

1 LiNa

Table 1: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiNa states in the framework of pure Hund's coupling case "a".

State	R_e	T_e	Method	Ref.
$A^1\Sigma^+$	3.38	14228	CI-CPP	This work
	3.36	14101	CI- l -CPP	[13]
	<i>3.371</i>	<i>14205.28</i>	Exp.	[4]
$C^1\Sigma^+$	4.15	19633	CI-CPP	This work
	4.16	19675	CI- l -CPP	[13]
	<i>4.138</i>	<i>19610.93</i>	Exp.	[3]
$a^3\Sigma^+$	4.77	6887	CI-CPP	This work
	4.72	6834	CI- l -CPP	[13]
	<i>4.706</i>	<i>6871.483</i>	Exp.	[20]
$c^3\Sigma^+$	3.45	17237	CI-CPP	This work
	3.44	17160	CI- l -CPP	[13]
$e^3\Sigma^+$	3.33	26282	CI-CPP	This work
$B^1\Pi$	3.22	20087	CI-CPP	This work
	3.23	20239	CI- l -CPP	[13]
	<i>3.208</i>	<i>20088</i>	Exp.	[3]
$D^1\Pi$	3.76	22296	CI-CPP	This work
	3.73	22300	CI- l -CPP	[13]
	<i>3.761</i>	<i>22299.66</i>	Exp.	[1]
$b^3\Pi$	2.86	12275	CI-CPP	This work
	2.84	12255	CI- l -CPP	[13]

Table 2: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiNa states in the framework of pure Hund's coupling case "c".

State	R_e	T_e	Method	Ref.
(2)0 ⁺	2.85	12216	FS-RCC	This work
(3)0 ⁺	3.38	14170	FS-RCC	This work
(4)0 ⁺	4.18	19573	FS-RCC	This work
	<i>4.138</i>	<i>19610.93</i>	Exp.	[3]
(1)0 ⁻ , 1	4.71	6879	FS-RCC	This work
	<i>4.706</i>	<i>6871.483</i>	Exp.	[20]
(2)0 ⁻	2.85	12216	FS-RCC	This work
(3)0 ⁻	3.46	17194	FS-RCC	This work
(5)0 ⁻	3.33	26235	FS-RCC	This work
(2)1	2.85	12219	FS-RCC	This work
(3)1	3.46	17194	FS-RCC	This work
(4)1	3.22	20053	FS-RCC	This work
	<i>3.208</i>	<i>20088</i>	Exp.	[3]
(5)1	3.75	22223	FS-RCC	This work
	<i>3.761</i>	<i>22299.66</i>	Exp.	[1]
(7)1	3.33	26235	FS-RCC	This work
(1)2	2.85	12222	FS-RCC	This work

2 LiK

Table 3: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiK states in the framework of pure Hund's coupling case "a".

State	R_e , \AA	T_e , cm^{-1}	Method	Ref.
$A^1\Sigma^+$	3.96	12199	CI-CPP	This work
	3.92	12056	CI-l-CPP	[17]
	3.95	12026	FS-RCC	[15]
	<i>3.947</i>	<i>12097.11</i>	Exp.	[7]
$C^1\Sigma^+$	4.19	17545	CI-CPP	This work
	4.13	17647	CI-l-CPP	[17]
	4.15	17669	FS-RCC	[15]
	<i>4.190</i>	<i>17501.178</i>	Exp.	[16]
$a^3\Sigma^+$	5.06	5960	CI-CPP	This work
	4.97	5947	CI-l-CPP	[17]
	<i>4.993</i>	<i>5929.868</i>	Exp	[24]
$c^3\Sigma^+$	3.95	15049	CI-CPP	This work
	3.93	14961	FS-RCC	[15]
	3.92	14931	CI-l-CPP	[17]
$e^3\Sigma^+$	3.80	22096	CI-CPP	This work
$B^1\Pi$	3.70	17607	CI-CPP	This work
	3.76	17725	CI-l-CPP	[17]
	3.73	17732	FS-RCC	[15]
	<i>3.713</i>	<i>17572.760</i>	Exp.	[16]
$D^1\Pi$	4.07	19500	CI-CPP	This work
	4.02	19541	CI-l-CPP	[17]
	4.00	19356	FS-RCC	[15]
	<i>4.043</i>	<i>19455.73</i>	Exp.	[5]
$b^3\Pi$	3.26	10565	CI-CPP	This work
	3.23	10475	CI-l-CPP	[17]
	3.24	10525	FS-RCC	[15]
$d^3\Pi$	4.12	20479	CI-CPP	This work
	4.02	20388	CI-l-CPP	[17]
	4.11	20365	FS-RCC	[15]

Table 4: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiK states in the framework of pure Hund's coupling case “c”.

