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Structural and physical properties of a new reversible and continuous thermochromic ionic liquid in a wide temperature interval: $[BMIM]_4[Ni(NCS)_6]$

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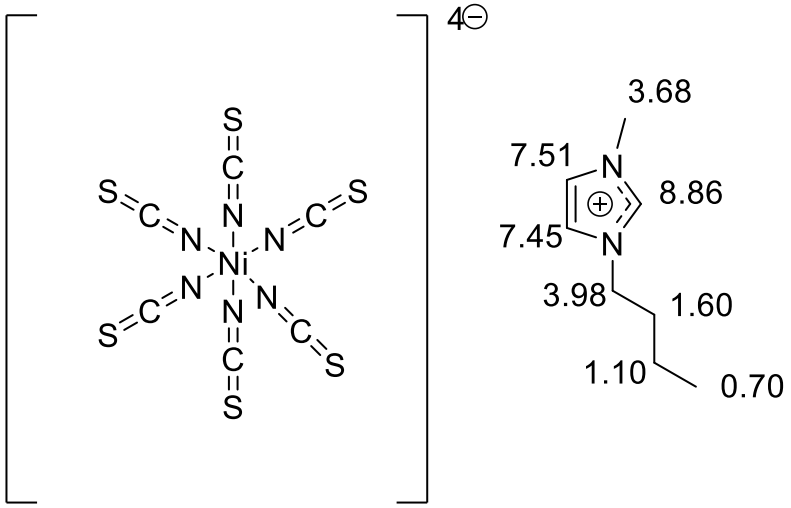

