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

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

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 Correction for 'Modelling and prediction of the thermophysical properties of aqueous mixtures of choline geranate and geranic acid (CAGE) using SAFT- $\gamma$  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- $\gamma$  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.

<sup>a</sup>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

<sup>b</sup>Department of Chemistry, Molecular Sciences Research Hub, White City Campus, Imperial College London, London W12 0BZ, UK

<sup>c</sup>Chemical Development, GSK, 1250 S Collegeville Rd, Collegeville, PA, 19426, USA

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

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



**Table 3** Unlike dispersion interaction energies ( $\epsilon_{kl}/k_B$ )/K and repulsive exponents  $\lambda_{kl}^r$  for use within the SAFT- $\gamma$  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  $\lambda_{kl}^r$  is given in eqn (6). The unlike group diameters  $\sigma_{kl}$  are obtained using the combining rule given in eqn (5) in all cases

Group k	Group l	( $\epsilon_{kl}/k_B$ )/K	$\lambda_{kl}^r$	Ref.	Group k	Group l	( $\epsilon_{kl}/k_B$ )/K	$\lambda_{kl}^r$	Ref.
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	256.77	15.050	17	CH=	Cl <sup>-</sup>	CR	CR	This work
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	350.77	CR	17	COOH	COOH	405.78	8.0000	18
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	CH <sub>2</sub> =	333.48	CR	18	COOH	H <sub>2</sub> O	289.76	CR	19
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	CH=	252.41	CR	18	COOH	CH <sub>2</sub> OH	656.80	CR	19
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	COOH	255.99	CR	18	COOH	C=	609.87	CR	This work
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	H <sub>2</sub> O	358.18	100.00	19	COOH	COO <sup>-</sup>	405.78	8.0000	This work
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	CH <sub>2</sub> OH	333.20	CR	19	COOH	N <sup>+</sup>	CR	CR	This work
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	C=	281.40	CR	69	COOH	Na <sup>+</sup>	CR	CR	This work
CH <sub>3</sub>	COO <sup>-</sup>	255.99	CR	This work	COOH	K <sup>+</sup>	CR	CR	This work
<sup>adj</sup> CH <sub>3</sub>	COO <sup>-</sup>	509.37	CR	This work	COOH	Cl <sup>-</sup>	CR	CR	This work
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	N <sup>+</sup>	462.18	CR	This work	H <sub>2</sub> O	H <sub>2</sub> O	266.68	17.020	68
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	Na <sup>+</sup>	CR	CR	This work	H <sub>2</sub> O	CH <sub>2</sub> OH	353.37	CR	19
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	K <sup>+</sup>	CR	CR	This work	H <sub>2</sub> O	C=	310.91	8.0000	This work
CH <sub>3</sub> <sup>adj</sup> CH <sub>3</sub>	Cl <sup>-</sup>	CR	CR	This work	H <sub>2</sub> O	COO <sup>-</sup>	171.61	CR	This work
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	473.39	19.871	17	H <sub>2</sub> O	N <sup>+</sup>	1481.3	21.217	This work
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	CH <sub>2</sub> =	386.80	CR	18	H <sub>2</sub> O	Na <sup>+</sup>	539.68	CR	20
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	CH=	459.40	CR	18	H <sub>2</sub> O	K <sup>+</sup>	376.25	CR	20
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	COOH	413.74	CR	18	H <sub>2</sub> O	Cl <sup>-</sup>	95.406	CR	20
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	H <sub>2</sub> O	423.63	100.00	19	CH <sub>2</sub> OH	CH <sub>2</sub> OH	407.22	22.699	19
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	CH <sub>2</sub> OH	423.17	CR	19	CH <sub>2</sub> OH	C=	799.66	CR	This work
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	C=	286.58	CR	69	CH <sub>2</sub> OH	COO <sup>-</sup>	656.80	CR	This work
CH <sub>2</sub>	COO <sup>-</sup>	413.74	CR	This work	CH <sub>2</sub> OH	N <sup>+</sup>	440.99	CR	This work
<sup>adj</sup> CH <sub>2</sub>	COO <sup>-</sup>	780.24	CR	This work	CH <sub>2</sub> OH	Na <sup>+</sup>	CR	CR	This work
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	N <sup>+</sup>	348.30	CR	This work	CH <sub>2</sub> OH	K <sup>+</sup>	CR	CR	This work
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	Na <sup>+</sup>	CR	CR	This work	CH <sub>2</sub> OH	Cl <sup>-</sup>	CR	CR	This work
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	K <sup>+</sup>	CR	CR	This work	C=	C=	1500.0	8.0000	69
CH <sub>2</sub> <sup>adj</sup> CH <sub>2</sub>	Cl <sup>-</sup>	CR	CR	This work	C=	COO <sup>-</sup>	609.87	CR	This work
CH <sub>2</sub> =	CH <sub>2</sub> =	300.90	20.271	18	C=	N <sup>+</sup>	CR	CR	This work
CH <sub>2</sub> =	CH=	275.75	CR	18	C=	Na <sup>+</sup>	CR	CR	This work
CH <sub>2</sub> =	COOH	<b>CR</b>	<b>CR</b>	This work	C=	K <sup>+</sup>	CR	CR	This work
CH <sub>2</sub> =	H <sub>2</sub> O	<b>387.25</b>	<b>94.463</b>	This work	C=	Cl <sup>-</sup>	CR	CR	This work
CH <sub>2</sub> =	CH <sub>2</sub> OH	<b>375.51</b>	CR	This work	COO <sup>-</sup>	COO <sup>-</sup>	<b>21.264</b>	8.0000	This work
CH <sub>2</sub> =	C=	<b>203.76</b>	CR	This work	COO <sup>-</sup>	N <sup>+</sup>	24.280	CR	This work
CH <sub>2</sub> =	COO <sup>-</sup>	CR	CR	This work	COO <sup>-</sup>	Na <sup>+</sup>	9.9125	CR	This work
CH <sub>2</sub> =	N <sup>+</sup>	CR	CR	This work	COO <sup>-</sup>	K <sup>+</sup>	23.999	CR	This work
CH <sub>2</sub> =	Na <sup>+</sup>	CR	CR	This work	COO <sup>-</sup>	Cl <sup>-</sup>	<b>47.154</b>	CR	This work
CH <sub>2</sub> =	K <sup>+</sup>	CR	CR	This work	N <sup>+</sup>	N <sup>+</sup>	<b>62.971</b>	<b>8.8971</b>	This work
CH <sub>2</sub> =	Cl <sup>-</sup>	CR	CR	This work	N <sup>+</sup>	Na <sup>+</sup>	CR	CR	This work
CH=	CH=	952.54	15.974	18	N <sup>+</sup>	K <sup>+</sup>	CR	CR	This work
CH=	COOH	453.13	CR	This work	N <sup>+</sup>	Cl <sup>-</sup>	61.989	CR	This work
CH=	H <sub>2</sub> O	332.21	17.309	This work	Na <sup>+</sup>	Na <sup>+</sup>	31.711	12.000	20
CH=	CH <sub>2</sub> OH	414.91	CR	This work	Na <sup>+</sup>	K <sup>+</sup>	CR	CR	This work
CH=	C=	1195.3	CR	69	Na <sup>+</sup>	Cl <sup>-</sup>	27.938	CR	20
CH=	COO <sup>-</sup>	453.13	CR	This work	K <sup>+</sup>	K <sup>+</sup>	90.097	12.000	20
CH=	N <sup>+</sup>	CR	CR	This work	K <sup>+</sup>	Cl <sup>-</sup>	61.010	CR	20
CH=	Na <sup>+</sup>	CR	CR	This work	Cl <sup>-</sup>	Cl <sup>-</sup>	113.77	12.000	20
CH=	K <sup>+</sup>	CR	CR	This work					



