

Supporting information

Screening of ionic liquids for keratin dissolution by means of COSMO-RS and experimental verification

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Number of figures: 4

Number of tables: 5

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1. Synthesis and characterization of ILs

1.1 Properties of ten ILs

Table S1. Properties of ten ILs

ILs	cation(m/z)	negion(m/z)	Water content(ppm)	Purity
EmimAc	111.0931	---	2890	99%
EmimDEP	111.0917	153.0311	1310	---
AmimCl	123.0930	---	2508	99%
EmimCl	111.0931	---	1163	98%
BmimCl	139.1247	---	2727	98%
HOEtMimCl	127.0896	---	9001	99%
BmimDCA	139.1253	---	4237	---
BmimSCN	139.1264	---	2606	---
BmpyrrCl	142.1629	---	9661	99%
BpyCl	136.1158	---	2200	99%

1.2 NMR analysis and Electronic spray mass spectrum of three synthesis ILs

EmimDEP: ^1H NMR (d_6 -DMSO): 9.32[s, 1H, (Im)], 7.86[t, J=1.7 Hz, 1H, (Im)], 7.76[t, J=1.6 Hz, 1H, (Im)], 4.23[q, J=7.3 Hz, 2H, $\text{CH}_2\text{-CH}_3$], 3.88[s, 3H, N- CH_3], 3.62[p, J=7.0 Hz, 4H,

2(O-CH₂)], 1.40[t, J=7.3 Hz, 3H,CH₂-CH₃], 1.07[t, J=7.1 Hz, 6H, 2(O-CH₂-CH₃)]; ¹³C NMR: 136.86, 123.51, 121.94, 58.98, 43.98, 35.55, 16.68, 15.14.

S2

BmimSCN: ¹H NMR (d₆-DMSO): 9.10[d, J=1.9 Hz, 1H, (Im)], 7.77[d, J=1.9 Hz, 1H, (Im)], 7.70[d, J=1.9Hz, 1H, (Im)], 3.85[s, J=7.3 Hz, 2H, N-CH₂-], 3.34[s, 3H, N-CH₃], 1.76[m, J=7.3 Hz, 2H, -CH₂-CH₂-CH₃], 1.26[q, J=7.4 Hz, 2H,CH₂-CH₃], 0.90[t, J=7.4 Hz, 3H, -CH₃]; ¹³C NMR: 136.67, 123.95, 122.52, 48.97, 36.26, 31.80, 18.93, 13.41.

BmimDCA: ¹H NMR (d₆-DMSO): 9.10[d, J=1.7 Hz, 1H, (Im)], 7.76[t, J=1.8 Hz, 1H, (Im)], 7.70[t, J=1.9Hz, 1H, (Im)], 3.84[t, J=7.3 Hz, 2H, N-CH₂-], 3.31[s, 3H, N-CH₃], 1.76[m, J=7.3 Hz, 2H, -CH₂-CH₂-CH₃], 1.25[m, J=7.1 Hz, 2H,CH₂-CH₃], 0.90[t, J=7.4 Hz, 3H, -CH₃]; ¹³C NMR: 137.12, 123.80, 122.74, 48.97, 36.26, 31.64, 18.93, 13.41.

Electronic spray mass spectrum

EmimDEP:

Cation:

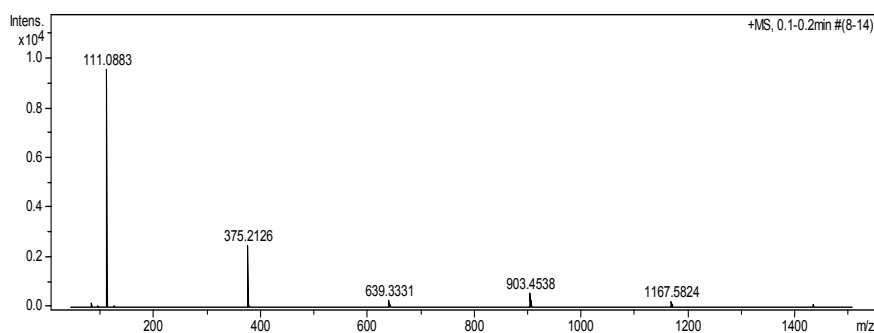


Figure S1. Electronic spray mass spectrum of [Emim]⁺

Anion:

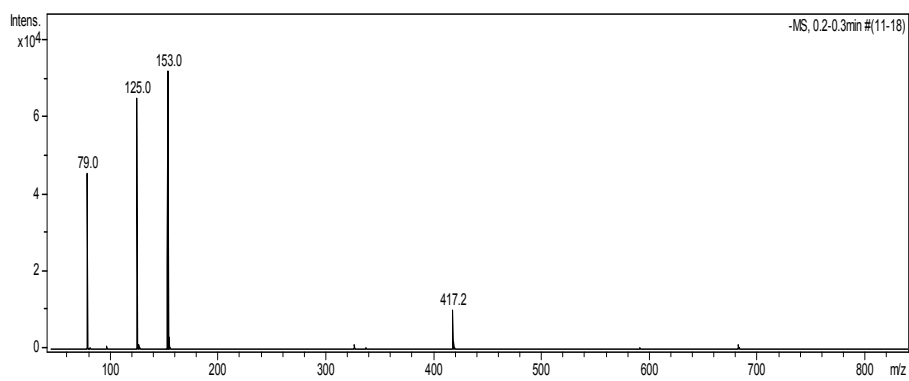


Figure S2. Electronic spray mass spectrum of [DEP]⁻

S3

BmimDCA:

Cation:

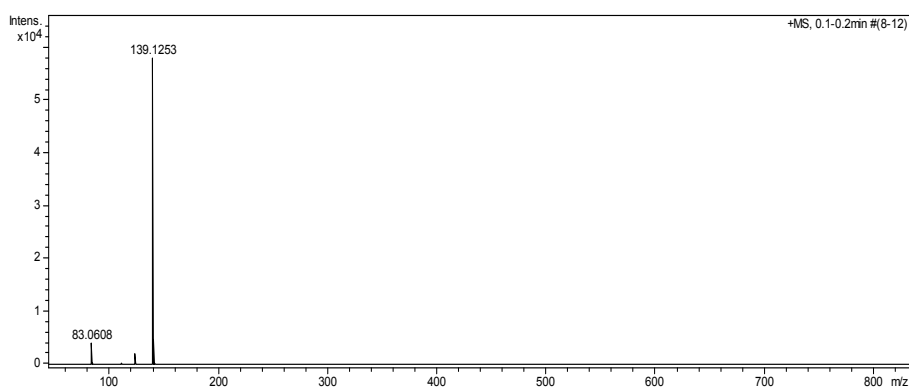


Figure S3. Electronic spray mass spectrum of [Bmim]⁺

BmimSCN:

Cation:

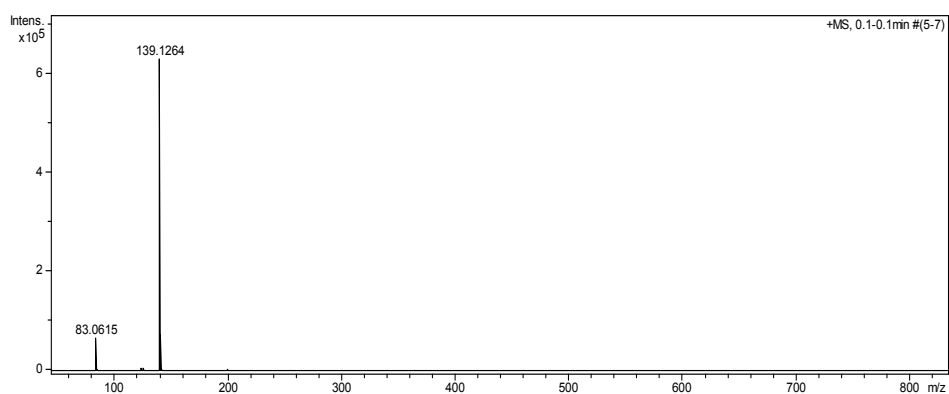


Figure S4. Electronic spray mass spectrum of [Bmim]⁺

2. Literature values of keratin dissolution in ionic liquids

Table of S2 The literature values of keratin dissolution in ionic liquids

Material	ILs	Conditions					Ref
		Temperature (°C)	Solid:liquid	Time	Solubility (wt%)	Yield of keratin	
Wool	AmimCl	130	--	640min	21%	--	1 ¹
Wool	BmimCl	130	--	535min	15%	--	1
Wool	BmimCl	120	1:6	30min	--	57%	2 ²
Wool	BmimCl	150	1:6	30min	--	35%	2
Wool	BmimCl	180	1:6	30min	--	18%	2
Feathers	BmimCl	130	1:2	10h	50%	60%	3 ³
Feathers	AmimCl	130	1:2	10h	50%	60%	3
Feathers	Choline thioglycolate	130	1:2	10h	45%	55%	3
Wool	BmimOAc	130	1:12.5	10min	--	--	4 ⁴
Wool	BmimSCN	130	1:12.5	900min	--	--	4
Wool	BmimFeCl ₄	130	1:12.5	nd ^a	--	--	4
Wool	BmimDMP	130	1:12.5	90min	--	--	4
Wool	EmimDMP	130	1:12.5	90min	--	--	4
Wool	BmimCl	130	1:12.5	300min	--	--	4
Wool	P ₄₄₄₄ Cl	130	1:12.5	nd ^a	--	--	4
Wool	N ₄₄₄₄ Cl	130	1:12.5	nd ^a	--	--	4
Wool	N ₂₂₂₁ DMP	130	1:12.5	180min	--	--	4
Wool	EmimDEP	120	1:12.5	90min	--	0.3553g/g	5 ⁵
Wool	EmimDMP	120	1:12.5	150min	--	0.3118g/g	5
Wool	DBNEDEP	120	1:12.5	180min	--	0.4471g/g	5
Wool	DBNMDMP	120	1:12.5	210min	--	0.4000g/g	5
Wool	DBNHOOAc	120	1:12.5	30min	--	0.1697g/g	5

