

# Additional parameters used in An approach for modelling simultaneous fluid-phase and chemical reaction equilibria in multicomponent systems via Lagrangian duality: The reactive HELD algorithm.

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Table 1: Like Group parameters for use within the SAFT -  $\gamma$  Mie

Group $k$	$v_k$	$S_k$	$\lambda_{kk}^r$	$\lambda_{kk}^a$	$\sigma_{kk}/\text{\AA}$	$\left(\frac{\varepsilon_{kk}}{k_B}\right)/K$	$N_{ST,k}$	$n_{k,H}$	$n_{k,e1}$	$n_{k,e2}$	Ref.
CH3COOH	1	0.6547	11.649	6	3.9500	318.42	3	1	2	2	[1]

Table 2: Group-group dispersion energies,  $\epsilon_{kl}$  and repulsive exponent  $\lambda_{kl}^r$  relevant to mixtures studied here for use within the SAFT- $\gamma$  Mie approach. CR indicates that the unlike repulsive exponent  $\lambda_{kl}^r$ . The  $\dagger$  indicates that the parameter is developed in the current work.

group $k$	group $l$	$\left(\frac{\varepsilon_{kl}}{k_B}\right)/K$	$\lambda_{kl}^r$	Ref.
CH <sub>3</sub>	CH <sub>3</sub> COOH	431.93	24.162	$\dagger$
CH <sub>2</sub> OH	CH <sub>3</sub> COOH	312.48	CR	$\dagger$
CH <sub>3</sub> COOH	COO	405.16	9.7616	$\dagger$
CH <sub>2</sub> OH	COO	533.65	CR	$\dagger$

Table 3: Unlike association energies  $\varepsilon_{kl,ab}^{HB}$  and bonding volume  $K_{kl,ab}$  parameters relevant to mixtures studied here for use within the SAFT- $\gamma$  Mie approach. The † indicates that the parameter is developed in the current work.

group $k$	site $a$	group $k$	group $l$	site $b$	group $l$	$\varepsilon_{kl,ab}^{HB} / \text{K}$	$K_{kl,ab} / \text{\AA}^3$	Ref.
CH <sub>2</sub> OH	H		CH <sub>3</sub> COOH	e1		1917.6	40.221	†
CH <sub>2</sub> OH	H		CH <sub>3</sub> COOH	e2		2905.1	4.2324	†
CH <sub>2</sub> OH	e		CH <sub>3</sub> COOH	H		2895.8	337.33	†
CH <sub>3</sub> COOH	H		COO	e		2678.3	85.450	†
COO	e		CH <sub>2</sub> OH	H		1240.9	385.39	†
CH <sub>3</sub> COOH	H		CH <sub>3</sub> COOH	H		5959.5	8.0000	[1]

## References

- [1] Z. Fan, M. Heiling, F.A. Perdomo, and G. Jackson, 2019. Application of PC-SAFT and SAFT- $\gamma$ -Mie equations of state in thermodynamic properties of aqueous systems comprising low molecular weight carboxylic acids, MRes dissertation, Imperial College London.