SPECTROSCOPIC IMPLICATIONS OF THE "STRUCTURE" OF HELIUM DIHALOGEN COMPLEXES

SARA E. RAY and ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*; JOHN M. HERBERT, *Department of Chemistry, University of California, Berkeley, CA 94720*.

The rovibronic ($\tilde{B} \leftarrow \tilde{X}$) transitions of He·$Br_2$ and He·I_2 have been studied through calculations of the energies of the bound states on the X and B state potential surfaces. In these studies, literature potentials are used for all but the X-state of He·Br_2.[ab] In that case, we calculated the potential at the CCSD(T) level of theory using the SDD+G($3df$) basis for Br, the aug- cc-pVQZ basis for He, and a $3s3p2d2f1g$ set of bond functions, optimized for rare-gas molecule interactions,[c] centered at the midpoint between He and the Br_2 center of mass. Using these potentials, the energies and wave functions of the bound states of the complexes are generated for $J \leq 9$. From these results, the vibronic spectra are computed over a range of temperatures from 0.1 to 2.5 K. Excellent agreement with the reported spectra is obtained.

[a] M. P. de Lara-Castells, A. A. Buchachenko, G. Delgado-Barrio, and P. Villarreal, J. Chem. Phys. 120, 2182 (2004).
[b] R.Prosmiti, A. Valdes, P. Villarreal, and G. Delgado-Barrio, J. Chem. Phys. 108, 6065 (2004).
[c] S. M. Cybulski and R. R. Toczylowski, J. Chem. Phys. 111, 10520 (1999).