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High resolution Fourier transform infrared emission spectra of lithium iodide

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The high resolution infrared emission spectrum of lithium iodide has been recorded with a Fourier transform spectrometer. A total of 1024 transmissions with $\Delta v = 1$ for ^{7}LiI (from $v = 1 \rightarrow 0$ to $v = 8 \rightarrow 7$), 387 transitions with $\Delta v = 2$ ($v = 2 \rightarrow 0$ to $v = 6 \rightarrow 4$) and 504 transitions with $\Delta v = 1$ for ^{6}LiI ($v = 1 \rightarrow 0$ to $v = 5 \rightarrow 4$) have been assigned. The infrared data have been used to determine improved mass-dependent Dunham Y_{lm} coefficients for the ground $X^1\Sigma^+$ electronic state. The mass-independent Dunham U_{lm} coefficients were obtained along with Born–Oppenheimer breakdown constants. Finally, all of the data were fitted to the eigenvalues of the radial Schrödinger equation containing a modified Morse potential function to determine the parameters of an effective ground state potential.

1. Introduction

As classical examples of ionic bonding, the alkali halides have been studied extensively in the past. The microwave absorption spectra of LiI and several other alkali halides were observed by Honig *et al.* [1] in 1954 when they reported values for the rotational constants of ^{7}LiI and ^{6}LiI, the electric quadrupole coupling constants for ^{127}I and the electric dipole moment for ^{7}LiI. In 1962, Rusk and Gordy [2] reported on millimetre wave spectra. Breivogel *et al.* [3] studied radiofrequency and microwave spectra of ^{6}LiI using the molecular beam electric-resonance method, and measured the electric dipole moment for ^{6}LiI. Jacobson and Ramsey [4] studied the hyperfine structure of ^{7}LiI in a molecular beam and reported spin–rotation constants for both iodide and lithium, and also nuclear spin–spin coupling constants. High resolution laser excitation and fluorescence spectra of the $A0^+$-$X^1\Sigma^+$ electronic transition were measured by Schaefer and coworkers [5]. An overview of the earlier literature of LiI was provided by Berry [6a] and Dyke [6b] in 1979.

In the infrared region, some LiI bandheads were measured by Klemperer *et al.* [7] and estimates of the vibrational constants were made. The high resolution infrared spectrum of the $\Delta v = 2$ transitions of ^{7}LiI was recorded by Thompson *et al.* [8] using a diode laser, and a total of 109 transitions was reported. The microwave and infrared diode laser data were used by Coxon and Hajigeorgiou [9] to determine an effective potential energy curve for the ground states of ^{7}LiI. However, this analysis was limited by the small number of overtone transitions available and the lack of infrared data for the minor ^{6}LiI isotopomer.

We report here our high resolution infrared emission spectrum of LiI recorded with a Bruker Fourier transform spectrometer. The infrared data were used to determine improved mass-dependent Dunham U_{lm} constants for the ground $X^1\Sigma^+$ electronic state. The mass-independent Dunham U_{lm} constants also were obtained along with Born–Oppenheimer breakdown constants. Finally, all of the data were fitted using the eigenvalues of the radial Schrödinger equation containing a modified Morse potential function to determine an effective ground state potential.

2. Experimental details

The high resolution infrared emission spectrum of lithium iodide was recorded with the Bruker IFS 120 HR Fourier transform spectrometer at the University of Waterloo. The $\Delta v = 1$ vibrational bands were recorded with a liquid helium cooled Si:B detector and a KBr beamsplitter at a resolution of $0{\cdot}005\,\mathrm{cm}^{-1}$. The spectral bandpass was limited to ~ 400-$760\,\mathrm{cm}^{-1}$ by a cold filter for the upper wavenumber limit and by the beamsplitter cutoff for the lower limit. The $\Delta v = 2$ vibrational bands were obtained with the same setup except that a bandpass filter was used which limited the spectra to the range 750-$1250\,\mathrm{cm}^{-1}$ and the resolution was $0{\cdot}01\,\mathrm{cm}^{-1}$.

The experimental setup was similar to that described earlier [10, 11]. Gas-phase lithium iodide molecules were produced in a tube furnace by gradually heating up

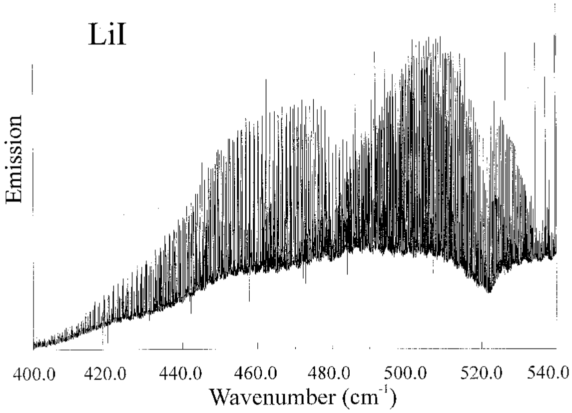

Figure 1. An overview of the $\Delta v = 1$ vibrational bands of LiI. The strong headband is the $v = 1 \rightarrow 0$ fundamental of ^{7}LiI.

lithium metal chips while I_2 vapour flowed into the system. The lithium metal pieces were contained in a carbon boat lying in the central part of a 1·2 m long and 5 cm diameter mullite tube which was sealed with a KBr window at each end. The tube was heated by a commercial furnace. The ends of the mullite tube were water cooled in order to prevent condensation on the windows. After the sample was loaded, the mullite tube was pumped and heated to about 150 °C overnight in order to remove residual water from inside the tube. About 10 Torr of argon gas was introduced into the tube before the temperature was increased. The 400- 750 cm^{-1} spectral region was monitored as the temperature was increased. When the temperature reached about 640°C, emission from LiI was noted. The temperature was then increased to 710°C, and the spectrum was taken with the coaddition of 100 scans. Figure 1 shows an overview of the fundamental and related hot bands of lithium iodide. The $\Delta v = 2$ bands were recorded at the same temperature with 60 scans coadded.

3. Results and discussion

The program 'PC-Decomp', developed by J. W. Brault, was used for the spectral line measurement. Using this program, the spectral line profiles were fitted using Voigt lineshape functions. The signal to noise ratio was as high as 30:1 for the unblended lines. Even with an abundance of 7·3%, ^{6}LiI yielded a good emission spectrum. The $\Delta v = 2$ bands, however, are much weaker and share the same spectral region as the much stronger CO_2 emission bands. The strong CO_2 lines were present also in the $\Delta v = 1$ band region, presumably as an impurity from the carbon liner. The measured spectral lines were calibrated with CO_2 line positions taken from the literature [12, 13]. The precision of the line position measurement is better than $\pm$0·0005 cm^{-1} for most of the strong and unblended lines. However, many of the weaker lines and the blended features were determined only to a lesser precision of about $\pm$0·001 cm^{-1}.

The vibrational bands LiI were identified and sorted using an interactive colour Loomis–Wood program. The rotational assignments were made by predicting the vibration–rotation line positions using the previous rotational and vibrational constants [3]. In total, 1915 vibration–rotational transitions were assigned to the two isotopomers and the transitions are listed in tables 1 (^{6}LiI) and 2 (^{7}LiI).

3.1. *Dunham model*

The line positions of each isotopomer were fitted to the Dunham energy level expression [14]

$$F(v, J) = \sum_{l,m} Y_{lm}(v + \tfrac{1}{2})^l [J(J+1)]^m. \qquad (1)$$

The pure rotational transitions [1–3] were included in the fit after correction for the effects of electric fields and hyperfine structure. The Dunham constants are listed in table 3 for each isotopomer, and depend on the isotopic masses, varying approximately with powers of the reduced mass ratio μ / μ^{i},

$$Y^{i}_{lm} = Y_{lm}\left(\frac{\mu}{\mu^{i}}\right)^{(\frac{l}{2}+m)}, \qquad (2)$$

where the i designates an isotopic species. All of the assigned infrared vibration–rotation transitions were fitted also to the mass-independent Dunham expression:

$$F(v, J) = \sum_{l,m} \mu^{-(\frac{l}{2}+m)} U_{lm}\left(1 + \frac{m_e}{M_{Li}}\Delta^{Li}_{lm}\right) \times (v + \tfrac{1}{2})^l [J(J+1)]^m, \qquad (3)$$

where m_e is the electron mass, M_{Li} is the Li atomic mass, and the Δ_{lm} are Born–Oppenheimer breakdown constants. Since only one naturally occurring isotope of iodine exists, all information on Born–Oppenheimer breakdown is confined to the lithium atom. Finally, a set of 'constrained' U_{lm} values was obtained from a fit where all U_{lm} for $m \leqslant 1$ were treated as independent parameters while all remaining U_{lm} were fixed to values determined from the constraint relations implicit in the Dunham model [10, 14]. The 'constrained' mass-independent Dunham coefficients and Born–Oppenheimer breakdown constants are listed in table 4.

