Table I. Parameters of the MLR potential energy functions for LiRb ($X^1\Sigma^+$, $b^3\Pi_0$, $b^3\Pi_1$, and $b^3\Pi_2$); (D_e, C_6, C_8, C_{10}, and RMS are in cm^{-1} and R_e in Å).

	$X^1\Sigma^+$	$b^3\Pi_0$	$b^3\Pi_1$	$b^3\Pi_2$
Φ_1	$-1.65954937025401\times10^{-1}$	$-3.78398704267304\times10^{-1}$	$-4.049457391207\times10^{-1}$	$-3.96253964468881\times10^{-1}$
Φ_2	-1.47307939648485	-2.08602333963445	-2.215351035993	-2.20213436424538
Φ_3	-1.97338379582326	-2.56927140910410	-3.264558950536	-2.35173837004823
Φ_4	-1.38027909025489	-1.43049147334407	-3.050086921839	$-5.91220913105060\times10^{-1}$
Φ_5	-3.10008460420709	1.78225976899681	-1.710834154652	2.46508485791987
Φ_6	$2.76700727829455\times10^{-2}$	7.66451872829829	5.081856378213	$2.57455631974559\times10^{-2}$
Φ_7	$3.87369094379414\times10^{1}$	-7.14854447188408	7.086886475278	$-2.64447134485736\times10^{1}$
Φ_8	$2.53584028381134\times10^{1}$	$-5.08900091944738\times10^{1}$	$-2.778706352292\times10^{1}$	$-3.50882103348123\times10^{1}$
Φ_9	$-2.00382611469885\times10^{2}$	$2.49125186839839\times10^{1}$	$-1.421723602772\times10^{-3}$	$8.31944656218654\times10^{1}$
Φ_{10}	$-1.70200286729326\times10^{2}$	$1.93081077883750\times10^{2}$	$1.556169646790\times10^{2}$	$1.35634319407802\times10^{2}$
Φ_{11}	$5.65969408006438\times10^{2}$	$-7.22734817151931\times10^{1}$	$-3.085538829674\times10^{1}$	$-2.11914011262861\times10^{2}$
Φ_{12}	$6.31900726303575\times10^{2}$	$-4.97189489019564\times10^{2}$	$-4.960255896665\times10^{2}$	$-3.80469263366913\times10^{2}$
Φ_{13}	$-7.01912308117566\times10^{2}$	$-2.68640518836253\times10^{-4}$	$-8.906121300635\times10^{1}$	$2.31105600260294\times10^{2}$
Φ_{14}	$-1.06930287706414\times10^{3}$	$6.62350529372493\times10^{2}$	$6.889317536016\times10^{2}$	$5.68694739304169\times10^{2}$
Φ_{15}	$1.93617920751443\times10^{2}$	$2.06562155454963\times10^{2}$	$2.994276912088\times10^{2}$	$-2.55452230898177\times10^{-5}$
Φ_{16}	$7.37566903911735\times10^{2}$	$-3.46134451649826\times10^{2}$	$-3.600138450378\times10^{2}$	$-3.55020831467025\times10^{2}$
Φ_{17}	$2.61902215894053\times10^{2}$	$-1.85137632969633\times10^{2}$	$-2.204552708352\times10^{2}$	$-1.44189857126391\times10^{2}$
D_e	$5.92248703376990\times10^{3}$	$8.12171680858926\times10^{3}$	$8.173948239463\times10^{3}$	$8.13029649310318\times10^{3}$
R_{ef}	4.17455163720961	4.83710057104409	4.524140514933	5.19631239923550
R_e	3.50842065424474	3.42298734382155	3.425183001402	3.42521229008978
C_6	$1.40363992679874\times10^{7}$	$2.10300247441515\times10^{7}$	$2.008398463231\times10^{7}$	$1.62123027435094\times10^{7}$
C_8	$3.15014624259183\times10^{8}$	$2.06762595786173\times10^{8}$	$2.389271963868\times10^{8}$	$1.92915092290023\times10^{8}$
C_{10}	$1.38241918191638\times10^{10}$	$1.33307197656858\times10^{10}$	$1.633636391834\times10^{10}$	$1.33307197424527\times10^{10}$
RMS	0.913	0.293	0.408	0.671

Table II. Parameters of the MLR potential energy functions for KRb ($X^1\Sigma^+$, $b^3\Pi_0$, $b^3\Pi_1$, and $b^3\Pi_2$); (D_e, C_6, C_8, C_{10}, and RMS are in cm^{-1} and R_e in Å).

