	1.31	238.97	16.16	0.01

TABLE CXIII: 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)								
	$R(J^e)$ / $R(J^f)$			$P(J^e)$ / $P(J^f)$			$Q(J^e)$ / $Q(J^f)$			$R(J^e)$ / $R(J^f)$			$P(J^e)$ / $P(J^f)$			$Q(J^e)$ / $Q(J^f)$		
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
2	343.04	6.48	9.79				334.48	7.02	20.47									
	343.04	6.48	9.79				334.48	7.02	20.47									
3	345.27	6.32	16.58	325.31	7.59	10.19	333.87	7.03	13.70	347.07	6.29	2.36				335.73	7.01	7.53
	345.27	6.32	16.58	325.31	7.59	10.19	333.87	7.03	13.70	347.07	6.29	2.36				335.73	6.99	7.51
4	347.29	6.16	21.51	321.65	7.81	17.49	333.05	7.06	9.95	349.10	6.12	3.99	323.61	7.72	2.47	334.95	7.03	5.47
	347.28	6.16	21.51	321.66	7.81	17.49	333.06	7.06	9.95	349.10	6.12	3.99	323.61	7.74	2.48	334.95	7.02	5.47
5	349.08	6.01	24.92	317.81	8.04	23.00	332.03	7.08	7.53	350.92	5.95	5.10	319.81	7.93	4.25	333.96	7.04	4.14
	349.08	6.01	24.92	317.81	8.04	23.00	332.04	7.08	7.53	350.92	5.95	5.10	319.81	7.94	4.25	333.96	7.04	4.13
6	350.65	5.87	26.98	313.77	8.27	27.01	330.80	7.11	5.81	352.53	5.76	5.78	315.83	8.13	5.51	332.79	7.06	3.19
	350.65	5.87	26.98	313.77	8.27	27.01	330.82	7.11	5.81	352.53	5.76	5.78	315.83	8.13	5.51	332.79	7.06	3.19
7	351.99	5.73	27.85	309.53	8.52	29.66	329.36	7.15	4.53	353.94	5.54	6.07	311.67	8.31	6.33	331.42	7.06	2.48
	351.99	5.73	27.85	309.55	8.52	29.66	329.40	7.15	4.53	353.94	5.54	6.07	311.67	8.31	6.33	331.42	7.06	2.48
8	353.10	5.59	27.67	305.11	8.78	31.05	327.70	7.19	3.54	355.15	5.27	6.00	307.34	8.46	6.76	329.86	7.04	1.92
	353.10	5.59	27.68	305.13	8.78	31.05	327.77	7.18	3.54	355.15	5.27	6.00	307.34	8.46	6.76	329.86	7.04	1.92
9	353.96	5.45	26.64	300.50	9.06	31.31	325.83	7.23	2.77	356.18	4.88	5.57	302.84	8.56	6.83	328.13	6.96	1.48
	353.96	5.45	26.65	300.53	9.06	31.31	325.93	7.23	2.77	356.19	4.89	5.58	302.85	8.56	6.83	328.13	6.96	1.48
10	354.59	5.32	24.93	295.70	9.35	30.59	323.74	7.28	2.16	357.08	4.29	4.76	298.20	8.53	6.56	326.26	6.75	1.11
	354.59	5.32	24.95	295.74	9.34	30.59	323.88	7.27	2.16	357.08	4.30	4.77	298.20	8.54	6.56	326.25	6.74	1.11
11	354.96	5.19	22.76	290.71	9.65	29.07	321.42	7.34	1.67	357.92	3.39	3.55	293.43	8.27	5.92	324.27	6.28	0.80
	354.97	5.20	22.79	290.77	9.65	29.08	321.62	7.32	1.67	357.92	3.43	3.59	293.44	8.29	5.93	324.26	6.27	0.80
12	355.07	5.07	20.29	285.53	9.98	26.95	318.88	7.40	1.29	358.76	2.35	2.27	288.59	7.57	4.91	322.25	5.38	0.52
	355.09	5.07	20.33	285.62	9.97	26.97	319.15	7.37	1.29	358.76	2.41	2.33	288.59	7.59	4.92	322.24	5.33	0.52
13	354.92	4.95	17.71	280.17	10.32	24.42	316.10	7.46	0.98	355.51	3.46	2.97	283.75	6.16	3.54	320.27	4.16	0.31
	354.95	4.95	17.75	280.28	10.31	24.44	316.47	7.42	0.98	355.48	3.39	2.91	283.75	6.23	3.58	320.26	4.06	0.30
14	354.50	4.82	15.13	274.61	10.68	21.67	313.10	7.53	0.74	355.31	3.88	2.94	278.99	4.33	2.15	314.21	4.48	0.25
	354.55	4.83	15.18	274.76	10.67	21.69	313.57	7.48	0.74	355.29	3.81	2.89	278.98	4.46	2.22	314.22	4.59	0.25
15	353.80	4.71	12.68	268.87	11.07	18.84	309.85	7.60	0.56	354.73	4.08	2.67	270.21	8.27	3.42	311.28	5.32	0.22
	353.87	4.71	12.72	269.05	11.06	18.87	310.46	7.54	0.56	354.75	4.02	2.63	270.17	8.12	3.36	311.27	5.44	0.22
16	352.82	4.59	10.42	262.94	11.48	16.07	306.36	7.68	0.41	353.79	4.15	2.30	264.57	9.68	3.31	308.04	5.88	0.18
	352.92	4.60	10.47	263.17	11.47	16.10	307.12	7.60	0.41	353.86	4.10	2.27	264.54	9.55	3.27	307.99	5.99	0.18
17	351.54	4.47	8.41	256.82	11.92	13.46	302.62	7.77	0.30	352.48	4.14	1.90	258.64	10.72	2.98	304.51	6.26	0.14
	351.67	4.48	8.46	257.10	11.90	13.49	303.56	7.65	0.30	352.64	4.11	1.89	258.64	10.59	2.94	304.39	6.36	0.14
18	349.95	4.35	6.67	250.51	12.40	11.08	298.63	7.85	0.22	350.72	4.05	1.52	252.46	11.54	2.55	300.71	6.53	0.10
	350.13	4.36	6.71	250.85	12.37	11.11	299.76	7.71	0.22	351.08	4.07	1.53	252.50	11.43	2.53	300.46	6.60	0.10
19	348.04	4.24	5.19	244.01	12.91	8.96	294.38	7.95	0.16	348.35	3.80	1.15	246.00	12.24	2.11	296.62	6.73	0.08
	348.28	4.25	5.23	244.41	12.88	9.00	295.73	7.77	0.16	349.17	4.01	1.21	246.13	12.17	2.10	296.14	6.71	0.08
20	345.81	4.12	3.97	237.32	13.46	7.13	289.87	8.04	0.11	344.94	3.14	0.74	239.22	12.80	1.69	292.25	6.88	0.06
	346.12	4.13	4.01	237.79	13.42	7.17	291.45	7.83	0.11	346.87	3.92	0.94	239.53	12.87	1.70	291.27	6.53	0.05
21	343.23	4.00	2.99	230.42	14.05	5.59	285.09	8.14	0.08	348.77	1.80	0.34	231.95	12.94	1.29	287.56	6.98	0.04
	343.62	4.02	3.03	230.99	14.01	5.62	286.93	7.89	0.08	344.13	3.78	0.70	232.70	13.54	1.35	285.40	5.55	0.03
22	340.30	3.87	2.21	223.33	14.70	4.31	280.03	8.25	0.06	344.95	2.52	0.37	223.78	11.72	0.86	282.51	7.01	0.03
	340.79	3.90	2.24	223.99	14.64	4.34	282.13	7.94	0.05	340.83	3.58	0.51	225.61	14.20	1.05	286.83	3.40	0.01
23	336.99	3.75	1.61	216.03	15.40	3.27	274.69	8.35	0.04	341.38	2.80	0.31	223.00	6.45	0.36	277.00	6.89	0.02
	337.59	3.77	1.64	216.80	15.33	3.30	277.07	7.99	0.04	336.75	3.20	0.34	218.22	14.80	0.80	280.66	5.04	0.01
24	333.29	3.62	1.15	208.53	16.17	2.45	269.05	8.46	0.03	337.74	2.84	0.23	214.75	9.72	0.39	270.83	6.42	0.01
	334.02	3.65	1.17	209.41	16.08	2.48	271.71	8.04	0.03	331.42	2.52	0.20	210.42	15.19	0.59	274.79	5.88	0.01

TABLE CXIII: 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										491.20	0.99	2.69						
1	427.11	0.46	0.22	418.24	0.33	0.31	421.10	0.37	0.53	493.88	1.08	4.36				488.26	0.90	3.58
2	429.92	0.50	0.47	415.15	0.29	0.40	420.76	0.37	0.85	496.36	1.17	6.17	481.97	0.73	0.93	488.13	0.90	5.79
3	432.65	0.55	0.75	412.00	0.26	0.44	420.25	0.36	1.12	498.63	1.27	8.01	478.50	0.65	1.56	487.94	0.90	7.73
4	435.29	0.59	1.03	408.79	0.22	0.45	419.58	0.36	1.34	500.70	1.36	9.79	474.85	0.57	1.93	487.69	0.89	9.33
5	437.85	0.64	1.30	405.52	0.19	0.42	418.73	0.36	1.49	502.56	1.46	11.39	471.02	0.50	2.06	487.37	0.89	10.55
6	440.32	0.69	1.55	402.19	0.16	0.38	417.71	0.35	1.58	504.21	1.55	12.74	467.01	0.43	2.01	486.99	0.89	11.35
7	442.68	0.73	1.76	398.79	0.14	0.32	416.52	0.34	1.60	505.66	1.65	13.76	462.82	0.37	1.83	486.55	0.88	11.74
8	444.93	0.78	1.91	395.34	0.11	0.26	415.15	0.34	1.57	506.89	1.74	14.40	458.46	0.31	1.56	486.03	0.88	11.74
9	447.07	0.83	2.02	391.83	0.09	0.20	413.61	0.33	1.49	507.91	1.83	14.64	453.94	0.25	1.27	485.45	0.87	11.41
10	449.09	0.88	2.06	388.25	0.07	0.15	411.89	0.32	1.37	508.72	1.92	14.48	449.26	0.20	0.97	484.80	0.87	10.79
11	450.97	0.92	2.04	384.61	0.05	0.10	410.00	0.31	1.22	509.32	2.00	13.94	444.43	0.16	0.70	484.08	0.86	9.97
12	452.72	0.97	1.98	380.91	0.04	0.07	407.92	0.30	1.07	509.73	2.06	12.96	439.45	0.12	0.48	483.29	0.86	9.00
13	454.31	1.01	1.86	377.13	0.03	0.04	405.67	0.29	0.91	510.03	1.89	10.55	434.33	0.08	0.30	482.42	0.85	7.96
14	455.75	1.05	1.72	373.29	0.02	0.02	403.22	0.27	0.75	509.51	1.84	8.94	429.09	0.05	0.17	481.48	0.84	6.89
15	457.02	1.09	1.55	369.37	0.01	0.01	400.60	0.26	0.61	509.38	2.23	9.28	423.82	0.03	0.08	480.45	0.83	5.86
16	458.11	1.12	1.36	365.37	0.00	0.00	397.79	0.25	0.48	508.92	2.35	8.21	417.84	0.01	0.02	479.34	0.82	4.89
17	459.02	1.16	1.18	361.30	0.00	0.00	394.79	0.23	0.37	508.22	2.43	7.01	412.32	0.00	0.01	478.15	0.81	4.00
18	459.72	1.19	1.00	357.14	0.00	0.00	391.60	0.22	0.28	507.30	2.49	5.84	406.58	0.00	0.00	476.86	0.80	3.22
19	460.22	1.21	0.82	352.89	0.00	0.00	388.22	0.20	0.21	506.15	2.53	4.77	400.72	0.00	0.00	475.47	0.79	2.55
20	460.49	1.23	0.67	348.54	0.01	0.00	384.65	0.19	0.15	504.77	2.57	3.82	394.74	0.01	0.01	473.99	0.77	1.98
21	460.53	1.24	0.53	344.11	0.01	0.00	380.88	0.17	0.11	503.16	2.59	3.00	388.65	0.02	0.01	472.39	0.76	1.51
22	460.33	1.25	0.42	339.57	0.02	0.00	376.92	0.16	0.07	501.30	2.60	2.31	382.46	0.03	0.02	470.69	0.74	1.14
23	459.86	1.26	0.32	334.93	0.03	0.00	372.77	0.14	0.05	499.21	2.59	1.74	376.18	0.05	0.02	468.86	0.72	0.84
24	459.11	1.25	0.24	330.17	0.04	0.00	368.42	0.13	0.03	496.86	2.57	1.29	369.80	0.07	0.02	466.92	0.70	0.61
25	458.08	1.24	0.18	325.31	0.05	0.00	363.87	0.11	0.02	494.25	2.52	0.93	363.34	0.10	0.02	464.85	0.67	0.43

