ELECTRONIC STRUCTURE OF PA$^{n+;n=1-4}$ IONS: LOOKING FOR CLARITY IN ACTINIDE ELECTRONIC STRUCTURE

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Since the identification of f-orbital contribution to the bonding in PaO$^+$, investigation into Pa cations have hoped to characterize as many of the electronic states possible.[1] Electronic states of the Pa$^{n+;n=1-4}$ ions have been investigated using multi-reference spin-orbit configuration interaction ($MR-SOCI$). Each additional electron in the series adds increased complexity and difficulty in evaluation of electronic states. Comparison of results with data at NIST and its institutional analog in France, or lack there of, indicate that $L-S$ coupling does not adequately describe all the complexity present in these ions. Instead of $L-S$ or a ω-ω coupling we propose that states of the Pa$^{n+;n=1-4}$ ions would be better described using a $J-j$ labeling of states.

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