THE LOW-LYING XCN BENDING MODES OF THE QUASILINEAR MOLECULES ClCNO AND BrCNO

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From the satellite structures in the a-type rotational spectra, the halofulminates ClCNO and BrCNO have been shown to be extremely quasilinear molecules, definitely more quasilinear than fulminic acid HCNO and roughly comparable to carbon suboxide OCCCO[ab]. In order to obtain a more fundamental description of the quasilinear dynamics, we have determined effective bending potentials for the anharmonic XCN bending modes of the two molecules by *semirigid bender* analyses of the a-type rotational data. Fitting Barrow-Dixon-Duxbury potential functions[c], the effective barriers to linearity have been determined to be 167 and 131 cm^{-1}, the origins of the ${}^{r}Q_0$ branches in the vibrational ground states to be 17.7 and 16.0 cm^{-1}, and the quasilinearity parameters ${\gamma_0}^{d}$ to be +0.416 and +0.362, respectively. These results will be compared to some results published for several other chain molecules.

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