Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information to: Theoretical study of the Coriolis effect in LiNa, LiK, and LiRb molecules†

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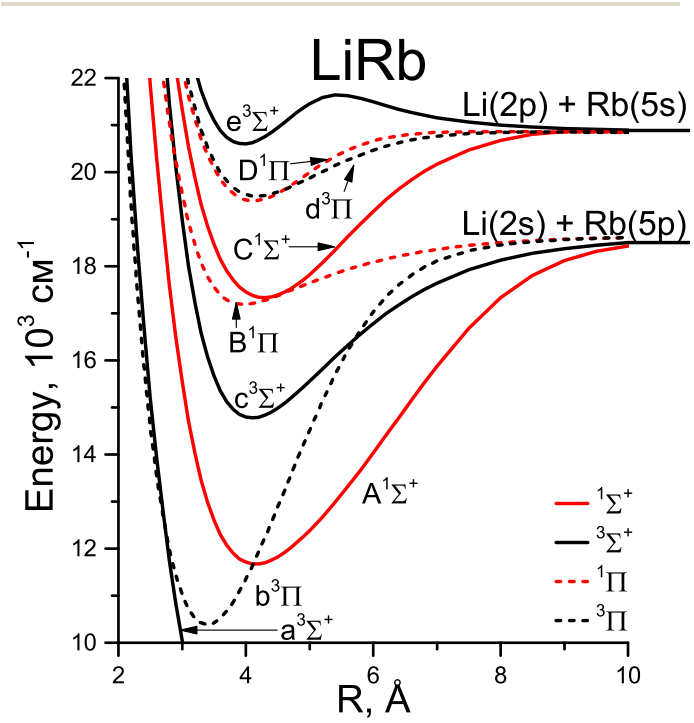

Fig. 1 The potential energy curves of LiRb for states converging to the second and third dissociation limit. The data to construct these curves was taken from Ref. [15] of the main text.

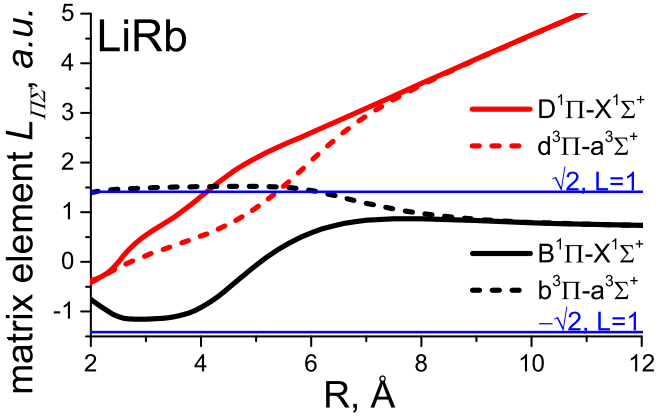

Fig. 2 The singlet-singlet and triplet-triplet $L_{\Pi\Sigma}(R)$ functions between the ground singlet and triplet states and Π states converging to the second an third dissociation limit in the LiRb molecule. The blue lines correspond to $\sqrt{L(L+1)}$ for different values of L.

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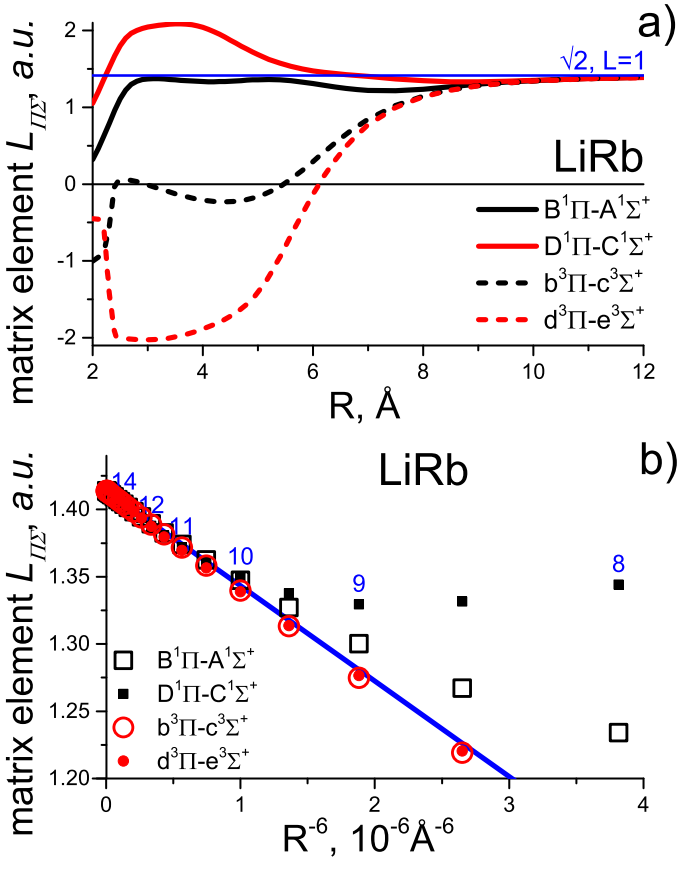

