CORRELATED AB INITIO STUDY OF THE GROUND ELECTRONIC STATE OF THE H_2–O_2^- COMPLEX

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The H_2–O_2^- $(X^2\Pi_g)$ complex has been examined using the coupled-cluster theory at the CCSD(T)/aug-cc-pVDZ and CCSD(T)/aug-cc-pVTZ levels. Electronic structure calculations show that the global minimum energy structure corresponds to a planar bent geometry with a well depth of 1550 cm^{-1}. For this geometry, the distance between centers of masses of moieties of the complex is 2.57Å, angstroms and the angles between the internuclear axes of the superoxide radical and the hydrogen molecule with respect to the axis that connects their centers of masses are 104° and 165° , respectively. These results indicate that the hydrogen molecule and the superoxide radical are held together by a strong hydrogen bond within the complex. Results of the current work will be discussed and compared to results of our recent ab initio study[a] of the H_2–O_2 (X $^3\Sigma_g^-$) complex.

[a] Wafaa M. Fawzy, in preparation for publication