3. Logarithmic activity coefficients of three keratin models

S6

Table S4. Prediction Iny of GSSG by COMSO-RS

Cations/ anions	Ac	Dec	HCOO	Cl	DEP	DMP	BEN	DBP	DHP	Br	TOS	MeOET SO ₄	BaSO ₄	MeSO ₄	I	DCA	HSO ₄	SCN	BF ₄	ClO ₂	PF ₆	TF ₂ N	ACl ₄
HOEPip	(1.82)	(1.74)	(1.52)	(1.37)	(1.46)	(1.41)	(1.41)	(1.41)	(0.99)	(0.91)	(0.96)	(0.72)	(0.72)	(0.63)	(0.53)	(0.53)	(0.42)	(0.40)	(0.32)	(0.22)	(0.27)	(0.32)	(0.33)
HOEmor	(1.86)	(1.78)	(1.55)	(1.37)	(1.46)	(1.41)	(1.44)	(1.42)	(0.99)	(0.92)	(0.96)	(0.69)	(0.70)	(0.60)	(0.52)	(0.54)	(0.40)	(0.40)	(0.27)	(0.17)	(0.20)	(0.28)	(0.26)
HOEmim	(1.89)	(1.77)	(1.60)	(1.46)	(1.51)	(1.47)	(1.46)	(1.45)	(1.06)	(1.00)	(1.01)	(0.76)	(0.76)	(0.68)	(0.60)	(0.58)	(0.48)	(0.47)	(0.35)	(0.25)	(0.27)	(0.31)	(0.30)
Cl	(1.94)	(1.83)	(1.63)	(1.48)	(1.53)	(1.49)	(1.48)	(1.48)	(1.02)	(1.00)	(1.01)	(0.73)	(0.74)	(0.65)	(0.57)	(0.57)	(0.43)	(0.43)	(0.28)	(0.19)	(0.21)	(0.28)	(0.27)
TBDH	(2.05)	(1.77)	(1.81)	(1.72)	(1.63)	(1.64)	(1.55)	(1.50)	(1.25)	(1.28)	(1.14)	(0.90)	(0.86)	(0.86)	(0.87)	(0.76)	(0.70)	(0.66)	(0.55)	(0.39)	(0.35)	(0.26)	(0.27)
HOEmpyr	(2.13)	(1.91)	(1.84)	(1.72)	(1.66)	(1.65)	(1.62)	(1.56)	(1.22)	(1.23)	(1.13)	(0.85)	(0.84)	(0.80)	(0.78)	(0.71)	(0.62)	(0.57)	(0.42)	(0.31)	(0.26)	(0.27)	(0.23)
DBUH	(2.25)	(1.97)	(1.95)	(1.79)	(1.72)	(1.73)	(1.71)	(1.59)	(1.34)	(1.32)	(1.17)	(0.89)	(0.86)	(0.86)	(0.86)	(0.79)	(0.70)	(0.67)	(0.51)	(0.36)	(0.30)	(0.22)	(0.21)
ACH	(2.25)	(2.10)	(1.90)	(1.70)	(1.72)	(1.69)	(1.73)	(1.65)	(1.26)	(1.17)	(1.13)	(0.83)	(0.83)	(0.76)	(0.70)	(0.68)	(0.57)	(0.54)	(0.37)	(0.24)	(0.22)	(0.27)	(0.21)
EOmPy	(2.31)	(2.12)	(1.98)	(1.79)	(1.78)	(1.76)	(1.76)	(1.69)	(1.36)	(1.25)	(1.18)	(0.90)	(0.89)	(0.84)	(0.79)	(0.72)	(0.66)	(0.61)	(0.47)	(0.33)	(0.30)	(0.29)	(0.25)
Buin	(2.33)	(2.05)	(2.03)	(1.86)	(1.78)	(1.78)	(1.76)	(1.65)	(1.40)	(1.34)	(1.19)	(0.93)	(0.89)	(0.80)	(0.88)	(0.79)	(0.75)	(0.67)	(0.54)	(0.39)	(0.32)	(0.24)	(0.22)
EOmMim	(2.33)	(2.09)	(2.01)	(1.84)	(1.79)	(1.78)	(1.77)	(1.68)	(1.38)	(1.31)	(1.19)	(0.91)	(0.89)	(0.87)	(0.84)	(0.76)	(0.70)	(0.64)	(0.50)	(0.35)	(0.30)	(0.26)	(0.22)
EOmMim	(2.34)	(2.13)	(2.00)	(1.82)	(1.80)	(1.78)	(1.77)	(1.70)	(1.36)	(1.27)	(1.19)	(0.92)	(0.90)	(0.86)	(0.80)	(0.72)	(0.68)	(0.60)	(0.49)	(0.35)	(0.32)	(0.28)	(0.26)
APy	(2.35)	(2.09)	(2.01)	(1.83)	(1.81)	(1.79)	(1.79)	(1.72)	(1.35)	(1.28)	(1.21)	(0.92)	(0.91)	(0.86)	(0.80)	(0.73)	(0.67)	(0.60)	(0.48)	(0.34)	(0.31)	(0.29)	(0.26)
Bpy	(2.34)	(2.10)	(2.03)	(1.85)	(1.79)	(1.78)	(1.78)	(1.68)	(1.42)	(1.32)	(1.19)	(0.92)	(0.90)	(0.89)	(0.86)	(0.77)	(0.74)	(0.66)	(0.52)	(0.37)	(0.30)	(0.25)	(0.20)