3.2. *Parameterized potential model*

In order to estimate energies of high lying vibration–rotational levels of the ground state, a reliable internuclear potential energy function is required. Such a

Table 1. ^{6}LiI infrared transitions (in cm^{-1}).[a]

Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ
						(1, 0) Band								
P(65)	442·8520	-5	P(64)	444·4169	-8	P(63)	445·9726	-33	P(62)	447·5268	-6	P(59)	452·1392	-6
P(57)	455·1791	-1	P(56)	456·6883	2	P(55)	458·1897	-1	P(54)	459·6871	32	P(53)	461·1709	0
P(52)	462·6496	-7	P(51)	464·1222	0	P(50)	465·5865	-1	P(49)	467·0431	-2	P(48)	468·4921	-3
P(47)	469·9347	9	P(46)	471·3675	1	P(45)	472·7927	-5	P(44)	474·2109	-2	P(43)	475·6208	-2
P(42)	477·0234	4	P(41)	478·4170	0	P(40)	479·8026	-2	P(39)	481·1807	2	P(38)	482·5489	-12
P(37)	483·9115	2	P(36)	485·2642	-1	P(35)	486·6090	1	P(34)	487·9450	-1	P(33)	489·2731	2
P(32)	490·5921	0	P(31)	491·9029	1	P(30)	493·2048	-1	P(29)	494·4985	1	P(28)	495·7834	4
P(27)	497·0589	-1	P(25)	499·5885	41	P(24)	500·8338	0	P(23)	502·0756	14	P(21)	504·5281	0
P(20)	505·7414	1	P(19)	506·9454	0	P(18)	508·1402	0	P(17)	509·3268	10	P(15)	511·6686	-5
P(14)	512·8271	3	P(13)	513·9749	0	P(12)	515·1140	5	P(11)	516·2422	-4	P(10)	517·3623	2
P(9)	518·4714	-6	P(7)	520·6633	7	P(6)	521·7433	1	P(5)	522·8153	13	P(4)	523·8747	-3
P(3)	524·9261	0	R(3)	532·0019	-1	R(4)	532·9737	17	R(5)	533·9314	-4	R(6)	534·8814	2
R(7)	535·8210	8	R(8)	536·7489	2	R(9)	537·6667	0	R(10)	538·5743	1	R(11)	539·4711	0
R(12)	540·3580	6	R(13)	541·2330	0	R(14)	542·0977	-3	R(15)	542·9523	2	R(16)	543·7955	1
R(17)	544·6278	-1	R(18)	545·4496	0	R(19)	546·2604	1	R(20)	547·0603	2	R(21)	547·8487	-1
R(22)	548·6266	0	R(23)	549·3929	-3	R(24)	550·1487	1	R(25)	550·8932	2	R(26)	551·6261	0
R(27)	552·3480	0	R(28)	553·0586	-1	R(29)	553·7580	0	R(30)	554·4450	-10	R(31)	555·1225	-1
R(32)	555·7870	-7	R(33)	556·4413	0	R(34)	557·0835	0	R(35)	557·7150	9	R(36)	558·3332	1
R(37)	558·9404	-2	R(38)	559·5362	-1	R(39)	560·1206	2	R(40)	560·6928	0	R(41)	561·2532	-1
R(42)	561·8020	-1	R(43)	562·3385	-6	R(44)	562·8633	-8	R(45)	563·3771	-2	R(46)	463·8787	2
R(47)	564·3682	3	R(48)	564·8455	4	R(49)	565·3104	1	R(50)	565·7636	1	R(51)	566·2046	0
R(52)	566·6327	-8	R(53)	567·0509	6	R(54)	567·4547	-1	R(55)	567·8473	1	R(56)	568·2277	4
R(57)	568·5953	2	R(58)	568·9507	2	R(59)	569·2923	-13	R(60)	569·6249	5	R(61)	569·9447	20
R(62)	570·2488	2	R(63)	570·5416	-4	R(64)	570·8228	-1	R(65)	571·0918	5	R(66)	571·3471	0
R(67)	571·5902	-2	R(68)	571·8213	3	R(69)	572·0390	0	R(70)	572·2443	-1	R(72)	572·6163	-6
R(74)	572·9419	34	R(75)	573·0783	-18									
						(2, 1) Band								
P(63)	440·2661	5	P(60)	444·8524	-26	P(55)	452·3637	2	P(54)	453·8464	28	P(53)	455·3164	0
P(52)	456·7817	-1	P(51)	458·2397	-1	P(50)	459·6871	-31	P(49)	461·1312	-20	P(48)	462·5689	3
P(47)	463·9964	1	P(46)	465·4158	-5	P(45)	466·8286	0	P(44)	468·2326	-5	P(43)	469·6280	-16
P(42)	471·0183	0	P(41)	472·4004	14	P(40)	473·7696	-21	P(39)	475·1355	-8	P(38)	476·4907	-21
P(37)	477·8402	-9	P(36)	479·1812	-1	P(35)	480·5129	-2	P(34)	481·8381	15	P(33)	433·1519	2
P(32)	484·4584	0	P(31)	485·7597	30	P(30)	487·0465	2	P(29)	488·3273	-1	P(28)	489·5997	-1
P(27)	490·8649	12	P(26)	492·1187	0	P(25)	493·3650	1	P(24)	494·6025	2	P(23)	495·8309	0
P(22)	497·0502	-2	P(21)	498·2613	2	P(20)	499·4627	1	P(19)	500·6551	-1	P(18)	501·8389	3
P(17)	503·0131	3	P(15)	505·3350	16	P(14)	506·4798	0	P(13)	507·6168	-1	P(12)	508·7431	-13
P(11)	509·8627	2	P(9)	512·0698	-3	P(8)	513·1600	3	P(7)	514·2391	-3	P(6)	515·3077	-18
P(5)	516·3701	2	P(4)	517·4202	-2	R(3)	525·4683	15	R(4)	526·4278	5	R(5)	527·3780	6
R(6)	528·3172	-1	R(7)	529·2464	-4	R(8)	530·1661	2	R(9)	531·0745	-2	R(10)	531·9735	5
R(11)	532·8623	15	R(12)	533·7416	36	R(13)	534·6046	-1	R(14)	535·4603	-3	R(15)	536·3036	-24
R(16)	537·1407	1	R(17)	537·9643	-2	R(18)	538·7777	1	R(19)	539·5773	-26	R(20)	540·3714	2
R(21)	541·1516	-1	R(22)	541·9213	1	R(23)	542·6800	2	R(24)	543·4272	-1	R(25)	544·1637	1
R(26)	544·8889	-1	R(27)	545·6031	1	R(28)	546·3065	5	R(29)	546·9978	1	R(30)	547·6783	1
R(31)	548·3472	-1	R(32)	549·0048	-3	R(33)	549·6515	0	R(34)	550·2867	2	R(35)	550·9103	3
R(36)	551·5222	1	R(37)	552·1227	1	R(38)	552·7115	-1	R(39)	553·2885	-4	R(40)	553·8547	0
R(41)	554·4087	0	R(42)	554·9510	0	R(43)	555·4809	-7	R(44)	556·0003	-1	R(45)	556·5077	3
R(46)	557·0026	0	R(47)	557·4860	1	R(48)	557·9574	1	R(49)	558·4167	0	R(50)	558·8638	-4
R(51)	559·2997	1	R(52)	559·7232	1	R(53)	560·1344	1	R(54)	560·5338	2	R(55)	560·9207	0
R(56)	561·2958	1	R(57)	561·6582	-1	R(58)	562·0090	1	R(59)	562·3447	-24	R(60)	562·6736	4
R(61)	562·9864	-4	R(62)	563·2882	1	R(63)	563·5770	0	R(64)	563·8537	1	R(65)	564·1175	-2
R(66)	564·3682	-12	R(67)	564·6081	-4	R(68)	564·8355	3	R(69)	565·0494	1	R(70)	565·2503	-5
R(72)	565·6133	-28												
						(3, 2) Band								
P(58)	442·1681	31	P(57)	443·6526	2	P(56)	445·1334	5	P(55)	446·6041	-20	P(51)	452·4263	-3
P(49)	455·2922	-3	P(48)	456·7157	15	P(47)	458·1244	-39	P(46)	459·5345	-4	P(45)	460·9336	-1
P(44)	462·3246	-2	P(43)	463·7078	-3	P(42)	465·0838	2	P(41)	466·4512	0	P(40)	467·8132	24
P(39)	469·1625	1	P(38)	470·5066	6	P(37)	471·8416	0	P(36)	473·1629	-60	P(35)	474·4879	-1
P(34)	475·7992	4	P(33)	477·1061	47	P(32)	478·3960	3	P(31)	479·6813	-2	P(30)	480·9587	-1
P(29)	482·2272	-5	P(28)	483·4884	4	P(27)	484·7396	0	P(26)	485·9829	2	P(25)	487·2169	0
P(24)	488·4438	14	P(23)	489·6600	8	P(22)	490·8649	-22	P(21)	492·0659	-2	P(20)	493·2558	-3
P(19)	494·4371	1	P(17)	496·7709	-10	P(16)	497·9310	54	P(15)	499·0706	5	P(14)	500·2055	2
P(13)	501·3311	-3	P(11)	503·5528	-24	P(10)	504·6535	5	P(9)	505·7414	1	P(8)	506·8199	-2
P(7)	507·8902	8	P(6)	508·9489	0	P(5)	509·9993	4	P(3)	512·0698	3	R(2)	518·0462	14
R(3)	519·0093	36	R(5)	520·8965	-5	R(6)	521·8288	13	R(7)	522·7483	7	R(8)	523·6577	2

(*continued*)

