How 2-periodic coordination networks are interweaved: entanglement isomerism and polymorphism

Eugeny V. Alexandrov,[1] *Vladislav A. Blatov*,[1] *Davide M. Proserpio*[2,1]

1) Samara Center for Theoretical Materials Science (SCTMS), Samara University, Ac. Pavlov Street 1, Samara 443011, Russia.
2) Dipartimento di Chimica, Università degli Studi di Milano, Via C. Golgi 19, 20133, Milano, Italy.

e-mail : E.V. A. aleksandrov_ev1@mail.ru, V.A.B. blatov@samsu.ru, D.M.P. davide.proserpio@unimi.it

SUPPLEMENTARY INFORMATIONS

Layer	Entang type	DOC, IS, Z	HRN	ERN	hits	RCSR
sql	ICAT	DOC 1/1 d/d	2C1	6T13	105	sql-c*
sql	ICAT	DOC 1/1 p/p	2C1	6-c sqc23	35	sql-c
sql	ICAT	DOC 2/2/2	2C1	6T225	3	sql-c3*
sql	ICAT	DOC 1/1/1	2C1	6T225	5	sql-c3
hcb	ICAT	DOC 1/1	2C1	8T190	13	hcb-c
hcb	ICAT	DOC 1/1/1	2C1	8T758	2	hcb-c3

Table S1: The correspondence between names ERN and RCSR for six entanglements of inclined polycatenation see http://rcsr.net/nets and C. Bonneau and M. O'Keeffe, *Acta Crystallogr*., *Sect. A*: *Found. Crystallogr*., 2015, **71**, 82.
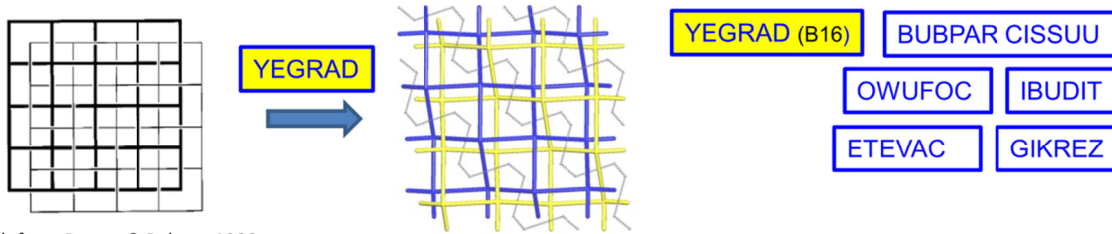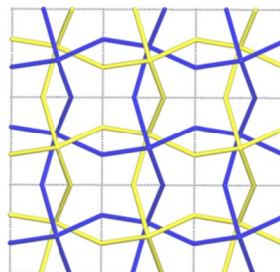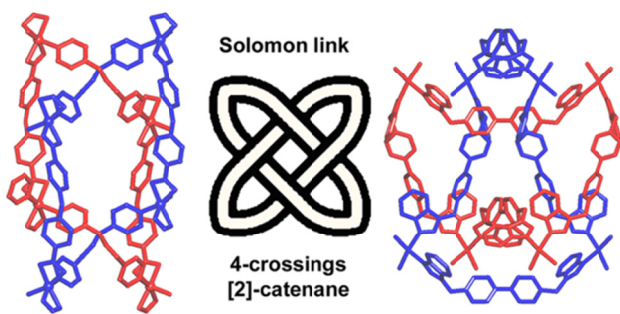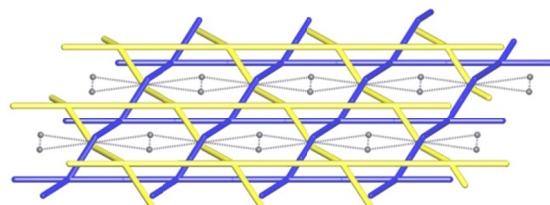
Figure 16b from Batten & Robson 1998: Schematic representation of the mode of interpenetration observed in YEGRAD

