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Supporting Information for

Ionic liquids from a fragmented perspective

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S1. Mean absolute differences and standard deviations of EFP polarization energy terms relative to SAPT2+3 for >180 ion pair configurations, from reference 24, with four different basis sets for EFP terms, both with and without the valence virtual orbital approximation. Units are in kcal/mol.

			ACCD[a]		ACCT[a]		6-311++G(d,p)		6-311++G(3df,2p)	
	Cations	Anions	CMO	VVO	CMO	VVO	CMO	VVO	CMO	VVO
Polarization	CnMIM	TILA	3.4 ± 1.4		3.7 ± 2.1		7.9 ± 3.3	7.9 ± 3.3	5.9 ± 3.1	5.9 ± 3.1
		TILA-tos	3.1 ± 1.4		3.4 ± 2.1		7.4 ± 3.2	7.4 ± 3.2	5.3 ± 2.8	5.3 ± 2.8
		Hal	1.6 ± 1.0		2.8 ± 4.3		1.8 ± 1.3	1.8 ± 1.3	1.7 ± 1.1	1.7 ± 1.1
		All	2.8 ± 1.5		3.4 ± 3.0		5.9 ± 4.0	5.9 ± 4.0	4.5 ± 3.3	4.5 ± 3.3
		All-tos	2.6 ± 1.4		3.2 ± 3.1		5.4 ± 3.8	5.4 ± 3.8	4.0 ± 2.9	4.0 ± 2.9
	CnMPyr	TILA	3.3 ± 1.5		3.8 ± 1.8		7.2 ± 2.3	7.2 ± 2.3	5.2 ± 2.1	5.2 ± 2.1
		TILA-tos	3.1 ± 1.5		3.7 ± 1.8		6.9 ± 2.2	6.9 ± 2.2	4.9 ± 2.0	4.9 ± 2.0
		Hal	1.2 ± 1.0		1.2 ± 0.8		1.3 ± 0.8	1.3 ± 0.8	1.6 ± 2.9	1.6 ± 2.9
		All	2.8 ± 1.7		3.2 ± 1.9		5.8 ± 3.2	5.8 ± 3.2	4.3 ± 2.7	4.3 ± 2.7
		All-tos	2.7 ± 1.7		3.1 ± 1.9		5.5 ± 3.2	5.5 ± 3.2	4.1 ± 2.7	4.1 ± 2.7
	All	TILA	3.3 ± 1.5		3.8 ± 1.9		7.5 ± 2.8	7.5 ± 2.8	5.5 ± 2.6	5.5 ± 2.6
		TILA-tos	3.1 ± 1.5		3.6 ± 1.9		7.1 ± 2.7	7.1 ± 2.7	5.1 ± 2.4	5.1 ± 2.4
		Hal	1.4 ± 1.0		2.1 ± 3.3		1.5 ± 1.1	1.5 ± 1.1	1.7 ± 2.1	1.7 ± 2.1
		All	2.8 ± 1.6		3.3 ± 2.5		5.8 ± 3.6	5.8 ± 3.6	4.4 ± 3.0	4.4 ± 3.0
		All-tos	2.6 ± 1.5		3.1 ± 2.5		5.5 ± 3.5	5.5 ± 3.5	4.0 ± 2.8	4.0 ± 2.8

[a]*SAPT2+3, EFP/ACCD and EFP/ACCT data taken from reference 24.*

S2. Mean absolute differences and standard deviations of EFP Electrostatic energy terms relative to SAPT2+3 for >180 ion pair configurations, from reference 24, with four different basis sets for EFP terms, both with and without the valence virtual orbital approximation. Units are in kcal/mol.

			ACCD[a]		ACCT[a]		6-311++G(d,p)		6-311++G(3df,2p)	
	Cations	Anions	CMO	VVO	CMO	VVO	CMO	VVO	CMO	VVO
Electrostatic	CnMIM	TILA	3.9 ± 6.4		2.2 ± 1.4		7.6 ± 17.9	7.6 ± 17.9	6.3 ± 16.6	6.3 ± 16.6
		TILA-tos	2.4 ± 1.3		2.0 ± 1.2		1.1 ± 1.2	1.1 ± 1.2	0.9 ± 0.6	0.9 ± 0.6
		Hal	2.5 ± 1.7		2.3 ± 2.2		3.3 ± 2.4	3.3 ± 2.4	2.8 ± 2.3	2.8 ± 2.3
		All	3.4 ± 5.3		2.2 ± 1.7		6.2 ± 14.8	6.2 ± 14.8	5.2 ± 13.6	5.1 ± 13.6
		All-tos	2.4 ± 1.4		2.1 ± 1.6		1.9 ± 2.0	1.9 ± 2.0	1.6 ± 1.7	1.6 ± 1.7
	CnMPyr	TILA	2.1 ± 1.8		1.1 ± 0.8		3.0 ± 6.9	3.0 ± 6.9	0.8 ± 1.4	0.8 ± 1.4
		TILA-tos	1.9 ± 1.3		1.0 ± 0.8		0.9 ± 0.7	0.9 ± 0.7	0.5 ± 0.4	0.5 ± 0.4
		Hal	4.4 ± 1.8		2.2 ± 1.1		2.2 ± 0.9	2.2 ± 0.9	2.2 ± 0.9	2.2 ± 0.9
		All	2.7 ± 2.0		1.3 ± 1.0		2.8 ± 6.1	2.8 ± 6.1	1.1 ± 1.4	1.1 ± 1.4
		All-tos	2.5 ± 1.8		1.3 ± 1.0		1.2 ± 1.0	1.2 ± 1.0	0.9 ± 0.9	0.9 ± 0.9
	All	TILA	2.9 ± 4.5		1.6 ± 1.2		5.0 ± 13.0	5.0 ± 13.0	3.2 ± 11.2	3.2 ± 11.2
		TILA-tos	2.1 ± 1.3		1.4 ± 1.1		1.0 ± 1.0	1.0 ± 1.0	0.7 ± 0.5	0.7 ± 0.5
		Hal	3.3 ± 1.9		2.2 ± 1.8		2.8 ± 2.0	2.8 ± 2.0	2.5 ± 1.8	2.5 ± 1.8
		All	3.0 ± 3.9		1.7 ± 1.4		4.4 ± 11.1	4.4 ± 11.1	3.0 ± 9.6	3.0 ± 9.6
		All-tos	2.5 ± 1.6		1.7 ± 1.4		1.5 ± 1.6	1.5 ± 1.6	1.2 ± 1.4	1.2 ± 1.4

[a]*SAPT2+3, EFP/ACCD and EFP/ACCT data taken from reference 24.*

S3. Mean absolute differences and standard deviations of EFP Exchange Repulsion energy terms relative to SAPT2+3 for >180 ion pair configurations, from reference 24, with four different basis sets for EFP terms, both with and without the valence virtual orbital approximation. Units are in kcal/mol.

			ACCD[a]		ACCT[a]		6-311++G(d,p)		6-311++G(3df,2p)	
	Cations	Anions	CMO	VVO	CMO	VVO	CMO	VVO	CMO	VVO
Exchange-Repulsion	CnMIM	TILA	2.0 ± 0.9		1.8 ± 0.8		3.0 ± 1.3	3.0 ± 1.3	2.2 ± 1.9	2.2 ± 1.9
		TILA-tos	1.9 ± 0.9		1.9 ± 0.8		2.6 ± 0.8	2.6 ± 0.8	1.7 ± 0.9	1.7 ± 0.9
		Hal	2.8 ± 1.7		2.9 ± 1.9		4.4 ± 3.3	4.4 ± 3.3	2.6 ± 1.6	2.6 ± 1.6
		All	2.3 ± 1.3		2.1 ± 1.4		3.5 ± 2.3	3.5 ± 2.3	2.3 ± 1.8	2.3 ± 1.8
		All-tos	2.2 ± 1.3		2.3 ± 1.4		3.3 ± 2.3	3.3 ± 2.3	2.0 ± 1.3	2.0 ± 1.3
	CnMPyr	TILA	1.9 ± 0.3		1.8 ± 0.3		2.8 ± 0.6	2.8 ± 0.6	2.1 ± 0.3	2.1 ± 0.3
		TILA-tos	1.9 ± 0.4		1.9 ± 0.3		2.7 ± 0.5	2.7 ± 0.5	2.1 ± 0.3	2.1 ± 0.3
		Hal	1.2 ± 0.7		0.7 ± 0.6		3.2 ± 1.4	3.2 ± 1.4	1.3 ± 1.0	1.3 ± 1.0
		All	1.7 ± 0.5		1.6 ± 0.6		2.9 ± 0.9	2.9 ± 0.9	1.9 ± 0.6	1.9 ± 0.6
		All-tos	1.7 ± 0.6		1.6 ± 0.6		2.8 ± 0.9	2.8 ± 0.9	1.9 ± 0.7	1.9 ± 0.7
	All	TILA	1.9 ± 0.6		1.8 ± 0.6		2.9 ± 1.0	2.9 ± 1.0	2.1 ± 1.3	2.1 ± 1.3
		TILA-tos	1.9 ± 0.6		1.9 ± 0.5		2.7 ± 0.7	2.7 ± 0.7	1.9 ± 0.7	1.9 ± 0.7
		Hal	2.1 ± 1.6		1.9 ± 1.8		3.9 ± 2.7	3.9 ± 2.7	2.0 ± 1.5	2.0 ± 1.5
		All	2.0 ± 1.0		1.8 ± 1.1		3.2 ± 1.7	3.2 ± 1.7	2.1 ± 1.3	2.1 ± 1.3
		All-tos	1.9 ± 1.0		1.9 ± 1.1		3.0 ± 1.7	3.0 ± 1.7	1.9 ± 1.0	1.9 ± 1.0

[a]*SAPT2+3, EFP/ACCD and EFP/ACCT data taken from reference 24.*

S4. Mean absolute differences and standard deviations of EFP Dispersion energy terms relative to SAPT2+3 for >180 ion pair configurations, from reference 24, with four different basis sets for EFP terms, both with and without the valence virtual orbital approximation. Units are in kcal/mol.