Table 1. *Continued.*

Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ
R(9)	524·5566	-4	R(10)	525·4466	4	R(11)	526·3283	34	R(12)	527·1929	-3	R(13)	528·0509	-1
R(14)	528·8980	-2	R(15)	529·7352	4	R(16)	530·5605	-3	R(17)	531·3759	-3	R(18)	532·1807	-1
R(19)	532·9737	-9	R(20)	533·7577	0	R(21)	534·5299	-1	R(22)	535·2913	-1	R(23)	536·0418	0
R(24)	536·7810	-3	R(25)	537·5097	-2	R(26)	538·2273	-2	R(27)	538·9334	-4	R(28)	539·6296	4
R(29)	540·3131	-2	R(30)	540·9859	-4	R(31)	541·6480	-1	R(32)	542·2985	-2	R(33)	542·9379	0
R(34)	543·5657	-1	R(35)	544·1825	1	R(36)	544·7876	1	R(37)	545·3810	-2	R(38)	545·9635	1
R(39)	546·5339	-2	R(40)	547·0932	-1	R(41)	547·6409	0	R(42)	548·1767	-2	R(43)	548·7012	0
R(44)	549·2136	-1	R(45)	549·7140	-6	R(47)	550·6841	30	R(48)	551·1467	0	R(49)	551·6004	-1
R(50)	552·0420	-2	R(51)	552·4720	-2	R(52)	552·8896	-5	R(53)	553·2944	-17	R(54)	553·6899	-2
R(55)	554·0720	0	R(56)	554·4450	31	R(57)	554·7995	-2	R(58)	555·1449	-3	R(59)	555·4809	22
R(61)	556·1095	5	R(62)	556·4059	0	R(63)	556·6900	-4	R(64)	556·9624	-2	R(65)	557·2227	2
R(66)	557·4711	10	R(67)	557·7094	41	R(68)	557·9280	0	R(70)	558·3334	-27			
						(4, 3) Band								
P(54)	442·3687	-1	P(53)	443·8143	6	P(45)	455·1078	0	P(44)	456·4854	-3	P(42)	459·2167	-14
P(39)	463·2563	-18	P(38)	464·5890	1	P(37)	465·9128	11	P(36)	467·2259	-3	P(35)	468·5327	-1
P(34)	469·8305	-6	P(33)	471·1215	3	P(32)	472·4004	-27	P(31)	473·6767	1	P(30)	474·9420	3
P(29)	476·1946	-38	P(28)	477·4483	18	P(26)	479·9172	-1	P(25)	481·1395	-2	P(24)	482·3538	3
P(23)	483·5591	6	P(22)	484·7544	-3	P(21)	485·9419	-2	P(20)	487·1256	49	P(18)	489·4507	-1
P(17)	490·6021	-4	P(16)	491·7449	-1	P(15)	492·8786	2	P(14)	494·0029	3	P(13)	495·1171	-5
P(12)	496·2232	-1	P(11)	497·3230	32	R(2)	511·6686	22	R(3)	512·6153	-23	R(5)	514·4903	3
R(7)	516·3216	-3	R(8)	517·2235	10	R(9)	518·1128	-1	R(13)	521·5686	-26	R(14)	522·4093	-3
R(15)	523·2400	24	R(16)	524·0550	-1	R(17)	524·8618	-1	R(18)	525·6574	-8	R(19)	526·4435	-3
R(20)	527·2183	-4	R(21)	527·9830	2	R(22)	528·7357	-4	R(23)	529·4782	-4	R(24)	530·2103	0
R(25)	530·9307	-3	R(26)	531·6404	-4	R(27)	532·3392	-4	R(28)	533·0271	-3	R(29)	533·7014	-28
R(30)	534·3693	-4	R(31)	535·0235	-7	R(32)	535·6672	-4	R(33)	536·3036	38	R(34)	536·9207	1
R(35)	537·5304	2	R(36)	538·1283	-3	R(37)	538·7151	-3	R(38)	539·2903	-7	R(39)	539·8534	-18
R(40)	540·4073	-6	R(41)	540·9483	-7	R(42)	541·4782	-5	R(43)	541·9967	0	R(44)	542·5028	-5
R(45)	542·9971	-10	R(46)	543·4809	-5	R(47)	543·9529	0	R(48)	544·4125	-2	R(49)	544·8605	-2
R(50)	545·2984	14	R(51)	545·7213	-1	R(52)	546·1341	1	R(53)	546·5339	-8	R(54)	546·9231	-3
R(55)	547·2998	-5	R(56)	547·6655	4	R(57)	548·0172	-8	R(59)	548·6880	5	R(60)	549·0048	6
R(61)	549·3091	4	R(62)	549·6003	-8	R(64)	550·1487	-5						
						(5, 4) Band								
P(47)	446·6041	60	P(42)	453·4215	3	P(35)	462·6496	29	P(34)	463·9356	30	P(32)	466·4827	28
P(31)	467·7434	23	P(30)	468·9940	-1	P(28)	471·4758	10	P(27)	472·7020	-6	P(25)	475·1355	31
P(22)	478·7130	4	P(21)	479·8881	-4	P(19)	482·2139	1	P(18)	483·3552	-80	P(17)	484·5060	23
P(16)	485·6359	8	P(15)	486·7569	-6	P(14)	487·8711	4	P(13)	488·9722	-26	P(12)	490·0702	4
R(17)	518·4146	-67	R(18)	519·2043	-48	R(21)	521·5074	-18	R(22)	522·2547	1	R(23)	522·9892	0
R(24)	523·7125	-6	R(25)	524·4255	-6	R(26)	525·1287	5	R(28)	526·4997	-1	R(29)	527·1695	3
R(30)	527·8276	1	R(33)	529·7352	-9	R(34)	530·3500	-1	R(35)	530·9527	-2	R(36)	531·5440	-4
R(37)	532·1243	-4	R(38)	532·6936	0	R(39)	533·2501	-11	R(41)	534·3320	-4	R(42)	534·8556	-2
R(43)	535·3685	7	R(44)	535·8679	-3	R(45)	536·3564	-7	R(46)	536·8356	11	R(48)	537·7550	6
R(49)	538·1967	0	R(51)	539·0468	3	R(52)	539·4544	6	R(53)	539·8534	41	R(54)	540·2323	-7
R(55)	540·6039	-8	R(56)	540·9656	10	R(58)	541·6480	-6	R(59)	541·9720	-8			

[a] Observed - calculated differences (columns labelled δ) are in units of 0·0001 cm^{-1}.

potential function can be determined from a least squares fit [10] of the combined ^{7}LiI and ^{6}LiI data set to the eigenvalues of the radial Schrödinger equation:

$$\left(\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} - U^{\text{eff}}(R) + E(v,J) - \frac{\hbar^2}{2\mu}[1 + q(R)] \times \frac{J(J+1)}{R^2}\right)\psi(R,v,J) = 0, \quad (4)$$

where the effective internuclear potential for vibrational motion is given by

$$U^{\text{eff}}(R) = U^{\text{BO}}(R) + \frac{U_{\text{Li}}(R)}{M_{\text{Li}}}, \quad (5)$$

and the form of the Born–Oppenheimer potential is chosen to be

$$U^{\text{BO}}(R) = D_e\left[\frac{1 - e^{-\beta(R)}}{1 - e^{-\beta(\infty)}}\right]^2, \quad (6)$$

with

$$\beta(R) = z\sum_{i=0}\beta_i z^i, \quad (7)$$

$$\beta(\infty) = \sum_{i=0}\beta_i, \quad (8)$$

and

$$z = \frac{R - R_e}{R + R_e}. \quad (9)$$

Table 2. ^{7}LiI infrared transitions (in cm^{-1}).[a]

Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ
							(1, 0) Band							
P(78)	400·8613	12	P(77)	402·2570	11	P(75)	405·0319	-2	P(74)	406·4144	20	P(73)	407·7880	6
P(72)	409·1570	-1	P(71)	410·5216	2	P(70)	411·8803	0	P(69)	413·2338	1	P(68)	414·5819	2
P(67)	415·9239	-2	P(66)	417·2613	3	P(65)	418·5924	2	P(64)	419·9177	-1	P(63)	421·2376	-1
P(62)	422·5519	1	P(61)	423·8601	-1	P(60)	425·1627	0	P(59)	426·4594	-1	P(58)	427·7514	12
P(57)	429·0353	3	P(56)	430·3139	0	P(55)	431·5866	-1	P(54)	432·8534	-1	P(53)	434·1139	-2
P(52)	435·3690	4	P(51)	436·6170	1	P(50)	437·8589	-1	P(49)	439·0947	-2	P(48)	440·3244	-1
P(47)	441·5475	-1	P(46)	442·7643	-1	P(45)	443·9746	-1	P(43)	446·3749	-11	P(42)	447·5666	-3
P(41)	448·7507	-4	P(40)	449·9287	-1	P(39)	451·0996	-2	P(38)	452·2640	-1	P(37)	453·4216	-1
P(36)	454·5723	-2	P(35)	455·7163	-1	P(34)	456·8535	-1	P(32)	459·1069	-2	P(31)	460·2234	0
P(30)	461·3327	-1	P(29)	462·4339	-11	P(28)	463·5301	-1	P(27)	464·6175	-7	P(26)	465·6991	-2
P(25)	466·7728	-2	P(24)	467·8394	-1	P(23)	468·8986	-2	P(22)	469·9506	-1	P(21)	470·9955	2
P(20)	472·0325	-1	P(19)	473·0624	0	P(18)	474·0846	-2	P(17)	475·0998	1	P(16)	476·1069	-2
P(15)	477·1061	-7	P(14)	478·0989	-2	P(13)	479·0836	-1	P(12)	480·0605	-2	P(11)	481·0299	0
P(10)	481·9914	0	P(9)	482·9451	-1	P(8)	483·8910	-1	P(7)	484·8291	-1	P(6)	485·7597	2
P(5)	486·6817	-1	P(4)	487·5960	-1	P(3)	488·5025	0	P(2)	489·4007	-2	P(1)	490·2912	0
R(0)	492·0479	2	R(1)	492·9136	-1	R(2)	493·7715	-1	R(3)	494·6213	2	R(4)	495·4625	0
R(6)	497·1206	2	R(7)	497·9373	5	R(8)	498·7440	-9	R(9)	499·5443	-2	R(10)	500·3356	-1
R(11)	501·1183	-1	R(12)	501·8926	-1	R(13)	502·6583	-1	R(14)	503·4155	0	R(15)	504·1638	-2
R(16)	504·9039	0	R(17)	505·6350	-1	R(18)	506·3574	-2	R(19)	507·0713	-1	R(20)	507·7763	-1
R(21)	508·4725	-1	R(22)	509·1599	-2	R(23)	509·8386	-1	R(24)	510·5077	-7	R(25)	511·1691	-1
R(26)	511·8209	-2	R(27)	512·4645	6	R(28)	513·0980	2	R(29)	513·7225	-1	R(30)	514·3383	-2
R(31)	514·9450	-2	R(33)	516·1311	-1	R(34)	516·7104	-2	R(35)	517·2805	-1	R(36)	517·8414	-1
R(37)	518·3930	-2	R(38)	518·9353	-1	R(39)	519·4685	0	R(40)	519·9923	1	R(41)	520·5064	-1
R(42)	521·0113	-1	R(43)	521·5069	0	R(44)	521·9929	-1	R(46)	522·9366	-1	R(47)	523·3943	0
R(48)	523·8422	-1	R(49)	524·2806	-1	R(50)	524·7095	-1	R(51)	525·1287	-1	R(52)	525·5383	-1
R(54)	526·3283	-2	R(55)	526·7089	-1	R(56)	527·0797	0	R(57)	527·4406	0	R(58)	527·7917	-2
R(59)	528·1331	-1	R(60)	528·4647	0	R(61)	528·7863	0	R(62)	529·0981	0	R(63)	529·3999	0
R(64)	529·6917	0	R(65)	529·9737	0	R(66)	530·2457	0	R(67)	530·5077	0	R(68)	530·7595	-1
R(69)	531·0015	0	R(70)	531·2333	-1	R(71)	531·4551	-1	R(72)	531·6667	0	R(73)	531·8682	0
R(74)	532·0595	-1	R(75)	532·2408	-1	R(76)	532·4119	0	R(77)	532·5725	-2	R(78)	532·7230	-2
R(79)	532·8623	-14	R(80)	532·9934	-3	R(81)	533·1134	-2	R(82)	533·2231	1	R(83)	533·3222	0
R(84)	533·4113	2	R(85)	533·4898	2	R(86)	533·5581	3	R(87)	533·6159	4	R(88)	533·6629	1
R(89)	533·7014	16	R(90)	533·7266	4	R(91)	533·7416	-6						
							(2, 1) Band							
P(74)	401·5492	9	P(72)	404·2673	-14	P(71)	405·6216	7	P(70)	406·9685	6	P(69)	408·3089	-4
P(68)	409·6457	3	P(67)	410·9761	1	P(66)	412·3013	3	P(65)	413·6207	1	P(64)	414·9345	1
P(63)	416·2428	2	P(62)	417·5451	-1	P(61)	418·8422	1	P(60)	420·1330	-1	P(59)	421·4180	-4
P(58)	422·6978	0	P(57)	423·9715	1	P(56)	425·2388	-1	P(55)	426·5004	-1	P(53)	429·0057	0
P(52)	430·2491	0	P(51)	431·4866	1	P(50)	432·7177	1	P(49)	433·9427	1	P(48)	435·1604	-9
P(47)	436·3736	0	P(46)	437·5797	0	P(45)	438·7794	0	P(44)	439·9727	0	P(43)	441·1596	1
P(42)	442·3398	0	P(41)	443·5136	0	P(40)	444·6809	-1	P(39)	445·8416	0	P(38)	446·9956	0
P(37)	448·1429	-1	P(36)	449·2829	-7	P(35)	450·4173	0	P(34)	451·5444	0	P(33)	452·6646	-1
P(32)	453·7779	0	P(31)	454·8843	-1	P(30)	455·9837	-2	P(29)	457·0745	-19	P(28)	458·1618	-1
P(27)	459·2402	0	P(26)	460·3114	-2	P(25)	461·3756	-2	P(23)	463·4825	-1	P(22)	464·5251	0
P(21)	465·5615	10	P(20)	466·5884	0	P(19)	467·6088	-2	P(18)	468·6227	4	P(17)	469·6280	0
P(16)	470·6257	-6	P(15)	471·6171	-1	P(13)	473·5758	-4	P(12)	474·5443	0	P(11)	475·5046	-2
P(10)	476·4576	-1	P(9)	477·4026	-1	P(8)	478·3401	0	P(7)	479·2695	-2	P(6)	480·1916	2
P(5)	481·1055	1	P(4)	482·0115	1	P(3)	482·9092	-2	P(2)	483·7995	-1	P(1)	484·6820	2
R(0)	486·4216	-4	R(1)	487·2800	0	R(2)	488·1300	0	R(3)	488·9722	5	R(4)	489·8052	-1
R(6)	491·4475	-2	R(7)	492·2567	2	R(8)	493·0572	2	R(9)	493·8491	0	R(10)	494·6332	4
R(11)	495·4081	-1	R(12)	496·1758	7	R(13)	496·9335	0	R(14)	497·6833	-2	R(15)	498·4251	2
R(16)	499·1578	2	R(17)	499·8818	0	R(18)	500·5973	-1	R(19)	501·3043	0	R(20)	502·0025	0
R(21)	502·6921	1	R(22)	503·3727	0	R(23)	504·0446	-1	R(24)	504·7077	-1	R(25)	505·3620	0
R(26)	506·0074	-1	R(27)	506·6416	-24	R(28)	507·2711	-4	R(29)	507·8902	0	R(30)	508·4998	0
R(31)	509·1003	-1	R(32)	509·6904	-15	R(33)	510·2743	-1	R(34)	510·8477	-1	R(35)	511·4119	-1
R(36)	511·9670	-1	R(37)	512·5129	-1	R(38)	513·0495	-1	R(39)	513·5770	-1	R(40)	514·0953	1
R(41)	514·6039	-2	R(42)	515·1040	5	R(43)	515·5938	0	R(44)	516·0745	-1	R(45)	516·5443	-16
R(46)	517·0079	0	R(47)	517·4608	4	R(48)	517·9034	-1	R(49)	518·3370	0	R(50)	518·7611	1
R(51)	519·1753	-1	R(52)	519·5803	1	R(53)	519·9757	1	R(54)	520·3610	-1	R(55)	520·7371	0
R(56)	521·1033	-1	R(57)	521·4603	3	R(58)	521·8070	1	R(59)	522·1441	1	R(60)	522·4700	-13
R(61)	522·7889	0	R(62)	523·0967	1	R(64)	523·6826	0	R(65)	523·9607	0	R(66)	524·2290	0
R(67)	524·4874	1	R(68)	524·7356	0	R(69)	524·9739	0	R(70)	525·2024	0	R(71)	525·4208	0
R(72)	525·6292	0	R(73)	525·8271	-3	R(74)	526·0156	-1	R(75)	526·1939	0	R(76)	526·3618	-1
R(77)	526·5199	1	R(78)	526·6677	1	R(79)	526·8050	-2	R(80)	526·9324	-1	R(81)	527·0497	0
R(82)	527·1567	0	R(83)	527·2537	3	R(84)	527·3397	-1	R(85)	527·4160	0	R(86)	527·4818	-2
R(87)	527·5373	-3	R(88)	527·5826	-2	R(89)	527·6173	-5	R(90)	527·6401	-23	R(91)	527·6562	-3

(*continued*)

