RSC Advances

CORRECTION

Cite this: *RSC Adv.*, 2020, **10**, 19463

Correction: Modelling and prediction of the thermophysical properties of aqueous mixtures of choline geranate and geranic acid (CAGE) using SAFT-γ Mie

Silvia Di Lecce, †[a] Georgia Lazarou,[a] Siti H. Khalit,[a] David Pugh,‡[b] Claire S. Adjiman, [a] George Jackson, [a] Amparo Galindo *[a] and Lisa McQueen[c]

DOI: 10.1039/d0ra90058c

rsc.li/rsc-advances

Correction for 'Modelling and prediction of the thermophysical properties of aqueous mixtures of choline geranate and geranic acid (CAGE) using SAFT-γ Mie' by Silvia Di Lecce *et al.*, *RSC Adv.*, 2019, **9**, 38017–38031. DOI: 10.1039/C9RA07057E

The authors regret the omission of one of the authors, David Pugh, from the original manuscript. The corrected list of authors and affiliations for this paper is as shown here.

In addition, we point readers to ref. 1 and 2, together with ref. 17–21 in the original paper, for a complete description of the association contribution to the SAFT-γ Mie equation of state.

The authors also wish to correct a number of typographical errors in Tables 3 and 4. The corrected Tables 3 and 4 are shown below; the letters and numbers in bold indicate the corrected values.

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

[a]*Department of Chemical Engineering, Centre for Process Systems Engineering, Institute for Molecular Science and Engineering, South Kensington Campus, Imperial College London, London SW7 2AZ, UK. E-mail: a.galindo@imperial.ac.uk*

[b]*Department of Chemistry, Molecular Sciences Research Hub, White City Campus, Imperial College London, London W12 0BZ, UK*

[c]*Chemical Development, GSK, 1250 S Collegeville Rd, Collegeville, PA, 19426, USA*

† Current address: Department of Chemistry, Molecular Sciences Research Hub, White City Campus, Imperial College London, London W12 0BZ, UK.

‡ Current address: Kings College London, Department of Chemistry, Britannia House, 7 Trinity Street, London SE1 1DB, UK.

Table 3 Unlike dispersion interaction energies (ε_{kl}/k_B)/K and repulsive exponents λ^r_{kl} for use within the SAFT-γ Mie group-contribution approach. CR indicates a combining rule is used to determine the value of the corresponding parameter. The unlike dispersion interactions indicated with CR are calculated using eqn (7) for uncharged groups and eqn (10) for charged groups. The combining rule is used to determine the value of λ^r_{kl} is given in eqn (6). The unlike group diameters σ_{kl} are obtained using the combining rule given in eqn (5) in all cases