			ACCD[a]		ACCT[a]		6-311++G(d,p)		6-311++G(3df,2p)	
	Cations	Anions	CMO	VVO	CMO	VVO	CMO	VVO	CMO	VVO
Dispersion	CnMIM	TILA	4.0 ± 1.5		4.1 ± 1.4		3.8 ± 1.4	3.8 ± 1.4	1.9 ± 1.9	1.9 ± 1.9
		TILA-tos	4.0 ± 1.6		4.0 ± 1.5		3.6 ± 1.4	3.6 ± 1.4	1.5 ± 1.2	1.5 ± 1.2
		Hal	2.1 ± 0.4		1.3 ± 1.1		5.4 ± 2.7	5.4 ± 2.7	2.9 ± 0.8	2.9 ± 0.8
		All	3.3 ± 1.5		3.2 ± 1.9		4.3 ± 2.1	4.3 ± 2.1	2.2 ± 1.7	2.2 ± 1.7
		All-tos	3.3 ± 1.6		3.0 ± 1.9		4.2 ± 2.1	4.2 ± 2.1	2.0 ± 1.3	2.0 ± 1.3
	CnMPyr	TILA	1.5 ± 0.6		1.6 ± 0.6		3.9 ± 1.3	3.9 ± 1.3	2.6 ± 1.2	2.6 ± 1.2
		TILA-tos	1.5 ± 0.7		1.6 ± 0.6		3.7 ± 1.1	3.7 ± 1.1	2.4 ± 1.0	2.4 ± 1.0
		Hal	2.3 ± 0.3		1.4 ± 0.2		5.2 ± 1.9	5.2 ± 1.9	3.3 ± 0.6	3.3 ± 0.6
		All	1.7 ± 0.7		1.6 ± 0.5		4.2 ± 1.5	4.2 ± 1.5	2.8 ± 1.1	2.8 ± 1.1
		All-tos	1.7 ± 0.7		1.5 ± 0.5		4.1 ± 1.5	4.1 ± 1.5	2.6 ± 1.0	2.6 ± 1.0
	All	TILA	2.5 ± 1.6		2.7 ± 1.6		3.9 ± 1.3	3.9 ± 1.3	2.3 ± 1.6	2.3 ± 1.6
		TILA-tos	2.6 ± 1.7		2.6 ± 1.6		3.7 ± 1.2	3.7 ± 1.2	2.0 ± 1.2	2.0 ± 1.2
		Hal	2.2 ± 0.4		1.3 ± 0.9		5.3 ± 2.3	5.3 ± 2.3	3.0 ± 0.7	3.0 ± 0.7
		All	2.5 ± 1.4		2.3 ± 1.6		4.3 ± 1.8	4.3 ± 1.8	2.5 ± 1.4	2.5 ± 1.4
		All-tos	2.5 ± 1.4		2.2 ± 1.5		4.2 ± 1.8	4.2 ± 1.8	2.3 ± 1.2	2.3 ± 1.2

[a]*SAPT2+3, EFP/ACCD and EFP/ACCT data taken from reference 24.*

S5. EFP Interaction Energies of 1-alkyl-3-methylimidazolium (CnMIM) cation and Typical ionic liquid anions (TILA) anion using canonical molecular orbitals with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1442	0.0238	-0.0140	-0.0154	-0.0029	-0.1528
1	dca	p1	-0.1477	0.0401	-0.0110	-0.0235	-0.0057	-0.1477
1	dca	p2	-0.1383	0.0376	-0.0156	-0.0146	-0.0052	-0.1361
1	mes	p1	-0.1633	0.0363	-0.0187	-0.0200	-0.0082	-0.1739
1	ntf2	p1	-0.1371	0.0375	-0.0126	-0.0256	-0.0065	-0.1426
1	ntf2	p2	-0.1341	0.0393	-0.0168	-0.0139	-0.0040	-0.1294
1	ntf2	p3	-0.1332	0.0307	-0.0152	-0.0169	-0.0029	-0.1372
1	pf6	p1	-0.1376	0.0227	-0.0120	-0.0154	-0.0038	-0.1461
1	tos	p1	-0.2063	0.0362	-0.0181	-0.0190	-0.0092	-0.2163
2	bf4	p1	-0.1431	0.0250	-0.0153	-0.0163	-0.0029	-0.1526
2	bf4	p2	-0.1428	0.0238	-0.0148	-0.0148	-0.0025	-0.1511
2	dca	p1	-0.1429	0.0390	-0.0130	-0.0234	-0.0084	-0.1486
2	dca	p2	-0.1413	0.0377	-0.0133	-0.0229	-0.0064	-0.1462
2	dca	p3	-0.1469	0.0428	-0.0132	-0.0236	-0.0069	-0.1478
2	dca	p4	-0.1446	0.0396	-0.0128	-0.0223	-0.0064	-0.1465
2	dca	p5	-0.1461	0.0408	-0.0115	-0.0233	-0.0057	-0.1458
2	dca	p6	-0.1444	0.0391	-0.0110	-0.0235	-0.0055	-0.1453
2	mes	p1	-0.1617	0.0379	-0.0212	-0.0213	-0.0077	-0.1740
2	mes	p2	-0.1610	0.0363	-0.0196	-0.0199	-0.0077	-0.1718
2	ntf2	p1	-0.1337	0.0392	-0.0135	-0.0293	-0.0072	-0.1445
2	ntf2	p2	-0.1314	0.0376	-0.0175	-0.0168	-0.0041	-0.1321
2	ntf2	p3	-0.1324	0.0325	-0.0162	-0.0178	-0.0031	-0.1371
2	ntf2	p4	-0.1333	0.0347	-0.0129	-0.0251	-0.0043	-0.1409
2	pf6	p1	-0.1370	0.0246	-0.0130	-0.0171	-0.0045	-0.1470
2	pf6	p2	-0.1361	0.0225	-0.0122	-0.0153	-0.0035	-0.1447
2	tos	p1	-0.0508	0.0313	-0.0064	-0.0119	-0.0072	-0.0449
2	tos	p2	-0.0165	0.0300	-0.0060	-0.0099	-0.0062	-0.0085
3	bf4	p1	-0.1429	0.0241	-0.0160	-0.0168	-0.0001	-0.1517
3	bf4	p2	-0.1451	0.0233	-0.0152	-0.0162	-0.0001	-0.1533
3	dca	p1	-0.1409	0.0384	-0.0136	-0.0237	-0.0016	-0.1413
3	dca	p2	-0.1412	0.0384	-0.0126	-0.0247	-0.0011	-0.1412
3	dca	p3	-0.1382	0.0375	-0.0149	-0.0187	-0.0019	-0.1363
3	dca	p4	-0.1467	0.0418	-0.0135	-0.0255	-0.0015	-0.1454
3	dca	p5	-0.1420	0.0381	-0.0112	-0.0238	-0.0011	-0.1400
3	dca	p6	-0.1420	0.0379	-0.0111	-0.0236	-0.0011	-0.1398
3	mes	p1	-0.1619	0.0384	-0.0230	-0.0224	-0.0012	-0.1700
3	mes	p2	-0.1589	0.0349	-0.0201	-0.0201	-0.0012	-0.1654
3	ntf2	p1	-0.1335	0.0407	-0.0139	-0.0307	-0.0073	-0.1448
3	ntf2	p2	-0.1311	0.0385	-0.0178	-0.0183	-0.0041	-0.1328
3	ntf2	p3	-0.1322	0.0334	-0.0167	-0.0186	-0.0032	-0.1374
3	ntf2	p4	-0.1296	0.0331	-0.0124	-0.0253	-0.0041	-0.1383
3	pf6	p1	-0.1320	0.0226	-0.0127	-0.0166	0.0000	-0.1388
3	pf6	p2	-0.1349	0.0218	-0.0122	-0.0153	0.0000	-0.1406
3	tos	p1	-0.2033	0.0373	-0.0193	-0.0308	-0.0011	-0.2173
3	tos	p2	-0.2091	0.0364	-0.0185	-0.0297	-0.0011	-0.2222
4	bf4	p1	-0.1432	0.0256	-0.0165	-0.0172	-0.0032	-0.1545
4	bf4	p2	-0.1423	0.0247	-0.0157	-0.0163	-0.0033	-0.1529
4	dca	p1	-0.1395	0.0396	-0.0136	-0.0242	-0.0091	-0.1467
4	dca	p2	-0.1474	0.0433	-0.0140	-0.0262	-0.0093	-0.1535
4	dca	p3	-0.1417	0.0387	-0.0113	-0.0239	-0.0058	-0.1440
4	mes	p1	-0.1623	0.0403	-0.0236	-0.0230	-0.0090	-0.1776
4	mes	p2	-0.1589	0.0364	-0.0204	-0.0201	-0.0079	-0.1709
4	pf6	p1	-0.1368	0.0257	-0.0142	-0.0184	-0.0050	-0.1486
4	pf6	p2	-0.1340	0.0224	-0.0126	-0.0153	-0.0036	-0.1431
4	tos	p1	-0.2135	0.0394	-0.0206	-0.0239	-0.0105	-0.2291
4	tos	p2	-0.2069	0.0376	-0.0205	-0.0205	-0.0110	-0.2212

S6. EFP Interaction Energies of CnMIM cation and TILA anion using Valance Virtual Orbital (VVO) Approximation with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1442	0.0238	-0.0140	-0.0154	0.0000	-0.1499
1	dca	p1	-0.1477	0.0401	-0.0110	-0.0235	-0.0018	-0.1438
1	dca	p2	-0.1383	0.0376	-0.0156	-0.0146	-0.0030	-0.1339
1	mes	p1	-0.1633	0.0363	-0.0187	-0.0200	-0.0015	-0.1672
1	ntf2	p1	-0.1371	0.0375	-0.0126	-0.0256	-0.0008	-0.1385
1	ntf2	p2	-0.1341	0.0393	-0.0168	-0.0139	-0.0026	-0.1281
1	ntf2	p3	-0.1332	0.0307	-0.0152	-0.0169	-0.0009	-0.1356
1	pf6	p1	-0.1376	0.0227	-0.0120	-0.0154	-0.0007	-0.1430
1	tos	p1	-0.2063	0.0362	-0.0181	-0.0190	-0.0016	-0.2088
2	bf4	p1	-0.1431	0.0250	-0.0153	-0.0163	0.0000	-0.1497
2	bf4	p2	-0.1428	0.0238	-0.0148	-0.0148	0.0000	-0.1486
2	dca	p1	-0.1429	0.0390	-0.0130	-0.0234	-0.0023	-0.1426
2	dca	p2	-0.1413	0.0377	-0.0133	-0.0229	-0.0021	-0.1418
2	dca	p3	-0.1469	0.0428	-0.0132	-0.0236	-0.0020	-0.1429
2	dca	p4	-0.1446	0.0396	-0.0128	-0.0223	-0.0020	-0.1421
2	dca	p5	-0.1461	0.0408	-0.0115	-0.0233	-0.0018	-0.1419
2	dca	p6	-0.1444	0.0391	-0.0110	-0.0235	-0.0017	-0.1415
2	mes	p1	-0.1617	0.0379	-0.0212	-0.0213	-0.0015	-0.1679
2	mes	p2	-0.1610	0.0363	-0.0196	-0.0199	-0.0014	-0.1656
2	ntf2	p1	-0.1337	0.0392	-0.0135	-0.0293	-0.0014	-0.1387
2	ntf2	p2	-0.1314	0.0376	-0.0175	-0.0168	-0.0024	-0.1305
2	ntf2	p3	-0.1324	0.0325	-0.0162	-0.0178	-0.0011	-0.1350
2	ntf2	p4	-0.1333	0.0347	-0.0129	-0.0251	-0.0010	-0.1376
2	pf6	p1	-0.1370	0.0246	-0.0130	-0.0171	0.0000	-0.1425
2	pf6	p2	-0.1361	0.0225	-0.0122	-0.0153	0.0000	-0.1411
2	tos	p1	-0.0508	0.0313	-0.0064	-0.0119	-0.0014	-0.0391
2	tos	p2	-0.0165	0.0300	-0.0060	-0.0099	-0.0012	-0.0036
3	bf4	p1	-0.1429	0.0241	-0.0160	-0.0168	-0.0001	-0.1517
3	bf4	p2	-0.1451	0.0233	-0.0152	-0.0162	-0.0001	-0.1533
3	dca	p1	-0.1409	0.0384	-0.0136	-0.0237	-0.0016	-0.1413
3	dca	p2	-0.1412	0.0384	-0.0126	-0.0247	-0.0011	-0.1412
3	dca	p3	-0.1382	0.0375	-0.0149	-0.0187	-0.0019	-0.1363
3	dca	p4	-0.1467	0.0418	-0.0135	-0.0255	-0.0015	-0.1454
3	dca	p5	-0.1420	0.0381	-0.0112	-0.0238	-0.0011	-0.1400
3	dca	p6	-0.1420	0.0379	-0.0111	-0.0236	-0.0011	-0.1398
3	mes	p1	-0.1619	0.0384	-0.0230	-0.0224	-0.0012	-0.1700
3	mes	p2	-0.1589	0.0349	-0.0201	-0.0201	-0.0012	-0.1654
3	ntf2	p1	-0.1335	0.0407	-0.0139	-0.0307	-0.0009	-0.1384
3	ntf2	p2	-0.1311	0.0385	-0.0178	-0.0183	-0.0022	-0.1309
3	ntf2	p3	-0.1322	0.0334	-0.0167	-0.0186	-0.0010	-0.1352
3	ntf2	p4	-0.1296	0.0331	-0.0124	-0.0253	-0.0008	-0.1351
3	pf6	p1	-0.1320	0.0226	-0.0127	-0.0166	0.0000	-0.1388
3	pf6	p2	-0.1349	0.0218	-0.0122	-0.0153	0.0000	-0.1406
3	tos	p1	-0.2033	0.0373	-0.0193	-0.0308	-0.0011	-0.2173
3	tos	p2	-0.2091	0.0364	-0.0185	-0.0297	-0.0011	-0.2222
4	bf4	p1	-0.1432	0.0256	-0.0165	-0.0172	0.0000	-0.1512
4	bf4	p2	-0.1423	0.0247	-0.0157	-0.0163	0.0000	-0.1497
4	dca	p1	-0.1395	0.0396	-0.0136	-0.0242	-0.0024	-0.1400
4	dca	p2	-0.1474	0.0433	-0.0140	-0.0262	-0.0023	-0.1465
4	dca	p3	-0.1417	0.0387	-0.0113	-0.0239	-0.0017	-0.1399
4	mes	p1	-0.1623	0.0403	-0.0236	-0.0230	-0.0016	-0.1702
4	mes	p2	-0.1589	0.0364	-0.0204	-0.0201	-0.0014	-0.1644
4	pf6	p1	-0.1368	0.0257	-0.0142	-0.0184	0.0000	-0.1436
4	pf6	p2	-0.1340	0.0224	-0.0126	-0.0153	0.0000	-0.1395
4	tos	p1	-0.2135	0.0394	-0.0206	-0.0239	-0.0019	-0.2205
4	tos	p2	-0.2069	0.0376	-0.0205	-0.0205	-0.0017	-0.2119

