Theor Chem Acc (2002) 107:318
DOI 10.1007/s00214-002-0328-z

Theoretical
Chemistry Accounts

Erratum

Fully relativistic correlated benchmark results for uranyl and a critical look at relativistic effective core potentials for uranium

W.A. de Jong, R.J. Harrison, J.A. Nichols, D.A. Dixon

Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA 99352, USA

Published online: 3 May 2002

Theor Chem Acc (2001) 107:22–26

After publication an error was found in the DHF bond length, originally published in Ref. [1]. This incorrect bond length was used to calculate frequencies at both the DHF and DHF + Gaunt level of theory, leading to erroneous frequencies in Table 1 of Theor Chem Acc (2001) 107:22–26. The bond length and frequencies have been recalculated and the corrected benchmark numbers are listed in Table 1 of this erratum.

Table 1. Corrected DHF bond length (r_e in Å), stretch and bending frequencies (in cm^{-1})

Calculation type	r_e	$\nu_{symmetric\ stretch}$	$\nu_{asymmetric\ stretch}$	ν_{bend}
DHF	1.659	1225	1300	238
DHF + Gaunt	1.659	1227	1302	240

Reference

1. de Jong WA, Visscher L, Nieuwpoort WC (1999) J Mol Struct 458:41