	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	572.46	1.61	3.37															
	572.36	1.61	3.37															
2	575.18	1.73	3.93				566.41	1.37	1.52	660.71	2.17	11.19						
	574.88	1.74	3.93				566.11	1.37	1.52	660.71	2.17	11.19						
3	577.79	1.85	4.54	557.36	1.02	0.21	566.12	1.36	2.54	663.11	2.37	12.33				651.54	1.58	2.69
	577.19	1.86	4.54	556.75	1.03	0.21	565.52	1.37	2.54	663.11	2.37	12.32				651.54	1.58	2.69
4	580.29	1.96	5.11	554.05	0.91	0.40	565.73	1.36	3.31	665.34	2.57	13.50	639.32	0.95	0.21	650.90	1.58	4.55
	579.29	1.98	5.11	553.05	0.92	0.40	564.72	1.37	3.31	665.34	2.57	13.49	639.33	0.95	0.21	650.90	1.58	4.55
5	582.68	2.07	5.59	550.66	0.80	0.52	565.23	1.35	3.87	667.39	2.77	14.54	635.65	0.83	0.41	650.09	1.57	5.86
	581.17	2.09	5.59	549.16	0.82	0.53	563.73	1.37	3.88	667.40	2.77	14.52	635.66	0.82	0.41	650.10	1.57	5.85
6	584.94	2.16	5.93	547.19	0.70	0.58	564.63	1.34	4.23	669.24	2.97	15.34	631.82	0.71	0.53	649.12	1.56	6.72
	582.83	2.19	5.93	545.09	0.72	0.58	562.54	1.36	4.24	669.26	2.97	15.32	631.83	0.71	0.53	649.13	1.55	6.70
7	587.06	2.24	6.09	543.62	0.60	0.57	563.91	1.32	4.39	670.89	3.18	15.84	627.84	0.60	0.58	647.97	1.54	7.20
	584.26	2.28	6.08	540.83	0.62	0.57	561.14	1.35	4.40	670.94	3.17	15.80	627.87	0.60	0.58	647.99	1.53	7.15
8	589.02	2.28	6.02	539.96	0.51	0.52	563.08	1.29	4.35	672.32	3.38	16.00	623.70	0.51	0.57	646.65	1.52	7.33
	585.44	2.34	6.02	536.39	0.53	0.53	559.53	1.32	4.37	672.42	3.36	15.95	623.75	0.50	0.56	646.67	1.50	7.23
9	590.81	2.26	5.68	536.21	0.41	0.43	562.11	1.24	4.13	673.50	3.56	15.74	619.40	0.43	0.51	645.15	1.50	7.17
	586.35	2.33	5.68	531.76	0.44	0.45	557.70	1.28	4.14	673.69	3.56	15.75	619.48	0.42	0.50	645.15	1.45	6.95
10	592.35	2.13	4.98	532.34	0.32	0.34	560.99	1.16	3.70	674.33	3.66	14.85	614.92	0.36	0.44	643.46	1.46	6.76
	586.93	2.21	4.98	526.94	0.35	0.35	555.63	1.21	3.71	674.74	3.74	15.21	615.06	0.34	0.42	643.41	1.36	6.30
11	593.58	1.81	3.88	528.35	0.23	0.23	559.65	1.02	3.04	674.58	3.42	12.52	610.24	0.30	0.36	641.57	1.42	6.16
	587.12	1.90	3.89	521.90	0.26	0.25	553.27	1.07	3.05	675.56	3.92	14.36	610.49	0.27	0.33	641.36	1.20	5.18
12	594.40	1.38	2.65	524.18	0.14	0.13	558.03	0.80	2.19	678.61	1.60	5.22	605.27	0.25	0.29	639.47	1.37	5.43
	586.83	1.46	2.66	516.60	0.17	0.15	550.53	0.84	2.18	676.13	4.08	13.25	605.77	0.21	0.25	638.78	0.84	3.33
13	598.90	1.80	3.08	519.75	0.06	0.05	556.04	0.55	1.34	678.34	2.69	7.63	599.79	0.21	0.23	637.14	1.30	4.61
	590.17	1.94	3.12	510.98	0.08	0.06	547.35	0.57	1.31	676.41	4.20	11.91	600.87	0.16	0.18	640.00	1.30	4.64
14	599.92	2.05	3.04	514.97	0.01	0.01	557.80	0.97	2.10	678.25	3.30	8.04	598.15	0.00	0.00	634.56	1.20	3.74
	589.93	2.27	3.15	504.95	0.02	0.01	547.82	1.06	2.13	676.37	4.26	10.36	595.79	0.12	0.12	636.99	1.54	4.82
15	600.83	2.12	2.69	513.96	0.21	0.14	556.07	1.10	2.04	678.08	3.67	7.54	592.29	0.01	0.01	631.67	1.07	2.87
	589.54	2.47	2.90	502.64	0.21	0.13	544.77	1.20	2.06	675.94	4.20	8.63	590.51	0.08	0.07	634.21	1.58	4.28
16	601.58	1.99	2.11	509.54	0.20	0.12	554.31	1.17	1.84	677.72	3.92	6.69	586.69	0.01	0.00	628.42	0.90	2.03
	588.97	2.56	2.50	496.84	0.19	0.10	541.60	1.29	1.85	675.01	3.96	6.75	584.99	0.06	0.04	631.39	1.57	3.59
17	602.04	1.47	1.29	505.11	0.22	0.10	552.48	1.21	1.58	677.13	4.10	5.73	581.10	0.00	0.00	624.72	0.68	1.27
	588.18	2.55	2.04	490.99	0.17	0.07	538.25	1.34	1.58	673.48	3.50	4.88	579.16	0.04	0.02	628.46	1.54	2.93
18	601.71	0.21	0.15	500.60	0.28	0.11	550.53	1.23	1.31	676.27	4.24	4.78	575.42	0.00	0.00	620.44	0.45	0.68
	587.15	2.39	1.54	485.06	0.17	0.06	534.62	1.35	1.29	680.10	1.93	2.19	572.94	0.02	0.01	625.35	1.51	2.33
19	604.82	7.01	4.05	495.91	0.58	0.18	548.44	1.24	1.07	675.11	4.33	3.88	569.60	0.00	0.00	624.35	1.24	1.54
	585.81	1.96	1.00	479.02	0.18	0.05	530.21	1.18	0.90	678.55	2.54	2.30	566.22	0.01	0.01	622.05	1.46	1.82
20	604.33	5.57	2.54	490.54	2.30	0.58	546.14	1.23	0.85	673.60	4.30	3.02	563.64	0.01	0.00	620.14	1.32	1.30
	591.43	8.32	3.38	472.87	0.23	0.05	529.25	0.89	0.54	676.91	3.02	2.14	567.76	0.04	0.01	618.52	1.41	1.39
21	604.05	5.03	1.79	488.71	2.28	0.45	543.42	1.17	0.63	671.87	4.43	2.40	557.49	0.03	0.01	615.88	1.34	1.02
	585.78	9.21	2.87	466.53	0.41	0.07	524.72	1.16	0.54	675.07	3.35	1.84	561.26	0.05	0.01	614.72	1.34	1.03
22	603.63	4.80	1.32	483.41	0.86	0.13	539.16	0.74	0.31	669.66	4.40	1.82	551.12	0.05	0.01	611.48	1.31	0.77
	582.51	7.10	1.68	459.81	1.25	0.16	520.44	1.23	0.44	672.98	3.53	1.48	554.78	0.08	0.02	610.77	1.28	0.76
23	602.98	4.70	0.98	478.44	0.57	0.07	540.51	0.94	0.30	667.05	4.30	1.34	544.67	0.09	0.01	606.88	1.25	0.55
	580.05	5.96	1.06	451.61	5.42	0.52	516.08	1.25	0.33	670.55	3.57	1.13	548.25	0.10	0.02	606.43	1.21	0.54
24	602.06	4.66	0.73	473.48	0.49	0.04	537.45	1.06	0.25	663.97	4.13	0.95	537.89	0.12	0.01	602.01	1.15	0.38
	577.58	5.47	0.72	449.07	1.67	0.12	511.55	1.24	0.25	667.71	3.47	0.81	541.60	0.13	0.02	601.77	1.12	0.37
25	600.81	4.66	0.54	468.43	0.49	0.03	534.46	1.09	0.19	660.37	3.89	0.66	530.86	0.15	0.01	596.80	1.03	0.25
	574.93	5.20	0.50	442.21	0.82	0.04	506.82	1.23	0.18	664.38	3.22	0.55	534.77	0.16	0.01	596.73	1.01	0.25

TABLE CXIII: 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 (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	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I	ν	$S_{\rm vib}$	I
0	632.00	1.32	4.86												
1	634.25	1.32	9.57	626.26	1.34	4.80	635.36	1.31	3.09				630.22	1.32	3.09
							635.52	1.31	3.09				630.03	1.32	3.08
2	636.07	1.31	13.94	622.77	1.35	9.34	637.15	1.31	5.34	624.08	1.34	3.01	629.57	1.32	1.66
							637.37	1.31	5.35	623.87	1.34	2.99	629.01	1.31	1.65
3	637.46	1.31	17.81	618.87	1.37	13.44	638.52	1.31	7.20	620.25	1.35	5.13	628.61	1.32	1.11
							638.78	1.31	7.23	619.91	1.35	5.10	627.48	1.30	1.09
4	638.42	1.31	21.02	614.56	1.38	16.95	639.47	1.31	8.73	616.02	1.37	6.83	627.32	1.33	0.81
							639.76	1.32	8.75	615.54	1.36	6.77	625.45	1.29	0.78
5	638.95	1.32	23.50	609.85	1.40	19.77	640.00	1.31	9.91	611.39	1.39	8.16	625.70	1.33	0.61
							640.30	1.33	9.93	610.75	1.38	8.06	622.91	1.28	0.58
6	639.03	1.32	25.19	604.73	1.43	21.82	640.09	1.32	10.73	606.36	1.41	9.13	623.76	1.33	0.47
							640.39	1.34	10.75	605.56	1.40	8.99	619.86	1.26	0.44
7	638.67	1.33	26.08	599.21	1.45	23.11	639.76	1.33	11.22	600.94	1.43	9.75	621.47	1.33	0.37
							640.03	1.35	11.21	599.96	1.43	9.57	616.30	1.24	0.34
8	637.86	1.34	26.23	593.28	1.48	23.64	638.98	1.35	11.37	595.12	1.46	10.04	618.85	1.32	0.29
							639.21	1.37	11.34	593.95	1.45	9.82	612.23	1.21	0.25
9	636.59	1.35	25.71	586.96	1.51	23.48	637.75	1.37	11.24	588.91	1.49	10.02	615.88	1.31	0.22
							637.92	1.39	11.17	587.53	1.48	9.76	607.66	1.17	0.19
10	634.85	1.37	24.61	580.23	1.55	22.73	636.08	1.39	10.85	582.30	1.52	9.74	612.56	1.30	0.17
							636.17	1.41	10.74	580.71	1.52	9.44	602.58	1.12	0.14
11	632.65	1.39	23.06	573.11	1.58	21.50	633.95	1.41	10.27	575.30	1.56	9.24	608.88	1.27	0.13
							633.93	1.44	10.11	573.48	1.56	8.92	596.99	1.06	0.10
12	629.96	1.41	21.18	565.58	1.63	19.90	631.36	1.45	9.55	567.90	1.60	8.58	604.84	1.24	0.10
							631.20	1.47	9.33	565.84	1.60	8.24	590.90	0.98	0.07
13	626.78	1.43	19.09	557.65	1.68	18.06	628.31	1.49	8.74	560.11	1.64	7.80	600.42	1.18	0.07
							627.98	1.51	8.46	557.79	1.64	7.46	584.31	0.86	0.05
14	623.10	1.46	16.91	549.32	1.73	16.08	624.79	1.54	7.90	551.93	1.69	6.96	595.61	1.10	0.05
							624.26	1.55	7.55	549.33	1.70	6.63	577.22	0.71	0.03
15	618.90	1.49	14.73	540.57	1.79	14.07	620.81	1.62	7.08	543.36	1.74	6.09	590.40	0.98	0.03
							620.02	1.60	6.64	540.46	1.75	5.78	569.64	0.49	0.01
16	614.19	1.53	12.62	531.42	1.85	12.11	616.40	1.73	6.36	534.41	1.79	5.23	584.80	0.82	0.02
							615.26	1.67	5.76	531.17	1.81	4.95	561.58	0.22	0.00
17	608.93	1.57	10.65	521.85	1.92	10.25	611.68	1.93	5.87	525.09	1.84	4.41			
							609.99	1.75	4.96	521.47	1.88	4.17			
18	603.13	1.61	8.86	511.85	2.00	8.55	607.15	2.30	5.71	515.43	1.88	3.62			
							604.19	1.87	4.26	511.35	1.95	3.46			
19	596.75	1.66	7.26	501.43	2.09	7.03	598.74	0.27	0.54	505.54	1.86	2.84			
							597.94	2.05	3.71	500.83	2.02	2.81			
20	589.78	1.72	5.87	490.56	2.18	5.70	593.87	0.47	0.74	495.97	1.50	1.79			
							591.43	2.39	3.38	489.91	2.09	2.25			
21	582.19	1.78	4.69	479.25	2.29	4.56	580.38	1.09	1.30	482.63	1.41	1.28			
							585.78	2.63	2.87	478.65	2.14	1.74			
22	573.96	1.85	3.70	467.47	2.41	3.60	573.48	1.41	1.28	472.94	1.34	0.92			
							573.92	0.62	0.51	467.28	2.03	1.24			
23	565.06	1.92	2.88	455.21	2.55	2.81	565.29	1.59	1.09	454.77	1.64	0.82			
							566.05	0.81	0.49	456.91	1.18	0.53			
24	555.45	2.01	2.22	442.46	2.70	2.16	556.12	1.73	0.87	443.33	2.23	0.82			
							558.06	0.65	0.29	440.49	1.98	0.64			
25	545.09	2.11	1.69	429.19	2.88	1.65	546.07	1.85	0.68	430.74	2.60	0.69			
							550.56	0.36	0.12	428.21	1.98	0.46			