AOPnum	(2.35)	(2.12)	(2.03)	(1.86)	(1.82)	(1.80)	(1.79)	(1.71)	(1.37)	(1.32)	(1.21)	(0.94)	(0.92)	(0.88)	(0.85)	(0.76)	(0.70)	(0.63)	(0.50)	(0.35)	(0.31)	(0.28)	(0.25)
Enim	(2.35)	(2.04)	(2.06)	(1.90)	(1.79)	(1.81)	(1.77)	(1.65)	(1.45)	(1.37)	(1.21)	(0.94)	(0.90)	(0.92)	(0.91)	(0.78)	(0.79)	(0.68)	(0.56)	(0.41)	(0.31)	(0.20)	(0.17)
Benor	(2.38)	(2.09)	(1.98)	(1.98)	(1.86)	(1.86)	(1.79)	(1.72)	(1.44)	(1.45)	(1.28)	(0.99)	(0.96)	(0.96)	(0.96)	(0.83)	(0.77)	(0.71)	(0.56)	(0.40)	(0.33)	(0.27)	(0.23)
DBNH	(2.39)	(2.15)	(2.06)	(1.89)	(1.84)	(1.83)	(1.81)	(1.73)	(1.41)	(1.35)	(1.22)	(0.94)	(0.92)	(0.90)	(0.86)	(0.77)	(0.72)	(0.65)	(0.52)	(0.37)	(0.32)	(0.27)	(0.24)
Anum	(2.39)	(2.16)	(2.06)	(1.87)	(1.82)	(1.81)	(1.82)	(1.71)	(1.41)	(1.33)	(1.20)	(0.90)	(0.88)	(0.86)	(0.84)	(0.78)	(0.70)	(0.64)	(0.46)	(0.32)	(0.25)	(0.24)	(0.17)
EOmMor	(2.39)	(2.21)	(2.08)	(1.90)	(1.87)	(1.85)	(1.84)	(1.77)	(1.35)	(1.33)	(1.25)	(0.95)	(0.94)	(0.89)	(0.84)	(0.75)	(0.70)	(0.60)	(0.49)	(0.34)	(0.31)	(0.29)	(0.25)
Epy	(2.42)	(2.21)	(2.08)	(1.90)	(1.87)	(1.85)	(1.84)	(1.77)	(1.35)	(1.33)	(1.25)	(0.95)	(0.94)	(0.89)	(0.84)	(0.75)	(0.70)	(0.60)	(0.49)	(0.34)	(0.31)	(0.29)	(0.25)
Aemor	(2.44)	(2.19)	(2.10)	(1.92)	(1.85)	(1.85)	(1.84)	(1.74)	(1.44)	(1.37)	(1.24)	(0.93)	(0.92)	(0.89)	(0.87)	(0.80)	(0.72)	(0.66)	(0.49)	(0.34)	(0.27)	(0.25)	(0.19)
Ampyr	(2.47)	(2.20)	(2.14)	(1.97)	(1.88)	(1.88)	(1.87)	(1.76)	(1.46)	(1.42)	(1.26)	(0.96)	(0.94)	(0.92)	(0.91)	(0.83)	(0.75)	(0.69)	(0.51)	(0.37)	(0.29)	(0.25)	(0.20)
Ampyr	(2.49)	(2.24)	(2.14)	(1.97)	(1.90)	(1.89)	(1.89)	(1.79)	(1.46)	(1.41)	(1.26)	(0.95)	(0.94)	(0.91)	(0.89)	(0.81)	(0.73)	(0.67)	(0.49)	(0.34)	(0.26)	(0.26)	(0.19)
Emor	(2.49)	(2.24)	(2.14)	(1.97)	(1.90)	(1.89)	(1.89)	(1.79)	(1.46)	(1.41)	(1.26)	(0.95)	(0.94)	(0.91)	(0.89)	(0.81)	(0.73)	(0.67)	(0.49)	(0.34)	(0.26)	(0.26)	(0.19)
DBUC	(2.57)	(2.21)	(2.26)	(2.11)	(1.94)	(1.97)	(1.92)	(1.78)	(1.59)	(1.56)	(1.32)	(1.02)	(0.97)	(1.01)	(1.04)	(0.90)	(0.88)	(0.78)	(0.60)	(0.43)	(0.31)	(0.19)	(0.13)
EOmMpyr	(2.57)	(2.26)	(2.24)	(2.07)	(1.94)	(1.95)	(1.94)	(1.80)	(1.55)	(1.51)	(1.32)	(1.00)	(0.97)	(0.97)	(0.98)	(0.88)	(0.81)	(0.74)	(0.55)	(0.39)	(0.28)	(0.14)	(0.16)
EOmMpyr	(2.58)	(2.24)	(2.26)	(2.10)	(1.94)	(1.97)	(1.94)	(1.79)	(1.57)	(1.54)	(1.32)	(1.01)	(0.97)	(0.99)	(1.01)	(0.90)	(0.84)	(0.77)	(0.57)	(0.41)	(0.29)	(0.20)	(0.14)
Bupyr	(2.58)	(2.24)	(2.26)	(2.10)	(1.94)	(1.97)	(1.94)	(1.79)	(1.57)	(1.54)	(1.32)	(1.01)	(0.97)	(0.99)	(1.01)	(0.90)	(0.84)	(0.77)	(0.57)	(0.41)	(0.29)	(0.20)	(0.14)
Empyr	(2.61)	(2.31)	(2.27)	(2.12)	(1.99)	(1.99)	(1.97)	(1.85)	(1.56)	(1.54)	(1.34)	(1.03)	(1.00)	(0.99)	(1.00)	(0.89)	(0.81)	(0.75)	(0.55)	(0.39)	(0.29)	(0.17)	(0.19)
Cations/ anions																							