Fig. 3 a) The singlet-singlet and triplet-triplet $L_{\Pi\Sigma}(R)$ functions between states converging to the the same dissociation limits in the LiRb molecule. The blue corresponds to $\sqrt{L(L+1)}$ for $L=1$. b) The linearization of the L-uncolupling functions in R^{-6}. The blue line shows the asymptote the functions converge to as $R\to\infty$. The blue numbers indicate the internuclear distance in Å.

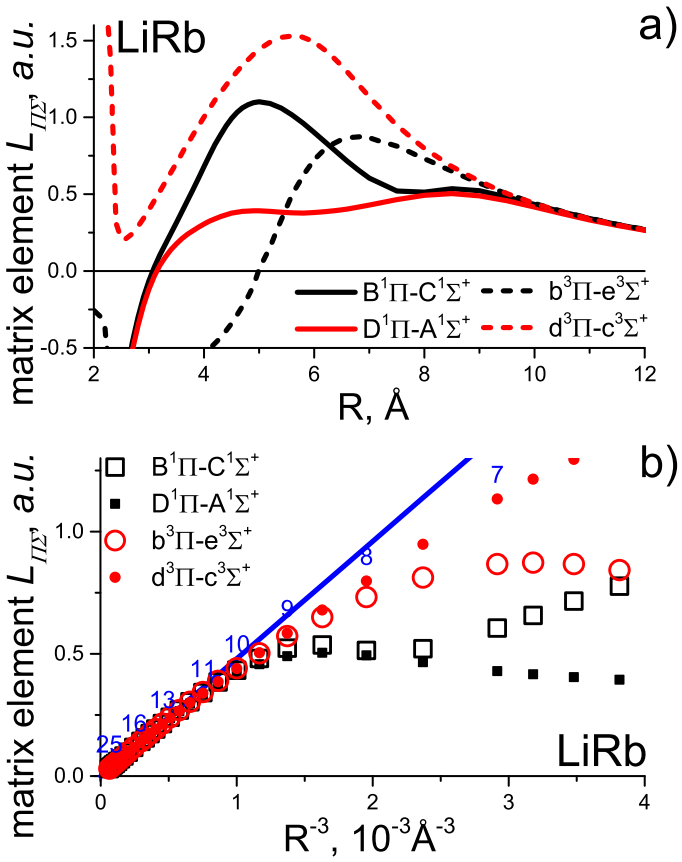

Fig. 4 a) The singlet-singlet and triplet-triplet $L_{\Pi\Sigma}(R)$ functions between states converging to different dissociation limits in LiRb. b) The linearization of the L-uncolupling functions in R^{-3}. The blue line shows the asymptote the functions converge to as $R\to\infty$. The blue numbers indicate the internuclear diustance in Å.