TABLE CXIII: D. continued

	K_a=2−2 $(b\,k)$=(2 2) → (2 2)								
2	640.07	1.22	4.05				632.14	1.30	8.54
	640.07	1.22	4.05				632.14	1.30	8.53
3	641.46	1.21	6.94	622.97	1.33	4.09	630.90	1.34	5.86
	641.46	1.21	6.94	622.97	1.33	4.09	630.90	1.34	5.86
4	642.41	1.21	9.13	618.69	1.35	7.00	629.24	1.39	4.39
	642.41	1.21	9.13	618.69	1.35	7.00	629.24	1.39	4.39
5	642.94	1.20	10.75	613.99	1.38	9.18	627.16	1.44	3.44
	642.94	1.20	10.75	614.00	1.38	9.18	627.17	1.44	3.44
6	643.02	1.20	11.87	608.89	1.40	10.76	624.66	1.50	2.76
	643.02	1.20	11.87	608.90	1.40	10.76	624.68	1.50	2.76
7	642.66	1.21	12.53	603.39	1.43	11.80	621.74	1.57	2.23
	642.67	1.21	12.52	603.41	1.43	11.80	621.77	1.57	2.23
8	641.84	1.22	12.77	597.48	1.46	12.33	618.38	1.63	1.81
	641.86	1.22	12.76	597.51	1.46	12.34	618.43	1.64	1.82
9	640.57	1.23	12.64	591.17	1.49	12.43	614.59	1.71	1.47
	640.59	1.23	12.63	591.21	1.49	12.44	614.67	1.71	1.47
10	638.82	1.24	12.20	584.44	1.52	12.15	610.37	1.78	1.19
	638.86	1.24	12.19	584.51	1.52	12.16	610.48	1.78	1.19
11	636.59	1.26	11.51	577.31	1.56	11.57	605.69	1.85	0.95
	636.66	1.26	11.50	577.40	1.56	11.58	605.85	1.86	0.96
12	633.88	1.28	10.64	569.76	1.60	10.76	600.57	1.93	0.76
	633.97	1.28	10.63	569.89	1.60	10.77	600.79	1.94	0.76
13	630.66	1.31	9.65	561.80	1.64	9.80	594.99	2.01	0.60
	630.79	1.30	9.64	561.97	1.64	9.81	595.28	2.02	0.60
14	626.93	1.34	8.59	553.42	1.69	8.75	588.94	2.09	0.47
	627.11	1.33	8.58	553.64	1.69	8.76	589.31	2.10	0.47
15	622.67	1.37	7.52	544.61	1.75	7.67	582.41	2.17	0.36
	622.91	1.36	7.51	544.89	1.75	7.69	582.89	2.19	0.37
16	617.87	1.40	6.48	535.37	1.81	6.61	575.40	2.26	0.28
	618.18	1.40	6.47	535.73	1.81	6.62	575.99	2.28	0.28
17	612.51	1.44	5.49	525.69	1.87	5.60	567.89	2.35	0.21
	612.91	1.44	5.48	526.14	1.87	5.62	568.61	2.37	0.21
18	606.57	1.49	4.58	515.57	1.95	4.68	559.87	2.45	0.16
	607.08	1.48	4.58	516.11	1.95	4.69	560.74	2.47	0.16
19	600.02	1.54	3.77	504.99	2.03	3.85	551.33	2.55	0.12
	600.67	1.53	3.77	505.65	2.03	3.86	552.35	2.57	0.12
20	592.85	1.59	3.05	493.94	2.13	3.12	542.25	2.65	0.09
	593.66	1.58	3.06	494.74	2.13	3.14	543.43	2.68	0.09
21	585.03	1.65	2.44	482.40	2.24	2.50	532.63	2.77	0.06
	586.02	1.64	2.45	483.37	2.23	2.51	533.97	2.80	0.06
22	576.52	1.71	1.92	470.38	2.36	1.97	522.43	2.89	0.04
	577.73	1.71	1.93	471.53	2.35	1.99	523.93	2.92	0.05
23	567.28	1.78	1.50	457.83	2.49	1.54	511.63	3.02	0.03
	568.76	1.78	1.51	459.19	2.48	1.55	513.29	3.04	0.03
24	557.27	1.86	1.15	444.75	2.65	1.19	500.22	3.17	0.02
	559.07	1.86	1.16	446.35	2.64	1.20	502.00	3.17	0.02
25	546.43	1.94	0.87	431.10	2.82	0.91	488.16	3.32	0.02
	548.62	1.94	0.89	432.98	2.81	0.92	490.03	3.31	0.02

TABLE CXIII: 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 (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	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	849.60	1.06	5.38												
1	852.22	1.04	10.45	843.67	1.09	5.44	875.07	0.94	3.17				869.89	1.04	3.49
							875.61	0.92	3.08				869.58	1.06	3.55
2	854.60	1.02	14.99	840.37	1.11	10.69	877.12	0.90	5.25	863.63	1.06	3.42	869.66	1.12	2.01
							878.06	0.85	4.92	863.54	1.08	3.48	868.73	1.17	2.10
3	856.75	1.00	18.83	836.84	1.13	15.52	878.83	0.86	6.74	859.97	1.08	5.89	869.30	1.24	1.50
							880.24	0.74	5.80	860.00	1.11	6.03	867.46	1.34	1.60
4	858.65	0.98	21.84	833.09	1.15	19.71	880.21	0.81	7.71	856.00	1.10	7.88	868.78	1.45	1.27
							882.01	0.51	4.79	856.23	1.13	8.07	865.76	1.58	1.37
5	860.30	0.97	23.95	829.13	1.17	23.11	881.24	0.76	8.17	851.71	1.10	9.39	867.95	1.68	1.11
							883.88	0.41	4.33	852.21	1.12	9.42	863.64	1.90	1.24
6	861.70	0.95	25.16	824.95	1.18	25.62	881.91	0.71	8.16	847.10	1.11	10.41	867.34	1.42	0.73
							884.62	0.25	2.92	847.81	0.94	8.76	861.10	2.32	1.17
7	862.84	0.93	25.51	820.56	1.20	27.20	882.21	0.64	7.66	842.18	1.10	10.92	865.71	2.36	0.94
							889.22	0.80	9.48	843.54	0.75	7.33	858.12	2.85	1.11
8	863.72	0.92	25.09	815.95	1.22	27.86	882.11	0.55	6.65	836.94	1.08	10.92	868.04	0.03	0.01
							890.28	0.90	10.69	838.18	0.69	6.86	854.69	3.47	1.05
9	864.32	0.90	24.04	811.12	1.24	27.67	881.53	0.43	5.06	831.36	1.05	10.39	866.95	0.09	0.02
							891.16	0.86	10.05	836.72	0.74	7.19	850.79	4.12	0.97
10	864.65	0.89	22.51	806.09	1.26	26.74	883.51	0.18	2.04	825.43	0.97	9.24	865.80	0.22	0.04
							891.87	0.85	9.36	831.77	0.92	8.54	846.36	4.54	0.83
11	864.68	0.88	20.69	800.84	1.27	25.23	881.64	0.33	3.43	819.08	0.83	7.32	864.59	0.33	0.05
							892.37	0.83	8.48	826.71	1.03	8.89	844.42	1.12	0.16
12	864.41	0.89	18.95	795.37	1.29	23.29	879.90	0.38	3.61	815.33	0.28	2.23	863.27	0.42	0.05
							892.62	0.80	7.48	821.54	1.10	8.64	838.59	3.58	0.39
13	864.07	0.61	11.63	789.69	1.32	21.10	877.96	0.38	3.22	807.80	0.59	4.21	861.83	0.52	0.05
							892.63	0.78	6.46	816.22	1.15	8.05	832.85	6.02	0.49
14	863.11	0.78	12.86	783.77	1.36	18.96	875.70	0.36	2.66	800.47	0.75	4.70	860.25	0.60	0.04
							892.37	0.76	5.47	810.75	1.20	7.27	826.87	8.35	0.51
15	861.94	0.78	11.05	777.87	1.03	12.29	873.08	0.33	2.09	793.02	0.81	4.38	858.51	0.69	0.04
							891.83	0.73	4.54	805.10	1.23	6.39	820.55	10.71	0.49
16	860.46	0.77	9.20	771.43	1.29	12.93	870.07	0.29	1.58	785.32	0.83	3.78	856.61	0.78	0.03
							891.00	0.71	3.70	799.28	1.26	5.49	813.85	13.23	0.45
17	858.65	0.75	7.49	764.88	1.32	10.96	866.65	0.26	1.15	777.36	0.83	3.11	854.51	0.88	0.02
							889.87	0.69	2.96	793.28	1.28	4.61	806.75	15.97	0.39
18	856.50	0.74	5.99	758.12	1.34	9.04	862.79	0.22	0.80	769.09	0.81	2.47	852.22	0.97	0.02
							888.42	0.67	2.33	787.09	1.31	3.80	799.23	18.97	0.34
19	854.02	0.72	4.71	751.14	1.36	7.30	858.47	0.18	0.54	760.52	0.78	1.91	849.71	1.07	0.02
							886.64	0.64	1.81	780.71	1.33	3.08	791.28	22.21	0.28
20	851.17	0.70	3.63	743.94	1.37	5.80	853.66	0.15	0.34	751.61	0.74	1.44	846.97	1.17	0.01
							884.51	0.62	1.38	774.14	1.34	2.45	782.90	25.70	0.23
21	847.97	0.69	2.75	736.52	1.38	4.53	848.32	0.11	0.20	742.35	0.70	1.05	843.97	1.28	0.01
							882.02	0.60	1.03	767.36	1.36	1.92	774.05	29.36	0.19
22	844.38	0.66	2.05	728.87	1.38	3.48	842.42	0.08	0.11	732.73	0.65	0.75	840.71	1.38	0.01
							879.14	0.58	0.76	760.37	1.37	1.48	764.72	33.10	0.15
23	840.41	0.64	1.50	720.99	1.38	2.63	835.89	0.05	0.05	722.72	0.60	0.52	837.14	1.50	0.01
							875.85	0.56	0.56	753.15	1.38	1.12	754.87	36.72	0.11
24	836.03	0.62	1.08	712.88	1.38	1.96	828.64	0.03	0.02	712.27	0.54	0.35	833.26	1.62	0.00
							872.14	0.52	0.39	745.71	1.39	0.84	744.45	39.92	0.08

