Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

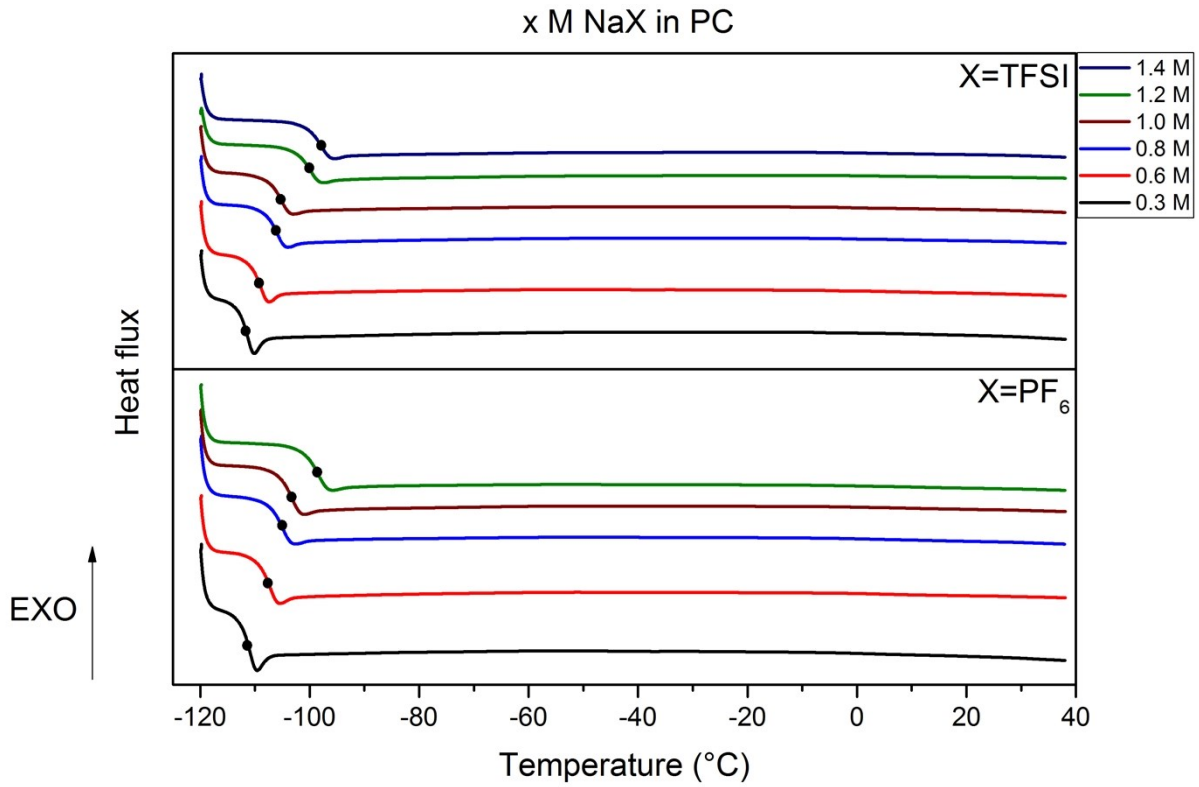

Fig. S1 DSC heating traces between -120°C - +40°C (right column) for (top) x M NaTFSI and (bottom) x M $NaPF_6$ in PC with x=0.3, 0.6, 0.8, 1.0, 1.2, 1.4. The T_gs (black dots) are within -115°C - -90°C.

