

THE SEARCH FOR A DOUBLE-STUFFED URANIUM METALLOCENE

J. L. SONNENBERG, J. ZHOU, H. B. SCHLEGEL, *Department of Chemistry, Wayne State University, Detroit, MI-48202.*

The discovery of $Zn(I)_2(\eta^5-C_5Me_5)^2$ has fundamentally changed the definition of metallocene by introducing dimetallic units to the middle of the classic sandwich complex. Since actinide metallocenes employing COT ($COT = [C_8H_8]^{2-}$) rings are well known, it occurred to us that uranium dimers may be stabilized by this new bonding motif. Scalar-relativistic density functional theory calculations have been employed to investigate the isomers of $[U(n)_2(COT)_2]^{2n-4}$ complexes where $n = 2$ or 3 . The IR and NMR vibrational signatures of these complexes is presented to facilitate experimental detection.