PRECISE DETERMINATION OF THE B AND C STATES OF XeF FROM A DEPERTURBATION ANALYSIS OF THE $B \rightarrow X$ SPECTRUM OF ^{136} XeF

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The B ($^1/_2$) and C ($^3/_2$) ion-pair excited states of XeF are coupled by the rotational Hamiltonian, producing perturbations in the rotational structure of $B \rightarrow X$ ($^2\Sigma^+$) transitions involving v' levels < 5. A number of $v' - v''$ bands in the $B \rightarrow X$ emission spectrum of the single isotopomer $^{136}Xe^{19}F$ are analyzed by a deperturbation model to yield improved spectroscopic descriptions of the low-v regions of the B and C states. The C state lies 797 cm^{-1} below the B state, with R_e = 2.473 Å. The electronic perturbative coupling element for B–C interactions is 6% below the simple Hund's case c-based prediction and just 3% greater than an estimate obtained from a more elaborate case-a approach.