UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI CHIMICA

Lucia Carlucci & Gianfranco Ciani

Davide M Proserpio

Entanglements in periodic structures: old and new views

Vladislav Blatov & Evgeny Alexandrov
Igor Baburin

Samara Center
for Theoretical Materials Science

A. F. Wells

1954 - 1979

Acta Cryst. (1954). 7, 535

The Geometrical Basis of Crystal Chemistry. Part 1

By A. F. Wells

Imperial Chemical Industries Limited (Dyestuffs Division), Hexagon House, Manchester 9, England

(*Received* 1 *January* 1954 *and in revised form* 1 *April* 1954)

An investigation is made of the periodic three-dimensional systems of points in which each point is connected to three others. These nets form the bases of the structures of a large number of crystals in which there are directed bonds or hydrogen bonds

Structural Inorganic Chemistry

4th Edition

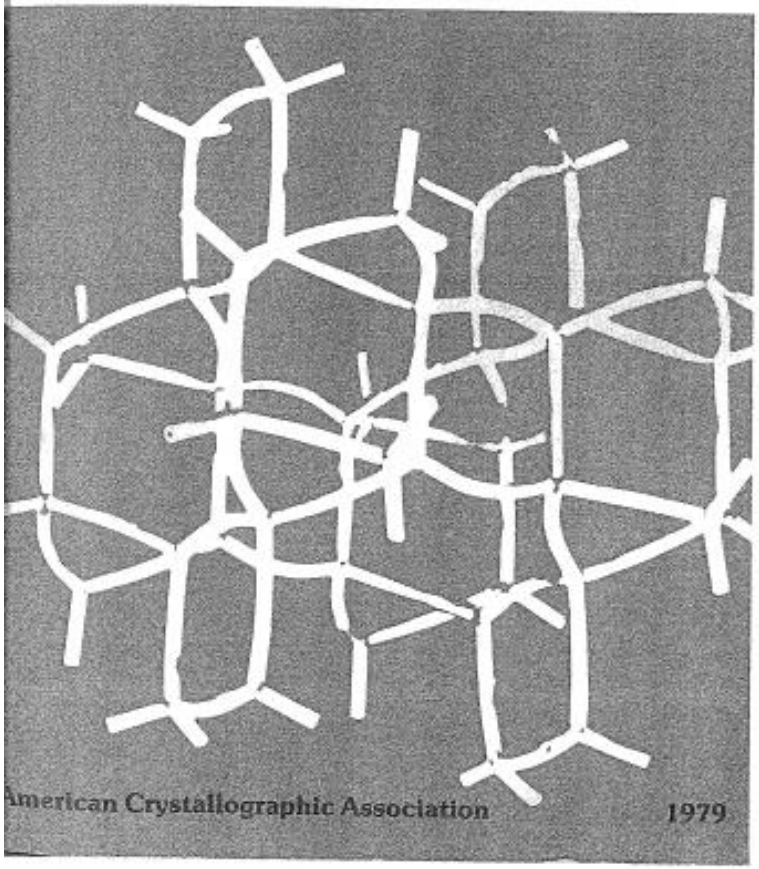
Three-dimensional nets and polyhedra

A. F. Wells

Department of Chemistry
and
Institute of Materials Science
University of Connecticut

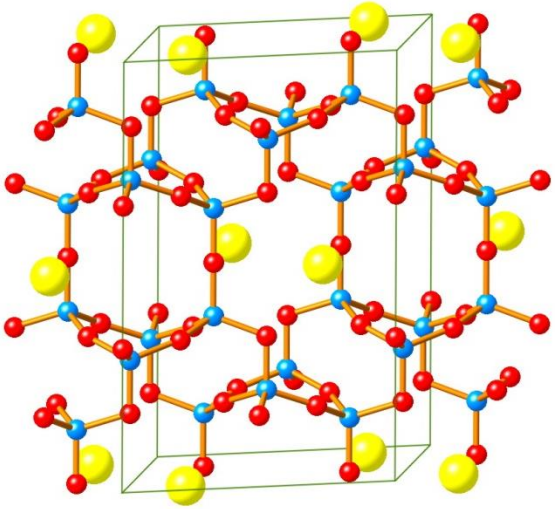
Further Studies of Three-dimensional Nets

A.F. Wells ACA Monograph No. 8

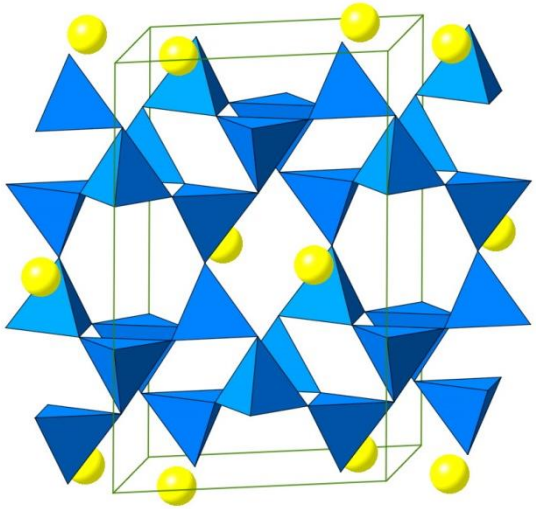


Three ways of drawing a feldspars

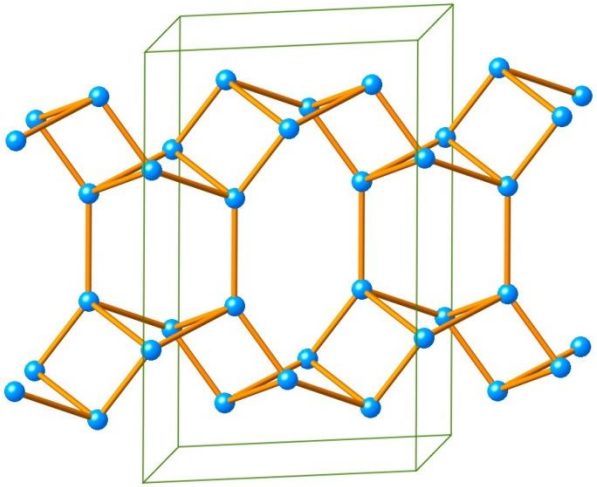
the most abundant minerals in the earth's crust $M[(Si/Al)_4O_8]$, e.g. albite, $Na(Si_3AlO_8)$, orthoclase, $K(Si_3AlO_8)$, anorthite, $Ca(Si_2Al_2O_8)$.



ball and stick



polyhedra



net

From the framework of alumino-silicates we get a **net** by **removing all 2-coordinated oxygen atoms -T-O-T-**

