VIBRONIC PERTURBATIONS IN THE ELECTRONIC SPECTRUM OF BeC

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Electronic spectra for BeC have been recorded over the range 30,500-40,000 cm^{-1}. Laser ablation and jet-cooling techniques were used to obtain rotationally resolved data. The vibronic structure consists of a large number of bands with erratic energy spacings. Two-color photoionization threshold measurements were used to show that the majority of these features originated from the ground state zero-point level. The rotational structures are mostly consistent with the bands of $^3\Pi$-$X^3\Sigma^-$ transitions. Theoretical calculations indicate that the erratic vibronic structure results from strong interactions between the four lowest energy $^3\Pi$ states. Adiabatic potential energy curves were obtained from dynamically weighted MRCI calculations. Diabatic potentials and coupling matrix elements were then reconstructed from these results, and used to compute the vibronic energy levels for the four interacting $^3\Pi$ states. The predictions were sufficiently close to the observed structure to permit assignment of the main features. Bands originating from the low-lying $^5\Sigma^-$ state were also identified, yielding a $^5\Sigma^-$ to $X^3\Sigma^-$ energy interval of 2200$\pm$50 cm^{-1}.