Supporting Information:

Physicochemical Properties of Imidazolium-derived Ionic Liquids with different C-2 Substitution

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ST1. Relative energies of three conformers of cation 1.

	C1	C2	C3
E (Hartree)	-615.73721	-615.73721	-615.73732
Δ *E* (kcal/mol)	0.07	0.07	0.00

ST2. Relative energies of three conformers of cation 2.

	C1	C2	C3
E (Hartree)	-422.76525	-422.76691	-422.76668
Δ *E* (kcal/mol)	1.04	0.00	0.14

ST3. Relative energies of three conformers of cation 3.

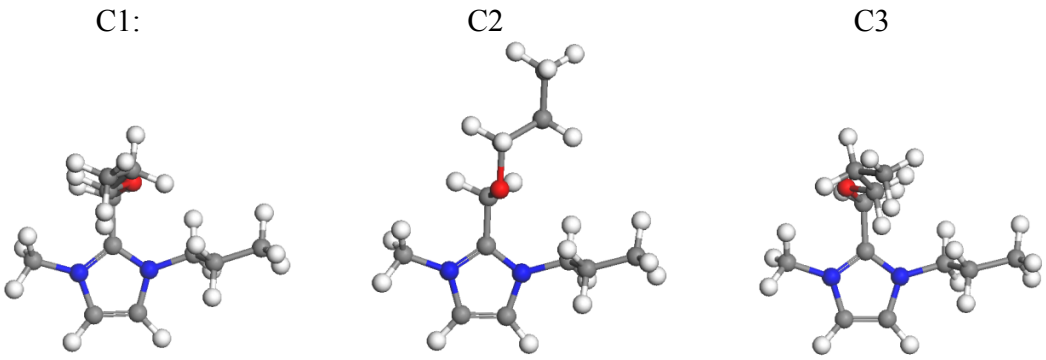
	C1	C2	C3
E (Hartree)	-752.65335	-752.65308	-752.65324
Δ *E* (kcal/mol)	0.00	0.17	0.07

ST4. Relative energies of three conformers of cation 4.

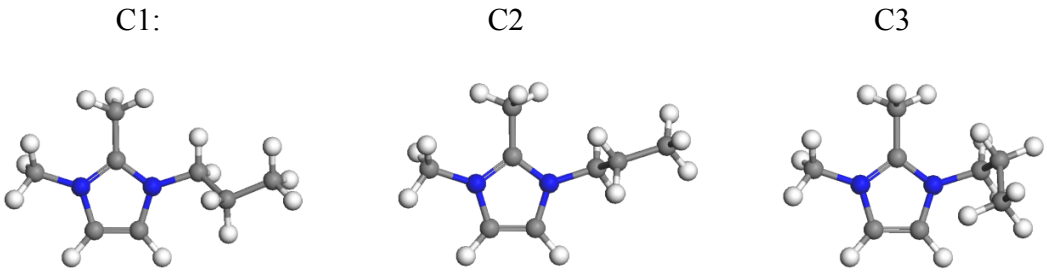
	C1	C2	C3
E (Hartree)	-984.90006	-984.90114	-984.89711
Δ *E* (kcal/mol)	0.68	0.00	2.53

ST5. Relative energies of three conformers of cation 5.

	C1	C2	C3
E (Hartree)	-475.63690	-475.63659	-475.63658
Δ *E* (kcal/mol)	0.00	0.19	0.20

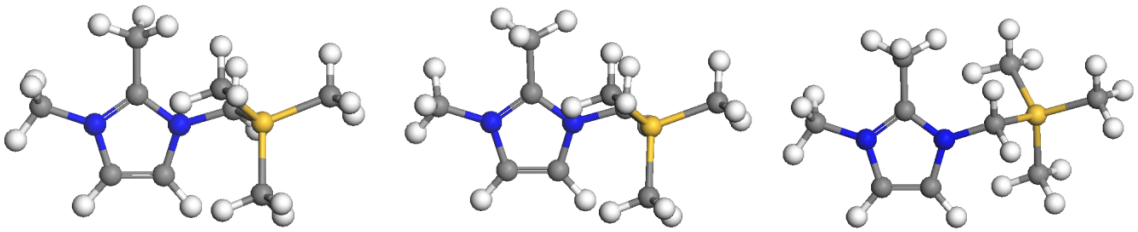


SF1: Three conformers of IL 1.



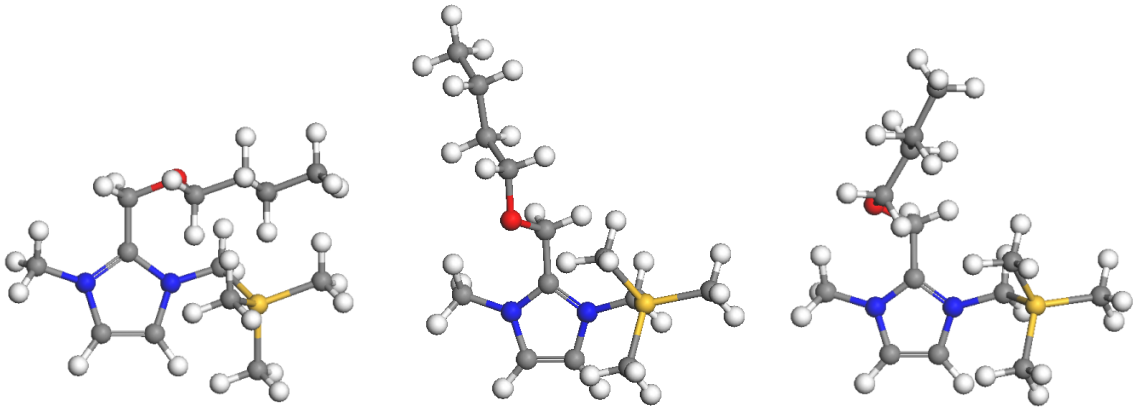
SF2: Three conformers of IL 2.

C1: C2 C3



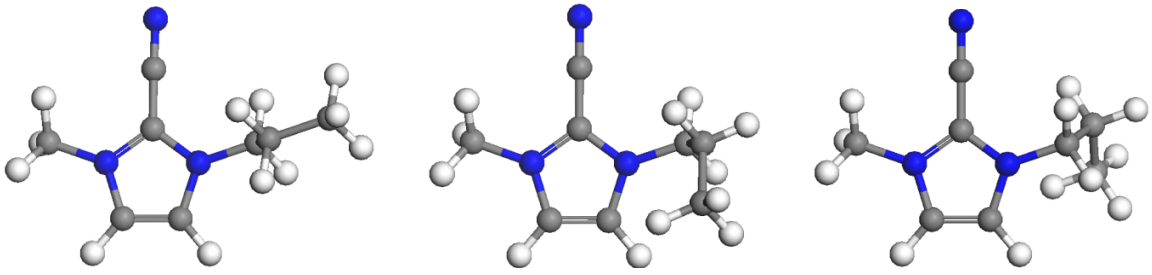
SF3: Three conformers of IL 3.

C1: C2 C3



SF4: Three conformers of IL 4.

C1: C2 C3



SF5: Three conformers of IL 5.