YEGRAD

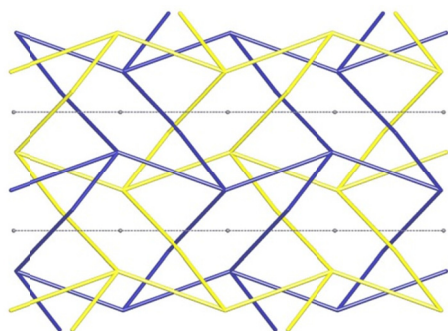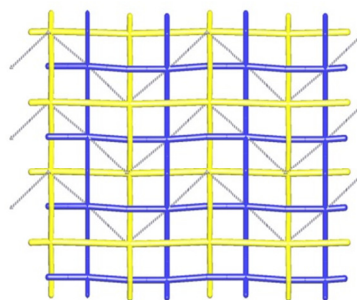YEGRAD (B16) BUBPAR CISSUU OWUFOC IBUDIT ETEVAC GIKREZ

Solomon link

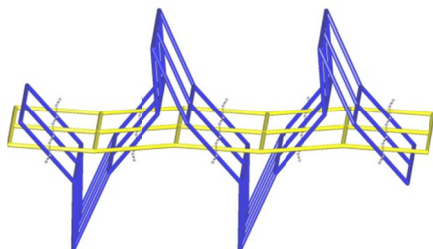4-crossings [2]-catenane

5 Solomon link A

2-fold interpenetration sql
8 less frequent patterns
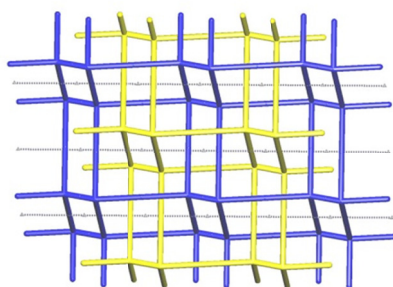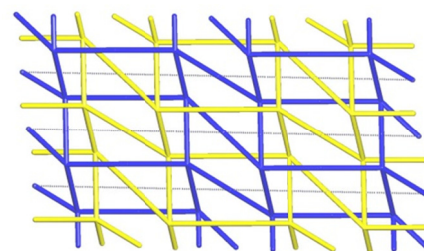
5 Solomon link B

BUBPAR, CISSUU

GIKREZ

OWUFUC

IBUDIT

ETEVAC

Figure S1. Eight less frequent patterns of catenation observed for 2-fold interpenetrated **sql**.

Interpenetration:
2-fold sql with 2-loops

48 *2-loop* **sql** 2-fold → **6 HRN** / **6 different** *2-periodic* →

6 Extended ring nets ERN

39 2,6L1 (B20) **81.2 %**

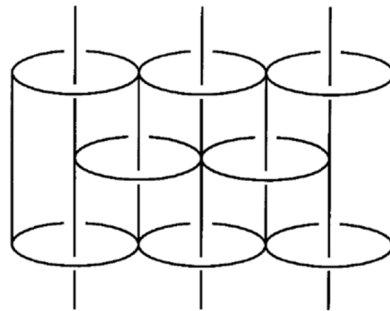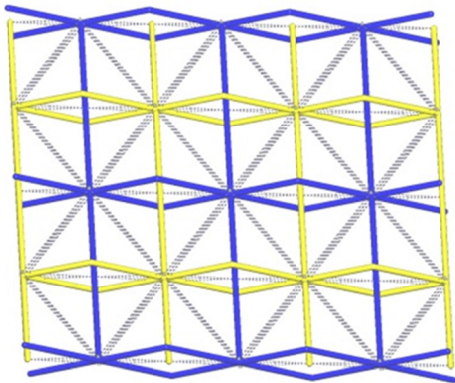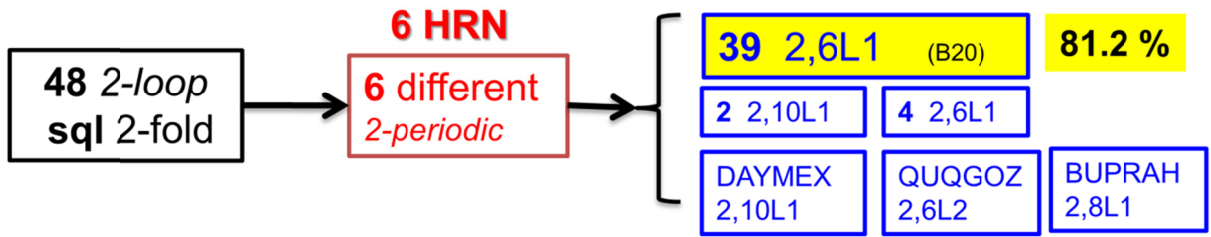**2** 2,10L1 | **4** 2,6L1

