Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

Spectroscopic Identification of Multiple Conformers of $o,p$-$\text{H}_2$ · · ·$\text{ICl}$ and $o,p$-$\text{H}_2$ · · ·$\text{I}_2$ Complexes JOSHUA DARR, RICHARD LOOMIS, Department of Chemistry Washington University in St. Louis — Laser-induced fluorescence and action spectroscopy experiments have identified ro-vibronic transitions associated with multiple conformers of the $o,p$-$\text{H}_2$ · · ·$\text{ICl}$($X,v=0$) and $o,p$-$\text{H}_2$ · · ·$\text{I}_2$($X,v=0$) complexes. For each complex, the conformers with the hydrogen molecule localized at the end of the dihalogen, with a $C_{2v}$ symmetry, are more stable than the conformers with the hydrogen molecule localized in the T-shaped well, which lies orthogonally about the dihalogen bond axis. Furthermore, the conformers containing $o$-$\text{H}_2$($j=1$) and $p$-$\text{D}_2$($j=1$) are found to be more strongly bound than those containing $p$-$\text{H}_2$($j=0$) and $o$-$\text{D}_2$($j=0$). The role of multi-pole electrostatic interactions is elucidated by comparing the binding energies of the $\text{H}_2$ · · ·$\text{ICl}$($X,v=0$) and $\text{H}_2$ · · ·$\text{I}_2$($X,v=0$) complexes with $C_{2v}$ symmetries. The relative populations of the $C_{2v}$ and T-shaped conformers can be altered by changing the properties of the supersonic expansion used to stabilize the complexes. The relative populations of the $o$-$\text{H}_2$ · · ·$\text{ICl}$($X,v=0$) and $p$-$\text{H}_2$ · · ·$\text{ICl}$($X,v=0$) conformers can also be manipulated, with a population ratio of 3:1 approached by decreasing the hydrogen concentration in helium.

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Date submitted: 22 Nov 2005  
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