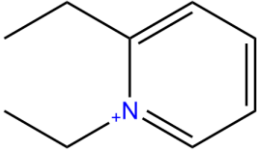
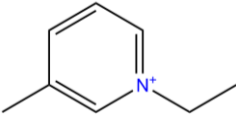
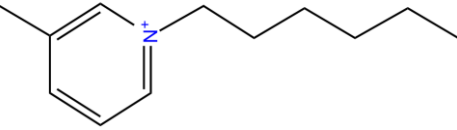
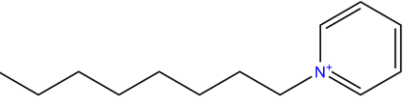
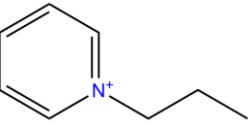
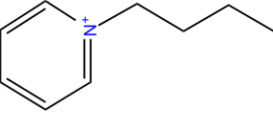
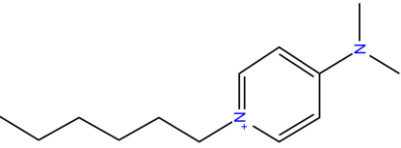
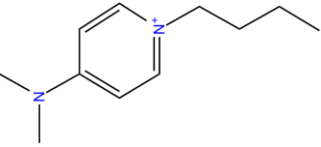
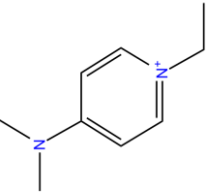
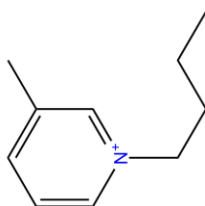


cations

K-1		$(C_2)_2Py$
	1,2-diethylpyridinium	
K-2		C_2MPy
	1-ethyl-3-methylpyridinium	
K-3		C_6MPy
	1-hexyl-3-methylpyridinium	
K-4		C_8Py
	1-octylpyridinium	
K-5		C_3Py
	1-propylpyridinium	
K-6		C_4Py
	1-butylpyridinium	
K-7		$C_6(CH_3NCH_3)Py$
	4-(dimethylamino)-1-hexylpyridinium	
K-8		$C_4(CH_3NCH_3)Py$
	n-butyl-4-(n',n'-dimethylammonium)pyridinium	
K-9		$C_2(CH_3NCH_3)Py$
	n-ethyl-4-(n',n'-dimethylammonium)pyridinium	