	$X^1\Sigma^+$	$b^3\Pi_0$	$b^3\Pi_1$	$b^3\Pi_2$
Φ_1	$1.715683332194\times10^{-7}$	$-8.026327323369\times10^{-1}$	$-7.030930216457\times10^{-1}$	$-8.252245908588\times10^{-1}$
Φ_2	$2.910825628023\times10^{-3}$	-4.963239574780	-6.011555023005	-5.754051354585
Φ_3	$8.964799417088\times10^{-1}$	-8.832726056703	$-1.043270036803\times10^{1}$	$-1.017830777296\times10^{1}$
Φ_4	2.286455141751	$-1.294831196322\times10^{1}$	$-1.469914785791\times10^{1}$	$-1.450478148265\times10^{1}$
Φ_5	4.747102006155	$-1.552121292253\times10^{1}$	$-1.763222805939\times10^{1}$	$-1.755518871064\times10^{1}$
Φ_6	-2.255859147812	$-2.078211039330\times10^{1}$	$-2.406492775135\times10^{1}$	$-2.522306755104\times10^{1}$
Φ_7	-3.918374417797×101	$-3.346609570984\times10^{1}$	$-3.255958806778\times10^{1}$	$-3.414496674951\times10^{1}$
Φ_8	$3.872867266058\times10^{1}$	$-1.791370269797\times10^{-5}$	$1.108525552957\times10^{1}$	$1.946689748004\times10^{1}$
Φ_9	$3.939721964050\times10^{2}$	$8.702239465175\times10^{1}$	$7.396373224446\times10^{1}$	$8.987905385713\times10^{1}$
Φ_{10}	$1.422315882231\times10^{2}$	$-6.816557317230\times10^{1}$	$-1.339887601156\times10^{2}$	$-1.591465425363\times10^{2}$
Φ_{11}	$-1.437320225593\times10^{3}$	$-4.525849115371\times10^{2}$	$-4.536199203378\times10^{2}$	$-5.217263023272\times10^{2}$
Φ_{12}	$-1.370602980416\times10^{3}$	$-1.534335647194\times10^{2}$	$-1.271898306412\times10^{1}$	$-2.224465632295\times10^{-3}$
Φ_{13}	$2.175423127586\times10^{3}$	$7.152874187306\times10^{2}$	$7.648149456145\times10^{2}$	$8.845841017115\times10^{2}$
Φ_{14}	$3.400823738586\times10^{3}$	$5.241810781065\times10^{2}$	$3.678642465431\times10^{2}$	$4.218059822592\times10^{2}$
Φ_{15}	$-3.433514638602\times10^{2}$	$-4.724866229763\times10^{2}$	$-5.703017603885\times10^{2}$	$-6.379874610370\times10^{2}$
Φ_{16}	$-2.491254021484\times10^{3}$	$-6.218924644594\times10^{2}$	$-5.724118331690\times10^{2}$	$-6.381349777965\times10^{2}$
Φ_{17}	$-1.035511984572\times10^{3}$	$-1.755752073924\times10^{2}$	$-1.370694368434\times10^{2}$	$-1.522923854416\times10^{2}$
D_e	$3.448802115964\times10^{3}$	$6.041207109500\times10^{3}$	$6.070473227620\times10^{3}$	$6.070128593453\times10^{3}$
R_{ef}	5.970357086365	7.289408879436	7.415067260591	7.408836214314
R_e	4.168255833410	4.173686985404	4.177248133287	4.182027322588
C_6	$3.206438724187\times10^{7}$	$9.358387394682\times10^{6}$	$7.226601885029\times10^{6}$	$6.782585935388\times10^{6}$
C_8	$3.169173120000\times10^{8}$	$3.133481705083\times10^{8}$	$9.274106105677\times10^{6}$	$1.805047335392\times10^{8}$
C_{10}	$1.333071974400\times10^{10}$	$1.333886564720\times10^{10}$	$1.548205956765\times10^{9}$	$8.941686782998\times10^{9}$
RMS	0.518	0.325	0.318	0.294

TABLE III. The vibrational levels ($N = 0$) for LiRb.

υ	$X^1\Sigma^+$	$b^3\Pi_0$	$b^3\Pi_1$	$b^3\Pi_2$	$B^1\Pi$
0	95.9	93.9	93.9	94.1	56.1
1	286.3	280.8	280.8	281.2	164.4
2	474.5	466.6	466.5	466.9	266.9
3	660.6	651.0	650.9	651.3	363.6
4	844.4	834.0	834.0	834.2	454.6
5	1026.1	1015.6	1015.5	1015.7	539.9
6	1205.5	1195.6	1195.6	1195.7	619.8
7	1382.8	1374.2	1374.1	1374.3	694.3
8	1557.8	1551.3	1551.1	1551.3	763.8
9	1730.6	1726.9	1726.5	1726.8	828.6
10	1901.1	1900.9	1900.3	1900.8	888.9
11	2069.2	2073.4	2072.7	2073.2	945.0
12	2235.0	2244.5	2243.5	2244.1	997.2
13	2398.3	2413.9	2412.7	2413.5	1045.7
14	2559.2	2581.9	2580.4	2581.3	1090.9
15	2717.6	2748.4	2746.6	2747.6	1132.9
16	2873.4	2913.3	2911.2	2912.3	1171.8
17	3026.6	3076.7	3074.3	3075.4	1207.7
18	3177.2	3238.5	3235.8	3236.9	1240.7
19	3325.1	3398.8	3395.7	3396.9	1270.7
20	3470.3	3557.5	3554.0	3555.2	1297.9
21	3612.6	3714.6	3710.6	3711.9	1322.1
22	3752.1	3870.1	3865.6	3867.0	1343.5
23	3888.5	4024.0	4018.9	4020.4	1361.9
24	4021.9	4176.2	4170.5	4172.1	1377.4
25	4152.1	4326.7	4320.3	4322.1	1390.0
26	4279.0	4475.5	4468.4	4470.4	1399.9
27	4402.4	4622.6	4614.8	4616.9	1407.0
28	4522.4	4767.9	4759.3	4761.7	1411.8
29	4638.7	4911.4	4901.9	4904.6	1414.4
30	4751.1	5053.1	5042.7	5045.6	–
31	4859.6	5192.8	5181.5	5184.8	–
32	4964.0	5330.7	5318.4	5322.0	–
33	5064.1	5466.5	5453.3	5457.2	–
34	5159.7	5600.4	5586.0	5590.4	–
35	5250.7	5732.1	5716.7	5721.5	–
36	5336.8	5861.6	5845.1	5850.5	–
37	5417.8	5988.9	5971.3	5977.2	–
38	5493.6	6113.8	6095.1	6101.7	–
39	5563.8	6236.4	6216.5	6223.8	–
40	5628.3	6356.4	6335.3	6343.4	–

