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Relativistic and nonrelativistic finite nucleus optimized double zeta basis sets for the 4*p*, 5*p* and 6*p* elements (Theor Chem Acc (1998) 99:366-371): addendum

Kenneth G. Dyall

Schrödinger, Inc., 1500 SW First Avenue, Suite 1180, Portland, OR 97201, USA

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Abstract. The coefficients of the atomic Foldy-Wouthuysen transformed large component, which can be used in scalar relativistic calculations, are provided in an internet archive for the relativistic double zeta basis sets for the 4*p*, 5*p* and 6*p* elements previously published by the author.

Key words: Gaussian basis sets – Relativistic basis sets – *p* Block – Double zeta – Contraction coefficients

This communication describes an addendum to the internet archive for the relativistic double zeta basis sets previously published by the author for the 4*p*, 5*p* and 6*p* elements [1]. The author recently developed a scalar relativistic approximation [2, 3], based on the modified Dirac equation [4], that is similar to the Douglas-Kroll-Hess approximation [5, 6]. In this approximation the scalar terms of the relativistic electron-electron interaction are approximated by the bare Coulomb operator, but evaluated with respect to the atomic Foldy-Wouthuysen transformed wave functions. The approximation neglects the commutator of the Coulomb operator with the atomic Foldy-Wouthuysen transformation. The neglected term is a renormalized two-electron Darwin term, which is expected to be small, and was shown to be small in numerical tests [2]. The benefit of the approximation is that two-electron integrals can be evaluated with the standard nonrelativistic integral procedures. The one-electron integrals are evaluated with respect to relativistic operators. The reader is referred to the paper describing the approximation for details.

The purpose of this communication is to make available the coefficients of the atomic Foldy-Wouthuysen transformed wave function, which can be used as contraction coefficients for the evaluation of the two-electron integrals. The atomic Foldy-Wouthuysen contraction coefficients for the primitive functions added for valence flexibility are 1, just as in nonrelativistic calculations. The coefficients of the large component and the pseudo-large component, which are used for the evaluation of the one-electron integrals, can be obtained from the original archive.

This communication contains an internet archive in ASCII format. The archive contains the Foldy-Wouthuysen transformed large component coefficients of the spin-free Dirac-Fock spinors for the double zeta basis sets for the 4*p*, 5*p* and 6*p* elements published by the author.

The electronic supplementary material to the original paper can be obtained by using the Springer Link server located at http://link.springer.de/link/service/journals/00214/supp/1998/m22/m22.htm.

Electronic supplementary material to this paper can be obtained by using the Springer Link server located at http://dx.doi.org/10.1007/s00214-002-0396-0.

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Correspondence to: K.G. Dyall
e-mail: dyall@schrodinger.com