Accurate Gaussian Basis Sets for New Material Quantum Chemical Calculations

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Theoretical chemistry has been used in the last decades as an important tool to investigate new materials. To understand what is going on at the molecular level is fundamental to characterize the electronic properties of a new material under study. In order to perform a quantum chemical calculation one needs to solve the Schrödinger equation $(H\Psi = E\Psi)$, where H represents the hamiltonian operator that acts over the wave function (Ψ) and E is the energy of the molecular system studied. The difficulty of solving the Schrödinger equation lies in knowing the radial part of the wave function (that is commonly known as basis function or basis set).

There are a lot of basis functions that can be used to perform quantum chemical calculations of new materials. Here, we are proposing a new set of basis sets that are able to obtain very accurate results with a very low computational cost, what is very important when we are calculating the electronic properties of a certain material. The basis sets proposed here are much better than the ones more commonly used in quantum chemical calculations and are also able to compete with the best basis sets available in the literature, but with a lower computational cost. Our basis sets were generated with the polynomial Generator Coordinate Hartree-Fock (pGCHF) method [1] and, as one example, Table 1 below shows a comparison between energy and CPU time obtained for the caffeine molecule with our basis sets (pGCHF) and the most commonly basis sets used in the literature nowadays, i.e, the basis sets of Pople (6-31G and 6-311G) and Dunning (cc-pVTZ and cc-pVQZ).

Table1: Energy and CPU time obtained with the DFT/B3LYP method for the caffeine molecule

Basis sets	Energy (hartree)	CPU time
pGCHF	-680.6761562	1 d 04 h 49 min
6-31G(3df,3pd)	-680.4553252	0 d 22 h 27 min
6-311G(3df,3pd)	-680.6060264	1 d 09 h 35 min
cc-pVTZ	-680.6176352	0 d 15 h 50 min
cc-pVQTZ	-680.6710062	8 d 16 h 49 min

Key words: Generator Coordinate method, Gaussian basis sets.

[1] R.C. BARBOSA and A.B.F. DA SILVA, *A new proposal for the discretization of the Griffin-Wheeler-Hartree-Fock equations.* Molecular Physics, 2003. **101**(8): p. 5.

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