HOEipy	(1.27)	(1.07)	(1.14)	(0.98)	(0.97)	(0.99)	(0.95)	(0.93)	(0.74)	(0.53)	(0.66)	(0.50)	(0.42)	(0.47)	(0.51)	(0.43)	(0.36)	(0.56)	(0.31)	(0.26)	(0.32)	(0.37)	(0.29)
HOEmor	(1.30)	(1.10)	(1.17)	(1.00)	(0.99)	(1.00)	(0.98)	(0.94)	(0.75)	(0.68)	(0.66)	(0.48)	(0.41)	(0.45)	(0.49)	(0.44)	(0.34)	(0.56)	(0.27)	(0.22)	(0.27)	(0.32)	(0.26)
HOEmim	(1.31)	(1.12)	(1.15)	(1.03)	(1.01)	(1.02)	(0.98)	(0.94)	(0.79)	(0.72)	(0.68)	(0.53)	(0.46)	(0.49)	(0.53)	(0.46)	(0.39)	(0.40)	(0.33)	(0.27)	(0.32)	(0.35)	(0.28)
Ch	(1.33)	(1.13)	(1.18)	(1.04)	(1.03)	(1.04)	(1.00)	(0.96)	(0.77)	(0.72)	(0.70)	(0.52)	(0.45)	(0.48)	(0.53)	(0.46)	(0.37)	(0.38)	(0.29)	(0.25)	(0.28)	(0.33)	(0.27)
TBDH	(1.37)	(1.21)	(1.07)	(1.16)	(1.08)	(1.06)	(1.00)	(0.91)	(0.89)	(0.87)	(0.74)	(0.61)	(0.63)	(0.60)	(0.58)	(0.56)	(0.52)	(0.51)	(0.45)	(0.36)	(0.36)	(0.30)	(0.22)
HOEmpyrr	(1.41)	(1.23)	(1.17)	(1.17)	(1.10)	(1.09)	(1.04)	(0.97)	(0.87)	(0.85)	(0.75)	(0.58)	(0.57)	(0.56)	(0.57)	(0.53)	(0.47)	(0.45)	(0.36)	(0.30)	(0.29)	(0.28)	(0.23)
DBUH	(1.48)	(1.30)	(1.18)	(1.23)	(1.14)	(1.11)	(1.08)	(0.97)	(0.95)	(0.90)	(0.76)	(0.60)	(0.62)	(0.59)	(0.57)	(0.57)	(0.52)	(0.50)	(0.41)	(0.32)	(0.31)	(0.25)	(0.18)
Benor	(1.49)	(1.32)	(1.15)	(1.26)	(1.15)	(1.11)	(1.06)	(0.95)	(0.98)	(0.91)	(0.74)	(0.59)	(0.62)	(0.60)	(0.55)	(0.52)	(0.54)	(0.47)	(0.41)	(0.32)	(0.28)	(0.18)	(0.12)
Bimim	(1.51)	(1.33)	(1.20)	(1.25)	(1.16)	(1.13)	(1.09)	(0.99)	(0.97)	(0.91)	(0.76)	(0.60)	(0.62)	(0.60)	(0.57)	(0.55)	(0.53)	(0.49)	(0.41)	(0.33)	(0.31)	(0.24)	(0.17)
Ach	(1.51)	(1.29)	(1.32)	(1.19)	(1.14)	(1.15)	(1.12)	(1.06)	(0.91)	(0.82)	(0.75)	(0.55)	(0.51)	(0.53)	(0.55)	(0.50)	(0.43)	(0.41)	(0.31)	(0.24)	(0.25)	(0.25)	(0.21)
AOPhim	(1.52)	(1.33)	(1.24)	(1.25)	(1.16)	(1.14)	(1.09)	(1.01)	(0.98)	(0.89)	(0.74)	(0.58)	(0.58)	(0.57)	(0.56)	(0.51)	(0.51)	(0.45)	(0.37)	(0.28)	(0.26)	(0.20)	(0.15)
Bpy	(1.52)	(1.33)	(1.23)	(1.25)	(1.16)	(1.14)	(1.10)	(1.00)	(0.97)	(0.90)	(0.77)	(0.60)	(0.60)	(0.60)	(0.58)	(0.54)	(0.53)	(0.48)	(0.41)	(0.32)	(0.31)	(0.25)	(0.18)
Apy	(1.52)	(1.32)	(1.28)	(1.23)	(1.17)	(1.16)	(1.11)	(1.05)	(0.95)	(0.87)	(0.77)	(0.60)	(0.57)	(0.58)	(0.59)	(0.51)	(0.49)	(0.44)	(0.39)	(0.31)	(0.31)	(0.28)	(0.22)
EOmPy	(1.52)	(1.31)	(1.30)	(1.22)	(1.16)	(1.16)	(1.11)	(1.06)	(0.95)	(0.86)	(0.77)	(0.59)	(0.55)	(0.57)	(0.58)	(0.51)	(0.48)	(0.45)	(0.37)	(0.29)	(0.30)	(0.27)	(0.22)