TABLE CXIII: E. continued

	K_a=2−2								
	$(b\,k)$=(2 2) → (4 2)								
2	928.47	0.81	4.06				920.13	0.92	9.08
	928.48	0.81	4.05				920.13	0.92	9.08
3	930.40	0.79	6.83	910.96	0.91	4.27	919.31	0.97	6.43
	930.43	0.79	6.83	910.96	0.91	4.27	919.30	0.97	6.43
4	932.04	0.77	8.80	907.09	0.93	7.32	918.21	1.05	5.03
	932.09	0.77	8.80	907.10	0.93	7.32	918.19	1.05	5.04
5	933.35	0.75	10.12	902.94	0.94	9.60	916.83	1.15	4.16
	933.46	0.75	10.12	902.97	0.94	9.61	916.79	1.15	4.17
6	934.34	0.73	10.85	898.52	0.95	11.21	915.18	1.27	3.56
	934.54	0.73	10.86	898.58	0.95	11.24	915.10	1.28	3.57
7	934.97	0.71	11.02	893.81	0.96	12.21	913.25	1.43	3.11
	935.32	0.71	11.09	893.93	0.96	12.28	913.09	1.44	3.13
8	935.16	0.67	10.55	888.80	0.96	12.62	911.03	1.62	2.76
	935.79	0.69	10.87	889.02	0.97	12.76	910.74	1.64	2.79
9	934.62	0.54	8.43	883.48	0.95	12.40	908.52	1.86	2.47
	935.93	0.66	10.26	883.86	0.97	12.73	907.99	1.87	2.48
10	936.23	0.41	6.05	877.76	0.90	11.34	905.70	2.14	2.21
	935.68	0.62	9.24	878.44	0.97	12.24	904.53	1.94	2.00
11	935.02	0.51	7.15	871.36	0.69	8.07	902.51	2.46	1.96
	934.84	0.53	7.38	872.74	0.96	11.30	903.26	1.30	1.04
12	933.71	0.52	6.65	867.18	0.81	8.67	898.75	2.64	1.62
	936.73	0.28	3.51	866.70	0.91	9.80	899.22	2.16	1.33
13	932.05	0.51	5.77	860.23	0.97	9.30	897.75	1.25	0.59
	935.04	0.42	4.73	860.15	0.74	7.17	895.11	2.75	1.29
14	929.90	0.46	4.59	853.25	1.00	8.40	893.18	2.57	0.92
	933.49	0.45	4.44	856.40	0.68	5.79	890.70	3.31	1.18
15	927.44	0.46	3.90	846.00	1.00	7.24	888.79	3.51	0.94
	931.76	0.44	3.75	849.14	0.93	6.78	885.85	3.74	1.00
16	924.37	0.43	3.08	838.34	0.94	5.72	884.25	4.34	0.86
	929.75	0.42	3.01	842.11	1.00	6.12	880.76	4.56	0.90
17	920.77	0.40	2.37	830.46	0.99	4.96	879.46	5.20	0.76
	927.42	0.38	2.31	834.98	1.02	5.16	875.11	5.32	0.77
18	916.60	0.37	1.77	822.07	0.97	3.96	874.37	6.15	0.65
	924.72	0.35	1.71	827.68	1.02	4.20	869.00	6.15	0.65
19	911.81	0.33	1.29	813.25	0.95	3.10	868.97	7.20	0.55
	921.62	0.31	1.21	820.16	1.01	3.33	862.38	7.07	0.54
20	906.37	0.30	0.92	803.97	0.92	2.37	863.21	8.37	0.46
	918.08	0.26	0.82	812.38	0.99	2.57	855.22	8.08	0.44

$\mathbf{Li^+–D_2}$ versus $\mathbf{Li^+–H_2}$

An analysis

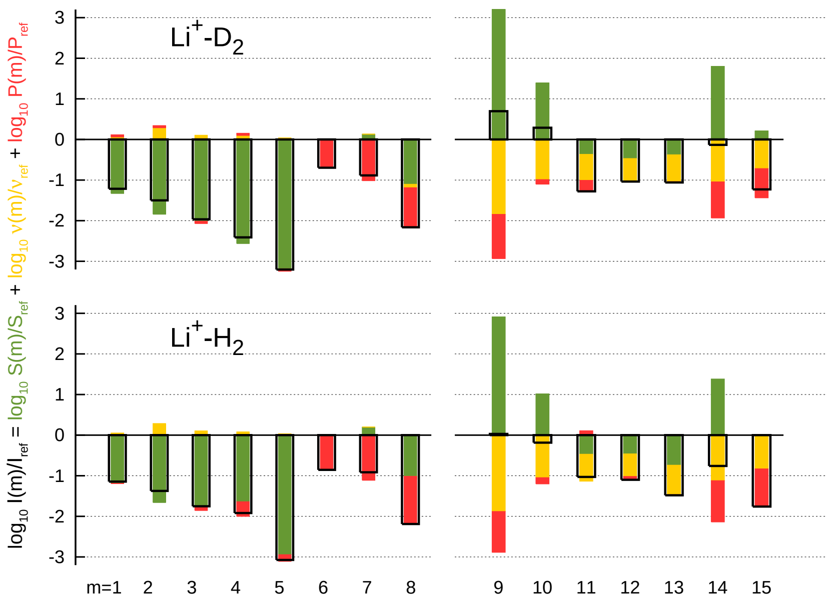
of

individual line strengths, intensities

and

integrated vibrational band intensities

Fig. C5. The most intense lines in different bands of the IR spectra.



The lines are specified in Table CXIV below. The intensities $I_{\mathrm{i}\to\mathrm{f}}(T{=}296\mathrm{K})$ of the eight lines in the near-infrared (m=1–8) and the seven lines in the far- and mid-infrared are shown relative to the intensity of the 'ref' line of each complex, which is the line in the $v_r{=}0{\to}1$ band. The colored bars show relations between the three factors of $I_{\mathrm{i}\to\mathrm{f}}$: the line strength $S_{\mathrm{i}\to\mathrm{f}}$, the transition frequency $\nu_{\mathrm{i}\to\mathrm{f}}$, and the population factor $P_{\mathrm{i}\to\mathrm{f}}{=}P_{\mathrm{i}}(T)[1-\exp(-hc\nu_{\mathrm{i}\to\mathrm{f}}/k_BT)]$, see Eq. (7).

TABLE CXIV. The most intense lines in several bands in the IR spectra of Li^+–D_2 and Li^+–H_2.

m	band	Li^+–D_2 subb[♭]	$B(J^p)$	E_{i}[♯] cm^{-1}	$\nu_{\mathrm{i}\to\mathrm{f}}$ cm^{-1}	$I_{\mathrm{i}\to\mathrm{f}}$[♮] cm/molecule	Li^+–H_2 subb[♭]	$B(J^p)$	E_{i}[♯] cm^{-1}	$\nu_{\mathrm{i}\to\mathrm{f}}$ cm^{-1}	$I_{\mathrm{i}\to\mathrm{f}}$[♮] cm/molecule
1	[0 0 0]→[1 1 0]	0–1	$Q(7^e)$	85.813	3403.81	1.85 (−21)[◇]	1–0	$Q(6^f)$	167.894	4586.96	7.86 (−21)
2	→[2 0 0]	0–0	$R(7^e)$	85.813	5733.73	9.55 (−22)	1–1	$R(6^e)$	164.797	7897.00	4.62 (−21)
3	→[1 2 0]	0–0	$P(9^e)$	137.528	3737.50	3.26 (−22)	1–1	$P(7^f)$	202.571	5197.45	1.93 (−21)
4	→[1 1 1]	0–1	$Q(7^e)$	85.813	3704.98	1.18 (−22)	1–0	$Q(10^f)$	335.079	4902.94	1.31 (−21)
5	→[1 0 1]	0–0	$P(9^e)$	137.528	3216.43	1.89 (−23)[†]	1–1	$P(8^f)$	242.039	4410.04	9.19 (−23)
6	[0 0 1]→[1 0 1]	0–0	$R(8^e)$	435.939	2943.46	6.10 (−21)	1–1	$R(6^e)$	563.594	4084.65	1.53 (−20)
7	[0 1 0]→[1 1 0]	1–1	$R(8^e)$	591.469	2942.65	3.94 (−21)	0–0	$R(6^e)$	691.524	4095.18	1.33 (−20)
8	[0 1 0]→[1 0 0]	1–0	$Q(7^f)$	572.358	2428.56	2.07 (−22)	0–1	$Q(6^e)$	691.521	3524.91	7.08 (−22)
9	[0 0 0]→[0 0 0]	0–0	$R(13^e)$	276.004	41.72	1.50 (−19)	1–1	$R(10^f)$	335.079	53.41	1.17 (−19)
10	→[0 0 1]	0–0	$P(8^e)$	110.186	303.03	5.87 (−20)	1–1	$P(7^e)$	198.466	365.13	7.13 (−20)
11	→[0 1 0]	2–3	$R(8^e)$	229.322	672.32	1.60 (−21)	1–2	$R(4^e)$	111.645	889.12	1.03 (−20)
12	→[0 2 0]	0–0	$P(8^e)$	110.186	815.95	2.79 (−21)	1–1	$P(7^f)$	202.571	1143.00	8.65 (−21)
13	→[0 0 2]	0–0	$R(8^e)$	110.186	637.86	2.62 (−21)	1–1	$R(6^f)$	167.894	765.39	3.59 (−21)
14	[0 0 1]→[0 0 2]	0–0	$P(9^e)$	461.425	263.06	2.23 (−20)	1–1	$P(7^e)$	594.265	308.13	1.91 (−20)
15	→[0 0 3]	0–0	$R(8^e)$	435.939	561.45	1.78 (−21)	1–1	$P(7^e)$	594.265	638.60	1.90 (−21)
ref	[0 0 0]→[1 0 0]	0–0	$R(8^e)$	110.186	2942.24	3.02 (−20)	1–1	$R(6^e)$	164.797	4082.01	1.09 (−19)
			$R(7^e)$*	85.813	2939.38	3.02 (−20)		$R(7^e)$*	198.466	4086.48	1.07 (−19)

[♭] The subband $K_a{=}k_{\mathrm{i}}-k_{\mathrm{f}}$. [♯] The energy of the initial state, i:=$[v_r\, v_\theta\, v_R]\, k\, J^p$, relative to the lowest level of the complex.

[♮] The used values of TIPS: $Z(296){=}4099.5$ for Li^+–D_2 and $Z(296){=}687.47$ — for Li^+–H_2. See Tables CV and BVII.

[◇] The numbers in parentheses are powers of 10.

[†] The most intense line in the subbands other than $K_a{=}3{-}3$ (which is heavily perturbed, see footnote g to Table CIII).

* The line of biggest height $\sigma(\nu{=}\nu_{\mathrm{i}\to\mathrm{f}}; 296)$ in the NIR; it is the reference line in the plots of the absorption cross-section of the complex, in Figs. 18, C4a–c — for Li^+–D_2 and in Figs. 17–18, B6a–e — for Li^+–H_2.

TABLE CXIVa. The ratios $\frac{\mathrm{Li}^+-\mathrm{H}_2}{\mathrm{Li}^+-\mathrm{D}_2}$ of intensities $I_{\mathrm{i}\to\mathrm{f}}(T{=}296\mathrm{K})$ and of three factors of the intensities for selected lines from Table CXIV. The factors are as defined in Fig. C5 and in the text below.

	Li^+–H_2/Li^+–D_2					Li^+–H_2/Li^+–D_2			
m	$I_{\mathrm{i}\to\mathrm{f}}$	$S_{\mathrm{i}\to\mathrm{f}}$ ($S^{\mathrm{vib}}_{\mathrm{i}\to\mathrm{f}}$ ♣)	$\nu_{\mathrm{i}\to\mathrm{f}}$	$P_{\mathrm{i}\to\mathrm{f}}$	m	$I_{\mathrm{i}\to\mathrm{f}}$	$S_{\mathrm{i}\to\mathrm{f}}$ ($S^{\mathrm{vib}}_{\mathrm{i}\to\mathrm{f}}$ ♣)	$\nu_{\mathrm{i}\to\mathrm{f}}$	$P_{\mathrm{i}\to\mathrm{f}}$
ref	3.61	1.140 (1.496[a])	1.387	2.286	9	0.78	0.218 (0.279[d])	1.280	2.787
5	4.86	1.977 (2.259)	1.371	1.794	10	1.21	0.482 (0.562[d])	1.205	2.092
1	4.25	1.576 (1.819[b])	1.348	2.001	11	6.41	0.894 (1.562)	1.322	5.419
3	5.94	1.964 (2.577)	1.391	2.173	12	3.11	1.148 (1.339)	1.401	1.932
2	4.84	1.729 (2.017[c])	1.377	2.031	13	1.37	0.496 (0.651[d])	1.200	2.301

[a], [b], [c] — close to the values of the mass factors c_1, c_1d_1, and c_2, respectively, defined in Fig. C4. [d] see comment (i) to Fig. C6b.