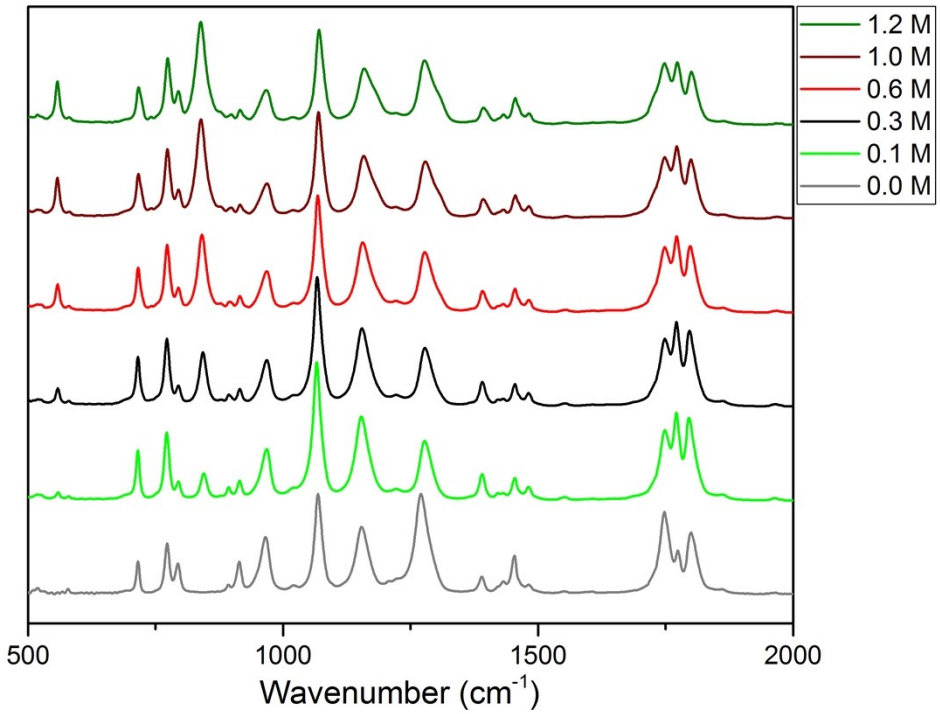

Fig. S2 IR spectra of x M $NaPF_6$ in EC:DMC (x=0.0-1.2) at room temperature in the spectral range 500-2000 cm^{-1}

Table. S1 DFT calculations of cation binding energies of Na(EC)x(DMC)y [x=0-6, y=0-6] complexes using the M06-2X and B3LYP functionals. Mixed refers to the M06-2X/6-311+G*// B3LYP/6-311+G* calculations.

ΔEbind - x+y=4					
x/n_{EC}	y/n_{DMC}	conformers	B3LYP	M06-2X	Mixed
0	4	AAAA	-506.0	-428.3	-509.1
0	4	AAAB	-505.9	-448.2	-508.6
0	4	AAAT	-509.3	-454.6	-511.8
0	4	AABB	-505.6	-429.2	-508.4
0	4	AABT	-510.6	-444.5	-513.0
0	4	AATT	-487.0	-488.2	-492.5
0	4	ABBB	-505.9	-456.1	-508.5
0	4	ABBT	-509.8	-437.7	-512.3
0	4	ABTT	-507.8	-452.9	-510.1
0	4	ATTT	-491.1	-464.5	-496.7
0	4	BBBB	-505.6	-423.9	-508.4
0	4	BBBT	-510.6	-465.4	-513.0
0	4	BBTT	-514.8	-488.9	-517.2
0	4	BTTT	-489.9	-509.8	-497.1

0	4	CAAA	-477.6	-433.9	-480.3
0	4	CAAB	-478.0	-449.7	-481.2
0	4	CAAT	-483.1	-454.7	-486.4
0	4	CABB	-477.3	-450.1	-480.2
0	4	CABT	-483.9	-467.6	-487.1
0	4	CATT	-487.4	-450.7	-490.6
0	4	CBBB	-477.7	-439.2	-481.2
0	4	CBBT	-483.1	-476.8	-486.5
0	4	CBTT	-487.4	-465.0	-490.9
0	4	CCAA	-453.9	-430.7	-456.1
0	4	CCAB	-450.6	-433.1	-454.1
0	4	CCAT	-456.6	-437.1	-460.2
0	4	CCBB	-449.3	-434.1	-453.3
0	4	CCBT	-456.5	-450.2	-460.1
0	4	CCCA	-430.0	-403.3	-432.2
0	4	CCCB	-426.5	-386.8	-429.8
0	4	CCCC	-407.9	-373.4	-409.4
0	4	CCCT	-434.7	-400.8	-437.3
0	4	CCTT	-461.3	-431.6	-464.9
0	4	CTTT	-492.6	-467.6	-495.8
0	4	TTTT	-495.0	-468.2	-502.0
1	3	AAA	-505.9	-433.8	-508.2
1	3	AAB	-505.4	-425.7	-507.8
1	3	AAT	-510.1	-463.0	-512.2
1	3	ABB	-505.3	-463.2	-507.6
1	3	ABT	-510.2	-427.1	-512.3
1	3	ATT	-513.6	-459.4	-515.8
1	3	BBB	-506.2	-470.5	-508.6
1	3	BBT	-510.7	-446.8	-512.9
1	3	BTT	-511.7	-471.6	-514.1
1	3	CAA	-478.6	-440.2	-481.0
1	3	CAB	-478.4	-436.9	-481.5
1	3	CAT	-482.9	-455.5	-485.6
1	3	CBB	-481.2	-468.3	-483.8
1	3	CBT	-483.1	-458.5	-486.6
1	3	CCA	-453.2	-432.4	-455.7
1	3	CCB	-452.1	-433.5	-455.4
1	3	CCC	-430.9	-406.7	-433.0
1	3	CCT	-456.7	-429.0	-460.1
1	3	CTT	-488.1	-463.0	-490.7
1	3	TTT	-516.6	-428.6	-518.7
2	2	AA	-505.6	-456.8	-507.6
2	2	AB	-505.8	-464.9	-507.8
2	2	AT	-509.9	-478.0	-511.9

