Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Proof of Ion-Pair Structures in Ammonium-Based Protic Ionic Liquids Using Combined NMR and DFT/PCM-Based Chemical Shift Calculations

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Table SI 1. Absolute[a)] and relative energies[b)] in the gas phase and the Boltzmann population[c,d)] for different relative dispositions of ions for the $[(C_2H_5)_3NH][TFSI]$ ion pair, calculated at the DFT-B3LYP/6-31G(d) and B3LYP/6-31++G(d,p) basis set levels of theory.

Ion pair	B3LYP/6-31G(d)				B3LYP/6-31++G(d,p)		
	absolute energy	relative energy	Boltzmann population		absolute energy	relative energy	Boltzmann population
1a	-2120.1532774	0.02	31.5	**1a**	-2120.2452567	0.16	24.8
1b	-2120.1533165	0.00	32.8	**1b**	-2120.2452695	0.15	25.2
1c	-2120.1457502	4.75		**1c**	-2120.2388727	4.17	
2a	-2120.1520576	0.79	8.6	**2a**	-2120.2449119	0.38	17.3
2b	-2120.1531347	0.11	27.0	**2b**	-2120.2455150	0.00	32.7
2c	-2120.1424046	6.85		**2c**	-2120.2373401	5.13	
3a	-2120.1356233	11.10		**3a**	-2120.2308122	9.23	
3b	-2120.1359798	10.88		**3b**	-2120.2313260	8.90	
4a	-2120.1342780	11.95		**4a**	-2120.2329624	7.88	
4b	-2120.1344654	11.83		**4b**	-2120.2324909	8.17	
5a	-2120.1369060	10.30		**5a**	-2120.2323680	8.25	
5b	-2120.1311791	13.89		**5b**	-2120.2337754	7.37	

[a)]in Hartrees; [b)]kcal*mol-1; [c)]percentages; [d)]where not specified, Boltzmann population of conformer is less than 0.05%.

Table SI 2. Relative energies[a)], experimental chemical shifts[b)] and calculated GIAO ^{1}H aliphatic chemical shifts[c,d)] at the DFT-B3LYP/6-31G(d) and the B3LYP/6-31++G(d,p) basis sets (shown in parentheses) with TMS[e)] used as the standard and chloroform used as the solvent (PCM) and experimental chemical shifts for the $[(C_2H_5)_3NH][TFSI]$ ion pair and its chloroform solvates.

complex	class of complex	ion pair of $[(C_2H_5)_3NH][TFSI]$		
		relative energy	CH_2	CH_3
1a	N^+-H ··· N^-	0.28 (0.72)	3.12 (3.11)	1.37 (1.38)
1b		0.24 (0.80)	3.08 (3.08)	1.39 (1.43)
1c		5.04 (4.76)	3.38 (3.41)	1.46 (1.43)
2a	N^+-H ··· O(=S)	0.00 (0.32)	3.07 (3.05)	1.38 (1.38)
2b		0.39 (0.00)	3.08 (3.05)	1.42 (1.40)
2c		5.69 (4.85)	3.37 (3.33)	1.48 (1.43)
average			**3.09 (3.06)**	**1.39 (1.40)**
solvates of the $[(C_2H_5)_3NH][TFSI]$ ion pair (6 $CHCl_3$ molecules)				
1a*6CHCl3	N^+-H ··· N^-	0.44 (0.90)	3.18 (3.15)	1.44 (1.45)
1b*6CHCl3		0.00 (0.81)	3.17 (3.11)	1.42 (1.50)
1c*6CHCl3		5.40 (4.80)	3.46 (3.43)	1.52 (1.48)
2a*6CHCl3	N^+-H ··· O(=S)	0.11 (0.00)	2.94 (3.04)	1.42 (1.43)
2b*6CHCl3		0.11 (0.21)	2.79 (3.07)	1.46 (1.47)
2c*6CHCl3		5.66 (4.70)	3.15 (3.33)	1.50 (1.42)
average			**3.01 (3.09)**	**1.43 (1.46)**
solvates of the $[(C_2H_5)_3NH][TFSI]$ ion pair (7 $CHCl_3$ molecules)				
1a*7CHCl3	N^+-H ··· N^-	0.43 (0.35)	3.37 (3.33)	1.48 (1.48)
1b*7CHCl3		0.09 (0.48)	3.34 (3.26)	1.48 (1.49)
2a*7CHCl3	N^+-H ··· O(=S)	0.00 (0.00)	3.30 (3.22)	1.46 (1.45)
2b*7CHCl3		0.17 (0.02)	3.34 (3.23)	1.51 (1.44)
average			**3.33 (3.25)**	**1.48 (1.46)**
exp.			**3.21 (q)**	**1.34 (t)**

[a)]in kcal/mol, in chloroform; [b)]in $CDCl_3$, room temperature; t-triplet, q-quartet; [c)]averages of the hydrogen atoms of the methylene (CH_2) and methyl groups (CH_3); [d)]Boltzmann's population-weighted average over all the relevant conformers; [e)]calculated average chemical shifts (δ) of TMS protons in chloroform are 32.1733 (31.6433) respectively; [f)]see text and Figure 1 for complex labels.

Table SI 3. Relative energies[a)], experimental chemical shifts[b)] and calculated GIAO ^{1}H aliphatic chemical shifts[c,d)] using the DFT-B3LYP/6-31G(d) and the B3LYP/6-31++G(d,p) basis sets (shown in parentheses) with TMS[e)] used as the standard and water used as the solvent (PCM) for the $[(C_2H_5)_3NH][TFSI]$ complexes and their hydrates.

complex	class of complex	ion pair of $[(C_2H_5)_3NH][TFSI]$		
		relative energy	CH_2	CH_3
1a	N^+-H ··· N^-	0.62 (0.81)	3.17 (3.16)	1.35 (1.36)
1b		0.48 (0.77)	3.14 (3.13)	1.36 (1.40)
1c		5.84 (5.32)	3.37 (3.38)	1.49 (1.46)
2a	N^+-H ··· O(=S)	0.00 (0.35)	3.13 (3.11)	1.45 (1.37)
2b		0.49 (0.00)	3.16 (3.11)	1.45 (1.37)
2c		5.88 (5.20)	3.36 (3.33)	1.65 (1.46)
3a	C^α-H ··· N^-	5.16 (2.28)	3.20 (3.38)	1.35 (1.37)
3b	C^α-H ··· O(=S) N^+-H ··· OH_2	4.65 (2.28)	3.21 (3.44)	1.35 (1.37)
4a	C^α-H ··· O(=S)	4.05 (2.38)	3.47 (3.38)	1.36 (1.35)
4b	N^+-H ··· OH_2	4.13 (2.20)	3.43 (3.40)	1.37 (1.36)
5a	C^α-H ··· $F(_3C)$	4.76 (3.05)	3.20 (3.21)	1.35 (1.37)
5b	N^+-H ··· OH_2	4.72 (2.97)	3.21 (3.21)	1.35 (1.37)
average			**3.14 (3.13)**	**1.42 (1.37)**
hydrate of the $[(C_2H_5)_3NH][TFSI]$ ion pair (6 water molecules)				
1a*6H2O g,h)	N^+-H ··· N^-	3.86 (2.10)	3.27 (3.24)	1.34 (1.38)
1b*6H2O g,h)		6.78 (4.56)	3.18 (3.10)	1.32 (1.37)
1c*6H2O g,h)		17.61 (14.07)	3.52 (3.52)	1.51 (1.48)
2a*6H2O	N^+-H ··· O(=S)	1.18 (1.77)	3.10 (3.07)	1.32 (1.37)
2b*6H2O h)		12.35 (6.48)	3.06 (3.10)	1.28 (1.36)
2c*6H2O h)		2.88 (1.26)	3.15 (3.19)	1.40 (1.45)
3a*6H2O h)	C^α-H ··· N^-	12.32 (7.58)	3.04 (3.51)	1.33 (1.36)
3b*6H2O h)	C^α-H ··· O(=S) N^+-H ··· OH_2	0.00 (0.00)	3.16 (3.14)	1.33 (1.32)
4a*6H2O g,h)	C^α-H ··· O(=S)	5.04 (2.39)	3.22 (3.18)	1.34 (1.33)
4b*6H2O g,h)	N^+-H ··· OH_2	5.47 (2.39)	3.19 (3.20)	1.34 (1.33)
5a*6H2O g,h)	C^α-H ··· $F(_3C)$	6.50 (2.39)	2.99 (3.18)	1.29 (1.33)
5b*6H2O h)	N^+-H ··· OH_2 N^+-H ··· N^-	6.43 (2.06)	3.00 (3.18)	1.28 (1.31)
average			**3.15 (3.15)**	**1.33 (1.34)**
exp.			**3.185 (q)**	**1.27 (t)**

[a)]in kcal/mol, in water; [b)]in D2O, room temperature; t-triplet, q-quartet; [c)]averages of the hydrogen atoms of the methylene (CH2) and methyl groups (CH3); [d)]Boltzmann's population-weighted average over all relevant conformers; [e)]calculated average chemical shifts (δ) of TMS protons in water 32.1685 (31.6428); [f)]see text and Figure 1 for complex labels; g) Cα-H … F(F2C) can also appear; h)the Cα-H … O(=S) feature can also appear.

