ACCURATE FIRST DISSOCIATION LIMIT OF THE OZONE MOLECULE FROM *AB INITIO* CALCULATIONS

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In this work a good agreement was achieved between the theoretical and the empirical value of the first dissociation limit (D_e) of $O_3(\tilde{X}^1A_1)$. The *ab initio* calculations were done with the extended CAS(24, 15) active space and with the inclusion of the spin-orbit coupling between the nine electronic states approaching in D_e. Finally, the full-dimensional potential energy surface was developed in the scattering (Jacobi) coordinates for the long-range region ($R_{O_2\text{-}O} \geq 5\ a_0$).

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