Theor Chem Acc (2012) 131:1283
DOI 10.1007/s00214-012-1283-y

ERRATUM

Erratum to: Computational ^{19}F NMR. 1. General features

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Erratum to: Theor Chem Acc (2012) 131:1140
DOI 10.1007/s00214-012-1140-z

Owing to an erroneous interchange of literature experimental data in the original publication, the interpretation of the computed results for uranium chlorofluorides should be partly modified as follows.

The ^{19}F spectra reported by Downs (ref. [17]) for UF_nCl_{6-n} could, in some cases, be assigned with confidence owing to their splitting patterns: this holds for UF_5Cl (A_4X), *cis*-UF_4Cl_2 (A_2X_2) and *mer*-UF_3Cl_3 (A_2X). (However, the assignment for *cis*-UF_4Cl_2 was only tentative)

However, we erroneously swapped the entries for each spin pair in the above compounds, which led to a seemingly better agreement with the calculations. In the paper we had suggested that, while the general performance of the calculations was unsatisfactory, individual trends in ^{19}F chemical shifts were correct for each of the above molecules. However, after reordering the data this appears not to be the case; the correlation is poor even for the above compounds. The affected items are Tables 1 and 4 (pairs of experimental shifts for UF_5Cl, *cis*-UF_4Cl_2 and *mer*-UF_3Cl_3 should be exchanged), and Fig. 5. For brevity, the revised situation is depicted in Fig. 1 (which replaces Fig. 5).

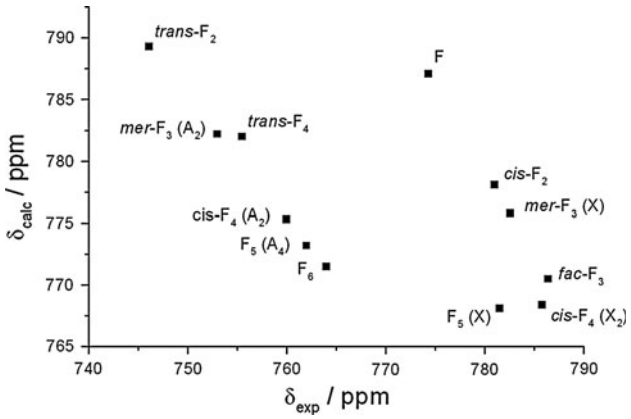

Fig. 5 Correlation of experimental with calculated ^{19}F chemical shifts of uranium chlorofluorides

General trends (Fig. 1) are unchanged since the interval spanned by UF_nCl_{6-n} is just ca. 40 ppm, over a full range of 1,300 ppm. The overall conclusions are, therefore, not affected.

Acknowledgments We thank Dr. Georg Schreckenbach for alerting us of this mistake.

The online version of the original article can be found under doi:10.1007/s00214-012-1140-z.

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Published online: 13 November 2012