EOmMim	(1.52)	(1.33)	(1.26)	(1.25)	(1.17)	(1.15)	(1.11)	(1.03)	(0.96)	(0.89)	(0.77)	(0.60)	(0.59)	(0.59)	(0.58)	(0.53)	(0.51)	(0.47)	(0.39)	(0.30)	(0.29)	(0.25)	(0.19)
Emim	(1.53)	(1.34)	(1.29)	(1.26)	(1.19)	(1.18)	(1.13)	(1.06)	(0.96)	(0.90)	(0.79)	(0.62)	(0.60)	(0.60)	(0.61)	(0.54)	(0.51)	(0.47)	(0.40)	(0.32)	(0.32)	(0.28)	(0.23)
DBNH	(1.53)	(1.35)	(1.24)	(1.30)	(1.21)	(1.19)	(1.12)	(1.05)	(0.99)	(0.97)	(0.83)	(0.66)	(0.67)	(0.65)	(0.63)	(0.59)	(0.56)	(0.52)	(0.44)	(0.34)	(0.32)	(0.26)	(0.21)
Anim	(1.54)	(1.35)	(1.28)	(1.27)	(1.19)	(1.18)	(1.12)	(1.05)	(0.98)	(0.91)	(0.78)	(0.62)	(0.60)	(0.60)	(0.60)	(0.54)	(0.52)	(0.47)	(0.40)	(0.31)	(0.31)	(0.26)	(0.20)
EOmMor	(1.55)	(1.36)	(1.29)	(1.27)	(1.18)	(1.17)	(1.13)	(1.04)	(0.98)	(0.91)	(0.77)	(0.59)	(0.59)	(0.58)	(0.57)	(0.54)	(0.50)	(0.46)	(0.35)	(0.27)	(0.24)	(0.20)	(0.16)
Epy	(1.56)	(1.36)	(1.33)	(1.28)	(1.21)	(1.21)	(1.15)	(1.09)	(0.95)	(0.90)	(0.81)	(0.63)	(0.59)	(0.60)	(0.62)	(0.53)	(0.50)	(0.45)	(0.39)	(0.31)	(0.31)	(0.28)	(0.23)
Aemor	(1.57)	(1.37)	(1.30)	(1.30)	(1.20)	(1.19)	(1.15)	(1.06)	(1.00)	(0.93)	(0.80)	(0.61)	(0.61)	(0.60)	(0.59)	(0.55)	(0.51)	(0.47)	(0.37)	(0.29)	(0.29)	(0.22)	(0.18)
AmPyrr	(1.58)	(1.39)	(1.30)	(1.32)	(1.22)	(1.20)	(1.16)	(1.07)	(1.01)	(0.96)	(0.81)	(0.63)	(0.64)	(0.62)	(0.61)	(0.58)	(0.54)	(0.50)	(0.40)	(0.31)	(0.29)	(0.24)	(0.19)
DBUE	(1.59)	(1.42)	(1.22)	(1.38)	(1.23)	(1.19)	(1.14)	(1.01)	(1.07)	(1.03)	(0.81)	(0.64)	(0.71)	(0.66)	(0.60)	(0.60)	(0.60)	(0.53)	(0.44)	(0.33)	(0.27)	(0.15)	(0.10)
Emor	(1.60)	(1.40)	(1.34)	(1.32)	(1.23)	(1.22)	(1.17)	(1.10)	(1.01)	(0.95)	(0.82)	(0.63)	(0.62)	(0.61)	(0.61)	(0.57)	(0.52)	(0.48)	(0.37)	(0.29)	(0.26)	(0.22)	(0.19)
BuPyrr	(1.61)	(1.43)	(1.25)	(1.38)	(1.25)	(1.21)	(1.16)	(1.04)	(1.06)	(1.02)	(0.83)	(0.64)	(0.69)	(0.65)	(0.61)	(0.61)	(0.59)	(0.53)	(0.42)	(0.32)	(0.27)	(0.17)	(0.13)
EOmmpyrr	(1.62)	(1.43)	(1.30)	(1.38)	(1.25)	(1.22)	(1.17)	(1.07)	(1.05)	(1.01)	(0.84)	(0.65)	(0.67)	(0.64)	(0.62)	(0.60)	(0.57)	(0.52)	(0.41)	(0.31)	(0.27)	(0.19)	(0.05)
EmPyrr	(1.65)	(1.45)	(1.35)	(1.40)	(1.28)	(1.26)	(1.21)	(1.12)	(1.06)	(1.03)	(0.86)	(0.67)	(0.69)	(0.66)	(0.65)	(0.61)	(0.57)	(0.53)	(0.42)	(0.33)	(0.28)	(0.22)	(0.09)
Cations / Anions	Ac	HCOO	Dec	Cl	DMP	DEP	BEN	DBP	DHP	Bn	TOS	MeOEtSO ₄	I	MeSO ₄	BuSO ₄	DCA	H ₂ SO ₄	SCN	BF ₄	ClO ₄	PF ₆	AlCl ₃	TfN