2	2	BB	-506.5	-470.6	-508.6
2	2	BT	-510.9	-470.5	-512.7
2	2	CA	-478.3	-446.7	-481.0
2	2	CB	-479.8	-457.7	-482.1
2	2	CC	-452.6	-435.2	-455.4
2	2	CT	-485.4	-466.4	-487.5
2	2	TT	-511.2	-452.7	-513.3
3	1	A	-506.3	-493.3	-508.0
3	1	B	-506.4	-468.9	-508.2
3	1	C	-480.1	-461.7	-482.0
3	1	T	-509.5	-442.2	-511.1
4	0		-506.0	-508.2	-507.3

ΔEbind - x+y=5

x/n_{EC}	y/n_{DMC}	conformers	B3LYP	M06-2X
0	5	AAAAA	-505.6	-479.3
0	5	AAAAB	-514.2	-483.9
0	5	AAAAT	-528.4	-452.7
0	5	AAABB	-525.0	-463.4
0	5	AAABT	-514.0	-493.0
0	5	AAATT	-514.4	-475.0
0	5	AABBB	-511.4	-493.8
0	5	AABBT	-521.0	-486.6
0	5	AABTT	-526.6	-478.3
0	5	AATTT	-524.3	-478.8
0	5	ABBBB	-517.4	-525.4
0	5	ABBBT	-525.3	-531.4
0	5	ABBTT	-529.8	-478.3
0	5	ABTTT	-520.7	-489.9
0	5	ATTTT	-533.3	-504.9
0	5	BBBBB	-507.9	-461.6
0	5	BBBBT	-560.0	-474.1
0	5	BBBTT	-519.4	-482.8
0	5	BBTTT	-524.2	-515.1
0	5	BTTTT	-547.2	-498.5
0	5	TTTTT	-531.4	-513.9
1	4	AAAA	-522.1	-480.9
1	4	AAAB	-519.1	-487.5
1	4	AAAT	-515.0	-460.6
1	4	AABB	-514.7	-487.8
1	4	AABT	-521.8	-452.3
1	4	AATT	-521.7	-485.8

1	4	ABBB	-534.4	-466.6
1	4	ABBT	-533.6	-467.2
1	4	ABTT	-518.1	-482.1
1	4	ATTT	-529.8	-501.6
1	4	BBBB	-563.8	-461.2
1	4	BBBT	-538.0	-563.0
1	4	BBTT	-525.8	-481.8
1	4	BTTT	-543.5	-494.2
1	4	TTTT	-544.7	-501.2
2	3	AAA	-507.5	-471.3
2	3	AAB	-519.8	-477.2
2	3	AAT	-517.0	-454.3
2	3	ABB	-530.3	-463.9
2	3	ABT	-539.6	-452.8
2	3	ATT	-526.1	-481.9
2	3	BBB	-542.5	-537.8
2	3	BBT	-519.4	-495.6
2	3	BTT	-522.9	-493.7
2	3	TTT	-533.5	-491.5
3	2	AA	-512.1	-436.8
3	2	AB	-537.0	-455.1
3	2	AT	-520.6	-493.1
3	2	BB	-519.8	-471.0
3	2	BT	-547.1	-490.2
3	2	TT	-530.3	-502.9
4	1	A	-525.3	-448.5
4	1	B	-542.6	-525.3
4	1	T	-539.9	-451.1
5	0		-525.2	-434.5