Table 2. *Continued*

Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ
							(3, 2) Band							
P(71)	400·7765	16	P(70)	402·1091	-8	P(69)	403·4400	5	P(68)	404·7635	-3	P(67)	406·0826	0
P(66)	407·3957	-2	P(65)	408·7038	1	P(64)	410·0059	-1	P(63)	411·3019	-8	P(62)	412·5934	-3
P(61)	413·8789	-3	P(60)	415·1585	-3	P(59)	416·4311	-16	P(58)	417·7008	0	P(57)	418·9637	6
P(56)	420·2197	2	P(55)	421·4701	1	P(54)	422·7143	-1	P(53)	423·9528	-2	P(52)	425·1852	-2
P(51)	426·4120	1	P(50)	427·6322	0	P(49)	428·8463	0	P(48)	430·0541	-1	P(47)	431·2559	0
P(46)	432·4512	-1	P(45)	433·6404	0	P(44)	434·8231	0	P(43)	435·9994	0	P(42)	437·1695	1
P(41)	438·3327	-1	P(40)	439·4897	0	P(39)	440·6400	-1	P(38)	441·7839	0	P(37)	442·9209	-1
P(36)	444·0515	-1	P(35)	445·1769	16	P(34)	446·2924	0	P(33)	447·4026	0	P(32)	448·5060	-1
P(31)	449·6021	-6	P(30)	450·6923	0	P(29)	451·7752	1	P(28)	452·8509	-1	P(27)	453·9197	-1
P(26)	454·9814	-2	P(25)	456·0361	-1	P(24)	457·0817	-21	P(23)	458·1244	2	P(22)	459·1574	0
P(21)	460·1836	1	P(20)	461·2021	-1	P(19)	462·2137	1	P(18)	463·2178	0	P(17)	464·2144	-1
P(16)	465·2039	1	P(15)	466·1857	-1	P(14)	467·1602	0	P(13)	468·1270	-1	P(12)	469·0865	0
P(11)	470·0382	-1	P(10)	470·9823	-2	P(9)	471·9189	0	P(8)	472·8476	-1	P(7)	473·7696	7
P(6)	474·6826	4	P(5)	475·5877	-1	P(4)	476·4837	-18	P(3)	477·3758	4	P(2)	478·2570	-4
P(1)	479·1319	4	R(1)	481·7055	-2	R(2)	482·5489	11	R(3)	483·3821	4	R(4)	484·2074	-1
R(5)	485·0266	14	R(6)	485·8350	3	R(7)	486·6359	0	R(8)	487·4289	0	R(9)	488·2136	1
R(10)	488·9900	1	R(11)	489·7578	-1	R(12)	490·5174	-1	R(13)	491·2687	0	R(14)	492·0115	0
R(15)	492·7456	-2	R(16)	493·4701	-15	R(17)	494·1889	1	R(18)	494·8974	-1	R(19)	495·5977	1
R(20)	496·2909	19	R(21)	496·9717	-1	R(22)	497·6458	0	R(23)	498·3109	-3	R(24)	498·9677	-2
R(25)	499·6156	-1	R(26)	500·2545	-2	R(27)	500·8852	4	R(28)	501·5062	0	R(29)	502·1183	-2
R(30)	502·7220	-1	R(31)	503·3159	-7	R(32)	503·9023	2	R(33)	504·4786	-1	R(34)	505·0460	-1
R(35)	505·6045	0	R(36)	506·1538	-2	R(37)	506·6940	-1	R(38)	507·2251	-1	R(39)	507·7470	0
R(40)	508·2598	1	R(41)	508·7631	0	R(42)	509·2573	0	R(43)	509·7422	0	R(44)	510·2178	-1
R(45)	510·6842	1	R(46)	511·1410	0	R(57)	511·5885	0	R(48)	512·0265	-1	R(49)	512·4554	1
R(50)	512·8747	2	R(51)	513·2840	-1	R(52)	513·6843	-1	R(53)	514·0751	1	R(54)	514·4554	-7
R(55)	514·8275	-1	R(56)	515·1895	0	R(57)	515·5425	7	R(58)	515·8844	0	R(59)	516·2174	1
R(61)	516·8541	0	R(62)	517·1578	0	R(63)	517·4523	4	R(64)	517·7361	0	R(65)	518·0104	-1
R(66)	518·2750	0	R(67)	518·5297	0	R(68)	518·7749	3	R(69)	519·0093	-3	R(70)	519·2344	-1
R(71)	519·4498	2	R(72)	519·6549	1	R(73)	519·8500	2	R(74)	520·0350	-1	R(75)	520·2102	0
R(77)	520·5305	2	R(78)	520·6750	-3	R(79)	520·8099	-2	R(80)	520·9350	1	R(81)	521·0496	1
R(82)	531·1538	-2	R(83)	521·2483	0	R(84)	521·3323	-1	R(85)	521·4062	-1	R(88)	521·5686	18
R(89)	521·5998	1												
							(4, 3) Band							
P(62)	407·6964	-4	P(61)	408·9711	3	P(60)	410·2398	6	P(59)	411·5018	0	P(58)	412·7582	-5
P(57)	414·0109	11	P(56)	415·2552	2	P(55)	416·4942	-3	P(54)	417·7273	-7	P(53)	418·9562	7
P(52)	420·1770	-1	P(51)	421·3924	-2	P(50)	422·6021	0	P(49)	423·8055	0	P(48)	425·0025	-2
P(47)	426·1937	0	P(46)	427·3786	0	P(45)	428·5571	0	P(44)	429·7295	1	P(43)	430·8953	0
P(42)	432·0547	-1	P(41)	433·2069	-11	P(40)	434·3543	-3	P(39)	435·4945	-2	P(38)	436·6288	4
P(37)	437·7555	1	P(36)	438·8758	-1	P(35)	439·9896	-1	P(34)	441·0966	-2	P(33)	442·1971	-1
P(32)	443·2907	-1	P(31)	444·3777	1	P(30)	445·4575	-1	P(29)	446·5307	0	P(28)	447·5969	0
P(27)	448·6561	-1	P(26)	449·7085	0	P(25)	450·7536	-1	P(24)	451·7920	0	P(23)	452·8230	0
P(22)	453·8464	-6	P(21)	454·8639	1	P(20)	455·8732	-2	P(19)	456·8772	15	P(18)	457·8706	-2
P(17)	458·8584	-2	P(16)	459·8387	-3	P(15)	460·8118	-3	P(14)	461·7776	0	P(13)	462·7357	-1
P(12)	463·6863	-1	P(11)	464·6277	-19	P(9)	466·4936	3	P(8)	467·4135	0	P(7)	468·3261	-2
P(6)	469·2312	-1	P(5)	470·1275	-10	P(4)	471·0183	2	P(3)	471·9007	9	P(2)	472·7737	0
R(2)	477·0234	-10	R(3)	477·8497	-9	R(4)	478·6682	-5	R(5)	479·4789	2	R(6)	480·2804	-2
R(7)	481·0743	0	R(8)	481·8598	0	R(9)	482·6370	-1	R(10)	483·4060	-1	R(11)	484·1668	0
R(12)	484·9191	-2	R(13)	485·6632	-1	R(14)	486·3990	0	R(15)	487·1256	-7	R(16)	487·8446	-5
R(17)	488·5557	2	R(18)	489·2574	1	R(19)	489·9507	1	R(20)	490·6345	-8	R(21)	491·3114	0
R(22)	491·9789	0	R(23)	492·6376	-2	R(24)	493·2878	-1	R(25)	493·9292	-1	R(26)	494·5622	2
R(27)	495·1862	3	R(28)	495·8010	0	R(29)	496·4073	0	R(30)	497·0046	-1	R(31)	497·5931	-1
R(32)	498·1727	-1	R(34)	499·3050	-2	R(35)	499·8577	-1	R(36)	500·4012	-2	R(37)	500·9359	-2
R(38)	501·4614	-1	R(39)	501·9779	0	R(40)	502·4851	-1	R(41)	502·9831	-1	R(42)	503·4720	-2
R(43)	503·9515	-3	R(44)	504·4221	-1	R(45)	504·8835	0	R(46)	505·3350	-3	R(47)	505·7777	-1
R(48)	506·2109	-1	R(50)	507·0494	0	R(51)	507·4542	-1	R(52)	507·8499	-1	R(53)	508·2361	0
R(54)	508·6126	-1	R(55)	508·9797	-1	R(56)	509·3376	2	R(58)	510·0237	-1	R(59)	510·3525	-1
R(60)	510·6720	2	R(61)	510·9804	-9	R(62)	511·2810	-2	R(63)	511·5715	1	R(64)	511·8518	0
R(65)	512·1224	-1	R(66)	512·3834	0	R(67)	512·6344	-2	R(70)	513·3291	0	R(71)	513·5410	0
R(72)	513·7428	0	R(73)	513·9350	1	R(74)	514·1170	0	R(75)	514·2898	7	R(78)	514·7452	-6
R(79)	514·8781	1	R(80)	515·0003	1	R(81)	515·1140	18	R(82)	515·2146	4	R(83)	515·3077	15
R(84)	515·3883	2	R(85)	515·4603	5	R(86)	515·5246	33	R(87)	515·5752	24			
							(5, 4) Band							
P(58)	407·8712	4	P(57)	409·1109	1	P(56)	410·3447	-3	P(55)	411·5737	2	P(54)	412·7956	-4
P(52)	415·2237	3	P(50)	417·6270	2	P(49)	418·8196	0	P(48)	420·0067	6	P(47)	421·1866	0
P(46)	422·3607	-2	P(45)	423·5283	-8	P(44)	424·6906	-3	P(43)	425·8458	-6	P(42)	426·9959	2