S7. EFP Interaction Energies of CnMIM cation and halide anion using canonical molecular orbitals with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1699	0.0807	-0.0286	-0.0195	-0.0286	-0.1658
1	br	p2	-0.1581	0.0604	-0.0311	-0.0111	-0.0063	-0.1463
1	cl	p1	-0.1773	0.0763	-0.0257	-0.0169	-0.0258	-0.1694
1	cl	p2	-0.1671	0.0654	-0.0321	-0.0097	-0.0083	-0.1517
2	br	p1	-0.1638	0.0798	-0.0267	-0.0199	-0.0231	-0.1537
2	br	p2	-0.1580	0.0613	-0.0332	-0.0114	-0.0045	-0.1458
2	br	p3	-0.1569	0.0611	-0.0329	-0.0123	-0.0073	-0.1483
2	br	p4	-0.1672	0.0787	-0.0283	-0.0201	-0.0300	-0.1669
2	cl	p1	-0.1710	0.0756	-0.0258	-0.0170	-0.0217	-0.1599
2	cl	p2	-0.1663	0.0640	-0.0326	-0.0100	-0.0078	-0.1526
2	cl	p3	-0.1655	0.0642	-0.0303	-0.0117	-0.0084	-0.1516
2	cl	p4	-0.1739	0.0739	-0.0279	-0.0165	-0.0268	-0.1712
3	br	p1	-0.1630	0.0806	-0.0292	-0.0204	-0.0247	-0.1567
3	br	p2	-0.1568	0.0582	-0.0419	-0.0096	-0.0018	-0.1519
3	br	p3	-0.1570	0.0659	-0.0291	-0.0143	-0.0078	-0.1422
3	br	p4	-0.1683	0.0792	-0.0348	-0.0198	-0.0403	-0.1840
3	cl	p1	-0.1687	0.0757	-0.0269	-0.0173	-0.0215	-0.1587
3	cl	p2	-0.1648	0.0673	-0.0316	-0.0101	-0.0074	-0.1467
3	cl	p3	-0.1649	0.0638	-0.0327	-0.0125	-0.0091	-0.1553
3	cl	p4	-0.1725	0.0767	-0.0285	-0.0178	-0.0356	-0.1776
4	br	p1	-0.1631	0.0780	-0.0331	-0.0199	-0.0272	-0.1654
4	br	p2	-0.1557	0.0664	-0.0301	-0.0119	-0.0057	-0.1370
4	br	p3	-0.1559	0.0644	-0.0335	-0.0152	-0.0135	-0.1537
4	br	p4	-0.1652	0.0810	-0.0294	-0.0212	-0.0509	-0.1858
4	cl	p1	-0.1682	0.0724	-0.0296	-0.0171	-0.0224	-0.1649
4	cl	p2	-0.1639	0.0623	-0.0385	-0.0084	-0.0072	-0.1558
4	cl	p3	-0.1637	0.0650	-0.0326	-0.0130	-0.0121	-0.1564
4	cl	p4	-0.1709	0.0796	-0.0269	-0.0179	-0.0437	-0.1797

S8. EFP Interaction Energies of CnMIM cation and halide anion using VVO Approximation with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1699	0.0807	-0.0286	-0.0195	-0.0040	-0.1412
1	br	p2	-0.1580	0.0604	-0.0311	-0.0111	-0.0035	-0.1434
1	cl	p1	-0.1773	0.0763	-0.0257	-0.0169	-0.0037	-0.1473
1	cl	p2	-0.1671	0.0654	-0.0321	-0.0097	-0.0039	-0.1472
2	br	p1	-0.1638	0.0798	-0.0267	-0.0199	-0.0034	-0.1341
2	br	p2	-0.1580	0.0613	-0.0332	-0.0114	-0.0036	-0.1449
2	br	p3	-0.1569	0.0611	-0.0329	-0.0123	-0.0031	-0.1441
2	br	p4	-0.1672	0.0787	-0.0283	-0.0201	-0.0041	-0.1410
2	cl	p1	-0.1710	0.0756	-0.0258	-0.0170	-0.0032	-0.1414
2	cl	p2	-0.1663	0.0640	-0.0326	-0.0100	-0.0039	-0.1488
2	cl	p3	-0.1655	0.0642	-0.0303	-0.0117	-0.0034	-0.1466
2	cl	p4	-0.1739	0.0739	-0.0279	-0.0165	-0.0038	-0.1482
3	br	p1	-0.1630	0.0806	-0.0292	-0.0204	-0.0030	-0.1351
3	br	p2	-0.1568	0.0582	-0.0419	-0.0096	-0.0035	-0.1537
3	br	p3	-0.1570	0.0659	-0.0291	-0.0143	-0.0027	-0.1371
3	br	p4	-0.1683	0.0792	-0.0348	-0.0198	-0.0040	-0.1477
3	cl	p1	-0.1687	0.0757	-0.0269	-0.0173	-0.0028	-0.1400
3	cl	p2	-0.1648	0.0673	-0.0316	-0.0101	-0.0039	-0.1432
3	cl	p3	-0.1649	0.0638	-0.0327	-0.0125	-0.0030	-0.1492
3	cl	p4	-0.1725	0.0767	-0.0285	-0.0178	-0.0037	-0.1457
4	br	p1	-0.1631	0.0780	-0.0331	-0.0199	-0.0029	-0.1411
4	br	p2	-0.1557	0.0664	-0.0301	-0.0119	-0.0032	-0.1345
4	br	p3	-0.1559	0.0644	-0.0335	-0.0152	-0.0026	-0.1428
4	br	p4	-0.1652	0.0810	-0.0294	-0.0212	-0.0045	-0.1393
4	cl	p1	-0.1682	0.0724	-0.0296	-0.0171	-0.0027	-0.1452
4	cl	p2	-0.1639	0.0623	-0.0385	-0.0084	-0.0035	-0.1520
4	cl	p3	-0.1637	0.0650	-0.0326	-0.0130	-0.0029	-0.1472
4	cl	p4	-0.1709	0.0796	-0.0269	-0.0179	-0.0041	-0.1402

S9. EFP Interaction Energies of CnMIM cation and TILA anion using canonical molecular orbitals with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1474	0.0214	-0.0118	-0.0119	-0.0042	-0.1539
1	dca	p1	-0.1463	0.0381	-0.0097	-0.0204	-0.0031	-0.1413
1	dca	p2	-0.1384	0.0341	-0.0135	-0.0127	-0.0032	-0.1336
1	mes	p1	-0.1642	0.0323	-0.0173	-0.0164	-0.0057	-0.1713
1	ntf2	p1	-0.1405	0.0299	-0.0116	-0.0232	-0.0038	-0.1492
1	ntf2	p2	-0.1425	0.0371	-0.0150	-0.0121	-0.0033	-0.1359
1	ntf2	p3	-0.1347	0.0251	-0.0149	-0.0136	-0.0019	-0.1401
1	pf6	p1	-0.1389	0.0204	-0.0105	-0.0113	-0.0027	-0.1429
1	tos	p1	-0.2668	0.0321	-0.0142	-0.0160	-0.0078	-0.2728
2	bf4	p1	-0.1443	0.0224	-0.0132	-0.0128	-0.0050	-0.1527
2	bf4	p2	-0.1449	0.0208	-0.0124	-0.0115	-0.0044	-0.1523
2	dca	p1	-0.1427	0.0365	-0.0114	-0.0204	-0.0043	-0.1423
2	dca	p2	-0.1397	0.0352	-0.0116	-0.0199	-0.0040	-0.1401
2	dca	p3	-0.1443	0.0394	-0.0114	-0.0204	-0.0034	-0.1400
2	dca	p4	-0.1448	0.0364	-0.0108	-0.0193	-0.0035	-0.1420
2	dca	p5	-0.1453	0.0385	-0.0100	-0.0203	-0.0030	-0.1401
2	dca	p6	-0.1425	0.0370	-0.0098	-0.0204	-0.0040	-0.1396
2	mes	p1	-0.1616	0.0343	-0.0199	-0.0175	-0.0063	-0.1711
2	mes	p2	-0.1629	0.0322	-0.0179	-0.0164	-0.0057	-0.1707
2	ntf2	p1	-0.1387	0.0321	-0.0124	-0.0256	0.0000	-0.1448
2	ntf2	p2	-0.1298	0.0331	-0.0167	-0.0144	-0.0030	-0.1309
2	ntf2	p3	-0.1369	0.0264	-0.0161	-0.0143	0.0003	-0.1405
2	ntf2	p4	-0.1319	0.0267	-0.0118	-0.0217	0.0007	-0.1381
2	pf6	p1	-0.1361	0.0222	-0.0116	-0.0125	-0.0035	-0.1414
2	pf6	p2	-0.1341	0.0199	-0.0108	-0.0111	-0.0028	-0.1390
2	tos	p1	-0.2527	0.0336	-0.0147	-0.0178	-0.0119	-0.2635
2	tos	p2	-0.2585	0.0313	-0.0135	-0.0157	-0.0092	-0.2655
3	bf4	p1	-0.1439	0.0229	-0.0140	-0.0132	-0.0051	-0.1533
3	bf4	p2	-0.1434	0.0218	-0.0134	-0.0126	-0.0046	-0.1522
3	dca	p1	-0.1415	0.0369	-0.0119	-0.0207	-0.0044	-0.1416
3	dca	p2	-0.1421	0.0364	-0.0110	-0.0216	-0.0031	-0.1413
3	dca	p3	-0.1374	0.0352	-0.0135	-0.0163	-0.0035	-0.1355
3	dca	p4	-0.1469	0.0388	-0.0125	-0.0219	-0.0048	-0.1473
3	dca	p5	-0.1430	0.0366	-0.0095	-0.0208	-0.0040	-0.1408
3	dca	p6	-0.1433	0.0368	-0.0099	-0.0205	-0.0047	-0.1417
3	mes	p1	-0.1621	0.0361	-0.0216	-0.0184	-0.0065	-0.1726
3	mes	p2	-0.1607	0.0323	-0.0184	-0.0165	-0.0071	-0.1704
3	ntf2	p1	-0.1406	0.0333	-0.0130	-0.0269	-0.0051	-0.1522
3	ntf2	p2	-0.1306	0.0333	-0.0172	-0.0157	-0.0047	-0.1349
3	ntf2	p3	-0.1327	0.0273	-0.0166	-0.0151	-0.0022	-0.1393
3	ntf2	p4	-0.1324	0.0250	-0.0115	-0.0219	-0.0040	-0.1448
3	pf6	p1	-0.1315	0.0200	-0.0112	-0.0120	-0.0024	-0.1372
3	pf6	p2	-0.1331	0.0198	-0.0110	-0.0112	-0.0031	-0.1385
3	tos	p1	-0.2434	0.0349	-0.0160	-0.0193	-0.0121	-0.2559
3	tos	p2	-0.2341	0.0327	-0.0140	-0.0178	-0.0135	-0.2467
4	bf4	p1	-0.1436	0.0229	-0.0146	-0.0134	-0.0053	-0.1540
4	bf4	p2	-0.1416	0.0217	-0.0137	-0.0127	-0.0047	-0.1510
4	dca	p1	-0.1409	0.0369	-0.0123	-0.0211	-0.0044	-0.1417
4	dca	p2	-0.1478	0.0394	-0.0124	-0.0228	-0.0046	-0.1481
4	dca	p3	-0.1431	0.0364	-0.0096	-0.0209	-0.0043	-0.1415
4	mes	p1	-0.1684	0.0363	-0.0224	-0.0190	-0.0070	-0.1805
4	mes	p2	-0.1605	0.0323	-0.0186	-0.0165	-0.0070	-0.1704
4	pf6	p1	-0.1366	0.0232	-0.0129	-0.0135	-0.0038	-0.1434
4	pf6	p2	-0.1316	0.0197	-0.0112	-0.0112	-0.0031	-0.1375
4	tos	p1	-0.2389	0.0356	-0.0163	-0.0202	-0.0153	-0.2552
4	tos	p2	-0.2038	0.0337	-0.0165	-0.0171	-0.0106	-0.2142

