Supplementary information

On the role of Fe-N-C geometry flip-flop on bistability in $Fe(tetrazol\text{-}2\text{-}yl)_4(C_2H_5CN)_2$ – type core based coordination network

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Contents:

Networks of intermolecular contacts involving perchlorate anions

In the complex **1** perchlorates participate in formation of intermolecular contacts (Table S2) with hydrogen atoms of ebtz (Fig. S1) as well as propionitrile molecules (Fig. S2). Each anion interacts with three propionitrile molecules coming from two neighboring layers and at the same time each propionitrile molecule interact with three anions. After HS→LS disordering of perchlorate anions disappears. In LS phase, intermolecular contacts C21-H21B...O2(1/2+x,1/2-y,1/2+z), C21-H21A...O3(-1/2+x,1/2-y,1/2+z), C21-H21A...O1(-1/2+x,1/2-y,1/2+z), C22-H22A...O1(x, y, 1+z) involving propionitrile molecule are shortened in relation to HS form.

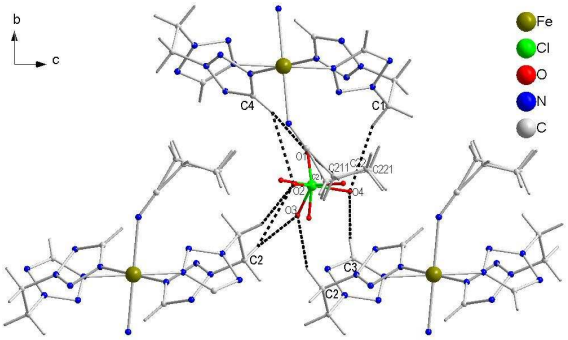

Figure S1. C-H···O intermolecular contacts (dotted lines) established between perchlorate anion and ebtz molecules in **1**. Only contacts involving major component of disordered anion was showed.

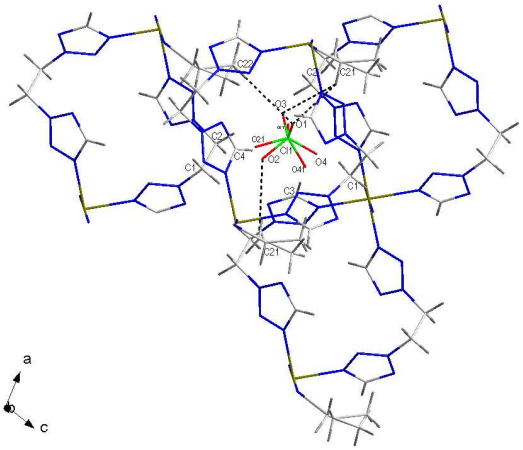

Figure S2. Network of $C_{propionitrile}$-H···O contacts (tick dotted lines) in **1** (250 K). Only contacts involving major component of disordered anion and propionitrile were showed.

Table. S1. Selected C-H···N interatomic distances [Å] and angles [°] for **1** (* - heating mode, ** - fast cooling).

	250(2) K		160(2) K		110(2) K		100(2) K**		80(2) K		110(2) K*		120(2) K*		160(2) K*	
	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A
C2-H2B...N1[a]	3.483(3)	122.1	3.447(3)	121.7	3.427(3)	121.8	3.439(2)	122.6	3.489(4)	116.3	3.493(4)	116.0	3.500(3)	116.2	3.444(4)	121.9
C1-H1A...N1[a]	3.562(3)	121.0	3.533(3)	120.5	3.524(3)	120.0	3.556(2)	119.9	3.420(4)	127.6	3.424(4)	127.7	3.430(4)	127.8	3.534(4)	120.4
C4-H4A...N3[b]	3.272(3)	117.2	3.271(3)	118.2	3.270(3)	118.8	3.302(2)	119.0	3.059(4)	114.6	3.064(4)	114.1	3.060(4)	114.2	3.271(4)	118.4
C21-H21B...N1[c] (***)	3.659(16)	154.8	3.565(11)	154.6	3.558(3)	153.8	3.561(3)	154.7	3.413(4)	131.0	3.425(4)	131.3	3.431(4)	144.9	3.560(4)	153.0
C211-H21D...N1[c] (***)	3.45(3)	136.2	3.59(6)	128.5												
C22-H22A-N5[c] (***)	3.687(9)	128.3	3.652(6)	123.7	3.638(3)	124.2	3.635(2)	123.2	3.496(4)	143.6	3.501(4)	144.2	3.460(10)	141.1	3.656(8)	125.4
C221-H22D...N5[c] (***)	3.389(19)	125.5	3.34(3)	129.4	3.28(5)	124.3									3.36(3)	125.1

[a]1-x,-y,2-z; [b]1-x,-y,1-z; [c]1/2-x,1/2+y,3/2-z

(***) atom names containing two digits were used for component with greater occupancy factor at given temperature

Table S2. Selected C-H···O interatomic contacts [Å] and angles [°] for **1** (* heating mode, ** - fast cooling).