Table 2. *Continued*

Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ
P(41)	428·1381	-4	P(40)	429·2751	1	P(39)	430·4049	-1	P(38)	431·5283	-2	P(37)	432·6455	0
P(36)	433·7562	2	P(35)	434·8598	-1	P(34)	435·9570	-1	P(33)	437·0476	-1	P(32)	438·1311	-4
P(31)	439·2087	0	P(30)	440·2789	-2	P(29)	441·3425	0	P(28)	442·3990	-2	P(27)	443·4491	1
P(26)	444·4917	-2	P(25)	445·5277	0	P(24)	446·5566	0	P(23)	447·5785	1	P(22)	448·5931	-1
P(20)	450·6016	3	P(19)	451·5945	-1	P(18)	452·5808	0	P(17)	453·5595	-1	P(16)	454·5314	2
P(15)	455·4989	35	P(14)	456·4522	0	P(13)	457·4017	-1	P(12)	458·3438	0	P(11)	459·2789	6
P(10)	460·2055	1	P(9)	461·1230	-19	P(8)	462·0368	-1	P(7)	462·9414	2	P(6)	463·8383	3
P(5)	464·7272	2	P(4)	465·6081	-3	P(3)	466·4827	7	P(2)	467·3478	0	R(0)	469·8996	13
R(2)	471·5608	16	R(3)	472·3802	26	R(4)	473·1863	-17	R(5)	473·9904	-2	R(6)	474·7847	-2
R(7)	475·5714	2	R(8)	476·3472	-21	R(10)	477·8810	1	R(11)	478·6345	0	R(12)	479·3796	-2
R(13)	480·1165	-3	R(14)	480·8458	4	R(15)	481·5657	0	R(16)	482·2781	5	R(17)	482·9797	-15
R(18)	483·6761	-1	R(19)	484·3622	-6	R(20)	485·0410	2	R(21)	485·7103	-1	R(22)	486·3713	0
R(23)	487·0237	0	R(24)	487·6673	-2	R(25)	488·3025	0	R(26)	488·9286	-4	R(27)	489·5465	-1
R(28)	490·1554	-2	R(29)	490·7557	-1	R(30)	491·3471	-1	R(31)	491·9296	-1	R(32)	492·5033	-1
R(33)	493·0686	3	R(34)	493·6240	-2	R(35)	494·1712	1	R(36)	494·7090	-1	R(37)	495·2379	-3
R(38)	495·7582	0	R(39)	496·2691	0	R(40)	496·7709	-1	R(41)	497·2636	-2	R(42)	497·7473	-1
R(43)	498·2218	-1	R(44)	498·6872	0	R(45)	499·1435	1	R(46)	499·5885	-18	R(47)	500·0278	-1
R(48)	500·4561	-2	R(49)	500·8758	4	R(50)	501·2851	0	R(51)	501·6853	-3	R(52)	502·0756	-9
R(53)	502·4578	-4	R(54)	502·8302	-1	R(55)	503·1935	3	R(56)	503·5460	-4	R(57)	503·8907	5
R(58)	504·2243	-2	R(59)	504·5491	-1	R(60)	504·8645	1	R(61)	505·1699	-1	R(62)	505·4661	1
R(63)	505·7524	1	R(64)	506·0291	0	R(65)	506·2965	4	R(66)	506·5534	-1	R(67)	506·8013	2
R(68)	507·0388	-2	R(70)	507·4854	-1	R(71)	507·6939	-3	R(73)	508·0819	0	R(75)	508·4302	-1
R(76)	508·5896	1	R(77)	508·7431	41	R(78)	508·8789	4	R(79)	509·0082	1	R(80)	509·1284	7
R(81)	509·2407	34												
							(6, 5) Band							
P(54)	407·9176	-4	P(53)	409·1230	-8	P(52)	410·3234	-3	P(51)	411·5176	-1	P(50)	412·7066	8
P(49)	413·8873	-6	P(48)	415·0642	3	P(47)	416·2339	-1	P(46)	417·3982	4	P(45)	418·5552	-2
P(44)	419·7067	-2	P(43)	420·8543	21	P(42)	421·9916	4	P(41)	423·1258	19	P(40)	424·2504	2
P(39)	425·3702	0	P(38)	426·4838	1	P(37)	427·5912	4	P(36)	428·6909	-4	P(35)	429·7860	7
P(34)	430·8728	1	P(33)	431·9536	0	P(32)	433·0278	1	P(31)	434·0954	2	P(29)	436·2099	0
P(28)	437·2573	1	P(27)	438·2977	2	P(26)	439·3313	3	P(25)	440·3580	4	P(24)	441·3773	1
P(23)	442·3903	5	P(22)	443·3954	-1	P(21)	444·3945	5	P(20)	445·3853	-2	P(18)	447·3474	4
P(17)	448·3171	1	P(15)	450·2353	1	P(14)	451·1836	2	P(13)	452·1245	2	P(12)	453·0575	-2
P(11)	453·9840	2	P(10)	454·8995	-29	P(9)	455·8141	6	P(8)	456·7157	-14	P(7)	457·6132	0
P(6)	458·5034	17	P(4)	460·2548	-10	R(2)	466·1526	12	R(3)	466·9628	5	R(4)	467·7650	-2
R(5)	468·5601	0	R(6)	469·3473	2	R(8)	470·8978	11	R(9)	471·6597	3	R(10)	472·4144	5
R(11)	473·1629	26	R(12)	473·8991	6	R(13)	474·6285	1	R(15)	476·0638	3	R(16)	476·7693	7
R(17)	477·4659	6	R(18)	478·1532	-4	R(19)	478·8329	-6	R(20)	479·5038	-12	R(21)	480·1682	3
R(22)	480·8225	0	R(23)	481·4685	1	R(24)	482·1059	1	R(25)	482·7345	-1	R(26)	483·3552	4
R(27)	483·9652	-12	R(28)	484·5692	0	R(29)	485·1634	0	R(30)	485·7505	18	R(31)	486·3254	0
R(32)	486·8933	0	R(33)	487·4524	1	R(34)	488·0026	1	R(35)	488·5442	4	R(36)	489·0763	0
R(37)	489·5997	-1	R(38)	490·1143	-1	R(39)	490·6230	30	R(40)	491·1164	-1	R(41)	491·6058	18
R(42)	492·0827	2	R(43)	492·5520	1	R(44)	493·0122	1	R(46)	493·9055	2	R(47)	494·3381	0
R(48)	494·7617	0	R(49)	495·1766	6	R(50)	495·5811	0	R(51)	495·9777	7	R(52)	496·3636	2
R(53)	496·7401	-5	R(54)	497·1091	7	R(55)	497·4670	0	R(56)	497·8160	0	R(57)	498·1561	4
R(58)	498·4861	3	R(59)	498·8066	1	R(60)	499·1181	4	R(61)	499·4193	-2	R(62)	499·7117	1
R(63)	499·9944	1	R(65)	500·5310	2	R(66)	500·7847	2	R(67)	501·0288	1	R(68)	501·2633	0
R(69)	501·4905	24	R(75)	502·6331	3	R(76)	502·7897	4	R(77)	502·9321	-40	R(78)	503·0729	0
							(7, 6) Band							
P(47)	411·3343	-8	P(46)	412·4873	-12	P(45)	413·6351	-8	P(44)	414·7756	-15	P(43)	415·9116	-5
P(41)	418·1629	-7	P(38)	421·4914	-19	P(37)	422·5905	1	P(36)	423·6804	-8	P(35)	424·7644	-9
P(33)	426·9127	-15	P(32)	427·9775	-12	P(30)	430·0877	-2	P(29)	431·1317	-7	P(28)	432·1693	-9
P(26)	434·2247	-7	P(25)	435·2412	-15	P(24)	436·2528	-3	P(23)	437·2558	-9	P(22)	438·2525	-7
P(21)	439·2421	-6	P(20)	440·2241	-11	P(19)	441·1989	-17	P(18)	442·1665	-24	P(17)	443·1292	-10
P(16)	444·0830	-12	P(15)	445·0300	-10	P(14)	445·9711	5	P(13)	446·9023	-5	P(12)	447·8257	-20
P(10)	449·6542	-14	P(7)	452·3369	-47	R(5)	463·1858	-10	R(6)	463·9647	-17	R(7)	464·7362	-17
R(8)	465·5009	-5	R(9)	466·2561	-8	R(10)	467·0032	-10	R(11)	467·7418	-18	R(12)	468·4740	-7
R(13)	469·1959	-18	R(14)	469·9117	-7	R(16)	471·3159	-14	R(17)	472·0093	20	R(18)	472·6875	-14
R(19)	473·3606	-16	R(20)	474·0256	-16	R(21)	474·6809	-27	R(22)	475·3311	-6	R(23)	475·9701	-13
R(24)	476·6012	-13	R(25)	477·2238	-12	R(26)	477·8386	-5	R(27)	478·4431	-14	R(28)	479·0399	-14
R(29)	479·6285	-9	R(30)	480·2078	-11	R(31)	480·7783	-14	R(32)	481·3404	-15	R(33)	481·8939	-13
R(34)	482·4385	-12	R(35)	482·9780	25	R(36)	483·5010	-13	R(37)	484·0190	-14	R(38)	484·5281	-14
R(40)	485·5197	-14	R(41)	486·0022	-12	R(42)	486·4755	-13	R(43)	486·9397	-14	R(44)	487·3951	-13
R(45)	487·8429	3	R(46)	488·2814	16	R(47)	488·7063	-15	R(48)	489·1253	-13	R(49)	489·5347	-16

(*continued*)