ΔEbind - x+y=6

x/n_{EC}	y/n_{DMC}	conformers	B3LYP	M06-2X
0	6	AAAAAA	-543.8	-523.9
0	6	AAAAAB	-541.5	-524.0
0	6	AAAAAT	-537.9	-499.6
0	6	AAAABB	-538.7	-527.5
0	6	AAAABT	-556.3	-516.2
0	6	AAAATT	-550.7	-502.2
0	6	AAABBB	-543.8	-535.2
0	6	AAABBT	-546.6	-521.2
0	6	AAABTT	-542.3	-508.2
0	6	AAATTT	-571.1	-528.0

0	6	AABBBB	-537.3	-527.6
0	6	AABBBT	-542.9	-531.1
0	6	AABBTT	-550.3	-537.4
0	6	AABTTT	-557.0	-552.4
0	6	AATTTT	-568.6	-535.0
0	6	ABBBBB	-540.1	-500.8
0	6	ABBBBT	-556.5	-544.2
0	6	ABBBTT	-543.8	-514.1
0	6	ABBTTT	-554.3	-542.9
0	6	ABTTTT	-554.7	-552.7
0	6	ATTTTT	-555.4	-521.8
0	6	BBBBBB	-536.0	-513.4
0	6	BBBBBT	-542.3	-545.7
0	6	BBBBTT	-547.7	-528.4
0	6	BBBTTT	-550.3	-546.6
0	6	BBTTTT	-566.9	-550.3
0	6	BTTTTT	-573.2	-527.3
0	6	TTTTTT	-538.8	-573.0
1	5	AAAAA	-518.8	-502.0
1	5	AAAAB	-536.3	-522.3
1	5	AAAAT	-542.2	-521.1
1	5	AAABB	-540.1	-492.6
1	5	AAABT	-560.8	-494.6
1	5	AAATT	-561.8	-545.8
1	5	AABBB	-536.3	-531.2
1	5	AABBT	-544.3	-528.9
1	5	AABTT	-552.2	-511.6
1	5	AATTT	-560.8	-546.2
1	5	ABBBB	-540.2	-542.7
1	5	ABBBT	-542.3	-548.9
1	5	ABBTT	-554.9	-548.1
1	5	ABTTT	-544.8	-526.2
1	5	ATTTT	-543.6	-532.4
1	5	BBBBB	-535.6	-525.8
1	5	BBBBT	-542.2	-516.8
1	5	BBBTT	-529.0	-542.2
1	5	BBTTT	-568.3	-540.3
1	5	BTTTT	-552.6	-536.2
1	5	TTTTT	-543.6	-552.4
2	4	AAAA	-542.3	-502.8
2	4	AAAB	-559.6	-493.1
2	4	AAAT	-550.1	-540.9
2	4	AABB	-541.6	-520.8
2	4	AABT	-550.1	-518.7

2	4	AATT	-551.5	-541.5
2	4	ABBB	-559.4	-508.6
2	4	ABBT	-554.0	-526.4
2	4	ABTT	-545.2	-522.2
2	4	ATTT	-546.3	-511.9
2	4	BBBB	-540.8	-499.3
2	4	BBBT	-523.7	-524.4
2	4	BBTT	-543.3	-526.4
2	4	BTTT	-547.4	-539.0
2	4	TTTT	-556.7	-559.0
3	3	AAA	-556.4	-485.1
3	3	AAB	-549.6	-516.3
3	3	AAT	-538.1	-515.0
3	3	ABB	-556.3	-511.3
3	3	ABT	-552.2	-529.1
3	3	ATT	-546.2	-520.2
3	3	BBB	-543.6	-528.2
3	3	BBT	-543.5	-520.7
3	3	BTT	-544.7	-502.3
3	3	TTT	-564.3	-506.1
4	2	AA	-533.3	-537.9
4	2	AB	-527.9	-528.3
4	2	AT	-542.9	-508.8
4	2	BB	-536.3	-487.6
4	2	BT	-515.8	-534.5
4	2	TT	-562.0	-540.7
5	1	A	-545.9	-514.8
5	1	B	-541.0	-529.4
5	1	T	-545.0	-550.2
6	0		-547.2	-489.6