Fig. S1: ^{1}H NMR assignments

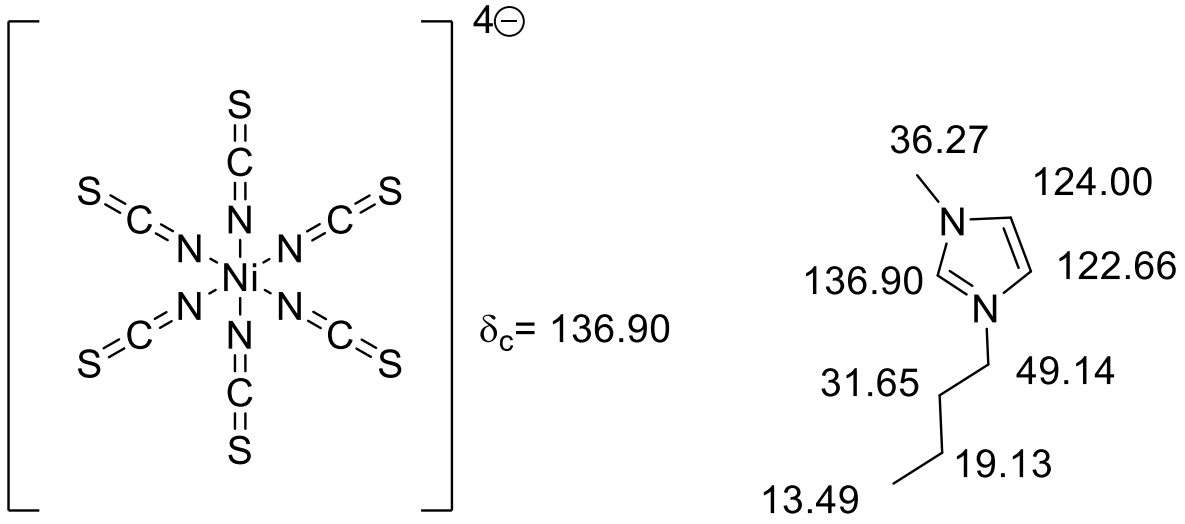

Fig. S2 ^{13}C NMR assignments

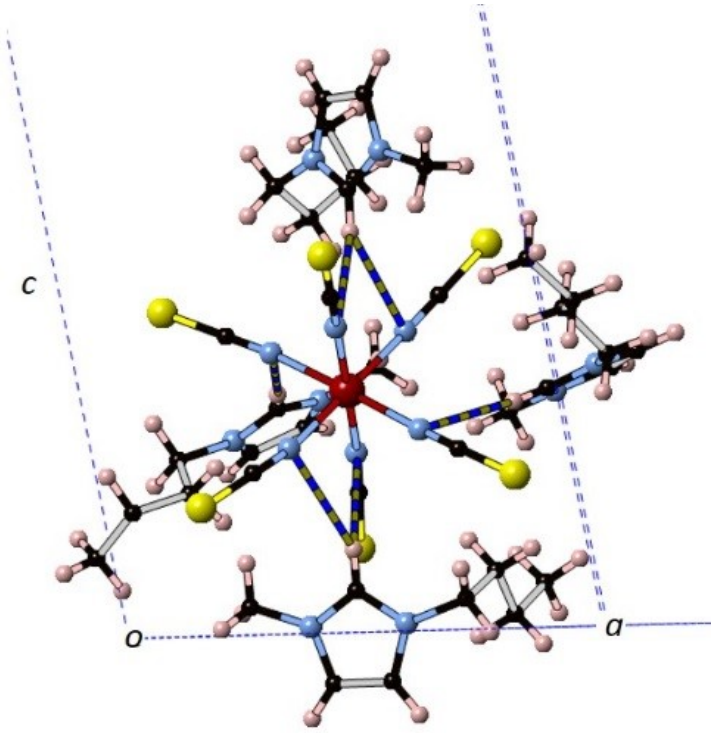

Fig. S3: Hydrogen bond interactions (dashed line) around $[Ni(SCN)_6]^-$ entity.

Table S1: Vibrational assignment (cm^{-1}) of Niquel (300 K) (sh-shoulder)

Assignment	Raman 300 K Frequency (cm^{-1})	IR 295 K Frequency (cm^{-1})
Ni-N sym-stretch	98.2	
Ni-N asym-Stretch	215.0	
CH3(N) bend, CH2(N) bend, CCCC bend	318.7 337.2 414.4	408.9 416.6 449.37
SCN–Ni–NCS stretch	 471.6 499.6	468.4 476.4 491.8
[Ring] op asym bend, N-CH_3 stretch	599.8	601.7
[Ring] op asym bend, N-CH_3 stretch	621.0	619.1
[Ring] op asym bend CH3(N),CH2(N) str		643.6 665 (sh)
[Ring] ip asym bend, N-CH-N bend	704.2 744.0	702 744.5
[CH_3(N)] stretch, [CH_2(N)] stretch, CCCC stretch	763.6 781.0	765.7
CCCH bend CCCC stretch [Ring]HCCH asym bend C-S strech		796.5
[SCN] S-C stretch	821.2	773
NC(H)N bend CCH bend		844.2
NC(H)N bend NH bending out of plane CCCC H bend		877.5 904.5
In plane ring vibration, stretching and bending; First overtone, 2Xδ(NCS) in plane bending		943.1 954.7
CCCC strech NC(H)N CH bend		977.8 987.5
CCCC stretch, [Ring] ip asym stretch	1016.7 1026.9 1051.5 1058.9	- 1026 1051.1 1062.7
[Ring] ip sym stretch, [Ring] C=C stretch	1091.4	1089.7
[CH_3(N)] H-C-H bend	1114.6	1114.8 1124.4
[CH_3(N)] stretch, [CH_2(N)] stretch, [Ring] ip asym stretch	1171.1	1168.7
CCCC stretch, [Ring] ip sym stretch	1210.6 1288 1299.8 1311.9	1207.3 1286.4 1303 (sh) 1311(sh)

