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Correction: A reduced radial potential energy function for the halogen bond and the hydrogen bond in complexes $B \cdots XY$ and $B \cdots HX$, where X and Y are halogen atoms†

Anthony C. Legon

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Correction for 'A reduced radial potential energy function for the halogen bond and the hydrogen bond in complexes $B \cdots XY$ and $B \cdots HX$, where X and Y are halogen atoms' by Anthony C. Legon, *Phys. Chem. Chem. Phys.*, 2014, 16, 12415–12421.

In the published version of the article *Phys. Chem. Chem. Phys.*, 2014, 16, 12415–12421, the following statement should have been made: 'In correcting the *ab initio*-calculated dissociation energies D_σ for basis set superposition error (BSSE), it was necessary for numerical stability to exclude the CABS singles correction term^{1,2} from the BSSE correction in the case of the complexes containing Br and I atoms (namely $B \cdots Br_2$, $B \cdots BrCl$, $B \cdots ICl$, $B \cdots HBr$ and $B \cdots HI$).' It has become possible recently to recalculate the BSSE corrections with inclusion of CABS singles. The changes that result are not significant, as indicated below.

The revised D_σ values that result when CABS singles are included for Br- and I-containing complexes are shown in the revised Tables 1', 2' and 3', available as ESI.† Complexes $B \cdots F_2$, $B \cdots Cl_2$, $B \cdots ClF$, $B \cdots HF$ and $B \cdots HCl$ did not require CABS singles exclusion and their D_σ values are accordingly as in the original versions of the tables. All the D_σ values for Br- and I-containing complexes are systematically increased, with an average increase of 0.3 kJ mol⁻¹. These increases have no visible effect on revised versions of Fig. 1, 2 and 3. This is clear when the results of revised linear least-squares fits, shown in eqn (3'), (4') and (5'), respectively, are compared with the original eqn (3), (4) and (5), both sets of which are given below.

$$D_\sigma/(\text{kJ mol}^{-1}) = 1.50(3)\{k_\sigma/(\text{N m}^{-1})\} - 0.29(23) \quad (3')$$

$$D_\sigma/(\text{kJ mol}^{-1}) = 1.47(3)\{k_\sigma/(\text{N m}^{-1})\} - 0.21(21) \quad (3)$$

$$D_\sigma/(\text{kJ mol}^{-1}) = 1.47(3)\{k_\sigma/(\text{N m}^{-1})\} - 0.02(36) \quad (4')$$

$$D_\sigma/(\text{kJ mol}^{-1}) = 1.45(3)\{k_\sigma/(\text{N m}^{-1})\} - 0.06(35) \quad (4)$$

$$D_\sigma/(\text{kJ mol}^{-1}) = 1.52(3)\{k_\sigma/(\text{N m}^{-1})\} - 1.94(36) \quad (5')$$

$$D_\sigma/(\text{kJ mol}^{-1}) = 1.53(3)\{k_\sigma/(\text{N m}^{-1})\} - 1.8(3) \quad (5)$$

All changes are less than the stated experimental error and none of the conclusions drawn in the article are affected.

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The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

- G. Knizia and H.-J. Werner, *J. Chem. Phys.*, 2008, 128, 154103.
- G. Knizia, T. B. Adler and H.-J. Werner, *J. Chem. Phys.*, 2009, 130, 054104.

School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK

† Electronic supplementary information (ESI) available. See DOI: 10.1039/c4cp90149e

