Electronic Supplementary Information for

Theoretical Investigations of Ferrocene/Ferrocenium Solvation in Imidazolium-Based Room-Temperature Ionic Liquids

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Results of NBO analysis are presented below. Table S1 shows orbital interactions for the Fc—BF_4^- and Fc^+—BF_4^-complexes. Figures S1 and S2 depict the electron density contour maps for the Fc^+—BF_4^- complexes.

Table S1. NBO analysis of orbital interactions for the Fc—BF_4^- and Fc^+—BF_4^-complexes.

Donor	Acceptor	E(2) (kcal/mol)
Fc—BF_4^- side		
LP(F23)	σ*(C3-H13)	0.74
LP(F23)	π*(C2-C3)	0.13
LP(F23)	σ*(C4-H14)	0.26
LP(F23)	π*(C4-C5)	0.10
LP(F24)	σ*(C10-H20)	0.73
LP(F24)	π*(C10-C11)	0.13
LP(F24)	σ*(C9-H19)	0.26
LP(F24)	π*(C8-C9)	0.10
LP(F25)	σ*(C9-H19)	1.87
LP(F25)	σ*(C4-H14)	1.88
	Total	**6.20**
Fc^+—BF_4^- side		
LP(F23)	σ*(C3-H13)	0.76
LP(F23)	π*(C2-C3)	0.20
LP(F23)	σ*(C4-H14)	0.72
LP(F23)	π*(C4-C5)	0.22
LP(F24)	σ*(C3-H13)	0.88
LP(F24)	π*(C3-C4)	0.04
LP(F24)	σ*(C10-H20)	0.94
LP(F24)	π*(C10-C11)	0.39
LP(F24)	π*(C8-C9)	0.16
LP(F25)	σ*(C4-H14)	1.89
LP(F25)	π*(C3-C4)	0.06
LP(F25)	σ*(C9-H19)	3.98
LP(F25)	π*(C9-C10)	0.06
	Total	**10.3**
Fc^+—BF_4^- top		
LP(F24)	π*(C2-C3)	1.30
LP(F26)	π*(C2-C3)	1.30
	Total	**2.60**

Note: For all atom labeling, please refer to Figures 5, 10, and 11 in the main context.

Figure Captions

Figure S1. Electron density contour map for the "side" binding Fc^{+}—BF_4^{-} projected on the plane defined by H14, H19, and F25.

Figure S2. Electron density contour map for the "top" binding Fc^{+}—BF_4^{-} projected on the plane defined by H12, H13, and F24.

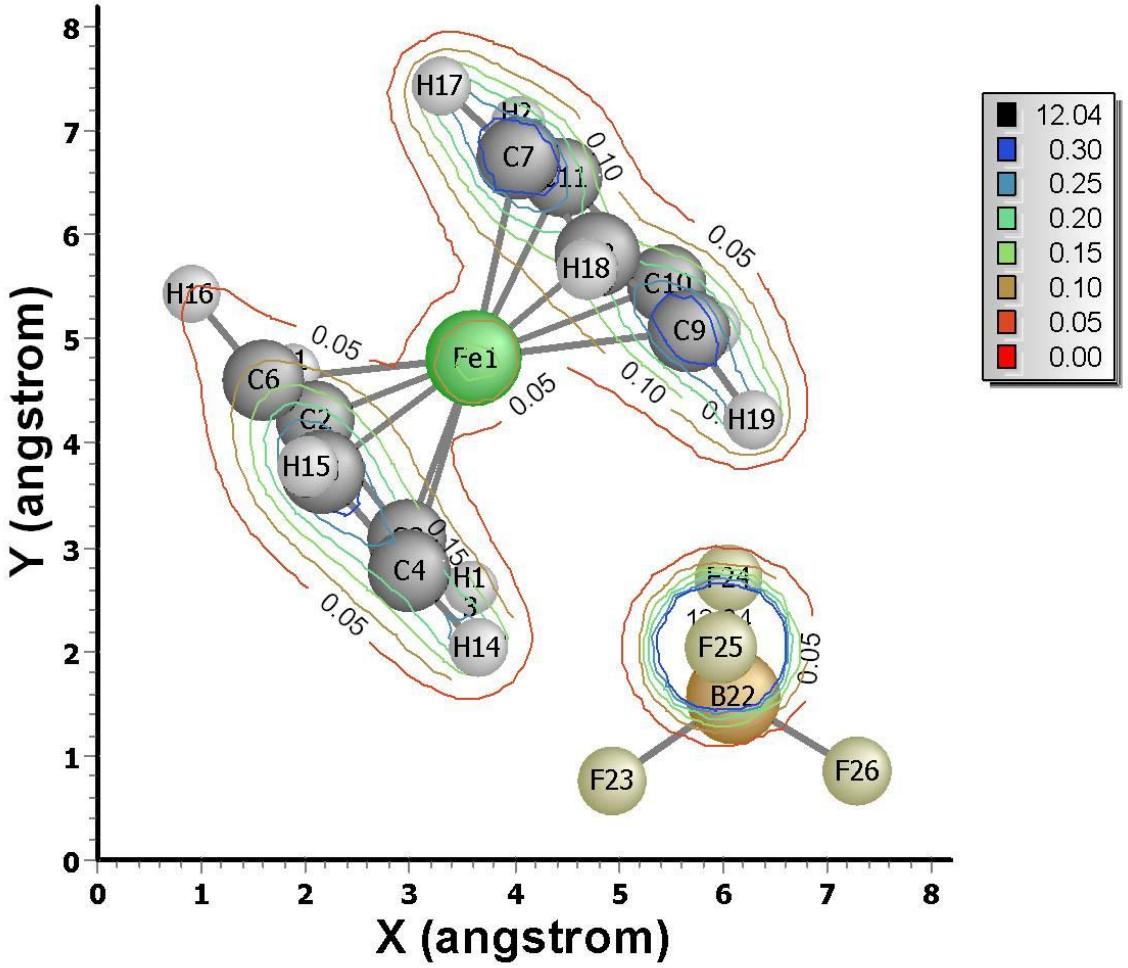
Y (angstrom)
X (angstrom)
0
1
2
3
4
5
6
7
8
H17
C7
H18
C10
C9
H19
H16
C6
C2
H15
Fe1
C4
H1
H14
F24
F25
B22
F23
F26
0.10
0.05
0.15
0.00
12.04
0.30
0.25
0.20
0.15
0.10
0.05
0.00