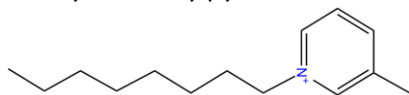
K-10



1-butyl-3-methylpyridinium

C₄MPy

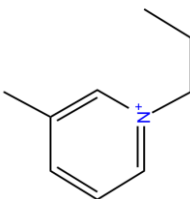
K-11



N-octyl-3-methylpyridinium

C₈MPy

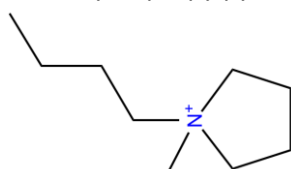
K-12



3-methyl-1-propylpyridinium

C₃MPy

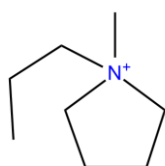
K-13



1-butyl-1-methylpyrrolidinium

C₄MPyr

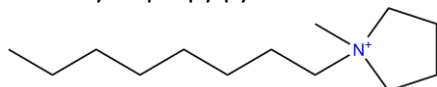
K-14



1-methyl-1-propylpyrrolidinium

C₃MPyr

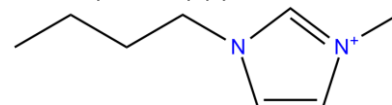
K-15



1-methyl-1-octylpyrrolidinium

C₈MPyr

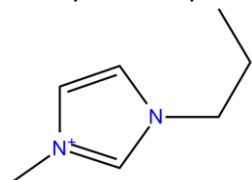
K-16



1-butyl-3-methylimidazolium

C₄MIm

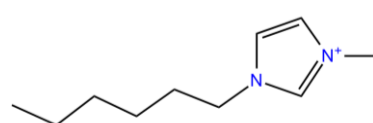
K-17



1-methyl-3-propylimidazolium

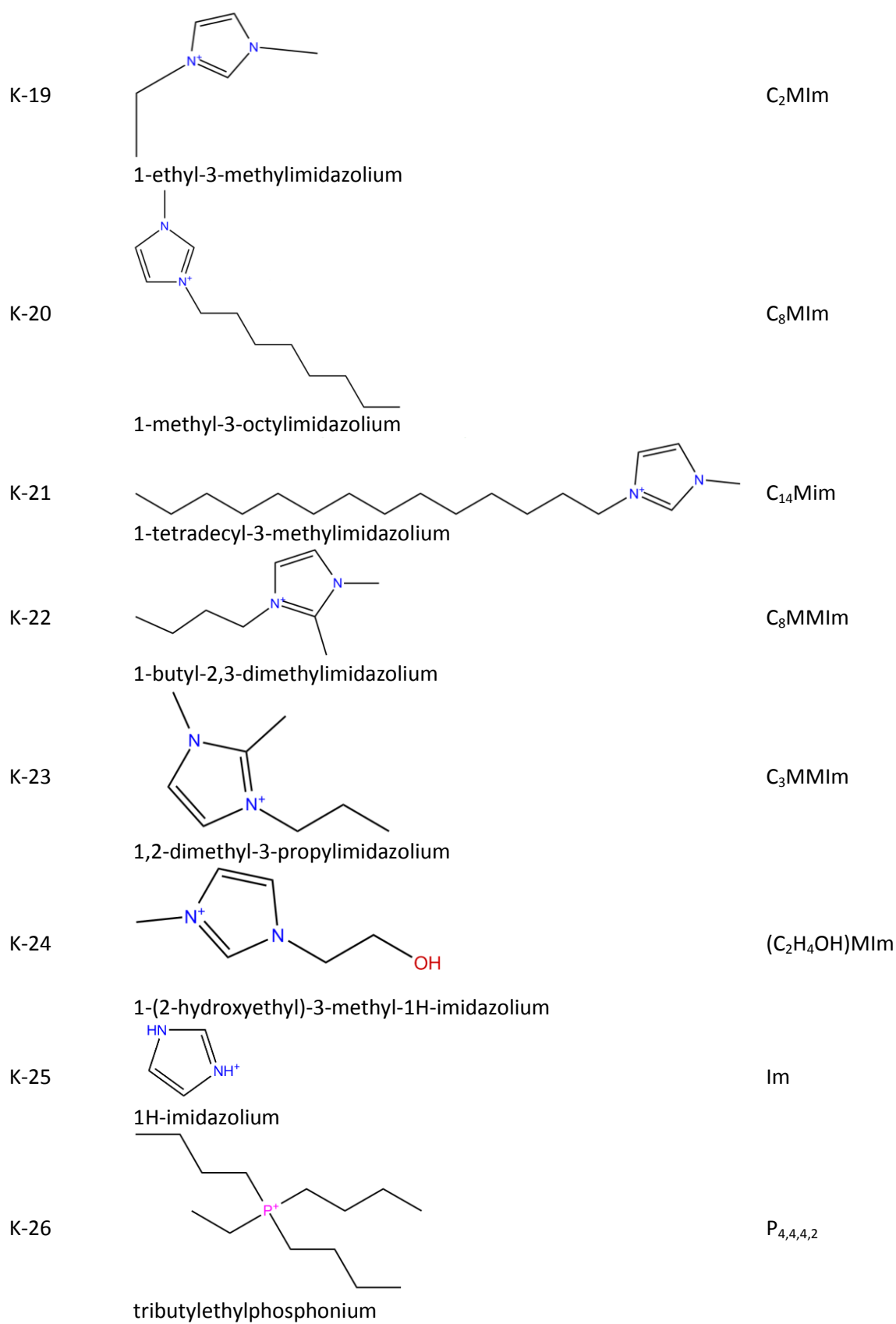
C₃MIm

K-18

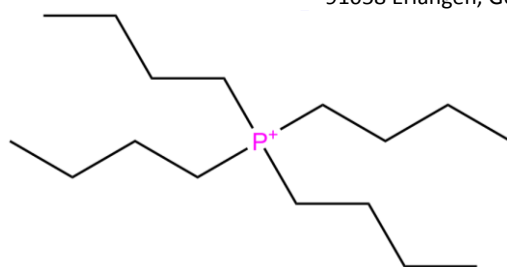


1-hexyl-3-methylimidazolium

C₆MIm