HOEtPy	(1.33)	(1.37)	(1.14)	(1.16)	(1.10)	(1.19)	(1.06)	(1.05)	(0.79)	(0.79)	(0.72)	(0.61)	(0.58)	(0.51)	(0.43)	(0.47)	(0.36)	(0.36)	(0.30)	(0.34)	(0.24)	(0.29)	(0.36)
HOEtMor	(1.38)	(1.41)	(1.18)	(1.19)	(1.13)	(1.22)	(1.09)	(1.09)	(0.80)	(0.81)	(0.74)	(0.60)	(0.57)	(0.50)	(0.43)	(0.48)	(0.35)	(0.36)	(0.27)	(0.31)	(0.20)	(0.24)	(0.31)
Ch	(1.37)	(1.37)	(1.18)	(1.20)	(1.14)	(1.22)	(1.11)	(1.09)	(0.81)	(0.82)	(0.77)	(0.62)	(0.59)	(0.52)	(0.45)	(0.50)	(0.36)	(0.38)	(0.28)	(0.33)	(0.22)	(0.26)	(0.33)
HOEtMim	(1.40)	(1.40)	(1.21)	(1.22)	(1.16)	(1.23)	(1.14)	(1.10)	(0.84)	(0.85)	(0.80)	(0.65)	(0.62)	(0.56)	(0.49)	(0.51)	(0.41)	(0.41)	(0.33)	(0.34)	(0.26)	(0.30)	(0.35)
TBDH	(1.46)	(1.37)	(1.29)	(1.28)	(1.25)	(1.25)	(1.25)	(1.14)	(0.96)	(0.94)	(0.95)	(0.73)	(0.74)	(0.68)	(0.66)	(0.63)	(0.55)	(0.54)	(0.46)	(0.35)	(0.37)	(0.38)	(0.37)
HOEtMpyrr	(1.48)	(1.43)	(1.30)	(1.29)	(1.25)	(1.28)	(1.26)	(1.16)	(1.17)	(0.92)	(0.92)	(0.70)	(0.69)	(0.63)	(0.59)	(0.59)	(0.49)	(0.48)	(0.37)	(0.34)	(0.30)	(0.30)	(0.32)
Ach	(1.61)	(1.61)	(1.40)	(1.38)	(1.32)	(1.38)	(1.31)	(1.26)	(0.99)	(0.94)	(0.91)	(0.70)	(0.68)	(0.61)	(0.55)	(0.58)	(0.46)	(0.45)	(0.33)	(0.32)	(0.25)	(0.25)	(0.29)
DBUH	(1.60)	(1.51)	(1.42)	(1.38)	(1.34)	(1.34)	(1.36)	(1.25)	(1.05)	(0.99)	(1.01)	(0.75)	(0.76)	(0.71)	(0.68)	(0.66)	(0.58)	(0.56)	(0.45)	(0.33)	(0.36)	(0.35)	(0.33)
DBNH	(1.62)	(1.53)	(1.43)	(1.41)	(1.38)	(1.39)	(1.40)	(1.26)	(1.06)	(1.02)	(1.04)	(0.79)	(0.79)	(0.74)	(0.70)	(0.67)	(0.59)	(0.56)	(0.46)	(0.35)	(0.37)	(0.35)	(0.33)
APy	(1.63)	(1.58)	(1.43)	(1.40)	(1.36)	(1.39)	(1.36)	(1.26)	(1.04)	(0.98)	(0.97)	(0.76)	(0.74)	(0.68)	(0.62)	(0.61)	(0.54)	(0.50)	(0.42)	(0.35)	(0.33)	(0.34)	(0.34)
EPy	(1.62)	(1.59)	(1.42)	(1.40)	(1.35)	(1.40)	(1.35)	(1.27)	(1.03)	(0.98)	(0.96)	(0.75)	(0.74)	(0.68)	(0.61)	(0.60)	(0.53)	(0.49)	(0.41)	(0.35)	(0.32)	(0.33)	(0.34)
Etompy	(1.63)	(1.58)	(1.43)	(1.40)	(1.36)	(1.39)	(1.37)	(1.27)	(1.05)	(0.98)	(0.98)	(0.75)	(0.74)	(0.68)	(0.63)	(0.61)	(0.55)	(0.50)	(0.42)	(0.34)	(0.33)	(0.33)	(0.33)
Enim	(1.63)	(1.58)	(1.43)	(1.41)	(1.36)	(1.39)	(1.37)	(1.27)	(1.04)	(0.99)	(0.99)	(0.76)	(0.75)	(0.69)	(0.64)	(0.62)	(0.55)	(0.51)	(0.42)	(0.35)	(0.33)	(0.33)	(0.34)
EtOMim	(1.64)	(1.58)	(1.45)	(1.41)	(1.37)	(1.39)	(1.39)	(1.28)	(1.07)	(1.00)	(1.01)	(0.76)	(0.76)	(0.70)	(0.65)	(0.64)	(0.56)	(0.52)	(0.43)	(0.34)	(0.34)	(0.33)	(0.32)
