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CORRECTION

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Correction: Scaling properties of information-theoretic quantities in density functional reactivity theory

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Correction for 'Scaling properties of information-theoretic quantities in density functional reactivity theory' by Chunying Rong *et al.*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 4977–4988.

The authors would like to amend the text by the following four points:

1. Eqn (19) of the text is in error. The correct formula is as follows:

$$S_\sigma = \frac{S_S}{N} + \ln N$$

2. Because of (1), numerical results of S_σ in Tables 1 and 2 (column 4) are incorrect. The correct results are shown in Table C1 below, where all data are found to be positive.

3. The correct correlation coefficient (R^2) and root-mean-square deviation (RMSD) values for S_σ from the least-square-fitting in Table 3 are shown in Table C2.

4. Correlation results of S_σ at atoms, molecules and atoms-in-molecules levels shown in Fig. 1a, 2a, 3a, 5a, and 6a are invalidated and should be replaced by the results in Table C2. However, as can be seen from the table, strong correlations at the atoms-in-molecules level are still observed.

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Table C1 Shannon entropy with the shape function for 36 neutral atoms and 42 molecular systems. Atomic units

Atom	S_σ	Molecule	S_σ
H	4.21	CH_2═CH_2	4.14
He	2.74	FHC═CH_2	3.95
Li	3.66	MeHC═CH_2	4.51
	3.60	CH_2═CH(CN)	4.33
B	3.38	CH_2═CH(CHO)	4.35
C	3.10	Butadiene	4.64
N	2.82	F_2C═CH_2	3.94
O	2.57	FHC═CHF	3.94
F	2.32	*trans*-MeHC═CHMe	4.78
Ne	2.08	*cis*-MeHC═CHMe	4.78
Na	2.32	Me_2C═CH_2	4.78
Mg	2.38	$(CH_3O)CH$═CH_2	4.52
Al	2.42	Cyclopentadiene	4.72
Si	2.41	Pyrrole	4.60
P	2.36	2-Methyl-butadiene	4.88
S	2.30	1-Methyl-butadiene	4.88
Cl	2.22	CH_2CH═$CHOBH_3$	4.77
Ar	2.14	CH_2═$CH(NO_2)$	4.33
K	2.28	F_2C═CHF	3.98
Ca	2.34	Me_2C═CHMe	4.99
Sc	2.28	$(Me)_2NCH$═CH_2	4.89
Ti	2.20	EtOCH═CH_2	4.78
V	2.12	$(CN)_2C$═CH_2	4.54
Cr	1.98	Benzene	4.82
Mn	1.96	CH_3COOCH═CH_2	4.70
Fe	1.81	CH_2═$C(NO_2)(NH_2)$	4.53
Co	1.73	F_2C═CF_2	4.05
Ni	1.66	Me_2C═CMe_2	5.17
Cu	1.58	Maleic anhydride	4.52
Zn	1.56	C_6H_5–Me	5.03
Ga	1.57	C_6H_5–F	4.76
Ge	1.57	C_6H_5–NH_2	4.94
As	1.55	C_6H_5–OH	4.85
Se	1.54	C_6H_5–CN	4.95
Br	1.51	C_6H_5–HCO	4.96
Kr	1.48	$(EtO)_2C$═CH_2	5.18
		$(CN)_2C$═$C(CN)_2$	4.88
		C_6H_5–NO_2	4.94
		C_6H_5–CF_3	4.92
		C_6H_5–$N(Me)_3$	5.40
		2,3-Diacetoxy-1,3-butadiene	5.31
		$(C_2H_5COO)_2C$═CH_2	5.38

Table C2 The correlation coefficient R^2 and root-mean-square deviation (RMSD) values for Shannon entropy with the shape function, S_σ, at atomic, molecular and atoms-in-molecules levels with AIM, Becke, and Hirshfeld partitioning schemes

			C			H		
S_σ	Atomic	Molecular	AIM	Becke	Hirshfeld	AIM	Becke	Hirshfeld
R^2	0.8010	0.4727	0.9700	0.9290	0.7501	0.9541	0.8956	0.6520
RMSD	0.2917	0.2750	0.0367	0.0295	0.0252	0.0262	0.0277	0.0307

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