

AIOMFAC main groups

		H <sup>+</sup>	Li <sup>+</sup>	Na <sup>+</sup>	K <sup>+</sup>	NH <sub>4</sub> <sup>+</sup>	Mg <sup>2+</sup>	Ca <sup>2+</sup>	Cl <sup>-</sup>	Br <sup>-</sup>	NO <sub>3</sub> <sup>-</sup>	HSO <sub>4</sub> <sup>-</sup>	SO <sub>4</sub> <sup>2-</sup>	CH <sub>n</sub>	CH <sub>n</sub> <sup>[alc]</sup>	CH <sub>n</sub> <sup>[alc-tail]</sup>	CH <sub>n</sub> <sup>[OH]</sup>	C=C	ACH <sub>n</sub>	OH	ACOH	CH <sub>n</sub> CO	CHO	CCOO	CH <sub>n</sub> O	COOH	CH <sub>n</sub> OOH[perox]	C(=O)OOH[perox]	CH <sub>n</sub> OOCH <sub>m</sub> [perox]	C(=O)OONO <sub>2</sub> [perox]	CH <sub>n</sub> ONO <sub>2</sub>	H <sub>2</sub> O
cations	H <sup>+</sup>																															
	Li <sup>+</sup>																															
	Na <sup>+</sup>																															
	K <sup>+</sup>																															
	NH <sub>4</sub> <sup>+</sup>																															
	Mg <sup>2+</sup>																															
	Ca <sup>2+</sup>																															
anions	Cl <sup>-</sup>																															
	Br <sup>-</sup>																															
	NO <sub>3</sub> <sup>-</sup>																															
	HSO <sub>4</sub> <sup>-</sup>		?		?		?	?																								
	SO <sub>4</sub> <sup>2-</sup>																															
alkyl (standard)	CH <sub>n</sub>																															
alkyl (in alcohols)	CH <sub>n</sub> <sup>[alc]</sup>																															
alkyl (in hydrophobic tails of alcohols)	CH <sub>n</sub> <sup>[alc-tail]</sup>																															
alkyl (bonded to hydroxyl group)	CH <sub>n</sub> <sup>[OH]</sup>																															
alkenyl	C=C																															
aromatic hydrocarbon	ACH <sub>n</sub>																															
hydroxyl	OH																															
aromatic carbon-alcohol	ACOH											?																				
ketone	CH <sub>n</sub> CO											?																				
aldehyde	CHO	?										?																				
ester	CCOO	?										?																				
ether	CH <sub>n</sub> O																															
carboxyl	COOH																															
hydroperoxide	CH <sub>n</sub> OOH[perox]																		?		?											
peroxyacid	C(=O)OOH[perox]																		?		?											
peroxide (organic)	CH <sub>n</sub> OOCH <sub>m</sub> [perox]																		?		?											
peroxyacyl nitrate	C(=O)OONO <sub>2</sub> [perox]	?	?	?	?	?	?	?	?	?	?	?	?					?		?												
organonitrate	CH <sub>n</sub> ONO <sub>2</sub>	?	?	?	?	?	?	?	?	?	?	?	?					?		?												
water	H <sub>2</sub> O																															

cation ↔ anion

middle-range parameters available

cation ↔ cation or anion ↔ anion

no specific interaction parameters

same main groups ("ideal mixing")

no specific interaction parameters

org. main group X ↔ main group Y

short-range parameters available

ion ↔ org. main group

middle-range parameters available

ion ↔ org. main group

available using analogy approach

water as the reference solvent for ions

no direct interaction parameters

?

missing interaction parameters

mixtures of these groups are not available