

## CORRECTION

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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

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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.



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**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.
$\text{CH}_3/\text{adjCH}_3$	$\text{CH}_3/\text{adjCH}_3$	256.77	15.050	17	$\text{CH}=\text{}$	$\text{Cl}^-$	CR	CR	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{CH}_2/\text{adjCH}_2$	350.77	CR	17	$\text{COOH}$	$\text{COOH}$	405.78	8.0000	18
$\text{CH}_3/\text{adjCH}_3$	$\text{CH}_2=\text{}$	333.48	CR	18	$\text{COOH}$	$\text{H}_2\text{O}$	289.76	CR	19
$\text{CH}_3/\text{adjCH}_3$	$\text{CH}=\text{}$	252.41	CR	18	$\text{COOH}$	$\text{CH}_2\text{OH}$	656.80	CR	19
$\text{CH}_3/\text{adjCH}_3$	$\text{COOH}$	255.99	CR	18	$\text{COOH}$	$\text{C}=\text{}$	609.87	CR	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{H}_2\text{O}$	358.18	100.00	19	$\text{COOH}$	$\text{COO}^-$	405.78	8.0000	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{CH}_2\text{OH}$	333.20	CR	19	$\text{COOH}$	$\text{N}^+$	CR	CR	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{C}=\text{}$	281.40	CR	69	$\text{COOH}$	$\text{Na}^+$	CR	CR	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{COO}^-$	255.99	CR	This work	$\text{COOH}$	$\text{K}^+$	CR	CR	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{COO}^-$	509.37	CR	This work	$\text{COOH}$	$\text{Cl}^-$	CR	CR	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{N}^+$	462.18	CR	This work	$\text{H}_2\text{O}$	$\text{H}_2\text{O}$	266.68	17.020	68
$\text{CH}_3/\text{adjCH}_3$	$\text{Na}^+$	CR	CR	This work	$\text{H}_2\text{O}$	$\text{CH}_2\text{OH}$	353.37	CR	19
$\text{CH}_3/\text{adjCH}_3$	$\text{K}^+$	CR	CR	This work	$\text{H}_2\text{O}$	$\text{C}=\text{}$	310.91	8.0000	This work
$\text{CH}_3/\text{adjCH}_3$	$\text{Cl}^-$	CR	CR	This work	$\text{H}_2\text{O}$	$\text{COO}^-$	171.61	CR	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{CH}_2/\text{adjCH}_2$	473.39	19.871	17	$\text{H}_2\text{O}$	$\text{N}^+$	1481.3	21.217	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{CH}_2=\text{}$	386.80	CR	18	$\text{H}_2\text{O}$	$\text{Na}^+$	539.68	CR	20
$\text{CH}_2/\text{adjCH}_2$	$\text{CH}=\text{}$	459.40	CR	18	$\text{H}_2\text{O}$	$\text{K}^+$	376.25	CR	20
$\text{CH}_2/\text{adjCH}_2$	$\text{COOH}$	413.74	CR	18	$\text{H}_2\text{O}$	$\text{Cl}^-$	95.406	CR	20
$\text{CH}_2/\text{adjCH}_2$	$\text{H}_2\text{O}$	423.63	100.00	19	$\text{CH}_2\text{OH}$	$\text{CH}_2\text{OH}$	407.22	22.699	19
$\text{CH}_2/\text{adjCH}_2$	$\text{CH}_2\text{OH}$	423.17	CR	19	$\text{CH}_2\text{OH}$	$\text{C}=\text{}$	799.66	CR	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{C}=\text{}$	286.58	CR	69	$\text{CH}_2\text{OH}$	$\text{COO}^-$	656.80	CR	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{COO}^-$	413.74	CR	This work	$\text{CH}_2\text{OH}$	$\text{N}^+$	440.99	CR	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{COO}^-$	780.24	CR	This work	$\text{CH}_2\text{OH}$	$\text{Na}^+$	CR	CR	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{N}^+$	348.30	CR	This work	$\text{CH}_2\text{OH}$	$\text{K}^+$	CR	CR	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{Na}^+$	CR	CR	This work	$\text{CH}_2\text{OH}$	$\text{Cl}^-$	CR	CR	This work