S10. EFP Interaction Energies of CnMIM cation and TILA anion using Valance Virtual Orbital (VVO) Approximation with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1474	0.0214	-0.0118	-0.0119	-0.0003	-0.1500
1	dca	p1	-0.1463	0.0381	-0.0097	-0.0204	-0.0009	-0.1391
1	dca	p2	-0.1384	0.0341	-0.0135	-0.0127	-0.0020	-0.1324
1	mes	p1	-0.1642	0.0323	-0.0173	-0.0164	-0.0011	-0.1667
1	ntf2	p1	-0.1405	0.0299	-0.0116	-0.0232	-0.0008	-0.1462
1	ntf2	p2	-0.1425	0.0371	-0.0150	-0.0121	-0.0025	-0.1351
1	ntf2	p3	-0.1347	0.0251	-0.0149	-0.0136	-0.0009	-0.1391
1	pf6	p1	-0.1389	0.0204	-0.0105	-0.0113	0.0000	-0.1402
1	tos	p1	-0.2668	0.0321	-0.0142	-0.0160	-0.0012	-0.2662
2	bf4	p1	-0.1443	0.0224	-0.0132	-0.0128	-0.0004	-0.1481
2	bf4	p2	-0.1449	0.0208	-0.0124	-0.0115	-0.0004	-0.1483
2	dca	p1	-0.1427	0.0365	-0.0114	-0.0204	-0.0013	-0.1392
2	dca	p2	-0.1397	0.0352	-0.0116	-0.0199	-0.0012	-0.1373
2	dca	p3	-0.1443	0.0394	-0.0114	-0.0204	-0.0010	-0.1377
2	dca	p4	-0.1448	0.0364	-0.0108	-0.0193	-0.0011	-0.1396
2	dca	p5	-0.1453	0.0385	-0.0100	-0.0203	-0.0009	-0.1380
2	dca	p6	-0.1425	0.0370	-0.0098	-0.0204	-0.0010	-0.1366
2	mes	p1	-0.1616	0.0343	-0.0199	-0.0175	-0.0012	-0.1659
2	mes	p2	-0.1629	0.0322	-0.0179	-0.0164	-0.0012	-0.1662
2	ntf2	p1	-0.1387	0.0321	-0.0124	-0.0256	-0.0008	-0.1455
2	ntf2	p2	-0.1298	0.0331	-0.0167	-0.0144	-0.0024	-0.1303
2	ntf2	p3	-0.1369	0.0264	-0.0161	-0.0143	-0.0010	-0.1419
2	ntf2	p4	-0.1319	0.0267	-0.0118	-0.0217	-0.0008	-0.1395
2	pf6	p1	-0.1361	0.0222	-0.0116	-0.0125	0.0000	-0.1379
2	pf6	p2	-0.1341	0.0199	-0.0108	-0.0111	0.0000	-0.1362
2	tos	p1	-0.2527	0.0336	-0.0147	-0.0178	-0.0017	-0.2533
2	tos	p2	-0.2585	0.0313	-0.0135	-0.0157	-0.0017	-0.2580
3	bf4	p1	-0.1439	0.0229	-0.0140	-0.0132	-0.0003	-0.1485
3	bf4	p2	-0.1434	0.0218	-0.0134	-0.0126	-0.0004	-0.1480
3	dca	p1	-0.1415	0.0369	-0.0119	-0.0207	-0.0012	-0.1385
3	dca	p2	-0.1421	0.0364	-0.0110	-0.0216	-0.0008	-0.1390
3	dca	p3	-0.1374	0.0352	-0.0135	-0.0163	-0.0015	-0.1336
3	dca	p4	-0.1469	0.0388	-0.0125	-0.0219	-0.0011	-0.1436
3	dca	p5	-0.1430	0.0366	-0.0095	-0.0208	-0.0009	-0.1376
3	dca	p6	-0.1433	0.0368	-0.0099	-0.0205	-0.0010	-0.1379
3	mes	p1	-0.1621	0.0361	-0.0216	-0.0184	-0.0012	-0.1673
3	mes	p2	-0.1607	0.0323	-0.0184	-0.0165	-0.0012	-0.1645
3	ntf2	p1	-0.1406	0.0333	-0.0130	-0.0269	-0.0008	-0.1479
3	ntf2	p2	-0.1306	0.0333	-0.0172	-0.0157	-0.0022	-0.1325
3	ntf2	p3	-0.1327	0.0273	-0.0166	-0.0151	-0.0010	-0.1382
3	ntf2	p4	-0.1324	0.0250	-0.0115	-0.0219	-0.0008	-0.1416
3	pf6	p1	-0.1315	0.0200	-0.0112	-0.0120	0.0000	-0.1348
3	pf6	p2	-0.1331	0.0198	-0.0110	-0.0112	0.0000	-0.1355
3	tos	p1	-0.2434	0.0349	-0.0160	-0.0193	-0.0016	-0.2454
3	tos	p2	-0.2341	0.0327	-0.0140	-0.0178	-0.0015	-0.2347
4	bf4	p1	-0.1436	0.0229	-0.0146	-0.0134	-0.0003	-0.1490
4	bf4	p2	-0.1416	0.0217	-0.0137	-0.0127	-0.0003	-0.1466
4	dca	p1	-0.1409	0.0369	-0.0123	-0.0211	-0.0012	-0.1386
4	dca	p2	-0.1478	0.0394	-0.0124	-0.0228	-0.0011	-0.1446
4	dca	p3	-0.1431	0.0364	-0.0096	-0.0209	-0.0008	-0.1381
4	mes	p1	-0.1684	0.0363	-0.0224	-0.0190	-0.0012	-0.1747
4	mes	p2	-0.1605	0.0323	-0.0186	-0.0165	-0.0012	-0.1645
4	pf6	p1	-0.1366	0.0232	-0.0129	-0.0135	0.0000	-0.1397
4	pf6	p2	-0.1316	0.0197	-0.0112	-0.0112	0.0000	-0.1343
4	tos	p1	-0.2389	0.0356	-0.0163	-0.0202	-0.0019	-0.2418
4	tos	p2	-0.2038	0.0337	-0.0165	-0.0171	-0.0015	-0.2051

S11. EFP Interaction Energies of CnMIM cation and halide anion using canonical molecular orbitals with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1702	0.0832	-0.0251	-0.0192	-0.0093	-0.1407
1	br	p2	-0.1578	0.0582	-0.0336	-0.0099	-0.0022	-0.1453
1	cl	p1	-0.1783	0.0777	-0.0216	-0.0079	-0.0126	-0.1427
1	cl	p2	-0.1667	0.0634	-0.0275	-0.0033	-0.0094	-0.1436
2	br	p1	-0.1631	0.0806	-0.0260	-0.0193	-0.0096	-0.1373
2	br	p2	-0.1577	0.0611	-0.0336	-0.0108	-0.0007	-0.1418
2	br	p3	-0.1560	0.0607	-0.0329	-0.0117	-0.0046	-0.1445
2	br	p4	-0.1667	0.0796	-0.0277	-0.0195	-0.0132	-0.1475
2	cl	p1	-0.1710	0.0734	-0.0227	-0.0079	-0.0131	-0.1413
2	cl	p2	-0.1661	0.0669	-0.0242	-0.0056	-0.0089	-0.1378
2	cl	p3	-0.1658	0.0658	-0.0222	-0.0063	-0.0097	-0.1381
2	cl	p4	-0.1733	0.0749	-0.0235	-0.0077	-0.0157	-0.1453
3	br	p1	-0.1646	0.0813	-0.0281	-0.0198	-0.0106	-0.1418
3	br	p2	-0.1537	0.0580	-0.0425	-0.0090	0.0020	-0.1453
3	br	p3	-0.1549	0.0656	-0.0293	-0.0137	-0.0037	-0.1360
3	br	p4	-0.1685	0.0802	-0.0305	-0.0194	-0.0145	-0.1527
3	cl	p1	-0.1701	0.0742	-0.0234	-0.0082	-0.0130	-0.1405
3	cl	p2	-0.1612	0.0641	-0.0282	-0.0043	-0.0079	-0.1374
3	cl	p3	-0.1640	0.0638	-0.0244	-0.0063	-0.0096	-0.1405
3	cl	p4	-0.1723	0.0763	-0.0237	-0.0083	-0.0175	-0.1454
4	br	p1	-0.1631	0.0785	-0.0328	-0.0194	-0.0127	-0.1496
4	br	p2	-0.1648	0.0662	-0.0299	-0.0114	-0.0108	-0.1507
4	br	p3	-0.1530	0.0641	-0.0335	-0.0146	-0.0051	-0.1421
4	br	p4	-0.1609	0.0819	-0.0269	-0.0206	-0.0253	-0.1518
4	cl	p1	-0.1693	0.0747	-0.0245	-0.0080	-0.0133	-0.1404
4	cl	p2	-0.1734	0.0701	-0.0233	-0.0053	-0.0075	-0.1394
4	cl	p3	-0.1625	0.0638	-0.0282	-0.0057	-0.0096	-0.1422
4	cl	p4	-0.1748	0.0768	-0.0232	-0.0083	-0.0266	-0.1560