Table SI 4. Comparison and assignment of the experimental proton chemical shifts[a)] of the (2-chloroethyl)diethylammonium bis(trifluoromethanesulfonyl) imide $[(C_2H_5)_2NH(C_2H_4Cl)][TFSI]$ neat and in dry $CDCl_3$, wet $CDCl_3$, and water.

Proton group	dry $CDCl_3$	wet $CDCl_3$ (reflected peak)	water	neat	multi-plicity[b)]
$C\mathbf{H_3}(CH_2N^+)$	1.40	1.40 (1.33)	1.31	1.22	*(t)*
$(CH_3)C\mathbf{H_2}(N^+)$	3.35	3.35 (3.28)	3.30	3.21	*(q)*
$(ClCH_2)C\mathbf{H_2}(N^+)$	3.54	3.54 (3.47)	3.56	3.40	*(t)*
$ClC\mathbf{H_2}(CH_2N^+)$	3.88	3.88 (3.82)	3.935	3.78	*(t)*

[a)]δ, TMS as a reference, room temperature; [b)]t-triplet, q-quartet;

Table SI 5. Calculated chemical shifts[a)] of the $[(C_2H_5)_2NH(C_2H_4Cl)][TFSI]$ models.

Proton group /model	**1**	**2**	**3**	**4**	**5**	**6**	experimental δ (wet $CDCl_3$)
$C\mathbf{H_3}(CH_2N^+)$	1.39	1.35	1.48	1.47	1.53	1.45	1.40 (1.33)
$(CH_3)C\mathbf{H_2}(N^+)$	3.48	3.57	3.18	3.38	3.18	3.11	3.35 (3.28)
$(ClCH_2)C\mathbf{H_2}(N^+)$	3.39	3.27	3.14	3.70	3.31	3.11	3.54 (3.47)
$ClC\mathbf{H_2}(CH_2N^+)$	3.86	3.65	4.08	3.78	3.64	3.71	3.88 (3.82)

[a)]δ, TMS as a reference;

Table SI 6. Calculated chemical shifts[a)] of the $[(C_2H_5)_2NH(C_2H_4Cl)][TFSI]$ associates of model 2 with a water molecule or hydronium ions.

Proton group /model	**2**$(H_5O_3)^+$	**2**$(H_5O_3)^+$	**2**(H_2O)	**2**$(H_2O$alt$)$	experimental δ (wet $CDCl_3$)
$C\mathbf{H_3}(CH_2N^+)$	1.42	1.53	1.49	1.55	1.40 (1.33)
$(CH_3)C\mathbf{H_2}(N^+)$	3.11	3.19	3.11	3.08	3.35 (3.28)
$(ClCH_2)C\mathbf{H_2}(N^+)$	3.00	3.05	3.05	3.06	3.54 (3.47)
$ClC\mathbf{H_2}(CH_2N^+)$	3.66	3.72	3.89	3.71	3.88 (3.82)

[a)]δ, TMS as a reference;

Table SI 7. Coordinates of the stable structures of $[(C_2H_5)_3NH][TFSI]$, its chloroform solvates and its hydrates as calculated at the DFT B3LYP/6-31++G(d,p) level of theory.

