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ERRATUM

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

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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).

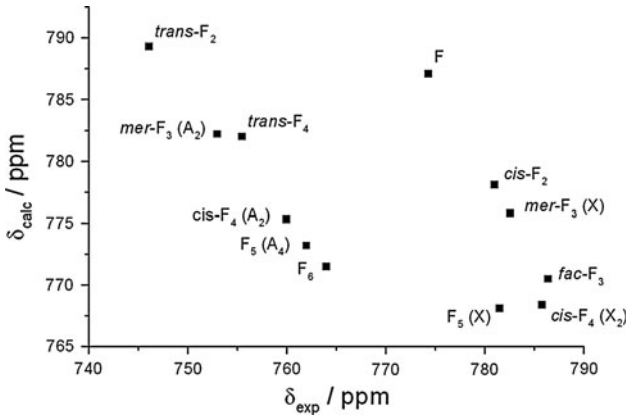

Fig. 5 Correlation of experimental with calculated ^{19}F chemical shifts of uranium chlorofluorides

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.

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