INSIGHTS INTO THE PA NEUTRAL ATOM: FROM AN EVALUATION OF PA^{2+} OUTER-CORE CORRELATION ENERGY CALCULATIONS

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Since the identification of f-orbital contribution to the bonding in PaO^{+}, investigations into Pa cations have hoped to characterize as many of the electronic states possible.[1] Electronic states of the Pa^{n+} (n=0-4) ions have been investigated using multi-reference spin-orbit configuration interaction ($MR-SOCI$). Initial investigations using Dunning style correlation consistent double-ζ basis sets are re-examined with a larger triple-ζ basis, with the hope of supporting the order of electronic states. Calculations using Hartree-Fock and CI calculations on the neutral atom did not produce the known order of states. A case study was deemed necessary on similar electron configurations present in the low energy states of Pa^{2+} more specifically those generated from the $5f^2 6d^1$ and $5f^1 6d^2$ configurations. Comparison in the Pa^{2+} ion is complicated by the lack of experimental results, but the states are presumed to be similar sequence as those in the neutral atom, with the addition of two electrons in the 7s shell. In evaluating the impact of inclusion of the outer core, calculations including valence-outer core correlation were completed for the 5d, 6s, and 6p shells of the Pa^{2+} ion. The magnitude of these individual shell correlation calculations will allow for identification of the energy level shifts associated with even and odd configurations, better describing the energy order in both the Pa^{2+} ion case study and for the neutral Pa atom. Upon completion of this aspect of the Pa neutral atom study, the knowledge of the energy levels in the Pa^{n+} (n=0-4) family of ions will be greatly expanded, and may yield a model for future studies of atomic actinide systems.

(1) Gibson $et\ al.$ $Organometallics$ 2007, 26, 3947-3956.