Assignment	Raman 300 K Frequency (cm^{-1})	IR 295 K Frequency (cm^{-1})
[Ring] ip asym stretch, CCCC stretch, CH3(N) CH2(N) CN strech		1326.9
[CH_3(N)] stretch, [CH_2(N)] stretch, [Ring] ip sym stretch	1343.4	1342.3
CH3(N) CH2(N) CN str		1359.7
CCCC stretch	1389.7	1388(sh)
[Ring] ip asym stretch, [Ring] N-CH_3 stretch	1412.9 1416.2 1425.9	1409(sh) 1415(sh) 1425.3
[butyl] H-C-H sym bend	1453.8 1475.5	1453.4 1469(sh) 1475(sh)
[Ring] ip asym stretch, [CH_3(N)] CN stretch, [CH_2(N)] CHstretch	1567.0	1573.5
[Ring] ip asym stretch, [CH_3(N)] HCH stretch, [CH_2(N)] HCH stretch		1613.3
[SCN] C-N stretch	2063.6 2099.1 2103.7 2121.6	2063(sh) 2094.5 2104(sh) 2121(sh)
[CH_2C(N)], terminal CH_3 sym stretch	2819.8	2821(sh)
[Bu] H-C-H sym stretch	2872.9	2869.8
Butyl H-C-H asym str		2918(sh)
[CH_3(N)] H-C-H sym stretch	2932.8	2931.6
[butyl] H-C-H asym stretch	2961.7	2956.6
[CH_2C(N)] H-C-H asym stretch	3006.0	3010(sh)
[CH_3(N)] H-C-H asym stretch	3074.9	3068.2
[CH_3(N)] H-C-H asym stretch	3089.4	3082
[Ring] HC=CH asym stretch	3140.9	3146.4
[Ring] HC=CH sym stretch, [Ring] ip sym stretch	3154.0	-

Table S2: Subtended angles between the different atoms at 200 K, 290 K AND 320 K

(N-Nitrogen, Ni-Nickel, C-Carbon)

Atoms			Angle (degree)		
Atom 1	Atom 2	Atom 3	T=320 K	T=290 K	T=200 K
N1	Ni1	N2	91.0(2)	90.7(2)	90.6(1)
N1	Ni1	N3	177.5(2)	177.3(1)	177.4(1)
N1	Ni1	N4	89.9(2)	90.2(1)	90.2(1)
N1	Ni1	N5	90.4(2)	90.1(2)	90.2(1)
N1	Ni1	N6	88.6(2)	88.4(1)	88.5(1)
N2	Ni1	N3	91.2(2)	91.8(2)	91.9(1)
N2	Ni1	N4	89.4(2)	89.5(1)	89.3(1)
N2	Ni1	N5	91.0(2)	91.0(2)	91.1(1)
N2	Ni1	N6	179.0(2)	178.9(2)	178.4(1)
N3	Ni1	N4	88.8(2)	88.9(1)	88.9(1)
N3	Ni1	N5	90.9(2)	90.9(2)	90.7(1)
N3	Ni1	N6	89.2(2)	89.1(1)	89.0(1)
N4	Ni1	N5	179.4(2)	179.5(2)	179.4(1)
N4	Ni1	N6	89.7(2)	89.8(1)	89.4(1)
N5	Ni1	N6	89.9(2)	89.7(2)	90.1(1)
Ni1	N1	C1	174.8(5)	174.4(4)	175.2(3)
N1	C1	S1	179.0(6)	178.7(4)	179.0(3)
Ni1	N2	C2	171.5(5)	170.5(4)	168.4(3)
N2	C2	S2	177.9(6)	178.5(5)	178.5(3)
Ni1	N3	C3	171.1(5)	172.0(4)	172.5(3)
N3	C3	S3	178.4(6)	179.1(5)	178.5(3)
Ni1	N4	C4	173.9(5)	173.3(4)	172.6(3)
N4	C4	S4	179.5(6)	179.5(4)	179.5(3)
Ni1	N5	C5	173.8(5)	173.9(4)	173.0(3)
N5	C5	S5	178.0(6)	178.8(5)	178.8(3)
Ni1	N6	C6	173.0(5)	170.9(4)	169.6(3)
N6	C6	S6	178.5(6)	179.6(4)	179.6(3)