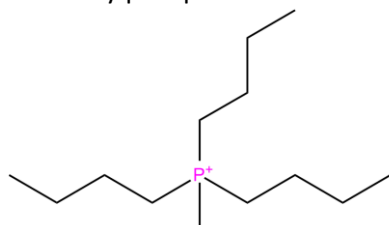
K-27



P_{4,4,4,4}

tetrabutylphosphonium

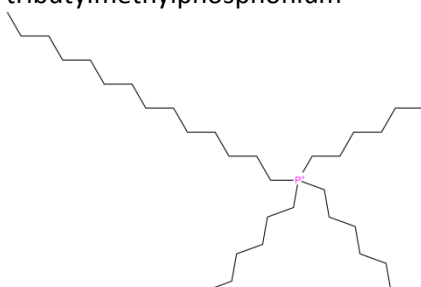
K-28



P_{4,4,4,1}

tributylmethylphosphonium

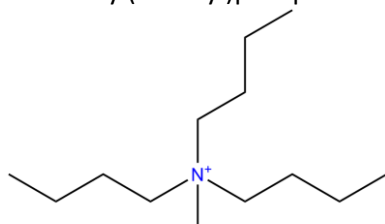
K-29



P_{14,6,6,6}

tetradecyl(trihexyl)phosphonium

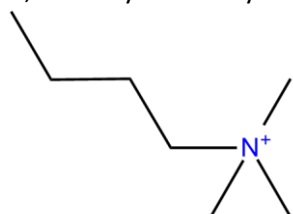
K-30



N_{4,4,4,1}

N,N-dibutyl-N-methyl-1-butanaminium

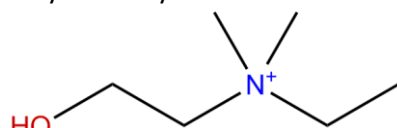
K-31



N_{4,1,1,1}

butyltrimethylammonium

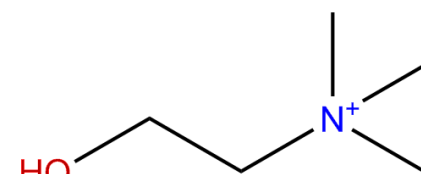
K-32



N_{C₂H₅OH,2,1,1}

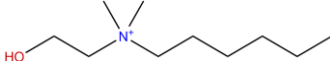
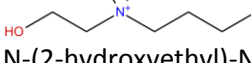
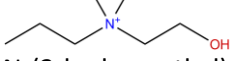
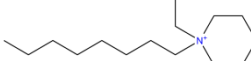
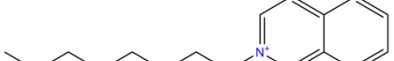
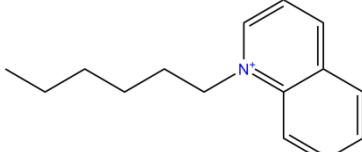
N-ethyl-2-hydroxy-N,N-dimethylethanaminium