$[(C_2H_5)_3NH][TFSI]$ ion pair **1a** B3LYP/6-31++(d,p) OPT \HF=-2120.2452567\	$[(C_2H_5)_3NH][TFSI]$ ion pair **1b** B3LYP/6-31++(d,p) OPT \HF=-2120.2452695\	$[(C_2H_5)_3NH][TFSI]$ ion pair **1c** B3LYP/6-31++(d,p) OPT \HF=-2120.2388727\	$[(C_2H_5)_3NH][TFSI]$ ion pair **2a** B3LYP/6-31++(d,p) OPT \HF=-2120.2449119\	$[(C_2H_5)_3NH][TFSI]$ ion pair **2b** B3LYP/6-31++(d,p) OPT \HF=-2120.245515\	$[(C_2H_5)_3NH][TFSI]$ ion pair **2c** B3LYP/6-31++(d,p) OPT \HF=-2120.2373401\
1 -1.123783 -1.899443 2.065816	1 2.706551 -1.631764 -2.961950	1 4.129170 -2.608802 -0.175652	1 -2.318061 -2.211007 2.710372	1 -1.214428 -2.357301 -1.288489	1 -4.909903 -1.605068 -0.542605
1 -1.672281 -0.287702 0.074991	1 1.635743 -0.365552 -0.089794	1 1.381313 -0.157334 -0.071395	1 -1.898520 -0.312097 -0.024584	1 -1.905388 -0.131150 -0.191864	1 -1.601277 0.364740 -0.289933
6 -3.519122 0.623374 -0.341426	6 3.269219 0.393338 -1.177965	6 2.845128 1.154840 -0.617587	6 -3.845627 -0.091505 -0.701783	6 -3.023651 -1.305487 1.140299	6 -2.820095 0.155781 1.327833
6 -3.495946 1.904463 0.483740	6 3.521518 1.788658 -0.615744	6 4.234092 1.290890 -1.232283	6 -4.117367 1.383171 -0.422750	6 -2.855019 -0.507765 2.429290	6 -4.069955 -0.537125 1.858049
7 -2.688682 -0.521199 0.212449	7 2.652183 -0.606834 -0.216326	7 2.432483 -0.225938 -0.142238	7 -2.817862 -0.742767 0.205972	7 -2.887905 -0.482993 -0.128115	7 -2.622968 0.164952 -0.181213
6 -2.914422 -0.709115 1.698108	6 2.699908 -2.007760 -0.794817	6 2.642435 -1.342540 -1.150596	6 -3.105190 -0.451420 1.665182	6 -3.125531 -1.318537 -1.367516	6 -2.778302 -1.179466 -0.870679
6 -2.186786 -1.898692 2.315369	6 2.105281 -2.124330 -2.193813	6 3.982971 -2.068851 -1.114640	6 -2.167515 -1.130121 2.657908	6 -2.271474 -2.579311 -1.450901	6 -4.175646 -1.557480 -1.348627
6 -2.936499 -1.802444 -0.561627	6 3.287402 -0.537616 1.158240	6 2.806934 -0.557091 1.293191	6 -2.708579 -2.230937 -0.064271	6 -3.771495 0.746975 -0.098742	6 -3.241243 1.344725 -0.907695
6 -2.779314 -1.658797 -2.072005	6 2.748055 -1.555353 2.157630	6 4.244743 -0.287352 1.721672	6 -2.440650 -2.586324 -1.522537	6 -3.693133 1.612308 -1.352641	6 -4.691216 1.685298 -0.582801
1 -4.538917 0.236474 -0.439240	1 2.582990 0.451563 -2.023561	1 2.707423 1.817341 0.238356	1 -4.757448 -0.690520 -0.607485	1 -2.246845 -2.065080 1.082727	1 -2.775399 1.202921 1.636133
1 -3.117197 0.828407 -1.332488	1 4.202826 -0.059890 -1.527185	1 2.089312 1.437372 -1.354599	1 -3.458360 -0.204551 -1.713652	1 -4.006528 -1.786191 1.088019	1 -1.930414 -0.339633 1.718858
1 -4.014169 2.675232 -0.094624	1 3.808901 2.432896 -1.452461	1 4.371061 2.341825 -1.505654	1 -4.756100 1.759443 -1.227723	1 -2.764146 -1.223139 3.251829	1 -4.062404 -0.431907 2.947425
1 -4.013738 1.808108 1.441251	1 2.629698 2.211065 -0.149630	1 5.039126 1.020591 -0.546895	1 -4.647841 1.549418 0.518051	1 -1.944446 0.096980 2.417020	1 -5.003104 -0.106091 1.490264
1 -2.476742 2.258612 0.647103	1 4.340750 1.807049 0.107316	1 4.340247 0.703504 -2.147842	1 -3.191943 1.962817 -0.434048	1 -3.709418 0.138140 2.647558	1 -4.064512 -1.608603 1.642322
1 -2.576099 0.214603 2.168204	1 3.751731 -2.312426 -0.774128	1 1.830934 -2.047388 -0.958929	1 -3.030799 0.630973 1.769767	1 -4.195695 -1.551126 -1.386153	1 -2.094338 -1.137644 -1.722843
1 -3.997901 -0.786593 1.838106	1 2.126547 -2.634692 -0.115113	1 2.464986 -0.891223 -2.130619	1 -4.147249 -0.741881 1.836028	1 -2.900715 -0.668283 -2.212914	1 -2.367627 -1.913266 -0.175896
1 -2.287578 -1.823301 3.402381	1 2.051718 -3.187452 -2.445426	1 3.972749 -2.816210 -1.914191	1 -1.119961 -0.931875 2.422480	1 -2.578761 -3.347781 -0.738030	1 -4.546754 -0.881347 -2.123628
1 -2.611796 -2.857994 2.010800	1 1.083850 -1.737645 -2.219507	1 4.840001 -1.413969 -1.282668	1 -2.382203 -0.720213 3.649586	1 -2.384029 -2.996627 -2.456053	1 -4.111508 -2.554375 -1.795874
1 -2.205451 -2.518856 -0.189818	1 4.365703 -0.657178 1.009207	1 2.125300 0.044371 1.899417	1 -1.880436 -2.581531 0.547800	1 -4.791194 0.394462 0.088417	1 -2.595339 2.192062 -0.665009
1 -3.944093 -2.135903 -0.291929	1 3.087831 0.469941 1.521527	1 2.532742 -1.605384 1.431902	1 -3.641887 -2.676718 0.295918	1 -3.441963 1.326517 0.763310	1 -3.110088 1.139260 -1.973242
1 -2.815111 -2.661244 -2.508252	1 3.172139 -1.315010 3.137126	1 4.339843 -0.602356 2.765566	1 -2.240215 -3.660642 -1.571045	1 -4.226469 2.545894 -1.150185	1 -4.978155 2.538919 -1.204930
1 -3.574056 -1.067750 -2.533108	1 1.660934 -1.498741 2.248784	1 4.984246 -0.840790 1.140261	1 -3.288834 -2.380200 -2.179858	1 -2.656521 1.863691 -1.591464	1 -5.385182 0.870680 -0.796877
1 -1.812814 -1.222975 -2.338516	1 3.029852 -2.583407 1.919381	1 4.489633 0.777091 1.685346	1 -1.550548 -2.080038 -1.904430	1 -4.164811 1.149118 -2.222816	1 -4.816558 1.990203 0.459074
8 1.447264 -1.583346 -1.936962	8 -1.553554 -1.509955 1.946586	8 -1.637314 -1.621193 1.949034	8 -0.981321 1.091047 -0.856378	8 0.059523 -1.701842 0.871776	8 -0.168539 -1.565386 0.907541
16 0.977175 -1.437215 -0.562176	16 -1.052882 -1.408977 0.578632	16 -1.042387 -1.508978 0.621764	16 0.426221 1.546908 -1.020637	16 1.465272 -1.242710 0.913750	16 1.308643 -1.459655 0.915713
7 0.166206 -0.050051 -0.242159	7 -0.179319 -0.061206 0.251998	7 -0.373314 -0.056289 0.263744	7 1.501997 0.364737 -1.103442	7 1.627804 0.361331 0.792688	7 1.851009 0.054355 0.756282
16 0.483390 1.395428 -0.955149	16 -0.432316 1.400681 0.954203	16 -0.817195 1.379545 0.927633	16 1.244675 -1.138312 -0.562249	16 0.390971 1.316315 0.436176	16 0.870501 1.272183 0.397822
6 2.535712 -1.408073 0.507936	6 -2.587377 -1.322459 -0.521517	6 -2.472508 -1.713090 -0.594897	6 0.773978 2.439308 0.608263	6 2.197490 -1.859570 -0.712944	6 1.830396 -2.267899 -0.708169
6 0.966348 2.425355 0.553606	6 -0.834475 2.445693 -0.567945	6 -1.354000 2.329645 -0.614795	6 2.844647 -1.403621 0.396682	6 1.358224 2.743240 -0.320346	6 2.153673 2.443443 -0.326663
8 0.160963 -2.497448 0.053505	8 -0.273854 -2.512670 -0.004657	8 -0.050691 -2.499260 0.168020	8 0.707386 2.550756 -2.039431	8 2.365077 -1.765674 1.934727	8 2.075245 -2.168379 1.933141
8 1.631185 1.450525 -1.854109	8 -1.589521 1.522818 1.833891	8 -1.979609 1.368481 1.808039	8 0.171347 -1.274598 0.451545	8 -0.494791 0.847377 -0.672612	8 -0.074808 1.025619 -0.735916
8 -0.812218 1.970303 -1.351231	8 0.885231 1.909970 1.371867	8 0.426361 2.059462 1.327711	8 1.275261 -2.125107 -1.644440	8 -0.317141 1.873395 1.599245	8 0.281816 1.964135 1.553461
9 3.140296 -2.599577 0.417070	9 -3.249203 -2.482921 -0.428537	9 -2.968219 -2.951752 -0.481499	9 -0.064003 3.483869 0.730718	9 2.144780 -3.202111 -0.741461	9 1.475606 -3.563842 -0.691927
9 3.381086 -0.457219 0.102549	9 -3.394333 -0.327374 -0.144372	9 -3.441198 -0.829037 -0.338093	9 0.574014 1.617159 1.655367	9 1.495234 -1.387695 -1.758783	9 1.221809 -1.676324 -1.750975
9 2.211980 -1.186194 1.792790	9 -2.229542 -1.132299 -1.802681	9 -2.042090 -1.534441 -1.854750	9 2.031590 2.886618 0.647310	9 3.470467 -1.474182 -0.841047	9 3.153207 -2.183982 -0.878303
9 1.171174 3.693135 0.176543	9 -0.986991 3.723553 -0.200319	9 -1.647384 3.589953 -0.274033	9 2.816366 -2.631731 0.939666	9 0.476723 3.686405 -0.695495	9 1.519408 3.565808 -0.704355
9 -0.024474 2.409110 1.470768	9 0.173322 2.378160 -1.464119	9 -0.356800 2.355325 -1.524169	9 3.905655 -1.309960 -0.407706	9 2.204217 3.270179 0.565834	9 3.079467 2.754049 0.581868
9 2.079118 1.955295 1.126131	9 -1.956392 2.025097 -1.160589	9 -2.427389 1.768757 -1.180359	9 2.958994 -0.502708 1.382504	9 2.037286 2.337254 -1.397472	9 2.743234 1.901177 -1.396151
$[(C_2H_5)_3NH][TFSI]$ ion pair **3a** B3LYP/6-31++(d,p) OPT \HF=-2120.2308122\	$[(C_2H_5)_3NH][TFSI]$ ion pair **3b** B3LYP/6-31++(d,p) OPT \HF=-2120.231326\	$[(C_2H_5)_3NH][TFSI]$ ion pair **4a** B3LYP/6-31++(d,p) OPT \HF=-2120.2329624\	$[(C_2H_5)_3NH][TFSI]$ ion pair **4b** B3LYP/6-31++(d,p) OPT \HF=-2120.2324909\	$[(C_2H_5)_3NH][TFSI]$ ion pair **5a** B3LYP/6-31++(d,p) OPT \HF=-2120.232368\	$[(C_2H_5)_3NH][TFSI]$ ion pair **5b** B3LYP/6-31++(d,p) OPT \HF=-2120.2337754\
1 -4.937360 1.922883 -0.662943	1 4.096579 -2.823349 0.582487	1 -5.118442 0.860346 -1.586127	1 4.357738 -2.396448 1.856953	1 4.030471 -0.099652 2.719033	1 3.584866 -0.510644 2.896034
1 -4.234405 -0.072610 0.584106	1 4.303043 0.005463 -0.205730	1 -4.227258 -1.191261 0.299253	1 4.236959 -1.235860 -0.261405	1 4.107584 -0.324735 0.290137	1 4.281319 -0.803028 0.199901
6 -2.400953 -0.418877 1.488856	6 2.886787 -0.216857 1.285965	6 -2.384823 -0.967456 1.221941	6 3.908379 0.795271 -0.034717	6 3.062989 0.711227 -1.169743	6 3.437880 1.080816 0.367393
6 -2.849576 0.391458 2.696716	6 3.576129 0.869828 2.097166	6 -3.066663 -1.196293 2.562302	6 5.012776 1.109631 -1.036069	6 4.077360 1.846502 -1.137831	6 4.715768 1.692461 -0.191389
7 -3.264602 -0.152996 0.261294	7 3.296469 -0.187648 -0.181245	7 -3.385260 -0.635381 0.117454	7 3.414646 -0.638416 -0.127917	7 3.118302 -0.167093 0.072084	7 3.339602 -0.412709 0.091214
6 -2.903638 1.167956 -0.403817	6 3.077854 -1.529389 -0.864954	6 -3.794728 0.827198 0.162473	6 2.756598 -1.077865 1.178124	6 2.499721 0.516813 1.284816	6 2.450979 -1.109991 1.117587
6 -4.036946 1.720941 -1.255770	6 4.127944 -2.562700 -0.478652	6 -5.133900 1.084528 -0.516256	6 3.788130 -1.525811 2.203701	6 2.940242 -0.115650 2.596868	6 3.211249 -1.412619 2.401313
6 -3.213610 -1.317404 -0.718733	6 2.604811 0.938103 -0.941224	6 -2.875543 -1.046326 -1.259565	6 2.518539 -0.852175 -1.343258	6 2.496629 -1.532204 -0.200414	6 2.912057 -0.691732 -1.344756
6 -4.128155 -2.460341 -0.298323	6 3.424652 1.411733 -2.132578	6 -2.991124 -2.545852 -1.489149	6 2.373171 -2.321835 -1.707663	6 3.478132 -2.477370 -0.878328	6 3.262617 -2.103863 -1.789846