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

Group k	Site <i>a</i> of group k	Group l	Site <i>b</i> of group l	$(\epsilon_{ab,kl}^{\text{HB}}/k_{\text{B}})/\text{K}$	$K_{ab,kl}^{\text{HB}}/\text{\AA}^3$	Ref.
COOH	H	COOH	H	6427.9	0.8062	18
COOH	e <sub>1</sub>	H <sub>2</sub> O	H	1451.8	280.89	19
COOH	e <sub>2</sub>	H <sub>2</sub> O	H	1252.6	150.98	19
COOH	H	H <sub>2</sub> O	e <sub>1</sub>	2567.7	270.09	19
COOH	e <sub>1</sub>	CH <sub>2</sub> OH	H	1015.5	21.827	19
COOH	e <sub>2</sub>	CH <sub>2</sub> OH	H	547.42	53.150	19
COOH	H	CH <sub>2</sub> OH	e <sub>1</sub>	524.04	14.017	19
H <sub>2</sub> O	e <sub>1</sub>	H <sub>2</sub> O	H	1985.4	101.69	68
H <sub>2</sub> O	e <sub>1</sub>	CH <sub>2</sub> OH	H	621.68	425.00	19
H <sub>2</sub> O	H	CH <sub>2</sub> OH	e <sub>1</sub>	2153.2	147.40	19
H <sub>2</sub> O	H	COO <sup>-</sup>	e <sub>1</sub>	802.21	52.555	This work
H <sub>2</sub> O	e <sub>1</sub>	N <sup>+</sup>	H	2783.7	15.536	This work
CH <sub>2</sub> OH	e <sub>1</sub>	CH <sub>2</sub> OH	H	2097.9	62.309	19
CH <sub>2</sub> OH	e <sub>1</sub>	N <sup>+</sup>	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.