State	R_e , \AA	T_e , cm^{-1}	Method	Ref.
(2)0 ⁺	3.24	10433	FS-RCC	This work
(3)0 ⁺	3.96	12018	FS-RCC	This work
(4)0 ⁺	4.13	17492	FS-RCC	This work
	<i>4.190</i>	<i>17501.178</i>	Exp.	[16]
(5)0 ⁺	4.06	20314	FS-RCC	This work
(1)0 ⁻ , (1)1	4.95	5935	FS-RCC	This work
	<i>4.993</i>	<i>5929.868</i>	Exp	[24]
(2)0 ⁻	3.24	10433	FS-RCC	This work
(3)0 ⁻	3.94	14945	FS-RCC	This work
(4)0 ⁻	4.06	20314	FS-RCC	This work
(5)0 ⁻	3.79	21893	FS-RCC	This work
(2)1	3.25	10443	FS-RCC	This work
(3)1	3.95	14945	FS-RCC	This work
(4)1	3.71	17528	FS-RCC	This work
	<i>3.713</i>	<i>17572.760</i>	Exp.	[16]
(5)1	4.02	19405	FS-RCC	This work
	<i>4.043</i>	<i>19455.73</i>	Exp.	[5]
(6)1	4.06	20322	FS-RCC	This work
(7)1	3.79	21893	FS-RCC	This work
(1)2	3.25	10454	FS-RCC	This work
(2)2	4.06	20330	FS-RCC	This work

3 LiRb

Table 5: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiRb states in the framework of pure Hund's coupling case "a".

state	$R_e, \text{\AA}$	T_e, cm^{-1}	Method	Ref.
$A^1\Sigma^+$	4.18	11789	CI-CPP	This work
	4.14	11639	CI-l-CPP	[10]
	—	<i>11677.8</i>	Exp.	[22]
$C^1\Sigma^+$	4.29	17274	CI-CPP	This work
	4.26	17348	CI-l-CPP	[10]
	<i>4.283</i>	<i>17230.571</i>	Exp.	[9]
$a^3\Sigma^+$	5.28	5686	CI-CPP	This work
	5.13	5678	CI-l-CPP	[10]
	<i>5.110</i>	<i>5650.529</i>	Exp.	[8]
$c^3\Sigma^+$	4.12	14806	CI-CPP	This work
	4.06	14719	CI-l-CPP	[10]
$e^3\Sigma^+$	3.95	20657	CI-CPP	This work
$B^1\Pi$	3.86	17134	CI-CPP	This work
	3.81	17205	CI-l-CPP	[10]
	<i>3.875</i>	<i>17110.406</i>	Exp.	[9]
$D^1\Pi$	4.15	19158	CI-CPP	This work
	4.10	19201	CI-l-CPP	[10]
	<i>4.115</i>	<i>19089.88</i>	Exp.	[9]
$b^3\Pi$	3.38	10301	CI-CPP	This work
	3.34	10233	CI-l-CPP	[10]
$d^3\Pi$	4.17	19531	CI-CPP	This work
	4.11	19484	CI-l-CPP	[10]

Table 6: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiRb states in the framework of pure Hund's coupling case “c”.