$\text{CH}_2/\text{adjCH}_2$	$\text{K}^+$	CR	CR	This work	$\text{C}=\text{}$	$\text{C}=\text{}$	1500.0	8.0000	69
$\text{CH}_2/\text{adjCH}_2$	$\text{Cl}^-$	CR	CR	This work	$\text{C}=\text{}$	$\text{COO}^-$	609.87	CR	This work
$\text{CH}_2=\text{}$	$\text{CH}_2=\text{}$	300.90	20.271	18	$\text{C}=\text{}$	$\text{N}^+$	CR	CR	This work
$\text{CH}_2=\text{}$	$\text{CH}=\text{}$	275.75	CR	18	$\text{C}=\text{}$	$\text{Na}^+$	CR	CR	This work
$\text{CH}_2=\text{}$	$\text{COOH}$	CR	CR	This work	$\text{C}=\text{}$	$\text{K}^+$	CR	CR	This work
$\text{CH}_2=\text{}$	$\text{H}_2\text{O}$	387.25	<b>94.463</b>	This work	$\text{C}=\text{}$	$\text{Cl}^-$	CR	CR	This work
$\text{CH}_2=\text{}$	$\text{CH}_2\text{OH}$	375.51	CR	This work	$\text{COO}^-$	$\text{COO}^-$	<b>21.264</b>	8.0000	This work
$\text{CH}_2=\text{}$	$\text{C}=\text{}$	203.76	CR	This work	$\text{COO}^-$	$\text{N}^+$	24.280	CR	This work
$\text{CH}_2=\text{}$	$\text{COO}^-$	CR	CR	This work	$\text{COO}^-$	$\text{Na}^+$	9.9125	CR	This work
$\text{CH}_2=\text{}$	$\text{N}^+$	CR	CR	This work	$\text{COO}^-$	$\text{K}^+$	23.999	CR	This work
$\text{CH}_2=\text{}$	$\text{Na}^+$	CR	CR	This work	$\text{COO}^-$	$\text{Cl}^-$	<b>47.154</b>	CR	This work
$\text{CH}_2=\text{}$	$\text{K}^+$	CR	CR	This work	$\text{N}^+$	$\text{N}^+$	<b>62.971</b>	<b>8.8971</b>	This work
$\text{CH}_2=\text{}$	$\text{Cl}^-$	CR	CR	This work	$\text{N}^+$	$\text{Na}^+$	CR	CR	This work
$\text{CH}=\text{}$	$\text{CH}=\text{}$	952.54	15.974	18	$\text{N}^+$	$\text{K}^+$	CR	CR	This work
$\text{CH}=\text{}$	$\text{COOH}$	453.13	CR	This work	$\text{N}^+$	$\text{Cl}^-$	61.989	CR	This work
$\text{CH}=\text{}$	$\text{H}_2\text{O}$	332.21	17.309	This work	$\text{Na}^+$	$\text{Na}^+$	31.711	12.000	20
$\text{CH}=\text{}$	$\text{CH}_2\text{OH}$	414.91	CR	This work	$\text{Na}^+$	$\text{K}^+$	CR	CR	This work
$\text{CH}=\text{}$	$\text{C}=\text{}$	1195.3	CR	69	$\text{Na}^+$	$\text{Cl}^-$	27.938	CR	20
$\text{CH}=\text{}$	$\text{COO}^-$	453.13	CR	This work	$\text{K}^+$	$\text{K}^+$	90.097	12.000	20
$\text{CH}=\text{}$	$\text{N}^+$	CR	CR	This work	$\text{K}^+$	$\text{Cl}^-$	61.010	CR	20
$\text{CH}=\text{}$	$\text{Na}^+$	CR	CR	This work	$\text{Cl}^-$	$\text{Cl}^-$	113.77	12.000	20
$\text{CH}=\text{}$	$\text{K}^+$	CR	CR	This work					

**Table 4** Association energy  $\varepsilon_{ab,kl}^{\text{HB}}/k_B$  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.,  $\varepsilon_{ab,kl}^{\text{HB}} = \varepsilon_{ba,lk}^{\text{HB}}$ . 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	$(\varepsilon_{ab,kl}^{\text{HB}}/k_B)/K$	$K_{ab,kl}^{\text{HB}}/\text{\AA}^3$	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

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