R. Robson 1989-

(Melbourne - Australia)

J. Am. Chem. Soc. **1989**, *111*, 5962–5964

Infinite Polymeric Frameworks Consisting of Three Dimensionally Linked Rod-like Segments

Bernard F. Hoskins and Richard Robson*

Department of Inorganic Chemistry
University of Melbourne
Parkville, Victoria, 3052, Australia

Received February 14, 1989

J. Am. Chem. Soc. **1990**, *112*, 1546–1554

Design and Construction of a New Class of Scaffolding-like Materials Comprising Infinite Polymeric Frameworks of 3D-Linked Molecular Rods. A Reappraisal of the $Zn(CN)_2$ and $Cd(CN)_2$ Structures and the Synthesis and Structure of the Diamond-Related Frameworks $[N(CH_3)_4][Cu^{I}Zn^{II}(CN)_4]$ and Cu^{I}[4,4′,4″,4‴-tetracyanotetraphenylmethane]$BF_4 \cdot xC_6H_5NO_2$

Scaffolding-Like Materials

Infinite Polymeric Frameworks

B. F. Hoskins and R. Robson*

> 1500 citations

Contribution from the Department of Inorganic Chemistry, University of Melbourne, Parkville, Victoria, 3052, Australia. Received July 12, 1989

A net-based approach to coordination polymers †

Richard Robson

School of Chemistry, University of Melbourne, Parkville, Victoria, 3052, Australia

Received 4th May 2000, Accepted 23rd June 2000
First published as an Advance Article on the web 9th October 2000
J. Chem. Soc., Dalton Trans., 2000, 3735–3744

DALTON PERSPECTIVE

early ´90

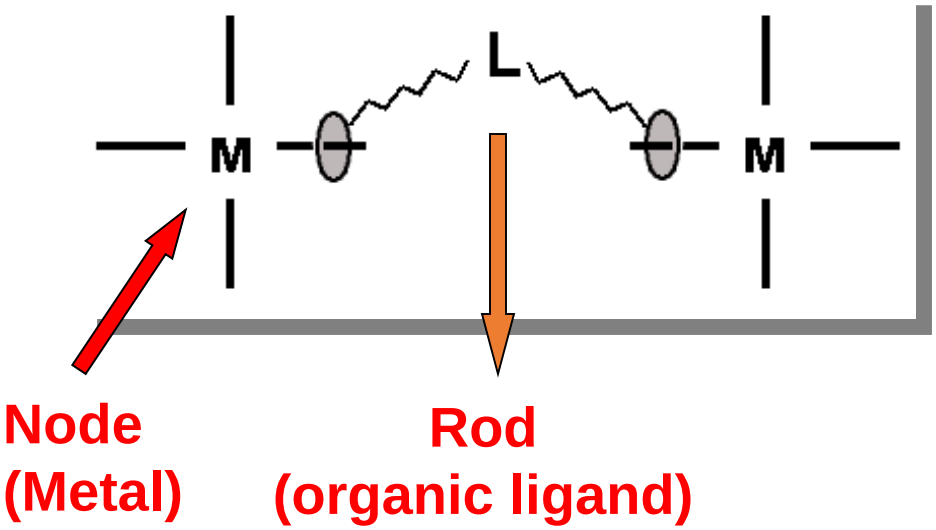
Infinite Polymeric Frameworks

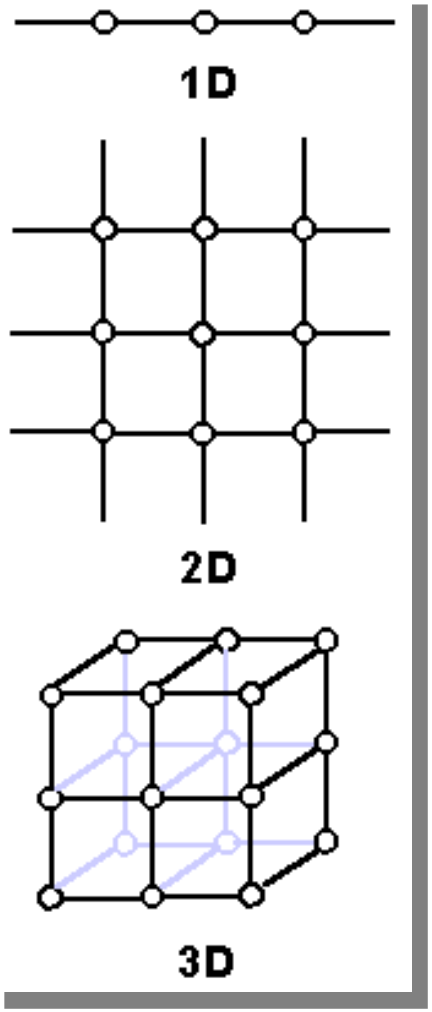
Organic/Inorganic Hybrid Materials

Coordination Polymers *(Networks)*

Metal Organic Frameworks (MOFs)