Figure S1

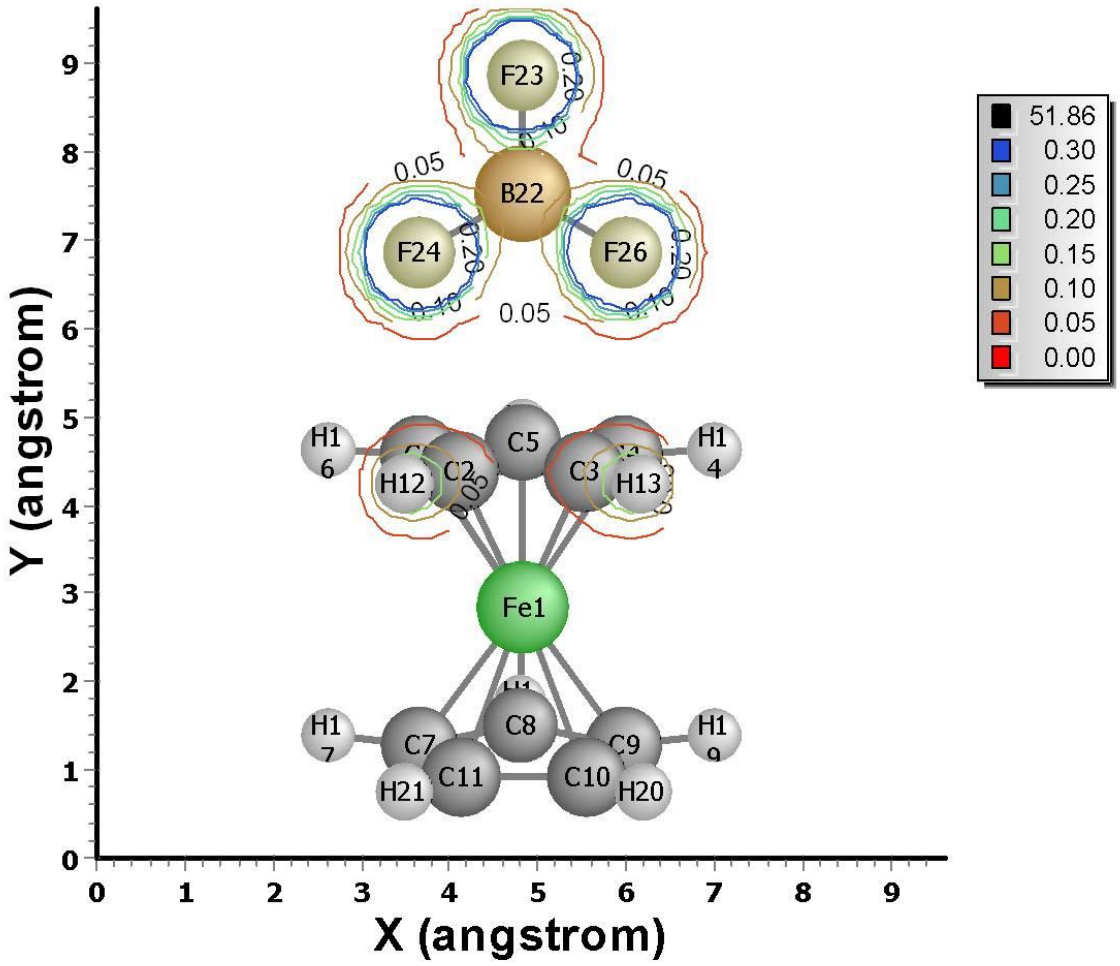
F23
B22
F24
F26
0.05
0.05
0.05
0.20
0.15
0.10
H16
C5
H14
H12
C2
C3
H13
Fe1
C8
H17
C7
C9
H19
C11
C10
H21
H20
51.86
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Y (angstrom)
X (angstrom)
0
1
2
3
4
5
6
7
8
9

Figure S2