



# Correction to: The Feynman dispersion correction for MNDO extended to F, Cl, Br and I

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A small coding error in the development version of EMPIRE led to some inconsistencies in the above article. They are corrected in this erratum.

## Introduction

Our recent description of MNDO-F for the halogens [1] was affected by a small coding error that was introduced into the code after the original MNDO-F article [2] and resulted in small deviations from the correct result. As this error was also present during the parameterization, we now present the correct parameters and results.

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The online version of the original article can be found at <https://doi.org/10.1007/s00894-019-4038-z>

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**Electronic supplementary material** The online version of this article (<https://doi.org/10.1007/s00894-019-4142-0>) contains supplementary material, which is available to authorized users.

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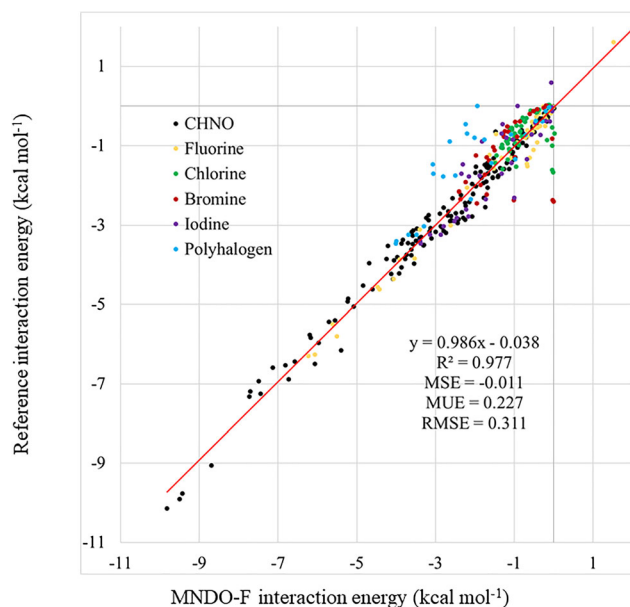
## Results

### Parameterization

Reparameterization using the correct code led to slightly better results for the training set, as shown in Fig. 1 and in the [Supporting Information](#).

The correct parameters are shown in Table 1:

The performance for the training set is marginally better than that reported in reference [1] with the exception of



**Fig. 1** Comparison of reference and MNDO-F interaction energies for the entire training set of C, H, N, O, F, Cl, Br and I compounds. The solid red line indicates the best-fit regression

**Table 1** The optimized parameters for MNDO-F for H, C, N, O, F, Cl, Br and I

Element	Original MNDO	MNDO-F			RMSD (kcal mol <sup>-1</sup> )
	$\alpha_A$	$\alpha_A$	$k_A$ (bohr <sup>6</sup> )	$r_{BJ}$ (bohr)	
H	2.544134	2.746420 (2.651305)	18.1663804 (22.749633)	3.5635804 (4.0216)	0.311
C	2.546380	2.640525 (2.58139)	7.752681 (7.971853)	5.385236 (4.0216)	
N	2.861342	3.031761 (3.012587)	3.564848 (4.387597)	4.425983 (4.0216)	
O	3.160604	3.125117 (3.201357)	8.823789 (7.416029)	3.644720 (4.0216)	
F	3.419661	3.228403	3.094361	3.538267	0.294
Cl	2.542201	2.575831	5.691735	4.341654	0.209
Br	2.44570512	2.331572	6.717021	4.627255	0.354
I	2.20732001	1.754901	29.413381	4.664481	0.525
				All halogen compounds	0.337
				Entire Dataset	0.313

The values in parentheses are those given in reference [2] for a single  $r_{BJ}$  value for H, C, N and O

**Table 2** Calculated complexation energies for 1,3,5-trihalogenated and perhalogenated benzenes complexed ( $\pi$ - $\pi$ ) to benzene

	MP2-cp	DFT-SAPT	MNDO-F
C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub> :C <sub>6</sub> H <sub>6</sub> (staggered)	-7.72	-4.22	-5.59
C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub> :C <sub>6</sub> H <sub>6</sub> (eclipsed)	-7.55	-4.23	-5.58
C <sub>6</sub> Cl <sub>6</sub> :C <sub>6</sub> H <sub>6</sub> (staggered)	-12.25	-6.21	-7.58
C <sub>6</sub> Cl <sub>6</sub> :C <sub>6</sub> H <sub>6</sub> (eclipsed)	-11.8	-6.29	-7.58
C <sub>6</sub> H <sub>3</sub> Br <sub>3</sub> :C <sub>6</sub> H <sub>6</sub> (staggered)	-8.4	-3.95	-6.66
C <sub>6</sub> Br <sub>6</sub> :C <sub>6</sub> H <sub>6</sub> (staggered)	-13.19	-5.08	-9.79
C <sub>6</sub> H <sub>3</sub> I <sub>3</sub> :C <sub>6</sub> H <sub>6</sub> (staggered)	-9.24	-4.52	-9.83
C <sub>6</sub> I <sub>6</sub> :C <sub>6</sub> H <sub>6</sub> (staggered)	-14.58	-7.04	-16.08

