ACCURATE REPS FOR THE SIXTH-ROW MAIN GROUP ELEMENTS

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Errors in predicted bond lengths in effective potential calculations involving heavy main-group elements are shown to be the result of the poor representation of the $f$-shell space. Test calculations for PbO and the hydrides of thallium, lead and bismuth demonstrate that with the inclusion of the $5d$, $6s$ and $6p$ subshells in the valence space and the proper partitioning of the $f$-shell valence spinors to form pseudospinors, accurate bond lengths are attainable. The previous reasonable bond lengths from $6s6p$ potentials appear to be the result of fortuitous error cancellations. New REPs in standard form are provided for Tl, Pb, Bi, At and Rn in electronic format at www.clarkson.edu/∼pac/reps.html.