Coordination Networks
“Metal-organic Frameworks” MOF

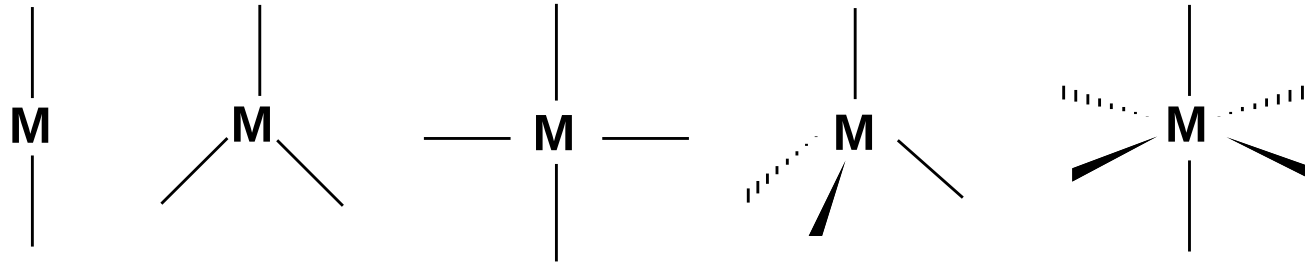




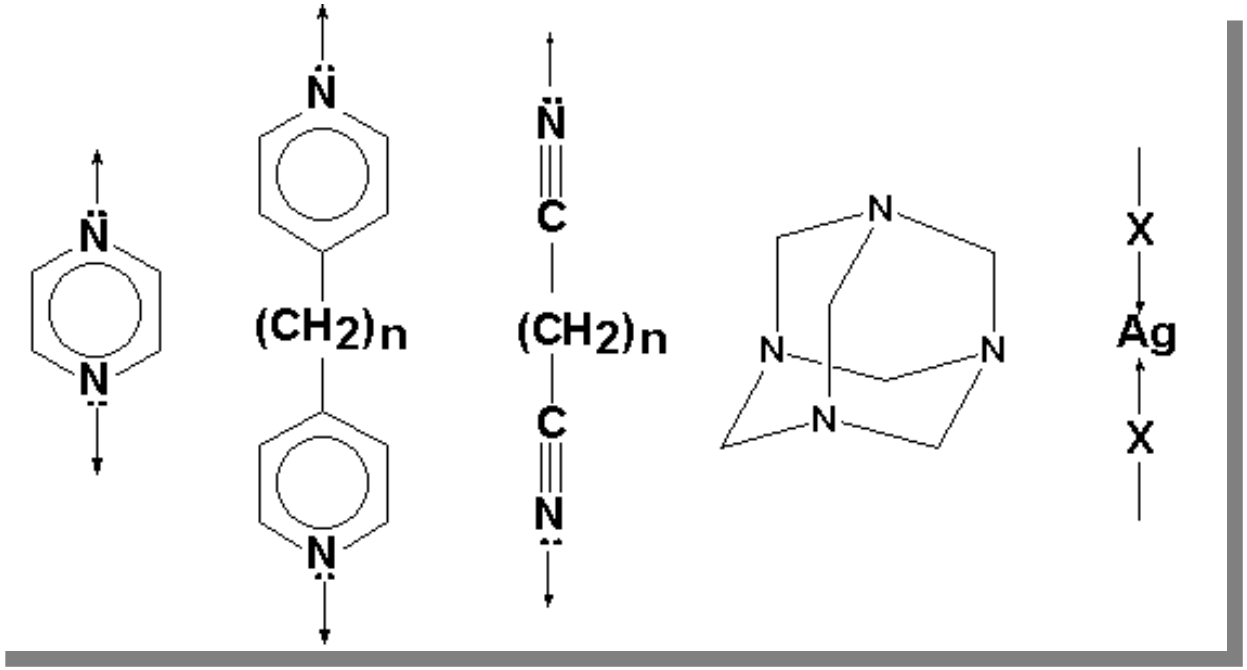
Different architectures could be obtained on varying the coordination geometry of the nodes...

Metal ions: Ag, Cu, Ni, Co, Zn, Cd…

coordination number and geometry



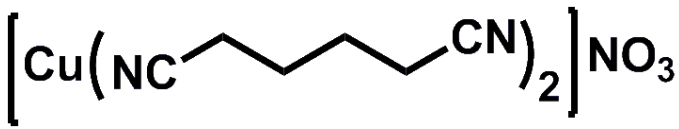
Ligands



donors: N, O, P, S
bi/polidentate
neutral/anionic
Length
rigidity/flexibility

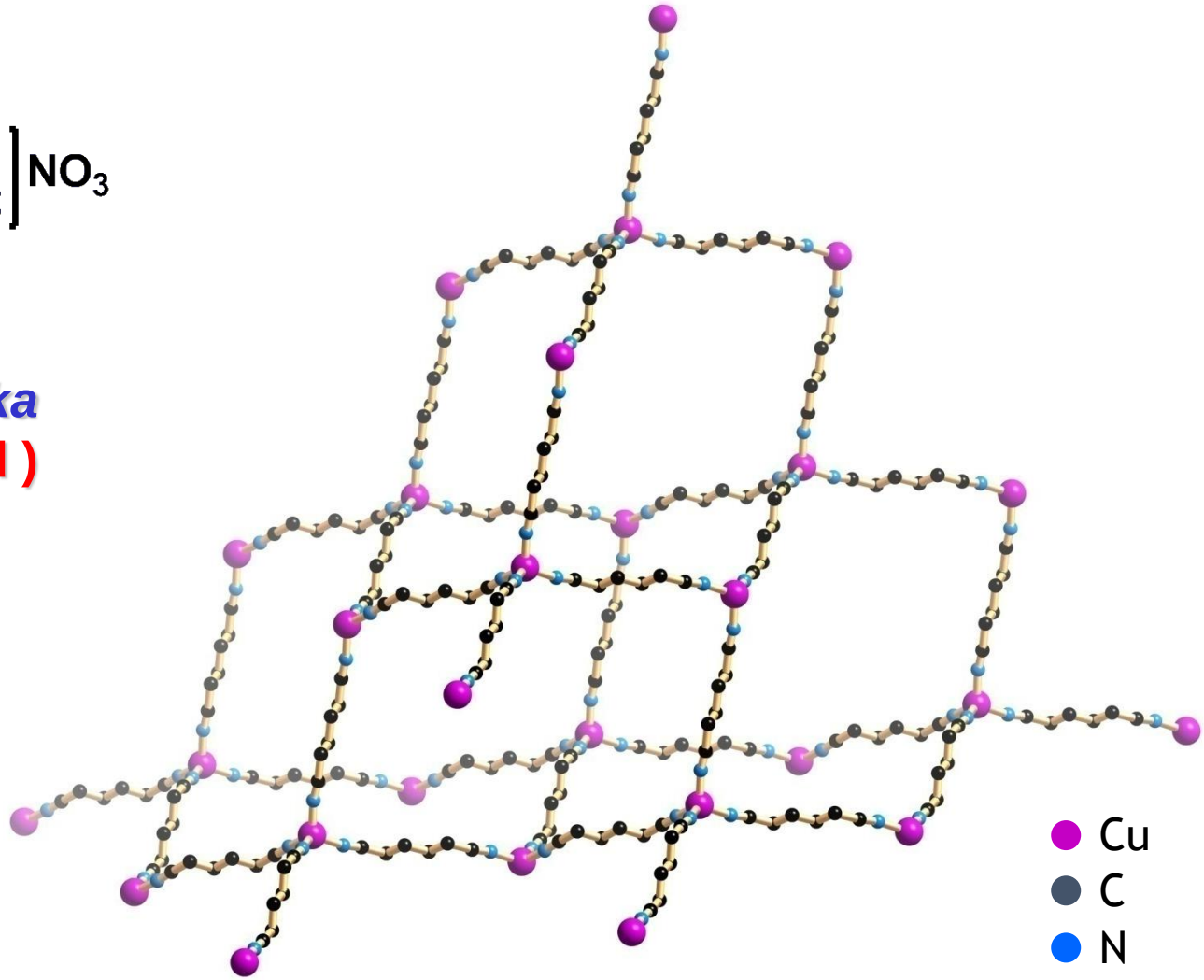
Coordination Network

1959



multiply intergrown *aka* interpenetrated (6-fold)