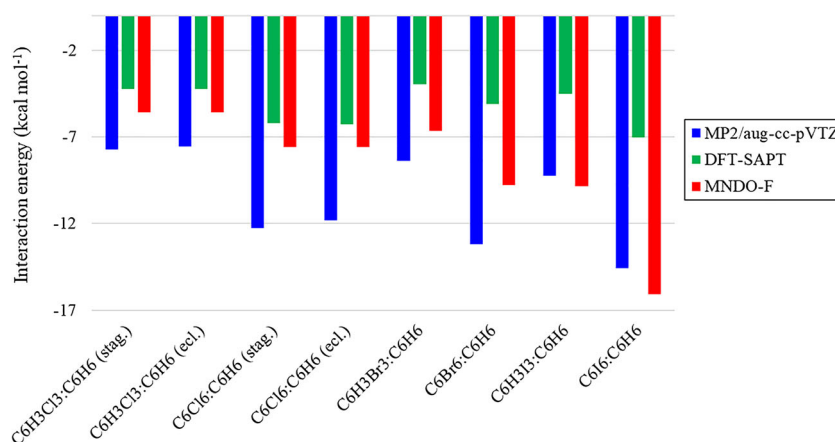
Complexation energies are given in kcal mol<sup>-1</sup> and abbreviations are those used in reference [1], Table 2

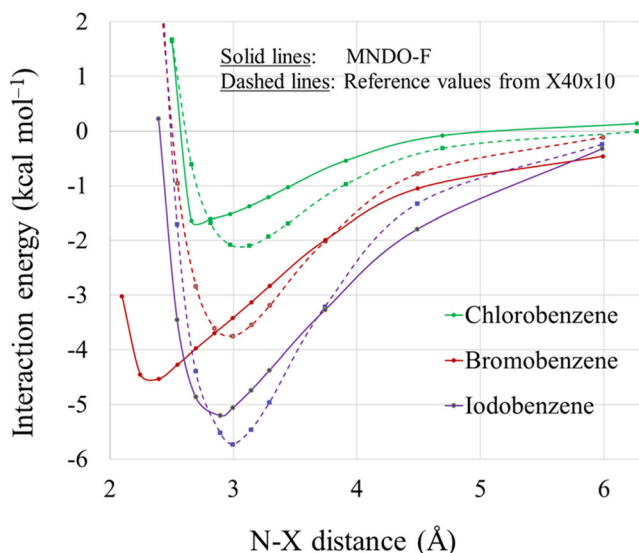
iodine compounds, which are slightly worse. The optimized parameters, however, have changed significantly, so that the correlation between the Feynman coefficient and the cube of the atomic polarizability reported in reference [1] is no longer as good. The detailed results are shown in the [ESM](#).

## Test complexes

### Complexes between 1,3,5-trihalo- and perhalobenzenes and benzene

Table 2 and Fig. 2 show comparisons of MP2, DFT-SAPT and MNDO-F complexation energies for these complexes.

**Fig. 2** A comparison of the MP2/aug-cc-pVTZ, DFT-SAPT (CBS) and MNDO-F interaction energies for the  $\pi$ - $\pi$  complexes of polyhalogenated benzenes with benzene



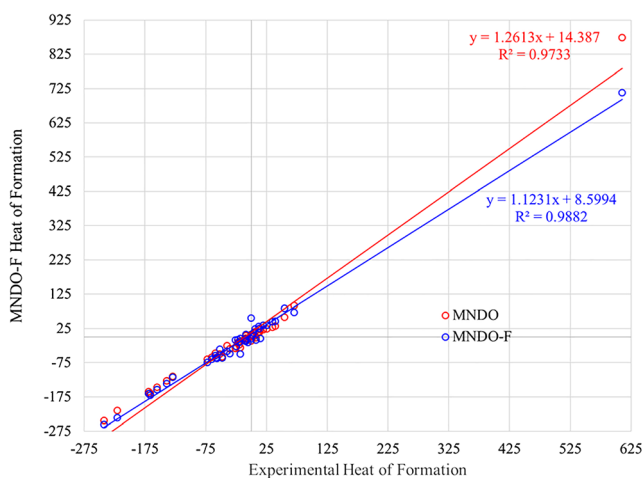
**Fig. 3** A comparison of the reference and MNDO-F interaction-energy curves for the halogen-bonded complexes of  $C_6H_5X$  ( $X = Cl, Br, I$ ) with trimethylamine

### Halogen-bonded complexes

Figure 3 shows the correct results for the complexes of  $C_6H_5X$  with methylamine shown in Fig. 4 of reference [1].