♣ Vibrational factors of line strengths

The vibrational factor of the strength $S_{\mathrm{i}\to\mathrm{f}}$ of transition from state i:=$[v_r\, v_\theta\, v_R]\; k\; J\; p$ to state f:=$[v_r'\, v_\theta'\, v_R']\; k'\; J'\; p'$ is defined in the paper (Fig. 15) as

$$S^{\mathrm{vib}}_{\mathrm{i}\to\mathrm{f}} = S_{\mathrm{i}\to\mathrm{f}}/S_{\mathrm{rot}}(Jk{\to}J'k')$$

$$\text{with} \qquad S_{\mathrm{rot}}(Jk{\to}J'k'){=}(2J{+}1)|C(J1J',k\,k'{-}k\,k')\,f^k_{k'-k}|^2\,. \tag{C16}$$

Here, it should be explained that the S_{rot} is the square of the coefficient in front of the term $\left[\mathbf{d}^\lambda_\Lambda(R)\right]_{v'j',vj}$ in the sum of Eq. (20) for the biggest of the matrix elements $\left[_{\mathrm{BF}}\mathbf{d}^{J_\mathrm{f}p_\mathrm{f},J_\mathrm{i}p_\mathrm{i}}(R)\right]_{v'j'\lambda',\,vj\lambda}$ which contribute to a given $S_{\mathrm{i}\to\mathrm{f}}$, namely, of the element with $\lambda{=}k$ and $\lambda'{=}k'$. Here $J_\mathrm{i}{=}J$, $J_\mathrm{f}{=}J'$, and obviously $\Lambda{=}k'{-}k$.

In subbands $K_a{=}k{\to}k$ (a-type transitions in asymmetric top molecules[6]),

$$S_{\mathrm{rot}}(Jk{\to}J'k) = J{+}1{-}\frac{k^2}{J{+}1}\,,\; J{-}\frac{k^2}{J}\,,\;\; \text{and}\;\; \frac{2J{+}1}{J^2{+}J}k^2\,, \tag{C17}$$

since $f^k_0{=}1$, and in subbands $K_a{=}k{\to}k{\pm}1$ (b-type transitions),

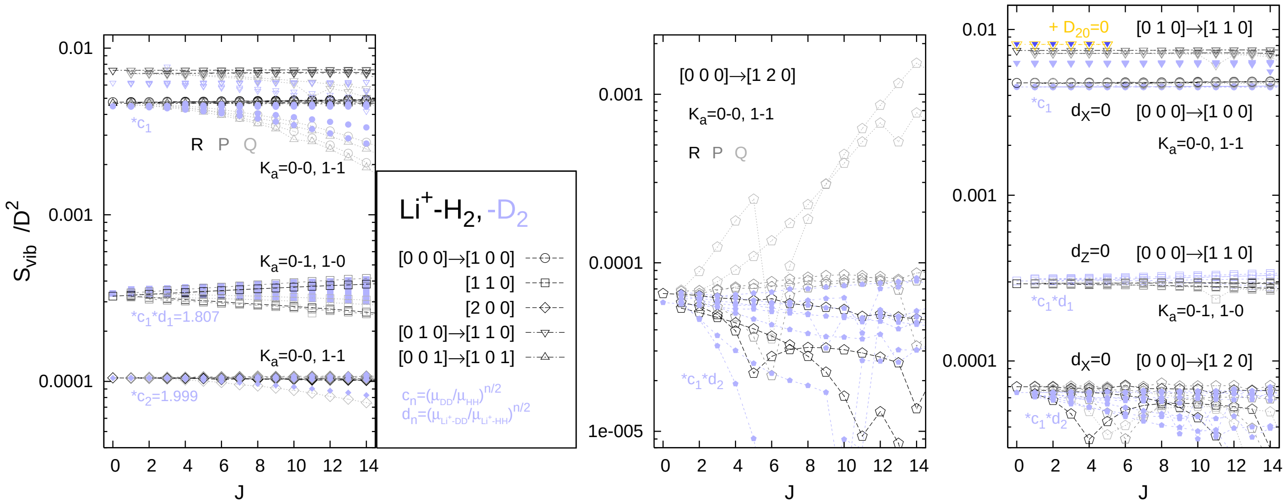
$$[f^k_{\pm1}]^{-2}\times S_{\mathrm{rot}}(Jk{\to}J'k{\pm}1) \;=\; \frac{(J{+}2{\pm}k)(J{+}1{\pm}k)}{2(J{+}1)}\,,\frac{(J{-}1{\mp}k)(J{\mp}k)}{2J}\,,$$

$$\text{and} \qquad \frac{(J{+}1{\pm}k)(J{\mp}k)(2J{+}1)}{2(J{+}1)} \tag{C18}$$

for $J'{=}J{+}1$, $J'{=}J{-}1$, and $J'{=}J$, respectively.

The S_{rot}s of Eq. (C17) are identical to the Hönl-London factors for parallel transitions in symmetric top molecules with $K{=}k$[6,8]. Formulas (C18) differ from the Hönl-London formulas for perpendicular transitions[8] by the presence of the factor $[f^k_{\pm1}]^2$ which, except for the cases $[f^0_1]^2{=}[f^1_{-1}]^2{=}1$, equals $\frac{1}{2}$.

Fig. C6. Vibrational factors of line strengths



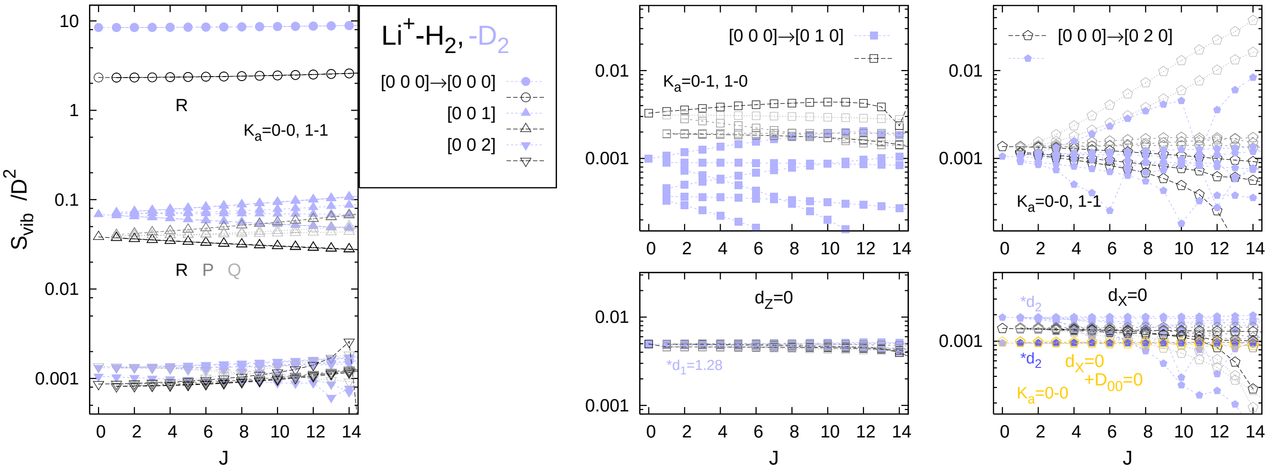
C6a. The factors $S^{\rm vib}_{\rm i\to f}$ of line strengths in the six most intense bands of the spectra of the Li^+–H_2 (D_2) complexes in the near-infrared range (the region of v_r=0→1, 2 excitations). The lines $R(J^p)$, $P(J^p)$ and $Q(J^p)$ for J<15 and $p=e,f$ in two most intense subbands K_a (=$k_{\rm i}\to k_{\rm f}$) of each band are shown. The strengths $S_{\rm i\to f}$ represented by the factors are determined by the complete dipole moment vector of each complex, cf. Eq. (18)–(22). The $S^{\rm vib}$s in the right panel represent the strengths obtained when the nominally less important dipole component, i.e. the d_X for a-type transitions and the d_Z — for b-type transitions, is neglected. The values of $S_{\rm vib}$s for Li^+–D_2 are multiplied by the mass factors $c_n d_m$ with the indices n and m adjusted to a given band $[v_r\, v_\theta\, v_R]\to[v'_r\, v'_\theta\, v'_R]$ as $n=v'_r-v_r$ and $m=|v'_\theta-v_\theta|+|v'_R-v_R|$.

Obviously, constant $S^{\rm vib}_{\rm i\to f}$s would testify on adequacy of the respective Hönl-London factors in describing the J- and k- dependence of line strengths in a given band. The feature may be expected to occur if the strengths are overwhelmingly determined by one dipole component, the ro-vibrational couplings in the initial and final states are relatively weak[9].

(i). In the a-type bands shown in the left panel, such situation occurs but only in the R- and P- branches. With growing J, the strengths of $Q(J^p)$ lines become more and more affected by the presence of d_X. This behavior may be described with Herman-Wallis coefficients for asymmetric top molecules[10], see Fig. C8.

(ii). In the panel for the [0 0 0]→[1 2 0] band, the curves formed by the $S^{\rm vib}$s as functions of J depart dramatically from straight horizontal lines and are not smooth. There are indeed cases of rather strong λ- and j-mixing in the functions of the terminal states. In particular, the energy proximity of the states [1 2 0] k=1 J^e with the states [1 1 2] k=0 J^e, and their crossing between J^e=5 and 6 (see Table BIV), is a favorable situation for the component d_X to contribute significant amounts to the strengths. The effect is the rapid growth which is seen for the Q-lines of the Li^+–H_2 complex.

(iii). The mass factors $c_n d_m$ (all >1) describe reasonably well the $S^{\rm vib}$s in the NIR spectrum of Li^+–H_2 relative to the $S^{\rm vib}$s in the corresponding bands in the spectrum of Li^+–D_2 provided the interference between (amplitudes of transitions mediated by) different components/parts of the dipole moment vector is not too big. (More on the interference in the part of further text marked with ♠ and in Figs. C6b and C7).



C6b. The factors $S^{\rm vib}_{\rm i\to f}$ of line strengths in selected bands in far- and mid-infrared ranges, in a purely rotational band, in the fundamental and first overtone bands in the R- and θ- modes.

The following observations should be made here:

(i). The relations between the $S^{\rm vib}_{\rm i\to f}$s in the bands $[0\,0\,0]\to[0\,0\,v'_R]$ for v'_R=0, 1, 2 of the spectra of the two complexes are qualitatively different from the relations observed in the bands associated with the excitation of the other, especially r-, modes. The values for Li^+–D_2 are bigger because of the dipole matrix element $\langle v{=}0|D_{00}(r,R)|0\rangle_r$ being decisive; it is bigger for the complex with the heavier diatom (see Fig. 1b in the paper) due to the larger distance of the Li^+ ion from the center-of-mass of the complex.

(ii). In the b-type band $[0\,0\,0]\to[0\,1\,0]$, the $S^{\rm vib}$s are affected by the nominally less important component d_Z much more than they are in the band $[0\,0\,0]\to[1\,1\,0]$. There are shifts between the values for the K_a=0−1 and 1−0 subbands which are so much different in the two complexes that undescribable by a single factor. However, the factor d_1 does fulfil such role very well if the $S^{\rm vib}_{\rm i\to f}$s are obtained with the d_Z set to zero.

(iii). The impact of d_Z–d_X interference on the $S^{\rm vib}$s of $Q(J^p)$-lines in the $[0\,0\,0]\to[0\,2\,0]$ band is similar to that observed in $[0\,0\,0]\to[1\,2\,0]$.

An additional observation to make, in both parts of the present figure, concerns possible interference between the anisotropic ($\sim D_{20}$) and isotropic ($\sim D_{00}$) parts of the component d_Z (see in Fig. 1b and Eqs. (18)–(22) in the paper). Namely, in the right panel of Fig. C6a and in the bottom right panel of Fig. C6b one observes that the role of this interference is:

(a) non-negligible (the shifts between the black and yellow symbols) and

(b) different in the two complexes (the shift between the black and light-blue versus the coincidence between the yellow and blue symbols).

TABLE CXV. Vibrational band strengths ($S_{[v]\to[v']}$ [a], in D^2) in the infra-red absorption spectra of Li^+–D_2 and Li^+–H_2. A demonstration of consistency with results of Ref. [11]. 'rdev' denotes relative percentage deviation.