1 -1.376524 -0.201392 1.179257	1 3.144204 -1.208019 1.660864	1 -1.673137 -0.142669 1.241369	1 4.273307 0.930002 0.985124	1 2.032821 1.068873 -1.251892	1 3.397505 1.199440 1.451211
1 -2.468826 -1.488037 1.691493	1 1.802932 -0.105121 1.291785	1 -1.837408 -1.851799 0.900354	1 3.023156 1.421324 -0.160218	1 3.261295 0.052003 -2.017059	1 2.534097 1.521857 -0.058864
1 -2.207642 0.131682 3.543149	1 3.264924 0.767981 3.140369	1 -2.293812 -1.429291 3.299796	1 5.342435 2.140340 -0.877372	1 4.007751 2.393740 -2.082069	1 4.732749 2.755641 0.064415
1 -2.757075 1.470069 2.543606	1 4.668853 0.777060 2.065454	1 -3.607916 -0.316804 2.924917	1 5.886118 0.461421 -0.896949	1 3.886899 2.565012 -0.336639	1 5.613304 1.235719 0.242954
1 -3.882636 0.162308 2.985594	1 3.285859 1.873735 1.778648	1 -3.758914 -2.046364 2.530387	1 4.681452 1.032323 -2.074783	1 5.106114 1.477684 -1.045190	1 4.778347 1.622163 -1.280770
1 -2.655495 1.863842 0.398080	1 2.063078 -1.844871 -0.605870	1 -3.845949 1.100335 1.217894	1 2.162558 -0.225589 1.508489	1 2.807447 1.562248 1.237520	1 1.595924 -0.451404 1.282159
1 -1.990334 0.995101 -0.973756	1 3.115231 -1.335025 -1.938545	1 -2.970053 1.380041 -0.290749	1 2.055547 -1.875428 0.938511	1 1.420900 0.458600 1.131308	1 2.079577 -2.021485 0.652366
1 -3.705149 2.669032 -1.687609	1 3.929508 -3.480332 -1.039404	1 -5.945390 0.513522 -0.049544	1 4.492043 -0.733520 2.478504	1 2.509286 0.465960 3.416618	1 2.528809 -1.903969 3.100304
1 -4.305326 1.064434 -2.088328	1 5.143229 -2.233895 -0.731973	1 -5.378439 2.145405 -0.411925	1 3.262517 -1.823077 3.115371	1 2.577501 -1.139800 2.711278	1 4.053288 -2.094269 2.229815
1 -3.511847 -0.922948 -1.690891	1 1.624393 0.548374 -1.217549	1 -3.472718 -0.494885 -1.987420	1 1.560449 -0.389910 -1.107585	1 2.154898 -1.930179 0.753927	1 1.839725 -0.503329 -1.387348
1 -2.168102 -1.630292 -0.763741	1 2.434535 1.746139 -0.230514	1 -1.843172 -0.702308 -1.312877	1 2.980879 -0.297095 -2.161364	1 1.606414 -1.337477 -0.797812	1 3.423003 0.047353 -1.963783
1 -4.049892 -3.257956 -1.042181	1 2.876761 2.215428 -2.632290	1 -2.646771 -2.763711 -2.503817	1 1.764022 -2.383877 -2.613090	1 2.973964 -3.431106 -1.057028	1 2.976081 -2.211216 -2.839655
1 -3.842649 -2.892202 0.664961	1 4.394504 1.819894 -1.823756	1 -2.354073 -3.118369 -0.811440	1 3.341742 -2.792357 -1.918801	1 3.826760 -2.107721 -1.847748	1 4.338429 -2.307163 -1.717243
1 -5.179709 -2.152083 -0.252159	1 3.596049 0.625669 -2.874414	1 -4.027069 -2.897841 -1.406577	1 1.847228 -2.891321 -0.938461	1 4.350555 -2.681616 -0.246162	1 2.712190 -2.866023 -1.233510
8 1.429406 -1.727930 -2.006256	8 -1.311014 -1.763834 1.905709	8 -0.733064 1.279300 -0.488219	8 0.768619 1.278051 0.428116	8 -2.558906 -0.699314 1.354677	8 -0.040884 -1.664957 -0.807463
16 0.871621 -1.510849 -0.672948	16 -0.901231 -1.545609 0.518685	16 0.686150 1.520345 -0.858443	16 -0.634473 1.511568 0.859777	16 -1.257860 -1.094822 0.819811	16 -1.464128 -1.261479 -0.885775
7 0.384617 -0.002639 -0.337637	7 -0.377794 -0.052709 0.162523	7 1.634188 0.236077 -0.693863	7 -1.575658 0.214784 0.773678	7 -0.445373 0.019013 -0.047712	7 -1.719368 0.309894 -0.622951
16 1.020778 1.358867 -0.975098	16 -0.838616 1.321670 0.906730	16 1.152755 -1.088968 0.101382	16 -1.147262 -1.117671 -0.039649	16 -1.102280 1.238024 -0.903549	16 -0.557877 1.274428 -0.064243
6 2.282244 -1.881459 0.528415	6 -2.461439 -1.807027 -0.513179	6 1.289135 2.713891 0.473713	6 -1.313841 2.675155 -0.462704	6 -1.630022 -2.467939 -0.427649	6 -2.241823 -2.086604 0.623248
6 1.393410 2.287346 0.626355	6 -1.413849 2.320558 -0.589002	6 2.790258 -2.013827 -0.011131	6 -2.844858 -1.933973 -0.037961	6 -1.331706 2.626220 0.362219	6 -1.605344 2.832750 0.077611
8 -0.214652 -2.387109 -0.188885	8 0.074592 -2.463663 -0.099326	8 0.975455 2.211285 -2.112290	8 -0.868177 2.223751 2.113637	8 -0.249321 -1.711092 1.700470	8 -2.279320 -1.723212 -2.004948
8 2.301751 1.240391 -1.667335	8 -1.991189 1.257905 1.802295	8 0.882907 -0.918876 1.540710	8 -0.792741 -0.923520 -1.458452	8 -0.011179 1.751143 -1.752091	8 -0.076861 0.996932 1.307079
8 -0.070898 2.148250 -1.570574	8 0.383309 2.032841 1.330415	8 0.182676 -1.917368 -0.649181	8 -0.276498 -2.030917 0.730424	8 -2.428927 1.008373 -1.470832	8 0.501639 1.599572 -1.047338
9 2.652417 -3.163361 0.396313	9 -2.887823 -3.068970 -0.360141	9 0.603122 3.867704 0.375829	9 -0.631270 3.834363 -0.423314	9 -2.163220 -3.516945 0.213565	9 -2.145284 -3.421864 0.494233
9 3.336684 -1.096731 0.286300	9 -3.430841 -0.970656 -0.126654	9 1.088822 2.205252 1.698294	9 -1.177134 2.144291 -1.685811	9 -2.474855 -2.058719 -1.374731	9 -1.601746 -1.724390 1.747592
9 1.879056 -1.682930 1.797314	9 -2.203100 -1.597319 -1.815127	9 2.591872 2.975428 0.321411	9 -2.608473 2.932379 -0.244778	9 -0.486445 -2.878245 -1.025875	9 -3.533138 -1.758611 0.738679
9 1.872246 3.504349 0.336956	9 -1.747682 3.556899 -0.194200	9 2.628466 -3.202619 0.596226	9 -2.729130 -3.119644 -0.661233	9 -1.718793 3.742565 -0.269991	9 -0.802249 3.820828 0.513914
9 0.269063 2.441322 1.362908	9 -0.425896 2.423577 -1.504955	9 3.143986 -2.227537 -1.281932	9 -3.283911 -2.145070 1.206195	9 -2.240338 2.310333 1.286228	9 -2.116346 3.187170 -1.103792
9 2.294196 1.634326 1.370953	9 -2.473522 1.752568 -1.175493	9 3.763297 -1.342801 0.612417	9 -3.734117 -1.187114 -0.700149	9 -0.158829 2.880456 0.987868	9 -2.596310 2.666744 0.958135
[$(C_2H_5)_3$NH][TFSI] solvate **1a•7CHCl3** B3LYP/6-31++(d,p) OPT SCRF=(PCM,Solvent=CHLOROFORM) \HF=-12055.2942499\	[$(C_2H_5)_3$NH][TFSI] solvate **1b•7CHCl3** B3LYP/6-31++(d,p) OPT SCRF=(PCM,Solvent=CHLOROFORM) \HF=-12055.294052\	[$(C_2H_5)_3$NH][TFSI] solvate **2a•7CHCl3** B3LYP/6-31++(d,p) OPT SCRF=(PCM, Solvent=CHLOROFORM) \HF= -12055.2948091\	[$(C_2H_5)_3$NH][TFSI] solvate **2b•7CHCl3** B3LYP/6-31++(d,p) OPT SCRF=(PCM, Solvent=CHLOROFORM) \HF=-12055.2947772\		
1 -2.939651 1.043744 -2.658412	8 -0.298512 2.226946 1.704841	17 -8.700336 -1.454506 0.111338	1 -1.986959 -2.352603 -2.350868		
1 -2.756831 -0.648107 -0.725891	16 -0.770792 2.000385 0.336696	6 -9.033197 -1.949087 -1.576882	1 -3.110480 -0.322864 -1.206583		
6 -3.897346 -2.363279 -0.375741	7 -0.785465 0.447869 -0.154373	17 -8.166703 -3.460558 -1.987729	6 -4.255670 -1.665264 -0.108282		
6 -3.180022 -3.418909 -1.207718	16 0.289320 -0.672443 0.345241	17 -8.624457 -0.639315 -2.724619	6 -4.270974 -0.921087 1.221108		
7 -3.743188 -0.935073 -0.874508	6 0.472431 2.910426 -0.762153	1 -10.097536 -2.144484 -1.660290	7 -4.035107 -0.773081 -1.316605		
6 -4.024674 -0.823699 -2.361639	6 1.115781 -1.144269 -1.287505	1 -4.452752 0.483683 -3.175746	6 -4.004269 -1.572560 -2.606561		
6 -3.897519 0.588270 -2.921512	8 -2.066656 2.557834 -0.082067	1 -2.902284 -0.989180 -0.623565	6 -2.984222 -2.704348 -2.625641		
6 -4.604462 0.024214 -0.069603	8 1.376645 -0.188231 1.207851	6 -4.326385 -2.291809 0.119533	6 -5.066014 0.341395 -1.378785		
6 -4.399092 -0.066009 1.437596	8 -0.443711 -1.888010 0.728418	6 -3.679375 -3.627003 -0.229589	6 -4.927549 1.266278 -2.582410		
1 -4.973037 -2.553770 -0.336480	9 0.384200 4.221547 -0.512054	7 -3.913060 -1.137484 -0.778246	1 -3.438150 -2.382774 -0.113962		
1 -3.507306 -2.367008 0.641146	9 1.721585 2.499665 -0.505952	6 -4.123967 -1.472960 -2.243786	1 -5.195662 -2.194093 -0.286835		
1 -3.246240 -4.364355 -0.661617	9 0.198523 2.693542 -2.055332	6 -3.757300 -0.357237 -3.214790	1 -4.260481 -1.668713 2.019129		
1 -3.637867 -3.574247 -2.186741	9 2.017448 -2.104642 -1.051740	6 -4.614177 0.151629 -0.388239	1 -3.378876 -0.301143 1.344353		
1 -2.119873 -3.187962 -1.332257	9 0.203989 -1.605834 -2.155369	6 -4.432790 0.538333 1.074751	1 -5.161478 -0.304559 1.359188		
1 -3.307503 -1.480765 -2.852081	9 1.732322 -0.087383 -1.827693	1 -5.416959 -2.345092 0.065169	1 -5.021609 -1.942293 -2.760183		
1 -5.027947 -1.230051 -2.516451	17 0.985419 2.554349 5.165212	1 -4.043358 -2.000671 1.130048	1 -3.774669 -0.858494 -3.396390		
1 -3.949871 0.518697 -4.011759	6 0.717842 0.924114 4.476795	1 -3.917997 -4.329935 0.573573	1 -3.256947 -3.536439 -1.973300		
1 -4.702554 1.249590 -2.594965	17 -0.906572 0.302378 4.912767	1 -4.056101 -4.054211 -1.161239	1 -2.936721 -3.089691 -3.648223		
1 -4.343582 1.022677 -0.415782	17 1.997469 -0.211543 5.001422	1 -2.590653 -3.543129 -0.282490	1 -6.043729 -0.147808 -1.356020		
1 -5.639965 -0.188919 -0.348487	1 0.757427 1.007351 3.394572	1 -3.509570 -2.350910 -2.440721	1 -4.944752 0.913293 -0.459688		
1 -4.937984 0.767852 1.895836	17 4.541437 -4.895007 -2.222183	1 -5.174509 -1.759697 -2.340730	1 -5.600811 2.113950 -2.426898		