The performance is generally similar to that reported in reference [1] except that the energy profile for iodobenzene is considerably improved.

All other test-set results are shown in the ESI.



**Fig. 4** MNDO and MNDO-F calculated Heats of Formation ( $kcal\ mol^{-1}$ ) compared to experiment. The isolated point is  $C_{60}$ -fullerene. The MNDO and MNDO-F regression lines and equations are shown

**Table 3** MNDO and MNDO-F parameters for heats of formation

Element	$E_{isol}$ (eV)		$\Delta H_{atom}$ ( $kcal\ mol^{-1}$ )
	MNDO	MNDO-F	
H	-11.906276	-12.58265	52.102
C	-120.500606	-122.22010	170.89
N	-202.566201	-205.21905	113.00
O	-317.868506	-319.63700	59.559
F	-476.683781	-476.86600	18.86
Cl	-353.1176787	-353.71210	28.99
Br	-346.68144152	-346.63050	26.74
I	-340.5984282	-339.91580	25.517

$E_{isol}$  is the total energy of the isolated atom and  $\Delta H_{atom}$  its Heat of Formation.  $E_{isol}$  is a variable parameter in MNDO-F. The numbers of significant figures are those used in the EMPIRE program

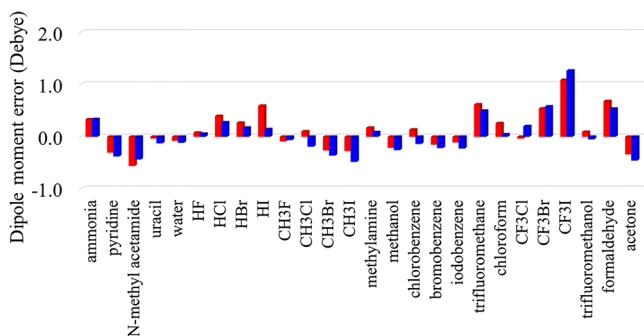
### Heats of formation

Table 3 shows the MNDO and MNDO-F values for  $E_{isol}$  (eV) and the heats of formation of the atoms ( $kcal\ mol^{-1}$ ). The individual results are shown in the ESI and graphically in Fig. 4.

The results are comparable to those reported in reference [1] (slightly worse than MNDO) but the excellent agreement found previously for  $C_{60}$ -fullerene is no longer as good.

### Dipole moments

Figure 5 show a comparison of MNDO and MNDO-F calculated dipole moments with experiment.



**Fig. 5** Errors (calculated – experimental dipole moment, Debye) in MNDO and MNDO-F calculated dipole moments

## Conclusions

The effect of the small program error present in reference [1] has been corrected. In general, MNDO-F performs as well or better than reported previously. The parameters reported in this erratum should be used for MNDO-F calculations.

The correct version of MNDO-F is available in the newest version of EMPIRE [3–5].

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## References

1. Kriebel M, Heßelmann A, Hennemann M, Clark T (2019) The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. *J. Mol. Model.* 25:156. <https://doi.org/10.1007/s00894-019-4038-z>
2. Kriebel M, Weber K, Clark T (2018) A Feynman dispersion correction: a proof of principle for MNDO. *J. Mol. Model.* 24:338. <https://doi.org/10.1007/s00894-018-3874-6>
3. Hennemann M, Clark T (2014) EMPIRE: a highly parallel semiempirical molecular orbital program: 1: self-consistent field calculations. *J. Mol. Model.* 20:2331. <https://doi.org/10.1007/s00894-014-2331-4>
4. Margraf JT, Hennemann M, Meyer B, Clark T (2015) EMPIRE: a highly parallel semiempirical molecular orbital program: 2: periodic boundary conditions. *J. Mol. Model.* 21:144. <https://doi.org/10.1007/s00894-015-2692-3>
5. Cepas InSilico GmbH (2018) EMPIRE software. Cepas InSilico GmbH, Erlangen. <http://www.ceposinsilico.de/products/empire.htm>. Accessed 16<sup>th</sup> July 2019

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