APPLICATION OF A DIRECT POTENTIAL FITTING METHOD TO THE $B^1\Sigma^+$ AND $X^1\Sigma^+$ ELECTRONIC STATES OF HF AND DF

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A collection of 6070 spectroscopic line positions for hydrogen fluoride and deuterium fluoride, which consists of all microwave and infrared $X^1\Sigma^+$ ground electronic state data, and the $B^1\Sigma^+$ - $X^1\Sigma^+$ emission band system data, has been employed in a weighted least-squares fit directly to the radial Hamiltonian operators of the $B^1\Sigma^+$ and $X^1\Sigma^+$ electronic states. The radial Hamiltonian operator model includes first- and second-order corrections to the Born-Oppenheimer approximation and was derived from the landmark theoretical work of Watson[a]. The $principle\ isotopomer$ fitting strategy of Le Roy[b] was incorporated in the least-squares fit. A total of 54 adjustable parameters was required to obtain a satisfactory representation of the experimental data, with a reduced standard deviation of 1.03. In addition, a collection of highly accurate quantum-mechanically meaningful rotational and centrifugal distortion constants was calculated from the derived Hamiltonian operators of the two electronic states.

[a] J. K. G. Watson, J. Mol. Spectrosc. 80, 411 (1980).
[b] R. J. Le Roy, J. Mol. Spectrosc. 194, 189 (1999).