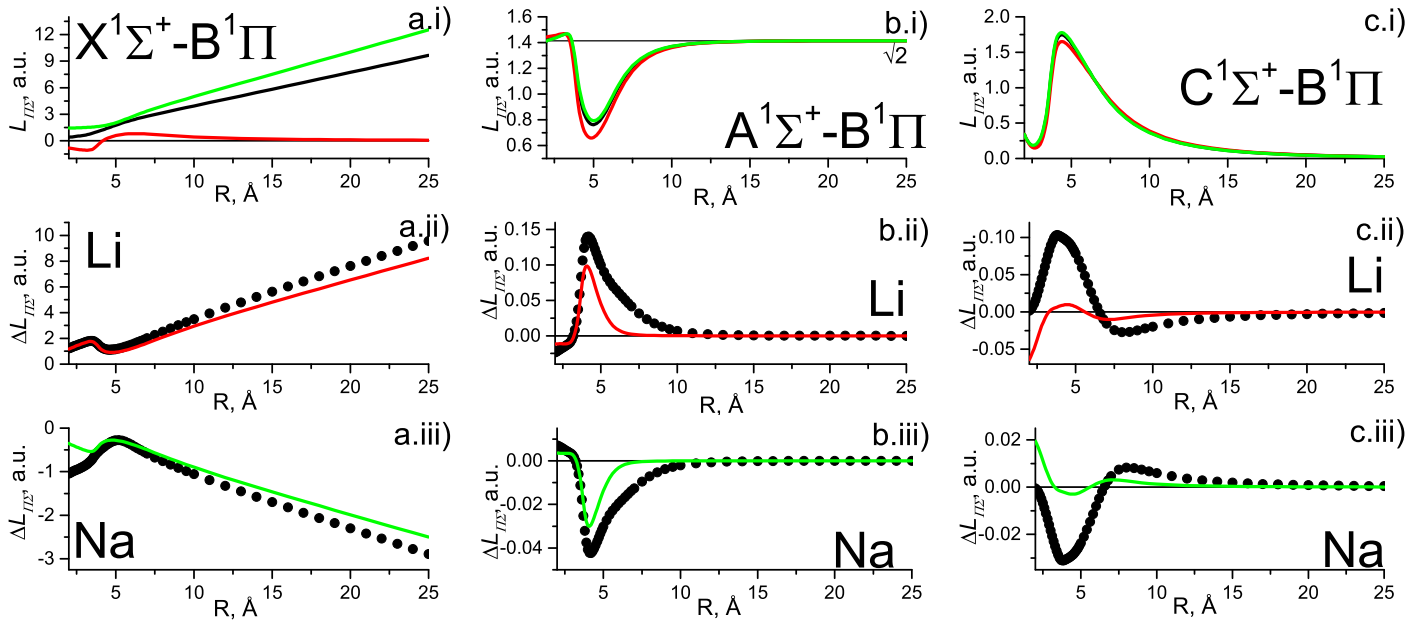

Fig. 5 Singlet-singlet L-uncoupling matrix elements in LiNa. Subfigures a.i-a.iii) between the $X^1\Sigma^+$ and $B^1\Pi$ states; Subfigures b.i-b.iii) between the $A^1\Sigma^+$ and $B^1\Pi$ states; Subfigures c.i-c.iii) between the $C^1\Sigma^+$ and $B^1\Pi$ states. The top row of subfigures (i) show the L-uncoupling matrix elements calculated with the origin of electronic coordinates located at the Li atom (red), Na atom (green), and the center of mass (black). The second (ii) and third (iii) row of sub figures show the results of calculating the correction according to formula (9) of the main manuscript as a line, and the difference between the ab initio calculations with the origin of electronic coordinates located at the center of mass and at the Li (ii) and Na (iii) atoms as black circles, respectively.