1 -4.790939 -0.989274 1.868972	6 5.396560 -3.379406 -2.636886	1 -2.743746 0.013378 -3.044766	1 -3.911875 1.660465 -2.671222		
1 -3.345227 0.034917 1.711633	17 4.653911 -2.588270 -4.061338	1 -3.801607 -0.773485 -4.225365	1 -5.214088 0.789411 -3.522011		
8 -0.264057 1.948713 1.392650	17 7.141797 -3.672775 -2.899421	1 -4.190252 0.924112 -1.026957	8 -1.066762 -1.493733 0.023349		
16 -0.804467 1.691631 0.053689	1 5.298341 -2.700975 -1.795085	1 -5.668769 0.017808 -0.644650	16 0.282738 -0.935582 0.192540		
7 -0.857466 0.128665 -0.392977	17 -3.316321 6.549822 -0.517072	1 -4.810637 1.556886 1.199833	7 0.375518 0.673386 0.182825		
16 0.238691 -0.994253 0.054048	6 -3.888412 5.177238 0.477732	1 -4.988542 -0.106157 1.758919	16 -0.702842 1.659945 -0.491873		
6 0.396337 2.563154 -1.120162	17 -5.425625 4.513423 -0.172342	1 -3.378074 0.540266 1.363410	6 1.232394 -1.500568 -1.339888		
6 0.942813 -1.500703 -1.624521	17 -4.072389 5.652755 2.191566	8 -1.217621 -1.366354 0.369878	6 0.391192 2.651998 -1.665116		
8 -2.114824 2.251198 -0.314838	1 -3.144361 4.386827 0.422107	16 0.215226 -1.011478 0.362557	8 1.112342 -1.423002 1.305307		
8 1.386952 -0.517896 0.832724	17 5.063852 -2.108334 1.834606	7 0.546944 0.556209 0.278920	8 -1.722778 1.046859 -1.368561		
8 -0.489519 -2.191756 0.500478	6 4.682621 -0.417805 1.388651	16 -0.405344 1.660905 -0.423803	8 -1.160627 2.654897 0.494218		
9 0.333412 3.880286 -0.891087	17 5.233031 -0.058022 -0.283086	6 0.868988 -1.795466 -1.228946	9 1.321723 -2.837115 -1.333134		
9 1.648635 2.141335 -0.915580	17 5.392827 0.735833 2.553250	6 0.777772 2.387368 -1.702206	9 0.591880 -1.115361 -2.453600		
9 0.055557 2.325456 -2.393484	1 3.602282 -0.303091 1.410062	8 1.071942 -1.596460 1.404847	9 2.465461 -0.980778 -1.345145		
9 1.837434 -2.478796 -1.439286	17 -1.862642 -4.729961 3.183575	8 -1.549161 1.148858 -1.195817	9 -0.356095 3.595258 -2.252306		
9 -0.036523 -1.951929 -2.422915	6 -0.226178 -4.632802 2.456664	8 -0.640522 2.777150 0.509076	9 1.387012 3.240926 -0.991193		
9 1.543614 -0.464534 -2.219158	17 -0.022602 -5.866594 1.173001	9 0.722647 -3.125544 -1.150530	9 0.911277 1.857540 -2.607387		
17 -2.167889 2.404300 5.002942	17 1.041528 -4.790489 3.707055	9 0.183685 -1.347605 -2.290496	17 -0.844851 4.200970 4.204012		
6 -0.636217 1.557315 4.614845	1 -0.129059 -3.655056 1.992485	9 2.165267 -1.509068 -1.392722	6 -0.071239 2.690486 3.628604		
17 -0.795104 -0.206849 4.883260	17 6.111561 4.667378 -1.199705	9 0.155484 3.385233 -2.342672	17 -0.776825 1.259157 4.443224		
17 0.726176 2.231597 5.557388	6 4.920815 3.763396 -2.180534	9 1.874437 2.870111 -1.104581	17 1.701755 2.750202 3.855280		
1 -0.430201 1.714237 3.559770	17 5.734372 2.679552 -3.349698	9 1.138813 1.455996 -2.592812	1 -0.274758 2.600415 2.564895		
17 5.440131 -4.910356 -1.059680	17 3.790830 4.875441 -3.011894	17 0.126872 4.871872 3.844293	17 5.139220 -5.041308 -1.949433		
6 6.220036 -3.462351 -1.763079	1 4.337670 3.143948 -1.506494	6 0.822071 3.277681 3.413106	6 5.675506 -3.350583 -2.188526		
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1 5.915240 -2.602213 -1.175052	6 -3.482717 -1.655118 -2.028737	1 0.408563 2.986840 2.450917	1 5.294168 -2.763765 -1.358504		
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17 -3.573879 5.981013 1.403045	6 -4.219900 0.721495 -1.719585	17 3.350746 -4.084925 -4.005546	17 -4.846716 4.291072 1.091556		
17 -3.688230 5.859448 -1.543821	6 -3.485958 1.157747 -2.981894	17 5.719724 -5.315589 -2.746033	17 -2.911949 6.519352 1.144743		
1 -3.151881 4.137030 -0.017806	6 -4.421302 -0.909310 0.181170	1 3.958797 -4.126832 -1.724731	1 -2.609976 4.316529 0.335913		
17 5.280712 -1.193181 2.212474	6 -4.617406 0.202912 1.203951	17 -3.528544 4.986611 -1.589175	17 4.921004 -2.553731 1.692176		
6 4.529695 0.164812 1.325081	1 -2.770577 -1.317145 -2.781057	6 -2.825170 5.208705 0.044905	6 4.242090 -0.970606 2.197005		
17 5.149475 0.248230 -0.361276	1 -4.459651 -1.767884 -2.506275	17 -4.082226 5.029607 1.310192	17 5.015966 0.370835 1.298991		
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1 3.460952 -0.019407 1.266799	1 -2.104471 -2.837726 -0.818209	1 -2.086099 4.426001 0.197330	1 3.183289 -0.976011 1.950930		
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6 0.045495 -4.916519 2.181901	1 -5.266095 0.479373 -1.924086	6 4.367950 -1.648153 1.738618	6 -0.038476 -3.814181 3.298452		
17 0.244799 -6.184276 0.931211	1 -4.179149 1.518845 -0.980653	17 5.198020 -0.473961 0.673344	17 -0.290517 -5.236093 2.237823		
17 1.414066 -4.926195 3.331890	1 -3.888408 2.129949 -3.280010	17 4.829077 -1.405880 3.448543	17 1.191259 -4.157389 4.551141		
1 0.029992 -3.953597 1.678183	1 -2.415826 1.288051 -2.799535	1 3.296562 -1.487467 1.650234	1 0.328324 -2.998999 2.679598		
17 4.421188 5.329917 -1.561227	1 -5.378196 -1.289435 -0.187505	17 -1.722531 -2.866332 4.364653	17 4.467495 4.790375 -3.393924		
6 5.583811 3.986605 -1.770318	1 -3.874627 -1.734989 0.634566	6 -0.094030 -3.440977 3.880948	6 4.873657 3.425770 -2.308127		
17 7.251665 4.509072 -1.386348	1 -5.081851 -0.241257 2.088949	17 -0.174310 -5.103038 3.216467	17 6.217318 3.854785 -1.208169		
17 5.486564 3.299622 -3.420606	1 -3.666414 0.642842 1.514559	17 1.048990 -3.351406 5.252822	17 5.248902 1.947239 -3.242335		
1 5.314690 3.201031 -1.070998	1 -5.276096 0.998137 0.849412	1 0.269615 -2.785993 3.092983	1 3.999690 3.219260 -1.698799		
17 -8.123905 -3.181024 -3.519031	17 -8.689275 -2.224246 -0.376799	17 4.376444 5.013794 -3.569455	17 -8.540884 -2.487250 -0.158010		
6 -9.075652 -2.208936 -2.356789	6 -9.197758 -2.693697 -2.028480	6 5.161480 3.855984 -2.452166	6 -8.618011 -3.289517 -1.756304		
17 -8.475016 -0.523201 -2.283056	17 -8.118188 -3.951573 -2.702447	17 6.416666 4.661552 -1.465023	17 -7.306447 -4.493830 -1.936978		
17 -9.081285 -2.962602 -0.734802	17 -9.281992 -1.268860 -3.106529	17 5.836209 2.457377 -3.341678	17 -8.577492 -2.088200 -3.082120		
1 -10.100599 -2.177481 -2.712309	1 -10.195060 -3.116085 -1.958129	1 4.398539 3.481176 -1.777548	1 -9.564131 -3.817908 -1.816148		

