XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

All-electron Gaussian basis sets of double zeta quality for the actinides

L. S. C. Martins, F. E. Jorge, M. L. Franco, and I. B. Ferreira

Departamento de Física, Universidade Federal do Espírito Santo, 29060-900 Vitória, Espíirito Santo, Brazil
Unidade Acadêmica de Física, Universidade Federal de Campina Grande, 58429-900 Campina Grande, Brazil

Abstract: For the actinides, two segmented all-electron basis sets of valence double zeta quality plus polarization functions (DZP) are developed. One of them must be used along with the non-relativistic Hamiltonian, whereas the other with the Douglas-Kroll-Hess (DKH) [1,2] one. Adding diffuse functions of s, p, d, f, and g symmetries to the non-relativistic and relativistic sets, augmented basis sets are developed. These functions are essential to describe correctly electrons far away from the nuclei. For some compounds, geometric parameters, atomic charges and valence orbital populations of the actinides, and bond dissociation energies are calculated using the Becke 3-parameter (exchange) [3] and the Lee, Yang, and Parr (correlation) [4] functional in conjunction with the DZP-DKH basis set. For Am and No, the static electric mean dipole polarizabilities are also reported. Comparison with benchmark theoretical [5-10] and experimental [11-14] values found in the literature is carried out. It is verified that the performances of the relativistic compact size basis sets generated in this work are regular, efficient, and reliable. They will be extremely helpful in molecular property calculations that need explicitly to consider the core electrons.

Key-words: **Basis Sets; Actinides; DFT; DKH.**
Support: This work has been supported by CNPq, CAPES, and FAPES

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