S12. EFP Interaction Energies of CnMIM cation and halide anion using VVO Approximation with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1702	0.0832	-0.0251	-0.0192	-0.0019	-0.1333
1	br	p2	-0.1578	0.0582	-0.0336	-0.0099	-0.0031	-0.1462
1	cl	p1	-0.1783	0.0777	-0.0216	-0.0079	-0.0017	-0.1318
1	cl	p2	-0.1667	0.0634	-0.0275	-0.0033	-0.0035	-0.1377
2	br	p1	-0.1631	0.0806	-0.0260	-0.0193	-0.0018	-0.1296
2	br	p2	-0.1577	0.0611	-0.0336	-0.0108	-0.0033	-0.1444
2	br	p3	-0.1560	0.0607	-0.0329	-0.0117	-0.0030	-0.1429
2	br	p4	-0.1667	0.0796	-0.0277	-0.0195	-0.0025	-0.1368
2	cl	p1	-0.1710	0.0734	-0.0227	-0.0079	-0.0017	-0.1299
2	cl	p2	-0.1661	0.0669	-0.0242	-0.0056	-0.0037	-0.1326
2	cl	p3	-0.1658	0.0658	-0.0222	-0.0063	-0.0030	-0.1314
2	cl	p4	-0.1733	0.0749	-0.0235	-0.0077	-0.0023	-0.1319
3	br	p1	-0.1646	0.0813	-0.0281	-0.0198	-0.0015	-0.1327
3	br	p2	-0.1537	0.0580	-0.0425	-0.0090	-0.0029	-0.1502
3	br	p3	-0.1549	0.0656	-0.0293	-0.0137	-0.0023	-0.1347
3	br	p4	-0.1685	0.0802	-0.0305	-0.0194	-0.0020	-0.1402
3	cl	p1	-0.1701	0.0742	-0.0234	-0.0082	-0.0014	-0.1289
3	cl	p2	-0.1612	0.0641	-0.0282	-0.0043	-0.0032	-0.1328
3	cl	p3	-0.1640	0.0638	-0.0244	-0.0063	-0.0026	-0.1335
3	cl	p4	-0.1723	0.0763	-0.0237	-0.0083	-0.0019	-0.1297
4	br	p1	-0.1631	0.0785	-0.0328	-0.0194	-0.0016	-0.1384
4	br	p2	-0.1648	0.0662	-0.0299	-0.0114	-0.0024	-0.1422
4	br	p3	-0.1530	0.0641	-0.0335	-0.0146	-0.0022	-0.1392
4	br	p4	-0.1609	0.0819	-0.0269	-0.0206	-0.0028	-0.1293
4	cl	p1	-0.1693	0.0747	-0.0245	-0.0080	-0.0014	-0.1285
4	cl	p2	-0.1734	0.0701	-0.0233	-0.0053	-0.0026	-0.1345
4	cl	p3	-0.1625	0.0638	-0.0282	-0.0057	-0.0024	-0.1350
4	cl	p4	-0.1748	0.0768	-0.0232	-0.0083	-0.0027	-0.1321

S13. EFP Interaction Energies of N-alkyl-N-methylpyrodinium (CnPyr) cation and TILA anion using canonical molecular orbitals with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1407	0.0218	-0.0149	-0.0118	-0.0021	-0.1478
1	bf4	p2	-0.1392	0.0216	-0.0146	-0.0104	-0.0017	-0.1442
1	dca	p1	-0.1341	0.0282	-0.0134	-0.0142	-0.0033	-0.1368
1	dca	p2	-0.1346	0.0273	-0.0120	-0.0150	-0.0031	-0.1375
1	dca	p3	-0.1260	0.0266	-0.0146	-0.0130	-0.0036	-0.1306
1	dca	p4	-0.1359	0.0279	-0.0117	-0.0147	-0.0033	-0.1377
1	mes	p1	-0.1550	0.0325	-0.0212	-0.0142	-0.0066	-0.1644
1	mes	p2	-0.1539	0.0363	-0.0220	-0.0099	-0.0064	-0.1559
1	ntf2	p1	-0.1212	0.0210	-0.0130	-0.0153	-0.0028	-0.1313
1	ntf2	p2	-0.1205	0.0198	-0.0142	-0.0119	-0.0020	-0.1288
1	ntf2	p3	-0.1222	0.0238	-0.0135	-0.0142	-0.0028	-0.1288
1	ntf2	p5	-0.1219	0.0199	-0.0141	-0.0121	-0.0017	-0.1299
1	pf6	p1	-0.1309	0.0185	-0.0126	-0.0111	-0.0028	-0.1388
1	pf6	p2	-0.1298	0.0152	-0.0110	-0.0074	-0.0026	-0.1355
1	tos	p1	-0.1630	0.0315	-0.0220	-0.0128	-0.0058	-0.1721
1	tos	p2	-0.1447	0.0298	-0.0208	-0.0113	-0.0048	-0.1518
2	bf4	p1	-0.1380	0.0216	-0.0154	-0.0120	-0.0021	-0.1459
2	bf4	p2	-0.1342	0.0222	-0.0142	-0.0104	-0.0018	-0.1383
2	bf4	p3	-0.1377	0.0224	-0.0151	-0.0105	-0.0018	-0.1428
2	dca	p1	-0.1312	0.0279	-0.0136	-0.0143	-0.0033	-0.1345
2	dca	p2	-0.1314	0.0273	-0.0121	-0.0151	-0.0035	-0.1347
2	dca	p3	-0.1322	0.0273	-0.0124	-0.0152	-0.0033	-0.1357
2	mes	p1	-0.1527	0.0317	-0.0215	-0.0148	-0.0065	-0.1638
2	mes	p2	-0.1470	0.0301	-0.0195	-0.0128	-0.0054	-0.1547
2	mes	p3	-0.1521	0.0345	-0.0218	-0.0115	-0.0065	-0.1573
2	ntf2	p1	-0.1186	0.0193	-0.0126	-0.0158	-0.0025	-0.1301
2	ntf2	p2	-0.1188	0.0205	-0.0143	-0.0126	-0.0019	-0.1271
2	ntf2	p3	-0.1167	0.0200	-0.0120	-0.0149	-0.0024	-0.1261
2	ntf2	p4	-0.1196	0.0224	-0.0133	-0.0143	-0.0027	-0.1276
2	ntf2	p5	-0.1171	0.0192	-0.0130	-0.0131	-0.0017	-0.1257
2	ntf2	p6	-0.1181	0.0195	-0.0139	-0.0121	-0.0016	-0.1261
2	pf6	p1	-0.1285	0.0194	-0.0127	-0.0111	-0.0027	-0.1356
2	pf6	p2	-0.1243	0.0183	-0.0120	-0.0100	-0.0025	-0.1305
2	pf6	p3	-0.1279	0.0185	-0.0127	-0.0100	-0.0027	-0.1349
2	tos	p1	-0.1495	0.0308	-0.0220	-0.0133	-0.0062	-0.1601
2	tos	p2	-0.1496	0.0289	-0.0199	-0.0116	-0.0047	-0.1569
3	bf4	p1	-0.1360	0.0212	-0.0157	-0.0123	-0.0021	-0.1449
3	bf4	p2	-0.1318	0.0215	-0.0147	-0.0104	-0.0018	-0.1372
3	bf4	p3	-0.1367	0.0223	-0.0154	-0.0107	-0.0019	-0.1425
3	dca	p1	-0.1295	0.0283	-0.0134	-0.0150	-0.0037	-0.1332
3	dca	p2	-0.1300	0.0271	-0.0123	-0.0152	-0.0035	-0.1339
3	dca	p3	-0.1192	0.0237	-0.0129	-0.0126	-0.0031	-0.1240
3	dca	p4	-0.1279	0.0255	-0.0128	-0.0146	-0.0009	-0.1306
3	dca	p5	-0.1312	0.0263	-0.0126	-0.0153	-0.0009	-0.1337
3	mes	p1	-0.1507	0.0305	-0.0217	-0.0154	-0.0065	-0.1638
3	mes	p2	-0.1452	0.0299	-0.0200	-0.0127	-0.0055	-0.1535
3	mes	p3	-0.1506	0.0344	-0.0222	-0.0119	-0.0064	-0.1567
3	ntf2	p1	-0.1178	0.0197	-0.0129	-0.0165	-0.0025	-0.1300
3	ntf2	p2	-0.1165	0.0211	-0.0142	-0.0122	-0.0020	-0.1238
3	ntf2	p3	-0.1157	0.0205	-0.0123	-0.0150	-0.0025	-0.1250
3	ntf2	p4	-0.1194	0.0227	-0.0136	-0.0150	-0.0028	-0.1282
3	ntf2	p5	-0.1159	0.0188	-0.0130	-0.0131	-0.0017	-0.1248
3	ntf2	p6	-0.1168	0.0194	-0.0139	-0.0127	-0.0016	-0.1256
3	pf6	p1	-0.1273	0.0183	-0.0132	-0.0118	-0.0028	-0.1368
3	pf6	p2	-0.1224	0.0180	-0.0122	-0.0099	-0.0025	-0.1290
3	pf6	p3	-0.1270	0.0184	-0.0129	-0.0103	-0.0028	-0.1346
3	tos	p1	-0.1478	0.0298	-0.0221	-0.0142	-0.0056	-0.1599
3	tos	p2	-0.1541	0.0285	-0.0204	-0.0115	-0.0046	-0.1620
4	bf4	p1	-0.1349	0.0212	-0.0159	-0.0124	-0.0020	-0.1439
4	bf4	p2	-0.1301	0.0214	-0.0151	-0.0105	-0.0016	-0.1359
4	bf4	p3	-0.1357	0.0226	-0.0156	-0.0109	-0.0019	-0.1415
4	dca	p1	-0.1263	0.0241	-0.0119	-0.0145	-0.0035	-0.1321
4	dca	p2	-0.1293	0.0270	-0.0125	-0.0152	-0.0035	-0.1335
4	dca	p3	-0.1285	0.0274	-0.0134	-0.0154	-0.0035	-0.1335
4	dca	p4	-0.1313	0.0272	-0.0122	-0.0151	-0.0037	-0.1351
4	dca	p5	-0.1293	0.0270	-0.0126	-0.0154	-0.0036	-0.1339
4	mes	p1	-0.1492	0.0304	-0.0217	-0.0155	-0.0062	-0.1622
4	mes	p2	-0.1435	0.0296	-0.0204	-0.0130	-0.0052	-0.1524
4	mes	p3	-0.1493	0.0344	-0.0224	-0.0120	-0.0065	-0.1557
4	ntf2	p1	-0.1171	0.0201	-0.0132	-0.0166	-0.0024	-0.1293
4	ntf2	p2	-0.1182	0.0198	-0.0144	-0.0145	-0.0018	-0.1291
4	ntf2	p3	-0.1161	0.0215	-0.0128	-0.0154	-0.0025	-0.1253
4	ntf2	p4	-0.1176	0.0226	-0.0137	-0.0154	-0.0028	-0.1269
4	ntf2	p5	-0.1155	0.0186	-0.0131	-0.0134	-0.0016	-0.1250
4	ntf2	p6	-0.1162	0.0195	-0.0141	-0.0133	-0.0018	-0.1258
4	pf6	p1	-0.1267	0.0184	-0.0133	-0.0119	-0.0027	-0.1362
4	pf6	p2	-0.1210	0.0179	-0.0124	-0.0101	-0.0024	-0.1280
4	pf6	p3	-0.1267	0.0184	-0.0130	-0.0105	-0.0028	-0.1345
4	tos	p1	-0.1429	0.0298	-0.0216	-0.0144	-0.0058	-0.1549
4	tos	p2	-0.1368	0.0283	-0.0202	-0.0120	-0.0048	-0.1454

