DIRECT-POTENTIAL-FIT (DPF) ANALYSIS FOR THE $A\,^3\Pi_1 - X\,^1\Sigma^+$ SYSTEM OF $I^{35/37}Cl$.

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The goal of this research is to obtain an optimal, portable, global description of, and summary of the dynamical properties of, the $A\,^3\Pi_1$ and $X\,^1\Sigma^+$ states of $I^{35/37}Cl$, by using 'direct potential fits' (DPFs) to all of the available spectroscopic data for this system to determine optimal analytic potential energy functions for these two states that represent all of those data (on average), within the experimental uncertainties. The DPF method compares observed spectroscopic data with synthetic data generated by solving the radial Schrödinger equation for the upper and lower level of every observed transition for some parameterized analytic potential function(s), and using least-squares fits to the data to optimize those parameters. The present work uses the Morse/Long-Range (MLR) potential function form because it is very flexible, can incorporate the correct theoretically known inverse-power-sum long-range behaviour, is everywhere continuous and differentiable to all orders, and has robust extrapolation properties at both large and small distances. The DPF approach also tends to require fewer fitting parameters than do traditional Dunham analyses, as well as having much more robust extrapolation properties in both the v and J domains. The present work combines the data for the $A\,^3\Pi_1$ and $X\,^1\Sigma^+$ states obtained in 1980 by Coxon *et al.*[a] using UV and near-infrared grating spectrometers, with our measurements in the 0.7-0.8μm region, obtained using a CW Ti:Sapphire Ring Laser.[b] The results of this study and our new fully analytic potential energy functions for the $A\,^3\Pi_1$ and $X\,^1\Sigma^+$ states of ICl will be presented.

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[a] J.A. Coxon, R.M. Gordon and M.A. Wickramaaratchi, *J. Mol. Spectrosc.* **79** (1980) 363 and 380.

[b] T.Yukiya, N. Nishimiya and M. Suzuki, *J. Mol. Spectrosc.* **269** (2011) 193.