Electronic Supplementary Material (ESI) for RSC Advances.

Table S1. Final refined positional coordinates from synchrotron powder X Ray diffraction pattern of Edimim[$FeCl_4$] at 100 K.

Edimim[$FeCl_4$] at 100K			
Atom	*x/a*	*y/b*	*z/c*
Fe	0.5300(2)	1.7467(2)	1.2536(4)
Cl1	0.4423(3)	1.7756(3)	1.4559(4)
Cl2	0.3625(3)	1.7637(3)	1.0826(4)
Cl3	0.7005(4)	1.8427(3)	1.2174(4)
Cl4	0.6017(4)	1.6007(2)	1.2449(4)
C1''	0.0713(11)	0.8728(7)	1.3526(4)
H1A''	0.0102	0.8231	1.2918
H1B''	0.0047	0.9155	1.4102
H1C''	0.1432	0.837	1.4238
C1'	0.3789(10)	1.1206(7)	1.1917(4)
H1A'	0.3666	1.1675	1.2769
H1B'	0.3614	1.1545	1.0923
C2'	0.5220(11)	1.0850(7)	1.1970(4)
H2A'	0.5431	1.0507	1.2955
H2B'	0.592	1.1423	1.1893
H2C'	0.5352	1.0369	1.1138
C1'''	0.2771(11)	1.0208(8)	1.4519(4)
H1A'''	0.3459	1.0794	1.4568
H1B'''	0.3303	0.9612	1.4962
H1C'''	0.1893	1.0359	1.5097
C2	0.2343(11)	1.0012(8)	1.3040(4)
N3	0.1463(9)	0.9324(7)	1.2623(4)
N1	0.2778(9)	1.0443(7)	1.1936(4)
C5	0.2095(11)	1.0065(8)	1.0721(4)
H5	0.2187	1.0261	0.9695
C4	0.1287(11)	0.9365(7)	1.1165(4)
H4	0.0632	0.8956	1.0525

Full occupancies for all atoms.
a = 9.6703(1) Å, b = 14.3513(2) Å, c = 9.5744(1) Å, $\alpha = \gamma = 90^{o}$, β = 94.261(1)º, s.g. $P2_1/n$, B_{Fe} = 2.5(2) Å^2, B_{Cl} = 2.9(1) Å^2, B_{Edimim} = 3.2(2) Å^2

Table S2. Final refined positional coordinates obtained from X Ray single crystal diffraction of Edimim[$FeBr_4$] at 100 K.

Edimim[$FeBr_4$] at 100K			
Atom	*x/a*	*y/b*	*z/c*
Fe	0.2999(3)	0.73410(14)	0.7427(3)
Br1	0.4534(2)	0.62359(11)	0.5637(3)
Br2	0.4247(2)	0.73187(12)	1.0494(2)
Br3	0.3449(2)	0.87866(10)	0.6117(2)
Br4	-0.0321(2)	0.70335(11)	0.7492(2)
C1''	1.088(3) -	1.1013(15)	0.263(3)
H1A''	0.9990	1.1233	-0.3584
H1B''	1.2036	1.0768	-0.3211
H1C''	1.1248	1.1512	-0.1806
C1'	0.948(2)	0.8567(10)	0.200(2)
H1A'	1.0849	0.8491	0.2369
H1B'	0.8960	0.7971	0.1629
C2'	0.836(3)	0.8954(19)	0.354(3)
H2A'	0.8430	0.8546	0.4606
H2B'	0.7019	0.9028	0.3146
H2C'	0.8899	0.9543	0.3885
C1'''	1.260(4)	1.003(2)	0.086(5)
H1A'''	1.2890	0.9614	0.1889
H1B'''	1.2572	1.0649	0.1320
H1C'''	1.3599	0.9970	-0.0078
C2	1.063(3)	0.9783(19)	0.000(4)
N3	0.991(4)	1.0267(17)	-0.150(4)
N1	0.930(3)	0.9221(14)	0.045(3)
C5	0.789(4)	0.9298(19)	-0.078(5)
H5	0.6857	0.8882	-0.0849
C4	0.804(4)	-1.000(2)	0.190(5)
H4	0.7119	1.0249	-0.2740

Full occupancies for all atoms.
a = 6.957(6) Å, *b* = 14.804(12) Å, *c* = 7.232(6) Å, α = γ = 90º, β = 90.728(14) º, s.g. $P2_1$,

Table S3. Anisotropic displacement parameters ($Å^2x10^3$) for Edimim[$FeBr_4$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2a^{*2}U_{11} + ... + 2\, h\, k\, a^*\, b^*\, U_{12}\,]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br(1)	26(1)	43(1)	47(1)	0(1)	7(1)	-8(1)
Br(2)	36(1)	42(1)	33(1)	4(1)	0(1)	3(1)
Br(3)	33(1)	30(1)	39(1)	6(1)	5(1)	-6(1)
Br(4)	38(1)	38(1)	48(1)	-11(1)	6(1)	11(1)
Fe(1)	26(1)	24(1)	32(1)	2(1)	4(1)	1(1)
C(1A)	49(10)	82(16)	30(12)	12(10)	5(9)	-7(10)
C(5A)	27(7)	33(9)	25(9)	5(7)	10(6)	-2(6)
C(6A)	43(10)	130(20)	62(17)	52(15)	26(9)	44(12)
C(3A)	32(13)	49(18)	42(19)	-20(16)	-8(13)	26(12)
C(2A)	31(8)	29(9)	28(11)	1(7)	2(8)	15(8)
N(1A)	45(9)	37(8)	28(10)	-1(7)	-12(8)	16(9)
N(2A)	25(8)	20(7)	37(10)	4(7)	-4(8)	5(7)
C(4A)	33(9)	32(10)	23(11)	-1(9)	-11(8)	3(8)
C(7A)	40(9)	35(10)	23(10)	-6(8)	-7(8)	8(8)
C(1B)	49(10)	82(16)	30(12)	12(10)	5(9)	-7(10)
C(5B)	27(7)	33(9)	25(9)	5(7)	10(6)	-2(6)
C(6B)	43(10)	130(20)	62(17)	52(15)	26(9)	44(12)
C(3B)	32(13)	49(18)	42(19)	-20(16)	-8(13)	26(12)
C(2B)	31(8)	29(9)	28(11)	1(7)	2(8)	15(8)
N(1B)	45(9)	37(8)	28(10)	-1(7)	-12(8)	16(9)
N(2B)	25(8)	20(7)	37(10)	4(7)	-4(8)	5(7)
C(4B)	33(9)	32(10)	23(11)	-1(9)	-11(8)	3(8)
C(7B)	40(9)	35(10)	23(10)	-6(8)	-7(8)	8(8)