ACCURATE ANALYTIC POTENTIALS FOR THE $A\,^3\Pi_1$ and $X\,^1\Sigma^+$ STATES OF IBr FROM A COMBINED-ISOTOPOLOGUE DIRECT-POTENTIAL-FIT DATA ANALYSIS

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Iodine monobromide has been studied in various wavelength regions by researchers using diffraction grating, microwave, and high-resolution laser techniques combined with a Fourier transform spectrometer. Differences in predictions generated from parameters for the $A\,^3\Pi_1$ and $X\,^1\Sigma^+$ states obtained from some of these studies show that it can be difficult to make reliable predictions outside the data region, especially if one is using conventional Dunham expansions. In the present work, high resolution absorption[a] and laser excitation[b] data for the $X\,^1\Sigma^+ - A\,^3\Pi_1$ system of $I^{79}Br$ and $I^{81}Br$, together with earlier microwave, infrared, and fluorescence progression data, are analyzed using a direct-potential-fit (DPF) procedure to obtain accurate analytic potential energy functions for the two states that provide a compact unified description of all of the available data, as well as realistic predictions for the unobserved levels of this species.

[a] N. Nishimiya, T. Yukiya and M. Suzuki, J. Mol. Spectrosc. **173**, 8 (1995).
[b] D.R.T. Appadoo, P.F. Bernath, and R.J. Le Roy, Can. J. Phys. **72**, 1265 (1994).