

NEW RESULTS FROM THE ROTATIONAL SPECTRA OF THE HALOGEN MONOXIDES. INTERATOMIC POTENTIALS, FINE AND HYPERFINE INTERACTIONS.

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Last year we reported the IO rotational spectrum in vibrational levels up to $v = 13$ for the $X_1 \ ^2\Pi_{3/2}$ state and to $v = 9$ for the $X_2 \ ^2\Pi_{1/2}$ state. In comparison, previous studies of BrO were limited to $v = 2$ for X_1 and $v = 1$ for the X_2 state. Using the DC discharge cell that was so effective for vibrational excitation of IO, measurements of BrO have now been extended up to $v = 8$ and $v = 7$ for the X_1 and X_2 states, respectively. Excited vibrational levels of ClO were not obtained with these methods, however good signal to noise at thermal populations allowed measurements for the $v = 2$ levels of both the X_1 and X_2 states as well as ^{18}O in natural abundance. The Hamiltonian of Brown, *et. al.*^a, with explicit isotope dependencies for each parameter, has provided a set of mass and nuclear moment independent parameters for each of the halogen monoxide species. The electron spin-rotation constant, γ , and the centrifugal distortion of the spin-orbit splitting, A_D , which are normally correlated, have been separately determined by the isotope dependence of their contributions to the spectrum. Interatomic potentials have been derived from the mass-independent parameters that are accurate up to the observed excitation energies for each molecule. Analyses of the fine-structure parameters indicate that these molecules are close to the single perturber limit. The hyperfine parameters will be compared with the literature values^{b,c,d} of the appropriate calculated relativistic radial integrals of the halogens.

^aJ. M. Brown and J. K. G. Watson, *J. Mol. Spec.* **148**, 371 (1991).

^bP. Pyykkö, M. Seth, *Theor. Chem. Acc.* **96**, 92-104 (1997).

^cI. Lindgren and A. Rosén, *Case Studies in Atomic Physics*, **4**, 197-298 (1974).

^dP. Pyykkö and L. Wiesenfeld, *Mol. Phys.* **43**, 557-580 (1981).