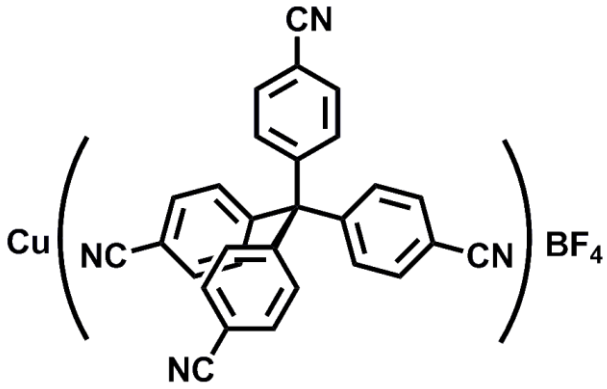
underlying net: diamondoid (dia)

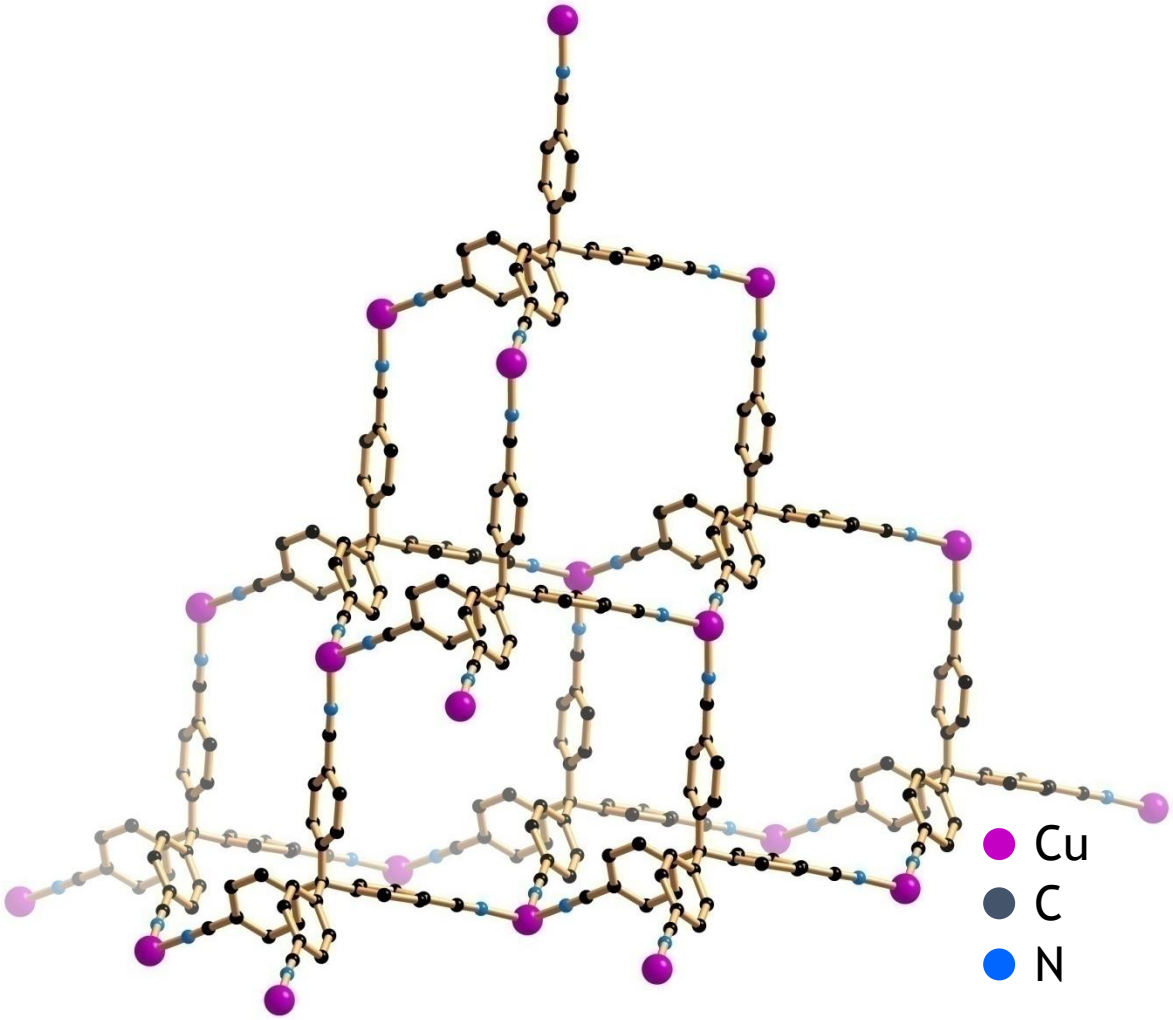


Kinoshita, Y., Matsubara, I., Higuchi, T. and Saito, Y. *Bull. Chem. Soc. Jpn* **1959**, 32, 1221

Coordination Network with polytopic links

1989





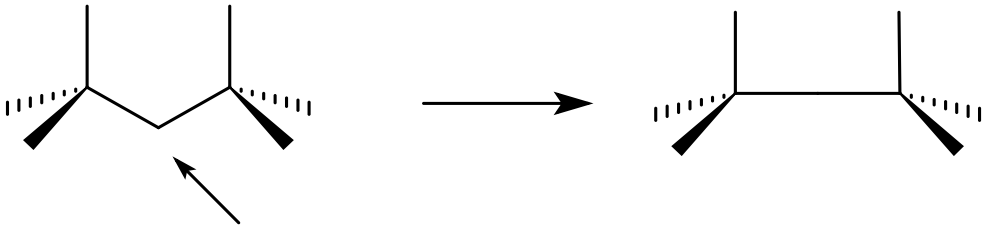
underlying net: dia

Hoskins, B. F. and Robson, R. *J. Am. Chem. Soc.* **1989**, 111, 5962–5964

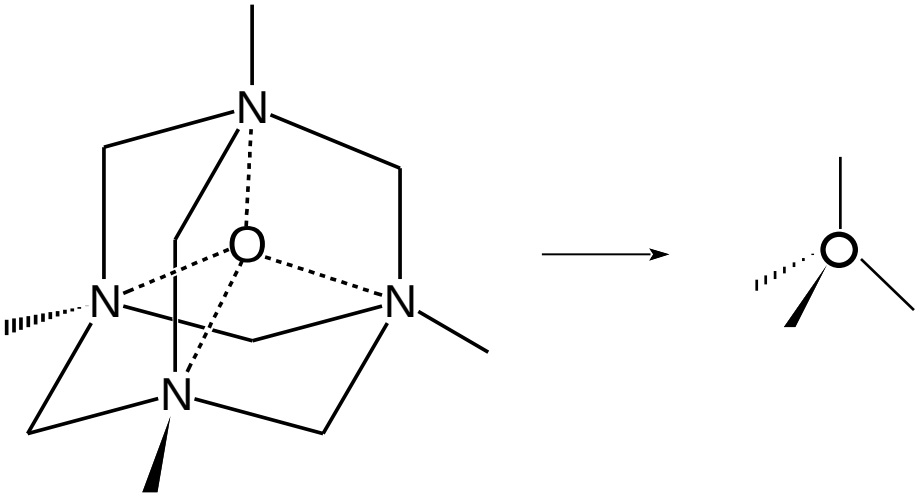
Simplifications:

