

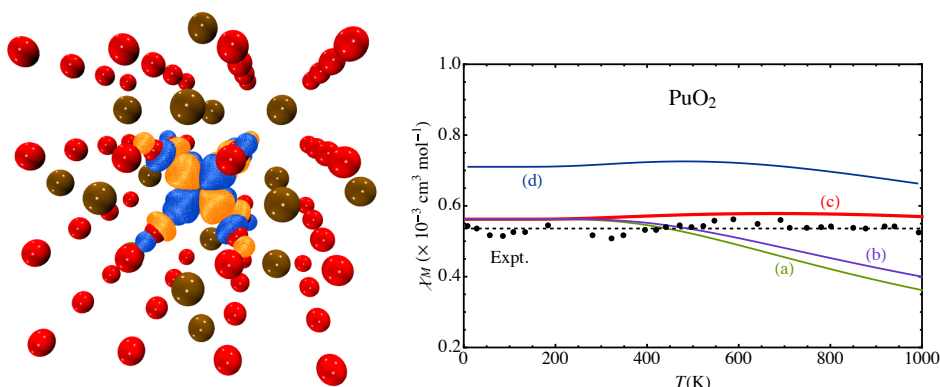
Influence of Covalent effects on Magnetic Properties of Actinide Complexes

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Abstract: For a long period of time, the Seaborg concept has driven our knowledge of the nature of the chemical bond in actinide complexes. The radial extension of the 5f orbitals decreases for the heaviest elements, leading to electrostatic chemical bonds similar to what is observed with lanthanide complexes. However, recent combined experimental and theoretical studies tend to suggest that this picture might not be that simple.¹ From a theoretical point of view, covalent effects can be evaluated using perturbation molecular orbital theory. However, such approach suffers from the nature of the orbitals used in these analyses and can lead to surprising situation where covalent bonds are obtained without any overlap. In this talk we will present another way to probe the nature of the chemical bond in actinide complexes by using multi-reference calculations to characterize different magnetic properties such as EPR g-factors, magnetic susceptibility, NMR chemical shifts or MCD C-terms.



Calculated and experimental magnetic susceptibility (χT) of solid PuO₂ from Ref 2.

References

- (1) Gendron, F.; Autschbach, J. Electronic Structure of the Actinide Elements. In *The Heaviest Metals: Science and Technology of the Actinides and Beyond*; Hanusa, T. P.; Evans, W. J., Eds.; Encyclopedia of Inorganic and Bioinorganic Chemistry John Wiley & Sons: Chichester, UK, page in press.
- (2) Gendron, F.; Autschbach, J. *J. Phys. Chem. Lett.* **2017**, *8*, 673-678.