



Cite this: *Phys. Chem. Chem. Phys.*, 2014, 16, 25199

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

DOI: 10.1039/c4cp90149e

www.rsc.org/pccp

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.

I thank Dr Grant Hill (University of Sheffield) for help with the calculation of the BSSE corrections in which CABS singles were included.

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

References

- 1 G. Knizia and H.-J. Werner, *J. Chem. Phys.*, 2008, 128, 154103.
- 2 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

