A Detailed Assignment of NEXAFS Resonances of Imidazolium Based Ionic Liquids

Supporting Information

Christopher Ehlert[1,2], Markus Holzweber[1],
Andreas Lippitz[1], Wolfgang E.S. Unger[1], Peter Saalfrank[2]

[1] *BAM Bundesanstalt für Materialforschung und –prüfung, D-12203 Berlin, Germany*

[2] *Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany*

January 25, 2016

1 Structures

Fig.1 gives the unit cells of the ILs $[C_1C_1im]^+[NTf_2]^-$ and $[C_4C_1im]^+[I]^-$ used to construct the single-ion pair models used in this work (see main text).

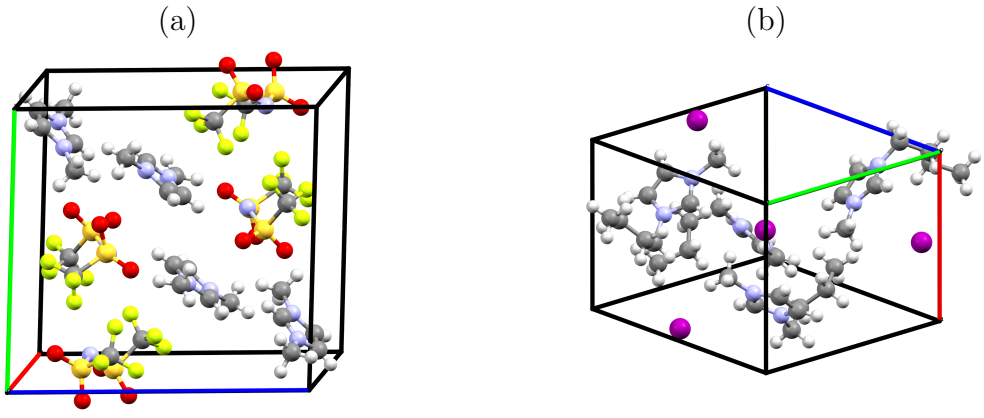

Figure 1: Unit cells of experimental crystal structures of $[C_1C_1im]^+[NTf_2]^-$ (a) according to Ref.[1], and of $[C_4C_1im]^+[I]^-$ (b) according to Ref.[2]. Color code: red for oxygen, orange for sulfur, yellow for fluorine, grey for carbon, white for hydrogen, light blue for nitrogen, purple for iodine. The cell of the $[C_1C_1im]^+[NTf_2]^-$ is characterized by three lattice constants and angles: $a = 8.535$Å, $b = 12.681$Å, $c = 13.502$Å, $\alpha = 88.06°$, $\beta = 80.18°$, $\gamma = 79.77°$. The cell of the $[C_4C_1im]^+[I]^-$ system is orthorhombic with lattice constants $a = 8.281$Å, $b = 10.789$Å,$c = 11.999$Å.

The following two tables give the Cartesian coordinates (x, y, z) in Å, for the dimer models of the two ILs which were studied theoretically in this work.

I	4.931525	7.364820	9.533205
N	8.360185	8.212360	7.472945
N	6.931785	9.836250	7.606135
C	7.824435	9.119890	8.292445
C	6.869685	9.356160	6.321095
C	7.772265	8.333410	6.234705
C	6.082195	10.875180	8.182055
C	9.396095	7.226510	7.858095
C	8.795745	6.037620	8.604405
C	7.853415	5.197190	7.738115
C	7.274605	3.991040	8.484425
H	8.041385	9.235330	9.209125
H	6.306605	9.673340	5.623975
H	7.958585	7.806930	5.466795
H	5.244195	10.474930	8.496415
H	5.885945	11.551620	7.501745
H	6.545905	11.295930	8.936765
H	10.068475	7.667760	8.435225
H	9.857325	6.901780	7.044605
H	8.297255	6.370980	9.391505
H	9.530235	5.461510	8.933165
H	8.346945	4.876770	6.941415
H	7.108995	5.768980	7.423755
H	8.006605	3.448380	8.845575
H	6.741335	3.449460	7.865295
H	6.706555	4.302830	9.218725

Table 1: Cartesian coordinates (in Å) of the cluster model for the $[C_4C_1im]^+$ $[I]^-$ system.

S	10.203500	11.604500	8.101500
S	7.644500	11.171500	9.180500
F	12.370500	12.453500	9.236500
F	10.813500	11.965500	10.632500
F	10.691500	13.778500	9.479500
F	8.152500	12.962500	11.036500
F	6.202500	12.063500	11.157500
F	6.621500	13.537500	9.643500
O	10.669500	12.251500	6.918500
O	10.566500	10.236500	8.323500
O	6.458500	10.887500	8.439500
O	8.172500	10.142500	10.024500
N	8.680500	11.937500	8.262500
C	11.061500	12.514500	9.441500
C	7.133500	12.518500	10.314500
N	10.140500	7.487500	11.727500
N	12.077500	8.255500	11.153500
C	10.771500	8.343500	10.927500
H	10.362500	8.894500	10.340500
C	12.284500	7.304500	12.129500
H	13.135500	7.054500	12.456500
C	11.081500	6.828500	12.486500
H	10.924500	6.221500	13.081500
C	8.707500	7.194500	11.695500
H	8.197500	7.860500	11.285500
H	8.419500	7.054500	12.629500
H	8.586500	6.301500	11.219500
C	13.115500	9.055500	10.484500
H	12.803500	9.353500	9.662500
H	13.797500	8.530500	10.247500
H	13.406500	9.720500	11.139500

Table 2: Cartesian coordinates (in Å) of the cluster model for the $[C_1C_1im]^+ [NTf_2]^-$ system.

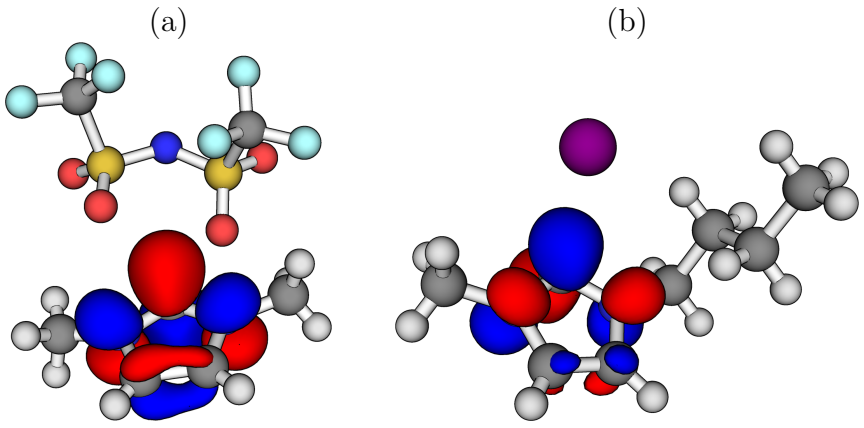

Figure 2: The lowest unoccupied molecular orbital (LUMO) belonging to the groundstate of (a) $[C_1C_1im]^+ [NTf_2]^-$ and (b) $[C_4C_1im]^+ [I]^-$. We used a contour value of 0.05 for the positive (blue) and -0.05 for the negative (red) isosurface.

References

[1] J. D. Holbrey; W. M. Reichert; R. D. Rogers. *Dalton Trans.*, 15, 2267, **2004**.

[2] M. Nakakoshi; M. Shiro; T. Fujimoto; T. Machinami; H. Seki; M. Tashiro; K. Nishikawa. *Chem. Lett.*, 35, 1400, **2006**.