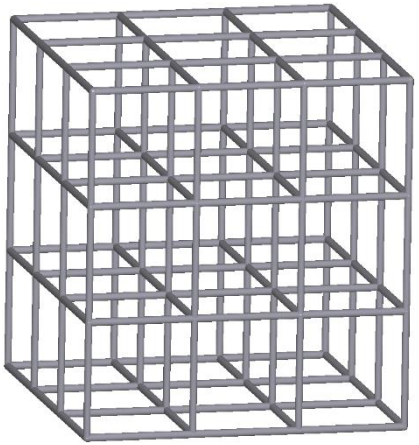
Keep only atoms with cooordination/connectivity > 2

Nodes/Vertex of the Net



Simplification of polydentate groups with centres of the same coord/conn





H. Li, M Eddaoudi, M. O'Keeffe, O.M. Yaghi

Nature 1999 **MOF-5**

(Metal-Organic Framework-5)

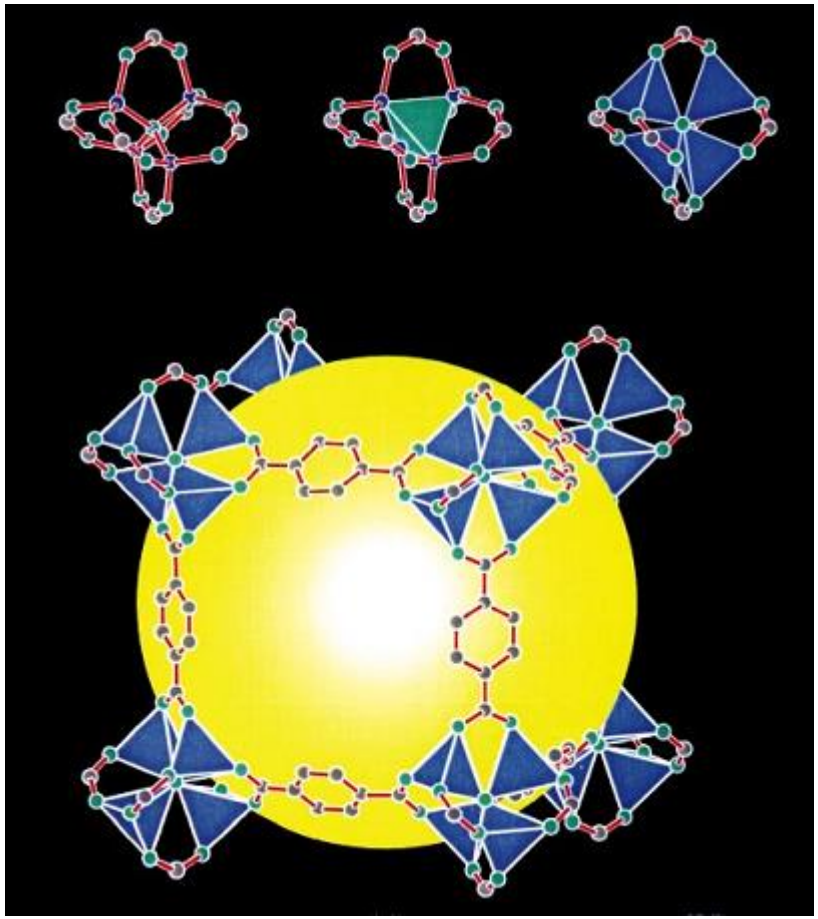
underlying net: pcu

Design and synthesis of an exceptionally stable and highly porous metal-organic framework