	Li^+–H_2			Li^+–D_2		
[v] → [v′]	this work	Ref. [11]	rdev	this work	Ref. [11]	rdev
[0 0 0]→[0 0 0]	∗2.326	2.342	−0.7	8.436	8.423	0.2
[0 0 1]→[0 0 1]	∗2.935	2.987	−1.7	9.690	9.745	−2.9
[0 1 0]→[0 1 0]	∗2.517	2.529	−0.5	8.897	8.886	0.1
[0 0 0]→[0 0 1]	∗3.830 (−2)	3.889 (−2)	−1.5	∗6.829 (−2)	6.942 (−2)	−1.5
[0 0 1]→[0 0 2]	∗8.667 (−2)	8.930 (−2)	−2.9	∗1.485 (−1)	1.525 (−1)	−2.6
[0 1 0]→[0 1 1]	∗4.353 (−2)	4.436 (−2)	−1.9	∗7.389 (−2)	7.534 (−2)	−1.9
[0 0 0]→[0 2 0]	1.368 (−3)	1.603 (−3)	−14.7	1.056 (−3)	1.272 (−3)	−17.0
	1.396 (−3) [b]		−12.9	1.139 (−3)		−10.5
[0 1 0]→[0 3 0]	4.013 (−3)	6.009 (−3)	−33.2	2.524 (−3)	3.953 (−3)	−36.1
	4.669 (−3) [b]		−22.3	3.467 (−3)		−12.3
[0 0 0]→[0 0 2]	8.663 (−4)	9.442 (−4)	−8.2	1.322 (−3)	1.514 (−3)	−12.7
	8.648 (−4) [b]		−8.4	1.326 (−3)		−12.4
[0 0 0]→[0 0 3]	5.752 (−5)	9.229 (−5)	−37.7	5.094 (−5)	6.803 (−5)	−25.1
	6.797 (−5) [b]		−26.4	5.066 (−5)		−25.5
[0 0 0]→[0 1 0]	3.278 (−3)			9.888 (−4)		
	4.972 (−3) [c]			3.856 (−3) [c]		
[0 0 0]→[1 0 0]	4.73 (−3)	5.02 (−3)	−5.8	3.17 (−3)	3.32 (−3)	−4.8
[0 0 1]→[1 0 1]	4.66 (−3)	4.97 (−3)	−6.3	3.12 (−3)	3.30 (−3)	−5.4
[0 1 0]→[1 1 0]	7.36 (−3)	8.02 (−3)	−8.2	4.39 (−3)	4.68 (−3)	−6.3
[0 0 0]→[2 0 0]	1.05 (−4)	7.90 (−5)	32.9	5.24 (−5)	3.96 (−5)	32.4
[0 0 0]→[1 2 0]	6.57 (−5)	1.02 (−4)	−35.3	2.52 (−5)	4.05 (−5)	−37.8
[0 0 1]→[1 0 0]	1.03 (−5)	1.32 (−5)	−21.9	5.05 (−6)	5.66 (−6)	−10.8
[0 0 0]→[1 0 1]	2.40 (−6)	3.47 (−6)	−30.9	1.32 (−6)	1.91 (−6)	−30.7
[0 0 0]→[1 0 2]	1.78 (−6)	2.58 (−6)	−31.0	8.89 (−7)	1.21 (−6)	−26.5
[0 0 0]→[1 1 0]	3.25 (−4)			1.87 (−4)		
	2.93 (−4) [c]			1.68 (−4) [c]		
[0 0 0]→[1 1 1]	2.54 (−5)			1.09 (−5)		
[0 1 0]→[1 0 0]	5.10 (−4)			3.05 (−4)		

[a] The numbers in columns 'this work' are the factors $S^{\rm vib}$ of the strengths of $R(0)$ lines in the shown vibrational bands. The factors are actually the total strengths of these lines since $S_{\rm rot}(0\,0\to1\,0)=1$ in the bands with $\Delta v_\theta=0,2$, formed of a-type transitions, and $S_{\rm rot}(0\,0\to1\,1)=1$ — in the bands with $\Delta v_\theta=\pm1$.
The numbers listed in columns 'Ref. [11]' represent values of the strength $\left[\langle i|d_Z|f\rangle^2+\langle i|d_X|f\rangle^2\right]$ used to obtain the intensities reported in Table 4 of that paper or the squares on the averages $\langle i|d_Z|i\rangle$ described in the text. Both $|i\rangle$ and $|f\rangle$ were taken there as purely vibrational bound state functions.

[b] The numbers in the second lines are sums of the strengths obtained from two separate calculations in which one of the dipole components, d_X or d_Z, was set to zero. Not accounting for interference of amplitudes of transitions mediated by the two components, these numbers give approximate strengths, which are called 'direct'♠. The 'direct' parts are actually the proper counterparts of the strengths generated in Ref. 11. The fact becomes visible in 'rdev' values when the interference plays a role, particularly in the bands with $\Delta v_\theta=2$.

[c] Obtained from calculations with $d_Z=0$. See Figs. C6a,b, and C9.

* Counterparts of these numbers in Tables 6 and 7 of Ref. 3, obtained from an analytical fit to the ab initio data for the dipole component d_Z (the same data as used in this work), are substantially larger; their relative deviations from results of Ref. 11 range from above 50 to above 250% (when treating the factor of 10^{-4} in the unit given in the captions of the tables as a misprint). Certainly, the omission of d_X cannot explain such a big discrepancy. The fit of Ref. 3 turns out to be incorrect.

♠ 'Direct' and d_Z–d_X interference parts of line strengths

Since the transition amplitude vector $\mathbf{T}$ defined in Eqs. (19)–(20) can be written as the sum $\mathbf{T}{=}\mathbf{T}(d_Z){+}\mathbf{T}(d_X)$, the strength $S_{\mathrm{i}\to\mathrm{f}}$ can be resolved as

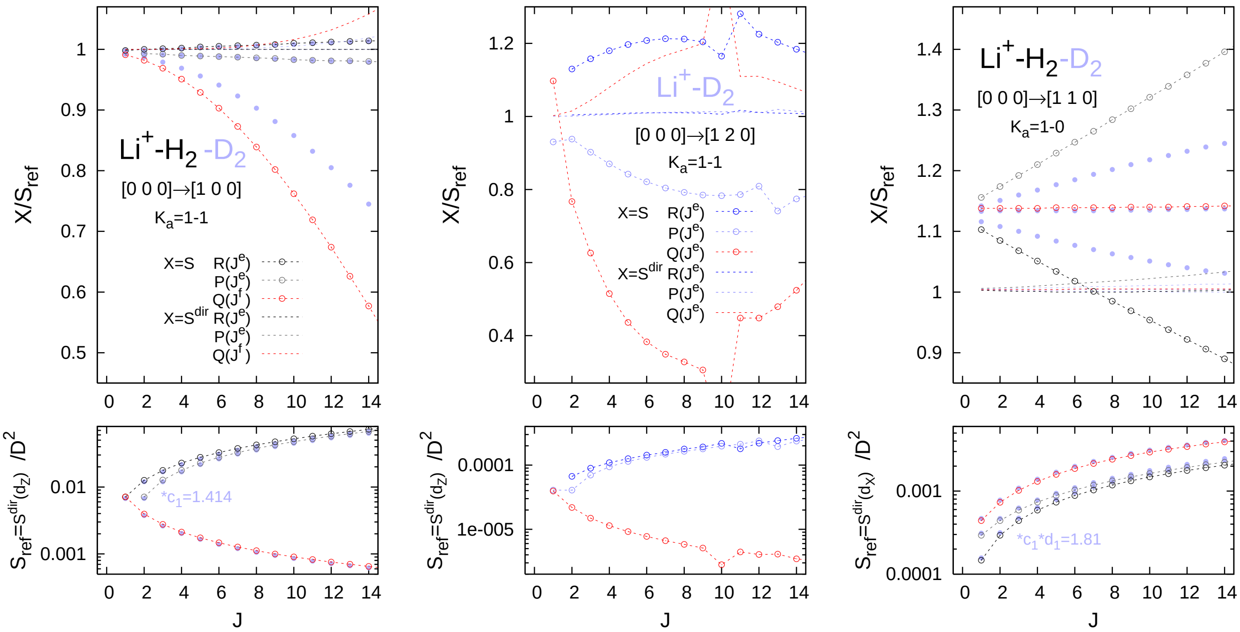
$$S_{\mathrm{i}\to\mathrm{f}} = S^{\mathrm{dir}}_{\mathrm{i}\to\mathrm{f}} + S^{\mathrm{intf}}_{\mathrm{i}\to\mathrm{f}}\,, \tag{C19}$$

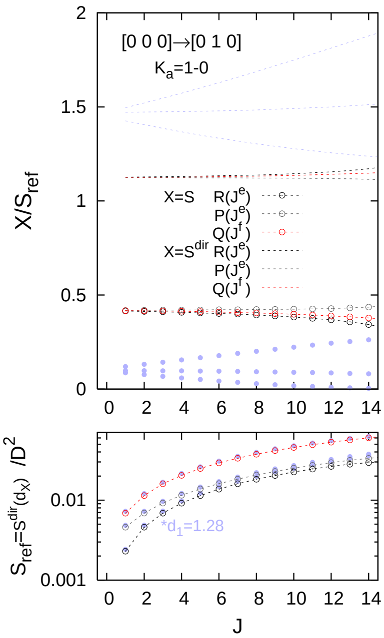
$$\text{where}\quad S^{\mathrm{dir}}_{\mathrm{i}\to\mathrm{f}} = \tfrac{\pi}{2}\Gamma\left[\mathbf{T}^{\dagger}(d_Z)\mathbf{T}(d_Z){+}\mathbf{T}^{\dagger}(d_X)\mathbf{T}(d_X)\right]{=}S^{\mathrm{dir}}_{\mathrm{i}\to\mathrm{f}}(d_Z){+}S^{\mathrm{dir}}_{\mathrm{i}\to\mathrm{f}}(d_X)$$

$$\text{and}\quad S^{\mathrm{intf}}_{\mathrm{i}\to\mathrm{f}} = \tfrac{\pi}{2}\Gamma\left[\mathbf{T}^{\dagger}(d_X)\mathbf{T}(d_Z){+}\mathbf{T}^{\dagger}(d_Z)\mathbf{T}(d_X)\right].$$

Obviously, the resolution applies also to bound→bound transitions, in which cases the vector $\mathbf{T}$ contains one element $T{=}T(E^B_{\mathrm{f}}J_{\mathrm{f}}p_{\mathrm{f}};E^B_{\mathrm{i}}J_{\mathrm{i}}p_{\mathrm{i}})$ and the factor $\frac{\pi}{2}\Gamma$ does not occur in the formulas for $S_{\mathrm{i}\to\mathrm{f}}$ and for its 'dir' and 'intf' parts.

Fig. C7. Line strengths. Contributions of d_Z–d_X interference.





For the sake of clarity of the plots, the strengths are shown only for lines in one subband $K_a{=}k_{\mathrm{i}}{-}k_{\mathrm{f}}$ of each of the four selected bands and only for one parity p of the initial states in each branch (only one is possible if k_{i} and/or $k_{\mathrm{f}}{=}0$).

S_{ref} — the largest contribution to the line strengths in a given band, which is the $S^{\mathrm{dir}}(d_Z)$ in the a- and the $S^{\mathrm{dir}}(d_X)$ in the b-type bands.

$S^{\mathrm{dir}}/S_{\mathrm{ref}}$ — shows the increase of the 'dir' parts of the strengths due to the inclusion of the second dipole component. The increase is: entirely negligible in the cases of $R(J)$ and $P(J)$ lines in the two a-type bands, rather small for all lines in the [0 0 0]→[1 1 0] band, and much bigger in the corresponding band in the FIR range.

The contribution of the d_Z–d_X interference is shown by $S/S_{\mathrm{ref}}{-}S^{\mathrm{dir}}/S_{\mathrm{ref}}$, i.e. by the distance between the lines of the same color with and without circles. In absolute value, the 'intf' contribution nearly always overwhelms the 'dir' contribution of the nominally less important dipole moment component.