S14. EFP Interaction Energies of CnPyr cation and TILA anion using VVO Approximation with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1407	0.0218	-0.0149	-0.0118	-0.0005	-0.1462
1	bf4	p2	-0.1392	0.0216	-0.0146	-0.0104	-0.0005	-0.1430
1	dca	p1	-0.1341	0.0282	-0.0134	-0.0142	-0.0016	-0.1351
1	dca	p2	-0.1346	0.0273	-0.0120	-0.0150	-0.0015	-0.1358
1	dca	p3	-0.1260	0.0266	-0.0146	-0.0130	-0.0017	-0.1287
1	dca	p4	-0.1359	0.0279	-0.0117	-0.0147	-0.0010	-0.1354
1	mes	p1	-0.1550	0.0325	-0.0212	-0.0142	-0.0019	-0.1597
1	mes	p2	-0.1539	0.0363	-0.0220	-0.0099	-0.0022	-0.1518
1	ntf2	p1	-0.1212	0.0210	-0.0130	-0.0153	-0.0011	-0.1296
1	ntf2	p2	-0.1205	0.0198	-0.0142	-0.0119	0.0000	-0.1268
1	ntf2	p3	-0.1222	0.0238	-0.0135	-0.0142	-0.0012	-0.1273
1	ntf2	p5	-0.1219	0.0199	-0.0141	-0.0121	0.0000	-0.1282
1	pf6	p1	-0.1309	0.0185	-0.0126	-0.0111	-0.0009	-0.1370
1	pf6	p2	-0.1298	0.0152	-0.0110	-0.0074	-0.0009	-0.1338
1	tos	p1	-0.1630	0.0315	-0.0220	-0.0128	-0.0018	-0.1681
1	tos	p2	-0.1447	0.0298	-0.0208	-0.0113	-0.0018	-0.1489
2	bf4	p1	-0.1380	0.0216	-0.0154	-0.0120	-0.0005	-0.1442
2	bf4	p2	-0.1342	0.0222	-0.0142	-0.0104	-0.0005	-0.1371
2	bf4	p3	-0.1377	0.0224	-0.0151	-0.0105	-0.0005	-0.1415
2	dca	p1	-0.1312	0.0279	-0.0136	-0.0143	-0.0015	-0.1327
2	dca	p2	-0.1314	0.0273	-0.0121	-0.0151	-0.0017	-0.1329
2	dca	p3	-0.1322	0.0273	-0.0124	-0.0152	-0.0015	-0.1339
2	mes	p1	-0.1527	0.0317	-0.0215	-0.0148	-0.0018	-0.1591
2	mes	p2	-0.1470	0.0301	-0.0195	-0.0128	-0.0017	-0.1509
2	mes	p3	-0.1521	0.0345	-0.0218	-0.0115	-0.0021	-0.1530
2	ntf2	p1	-0.1186	0.0193	-0.0126	-0.0158	0.0000	-0.1276
2	ntf2	p2	-0.1188	0.0205	-0.0143	-0.0126	0.0000	-0.1252
2	ntf2	p3	-0.1167	0.0200	-0.0120	-0.0149	-0.0009	-0.1246
2	ntf2	p4	-0.1196	0.0224	-0.0133	-0.0143	-0.0012	-0.1261
2	ntf2	p5	-0.1171	0.0192	-0.0130	-0.0131	0.0000	-0.1240
2	ntf2	p6	-0.1181	0.0195	-0.0139	-0.0121	0.0000	-0.1246
2	pf6	p1	-0.1285	0.0194	-0.0127	-0.0111	0.0000	-0.1329
2	pf6	p2	-0.1243	0.0183	-0.0120	-0.0100	-0.0008	-0.1289
2	pf6	p3	-0.1279	0.0185	-0.0127	-0.0100	-0.0009	-0.1331
2	tos	p1	-0.1495	0.0308	-0.0220	-0.0133	-0.0019	-0.1558
2	tos	p2	-0.1495	0.0289	-0.0199	-0.0116	-0.0017	-0.1539
3	bf4	p1	-0.1360	0.0212	-0.0157	-0.0123	-0.0004	-0.1433
3	bf4	p2	-0.1318	0.0215	-0.0147	-0.0104	-0.0005	-0.1359
3	bf4	p3	-0.1367	0.0223	-0.0154	-0.0107	-0.0005	-0.1411
3	dca	p1	-0.1295	0.0283	-0.0134	-0.0150	-0.0015	-0.1310
3	dca	p2	-0.1300	0.0271	-0.0123	-0.0152	-0.0017	-0.1321
3	dca	p3	-0.1192	0.0237	-0.0129	-0.0126	-0.0014	-0.1224
3	dca	p4	-0.1279	0.0255	-0.0128	-0.0146	-0.0009	-0.1306
3	dca	p5	-0.1312	0.0263	-0.0126	-0.0153	-0.0009	-0.1337
3	mes	p1	-0.1507	0.0305	-0.0217	-0.0154	-0.0017	-0.1590
3	mes	p2	-0.1452	0.0299	-0.0200	-0.0127	-0.0017	-0.1497
3	mes	p3	-0.1506	0.0344	-0.0222	-0.0119	-0.0021	-0.1524
3	ntf2	p1	-0.1178	0.0197	-0.0129	-0.0165	0.0000	-0.1275
3	ntf2	p2	-0.1165	0.0211	-0.0142	-0.0122	0.0000	-0.1218
3	ntf2	p3	-0.1157	0.0205	-0.0123	-0.0150	-0.0009	-0.1235
3	ntf2	p4	-0.1194	0.0227	-0.0136	-0.0150	0.0000	-0.1254
3	ntf2	p5	-0.1159	0.0188	-0.0130	-0.0131	0.0000	-0.1231
3	ntf2	p6	-0.1168	0.0194	-0.0139	-0.0127	0.0000	-0.1240
3	pf6	p1	-0.1273	0.0183	-0.0132	-0.0118	-0.0009	-0.1349
3	pf6	p2	-0.1224	0.0180	-0.0122	-0.0099	-0.0008	-0.1273
3	pf6	p3	-0.1270	0.0184	-0.0129	-0.0103	0.0000	-0.1318
3	tos	p1	-0.1478	0.0298	-0.0221	-0.0142	-0.0018	-0.1561
3	tos	p2	-0.1541	0.0285	-0.0204	-0.0115	-0.0017	-0.1591
4	bf4	p1	-0.1349	0.0212	-0.0159	-0.0124	-0.0004	-0.1423
4	bf4	p2	-0.1301	0.0214	-0.0151	-0.0105	-0.0005	-0.1347
4	bf4	p3	-0.1357	0.0226	-0.0156	-0.0109	-0.0005	-0.1401
4	dca	p1	-0.1263	0.0241	-0.0119	-0.0145	0.0000	-0.1286
4	dca	p2	-0.1293	0.0270	-0.0125	-0.0152	-0.0016	-0.1316
4	dca	p3	-0.1285	0.0274	-0.0134	-0.0154	-0.0013	-0.1313
4	dca	p4	-0.1313	0.0272	-0.0122	-0.0151	0.0000	-0.1314
4	dca	p5	-0.1293	0.0270	-0.0126	-0.0154	-0.0014	-0.1318
4	mes	p1	-0.1492	0.0304	-0.0217	-0.0155	-0.0017	-0.1576
4	mes	p2	-0.1435	0.0296	-0.0204	-0.0130	-0.0016	-0.1488
4	mes	p3	-0.1493	0.0344	-0.0224	-0.0120	-0.0020	-0.1513
4	ntf2	p1	-0.1171	0.0201	-0.0132	-0.0166	0.0000	-0.1269
4	ntf2	p2	-0.1182	0.0198	-0.0144	-0.0145	0.0000	-0.1273
4	ntf2	p3	-0.1161	0.0215	-0.0128	-0.0154	-0.0010	-0.1238
4	ntf2	p4	-0.1176	0.0226	-0.0137	-0.0154	-0.0011	-0.1253
4	ntf2	p5	-0.1155	0.0186	-0.0131	-0.0134	0.0000	-0.1234
4	ntf2	p6	-0.1162	0.0195	-0.0141	-0.0133	0.0000	-0.1240
4	pf6	p1	-0.1267	0.0184	-0.0133	-0.0119	-0.0008	-0.1343
4	pf6	p2	-0.1210	0.0179	-0.0124	-0.0101	-0.0008	-0.1264
4	pf6	p3	-0.1267	0.0184	-0.0130	-0.0105	0.0000	-0.1318
4	tos	p1	-0.1429	0.0298	-0.0216	-0.0144	-0.0017	-0.1508
4	tos	p2	-0.1368	0.0283	-0.0202	-0.0120	-0.0017	-0.1423

S15. EFP Interaction Energies of CnPyr cation and halide anion using canonical molecular orbitals with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1545	0.0569	-0.0329	-0.0131	-0.0088	-0.1523
1	br	p2	-0.1537	0.0569	-0.0284	-0.0123	-0.0071	-0.1446
1	cl	p1	-0.1575	0.0516	-0.0276	-0.0111	-0.0086	-0.1532
1	cl	p2	-0.1573	0.0519	-0.0252	-0.0104	-0.0061	-0.1473
2	br	p1	-0.1520	0.0572	-0.0335	-0.0135	-0.0083	-0.1501
2	br	p2	-0.1477	0.0564	-0.0292	-0.0122	-0.0069	-0.1397
2	br	p3	-0.1517	0.0590	-0.0267	-0.0131	-0.0053	-0.1377
2	cl	p1	-0.1550	0.0514	-0.0272	-0.0112	-0.0088	-0.1509
2	cl	p2	-0.1503	0.0500	-0.0262	-0.0102	-0.0065	-0.1432
2	cl	p3	-0.1546	0.0503	-0.0267	-0.0106	-0.0066	-0.1482
3	br	p1	-0.1630	0.0806	-0.0292	-0.0204	-0.0247	-0.1567
3	br	p2	-0.1452	0.0542	-0.0294	-0.0119	-0.0043	-0.1366
3	br	p3	-0.1508	0.0590	-0.0270	-0.0129	-0.0060	-0.1377
3	cl	p1	-0.1529	0.0508	-0.0284	-0.0115	-0.0093	-0.1512
3	cl	p2	-0.1488	0.0489	-0.0281	-0.0100	-0.0068	-0.1448
3	cl	p3	-0.1530	0.0519	-0.0251	-0.0105	-0.0074	-0.1441
4	br	p1	-0.1495	0.0592	-0.0309	-0.0139	-0.0103	-0.1454
4	br	p2	-0.1423	0.0552	-0.0290	-0.0120	-0.0059	-0.1340
4	br	p3	-0.1496	0.0568	-0.0296	-0.0129	-0.0096	-0.1449
4	cl	p1	-0.1518	0.0505	-0.0293	-0.0114	-0.0091	-0.1511
4	cl	p2	-0.1473	0.0493	-0.0277	-0.0106	-0.0071	-0.1433
4	cl	p3	-0.1513	0.0512	-0.0256	-0.0107	-0.0080	-0.1445

S16. EFP Interaction Energies of CnPyr cation and halide anion using VVO Approximation with 6-311++G(3df2p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1545	0.0569	-0.0329	-0.0131	-0.0022	-0.1457
1	br	p2	-0.1537	0.0569	-0.0284	-0.0123	-0.0019	-0.1394
1	cl	p1	-0.1575	0.0516	-0.0276	-0.0111	-0.0021	-0.1467
1	cl	p2	-0.1573	0.0519	-0.0252	-0.0104	-0.0018	-0.1429
2	br	p1	-0.1520	0.0572	-0.0335	-0.0135	-0.0023	-0.1441
2	br	p2	-0.1477	0.0564	-0.0292	-0.0122	-0.0026	-0.1354
2	br	p3	-0.1517	0.0590	-0.0267	-0.0131	-0.0028	-0.1353
2	cl	p1	-0.1550	0.0514	-0.0272	-0.0112	-0.0021	-0.1441
2	cl	p2	-0.1503	0.0500	-0.0262	-0.0102	-0.0018	-0.1384
2	cl	p3	-0.1546	0.0503	-0.0267	-0.0106	-0.0025	-0.1441
3	br	p1	-0.1630	0.0806	-0.0292	-0.0204	-0.0030	-0.1351
3	br	p2	-0.1452	0.0542	-0.0294	-0.0119	-0.0017	-0.1341
3	br	p3	-0.1508	0.0590	-0.0270	-0.0129	-0.0020	-0.1337
3	cl	p1	-0.1529	0.0508	-0.0284	-0.0115	-0.0020	-0.1440
3	cl	p2	-0.1488	0.0489	-0.0281	-0.0100	-0.0017	-0.1398
3	cl	p3	-0.1530	0.0519	-0.0251	-0.0105	-0.0017	-0.1385
4	br	p1	-0.1495	0.0592	-0.0309	-0.0139	-0.0020	-0.1371
4	br	p2	-0.1423	0.0552	-0.0290	-0.0120	-0.0020	-0.1301
4	br	p3	-0.1496	0.0568	-0.0296	-0.0129	-0.0020	-0.1373
4	cl	p1	-0.1518	0.0505	-0.0293	-0.0114	-0.0018	-0.1438
4	cl	p2	-0.1473	0.0493	-0.0277	-0.0106	-0.0018	-0.1380
4	cl	p3	-0.1513	0.0512	-0.0256	-0.0107	-0.0017	-0.1383

