CORRELATED AB INITIO STUDY OF THE GROUND ELECTRONIC STATE OF THE $O_2$-HCN COMPLEX

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The potential energy surface of the $O_2(X^3\Sigma_g^-)$-HCN complex has been investigated using the CCSD(T) level of theory with the aug-cc-pVDZ and aug-cc-pVTZ basis sets. Results of calculations with the aug-cc-pVTZ basis set provided a minimum energy structure of a planar bent geometry with a well depth of about 320 $\mathrm{cm}^{-1}$. In Jacobi coordinates, the angles between the internuclear axes of the $O_2$ and the HCN monomers with respect to the axis that connects their centers of masses in the complex are $48^\circ$ and $6^\circ$, respectively. The distance between centers of masses of moieties of the complex is 3.9 Å. Currently, calculations with the aug-cc-pVQZ basis set as well as effects of the BSSE corrections are being investigated. Results of the current work will be discussed and compared to results of our previous ab initio study of the $O_2(X^3\Sigma_g^-)$-$H_2$ and $O_2(X^3\Sigma_g^-)$-HF complexes.