	250(2) K		160(2) K		110(2) K		100(2) K**		80(2) K		110(2) K*		120(2) K*		160(2) K*	
	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A	D···A	<D-H···A
C1-H1A···O2[a]	3.157(5)	115.6	3.133(3)	114.7	3.124(3)	114.7	3.129(2)	114.4	3.104(3)	108.9	3.112(3)	109.1	3.118(3)	109.4	3.127(4)	114.6
C1-H1B...O1[b]	3.589(3)	152.4	3.588(3)	149.9	3.588(3)	148.8	3.631(2)	147.5	3.520(3)	152.4	3.529(4)	152.7	3.531(3)	152.7	3.587(4)	150.1
C1-H1B···O4[b]	3.476(5)	151.1	3.437(4)	152.9	3.415(3)	153.8	3.424(2)	155.0	3.396(4)	147.5	3.403(4)	147.7	3.414(3)	147.8	3.436(4)	152.4
C2-H2A···O2[a]	3.358(5)	124.2	3.324(4)	124.0	3.297(3)	124.1	3.300(2)	124.0	3.391(3)	121.9	3.396(4)	122.0	3.399(3)	122.2	3.313(4)	124.1
C2-H2A···O3[a]	3.526(6)	172.8	3.490(4)	173.8	3.470(3)	174.6	3.460(2)	173.9	3.448(3)	168.9	3.451(4)	168.9	3.458(3)	168.8	3.488(4)	173.8
C2-H2B···O3[c]	3.192(6)	117.4	3.173(4)	117.6	3.160(3)	117.8	3.172(2)	118.2	3.183(3)	116.6	3.182(4)	116.7	3.189(3)	116.7	3.181(4)	117.3
C3-H3A···O4[d]	3.287(5)	173.0	3.270(4)	173.2	3.269(3)	172.8	3.250(2)	173.2	3.187(4)	178.9	3.195(4)	179.2	3.197(4)	178.8	3.272(4)	173.0
C4-H4A···O1[e]	3.409(3)	149.4	3.352(3)	148.7	3.314(3)	148.3	3.301(2)	148.4	3.415(3)	145.6	3.411(4)	145.2	3.409(3)	145.4	3.354(4)	148.6
C4-H4A···O2[e]	3.612(7)	143.5	3.586(4)	142.7	3.589(4)	142.6	3.597(2)	142.8	3.435(4)	141.8	3.441(4)	142.6	3.452(4)	142.3	3.589(5)	142.6
C1-H1B···O41[b]	3.38(2)	141.3	3.35(3)	142.1	3.42(5)	144.7									3.36(4)	141.5
C2-H2A···O21[a]	3.32(3)	128.9	3.23(4)	128.8	3.21(5)	127.2									3.34(5)	129.3
C2-H2A···O31[a]	3.50(3)	160.2	3.46(5)	162.0	3.40(6)	162.0									3.58(6)	160.3
C3-H3A···O41[d]	3.17(2)	160.6	3.09(3)	162.2	2.99(5)	167.1									3.12(4)	160.3
C4-H4A···O21[e]	3.30(3)	137.4	3.31(4)	135.8	3.22(5)	133.8									3.22(5)	137.0
C21-H21B...O2[b]	3.58(2)	106.3	3.609(11)	104.0	3.594(4)	127.6	3.600(3)	102.2	3.314(4)	129.7	3.314(4)	129.6	3.317(4)	131.1	3.564(5)	124.8
C21-H21A...O3[f]	3.653(19)	131.8	3.569(10)	128.4	3.574(4)	164.5	3.563(2)	123.8	3.510(4)	176.7	3.511(4)	177.7	3.526(4)	174.2	3.589(5)	161.9
C21-H21A···O1[f]	3.425(18)	134.3	3.399(10)	131.1	3.403(3)	130.4	3.387(2)	128.4	3.327(4)	123.2	3.327(4)	124.2	3.341(4)	139.0	3.417(4)	131.9
C22-H22A...O1[g]	3.610(8)	132.3	3.595(5)	135.1	3.577(3)	134.8	3.589(2)	135.6	3.513(4)	121.0	3.514(4)	120.7	3.55(5)	130.6	3.590(7)	134.0
C22-H22B···O41[b]	3.14(3)	160.9	3.13(4)	163.4	3.25(7)	163.2									3.11(3)	160.2
C211-H21C···O1[f]	3.46(4)	119.4	3.48(6)	115.4												
C221-H22F···O21[g]	3.31(4)	123.3	3.22(6)	128.2	2.97(9)	121.9									3.27(7)	126.8
C221-H22D···O1[g]	3.53(2)	124.8	3.40(3)	116.2	3.24(5)	125.1							3.522(8)	117.1	3.43(3)	121.3
C211-H21D···O2[b]	3.42(4)	130.8	3.35(5)	140.2												

[a] 1+x,y,1+z; [b] 1/2+x,1/2-y,1/2+z; [c] 1-x,-y,1-z; [d] -x,-y,1-z; [e] 1/2-x,-1/2+y,1/2-z; [f] -1/2+x,1/2-y,1/2+z; [g] x, y, 1+z