Table 2. *Continued*

Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ
R(51)	490·3270	−11	R(52)	490·7087	−15	R(53)	491·0816	−13	R(54)	491·4458	−7	R(55)	491·7993	−14
R(56)	492·1443	−12	R(57)	492·4799	−11	R(58)	492·8062	−10	R(59)	493·1225	−14	R(60)	493·4300	−13
R(61)	493·7278	−13	R(62)	494·0160	−15	R(63)	494·2952	−12	R(65)	494·8244	−13	R(66)	495·0747	−14
R(67)	495·3153	−15	R(68)	495·5470	−10	R(73)	496·5586	−8	R(75)	496·8949	−13			
							(8, 7) Band							
P(41)	413·2563	−6	P(37)	417·6442	1	P(36)	418·7251	1	P(31)	424·0318	−6	P(30)	425·0746	4
P(24)	431·1837	−1	P(23)	432·1795	12	P(21)	434·1447	−16	P(20)	435·1216	17	P(19)	436·0862	−4
P(17)	437·9979	−6	P(16)	438·9421	−17	P(15)	439·8840	20	P(14)	440·8130	0	R(12)	463·1098	19
R(13)	463·8246	7	R(15)	465·2308	−8	R(16)	465·9234	3	R(18)	467·2810	−6	R(19)	467·9479	−4
R(21)	469·2565	−3	R(22)	469·8979	−6	R(23)	470·5315	−3	R(24)	471·1562	−5	R(25)	471·7722	−8
R(26)	472·3785	−24	R(27)	472·9789	−15	R(28)	473·5741	29	R(29)	474·1533	−1	R(30)	474·7265	−6
R(31)	475·2918	−3	R(32)	475·8479	−6	R(33)	476·3966	5	R(34)	476·9342	−9	R(35)	477·4642	−11
R(36)	477·9860	−7	R(37)	478·4986	−7	R(38)	479·0027	−5	R(40)	479·9839	−3	R(41)	480·4602	−12
R(42)	480·9293	−4	R(43)	481·3882	−9	R(44)	481·8364	−29	R(46)	482·7126	−4	R(47)	483·1360	−2
R(48)	483·5504	−1	R(51)	484·7379	−4	R(52)	485·1156	−4	R(53)	485·4837	−7	R(55)	486·1938	1
R(56)	486·5334	−10	R(57)	486·8655	−4	R(58)	487·1863	−16	R(59)	487·5006	−1	R(60)	487·8038	−4
R(61)	488·0983	−1	R(62)	488·3817	−13	R(63)	488·6573	−10	R(64)	488·9268	27	R(65)	489·1798	−7
R(66)	489·4275	1	R(68)	489·8936	9	R(69)	490·1126	15	R(70)	490·3209	10	R(71)	490·5157	−34
R(72)	490·7087	0												
							(2, 0) Band							
P(65)	887·4996	−25	P(62)	892·9639	−17	P(57)	901·8008	11	P(56)	903·5280	27	P(52)	910·2881	−5
P(51)	911·9464	19	P(50)	913·5860	−2	P(49)	915·2147	9	P(48)	916·8269	−3	P(47)	918·4256	−7
P(45)	921·5836	18	P(44)	923·1389	9	P(43)	924·6794	−3	P(42)	926·2085	14	P(41)	927·7225	26
P(40)	929·2185	4	P(39)	930·7021	4	P(38)	932·1704	−3	P(37)	933·6280	30	P(35)	936·4912	18
P(33)	939·2976	31	P(32)	940·6748	2	P(30)	943·3911	9	P(29)	944·7268	14	P(28)	946·0468	12
P(27)	947·3498	−8	P(26)	948·6407	2	P(25)	949·9176	24	P(24)	951·1761	14	P(23)	952·4198	9
P(22)	953·6508	31	P(21)	954·8628	16	P(19)	957·2425	5	P(18)	958·4110	18	P(16)	960·6979	9
P(15)	961·8106	−69	P(12)	965·0932	80	P(11)	966·1426	−4	P(8)	969·2255	40	P(5)	972·1646	74
R(9)	984·6506	−70	R(11)	986·0456	−9	R(12)	986·7172	12	R(13)	987·3713	22	R(15)	988·6272	20
R(16)	989·2287	4	R(17)	989·8153	6	R(18)	990·3859	15	R(19)	990·9372	−1	R(20)	991·4745	10
R(21)	991·9935	7	R(22)	992·4997	44	R(23)	992·9800	−9	R(24)	993·4503	7	R(25)	993·9033	18
R(26)	994·3362	−2	R(27)	994·7531	−12	R(28)	995·1554	1	R(29)	995·5395	3	R(30)	995·9063	3
R(31)	996·2560	1	R(32)	996·5904	18	R(33)	996·9061	18	R(34)	997·2027	0	R(35)	997·4851	11
R(36)	997·7472	−9	R(37)	997·9980	29	R(38)	998·2240	−7	R(39)	998·4380	9	R(40)	998·6336	13
R(41)	998·8104	1	R(42)	998·9725	17	R(43)	999·1118	−22	R(44)	999·2394	−4	R(45)	999·3509	25
R(46)	999·4415	20	R(47)	999·5145	14	R(48)	999·5702	7	R(49)	999·6129	47			
							(3, 1) Band							
P(62)	882·5135	−5	P(61)	884·2949	19	P(58)	889·5500	15	P(57)	891·2750	18	P(56)	892·9894	53
P(55)	894·6821	7	P(53)	898·0353	9	P(52)	899·6902	1	P(51)	901·3291	−27	P(50)	902·9594	−2
P(49)	904·5730	−3	P(48)	906·1744	13	P(46)	909·3325	25	P(45)	910·8890	18	P(44)	912·4290	−12
P(43)	913·9593	5	P(42)	915·4738	7	P(41)	916·9733	3	P(40)	918·4573	−11	P(39)	919·9282	−12
P(38)	921·3933	75	P(37)	922·8283	7	P(36)	924·2558	9	P(35)	925·6684	10	P(34)	927·0654	0
P(33)	928·4506	22	P(32)	929·8178	10	P(31)	931·1757	44	P(30)	932·5107	18	P(29)	933·8334	8
P(28)	935·1421	7	P(27)	936·4344	−8	P(26)	937·7147	8	P(25)	938·9768	−7	P(24)	940·2279	19
P(23)	941·4603	9	P(22)	942·6786	11	P(21)	943·8794	−10	P(20)	945·0689	8	P(19)	946·2426	22
P(18)	947·4035	61	P(17)	948·5392	2	P(16)	949·6663	12	P(15)	950·7774	17	P(14)	951·8726	17
P(13)	952·9507	3	P(12)	954·0077	−67	P(11)	955·0641	13	P(10)	956·0960	5	P(9)	957·1146	20
P(5)	961·0162	−68	R(3)	968·8921	27	R(5)	970·4632	29	R(7)	971·9683	20	R(8)	972·6957	8
R(9)	973·4051	−20	R(10)	974·1043	13	R(11)	974·7844	19	R(12)	975·4470	15	R(13)	976·0935	14
R(14)	976·7225	4	R(15)	977·3378	20	R(16)	977·9331	3	R(17)	978·5134	2	R(18)	979·0786	14
R(19)	979·6261	18	R(20)	980·1574	25	R(21)	980·6682	−6	R(22)	981·1661	1	R(23)	981·6466	2
R(24)	982·1115	15	R(25)	982·5589	20	R(26)	982·9875	5	R(27)	983·4017	15	R(28)	983·7970	4
R(29)	984·1780	20	R(30)	984·5404	18	R(31)	984·8844	2	R(32)	985·2137	9	R(33)	985·5243	−2
R(34)	985·8190	−2	R(35)	986·0971	4	R(36)	986·3568	−5	R(37)	986·6005	−2	R(38)	986·8287	16
R(39)	987·0386	23	R(40)	987·2289	5	R(41)	987·4043	10	R(42)	987·5629	19	R(43)	987·7018	2
R(44)	987·8257	8	R(45)	987·9322	12	R(46)	988·0185	−12	R(47)	988·0918	5	R(48)	988·1455	0
R(49)	988·1861	37												
							(4, 2) Band							
P(63)	870·3989	2	P(59)	877·4289	18	P(56)	882·5559	−10	P(54)	885·9095	8	P(53)	887·5640	−1
P(52)	889·2069	11	P(50)	892·4471	−4	P(48)	895·6340	5	P(47)	897·2045	−11	P(46)	898·7650	14
P(45)	900·3082	7	P(44)	901·8416	44	P(43)	903·3537	9	P(42)	904·8559	18	P(41)	906·3422	10
P(40)	907·8110	−28	P(39)	909·2732	10	P(37)	912·1459	3	P(36)	913·5622	16	P(35)	914·9625	15
P(34)	916·3454	−14	P(33)	917·7164	−17	P(32)	919·0731	−15	P(31)	920·4156	−9	P(30)	921·7440	4
P(29)	923·0564	6	P(28)	924·3570	38	P(27)	925·6367	9	P(26)	926·9033	−1	P(25)	928·1556	−4
P(24)	929·3926	−11	P(23)	930·6163	0	P(22)	931·8241	3	P(21)	933·0183	21	P(20)	934·1916	−18

Table 2. *Continued*

Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ	Line	Observed	δ
P(19)	935·3523	−32	P(17)	937·6350	13	P(16)	938·7503	4	P(15)	939·8534	27	P(14)	940·9354	−8
P(11)	944·0980	−18	P(9)	946·1316	5	P(8)	947·1205	−29	P(7)	948·0990	−10	R(3)	957·8018	17
R(5)	959·3582	19	R(6)	960·1121	18	R(7)	960·8473	−7	R(8)	961·5692	−4	R(9)	962·2734	−16
R(10)	962·9700	59	R(11)	963·6332	−37	R(12)	964·2989	53	R(13)	964·9326	−11	R(14)	965·5605	29
R(15)	966·1649	−1	R(16)	966·7561	0	R(17)	967·3308	2	R(18)	967·8879	−9	R(19)	968·4304	1
R(20)	968·9555	2	R(21)	969·4651	12	R(22)	969·9558	1	R(23)	970·4320	10	R(24)	970·8906	9
R(25)	971·3321	5	R(26)	971·7562	−8	R(27)	972·1646	−9	R(28)	972·5575	2	R(29)	972·9314	−9
R(30)	973·2896	−11	R(31)	973·6310	−11	R(32)	973·9581	14	R(33)	974·2629	−15	R(34)	974·5545	−7
R(35)	974·8294	3	R(36)	975·0872	10	R(37)	975·3275	13	R(38)	975·5509	16	R(39)	975·7582	28
R(40)	975·9474	29	R(41)	976·1187	22	R(42)	976·2745	30	R(43)	986·4120	26	R(44)	976·5337	35
R(45)	976·6357	19	R(46)	976·7225	22	R(47)	986·7929	32						
						(5, 3) Band								
P(48)	885·2063	−10	P(47)	886·7636	−23	P(46)	888·3049	−57	P(45)	889·8403	−10	P(44)	891·3533	−47
P(43)	892·8587	−18	P(42)	894·3480	−9	P(41)	895·8232	0	P(40)	897·2855	22	P(39)	898·7302	10
P(38)	900·1615	9	P(37)	901·5774	−4	P(36)	902·9807	1	P(35)	904·3760	71	P(34)	905·7446	17
P(33)	907·1018	−4	P(32)	908·4457	−14	P(31)	909·7780	7	P(30)	911·0937	9	P(29)	912·3931	−6
P(28)	913·6804	6	P(27)	914·9483	−30	P(26)	916·2098	20	P(25)	917·4505	10	P(24)	918·6770	6
P(23)	919·8879	−4	P(22)	921·0836	−16	P(21)	922·2702	30	P(20)	923·4326	−15	P(19)	924·5858	−1
P(18)	925·7187	−38	P(17)	926·8419	−22	P(16)	927·9509	5	P(15)	929·0408	−6	P(14)	930·1156	−16
P(13)	931·1747	−30	R(5)	948·3744	52	R(8)	950·5643	28	R(10)	951·9410	−14	R(11)	952·6064	−24
R(13)	953·8961	33	R(14)	954·5141	36	R(15)	955·1114	−3	R(16)	955·6954	−14	R(17)	956·2650	−7
R(19)	957·3552	12	R(20)	957·8751	15	R(21)	958·3759	−8	R(22)	958·8634	0	R(23)	959·3351	15
R(24)	959·7880	7	R(25)	960·2240	−4	R(26)	960·6450	1	R(27)	961·0508	19	R(28)	961·4362	0
R(29)	961·8106	37	R(30)	962·1615	5	R(31)	962·4991	8	R(32)	962·8195	6	R(33)	963·1245	17
R(34)	963·4112	13	R(35)	963·6801	−1	R(36)	963·9331	−7	R(37)	964·1714	9	R(38)	964·3902	−1
R(40)	964·7736	−57	R(41)	964·9502	17	R(43)	963·2375	15	R(44)	965·3556	12	R(45)	965·4490	−67
R(46)	965·5376	−24	R(47)	965·6037	−36	R(48)	965·6549	−26						
						(6, 4) Band								
P(60)	855·2885	−10	P(58)	858·6927	16	P(51)	870·1773	21	P(50)	871·7609	−7	P(46)	877·9748	48
P(43)	882·4772	−36	P(42)	883·9591	26	P(41)	885·4205	24	P(39)	888·3049	60	P(38)	889·7195	15
P(37)	891·1238	8	P(35)	893·8905	4	P(34)	895·2510	−11	P(33)	896·5938	−59	P(32)	897·9343	15
P(31)	899·2524	9	P(30)	900·5554	−2	P(29)	901·8416	−36	P(28)	903·1189	−12	P(27)	904·3760	−44
P(24)	908·0723	−7	P(23)	909·2732	−11	P(22)	910·4582	−25	P(19)	913·9338	32	P(18)	915·0588	17
P(16)	917·2661	9	R(13)	942·9669	−12	R(14)	943·5797	2	R(15)	944·1761	12	R(16)	944·7579	39
R(19)	946·3932	−10	R(20)	946·9076	−7	R(21)	947·4035	−27	R(22)	947·8894	17	R(23)	948·3539	10
R(24)	948·8010	−6	R(25)	949·2358	18	R(26)	949·6500	2	R(27)	950·0485	−8	R(28)	950·4332	10
R(29)	950·7981	−4	R(30)	951·1492	8	R(31)	951·4767	−50	R(32)	951·7987	4	R(33)	952·0978	−6
R(34)	952·3844	26	R(35)	952·6494	8	R(36)	952·8999	12	R(37)	953·1324	3	R(38)	953·3512	24
R(39)	953·5496	10	R(40)	953·7365	47	R(41)	953·8961	−21	R(42)	954·0475	−2	R(43)	954·1836	31
R(44)	954·3026	62	R(45)	954·3925	−29	R(46)	954·4787	12	R(47)	954·5450	22	R(48)	954·5904	−7

