

PURE MW DATA FOR $v = 0 - 6$ OF PbI GIVE VIBRATIONAL SPACINGS AND A FULL ANALYTIC POTENTIAL ENERGY FUNCTION

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At last year's ISMS meeting, Zaleski *et al.* reported new broadband MW spectroscopy measurements of pure rotational transitions in the $v = 0 - 6$ levels of the $^2\Pi_{1/2}$ ground electronic state of PbI.^a The analysis presented at that time was a conventional v -level by v -level 'band-constant' analysis performed using the PGopher program.^b That level-by-level PGopher analysis yielded values of B_v , D_v and five spin-splitting parameters for each vibrational level of each isotopologue. Ignoring the spin-splitting information, the B_v and D_v values were used to generate a set of synthetic pure $R(0)$ transitions for each level that were taken to represent the "mechanical" information about the molecule contained in these spectra. A standard direct-potential-fit (DPF) analysis^c was then used to fit these data to an "Expanded Morse Oscillator" (EMO) potential function form. The well-depth parameter \mathcal{D}_e was fixed at the literature value, while values of the equilibrium distance r_e and three EMO exponent-coefficient expansion 'potential shape' parameters are determined from the fits. The best fits to the data yield potentials whose fundamental vibrational spacings are in excellent agreement with experiment^d together with reliable predictions for the first five overtone energies.

^a D.P. Zaleski, H. Köckert, S.L. Stephens, N. Walker, L.-M. Dickens, and C. Evans, paper RE08 at the 69th International Symposium on Molecular Spectroscopy, University of Illinois (2014).

^b **PGopher** - a Program for Simulating Rotational Structure, C. M. Western, University of Bristol, <http://pgopher.chm.bris.ac.uk>

^c **DPotFit 2.0**: A Computer Program for fitting Diatomic Molecule Spectra to Potential Energy Functions, R.J. Le Roy, J. Seto and Y. Huang, University of Waterloo Chemical Physics Research Report CP-667 (2013); see <http://leroy.uwaterloo.ca/programs/>.

^d K. Ziebarth, R. Breidohr, O. Shestakov and E.H. Fink, *Chem. Phys. Lett.* **190**, 271 (1992).