S17. EFP Interaction Energies of N-alkyl-N-methylpyrodinium (CnPyr) cation and TILA anion using canonical molecular orbitals with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1400	0.0189	-0.0129	-0.0094	-0.0051	-0.1485
1	bf4	p2	-0.1388	0.0186	-0.0126	-0.0082	-0.0045	-0.1455
1	dca	p1	-0.1321	0.0255	-0.0125	-0.0123	-0.0032	-0.1346
1	dca	p2	-0.1344	0.0251	-0.0109	-0.0131	-0.0022	-0.1354
1	dca	p3	-0.1275	0.0241	-0.0144	-0.0115	-0.0043	-0.1336
1	dca	p4	-0.1352	0.0256	-0.0104	-0.0129	-0.0023	-0.1351
1	mes	p1	-0.1569	0.0288	-0.0200	-0.0117	-0.0068	-0.1666
1	mes	p2	-0.1566	0.0326	-0.0209	-0.0077	-0.0067	-0.1594
1	ntf2	p1	-0.1245	0.0157	-0.0125	-0.0134	-0.0027	-0.1374
1	ntf2	p2	-0.1207	0.0162	-0.0143	-0.0097	-0.0015	-0.1300
1	ntf2	p3	-0.1242	0.0181	-0.0131	-0.0125	-0.0028	-0.1345
1	ntf2	p5	-0.1227	0.0159	-0.0143	-0.0099	-0.0012	-0.1321
1	pf6	p1	-0.1307	0.0156	-0.0112	-0.0083	-0.0028	-0.1374
1	pf6	p2	-0.1298	0.0152	-0.0110	-0.0074	-0.0026	-0.1355
1	tos	p1	-0.2004	0.0277	-0.0191	-0.0106	-0.0077	-0.2101
1	tos	p2	-0.1741	0.0264	-0.0204	-0.0094	-0.0062	-0.1838
2	bf4	p1	-0.1379	0.0188	-0.0135	-0.0095	-0.0053	-0.1474
2	bf4	p2	-0.1348	0.0192	-0.0125	-0.0082	-0.0048	-0.1411
2	bf4	p3	-0.1375	0.0193	-0.0132	-0.0083	-0.0051	-0.1447
2	dca	p1	-0.1297	0.0254	-0.0126	-0.0124	-0.0033	-0.1326
2	dca	p2	-0.1308	0.0243	-0.0106	-0.0131	-0.0024	-0.1327
2	dca	p3	-0.1322	0.0251	-0.0111	-0.0133	-0.0024	-0.1339
2	mes	p1	-0.1542	0.0280	-0.0205	-0.0123	-0.0069	-0.1658
2	mes	p2	-0.1489	0.0266	-0.0186	-0.0105	-0.0055	-0.1568
2	mes	p3	-0.1545	0.0309	-0.0206	-0.0093	-0.0067	-0.1603
2	ntf2	p1	-0.1212	0.0143	-0.0122	-0.0138	-0.0022	-0.1351
2	ntf2	p2	-0.1184	0.0170	-0.0145	-0.0103	-0.0015	-0.1277
2	ntf2	p3	-0.1189	0.0145	-0.0115	-0.0131	-0.0020	-0.1309
2	ntf2	p4	-0.1230	0.0167	-0.0130	-0.0126	-0.0027	-0.1345
2	ntf2	p5	-0.1182	0.0153	-0.0130	-0.0109	-0.0012	-0.1280
2	ntf2	p6	-0.1182	0.0157	-0.0144	-0.0099	-0.0012	-0.1279
2	pf6	p1	-0.1290	0.0166	-0.0115	-0.0082	-0.0029	-0.1350
2	pf6	p2	-0.1249	0.0156	-0.0107	-0.0074	-0.0025	-0.1299
2	pf6	p3	-0.1284	0.0155	-0.0113	-0.0075	-0.0028	-0.1344
2	tos	p1	-0.1753	0.0272	-0.0194	-0.0112	-0.0072	-0.1859
2	tos	p2	-0.1869	0.0257	-0.0178	-0.0096	-0.0061	-0.1948
3	bf4	p1	-0.1364	0.0184	-0.0139	-0.0097	-0.0051	-0.1467
3	bf4	p2	-0.1336	0.0184	-0.0129	-0.0082	-0.0047	-0.1410
3	bf4	p3	-0.1365	0.0192	-0.0133	-0.0085	-0.0050	-0.1442
3	dca	p1	-0.1283	0.0254	-0.0118	-0.0130	-0.0031	-0.1308
3	dca	p2	-0.1303	0.0241	-0.0109	-0.0132	-0.0023	-0.1326
3	dca	p3	-0.1220	0.0207	-0.0123	-0.0110	-0.0034	-0.1280
3	dca	p4	-0.1279	0.0255	-0.0128	-0.0146	-0.0009	-0.1306
3	dca	p5	-0.1312	0.0263	-0.0126	-0.0153	-0.0009	-0.1337
3	mes	p1	-0.1517	0.0270	-0.0206	-0.0128	-0.0064	-0.1646
3	mes	p2	-0.1476	0.0263	-0.0190	-0.0104	-0.0054	-0.1560
3	mes	p3	-0.1526	0.0308	-0.0207	-0.0096	-0.0063	-0.1585
3	ntf2	p1	-0.1208	0.0144	-0.0127	-0.0144	-0.0022	-0.1357
3	ntf2	p2	-0.1162	0.0177	-0.0144	-0.0098	-0.0014	-0.1241
3	ntf2	p3	-0.1181	0.0149	-0.0117	-0.0131	-0.0020	-0.1301
3	ntf2	p4	-0.1181	0.0168	-0.0131	-0.0131	-0.0025	-0.1300
3	ntf2	p5	-0.1184	0.0149	-0.0129	-0.0108	-0.0010	-0.1283
3	ntf2	p6	-0.1162	0.0160	-0.0140	-0.0104	-0.0011	-0.1256
3	pf6	p1	-0.1277	0.0155	-0.0119	-0.0088	-0.0029	-0.1358
3	pf6	p2	-0.1232	0.0152	-0.0109	-0.0073	-0.0025	-0.1286
3	pf6	p3	-0.1267	0.0155	-0.0114	-0.0077	-0.0027	-0.1330
3	tos	p1	-0.1864	0.0263	-0.0207	-0.0120	-0.0073	-0.2000
3	tos	p2	-0.1795	0.0253	-0.0183	-0.0095	-0.0062	-0.1884
4	bf4	p1	-0.1361	0.0184	-0.0142	-0.0098	-0.0051	-0.1468
4	bf4	p2	-0.1313	0.0184	-0.0133	-0.0083	-0.0047	-0.1391
4	bf4	p3	-0.1359	0.0195	-0.0136	-0.0086	-0.0053	-0.1440
4	dca	p1	-0.1271	0.0226	-0.0112	-0.0127	-0.0019	-0.1303
4	dca	p2	-0.1280	0.0239	-0.0110	-0.0132	-0.0022	-0.1306
4	dca	p3	-0.1281	0.0243	-0.0119	-0.0134	-0.0028	-0.1319
4	dca	p4	-0.1324	0.0249	-0.0109	-0.0132	-0.0021	-0.1338
4	dca	p5	-0.1297	0.0247	-0.0114	-0.0135	-0.0024	-0.1323
4	mes	p1	-0.1517	0.0269	-0.0209	-0.0129	-0.0064	-0.1651
4	mes	p2	-0.1445	0.0261	-0.0193	-0.0107	-0.0052	-0.1535
4	mes	p3	-0.1511	0.0308	-0.0210	-0.0098	-0.0066	-0.1577
4	ntf2	p1	-0.1198	0.0147	-0.0131	-0.0145	-0.0024	-0.1351
4	ntf2	p2	-0.1174	0.0163	-0.0148	-0.0119	-0.0014	-0.1292
4	ntf2	p3	-0.1176	0.0158	-0.0122	-0.0134	-0.0021	-0.1296
4	ntf2	p4	-0.1159	0.0168	-0.0132	-0.0134	-0.0027	-0.1284
4	ntf2	p5	-0.1157	0.0147	-0.0130	-0.0111	-0.0010	-0.1261
4	ntf2	p6	-0.1169	0.0160	-0.0143	-0.0109	-0.0014	-0.1274
4	pf6	p1	-0.1268	0.0156	-0.0122	-0.0088	-0.0029	-0.1351
4	pf6	p2	-0.1208	0.0152	-0.0111	-0.0075	-0.0024	-0.1266
4	pf6	p3	-0.1255	0.0154	-0.0116	-0.0078	-0.0028	-0.1323
4	tos	p1	-0.2225	0.0263	-0.0196	-0.0122	-0.0079	-0.2359
4	tos	p2	-0.1704	0.0250	-0.0175	-0.0100	-0.0075	-0.1804