[a] Observed–calculated differences (columns labelled δ) are in units of 0·0001 cm^{-1}.

Table 3. Mass-dependent Dunham constants (in cm^{-1}).

	^{6}LiI	^{7}LiI
Y_{10}	534·586 010(165)	496·848 333(62)
Y_{20}	−3·303 512(109)	−2·853 706 3(265)
$10^{2} Y_{30}$	1·248 72(284)	1·006 418(458)
$10^{5} Y_{40}$	−2·911(251)	−2·488 6(275)
Y_{01}	0·513 057 887(313)	0·443 175 934(334)
$10^{3} Y_{11}$	−5·090 024(102)	−4·086 252 0(422)
$10^{5} Y_{21}$	2·005 65(312)	1·499 781(681)
$10^{8} Y_{31}$	−1·699(330)	−1·383 5(469)
$10^{6} Y_{02}$	−1·891 104(186)	−1·410 476(135)
$10^{9} Y_{12}$	8·548 0(234)	5·844 5(123)
$10^{11} Y_{22}$	4·489(433)	2·514 4(684)
$10^{12} Y_{03}$	2·051 3(380)	1·221 6(162)
$10^{14} Y_{13}$		1·492(138)

The final term in equation (5) is a correction term for the Li nucleus which takes into account the Born–Oppenheimer breakdown and homogeneous non-adiabatic mixing from distant Σ electronic states, and is represented by the power series expansion

$$U_{\mathrm{Li}}(R) = \sum_{i=1} u_i^{\mathrm{Li}} (R - R_e)^i \qquad (10)$$

Similarly, effects from the rotational motion, namely J-dependent Born–Oppenheimer breakdown and heterogeneous non-adiabatic mixing from distant Π electronic states, are accounted for by the $q(R)$ term in equation (3), where

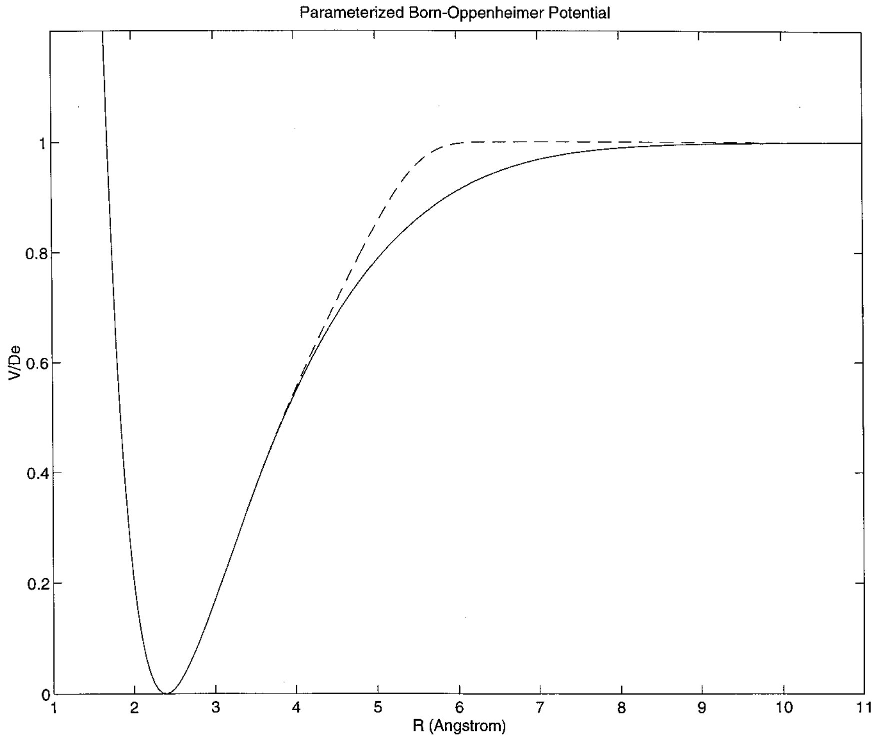

Figure 2. The parameterized Born–Oppenheimer potential of LiI plotted using the parameters obtained by fitting the experimental data: solid line, this work; dashed line, reference [9].

Table 4. Mass-independent Dunham constants (in cm^{-1}).

U_{10}	1281·100 71(39)	$10^{10}U_{03}$	3·655 535 95
U_{20}	−18·972 779(150)	$10^{11}Y_{13}$	1·250 763 30
U_{30}	0·172 534 8(703)	$10^{13}U_{23}$	−4·870 216 02
$10^{3}U_{40}$	−1·100 9(114)	$10^{15}U_{04}$	−5·617 536 79
U_{01}	2·946 333 19(853)	$10^{17}U_{14}$	−9·667 560 20
$10^{2}U_{11}$	−7·004 429 (125)	$10^{17}U_{24}$	−1·836 821 53
$10^{4}U_{21}$	6·618 50(229)	$10^{19}U_{05}$	1·633 533 43
$10^{6}U_{31}$	−1·254 7(611)	$10^{22}U_{15}$	−1·956 016 80
$10^{5}U_{02}$	−6·233 601 31	$10^{24}U_{06}$	−1·835 139 20
$10^{7}U_{12}$	6·625 218 29	$10^{25}U_{16}$	−5·813 369 17
$10^{9}U_{22}$	9·367 163 45	$10^{29}U_{07}$	5·407 320 41
$10^{10}U_{32}$	−4·593 862 55	$10^{33}U_{08}$	−3·018 234 98
Δ^{Li}_{10}	0·013 65(349)		
Δ^{Li}_{01}	0·417 4(340)		
Δ^{Li}_{11}	0·638(197)		
Δ^{Li}_{02}	4·145(502)		
Δ^{Li}_{03}	377·5(536)		

Table 5. Derived parameter values for the modified Morse potential.

D_e cm^{-1}	288 39.0
R_e A	2·391 981 00(338)
β_0	3·394 922 75(595)
β_1	2·086 096 6(992)
β_2	2·919 149(628)
β_3	9·036 44(578)
β_4	7·7780(470)
β_5	26·707(450)
u_1^{Li} cm^{-1} u $Å^{-1}$	13·63(107)
u_2^{Li} cm^{-1} u $Å^{-2}$	−21·31(178)
u_3^{Li} cm^{-1} u $Å^{-3}$	10·75(126)
q_1^{Li} u $Å^{-1}$	−0·000 264 5(625)
q_2^{Li} u $Å^{-2}$	0·000 573 3(956)
M (^{6}Li) u	6·015 121 4
M (^{7}Li) u	7·016 003 0
M (^{127}I) u	126·904 473

$$q(R) = \frac{1}{M_{Li}} \sum_{i=1} q_i^{Li}(R - R_e)^i. \qquad (11)$$

Our fitting procedure is similar to the method reported by Coxon and Hajigeorgiou [9, 15] and is described in greater detail elsewhere [10]. Results of the potential fit are given in table 5, where the value of D_e was fixed to that given in Huber and Herzberg [16] and the atomic masses were taken from Mills *et al.* [17]. In figure 2, we plot the potential using equation (6) and the Born–Oppenheimer parameters in table 5, and compare it with the potential reported by Coxon and Hajigeorgiou [9].

4. Conclusion

Fourier transform infrared emission spectroscopy is a very powerful technique for the study of alkali halide molecules. Our new infrared vibration–rotation data for the two isotopomers, ^{7}LiI and ^{6}LiI, were used to derive a set of improved spectroscopic constants as well as the parameters for a modified Morse potential for the ground state.

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