COMPARISON OF COMPUTED CONDON LOCI WITH FRANCK-CONDON FACTORS IN DESLANDRES TABLES OF MOLECULAR BAND SYSTEMS

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The literature often shows a Condon parabola not quite tracking the Franck-Condon factors for the strongest bands in the Deslandres table for a diatomic molecular band system [a]; often the parabola appears to have been hand-drawn [b]. We have calculated Condon loci, assuming originally that the lower and upper electronic potentials are simple harmonic potentials, and assuming now that they are Morse potentials. In the harmonic case the Condon loci are parabolas. These calculations are for small vibrational quantum numbers, where the Morse loci also begin as parabolas. We will present these loci for representative molecular band systems and discuss the extent to which the loci track the strongest Franck-Condon factors. In the event that neither does, calculations for arbitrary potentials are available. The importance of this study is that we have previously calculated the latera recta and the symmetry-axis angles of the harmonic oscillator parabolas in Deslandres tables appropriate to molecules in several isoelectronic sequences. We have found that the angle increases along the sequence until the species one proton-shift away from rare-gas molecules, such as LiNe, is reached. This phenomenon is a suggestion that diatomic molecules are periodic with respect to each of their two atoms.

[a] G. Herzberg, Molecular Spectra and Molecular Structure, 1950, pg. 197

[b] D. J. Flynn, R. J. Spindler; S. Fifer; M. Kelly, J. Quant. Spectr. Radiat. Transfer 4, 271-282, (1964); R. W. Nicholls, J. Quant. Spectr. Radiat. Transfer 28, 481-492, (1982).