S18. EFP Interaction Energies of CnPyr cation and TILA anion using VVO Approximation with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	bf4	p1	-0.1400	0.0189	-0.0129	-0.0094	-0.0008	-0.1442
1	bf4	p2	-0.1388	0.0186	-0.0126	-0.0082	-0.0008	-0.1418
1	dca	p1	-0.1321	0.0255	-0.0125	-0.0123	-0.0010	-0.1324
1	dca	p2	-0.1344	0.0251	-0.0109	-0.0131	-0.0009	-0.1341
1	dca	p3	-0.1275	0.0241	-0.0144	-0.0115	-0.0012	-0.1306
1	dca	p4	-0.1352	0.0256	-0.0104	-0.0129	-0.0010	-0.1338
1	mes	p1	-0.1569	0.0288	-0.0200	-0.0117	-0.0017	-0.1615
1	mes	p2	-0.1566	0.0326	-0.0209	-0.0077	-0.0021	-0.1548
1	ntf2	p1	-0.1245	0.0157	-0.0125	-0.0134	-0.0009	-0.1356
1	ntf2	p2	-0.1207	0.0162	-0.0143	-0.0097	0.0000	-0.1285
1	ntf2	p3	-0.1242	0.0181	-0.0131	-0.0125	-0.0011	-0.1328
1	ntf2	p5	-0.1227	0.0159	-0.0143	-0.0099	0.0000	-0.1309
1	pf6	p1	-0.1307	0.0156	-0.0112	-0.0083	-0.0007	-0.1352
1	pf6	p2	-0.1298	0.0152	-0.0110	-0.0074	-0.0007	-0.1336
1	tos	p1	-0.2004	0.0277	-0.0191	-0.0106	-0.0017	-0.2042
1	tos	p2	-0.1741	0.0264	-0.0204	-0.0094	-0.0016	-0.1792
2	bf4	p1	-0.1379	0.0188	-0.0135	-0.0095	-0.0007	-0.1429
2	bf4	p2	-0.1348	0.0192	-0.0125	-0.0082	-0.0008	-0.1371
2	bf4	p3	-0.1375	0.0193	-0.0132	-0.0083	-0.0008	-0.1405
2	dca	p1	-0.1297	0.0254	-0.0126	-0.0124	-0.0009	-0.1302
2	dca	p2	-0.1308	0.0243	-0.0106	-0.0131	-0.0010	-0.1313
2	dca	p3	-0.1322	0.0251	-0.0111	-0.0133	-0.0009	-0.1324
2	mes	p1	-0.1542	0.0280	-0.0205	-0.0123	-0.0016	-0.1605
2	mes	p2	-0.1489	0.0266	-0.0186	-0.0105	-0.0016	-0.1529
2	mes	p3	-0.1545	0.0309	-0.0206	-0.0093	-0.0020	-0.1556
2	ntf2	p1	-0.1212	0.0143	-0.0122	-0.0138	0.0000	-0.1329
2	ntf2	p2	-0.1184	0.0170	-0.0145	-0.0103	-0.0006	-0.1268
2	ntf2	p3	-0.1189	0.0145	-0.0115	-0.0131	-0.0007	-0.1296
2	ntf2	p4	-0.1230	0.0167	-0.0130	-0.0126	-0.0010	-0.1328
2	ntf2	p5	-0.1182	0.0153	-0.0130	-0.0109	-0.0005	-0.1274
2	ntf2	p6	-0.1182	0.0157	-0.0144	-0.0099	0.0000	-0.1267
2	pf6	p1	-0.1290	0.0166	-0.0115	-0.0082	0.0000	-0.1321
2	pf6	p2	-0.1249	0.0156	-0.0107	-0.0074	-0.0007	-0.1281
2	pf6	p3	-0.1284	0.0155	-0.0113	-0.0075	-0.0007	-0.1324
2	tos	p1	-0.1753	0.0272	-0.0194	-0.0112	-0.0017	-0.1804
2	tos	p2	-0.1869	0.0257	-0.0178	-0.0096	-0.0015	-0.1902
3	bf4	p1	-0.1364	0.0184	-0.0139	-0.0097	-0.0006	-0.1422
3	bf4	p2	-0.1336	0.0184	-0.0129	-0.0082	-0.0008	-0.1370
3	bf4	p3	-0.1365	0.0192	-0.0133	-0.0085	-0.0008	-0.1399
3	dca	p1	-0.1283	0.0254	-0.0118	-0.0130	-0.0008	-0.1284
3	dca	p2	-0.1303	0.0241	-0.0109	-0.0132	-0.0009	-0.1313
3	dca	p3	-0.1220	0.0207	-0.0123	-0.0110	-0.0009	-0.1255
3	dca	p4	-0.1279	0.0255	-0.0128	-0.0146	-0.0007	-0.1304
3	dca	p5	-0.1312	0.0263	-0.0126	-0.0153	-0.0008	-0.1336
3	mes	p1	-0.1517	0.0270	-0.0206	-0.0128	-0.0014	-0.1596
3	mes	p2	-0.1476	0.0263	-0.0190	-0.0104	-0.0015	-0.1521
3	mes	p3	-0.1526	0.0308	-0.0207	-0.0096	-0.0018	-0.1540
3	ntf2	p1	-0.1208	0.0144	-0.0127	-0.0144	0.0000	-0.1335
3	ntf2	p2	-0.1162	0.0177	-0.0144	-0.0098	0.0000	-0.1227
3	ntf2	p3	-0.1181	0.0149	-0.0117	-0.0131	-0.0007	-0.1288
3	ntf2	p4	-0.1181	0.0168	-0.0131	-0.0131	-0.0009	-0.1284
3	ntf2	p5	-0.1184	0.0149	-0.0129	-0.0108	0.0000	-0.1273
3	ntf2	p6	-0.1162	0.0160	-0.0140	-0.0104	0.0000	-0.1246
3	pf6	p1	-0.1277	0.0155	-0.0119	-0.0088	-0.0006	-0.1335
3	pf6	p2	-0.1232	0.0152	-0.0109	-0.0073	-0.0006	-0.1268
3	pf6	p3	-0.1267	0.0155	-0.0114	-0.0077	0.0000	-0.1303
3	tos	p1	-0.1864	0.0263	-0.0207	-0.0120	-0.0014	-0.1942
3	tos	p2	-0.1795	0.0253	-0.0183	-0.0095	-0.0014	-0.1836
4	bf4	p1	-0.1361	0.0184	-0.0142	-0.0098	-0.0006	-0.1423
4	bf4	p2	-0.1313	0.0184	-0.0133	-0.0083	-0.0007	-0.1352
4	bf4	p3	-0.1359	0.0195	-0.0136	-0.0086	-0.0008	-0.1394
4	dca	p1	-0.1271	0.0226	-0.0112	-0.0127	0.0000	-0.1283
4	dca	p2	-0.1280	0.0239	-0.0110	-0.0132	-0.0009	-0.1293
4	dca	p3	-0.1281	0.0243	-0.0119	-0.0134	-0.0006	-0.1297
4	dca	p4	-0.1324	0.0249	-0.0109	-0.0132	-0.0009	-0.1326
4	dca	p5	-0.1297	0.0247	-0.0114	-0.0135	-0.0008	-0.1307
4	mes	p1	-0.1517	0.0269	-0.0209	-0.0129	-0.0014	-0.1601
4	mes	p2	-0.1445	0.0261	-0.0193	-0.0107	-0.0015	-0.1498
4	mes	p3	-0.1511	0.0308	-0.0210	-0.0098	-0.0019	-0.1530
4	ntf2	p1	-0.1198	0.0147	-0.0131	-0.0145	0.0000	-0.1327
4	ntf2	p2	-0.1174	0.0163	-0.0148	-0.0119	0.0000	-0.1278
4	ntf2	p3	-0.1176	0.0158	-0.0122	-0.0134	-0.0008	-0.1282
4	ntf2	p4	-0.1159	0.0168	-0.0132	-0.0134	-0.0009	-0.1267
4	ntf2	p5	-0.1157	0.0147	-0.0130	-0.0111	0.0000	-0.1251
4	ntf2	p6	-0.1169	0.0160	-0.0143	-0.0109	0.0000	-0.1260
4	pf6	p1	-0.1268	0.0156	-0.0122	-0.0088	-0.0006	-0.1328
4	pf6	p2	-0.1208	0.0152	-0.0111	-0.0075	-0.0006	-0.1248
4	pf6	p3	-0.1255	0.0154	-0.0116	-0.0078	0.0000	-0.1295
4	tos	p1	-0.2225	0.0263	-0.0196	-0.0122	-0.0014	-0.2295
4	tos	p2	-0.1704	0.0250	-0.0175	-0.0100	-0.0017	-0.1746

S19. EFP Interaction Energies of CnPyr cation and halide anion using canonical molecular orbitals with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1531	0.0585	-0.0299	-0.0131	-0.0081	-0.1457
1	br	p2	-0.1541	0.0561	-0.0291	-0.0119	-0.0054	-0.1443
1	cl	p1	-0.1570	0.0491	-0.0249	-0.0051	-0.0112	-0.1491
1	cl	p2	-0.1576	0.0511	-0.0206	-0.0053	-0.0082	-0.1406
2	br	p1	-0.1513	0.0571	-0.0340	-0.0135	-0.0086	-0.1503
2	br	p2	-0.1469	0.0531	-0.0327	-0.0115	-0.0047	-0.1427
2	br	p3	-0.1520	0.0560	-0.0310	-0.0118	-0.0043	-0.1431
2	cl	p1	-0.1544	0.0523	-0.0213	-0.0059	-0.0119	-0.1411
2	cl	p2	-0.1500	0.0491	-0.0217	-0.0050	-0.0090	-0.1365
2	cl	p3	-0.1548	0.0502	-0.0221	-0.0048	-0.0088	-0.1403
3	br	p1	-0.1498	0.0587	-0.0294	-0.0135	-0.0088	-0.1428
3	br	p2	-0.1474	0.0559	-0.0262	-0.0127	-0.0026	-0.1330
3	br	p3	-0.1495	0.0543	-0.0322	-0.0122	-0.0035	-0.1431
3	cl	p1	-0.1527	0.0513	-0.0227	-0.0056	-0.0113	-0.1411
3	cl	p2	-0.1496	0.0490	-0.0217	-0.0047	-0.0087	-0.1357
3	cl	p3	-0.1531	0.0501	-0.0214	-0.0052	-0.0085	-0.1381
4	br	p1	-0.1486	0.0564	-0.0355	-0.0133	-0.0091	-0.1502
4	br	p2	-0.1428	0.0556	-0.0267	-0.0128	-0.0029	-0.1297
4	br	p3	-0.1480	0.0534	-0.0332	-0.0122	-0.0071	-0.1471
4	cl	p1	-0.1525	0.0511	-0.0223	-0.0059	-0.0115	-0.1410
4	cl	p2	-0.1473	0.0470	-0.0246	-0.0046	-0.0087	-0.1382
4	cl	p3	-0.1525	0.0499	-0.0219	-0.0050	-0.0093	-0.1388

S20. EFP Interaction Energies of CnPyr cation and halide anion using VVO Approximation with 6-311++G(d,p) basis set. Units are in Hartree.

Chain	Anion	Conf	Electrostatic	Exchange Repulsion	Polarization	Dispersion(6,7,8)	Charge Transfer	Total Energy
1	br	p1	-0.1531	0.0585	-0.0299	-0.0131	-0.0022	-0.1398
1	br	p2	-0.1541	0.0561	-0.0291	-0.0119	-0.0019	-0.1408
1	cl	p1	-0.1570	0.0491	-0.0249	-0.0051	-0.0019	-0.1399
1	cl	p2	-0.1576	0.0511	-0.0206	-0.0053	-0.0017	-0.1341
2	br	p1	-0.1513	0.0571	-0.0340	-0.0135	-0.0021	-0.1437
2	br	p2	-0.1469	0.0531	-0.0327	-0.0115	-0.0019	-0.1398
2	br	p3	-0.1520	0.0560	-0.0310	-0.0118	-0.0018	-0.1406
2	cl	p1	-0.1544	0.0523	-0.0213	-0.0059	-0.0019	-0.1311
2	cl	p2	-0.1500	0.0491	-0.0217	-0.0050	-0.0017	-0.1293
2	cl	p3	-0.1548	0.0502	-0.0221	-0.0048	-0.0016	-0.1331
3	br	p1	-0.1498	0.0587	-0.0294	-0.0135	-0.0017	-0.1357
3	br	p2	-0.1474	0.0559	-0.0262	-0.0127	-0.0015	-0.1319
3	br	p3	-0.1495	0.0543	-0.0322	-0.0122	-0.0016	-0.1412
3	cl	p1	-0.1527	0.0513	-0.0227	-0.0056	-0.0015	-0.1313
3	cl	p2	-0.1496	0.0490	-0.0217	-0.0047	-0.0015	-0.1285
3	cl	p3	-0.1531	0.0501	-0.0214	-0.0052	-0.0015	-0.1311
4	br	p1	-0.1486	0.0564	-0.0355	-0.0133	-0.0016	-0.1427
4	br	p2	-0.1428	0.0556	-0.0267	-0.0128	-0.0016	-0.1283
4	br	p3	-0.1480	0.0534	-0.0332	-0.0122	-0.0017	-0.1417
4	cl	p1	-0.1525	0.0511	-0.0223	-0.0059	-0.0014	-0.1309
4	cl	p2	-0.1473	0.0470	-0.0246	-0.0046	-0.0016	-0.1312
4	cl	p3	-0.1525	0.0499	-0.0219	-0.0050	-0.0015	-0.1311