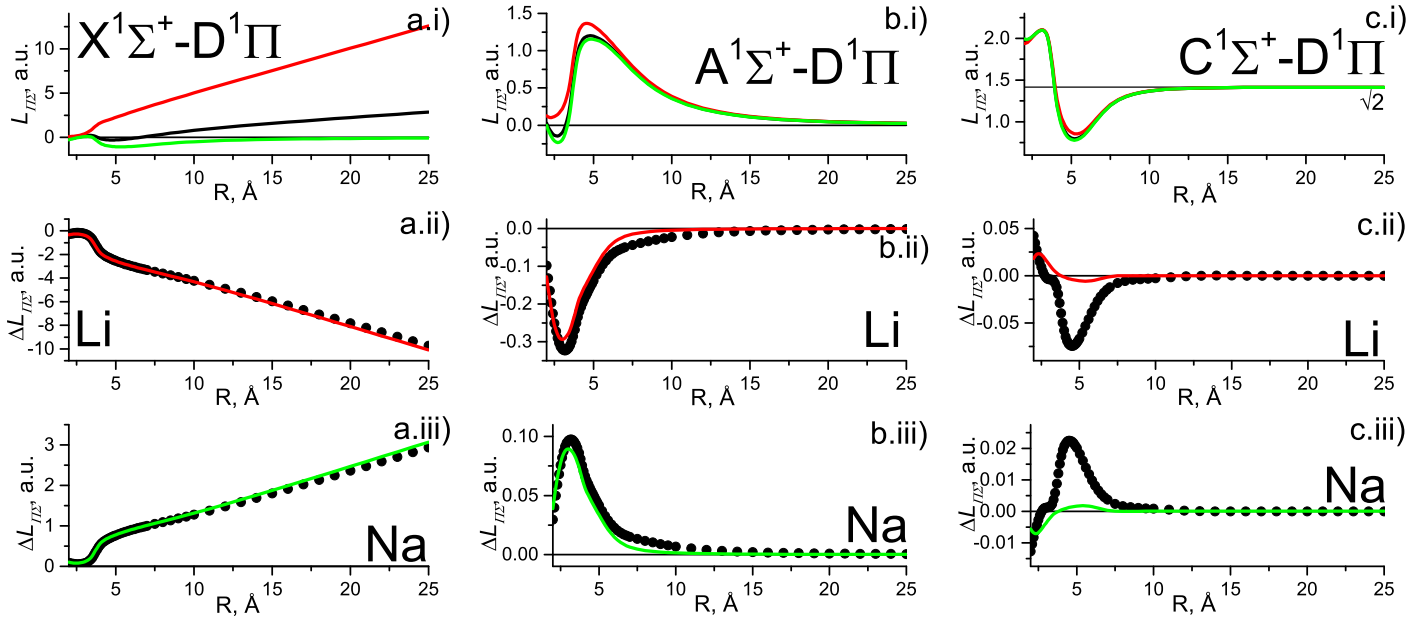

Fig. 6 Singlet-singlet L-uncoupling matrix elements in LiNa. Subfigures a.i-a.iii) between the $X^1\Sigma^+$ and $D^1\Pi$ states; Subfigures b.i-b.iii) between the $A^1\Sigma^+$ and $D^1\Pi$ states; Subfigures c.i-c.iii) between the $C^1\Sigma^+$ and $D^1\Pi$ states. The top row of subfigures (i) show the L-uncoupling matrix elements calculated with the origin of electronic coordinates located at the Li atom (red), Na atom (green), and the center of mass (black). The second (ii) and third (iii) row of sub figures show the results of calculating the correction according to formula (9) of the main manuscript as a line, and the difference between the ab initio calculations with the origin of electronic coordinates located at the center of mass and at the Li (ii) and Na (iii) atoms as black circles, respectively.