Bnim	(1.65)	(1.55)	(1.46)	(1.41)	(1.38)	(1.38)	(1.41)	(1.28)	(1.09)	(1.01)	(1.04)	(0.78)	(0.78)	(0.73)	(0.69)	(0.66)	(0.60)	(0.56)	(0.47)	(0.34)	(0.37)	(0.36)	(0.34)
Bpy	(1.66)	(1.57)	(1.47)	(1.42)	(1.39)	(1.39)	(1.41)	(1.29)	(1.09)	(1.01)	(1.03)	(0.78)	(0.78)	(0.73)	(0.68)	(0.65)	(0.60)	(0.55)	(0.46)	(0.35)	(0.37)	(0.36)	(0.34)
Amim	(1.65)	(1.59)	(1.46)	(1.43)	(1.38)	(1.41)	(1.40)	(1.28)	(1.07)	(1.01)	(1.02)	(0.78)	(0.77)	(0.71)	(0.66)	(0.63)	(0.57)	(0.52)	(0.44)	(0.35)	(0.34)	(0.34)	(0.33)
Bemor	(1.67)	(1.54)	(1.49)	(1.43)	(1.41)	(1.38)	(1.45)	(1.29)	(1.13)	(1.03)	(1.07)	(0.79)	(0.80)	(0.76)	(0.73)	(0.67)	(0.64)	(0.57)	(0.49)	(0.33)	(0.39)	(0.36)	(0.31)
Asprim	(1.69)	(1.61)	(1.49)	(1.44)	(1.41)	(1.42)	(1.43)	(1.31)	(1.12)	(1.02)	(1.04)	(0.78)	(0.78)	(0.72)	(0.68)	(0.65)	(0.60)	(0.54)	(0.44)	(0.33)	(0.34)	(0.33)	(0.30)
EtOMemor	(1.69)	(1.63)	(1.49)	(1.45)	(1.41)	(1.43)	(1.43)	(1.32)	(1.10)	(1.02)	(1.04)	(0.77)	(0.76)	(0.70)	(0.66)	(0.65)	(0.57)	(0.53)	(0.41)	(0.32)	(0.31)	(0.29)	(0.29)
Aemor	(1.70)	(1.63)	(1.50)	(1.46)	(1.42)	(1.43)	(1.44)	(1.32)	(1.10)	(1.03)	(1.05)	(0.78)	(0.77)	(0.72)	(0.67)	(0.66)	(0.58)	(0.54)	(0.42)	(0.33)	(0.33)	(0.31)	(0.30)
Ampyrr	(1.70)	(1.61)	(1.50)	(1.46)	(1.42)	(1.43)	(1.45)	(1.32)	(1.11)	(1.04)	(1.07)	(0.79)	(0.79)	(0.73)	(0.70)	(0.68)	(0.60)	(0.56)	(0.44)	(0.34)	(0.35)	(0.33)	(0.31)
Femor	(1.71)	(1.65)	(1.51)	(1.47)	(1.43)	(1.45)	(1.46)	(1.33)	(1.11)	(1.04)	(1.06)	(0.79)	(0.78)	(0.72)	(0.68)	(0.66)	(0.58)	(0.54)	(0.42)	(0.33)	(0.32)	(0.30)	(0.30)
EtOMpyrr	(1.75)	(1.64)	(1.56)	(1.50)	(1.47)	(1.46)	(1.53)	(1.36)	(1.17)	(1.08)	(1.13)	(0.83)	(0.83)	(0.78)	(0.75)	(0.71)	(0.64)	(0.59)	(0.47)	(0.33)	(0.37)	(0.33)	(0.29)
Empyrr	(1.75)	(1.65)	(1.55)	(1.51)	(1.47)	(1.48)	(1.52)	(1.36)	(1.15)	(1.08)	(1.12)	(0.83)	(0.83)	(0.77)	(0.74)	(0.71)	(0.63)	(0.58)	(0.46)	(0.34)	(0.36)	(0.33)	(0.30)
Bmpyrr	(1.76)	(1.62)	(1.58)	(1.51)	(1.49)	(1.46)	(1.56)	(1.37)	(1.20)	(1.10)	(1.17)	(0.84)	(0.85)	(0.81)	(0.79)	(0.74)	(0.68)	(0.62)	(0.50)	(0.33)	(0.40)	(0.35)	(0.30)
DBUE	(1.77)	(1.61)	(1.59)	(1.52)	(1.50)	(1.45)	(1.57)	(1.37)	(1.22)	(1.11)	(1.19)	(0.85)	(0.87)	(0.83)	(0.82)	(0.75)	(0.71)	(0.64)	(0.53)	(0.33)	(0.42)	(0.37)	(0.30)
Cations / Anions	AC	DEC	HCOO	DEP	DMP	DBP	CI	BEN	DHP	TOS	Br	BuSO ₃	MeOEtSO ₃	MeSO ₃	I	DCA	HSO ₃	SCN	BF ₄	TF ₃ N	ClO ₄	PF ₆	AlCl ₄

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