[$(C_2H_5)_3NH$][TFSI] hydrate **1a·6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9775546\	[$(C_2H_5)_3NH$][TFSI] hydrate **1b·6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9736325\	[$(C_2H_5)_3NH$][TFSI] hydrate **1c·6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9584759\	[$(C_2H_5)_3NH$][TFSI] hydrate **2a·6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9780822\	[$(C_2H_5)_3NH$][TFSI] hydrate **2b·6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9705702\	[$(C_2H_5)_3NH$][TFSI] hydrate **2c·6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9788986\
1 3.284457 -0.004117 1.512096	1 4.965588 -0.996950 0.916309	1 4.813820 -0.328043 2.133074	1 4.464668 -2.262593 1.370142	1 -1.775580 -1.987041 -2.106099	1 5.583830 -1.995694 -1.581680
1 1.769164 1.353602 -0.094026	1 2.260083 0.657479 -0.168095	1 1.936241 -0.266833 -0.166299	1 3.056763 -0.043367 -0.075565	1 -2.365489 -1.217048 0.312879	1 3.587937 0.811178 0.176126
6 2.293577 2.894454 -1.395523	6 4.013968 0.438030 -1.266278	6 3.368571 -0.452900 -1.590259	6 4.164447 0.932853 -1.537899	6 -2.307979 -3.217146 0.855919	6 5.393158 1.180582 -0.680126
6 2.724741 2.120739 -2.635169	6 3.512975 0.718685 -2.678069	6 4.800298 -0.908173 -1.840454	6 3.107623 0.649090 -2.597677	6 -1.630118 -3.049535 2.209877	6 6.487278 0.604169 -1.571534
7 2.444255 2.135938 -0.084560	7 3.196724 1.092910 -0.163846	7 2.966597 -0.200263 -0.141095	7 4.056719 0.027781 -0.321559	7 -3.053298 -1.982781 0.377306	7 4.412260 0.199677 -0.062076
6 3.829219 1.530812 0.063512	6 3.797332 0.834920 1.209957	6 3.349497 -1.302315 0.841061	6 4.550087 -1.375010 -0.634543	6 -3.648426 -2.185622 -1.006750	6 3.816515 -0.814992 -1.023697
6 4.046293 0.765869 1.363184	6 4.117064 -0.627208 1.495202	6 4.724273 -1.206915 1.490567	6 4.071297 -2.421503 0.363342	6 -2.652947 -2.637582 -2.068236	6 4.569107 -2.128063 -1.203594
6 2.098173 3.017395 1.105924	6 3.016328 2.580926 -0.420782	6 3.203073 1.224917 0.351340	6 4.787429 0.615769 0.874303	6 -4.116372 -1.552562 1.375932	6 4.817270 -0.351407 1.294227
6 0.773126 3.758084 0.981393	6 2.250411 3.322887 0.665482	6 4.579064 1.826773 0.094451	6 4.064134 1.797693 1.505955	6 -4.894033 -0.305967 0.971877	6 6.239399 -0.880488 1.437668
1 2.873551 3.813328 -1.278367	1 3.986672 -0.631902 -1.065016	1 3.147119 0.475575 -2.119730	1 5.178641 0.802901 -1.922884	1 -1.558318 -3.426708 0.095728	1 5.817132 1.743451 0.154459
1 1.236312 3.147286 -1.473538	1 5.040147 0.788405 -1.130541	1 2.675268 -1.215056 -1.952187	1 4.064814 1.955317 -1.175549	1 -3.037894 -4.030307 0.864132	1 4.776630 1.871530 -1.260780
1 2.436629 2.717750 -3.505464	1 4.059990 0.058250 -3.356964	1 4.920620 -1.005366 -2.923611	1 3.232121 1.380317 -3.401264	1 -1.000463 -3.928446 2.375049	1 7.107586 1.440595 -1.907494
1 3.803699 1.962235 -2.689169	1 2.447257 0.499591 -2.786765	1 5.547632 -0.197458 -1.486411	1 3.204083 -0.345266 -3.040320	1 -0.980732 -2.169732 2.226009	1 7.136284 -0.104115 -1.054590
1 2.211735 1.158944 -2.712691	1 3.700828 1.745918 -2.996895	1 5.003812 -1.888122 -1.402775	1 2.097556 0.759005 -2.194432	1 -2.336915 -2.991144 3.039769	1 6.077649 0.124938 -2.463788
1 3.959190 0.860730 -0.784954	1 4.692291 1.458461 1.271830	1 2.578173 -1.266657 1.612417	1 4.186235 -1.616467 -1.632703	1 -4.459363 -2.907591 -0.884000	1 2.812730 -1.014030 -0.640294
1 4.535054 2.358759 -0.039125	1 3.064096 1.201862 1.926650	1 3.231084 -2.239151 0.292429	1 5.639993 -1.311198 -0.673889	1 -4.081037 -1.227138 -1.289549	1 3.704821 -0.290122 -1.975381
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1 2.073227 2.356191 1.970396	1 4.022590 2.986696 -0.551715	1 2.447987 1.826132 -0.161386	1 4.894634 -0.188823 1.600985	1 -4.774911 -2.414903 1.506131	1 4.663083 0.475069 1.992760
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1 0.569363 4.227638 1.947784	1 2.074406 4.340317 0.305310	1 4.577697 2.824642 0.543730	1 4.641036 2.118710 2.377712	1 -5.504704 -0.007455 1.828769	1 6.347084 -1.249681 2.462077
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1 -0.055096 3.079635 0.762840	1 2.803726 3.396253 1.603712	1 4.779450 1.954247 -0.971958	1 3.064638 1.518680 1.850489	1 -5.569736 -0.478745 0.131918	1 6.985506 -0.095013 1.296046
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16 -0.419988 -0.539594 1.436310	16 -0.452856 -0.395845 1.501258	16 -0.697462 -0.219440 1.399701	16 -1.809093 -0.676491 -1.227557	16 1.180272 -0.387595 -0.328235	16 -2.225926 0.167928 -1.323904
7 0.421573 -0.459650 0.053520	7 0.249339 -0.447881 0.041954	7 -0.144231 -0.515167 -0.092171	7 -1.479310 -0.615403 0.357729	7 0.748592 1.177099 -0.320887	7 -2.048256 -0.328163 0.205441
16 -0.027174 -1.199790 -1.324549	16 -0.494811 -0.845329 -1.346733	16 -0.970128 -0.340165 -1.485805	16 -0.080552 -0.025180 0.932160	16 -0.726057 1.719857 0.051074	16 -0.587475 -0.622439 0.861000
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6 1.479237 -2.283240 -1.674706	6 0.404306 -2.424392 -1.865304	6 -1.225466 -2.119366 -2.070430	6 -0.009167 -1.009947 2.541573	6 -1.554937 2.038296 -1.616187	6 -1.102429 -1.937928 2.112137
8 0.081873 0.539866 2.298665	8 0.396914 0.468491 2.340556	8 0.484084 0.079912 2.225156	8 -3.265930 -0.594947 -1.399442	8 2.275149 -0.598697 0.643901	8 -3.465701 0.953940 -1.412575
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8 -0.031123 -0.226710 -2.427894	8 -0.109662 0.135911 -2.374392	8 -0.043746 0.216175 -2.482980	8 -0.195251 1.388150 1.353068	8 -0.579495 3.062795 0.629471	8 -0.124389 0.515829 1.691122
9 -0.442184 -2.151785 3.530949	9 -0.582956 -2.056306 3.554835	9 -1.522645 -1.726450 3.403471	9 -1.689820 -2.625365 -3.013489	9 2.519953 -1.728596 -2.160255	9 -2.852068 -1.093709 -3.566605
9 -0.234629 -3.199091 1.630222	9 -1.017157 -2.995947 1.636153	9 -2.430932 -2.252753 1.494421	9 -0.102468 -2.707694 -1.520471	9 1.152834 -0.244699 -2.986821	9 -1.612888 -2.272860 -2.213988
9 1.463485 -2.121256 2.472629	9 1.040376 -2.511942 2.172345	9 -0.364786 -2.814529 1.909706	9 -2.129005 -3.308592 -0.989254	9 3.034013 0.389162 -2.084114	9 -3.728620 -1.982753 -1.778561
9 1.282258 -2.920687 -2.834860	9 -0.084387 -2.820897 -3.046148	9 -1.768628 -2.087494 -3.292726	9 1.100441 -0.646011 3.194883	9 -2.762785 2.574952 -1.407185	9 -0.005314 -2.315393 2.780319
9 2.585387 -1.536922 -1.768364	9 1.717570 -2.203705 -1.987112	9 -0.054860 -2.762391 -2.125502	9 -1.074422 -0.748924 3.303285	9 -0.816134 2.885225 -2.339773	9 -1.997692 -1.453618 2.977635
9 1.639710 -3.184814 -0.700465	9 0.203987 -3.389130 -0.961375	9 -2.047927 -2.769333 -1.241501	9 0.043347 -2.318800 2.281497	9 -1.695009 0.890528 -2.290619	9 -1.619653 -2.998085 1.484555
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1 -3.007611 -1.845602 -1.019748	1 -0.516665 2.096814 -2.204997	1 -3.794293 0.406378 0.881134	1 -3.546279 2.334853 0.966906	1 1.581196 2.440562 3.105729	1 -2.570025 2.948913 1.597357
1 -4.197901 -1.690508 -0.051275	1 -0.748761 3.349625 -1.295932	1 -4.707821 0.098478 -0.300959	1 -2.043628 2.339160 1.387260	1 0.349056 3.174938 2.523605	1 -1.190535 2.268540 1.876988
8 -1.035537 2.584531 -2.334716	8 -0.689861 3.138072 2.839779	8 1.379709 2.789080 -2.107189	8 0.940392 3.718700 -0.283056	8 6.502240 -2.792395 0.556518	8 2.316476 1.828969 0.624223
1 -0.770520 1.650899 -2.355703	1 -0.347602 2.226762 2.795617	1 0.886008 1.978159 -2.310013	1 0.620296 3.393839 -1.151107	1 5.554048 -2.830216 0.805353	1 1.832499 2.244796 -0.136172
1 -1.935432 2.592914 -1.951280	1 -1.364631 3.133983 3.532035	1 0.701223 3.424896 -1.800244	1 0.744454 2.992844 0.331421	1 6.513559 -2.694569 -0.404227	1 1.622970 1.370412 1.129052
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8 -4.796343 0.429814 -2.430390	8 -3.562858 3.079720 -1.299077	8 -3.069106 3.113384 -1.510484	8 -1.823592 4.700601 -0.595841	8 -1.181745 0.861195 3.885700	8 -0.560092 4.793956 0.062465