Hailian Li*, Mohamed Eddaoudi†, M. O'Keeffe* & O. M. Yaghi†

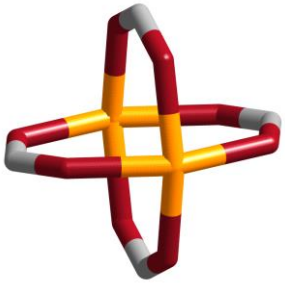
NATURE | VOL 402 | 18 NOVEMBER 1999 | w

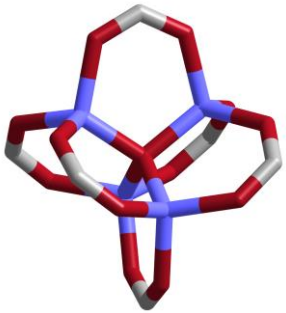
> 5000 citations



Reticular Chemistry

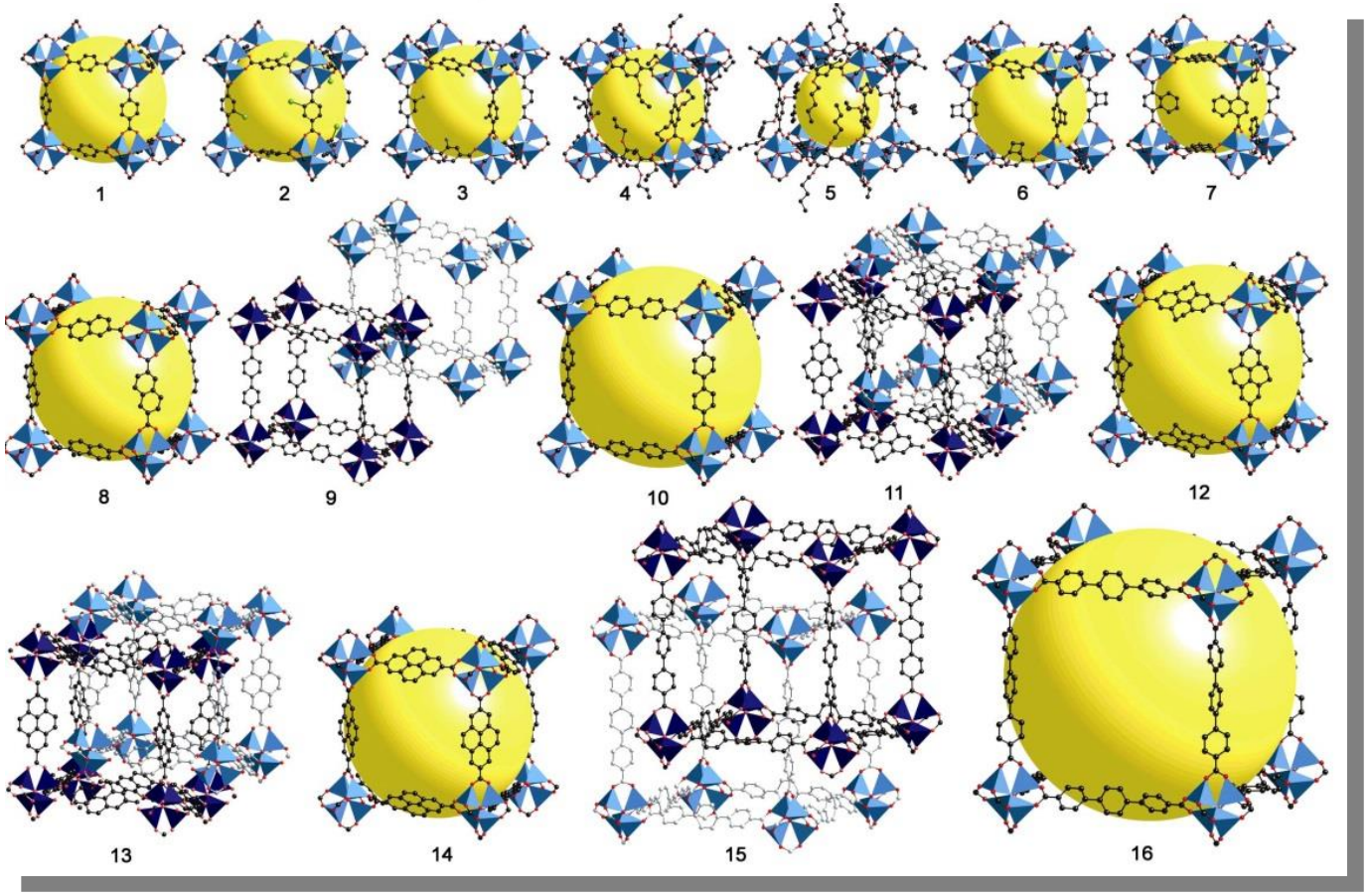
≈ 2000





O.M.Yaghi, M. O'Keeffe

Nature 2003 > 6500 citations



Why interest in Coordination Networks (MOFs) ?

Doubling time 3.9 yrs compared with 9.3 yrs for all CSD!

# of structures in CSD ≈ 900000

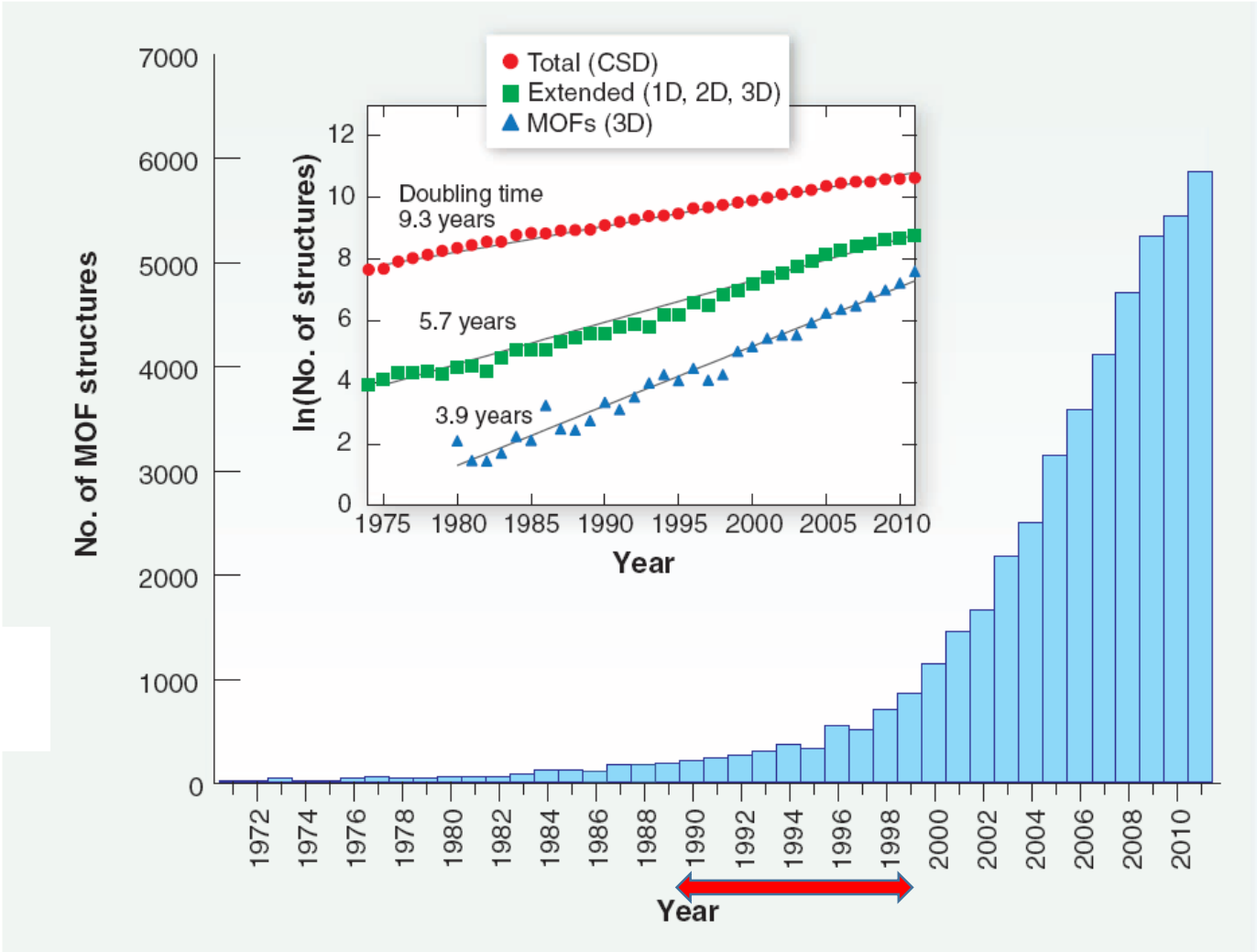


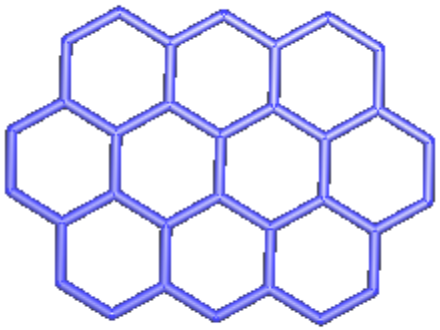
Fig. 1. Metal-organic framework structures (1D, 2D, and 3D) reported in the Cambridge Structural Database (CSD) from 1971 to 2011. The trend shows a striking increase during this period for all structure types. In particular, the doubling time for the number of 3D MOFs (inset) is the highest among all reported metal-organic structures.

