Prolapse-Free Relativistic Adapted Gaussian Basis Sets for $_{87}$Fr up to $_{118}$Uuo

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The variational prolapse problem in relativistic Gaussian basis sets is attributed to an ill description of atomic orbital symmetries close to the nucleus, which leads to increasing total energy values during the addition of tight functions and may result in total energies from Dirac-Fock-Coulomb (DFC) calculations below the correspondent ones from numerical Dirac-Fock (NDF) results [1, 2].

Hence, we generated relativistic adapted Gaussian basis sets (RAGBSs) for Francium through Ununoctium atoms without variational prolapse by means of a polynomial version of the Generator Coordinate Dirac-Fock (p-GCDF) method [3], where the resolution of Dirac-Fock integral equations is done through the integral discretization (ID) technique with a polynomial expansion for each *w* atomic orbital symmetry,

$$\Theta_i^{(w)} = \frac{\ln \gamma_i^{(w)}}{A} = \Theta_{\min}^{(w)} + \Delta\Theta_1^{(w)}(i-1) + \Delta\Theta_2^{(w)}(i-1)^2 + \ldots + \Delta\Theta_q^{(w)}(i-1)^q , \qquad (1)$$

in which $i = 1, 2, \ldots, N$ (N = number of discretization points), A is a scaling parameter and $\Theta_{\min}^{(w)}$ and $\Delta\Theta_q^{(w)}$ are parameters respectively known as the initial point of the mesh and the increment of order q applied to obtain discretization points. A slight adjustment of these parameters after an initial optimization process was capable to eliminate completely variational prolapse.

Two finite nucleus models were employed, the Gaussian and the uniform sphere models. The basis set sizes, for the 7*s*, 7*p*, 6*d* and 5*f* block elements are, respectively, 33s27p17d11f, 33s30p19d14f, 33s27p19d14f and 33s27p17d14f functions. The largest difference between the DFC energies obtained with our RAGBSs and NDF values is 15.4 mE_h for $_{118}$Uuo. Such study complements a series of prolapse-free relativistic Gaussian basis sets from $_1$H up to $_{118}$Uuo atoms obtained with the p-GCDF variant [4, 5].

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