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.