DIRECT-POTENTIAL-FIT DETERMINATION OF AN ACCURATE ANALYTICAL POTENTIAL FOR THE $B\,^1\Pi_u$ "BARRIER" STATE OF Li_2

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The potential energy curve for the $B\,^1\Pi_u$ state of Li_2 is known to have an unusual shape, in that its long-range interaction is dominated by a repulsive term which gives this potential a rotationless barrier which protrudes above its energy asymptote. We have used program DSPotFit[a] in a direct fit of available spectroscopic data for this state, including the observed Λ–doubling splittings and tunneling predissociation line widths, to determine an analytic potential energy function plus Born-Oppenheimer breakdown and Λ–doubling radial correction functions. Differences between this approach and a recent direct-potential-fit analysis[b] using a numerical model potential function will be critically examined.

[a] R.J. Le Roy, J.Y. Seto and Y. Huang, University of Waterloo Chemical Physics Research Report CP-651 (2001); also available through http://leroy.uwaterloo.ca.

[b] N. Bouloufa, P. Cacciani, R. Vetter, A. Yiannopoulou, F. Martin and A.J. Ross, *J. Chem. Phys.* (2001, in press).