State	R_e , \AA	T_e , cm^{-1}	Method	Ref.
(2)0 ⁺	3.37	10155	FS-RCC	This work
	3.29	10192	CI-l-CPP	[11]
	–	<i>10005.186</i>	Exp.	[22]
(3)0 ⁺	4.07	11625	FS-RCC	This work
(4)0 ⁺	4.27	17215	FS-RCC	This work
	4.21	17468	CI-l-CPP	[11]
(5)0 ⁺	4.12	19316	FS-RCC	This work
	4.06	19528	CI-l-CPP	[11]
	<i>4.19</i>	<i>19383.4</i>	Exp.	[21]
(2)0 [−] , (1)1	5.07	5635	FS-RCC	This work
	5.00	5856	CI-l-CPP	[11]
	<i>5.110</i>	<i>5650.529</i>	Exp.	[8]
(2)0 [−]	3.37	10156	FS-RCC	This work
	3.29	10194	CI-l-CPP	[11]
(3)0 [−]	4.13	14706	FS-RCC	This work
	4.03	14867	CI-l-CPP	[11]
(4)0 [−]	4.12	19315	FS-RCC	This work
	4.06	19564	CI-l-CPP	[11]
(5)0 [−]	3.92	20423	FS-RCC	This work
	3.87	20611	CI-l-CPP	[11]
(2)1	3.38	10195	FS-RCC	This work
	3.29	10226	CI-l-CPP	[11]
(3)1	4.13	14706	FS-RCC	This work
	4.03	14866	CI-l-CPP	[11]
(4)1	3.86	17089	FS-RCC	This work
	3.82	17315	CI-l-CPP	[11]
	<i>3.875</i>	<i>17110.406</i>	Exp.	[9]
(5)1	4.10	19028	FS-RCC	This work
	4.04	19341	CI-l-CPP	[11]
	<i>4.115</i>	<i>19089.88</i>	Exp.	[9]
(6)1	4.12	19352	FS-RCC	This work
	4.06	19586	CI-l-CPP	[11]
	<i>4.12</i>	<i>19420.7</i>	Exp.	[21]
(7)1	3.91	20423	FS-RCC	This work
	3.87	20608	CI-l-CPP	[11]
(1)2	3.38	10235	FS-RCC	This work
	3.28	10228	CI-l-CPP	[11]
(2)2	4.12	19386	FS-RCC	This work
	4.06	19625	CI-l-CPP	[11]
	–	<i>19453.2</i>	Exp.	[21]

4 LiCs

Table 7: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiCs states in the framework of pure Hund's coupling case "a".

state	R_e , \AA	T_e , cm^{-1}	Method	Ref.
$A^1\Sigma^+$	4.47	10777	CI-CPP	This work
	4.38	10715	CI-l-CPP	[14]
	<i>4.432</i>	<i>10657.41</i>	Exp.	[12]
$C^1\Sigma^+$	4.37	16846	CI-CPP	This work
	4.32	16932	CI-l-CPP	[14]
	<i>4.370</i>	<i>16786.43</i>	Exp.	[6]
$(4)^1\Sigma^+$	5.55	19021	CI-CPP	This work
	5.01	19081	CI-l-CPP	[14]
	<i>4.91</i>	<i>18848.4</i>	Exp.	[23]
$a^3\Sigma^+$	5.47	5636	CI-CPP	This work
	5.23	5725	CI-l-CPP	[14]
	<i>5.247</i>	<i>5566.090</i>	Exp.	[18]
$c^3\Sigma^+$	4.23	13828	CI-CPP	This work
	4.11	13730	CI-l-CPP	[14]
$e^3\Sigma^+$	4.19	17746	CI-CPP	This work
	4.16	17779	CI-l-CPP	[14]
	<i>4.314</i>	<i>17727.19</i>	Exp.	[6]
$(4)^3\Sigma^+$	4.35	22296	CI-CPP	This work
$B^1\Pi$	4.11	16055	CI-CPP	This work
	4.08	16165	CI-l-CPP	[14]
	<i>4.122</i>	<i>16012.217</i>	Exp.	[19]
$D^1\Pi$	4.06	18378	CI-CPP	This work
	4.02	18570	CI-l-CPP	[14]
	<i>4.062</i>	<i>18293.37</i>	Exp.	[19]
$(3)^1\Pi$	5.53	19998	CI-CPP	This work
	5.24	20123	CI-l-CPP	[14]
$b^3\Pi$	3.52	9295	CI-CPP	This work
	3.43	9063	CI-l-CPP	[14]
$d^3\Pi$	4.26	17389	CI-CPP	This work
	4.17	17287	CI-l-CPP	[14]
	<i>4.314</i>	<i>17368.12</i>	Exp.	[6]
$(1)^1\Delta$	3.96	18901	CI-CPP	This work
	3.94	18963	CI-l-CPP	[14]
$(1)^3\Delta$	4.15	19317	CI-CPP	This work
	4.13	19381	CI-l-CPP	[14]

