THE SEARCH FOR A DOUBLE-STUFFED URANIUM METALLOCENE

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The discovery of $\mathrm{Zn(I)_2(\eta^5\text{-}C_5Me_5)^2}$ 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 = $[\mathrm{C_8H_8}]^{2-}$) 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 $[\mathrm{U}(n)_2(\mathrm{COT})_2]^{2n-4}$ complexes where n = 2 or 3. The IR and NMR vibrational signatures of these complexes is presented to facilitate experimental detection.