

A Density Functional Theory Study of the $\text{Cu}^+ \cdot \text{O}_2$ and $\text{Cu}^+ \cdot \text{N}_2$ Adducts

Jamal N. Dawoud^a, Ismail I. Fafous^a, and Amin F. Majdalawieh^b

^a Department of Chemistry, Faculty of Science, Hashemite University, Zarqa 13115,
P. O. Box 150459, Jordan

^b Department of Biology, Chemistry and Environmental Sciences, Faculty of Arts and Sciences,
American University of Sharjah, Sharjah, P. O. Box 26666, United Arab Emirates

Reprint requests to Jamal N. Dawoud. E-mail: jamaldawoud@hu.edu.jo

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The geometries and harmonic vibration frequencies of the $\text{Cu}^+ \cdot \text{O}_2$ and $\text{Cu}^+ \cdot \text{N}_2$ are determined by various density functional theory (DFT) methods employing different basis sets. The potential energy surfaces (PES) are examined. The $\text{Cu}^+ \cdot \text{O}_2$ adduct exhibits a bent structure with a binding energy of $12.4 \text{ kcal mol}^{-1}$, whereas $\text{Cu}^+ \cdot \text{N}_2$ exhibits a linear configuration with a binding energy of $23.5 \text{ kcal mol}^{-1}$. The binding energy values for the two adducts agree well with the available published experimental and theoretical data and hence are reliable.

Key words: Copper Ion Complexes, Potential Energy Surface, Gas Separation, Binding Energies, NBO Analysis, Oxygen, Nitrogen