1 -4.546892 -0.375293 -1.914927	1 -3.803739 2.174962 -1.014158	1 -2.860905 2.175700 -1.661048	1 -0.897414 4.715611 -0.291429	1 -1.456976 0.686722 2.973479	1 -0.032438 5.482891 0.487489
1 -5.755005 0.394655 -2.546891	1 -2.767206 2.968133 -1.857550	1 -3.085799 3.203729 -0.534408	1 -2.275801 4.114550 0.055955	1 -0.489246 1.552608 3.795568	1 -0.940099 4.238965 0.791406
8 -3.675917 2.567414 -1.219765	8 -6.789602 -0.303967 -0.487133	8 -0.697378 4.488730 -1.185395	8 -4.038806 -0.933656 2.005371	8 3.035866 3.110779 0.013502	8 -4.598978 0.056960 1.832698
1 -4.162196 1.840352 -1.690777	1 -5.833608 -0.099141 -0.427686	1 -1.529921 4.092770 -1.536037	1 -3.173423 -1.001307 1.561454	1 2.223059 2.643165 -0.255665	1 -3.821219 -0.259387 1.336486
1 -4.163895 3.384054 -1.393466	1 -6.870744 -1.231845 -0.231325	1 -0.679012 5.407972 -1.484284	1 -4.456926 -1.799770 1.904366	1 2.809321 4.050757 0.026982	1 -5.351182 -0.449851 1.497284
[$(C_2H_5)_3NH$][TFSI] hydrate **3a•6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9688229\	[$(C_2H_5)_3NH$][TFSI] hydrate **3b•6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9809008\	[$(C_2H_5)_3NH$][TFSI] hydrate **4a•6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9770858\	[$(C_2H_5)_3NH$][TFSI] hydrate **4b•6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9770871\	[$(C_2H_5)_3NH$][TFSI] hydrate **5a•6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9770851\	[$(C_2H_5)_3NH$][TFSI] hydrate **5b•6H2O** B3LYP/6-31++G(d,p) OPT SCRF=(PCM, Solvent=WATER) \HF=-2578.9776175\
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1 -4.864142 0.039319 1.087700	1 4.583845 0.505664 -0.397075	1 4.957573 0.360035 -0.110948	1 4.928268 0.376536 -0.154458	1 4.958116 0.359734 -0.109716	1 5.400628 -0.292393 -0.480868
6 -3.050205 -0.978870 1.200821	6 2.608701 0.895174 -0.939990	6 3.779327 -1.004027 0.938096	6 3.772939 -1.317115 -0.539602	6 3.373445 1.453823 0.691364	6 4.566935 1.574848 -0.066785
6 -2.611138 -0.074386 2.346078	6 2.957883 0.880622 -2.423087	6 4.705924 -2.156898 0.572198	6 4.988898 -2.217444 -0.360711	6 4.238346 1.994514 1.823575	6 5.200112 2.177623 -1.315378
7 -4.211940 -0.404212 0.411508	7 3.643900 0.202450 -0.071913	7 3.939975 0.207073 0.037525	7 3.957810 0.067334 0.053675	7 3.940557 0.206270 0.038521	7 4.495945 0.057395 -0.107480
6 -3.729850 0.676036 -0.543678	6 3.502238 0.615531 1.382262	6 3.306056 -0.029732 -1.321598	6 3.003645 1.064179 -0.579848	6 3.780207 -1.005512 0.938283	6 4.318616 -0.518428 1.284869
6 -4.837448 1.624493 -0.987644	6 4.048307 2.008510 1.670778	6 3.832593 0.905263 -2.403892	6 3.420910 1.487495 -1.982643	6 4.707175 -2.157874 0.571748	6 5.600214 -0.512464 2.108530
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6 -5.815754 -2.371687 0.585832	6 4.849026 -2.017416 0.193081	6 4.239110 1.996709 1.820960	6 4.404179 1.249595 2.260412	6 3.832163 0.906672 -2.402288	6 3.582575 -1.854002 -1.508132
1 -2.244016 -1.150927 0.484048	1 2.536302 1.922202 -0.582130	1 2.725528 -1.285000 0.884620	1 3.562470 -1.181833 -1.600290	1 2.369290 1.190741 1.030352	1 5.160720 1.833691 0.810434
1 -3.372141 -1.945276 1.588070	1 1.656194 0.399804 -0.737164	1 3.988697 -0.668839 1.953575	1 2.879992 -1.732929 -0.067496	1 3.281307 2.201804 -0.095993	1 3.543374 1.928553 0.089343
1 -1.757816 -0.542464 2.844972	1 2.185623 1.440742 -2.957645	1 4.531939 -2.970443 1.282127	1 4.764714 -3.187318 -0.813517	1 3.773608 2.912261 2.194780	1 5.241097 3.262794 -1.184571
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1 -3.407815 0.043996 3.086267	1 2.983855 -0.126939 -2.845543	1 5.756918 -1.864464 0.649095	1 5.237523 -2.394162 0.688941	1 5.245561 2.244484 1.478533	1 4.623664 1.979593 -2.222712
1 -2.947766 1.235291 -0.027438	1 2.438797 0.537025 1.619414	1 3.516588 -1.064815 -1.590449	1 2.018526 0.593600 -0.568434	1 3.989397 -0.670910 1.953986	1 3.525197 0.065123 1.757241
1 -3.279575 0.147494 -1.387670	1 4.040764 -0.125955 1.972532	1 2.227980 0.073398 -1.179665	1 2.967702 1.930953 0.079367	1 2.726488 -1.286740 0.884491	1 3.960157 -1.540172 1.161580
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1 -6.376158 -3.070645 -0.041687	1 4.701718 -3.092299 0.055920	1 3.774662 2.914721 2.191872	1 4.274821 1.119938 3.338693	1 3.337888 0.649327 -3.343316	1 2.761794 -2.099334 -2.187948
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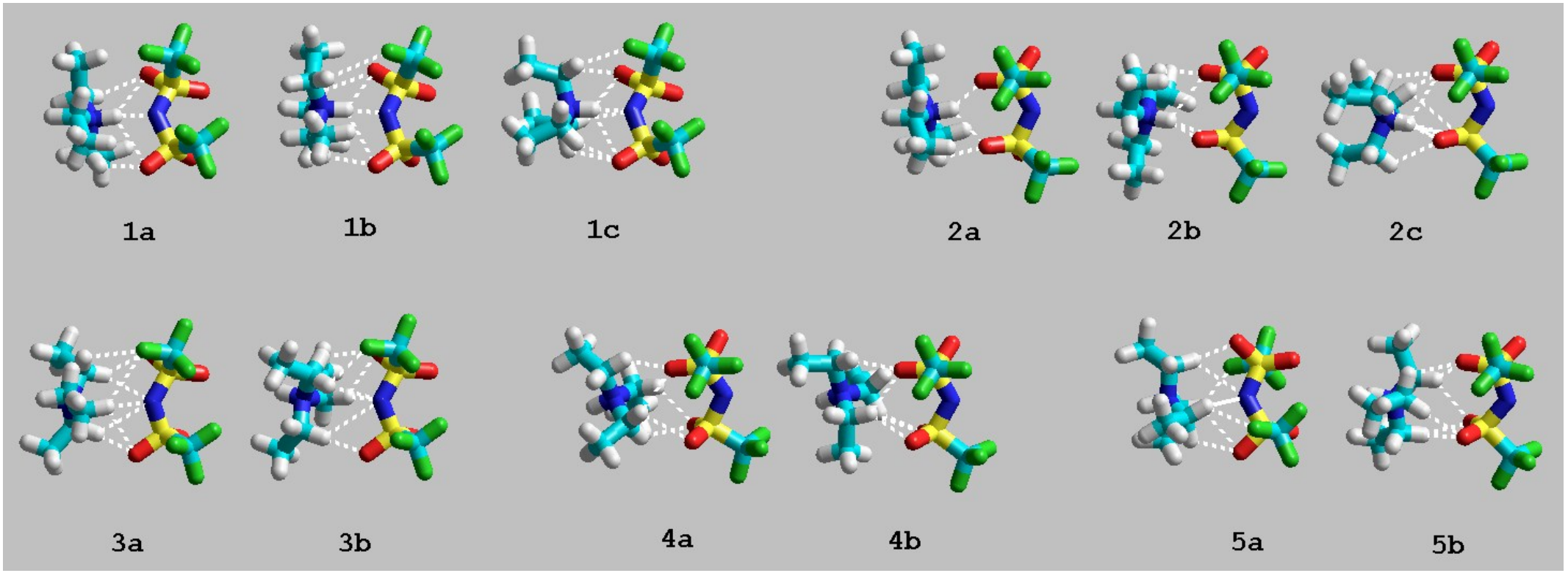