K-33

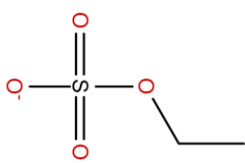
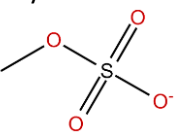
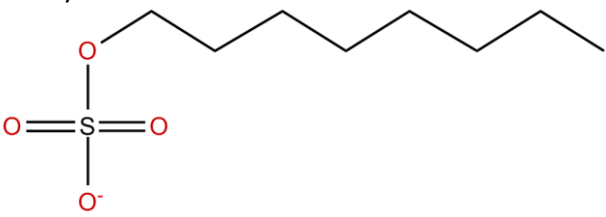
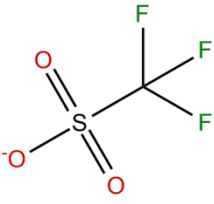
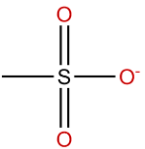
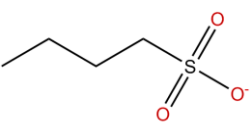
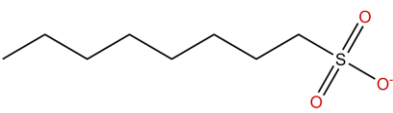
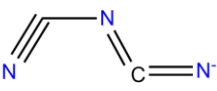


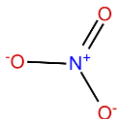
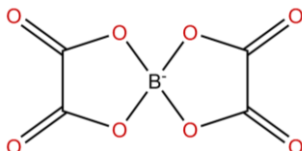
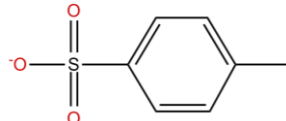
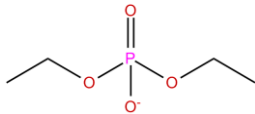
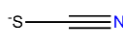
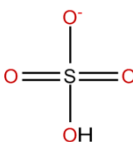
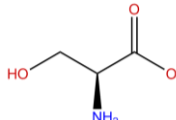
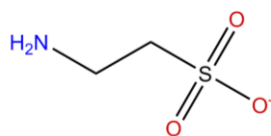
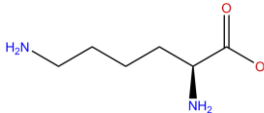
N_{C₂H₅OH,1,1,1}

2-hydroxy-N,N,N-trimethyl-ethanaminium

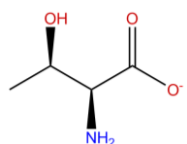
K-34	 N-(2-hydroxyethyl)-N,N-dimethylhexan-1-aminium	$N_{6,C_2H_5OH,1,1}$
K-35	 N-(2-hydroxyethyl)-N,N-dimethylbutanaminium	$N_{4,C_2H_5OH,1,1}$
K-36	 N-(2-hydroxyethyl)-N,N-dimethylpropanaminium	$N_{3,C_2H_5OH,1,1}$
K-37	 1-ethyl-1-octylpiperidinium	C_8C_2Pip
K-38	 2-octylisoquinolinium	C_8Quin
K-39	 1-hexylquinolinium	C_6Quin

anions

A-1		EtSO ₄
	ethylsulfate	
A-2		MeSO ₄
	methylsulfate	
A-3		C ₈ SO ₄
	octylsulfate	
A-4		CF ₃ SO ₃
	trifluoromethanesulfonate	
A-5		MeSO ₃
	methanesulfonate	
A-6		C ₄ SO ₃
	1-butanefulfonate	
A-7		C ₈ SO ₃
	1-octanesulfonate	
A-8		Dca
	dicyanamide	
A-9		Br
	bromide	