41	5686.8	6473.7	6451.5	6460.5	–
42	5739.0	6588.4	6564.9	6574.9	–
43	5784.8	6700.1	6675.5	6686.6	–
44	5824.0	6808.9	6783.1	6795.3	–
45	5856.6	6914.5	6887.6	6900.9	–
46	5882.4	7016.8	6988.7	7003.4	–
47	5901.4	7115.7	7086.5	7102.5	–
48	5913.6	7211.0	7180.6	7198.1	–
49	–	7302.4	7270.9	7290.0	–
50	–	7389.8	7357.2	7378.0	–
51	–	7473.1	7439.4	7461.8	–
52	–	7551.9	7517.2	7541.4	–
53	–	7626.1	7590.4	7616.4	–
54	–	7695.5	7658.8	7686.8	–
55	–	7759.8	7722.2	7752.1	–
56	–	7818.9	7780.4	7812.4	–
57	–	7872.5	7833.3	7867.3	–
58	–	7920.7	7880.8	7916.8	–
59	–	7963.2	7922.7	7960.7	–
60	–	8000.2	7959.0	7999.1	–
61	–	8031.6	7989.9	8031.9	–
62	–	8057.7	8015.4	8059.3	–
63	–	8078.5	8035.8	8081.5	–
64	–	8094.4	8051.4	8098.8	–
65	–	8105.9	8062.7	8111.5	–
66	–	8113.6	8070.2	8120.2	–
67	–	8118.2	8074.6	8125.7	–
68	–	8120.6	8076.9	8128.7	–
69	–	–	–	8130.1	–

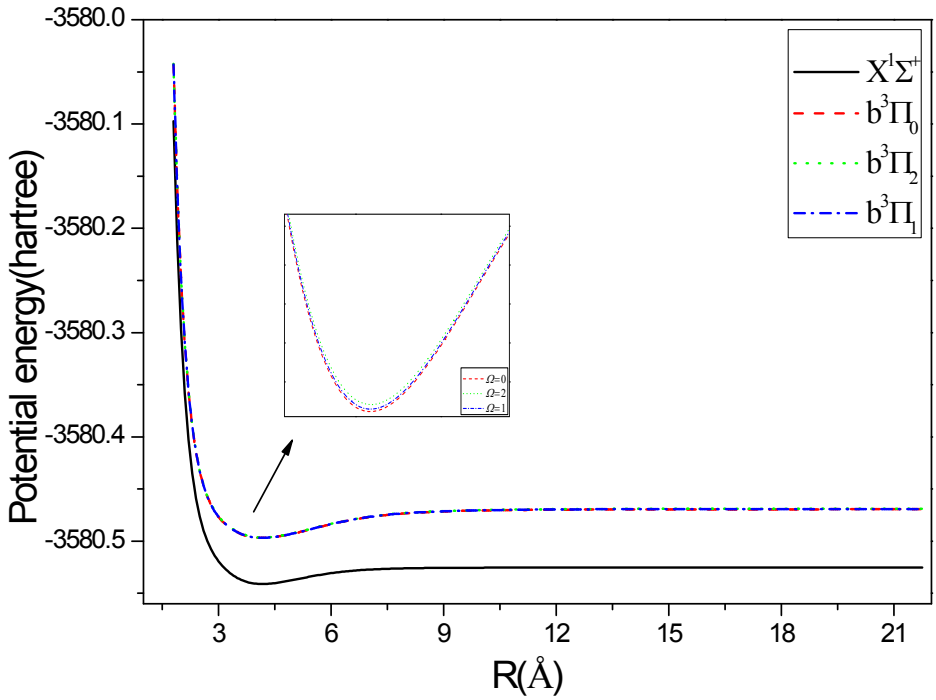

FIG. 1. *Ab initio* PECs of KRb for the ground state $X^1\Sigma^+$ and the SOC effect of the $b^3\Pi$ state. The inset figure shows the enlarged SOC effect of the $b^3\Pi$ state around the equilibrium position R_e.