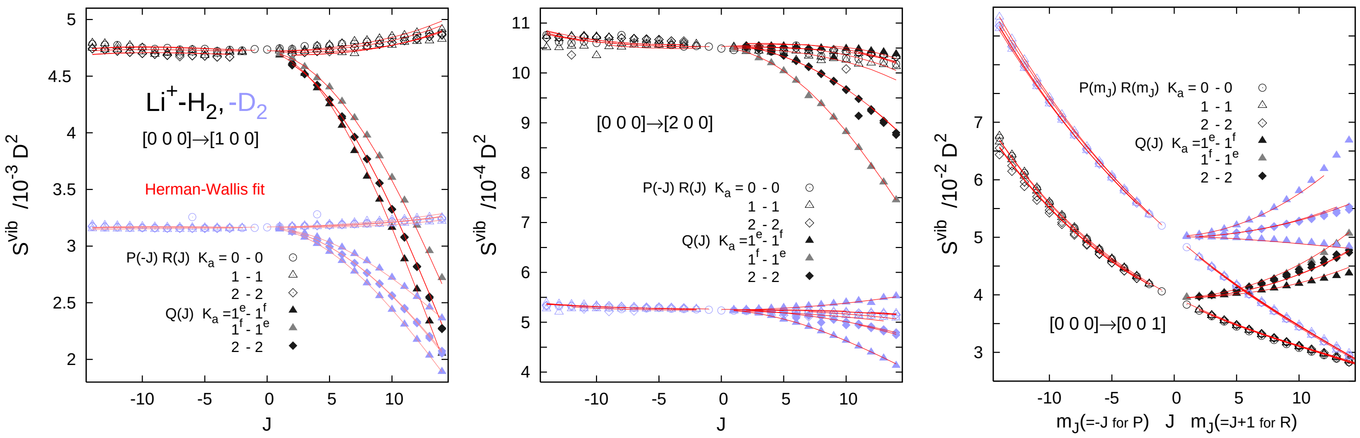
The largest interference (destructive, $S^{\mathrm{intf}}{<}0$) demonstrated in the figure occurs in the [0 0 0]→[0 1 0] band of Li^+–D_2. Its impact on the cross-section $\sigma(\nu;T)$ and on the integrated band intensity is seen in Figs. C4d and C9, respectively.

Fig. C8. Herman-Wallis type parametrization[10] of $S^{\rm vib}_{\rm i\to f}$s

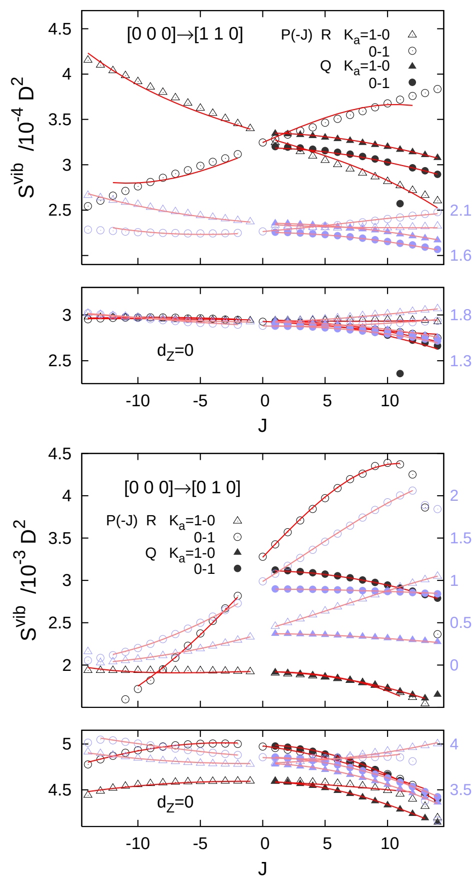
$$
\begin{aligned}
S^{\rm vib}_{\rm i\to f} &= \underbrace{S_{[\rm v]\to[\rm v']}(s_0)}\ \underbrace{F_{\rm HW}(kJp\to k'J'p';\{s_1,..\})} \\
&= \qquad s_0^2 \qquad \Big[1+\sum_{i=1}^{7} s_i f_i(kJp\to k'J'p')\Big]^2 , \qquad \text{(C20)}
\end{aligned}
$$

$$
\begin{aligned}
&f_1=\tfrac{1}{2}([J']-[J]) := m_J\,, \quad f_3=\tfrac{1}{2}([J']+[J])\,, \quad f_2=m_J^2\,,\\
&f_5=\tfrac{1}{2}(F'-F) \quad := m_F\,, \quad f_4=\tfrac{1}{2}(F'+F)\,, \quad f_7=m_F^2\,,\\
&f_6=m_J\,m_F\,,
\end{aligned}
$$

where $\quad [J] := J(J+1) \quad$ and $\quad F(kJp) := E([\rm v]kJp)-E([\rm v]J{=}0)\,.$



The red lines join values obtained using formula (C20) with the parameters s_i listed in Table CXVI. In each panel of the figure, one red curve connects the fitted $S^{\rm vib}$s of lines $B(J^p)$ for a given parity p in a given branch $B\,(=R,P,Q)$ of a given subband K_a of the band shown in the panel. The $p{=}e$ and $p{=}f$ curves are clearly distinguishable only in the Q branches of $K_a{=}1{-}1$ subbands. Obviously, only one value of p is possible in subbands 0−0, 0−1, and 1−0.



The set of $S^{\rm vib}$s represented by the symbols in each of the three panels in the row is the same as the set shown for the same band in Fig. 15 of the paper. Except for a few cases, the symbols lie on or very close to the fitted lines. For each of the three bands, the parameter s_0^2 of the fitted lines has indeed the meaning of the strength $S_{[\rm v]\to[\rm v']}$, as evidenced in Table CXVI. This provides a justification of the statement in the discussion of Fig. 15 that the strengths of lines in the three subbands of the three a-type bands can be well represented with the help of the Herman-Wallis coefficients derived in Ref. 10 for asymmetric top molecules.

Attempts to parametrize the entire set of $S^{\rm vib}$s shown in Fig. 15 for the band [0 0 0]→[1 1 0] were not successful because of too severely perturbed values occurring in the $K_a{=}1{-}2$ subband. The set was therefore limited to values for subbands $K_a{=}0{-}1$ and 1−0. The parametrization of this set is possible, as shown in the second panel in the column of the present figure and in the fifth column of Table CXVI, but its quality is definitely lower than in the cases of the a-type bands.

Though the bottom panels may seem to testify to the contrary, the parametrization (C20) is actually unsuitable for the band [0 0 0]→[0 1 0]. The argumentation is given in the comment to Table CXVI.

TABLE CXVI. Parameters $s_0, \ldots, s_7$ from least-squares fits of formula (C20) to the factors $S^{\rm vib}_{\rm i\to f}$ of line strengths in several bands of the IR spectra of the Li^+–H_2 (D_2) complexes.

	Li^+–H_2						
						d_Z=0	
	[000]→[100]	[000]→[200]	[000]→[001]	[000]→[110]	[000]→[010]	[000]→[110]	[000]→[010]
$N_{\rm fit}$[a]	187	181	187	79	73	83	80
$s_0\times\alpha$[b]	2.17384 (88)[f]	1.02619 (58)	1.9919 (14)	1.8244 (24)	1.53971 (99)	1.7038 (15)	2.1552 (12)
α	$10^{3/2}$	100	10	100	$10^{3/2}$	100	$10^{3/2}$
$s_1\times10^3$[c]	16.18 (40)	−24.30 (49)	−1.99 (55)	1.04 (13)	4.291 (77)	−0.613 (37)	−1.683 (34)
$s_2\times10^3$[c]	0.539 (22)	− 1.370 (32)	−0.606 (39)	–	−0.910 (12)	0.0348 (58)	–
$s_3\times10^3$[c]	− 0.895 (14)	− 1.820 (30)	−0.201 (34)	0.236 (18)	−0.1441 (83)	−0.2422 (53)	−0.2635 (47)
$s_4\times10^4$[d]	− 2.293 (56)	6.31 (13)	0.513 (44)	−2.007 (67)	–	–	–
$s_5\times10^3$[d]	− 6.64 (17)	9.90 (20)	−5.80 (23)	−0.313 (20)	3.141 (12)	−0.0642 (69)	0.4275 (59)
$s_6\times10^4$[d]	0.120 (79)	− 0.223 (60)	1.317 (66)	2.037 (31)	3.692 (20)	−0.371 (28)	−0.505 (18)
$s_7\times10^5$[e]	–	–	–	–	–	0.50 (6)	0.78 (4)
$\sigma\times\alpha^2\times10^3$[g,h]	24.6	7.8	36.3	40.5	15.4	12.1	17.0
$S_{[{\rm v}]\to[{\rm v}']}\times\alpha^2$[i,h]	4.725	1.053	3.968	3.328	2.371	2.903	4.644
$S^{\rm cal}_{[{\rm v}]\to[{\rm v}']}\times\alpha^2$[j,h]	4.735	1.049	3.830	3.246	3.278	2.926	4.972
	Li^+–D_2						
$N_{\rm fit}$	185	173	184	82	78	84	80
$s_0\times\alpha$	1.77971 (33)	2.29419 (64)	2.65049 (58)	1.38285 (67)	0.7759 (19)	1.3033 (10)	1.95454 (33)
α	$10^{3/2}$	$10^{5/2}$	10	100	$10^{3/2}$	100	$10^{3/2}$
$s_1\times10^3$	12.51 (20)	−22.67 (24)	3.93 (20)	0.879 (52)	31.17 (12)	0.116 (36)	−0.772 (19)
$s_2\times10^3$	1.184 (87)	–	− 0.717 (12)	–	–	0.2246 (81)	0.1673 (24)
$s_3\times10^3$	− 0.6322 (49)	− 1.007 (10)	− 0.5144 (90)	−0.1921 (75)	0.929 (19)	−0.2703 (46)	−0.2702 (22)
$s_4\times10^3$	− 0.2021 (28)	0.5579 (66)	0.0764 (24)	−0.0515 (45)	− 0.596 (12)	–	–
$s_5\times10^3$	− 8.05 (13)	14.62 (16)	−11.63 (13)	−0.819 (18)	13.170 (45)	−0.397 (14)	0.2781 (67)
$s_6\times10^3$	− 1.21 (11)	− 0.993 (15)	0.1381 (46)	0.1581 (27)	0.661 (17)	−0.0788 (85)	−0.0408 (10)
$s_7\times10^4$	4.18 (38)	3.162 (70)	–	–	− 0.356 (71)	0.111 (28)	–
$\sigma\times\alpha^2\times10^3$	7.2	19.3	20.5	9.3	4.2	6.1	7.0
$S_{[{\rm v}]\to[{\rm v}']}\times\alpha^2$	3.167	5.263	7.025	1.912	0.602	1.699	3.820
$S^{\rm cal}_{[{\rm v}]\to[{\rm v}']}\times\alpha^2$	3.166	5.237	6.829	1.865	0.989	1.682	3.856

[a] The number of $S^{\rm vib}_{\rm i\to f}$ values (i:=[v]kJp, f:=[v′]$k'J'p'$) used in the fit for a given band [v]→[v′]. The values concern lines $R(J^p)$, $P(J^p)$, and $Q(J^p)$ for J=0, ..., 14 and p=e, f from three subbands K_a=k→k' (0−0, 1−1, 2−2) in the cases of the three a-type bands shown and from two subbands, K_a=0−1 and 1−0, in the cases the two b-type bands. Some values from the specified ranges were rejected in order to assure reasonable uncertainties of the fitting parameters.

[b] The unit of the parameter s_0 is Debye. [c] Dimensionless parameters.

[d] Given in cm since the rotational energies $F(kJp)$ in the unit of cm^{-1} are inserted. [e] Given in cm^2.

[f] In parentheses are the estimated uncertainties of the parameters on the last decimal positions shown.

[g] Root-mean-square deviation between fitted and calculated $S^{\rm vib}_{\rm i\to f}$s. [h] In D^2.

[i] The vibrational band strength resulting from the fit.

[j] The calculated vibrational band strength; like in Table CXV, it is taken as the strength S of $R(0)$ line.

The strength of a given band [v]→[v′] obtained from the fit, $S_{[{\rm v}]\to[{\rm v}']}=p_0^2$, should be close to the calculated value $S^{\rm cal}_{[{\rm v}]\to[{\rm v}']}$ if the semi-rigid asymmetric top model, underlaying the fit, describes adequately the impact of vibration-rotation interactions in the initial and final states on the transition strengths in the band.

The agreement appears quite satisfactory for all bands shown in the table except for [0 0 0]→[0 1 0] (discrepancies of 28 and 39% for Li^+–H_2 and Li^+–D_2, respectively). The impact of the rotation-vibration interactions on the strength of this band, nominally driven by the d_X dipole component, is magnified by the size of the interfering d_Z (see the comments to Fig. C4d, B6d, and C6b). One should thus conclude that this impact is too big to be meaningfully described by formula (C20).

