

Supplementary material Dazem et al.

New 3-c binodal net noa

ToposPro output:

Coordination sequences

Node1: 1 2 3 4 5 6 7 8 9 10
Num 3 5 9 17 28 41 53 67 92 119
Cum 4 9 18 35 63 104 157 224 316 435

Node2: 1 2 3 4 5 6 7 8 9 10
Num 3 6 11 18 27 40 58 74 89 109
Cum 4 10 21 39 66 106 164 238 327 436

TD10=436

Vertex symbols for selected sublattice

Node 1 Point symbol:{4.8.10}
Extended point symbol:[4.8.10(3)]

Node 2 Point symbol:{8.10²}
Extended point symbol:[8.10.10]

Point symbol for net: {4.8.10}{8.10²}
3,3-c net with stoichiometry (3-c)(3-c); 2-nodal net

Systre optimised cell parameters and vertex positions

Ideal space group is Pmna.
Relaxed cell parameters:
a = 5.72536, b = 2.91682, c = 3.34772
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 55.90638
Relaxed positions:
Node 1: 0.41267 0.33705 0.04637
Node 2: 0.29381 0.10081 0.12080

New 3-c trinodal net daz

ToposPro output:

Coordination sequences

Node1: 1 2 3 4 5 6 7 8 9 10
Num 3 6 12 21 36 55 74 98 125 156
Cum 4 10 22 43 79 134 208 306 431 587

Node2: 1 2 3 4 5 6 7 8 9 10
Num 3 6 12 22 35 54 75 98 124 160
Cum 4 10 22 44 79 133 208 306 430 590

Node3: 1 2 3 4 5 6 7 8 9 10
Num 3 6 12 21 36 55 74 102 131 156
Cum 4 10 22 43 79 134 208 310 441 597

TD10=591

Vertex symbols for selected sublattice

Node1 Point symbol:{8³}
Extended point symbol:[8.8.8]

Node2 Point symbol:{8.10²}
Extended point symbol:[8(2).10.10]

Node3 Point symbol:{8³}
Extended point symbol:[8.8.8]

Point symbol for net: {8.10²}{8³}₂
3,3,3-c net with stoichiometry (3-c)(3-c)(3-c); 3-nodal net
Systre optimised cell parameters and vertex positions

Ideal space group is C222.
Relaxed cell parameters:
a = 4.86168, b = 1.88162, c = 3.37216
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 30.84800
Relaxed positions:
Node 1: 0.25000 0.25000 0.65320
Node 2: 0.25000 0.75000 0.05025
Node 3: 0.10284 0.00000 0.50000

Topological type: 3,3,3T12 (topos&RCSR.ttd) {8.10²}{8³}₂ -
VS [8.8.8] [8(2).10.10] [8.8.8]

New 3-c, 4-c binodal net mys

ToposPro output:

Coordination sequences

Node 1: 1 2 3 4 5 6 7 8 9 10
Num 4 8 14 28 46 62 82 112 140 168
Cum 5 13 27 55 101 163 245 357 497 665

Node 2: 1 2 3 4 5 6 7 8 9 10
Num 3 7 15 26 42 61 82 110 138 169
Cum 4 11 26 52 94 155 237 347 485 654

TD10=656

Vertex symbols for selected sublattice

Node 1 Point symbol:{6².8².10²}
Extended point symbol:[6.6.8(2).8(2).10(2).10(2)]

Node 2 Point symbol:{6.8²}
Extended point symbol:[6.8.8]

Point symbol for net: {6.8²}₄{6².8².10²}
3,4-c net with stoichiometry (3-c)₄(4-c); 2-nodal net

Systre optimised cell parameters and vertex positions

Ideal space group is Pmna.
Relaxed cell parameters:
a = 3.91944, b = 2.05102, c = 2.93442
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 23.5893
Relaxed positions:
Node 1: 0.32621 0.18200 0.11336
Node 2: 0.00000 0.50000 0.50000

