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Spectroscopic Identification of Multiple Conformers of o,p-$H_2\cdot\cdot\cdot$ICl and o,p-$H_2\cdots I_2$ 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-$H_2\cdot\cdot$ICl(X,v=0) and o,p-$H_2\cdot\cdot I_2$(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-H_2(j=1) and p-D_2(j=1) are found to be more strongly bound than those containing p-H_2(j=0) and o-D_2(j=0). The role of multi-pole electrostatic interactions is elucidated by comparing the binding energies of the $H_2\cdots$ICl(X,v=0) and $H_2\cdots I_2$(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-$H_2\cdot\cdot$ICl(X,v=0) and p-$H_2\cdots$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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