

DIRECT-POTENTIAL-FIT DETERMINATION OF AN ACCURATE ANALYTICAL POTENTIAL FOR THE $F(4)^1\Sigma_g^+$ “SHELF” STATE OF Li_2

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The $F(4)^1\Sigma^+$ state of Li_2 is known to have an unusual shape because of two (or three) avoided crossings with other states of the same symmetry. One of these avoided crossings gives rise to a well defined “shelf” in the effective adiabatic potential curve, which makes analysis of data for this state by traditional methods quite difficult, since conventional molecular constant expressions cannot describe the resulting level energy patterns. Recent experimental results^a have yielded precise measurements of selected vibration-rotation levels of this state spanning almost the entire interval from the potential minimum to dissociation. The present paper describes our use of “direct-potential-fit” (DPF) methods to quantitatively reanalyse those data and determine an accurate analytic potential energy function for this shelf-state system.

^a S. Antonova, G. Lazarov, K. Urbanski, A. M. Lyra, L. Li, G.-H. Jeung and W. C. Stwalley, *J. Chem. Phys.* **112** (2000).