Reactions of Laser-Ablated U Atoms with CO and Ar, Kr and Xe. Infrared Spectra and Density Functional Calculations for Triplet CUO

Lester Andrews* and Binyong Liang

University of Virginia, Department of Chemistry, Charlottesville, VA 22904-4319

Jun Li and Bruce E. Bursten

The Ohio State University, Department of Chemistry, Columbus, OH 43210

Abstract

Laser-ablated U atoms react with CO in excess argon to produce CUO, which is trapped in a bent triplet state in solid argon at 7 K, based on agreement between observed and relativistic density functional theory calculated isotopic frequencies ($^{12}C^{16}O$, $^{13}C^{16}O$, $^{12}C^{18}O$). This contrasts a recent neon matrix investigation, which trapped CUO in a linear singlet state calculated to be 1.6 kcal/mol lower in energy. The argon interaction with triplet CUO makes this species the global minimum energy trapped state in solid argon. Experiments with < 1% Ar in Ne and density functional calculations suggest that a single argon atom is sufficient to trap the triplet state CUO(Ar) complex. Similar krypton and xenon experiments give small shifts for CUO(Kr) and CUO(Xe) in the same triplet state trapped in solid argon.

New results with PtNN, $PtNN^-$ and $Pt(NN)_2^{+,0,-}$ will also be discussed

*Electronic mail: lsa@virginia.edu