

AIOMFAC main groups

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

cation ↔ anion

middle-range parameters available

?

cation ↔ anion

param. available using analogy approach

cation ↔ cation or anion ↔ anion

no specific (0) interaction parameters

∅

cation ↔ cation or anion ↔ anion

specific, non-zero interaction parameter

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

param. 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