Abstract Submitted
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Computational efficiences for calculating rare earth f^n energies[1]
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Recently[2], we have used new computational strategies to obtain wavefunctions and energies for Gd IV $4f^7$ and $4f^6 5d$ levels. Here we extend one of these techniques to allow efficent inclusion of $4f^2$ pair correlation effects using radial pair energies obtained from much simpler calculations[3] and angular factors which can be simply computed[4]. This is a re-vitalization of an older idea[5]. We display relationships between angular factors involving the exchange of holes and electrons (e.g. f^6 vs f^8, $f^{13}d$ vs fd^9). We apply the results to Tb IV and Gd IV, whose spectra is largely unknown, but which may play a role in MRI medicine as endohedral metallofullerenes (e.g. Gd_3N-C_{80}[6]). Pr III results are in good agreement (910 cm^{-1}) with experiment. Pu I $5f^2$ radial pair energies are also presented.

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[2]D. R. Beck and E. J. Domeier, Can. J. Phys. Walter Johnson issue, Jan. 2009.
[3]e.g. K. Jankowski *et al.*, Int. J. Quant. Chem. **XXVII**, 665 (1985).
[4]D. R. Beck and C. A. Nicolaides, Excited States in Quantum Chemistry, C. A. Nicolaides and D. R. Beck (editors), D. Reidel (1978), p. 105ff.
[5]I. Oksuz and O. Sinanoglu, Phys. Rev. **181**, 54 (1969).
[6]M. C. Qian and S. N. Khanna, J. Appl. Phys. **101**, 09E105 (2007).

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