DAYMEX 2,10L1 | QUQGOZ 2,6L2 | BUPRAH 2,8L1

Figure 20 from Batten & Robson 1998

Figure 20. Schematic representation of the two parallel interpenetrating (4,4) nets in [Mn(3)₃](ClO₄)₂ showing the polyrotaxane/polycatenane associations. Six-connected nodes are provided by six-coordinate Mn, and connections between the nodes by ligand **3**.
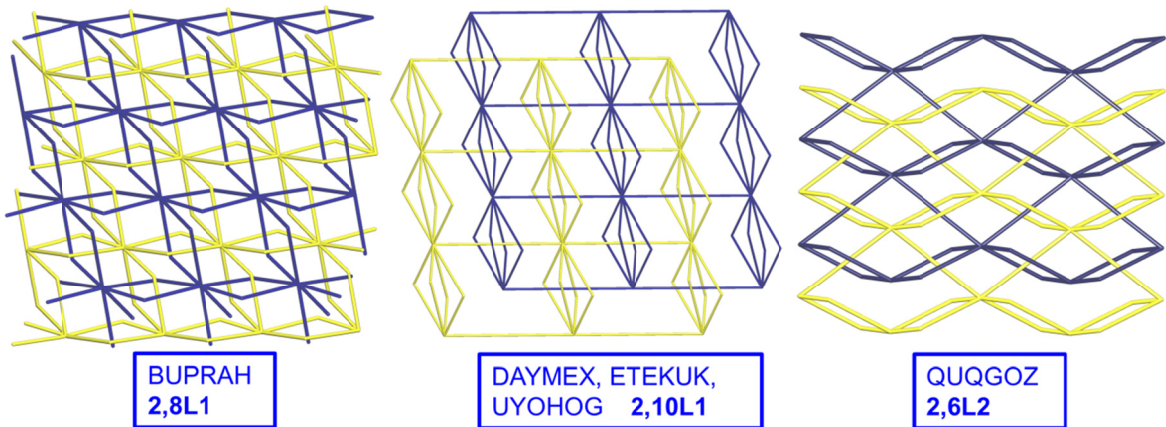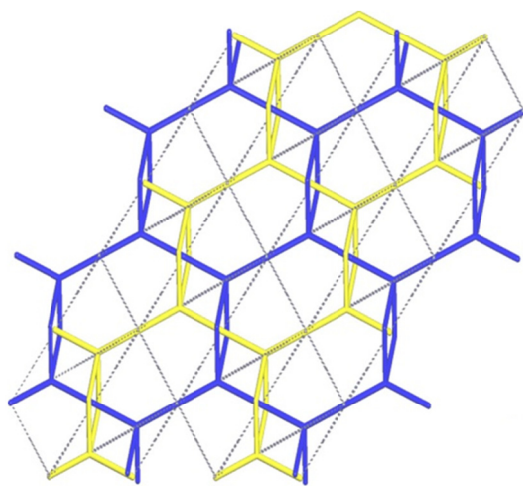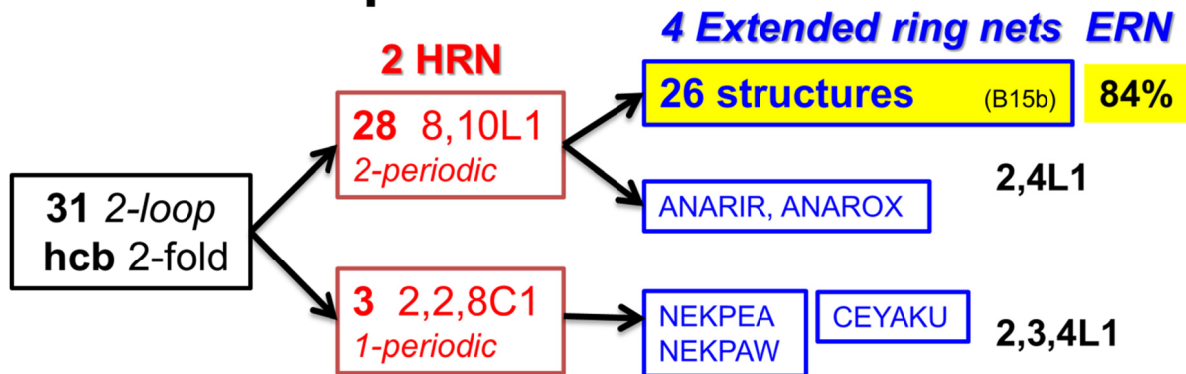

