

DIRECT-POTENTIAL-FIT DETERMINATION OF THE LiH ($C^1\Sigma^+$) DOUBLE MINIMUM POTENTIAL

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Empirical analyses of data involving states whose potential energy curves have double or multiple minima tend to be fragmentary or approximate, since conventional molecular constant expressions cannot describe their level energy patterns. The only accurate quantal way of analysing such data is to perform direct fits of the data to analytic expressions for the underlying potential energy curves. This paper describes our direct-potential-fit (DPF) analysis of recently published^a data for the $C^1\Sigma^+$ state of LiH which is known^b to have a shallow second potential well lying near dissociation on the inner potential wall. The resulting potential has the “MLJ” form $V(R) = \mathcal{D}_e[1 - (R_e/R)^n e^{-\beta(z)} z]^2$, where $z = (R - R_e)/(R + R_e)$ and $\beta(z)$ is a power series in z which has smooth monotonic behaviour across the region where the potential oscillates to support the two minima.^c

^a J.-J. Chen, W.-T. Luh and G.-H. Jeung, *J. Chem. Phys.* **110**, 4402 (1999)

^b A. Boutalib and F. X. Gadéa, *J. Chem. Phys.* **97**, 1144 (1992)

^c P. G. Hajigeorgiou and R. J. Le Roy, *J. Chem. Phys.* **112**, 3949 (2000).