Fig. C9. Integrated band intensities $I_{[\mathrm{v}]\to[\mathrm{v}']}(T)$

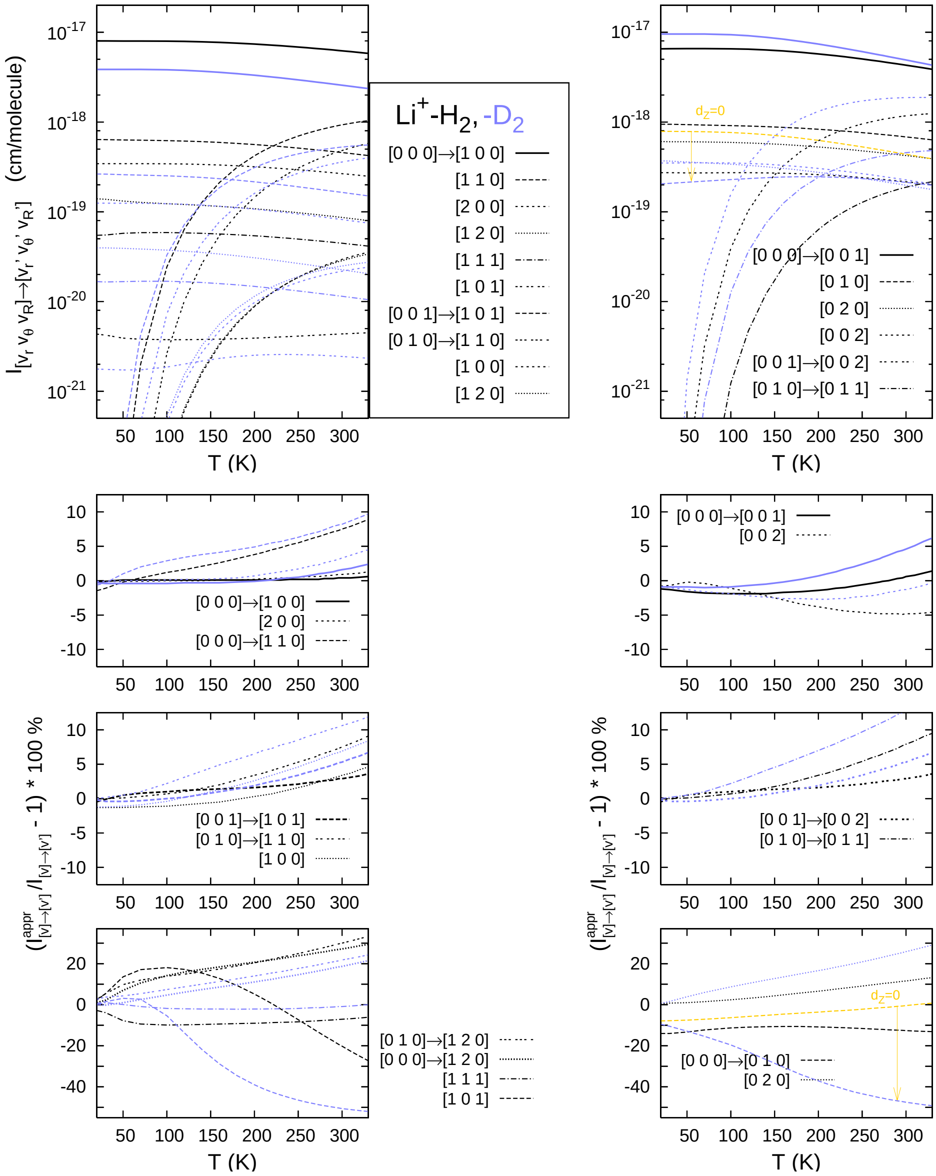


Table XII of the paper is appended here with a demonstration of temperature dependence of the integrated intensities of the various vibrational bands (the upper panels) and with information on adequacy of the following approximate formula[12] for the quantity in application to these bands,

$$
\begin{aligned}
I^{\mathrm{appr}}_{[\mathrm{v}]\to[\mathrm{v}']}(T) &= \left\{\tfrac{2\pi^2}{3hc\epsilon_0}\right\}\nu_{[\mathrm{v}]\to[\mathrm{v}']}\,S_{[\mathrm{v}]\to[\mathrm{v}']}\,\underbrace{P_{[\mathrm{v}]}(T)\left[1-\exp\!\left(-\frac{hc\nu_{[\mathrm{v}]\to[\mathrm{v}']}}{k_BT}\right)\right]} \\
&:= \left\{\qquad\right\}\nu_{[\mathrm{v}]\to[\mathrm{v}']}\,S_{[\mathrm{v}]\to[\mathrm{v}']}\qquad P_{[\mathrm{v}]\to[\mathrm{v}']}(T)\,, \qquad \text{(C21)}
\end{aligned}
$$

where $\nu_{[\mathrm{v}]\to[\mathrm{v}']}$ is the band center as defined in Table XII, $S_{[\mathrm{v}]\to[\mathrm{v}']}$ — the band strength as defined in Table CXV, and $P_{[\mathrm{v}]}(T)$ — the population of the initial vibrational state at temperature T, $P_{[\mathrm{v}]}(T){=}Z_{[\mathrm{v}]}(T)/Z(T)$ with $Z_{[\mathrm{v}]}$ denoting the sum of states belonging to [v], $\sum_{[\mathrm{v}]} Z_{[\mathrm{v}]}{=}Z$.

The simpler expression for $P_{[\mathrm{v}]}(T)$ which is obtained under the assumption $Z(T){\approx}Z_{\mathrm{vib}}(T)Z_{\mathrm{rot}}(T)$,

$$\widetilde{P}_{[\mathrm{v}]}(T){=}\exp\big(-[E([\mathrm{v}]\,J{=}0){-}E([0]\,0)]/k_BT\big)/Z_{\mathrm{vib}}(T)$$

with $Z_{\mathrm{vib}}(T){=}\sum_{[\mathrm{v}]}\exp\big(-[E([\mathrm{v}]\,J{=}0){-}E([0]\,0)]/k_BT\big)$, may be used in formula (C21) when [v]=[0 0 0] but rather not, and certainly not at low Ts (<100 K), when [v] is an excited state. A demonstration of this fact is given in Fig. C9a.

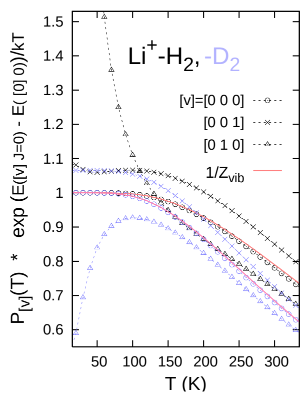


Fig. C9a. A comparison of populations $P_{[\mathrm{v}]}(T)$ with $\widetilde{P}_{[\mathrm{v}]}(T)$ at $T{\le}330$ K for [v]=[0 0 0], [0 0 1], and [0 1 0].

The approximate formula (C21) appears to work reasonably, the relative deviations $I^{\rm appr}_{[{\rm v}]\to[{\rm v}']}/I_{[{\rm v}]\to[{\rm v}']}-1$ within $\pm 10\,\%$, for ten bands (of the sixteen) examined in the figure. These seem to be the bands in which the line strengths are predominantly determined by one dipole component, i.e. no substantial λ- and j- mixing in the initial and final states of the transitions occurs ✠.
Thus, the temperature dependence of the 'exact' intensities $I_{[{\rm v}]\to[{\rm v}']}$ of these bands is reasonably represented by the factor $P_{[{\rm v}]\to[{\rm v}']}$ of Eq. (C21). The factor practically equals the population $P_{[{\rm v}]}$ for the bands in the near-infrared at temperatures of interest here.
Naturally, the comparison of the corresponding bands of the Li^+–H_2 and Li^+–D_2 complexes with respect to the rotationally averaged quantity $I_{[{\rm v}]\to[{\rm v}']}$, which is made in Table CXVII, shows smaller differences than those shown in Table CXIVa from the comparison of the $I_{\rm i\to f}$s of the most intense rotational lines in the bands. The ratios $\frac{{\rm Li^+-H_2}}{{\rm Li^+-D_2}}$ of the factors $P_{[{\rm v}]\to[{\rm v}']}$, much smaller than those of the $P_{\rm i\to f}$s, are mostly responsible for the fact.

TABLE CXVII. The ratios $\frac{{\rm Li^+-H_2}}{{\rm Li^+-D_2}}$ of intensities $I^{\rm appr}_{[{\rm v}]\to[{\rm v}']}$(296K) and of three their factors, Eq. C21.

	Li^+–H_2/Li^+–D_2			
[v]→[v′]	$I^{\rm appr}_{[{\rm v}]\to[{\rm v}']}$	$S_{[{\rm v}]\to[{\rm v}']}$	$\nu_{[{\rm v}]\to[{\rm v}']}$	$P_{[{\rm v}]\to[{\rm v}']}$
[0 0 0]→[1 0 0]	2.38 (2.40)[a]	1.496	1.390	1.146
→[2 0 0]	3.17 (3.24)	2.003	1.379	1.146
→[1 1 0]	2.76 (2.77)	1.740	1.382	1.146
→[0 0 1]	0.84 (0.87)	0.561	1.216	1.235
→[0 0 2]	0.92 (0.95)	0.655	1.192	1.172
[0 0 1]→[1 0 1]	1.72 (1.75)	1.491	1.399	0.823
→[0 0 2]	0.60 (0.63)	0.584	1.165	0.887
[0 1 0]→[1 1 0]	1.29 (1.33)	1.679	1.392	0.552
→[1 0 0]	1.29 (1.34)	1.670	1.404	0.552
→[0 1 1]	0.40 (0.41)	0.589	1.149	0.585

[a] in parentheses are the ratios of the respective $I_{[{\rm v}]\to[{\rm v}']}$es.

✠ The facts supporting the conjecture: (i) In the bottom panels of Fig. 9 collected are the bands [v]→[v′] for which large deviations $I^{\rm appr}_{[{\rm v}]\to[{\rm v}']}/I_{[{\rm v}]\to[{\rm v}']}-1$ were found. In three of these bands, [0 0 0]→[1 2 0], [0 0 0]→[0 2 0], and [0 0 0]→[0 1 0], strong d_Z–d_X interference and accidental-degeneracy effects on the line strengths were demonstrated in Figs. C6–C7.
(ii) In the right bottom panel of Fig. 9, there is an indication that the big error of $I^{\rm appr}$ in application to [0 0 0]→[0 1 0] of Li^+–D_2 (about −49% at $T{\approx}330$ K) stems from inability to fully account for the big d_X–d_Z interference in this band. Namely, the yellow curve drawn in this panel shows that the error decreases substantially (to 0.8 % at 330 K) when the band strength $S_{[{\rm v}]\to[{\rm v}']}$ inserted into formula (C21) comes from calculations with the component d_Z turned off.
(iii) In the band [0 0 0]→[1 0 1], on which formula (C21) fails most severely, all three parts of the dipole moment vector, $\propto D_{0,0}$, $\propto D_{2,0}$, and $\propto D_{2,1}$ (cf. Fig. 1b), contribute significantly or non-negligibly. As shown in Fig. C9b, the intensities $I_{[000]\to[101]}(T)$ produced by each of the dipole moment parts directly (i.e. excluding the interference with the other two parts) assume comparable sizes at $T{>}250$. Quite different relation is seen between the analogous intensities of the band [0 0 0]→[1 0 0], on which formula (C21) works very well. Namely, the intensity $I_{[000]\to[100]}(\propto D_{0,0})$ dominates over the $I_{[000]\to[100]}(\propto D_{2,0})$ in the entire temperature range by a factor $\gtrsim$10 and the intensity produced the component $d_X{\propto}D_{21}$ stays smaller by at least three orders of magnitude.

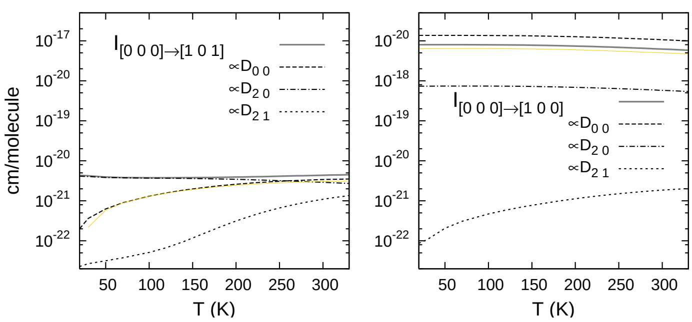


Fig. C9b. Integrated intensities of bands [0 0 0]→[1 0 1] and [0 0 0]→[1 0 0] of Li^+–H_2. A comparison of direct contributions to the intensities produced by the three parts of the dipole vector $\mathbf{d}(r,R,\theta)$, $D_{L|\Lambda|}(r,R)P_L^{|\Lambda|}(\cos\theta)$ for $(L\,|\Lambda|)$=(0 0), (2 0), and (2 1).

$$I_{[000]\to[10v_R]} = \sum_{L,|\Lambda|} I_{[000]\to[{\rm v}']}(\propto D_{L|\Lambda|}) + I^{\rm intf}_{[000]\to[{\rm v}']}\,;$$

the interference contributions $I^{\rm intf}\times(-1)$ are represented by the yellow lines in the figure.

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