

STATISTICAL ERROR PROPAGATION IN THE COMPUTATION OF RKR POTENTIAL CURVES, SPECTROSCOPIC CONSTANTS, AND FRANCK-CONDON FACTORS: THE  $D$  STATE OF  $I_2$

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Existing spectroscopic data for the  $D$  ion-pair state of  $I_2$  are reanalyzed with the primary goal of improving and extending to higher  $v$  the rotational constants  $B_v$ . The lack of rotational data for the  $v = 130$ -200 region makes the structure of this data set unusual, and has prompted a thorough study of the propagated statistical error in the directly fitted spectroscopic constants,  $T_v$  and  $B_v$ , and in the RKR potential curve calculated therefrom. For the first time, such error propagation computations have been extended to properties computed by numerical solution of the Schroedinger equation for the state in question: the quantum vibrational energy  $G_v$  and rotational constant  $B_v$ , centrifugal distortion constants  $D_v$  and  $H_v$ , and Franck-Condon factors for the  $D - X$  transition.