Group k	Group l	(ε_{kl}/k_B)/K	λ^r_{kl}	Ref.	Group k	Group l	(ε_{kl}/k_B)/K	λ^r_{kl}	Ref.
$CH_3/^{adj}CH_3$	$CH_3/^{adj}CH_3$	256.77	15.050	17	CH═	Cl^-	CR	CR	This work
$CH_3/^{adj}CH_3$	$CH_2/^{adj}CH_2$	350.77	CR	17	COOH	COOH	405.78	8.0000	18
$CH_3/^{adj}CH_3$	CH_2═	333.48	CR	18	COOH	H_2O	289.76	CR	19
$CH_3/^{adj}CH_3$	CH═	252.41	CR	18	COOH	CH_2OH	656.80	CR	19
$CH_3/^{adj}CH_3$	COOH	255.99	CR	18	COOH	C═	609.87	CR	This work
$CH_3/^{adj}CH_3$	H_2O	358.18	100.00	19	COOH	COO^-	405.78	8.0000	This work
$CH_3/^{adj}CH_3$	CH_2OH	333.20	CR	19	COOH	N^+	CR	CR	This work
$CH_3/^{adj}CH_3$	C═	281.40	CR	69	COOH	Na^+	CR	CR	This work
CH_3	COO^-	255.99	CR	This work	COOH	K^+	CR	CR	This work
$^{adj}CH_3$	COO^-	509.37	CR	This work	COOH	Cl^-	CR	CR	This work
$CH_3/^{adj}CH_3$	N^+	462.18	CR	This work	H_2O	H_2O	266.68	17.020	68
$CH_3/^{adj}CH_3$	Na^+	CR	CR	This work	H_2O	CH_2OH	353.37	CR	19
$CH_3/^{adj}CH_3$	K^+	CR	CR	This work	H_2O	C═	310.91	8.0000	This work
$CH_3/^{adj}CH_3$	Cl^-	CR	CR	This work	H_2O	COO^-	171.61	CR	This work
$CH_2/^{adj}CH_2$	$CH_2/^{adj}CH_2$	473.39	19.871	17	H_2O	N^+	1481.3	21.217	This work
$CH_2/^{adj}CH_2$	CH_2═	386.80	CR	18	H_2O	Na^+	539.68	CR	20
$CH_2/^{adj}CH_2$	CH═	459.40	CR	18	H_2O	K^+	376.25	CR	20
$CH_2/^{adj}CH_2$	COOH	413.74	CR	18	H_2O	Cl^-	95.406	CR	20
$CH_2/^{adj}CH_2$	H_2O	423.63	100.00	19	CH_2OH	CH_2OH	407.22	22.699	19
$CH_2/^{adj}CH_2$	CH_2OH	423.17	CR	19	CH_2OH	C═	799.66	CR	This work
$CH_2/^{adj}CH_2$	C═	286.58	CR	69	CH_2OH	COO^-	656.80	CR	This work
CH_2	COO^-	413.74	CR	This work	CH_2OH	N^+	440.99	CR	This work
$^{adj}CH_2$	COO^-	780.24	CR	This work	CH_2OH	Na^+	CR	CR	This work
$CH_2/^{adj}CH_2$	N^+	348.30	CR	This work	CH_2OH	K^+	CR	CR	This work
$CH_2/^{adj}CH_2$	Na^+	CR	CR	This work	CH_2OH	Cl^-	CR	CR	This work
$CH_2/^{adj}CH_2$	K^+	CR	CR	This work	C═	C═	1500.0	8.0000	69
$CH_2/^{adj}CH_2$	Cl^-	CR	CR	This work	C═	COO^-	609.87	CR	This work
CH_2═	CH_2═	300.90	20.271	18	C═	N^+	CR	CR	This work
CH_2═	CH═	275.75	CR	18	C═	Na^+	CR	CR	This work
CH_2═	COOH	**CR**	**CR**	This work	C═	K^+	CR	CR	This work
CH_2═	H_2O	**387.25**	**94.463**	This work	C═	Cl^-	CR	CR	This work
CH_2═	CH_2OH	**375.51**	CR	This work	COO^-	COO^-	**21.264**	8.0000	This work
CH_2═	C═	**203.76**	CR	This work	COO^-	N^+	24.280	CR	This work
CH_2═	COO^-	CR	CR	This work	COO^-	Na^+	9.9125	CR	This work
CH_2═	N^+	CR	CR	This work	COO^-	K^+	23.999	CR	This work
CH_2═	Na^+	CR	CR	This work	COO^-	Cl^-	**47.154**	CR	This work
CH_2═	K^+	CR	CR	This work	N^+	N^+	**62.971**	**8.8971**	This work
CH_2═	Cl^-	CR	CR	This work	N^+	Na^+	CR	CR	This work
CH═	**CH**═	952.54	15.974	18	N^+	K^+	CR	CR	This work
CH═	COOH	453.13	CR	This work	N^+	Cl^-	61.989	CR	This work
CH═	H_2O	332.21	17.309	This work	Na^+	Na^+	31.711	12.000	20
CH═	CH_2OH	414.91	CR	This work	Na^+	K^+	CR	CR	This work
CH═	C═	1195.3	CR	69	Na^+	Cl^-	27.938	CR	20
CH═	COO^-	453.13	CR	This work	K^+	K^+	90.097	12.000	20
CH═	N^+	CR	CR	This work	K^+	Cl^-	61.010	CR	20
CH═	Na^+	CR	CR	This work	Cl^-	Cl^-	113.77	12.000	20
CH═	K^+	CR	CR	This work					

Table 4 Association energy $\varepsilon^{HB}_{ab,kl}/k_B$ and bonding volume $K^{HB}_{ab,kl}$ parameters for use within the SAFT-γ Mie group-contribution approach. For groups with several site types, the interactions are symmetrical, *i.e.*, $\varepsilon^{HB}_{ab,kl} = \varepsilon^{HB}_{ba,lk}$. Interactions not reported here are set to zero

Group k	Site *a* of group k	Group l	Site *b* of group l	$(\varepsilon^{HB}_{ab,kl}/k_B)$/K	$K^{HB}_{ab,kl}$/Å^3	Ref.
COOH	H	COOH	H	6427.9	0.8062	18
COOH	e_1	H_2O	H	1451.8	280.89	19
COOH	e_2	H_2O	H	1252.6	150.98	19
COOH	H	H_2O	e_1	2567.7	270.09	19
COOH	e_1	CH_2OH	H	1015.5	21.827	19
COOH	e_2	CH_2OH	H	547.4**2**	53.150	19
COOH	H	CH_2OH	e_1	524.0**4**	14.017	19
H_2O	e_1	H_2O	H	1985.4	101.69	68
H_2O	e_1	CH_2OH	H	621.68	425.00	19
H_2O	H	CH_2OH	e_1	2153.2	147.40	19
H_2O	H	COO^-	e_1	802.2**1**	52.5**55**	This work
H_2O	e_1	N^+	H	2783.7	15.536	This work
CH_2OH	e_1	CH_2OH	H	2097.9	62.3**09**	19
CH_2OH	e_1	N^+	H	1247.2	286.83	This work

References

1 S. Dufal, T. Lafitte, A. J. Haslam, A. Galindo, G. N. Clark, C. Vega and G. Jackson, *Mol. Phys.*, 2015, **113**, 948–984.
2 S. Dufal, T. Lafitte, A. J. Haslam, A. Galindo, G. N. Clark, C. Vega and G. Jackson, *Mol. Phys.*, 2018, **116**, 283–285.