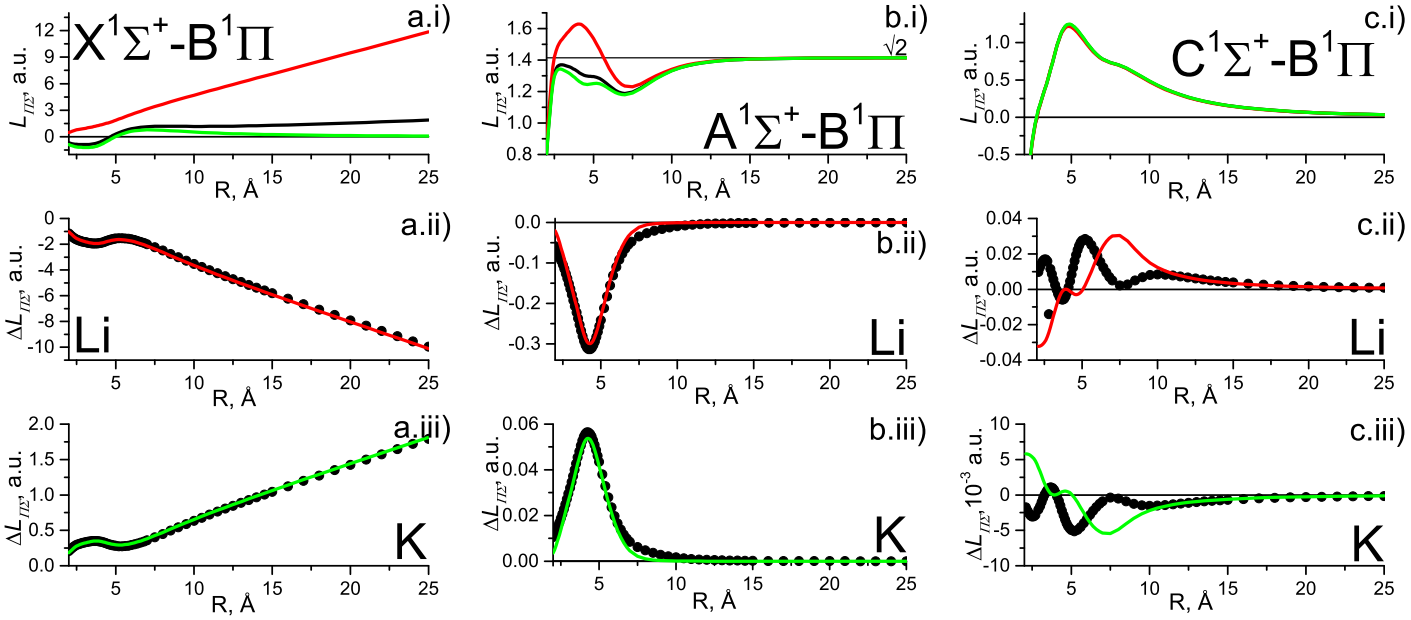

Fig. 7 Singlet-singlet L-uncoupling matrix elements in LiK. Subfigures a.i-a.iii) between the $X^1\Sigma^+$ and $B^1\Pi$ states; Subfigures b.i-b.iii) between the $A^1\Sigma^+$ and $B^1\Pi$ states; Subfigures c.i-c.iii) between the $C^1\Sigma^+$ and $B^1\Pi$ states. The top row of subfigures (i) show the L-uncoupling matrix elements calculated with the origin of electronic coordinates located at the Li atom (red), K atom (green), and the center of mass (black). The second (ii) and third (iii) row of sub figures show the results of calculating the correction according to formula (9) of the main manuscript as a line, and the difference between the ab initio calculations with the origin of electronic coordinates located at the center of mass and at the Li (ii) and K (iii) atoms as black circles, respectively.