Figure SI 1. $[(C_2H_5)_3NH][TFSI]$ in different dispositions and H-bonding modes. The N^+-H proton donor is directed to nitrogen and the nearest oxygen atoms (**1a** – **1c**) or exclusively to the oxygen sites due to the outward orientation of the imide nitrogen (pointing away from N^+-H into the bulk solvent) (**2a** – **2c**). The N^+-H proton in the outward orientation, away from the anion surface, is associated with the formation of both C-H···N and C-H···O (**3a** – **3b**) hydrogen bonding or of just C-H···O (**4a** – **4b**) hydrogen bonding. The N^+-H proton is in the same orientation as in **3a** – **4b**, but with extra C-H···F bonds (**5a** – **5b**).

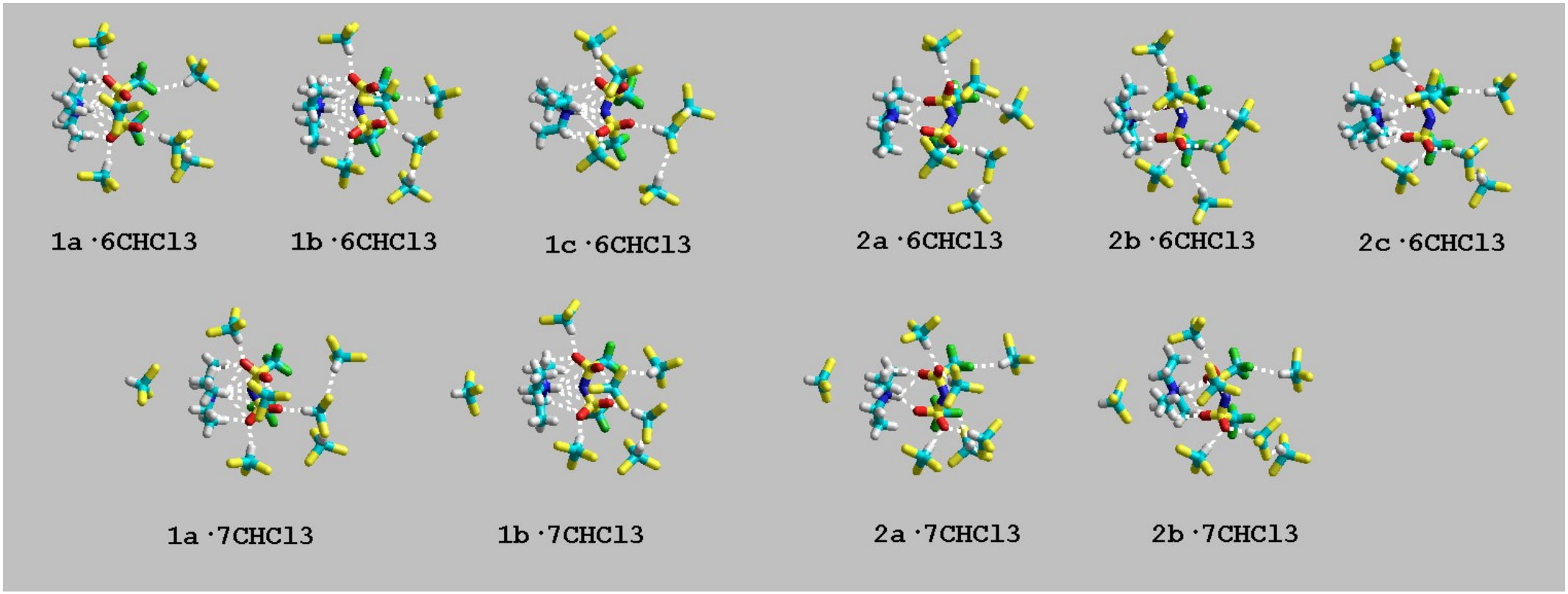

Figure SI 2. $[(C_2H_5)_3NH][TFSI]$ ion pairs as chloroform solvates with the coordination of six (**1a·6CHCl3**-**2c·6CHCl3**, top) or seven (**1a·7CHCl3-2b·7CHCl3**, bottom) molecules of solvent.

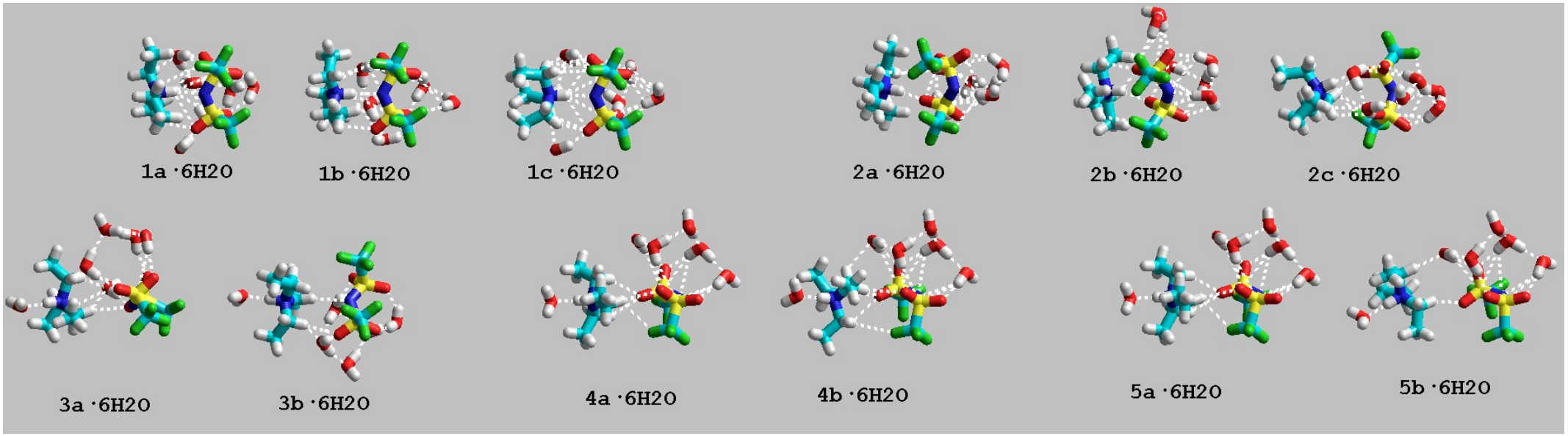

Figure SI 3. $[(C_2H_5)_3NH][TFSI]$ ion pairs as hydrates with the coordination of explicit solvent as a first hydration shell, with six (**1a·6H2O**-**2c·6H2O**, top) or seven (**1a·6H2O - 2b·6H2O**, bottom) molecules of solvent.