New 3-c 8-c binodal net hum

ToposPro output

Coordination sequences

Node1: 1 2 3 4 5 6 7 8 9 10
Num 8 22 54 84 146 186 284 330 468 514
Cum 9 31 85 169 315 501 785 1115 1583 2097

Node2: 1 2 3 4 5 6 7 8 9 10
Num 3 19 46 90 128 205 251 366 415 573
Cum 4 23 69 159 287 492 743 1109 1524 2097

TD10=2097

Vertex symbols for selected sublattice

Node1 Point symbol: {4⁴4.5⁶6.6¹⁰7⁵8²9}
Extended point
symbol: [4.4.4.4.5.5.5.5.5.6.6.6(3).6(3).6(3).6(4).6(4).6(4).6(4).7(2).7(4).7(4).7(4).7(4).8(5).8(5).9(24)]

Node2 Point symbol: {4²5}
Extended point symbol: [4.4.5(2)]

Point symbol for net: {4²5}2{4⁴4.5⁶6.6¹⁰7⁵8²9}
3,8-c net with stoichiometry (3-c)2(8-c); 2-nodal net

Systre optimised cell parameters and vertex positions

Ideal space group is Fddd.

Relaxed cell parameters:

a = 3.37171, b = 1.00000, c = 5.90566

alpha = 90.0000, beta = 90.0000, gamma = 90.0000

Cell volume: 19.91224

Relaxed positions:

Node 1: 0.12500 0.12500 0.12500

Node 2: 0.12500 0.12500 0.29433

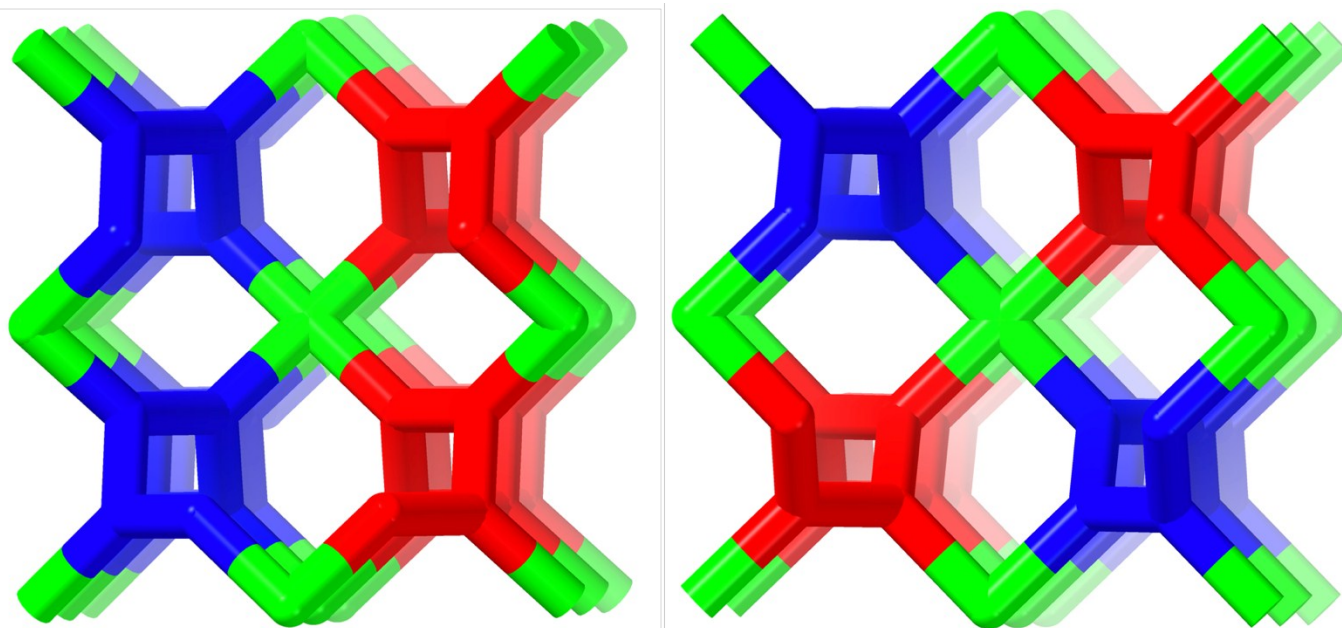


Fig. S1 The 3-c, 4-c **mys-net** left and the **jph-net** right

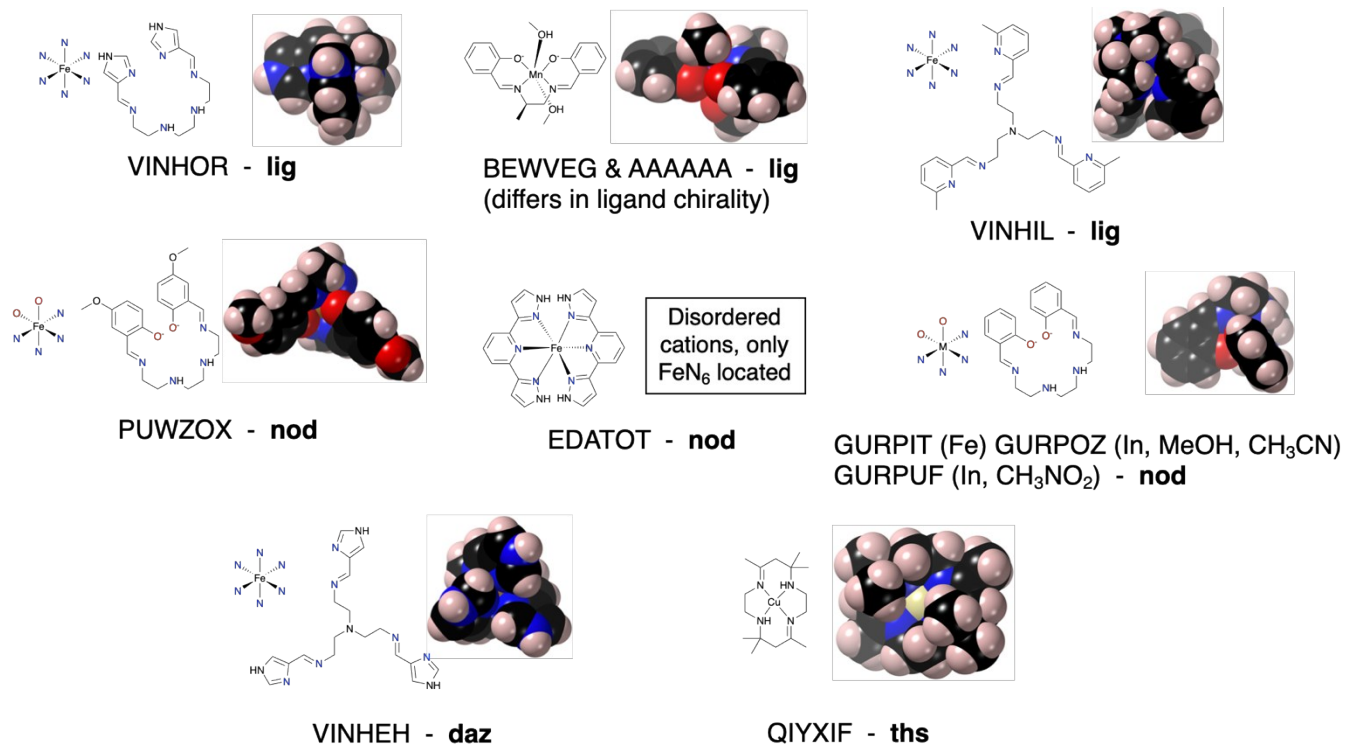


Fig. S2 Structure drawings and space filling models from the X-ray diffraction structures of selected counter ions in Table 1.