BUPRAH 2,8L1 | DAYMEX, ETEKUK, UYOHOG 2,10L1 | QUQGOZ 2,6L2

Figure S2. The classification of the patterns observed for the 48 2-fold interpenetrated **sql** with 2-loops. The most frequent one is illustrated side by side with the representation of Batten & Robson.

Interpenetration:
2-fold hcb with 2-loops

2 HRN

4 Extended ring nets ERN

31 *2-loop* **hcb** 2-fold

28 8,10L1
2-periodic

26 structures (B15b) **84%**

ANARIR, ANAROX

2,4L1

3 2,2,8C1
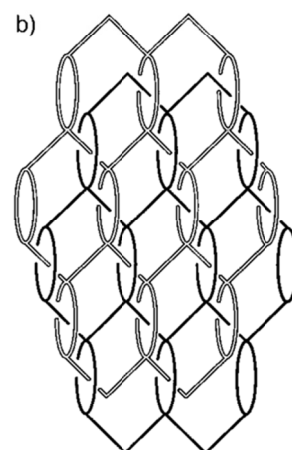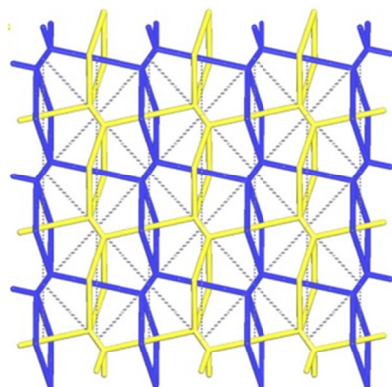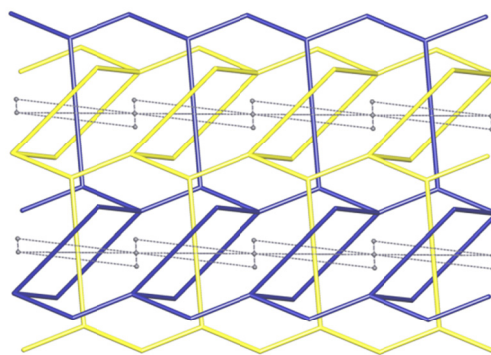*1-periodic*

NEKPEA NEKPAW   CEYAKU

2,3,4L1

2,4L1

b)

Figure 15b from Batten & Robson 1998:
Schematic representation of the two
interpenetrating nets observed in NEBSUI

ANARIR, ANAROX

2,4L1

NEKPEA, NEKPAW CEYAKU

2,3,4L1

Figure S3. The classification of the patterns observed for the 31 2-fold interpenetrated **hcb** with 2-loops. The most frequent one is illustrated in the middle side by side with the representation of Batten & Robson.