

QUANTITATIVE ANALYSIS OF NON-ADIABATIC PREDISSOCIATION OF Li₂ (*F* 1Σ_g⁺)

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Extensive recent measurements^a of the widths of predissociating levels of the *F*(4) 1Σ_g⁺ state of Li₂ are analysed within an adiabatic description of the interstate mixing of the *F*(4) and *E*(3) 1Σ_g⁺ states. The coupling operator driving the predissociation is the sum of two terms of the form $(-\hbar^2/2\mu) [2 W'_e(R) + W_e(R) \frac{d}{dR}]$, where each $W_e(R)$ function is a Lorentzian centred at one of the avoided crossings between the adiabatic *F*- and *E*-state potential energy curves.^b Application of an updated^c version of photodissociation code BCONT^d allows the parameters of the two Lorentzians defining this coupling operator to be quantitatively determined from a direct least-squares fit to the 274 measured^a line widths for ^{7,7}Li₂.

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

^b A. Bandrauk and M. S. Child, *Mol. Phys.* **19**, 95 (1970).

^c R. J. Le Roy, <http://theochem.uwaterloo.ca/~leroy> (2000).

^d R. J. Le Roy, *Comp. Phys. Comm.* **52**, 383 (1989).