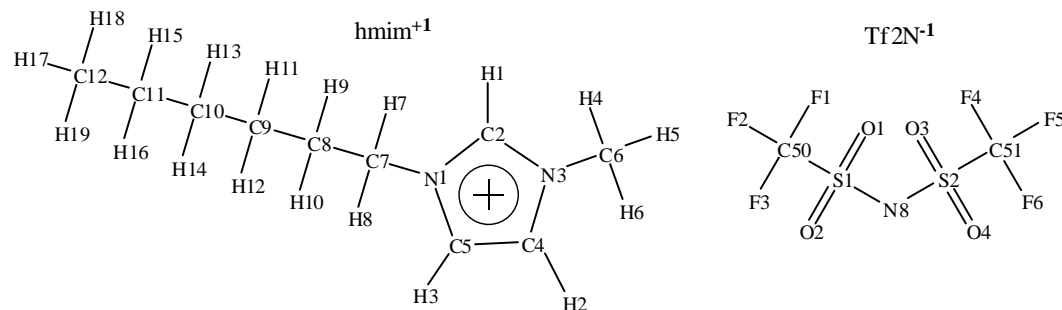


Atomistic Simulation of the Absorption of Carbon Dioxide and Water in the Ionic Liquid 1-n-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([hmim][Tf₂N])

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Supplemental information - Force field parameters and nomenclature



Partial Atomic Charges and Lennard-Jones Parameters

Atom ID	Type	q_i (e)	ϵ_i (kcal/mol)	R_{\min} (Å)
C5	CPH1	-0.125063	0.05	3.6
C4	CPH1	-0.127671	0.05	3.6
C2	CPH2	-0.064652	0.05	3.6
N1	NR1	0.096130	0.20	3.7
H3	HR3	0.208060	0.0078	2.936
H2	HR3	0.198397	0.0078	2.936
H1	HR1	0.202706	0.046	1.8
N3	NR1	0.144827	0.20	3.7
C6	CN7B	-0.196548	0.02	4.55
H4	HN7	0.133140	0.022	2.64
H5	HN7	0.133140	0.022	2.64
H6	HN7	0.133140	0.022	2.64
C7	CN7B	-0.068487	0.02	4.55
H7	HN7	0.086794	0.022	2.64
H8	HN7	0.086794	0.022	2.64
C8	CT2	0.075607	0.055	4.35
H9	HN7	-0.004141	0.022	2.64
H10	HN7	-0.004141	0.022	2.64
C9	CT2	0.021504	0.055	4.35
H11	HN7	0.014712	0.022	2.64
H12	HN7	0.014712	0.022	2.64
C10	CT2	-0.005004	0.055	4.35
H13	HN7	-0.008878	0.022	2.64
H14	HN7	-0.008878	0.022	2.64
C11	CT2	0.128765	0.055	4.35
H15	HN7	-0.016022	0.022	2.64
H16	HN7	-0.016022	0.022	2.64
C12	CT3	-0.152351	0.055	4.35
H17	HN7	0.039810	0.022	2.64
H18	HN7	0.039810	0.022	2.64
H19	HN7	0.039810	0.022	2.64
N8	NTF2	-0.66	0.17	3.648002

Bonds

Type	Type	k_b (kcal/mol Å ⁻²)	r_0 (Å)
CN7B	NR1	220.0	1.4762
CPH1	NR1	400.0	1.3819
CPH2	NR1	400.0	1.3366
CPH1	CPH1	410.0	1.3610
CPH2	HR1	340.0	1.0779
CPH1	HR3	365.0	1.0775
CN7B	HN7	309.0	1.0899
CT2	HN7	309.0	1.0954
CT3	HN7	322.0	1.0935
CN7B	CT2	200.0	1.5308
CT2	CT2	222.5	1.5373
CT2	CT3	222.5	1.5314
CN7B	CT3	200.0	1.5308
CTF2	FTF2	441.802	1.3230
CTF2	STF2	235.421	1.8180
STF2	OTF2	637.070	1.4420
NTF2	STF2	372.012	1.5700
O	C	1029.995	1.1600
OT	HT	450.0	1.0000

Atom ID	Type	q_i (e)	ϵ_i	R_{\min}
F5	FTF2	-0.16	0.053	3.311264
F6	FTF2	-0.16	0.053	3.311264
C (CO ₂)	C	0.70	0.053655	3.142894
O1 (CO ₂)	O	-0.35	0.156989	3.423509
O2 (CO ₂)	O	-0.35	0.156989	3.423509
O (H ₂ O)	OT	-0.82	0.155425	3.553145
H1 (H ₂ O)	HT	0.41	0.0	0.0
H2 (H ₂ O)	HT	0.41	0.0	0.0