Table 8: The electronic energies, T_e (in cm^{-1}), and equilibrium distances, R_e (in \AA), of theoretical and experimental interatomic potentials constructed for the excited LiCs states in the framework of pure Hund's coupling case “c”.

state	R_e , \AA	T_e , cm^{-1}	Method	Ref.
(2)0 ⁺	3.50	9085	FS-RCC	This work
	3.46	9192	CI-I-CPP	[2]
	<i>3.528</i>	<i>9175.05</i>	Exp.	[12]
(3)0 ⁺	4.25	10650	FS-RCC	This work
(4)0 ⁺	4.33	16727	FS-RCC	This work
	4.28	16847	CI-I-CPP	[2]
	<i>4.370</i>	<i>16786.43</i>	Exp.	[6]
(5)0 ⁺	4.24	17160	FS-RCC	This work
	4.12	17252	CI-I-CPP	[2]
	<i>4.353</i>	<i>17206.93</i>	Exp.	[6]
(6)0 ⁺	4.92	18789	FS-RCC	This work
	4.96	19004	CI-I-CPP	[2]
(7)0 ⁺	4.23	21460	FS-RCC	This work
	4.18	21620	CI-I-CPP	[2]
(1)0 ⁻ , (1)1	5.18	5580	FS-RCC	This work
	5.235	5689	CI-I-CPP	[2]
	<i>5.247</i>	<i>5566.090</i>	Exp.	[18]
(2)0 ⁻	3.50	9089	FS-RCC	This work
(3)0 ⁻	4.22	13690	FS-RCC	This work
	4.10	13683	CI-I-CPP	[2]
(4)0 ⁻	4.21	17098	FS-RCC	This work
	4.36	17194	CI-I-CPP	[2]
(5)0 ⁻	4.17	17583	FS-RCC	This work
	4.16	17768	CI-I-CPP	[2]
(6)0 ⁻	4.32	22277	FS-RCC	This work
	4.28	22449	CI-I-CPP	[2]
(7)0 ⁻	4.61	22386	FS-RCC	This work
(2)1	3.50	9168	FS-RCC	This work
(3)1	4.22	13684	FS-RCC	This work
	4.10	13683	CI-I-CPP	[2]
(4)1	4.11	15933	FS-RCC	This work
	4.09	16101	CI-I-CPP	[2]
	<i>4.122</i>	<i>16012.217</i>	Exp.	[19]
(5)1	4.21	17208	FS-RCC	This work
	4.21	17365	CI-I-CPP	[2]
	<i>4.314</i>	<i>17368.12</i>	Exp.	[6]
(6)1	4.17	17575	FS-RCC	This work
	4.18	17771	CI-I-CPP	[2]
	<i>4.314</i>	<i>17727.19</i>	Exp.	[6]
(7)1	4.01	18204	FS-RCC	This work
	4.00	18544	CI-I-CPP	[2]
	<i>4.062</i>	<i>18293.37</i>	Exp.	[19]
(8)1	4.09	19174	FS-RCC	This work
	4.16	19389	CI-I-CPP	[2]
(9)1	5.30	19905	FS-RCC	This work
(10)1	4.31	22279	FS-RCC	This work
	4.28	22452	CI-I-CPP	[2]
(11)1	4.62	22388	FS-RCC	This work
(1)2	3.51	9248	FS-RCC	This work
	3.45	9326	CI-I-CPP	[2]
(2)2	4.22	17306	FS-RCC	This work
	4.23	17506	CI-I-CPP	[2]
(3)2	3.92	18771	FS-RCC	This work
	3.97	19034	CI-I-CPP	[2]
(4)2	4.09	19206	FS-RCC	This work
	4.16	19436	CI-I-CPP	[2]
(1)3	4.01	19232	FS-RCC	This work
	4.16	19474	CI-I-CPP	[2]

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