A Net, as used in solid state chemistry, is a *n-periodic connected simple graph*

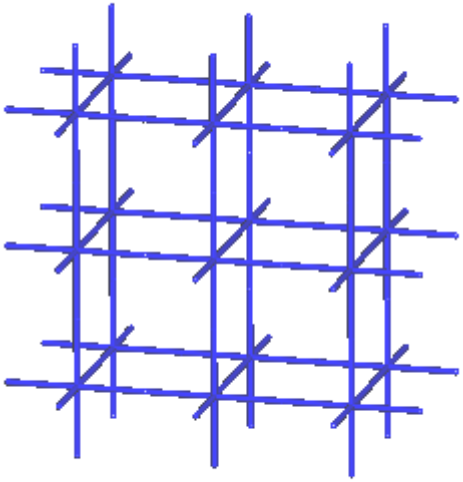
n-periodic **= has translational symmetry in *n*-independent directions**

connected **= there is a continuous path between every pair of vertices**

simple **= contains only simple edges**



2-p

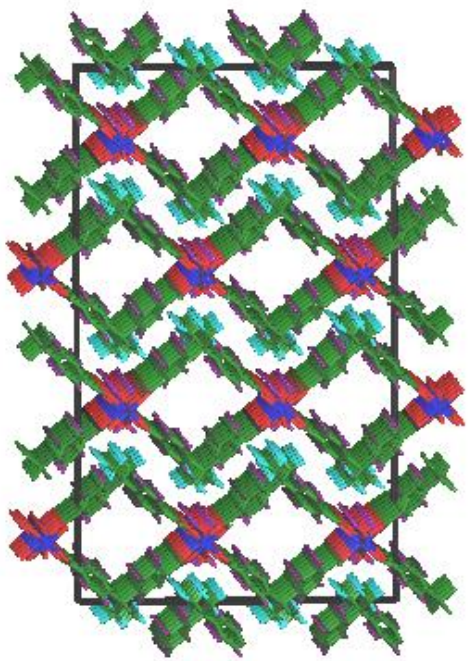


3-p

Periodic Structures and Crystal Chemistry

n-Periodic Structures

structures (as nets) that have **translational symmetry** in exactly *n* independent directions.



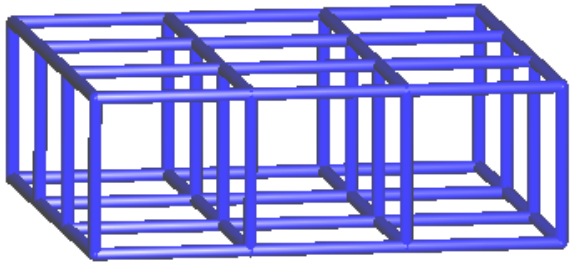
Any crystalline material is a 3D ordered arrangement of atoms

any crystal is a 3D supramolecular entity

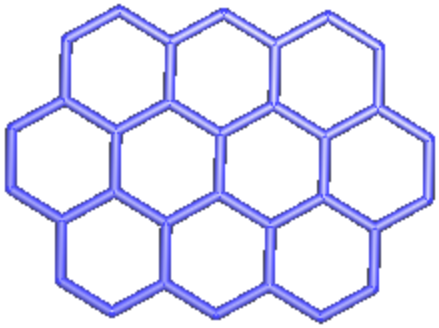
depending on the interactions considered we may "see" chains *1-periodic*, layers *2-periodic* or *3-periodic* netwoks

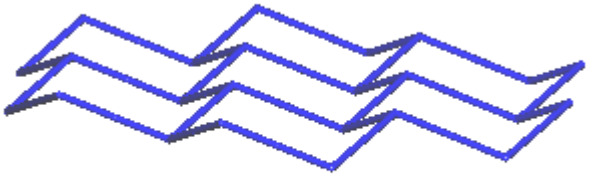
Double-layers are 3D 2-periodic

2-p 3D

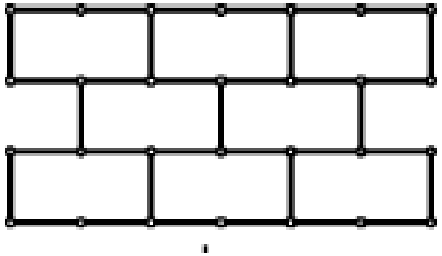


2-p 2D honeycomb layer

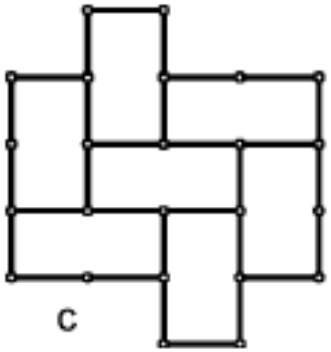




6^3-*hcb*



brick wall



parquet

Crystal Structures

↓

Underlying Net

↓

Entanglements

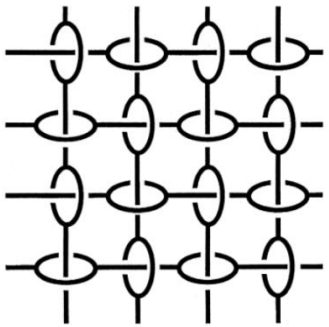
Angew. Chem. Int. Ed. **1998**, *37*, 1460 – 1494

