Gd IV $4f^7$ $J = 7/2$ Levels

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[1] DONALD R. BECK, Michigan Technological University — This is an ion of tremendous complexity for the *ab initio* computationalist, because a large energy matrix is required (well above 20 000) and a large number of basis functions (over 100 000 determinants in some cases) is needed to create its elements. Furthermore, $4f$ pair correlation converges rather slowly in angular space [2] in contrast, say, to that of d shell electrons. The ion is of potential interest for determination of the electron electric dipole moment and in PbF_2:Gd scintillators. We report energy differences between the 50 $4f^7$ $J = 7/2$ levels whose average error [3] for the bottom five levels is 1309 cm^{-1}, comparable to the best semi-empirical results [4]. Our values, however, are obtained by dividing the energy matrix up into about 50 pieces. Future work will focus on assembly (and diagonalization) of the full energy matrix.

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