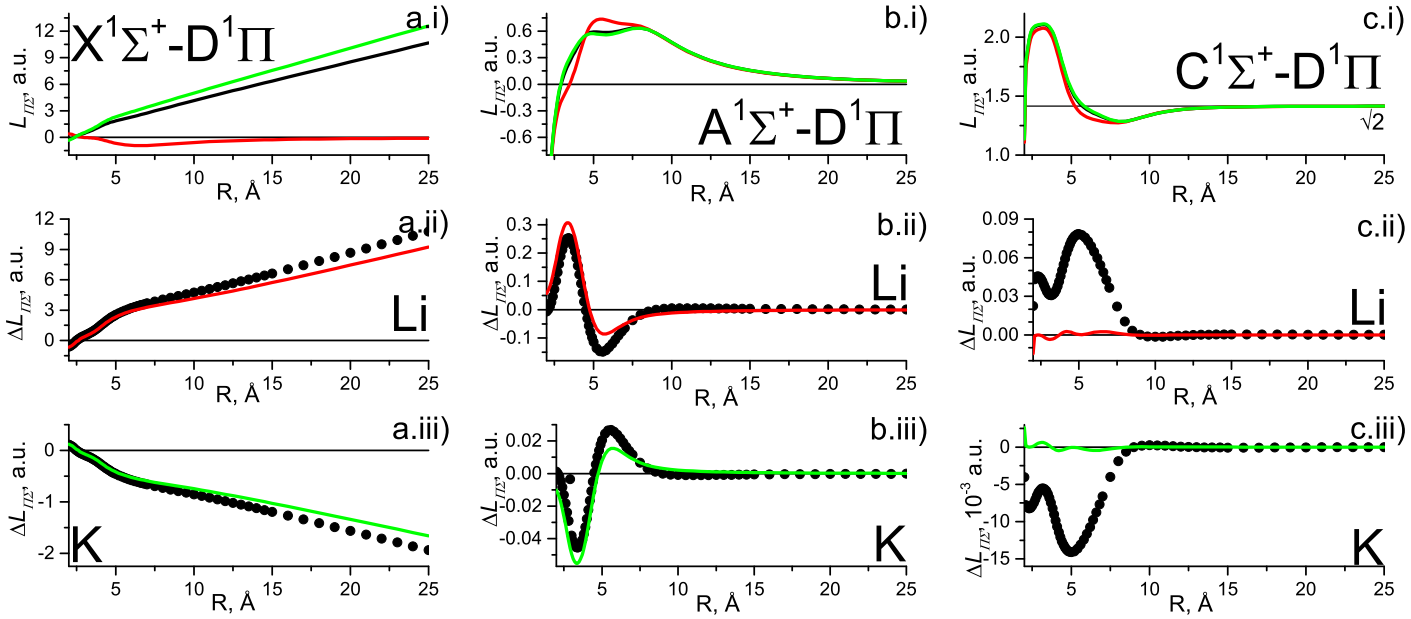

Fig. 8 Singlet-singlet L-uncoupling matrix elements in LiK. Subfigures a.i-a.iii) between the $X^1\Sigma^+$ and $D^1\Pi$ states; Subfigures b.i-b.iii) between the $A^1\Sigma^+$ and $D^1\Pi$ states; Subfigures c.i-c.iii) between the $C^1\Sigma^+$ and $D^1\Pi$ states. The top row of subfigures (i) show the L-uncoupling matrix elements calculated with the origin of electronic coordinates located at the Li atom (red), K atom (green), and the center of mass (black). The second (ii) and third (iii) row of sub figures show the results of calculating the correction according to formula (9) of the main manuscript as a line, and the difference between the ab initio calculations with the origin of electronic coordinates located at the center of mass and at the Li (ii) and K (iii) atoms as black circles, respectively.

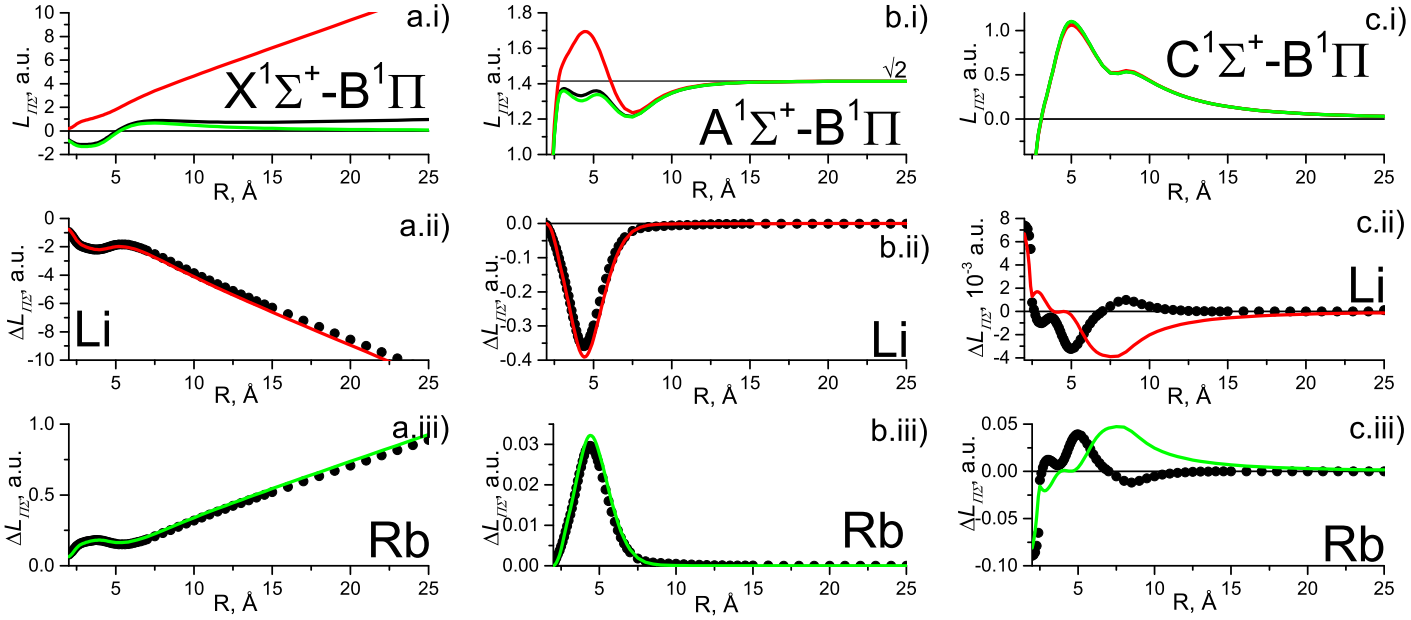

Fig. 9 Singlet-singlet L-uncoupling matrix elements in LiRb. Subfigures a.i-a.iii) between the $X^1\Sigma^+$ and $B^1\Pi$ states; Subfigures b.i-b.iii) between the $A^1\Sigma^+$ and $B^1\Pi$ states; Subfigures c.i-c.iii) between the $C^1\Sigma^+$ and $B^1\Pi$ states. The top row of subfigures (i) show the L-uncoupling matrix elements calculated with the origin of electronic coordinates located at the Li atom (red), Rb atom (green), and the center of mass (black). The second (ii) and third (iii) row of sub figures show the results of calculating the correction according to formula (9) of the main manuscript as a line, and the difference between the ab initio calculations with the origin of electronic coordinates located at the center of mass and at the Li (ii) and Rb (iii) atoms as black circles, respectively.