A-10		NO_3
	nitrate	
A-11		BF_4
	tetrafluoroborate	
A-12		C4O8B
	bis(oxalato)borate	
A-13		Tos
	tosylate	
A-14		NTF ₂
	bis[(trifluoromethyl)sulfonyl]imide	
A-15		$(\text{C}_2\text{H}_5)_2\text{PO}_4$
	diethylphosphate	
A-16		Tca
	thiocyanate	
A-17		HSO_4
	hydrogen sulfate	
A-18		Ser
	L-serinate	
A-19		Tau
	2-aminoethanesulfonate	
A-20		Lys
	L-lysinate	

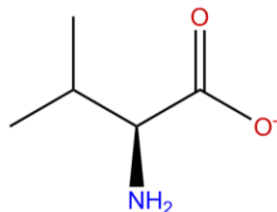
A-21



L-threoninate

Thr

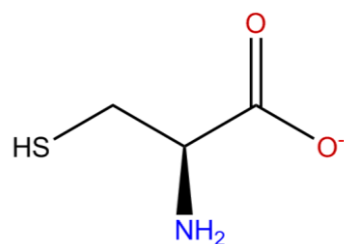
A-22



L-valinate

Val

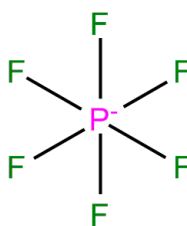
A-23



L-cysteinate

Cys

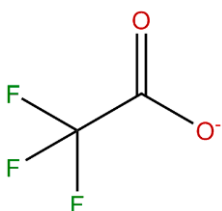
A-24



hexafluorophosphate

PF₆

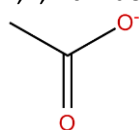
A-25



2,2,2-trifluoroacetate

OTfa

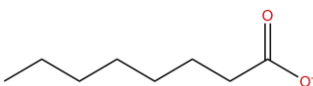
A-26



acetate

OAc

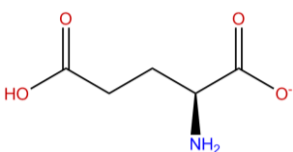
A-27



octanoate

OCE

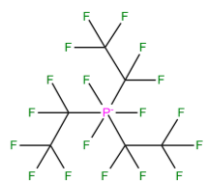
A-28



(S)-2-amino-4-carboxybutanoate

COB

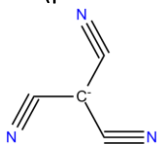
A-29



Fap

tris(pentafluoroethyl)trifluorophosphate

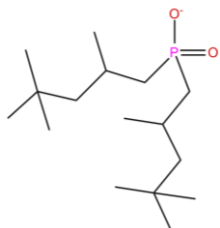
A-30



Tcm

tricyanomethanide

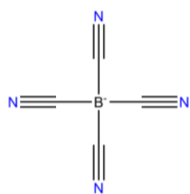
A-31



TMPP

bis(2,4,4-trimethylpentyl)phosphinate

A-32



(CN)₄B

tetracyanoborate

mathematical definitions of error types

Absolute average error (AAE):

$$AAE = \frac{1}{n} \sum_{i=1}^n |c_{P,i}^{exp.} - c_{P,i}^{calc.}|$$

Absolute average percentage error (AAPE):

$$AAPE = \frac{1}{n} \cdot 100\% \sum_{i=1}^n \frac{|c_{P,i}^{exp.} - c_{P,i}^{calc.}|}{c_{P,i}^{exp.}}$$

root mean square deviation (RMSD):

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (c_{P,i}^{exp.} - c_{P,i}^{calc.})^2}{n}}$$

combined uncertainty:

$$combined\ uncertainty = \frac{\sum_{i=1}^n \sqrt{\Delta c_{P,i}^{exp.-uncertainty^2} + \left(\frac{|c_{P,i}^{exp.} - c_{P,i}^{calc.}|}{c_{P,i}^{exp.}} \right)^2}}{n}$$