S1	STF2	1.02	0.25	3.984740
S2	STF2	1.02	0.25	3.984740
C50	CTF2	0.35	0.066	3.928618
C51	CTF2	0.35	0.066	3.928618
O1	OTF2	-0.53	0.21	3.322488
O2	OTF2	-0.53	0.21	3.322488
O3	OTF2	-0.53	0.21	3.322488
O4	OTF2	-0.53	0.21	3.322488
F1	FTF2	-0.16	0.053	3.311264
F2	FTF2	-0.16	0.053	3.311264
F3	FTF2	-0.16	0.053	3.311264
F4	FTF2	-0.16	0.053	3.311264

dihedrals

Type	Type	Type	Type	k_χ (kcal/mol)	n_θ	δ_θ (deg)
CPH2	NR1	CPH1	CPH1	14.0	2	180.0
NR1	CPH1	CPH1	NR1	14.0	2	180.0
NR1	CPH2	NR1	CPH1	14.0	2	180.0
HR1	CPH2	NR1	CPH1	3.0	2	180.0
HR3	CPH1	CPH1	HR3	2.0	2	180.0
CPH1	CPH1	NR1	CN7B	0.0	1	0.0
HR3	CPH1	NR1	CPH2	3.0	2	180.0
NR1	CPH1	CPH1	HR3	3.0	2	180.0
NR1	CPH2	NR1	CN7B	0.0	2	180.0
HR1	CPH2	NR1	CN7B	0.0	2	180.0
HR3	CPH1	NR1	CN7B	0.0	2	180.0
CPH2	NR1	CN7B	HN7	0.1950	2	180.0
CPH1	NR1	CN7B	HN7	0.0	3	0.0
CPH2	NR1	CN7B	CT2	0.1	3	180.0
CPH1	NR1	CN7B	CT2	0.2	4	0.0
NR1	CN7B	CT2	CT2	0.0	3	0.0
HN7	CT2	CT3	HN7	0.16	3	0.0
CT2	CT2	CT3	HN7	0.16	3	0.0
NR1	CN7B	CT2	HN7	0.0	3	0.0
CN7B	CT2	CT2	CT3	0.15	1	0.0
HN7	CN7B	CT2	HN7	0.195	3	0.0
HN7	CN7B	CT2	CT2	0.195	3	0.0
HN7	CT2	CT2	HN7	0.195	3	0.0
CN7B	CT2	CT2	HN7	0.195	3	0.0
HN7	CT2	CT2	CT3	0.195	3	0.0
CPH2	NR1	CN7B	CT3	0.1	3	180.0
CPH1	NR1	CN7B	CT3	0.2	4	0.0
NR1	CN7B	CT3	HN7	0.0	3	0.0
HN7	CN7B	CT3	HN7	0.195	3	0.0
CT2	CT2	CT2	CT2	0.195	3	0.0
CT2	CT2	CT2	CT3	0.195	3	0.0
CN7B	CT2	CT2	CT2	0.195	3	0.0
CT2	CT2	CT2	HN7	0.195	3	0.0
FTF2	CTF2	STF2	OTF2	0.1734	3	0.0
STF2	NTF2	STF2	OTF2	-0.0018	3	0.0
FTF2	CTF2	STF2	NTF2	0.158	3	0.0
STF2	NTF2	STF2	CTF2	7.8329	1	0.0
STF2	NTF2	STF2	CTF2	-2.4904	2	180.0
STF2	NTF2	STF2	CTF2	-0.7636	3	0.0

Angles

Type	Type	Type	k_θ (kcal/mol rad ⁻²)	θ_0 (deg)
CT2	CN7B	NR1	140.00	112.34
CPH1	NR1	CPH2	130.00	108.25
HN7	CN7B	NR1	30.00	109.41
HR1	CPH2	NR1	25.00	125.44
NR1	CPH1	CPH1	130.00	107.28
NR1	CPH2	NR1	130.00	109.11
HR3	CPH1	CPH1	25.00	130.74
NR1	CPH1	HR3	25.00	122.04
HN7	CN7B	HN7	35.50	108.44
HN7	CN7B	CT2	33.40	111.68
HN7	CT2	CN7B	33.40	109.13
CN7B	CT2	CT2	58.35	111.50
CT2	CT2	CT3	58.00	112.34
HN7	CT2	HN7	35.50	106.13
HN7	CT3	HN7	35.50	107.24
CT2	CT2	HN7	26.50	108.43
CT3	CT2	HN7	34.60	109.47
CT2	CT3	HN7	34.60	111.62
CN7B	NR1	CPH2	130.00	125.75
CN7B	NR1	CPH1	130.00	125.67
CT3	CN7B	NR1	140.00	112.34
HN7	CN7B	CT3	33.40	111.68
HN7	CT3	CN7B	33.40	109.13
CT2	CT2	CT2	58.35	114.27
FTF2	CTF2	FTF2	93.33	107.10
STF2	CTF2	FTF2	82.93	111.80
CTF2	STF2	OTF2	103.97	102.60
OTF2	STF2	OTF2	115.80	118.50
OTF2	STF2	NTF2	94.51	113.60
CTF2	STF2	NTF2	97.51	100.20
STF2	NTF2	STF2	80.19	125.60
O	C	O	56.0	180.00
HT	OT	HT	55.00	109.47

impropers

Note that there are only 5 impropers on each hmim. In terms of atom ID, they are shown as: C2-N1-N3-H1, N1,3-C5,4-C2-C7,6, and C4,5-C5,4-N3,1-H2,3

Type	Type	Type	Type	k_ψ (kcal/mol rad ⁻²)	ψ_0 (deg)
CPH2	NR1	NR1	HR1	0.5	0.0
NR1	CPH1	CPH2	CN7B	0.6	0.0
CPH1	CPH1	NR1	HR3	0.5	0.0