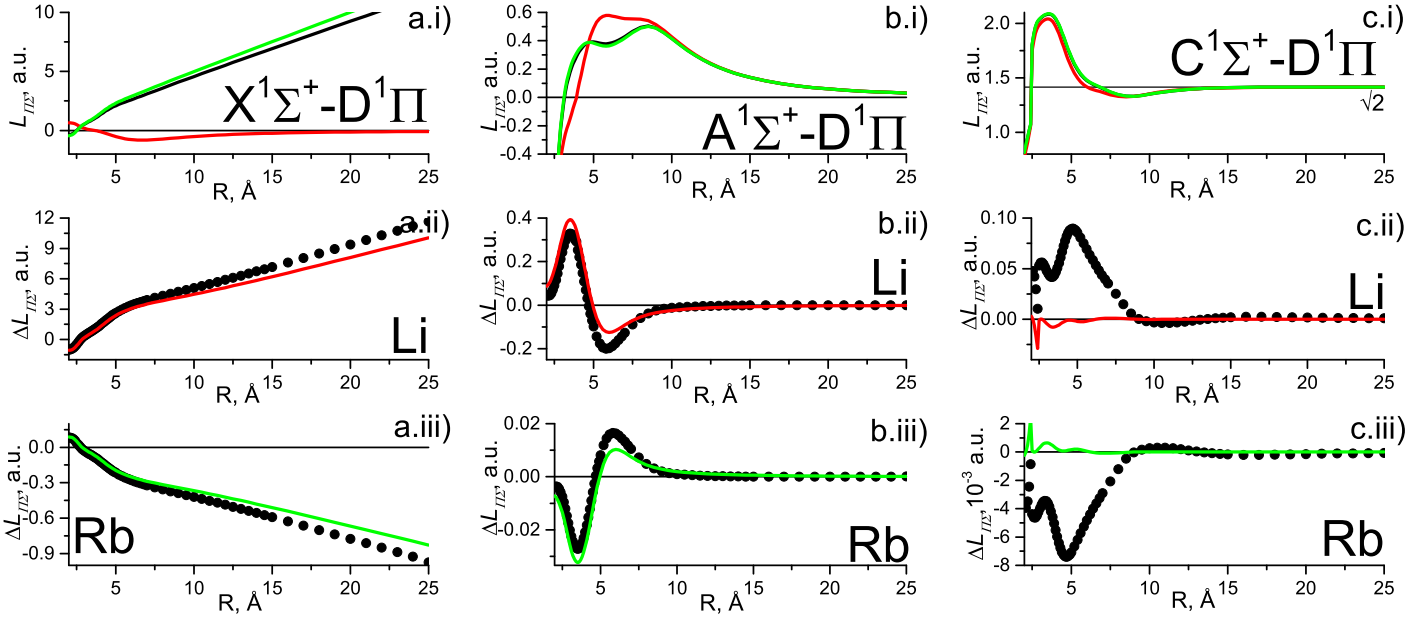

Fig. 10 Singlet-singlet L-uncoupling matrix elements in LiRb. Subfigures a.i-a.iii) between the $X^1\Sigma^+$ and $D^1\Pi$ states; Subfigures b.i-b.iii) between the $A^1\Sigma^+$ and $D^1\Pi$ states; Subfigures c.i-c.iii) between the $C^1\Sigma^+$ and $D^1\Pi$ states. The top row of subfigures (i) show the L-uncoupling matrix elements calculated with the origin of electronic coordinates located at the Li atom (red), Rb atom (green), and the center of mass (black). The second (ii) and third (iii) row of sub figures show the results of calculating the correction according to formula (9) of the main manuscript as a line, and the difference between the ab initio calculations with the origin of electronic coordinates located at the center of mass and at the Li (ii) and Rb (iii) atoms as black circles, respectively.