1998

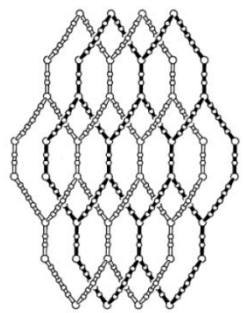
> 4500 citations

Interpenetrating Nets: Ordered, Periodic Entanglement

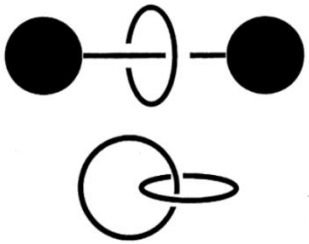
Stuart R. Batten and Richard Robson*



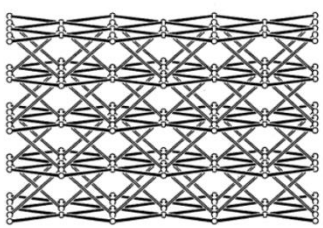
one-dimensional



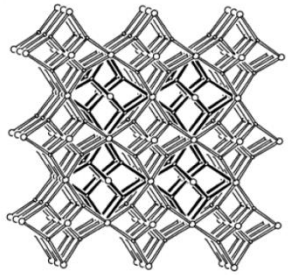
two-dimensional parallel



zero-dimensional



two-dimensional inclined



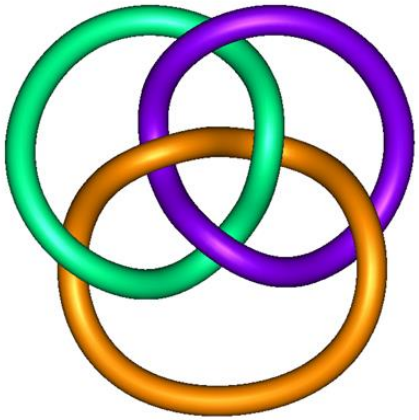
three-dimensional

Interpenetrating structures, are characterized by the presence of infinite structurally **regular motifs that must contain rings** through which independent components are inextricably entangled and that can be disentangled only by breaking internal connections

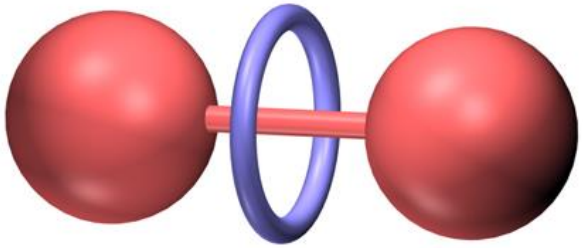
Hopf link

Geometrical requirement for Inextricable Entanglement

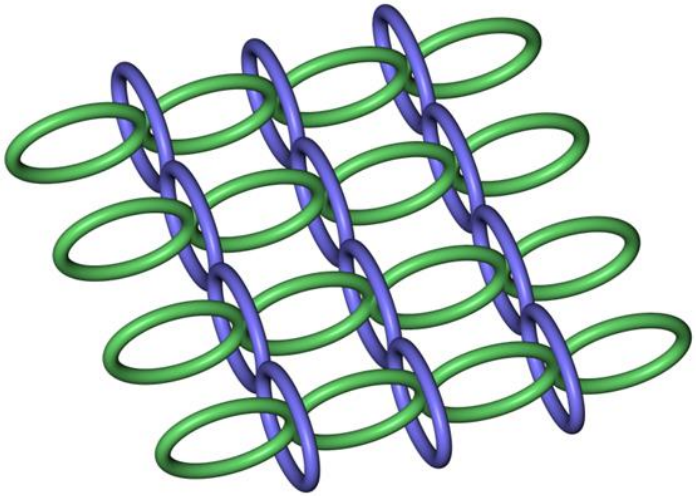
Hopf link



Borromean



[2]-rotaxane

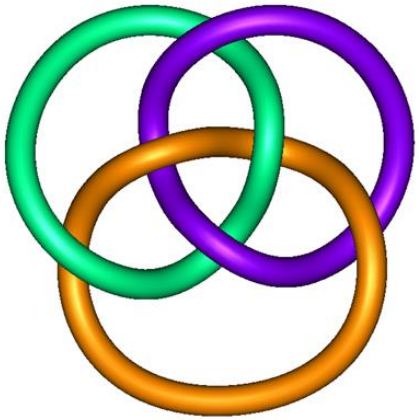


"Topological" Entanglement

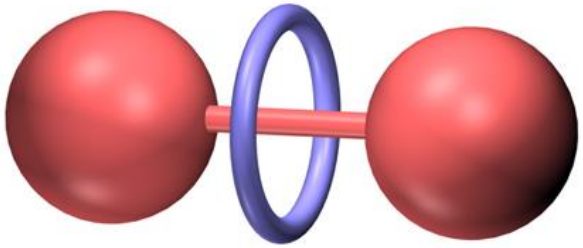
"Euclidean" Entanglement

Geometrical requirement for Inextricable Entanglement

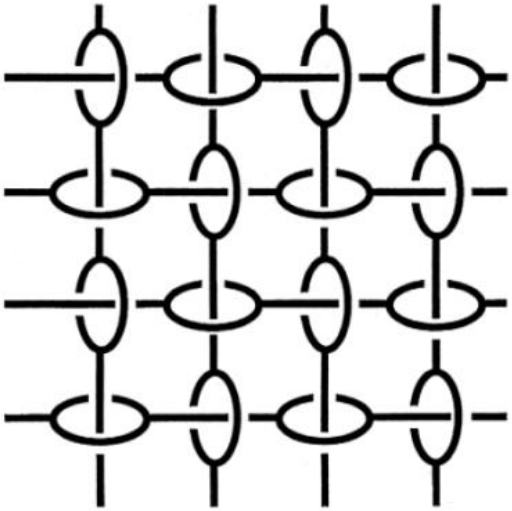
Hopf link



Borromean



[2]-rotaxane



"Topological" Entanglement

"Euclidean" Entanglement

interpenetration

Acta Cryst. (1954). **7**, 849

1954

The Geometrical Basis of Crystal Chemistry. Part 4

By A. F. Wells

Imperial Chemical Industries Limited (Dyestuffs Division), Hexagon House, Manchester 9, England

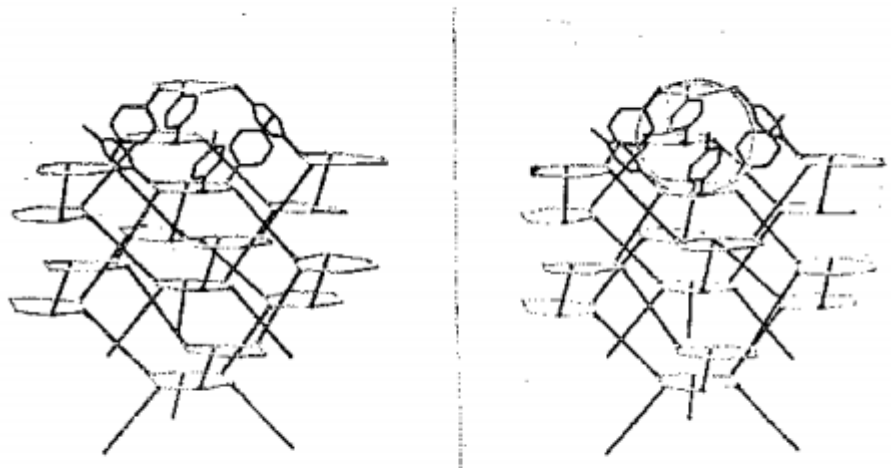
(*Received* 7 *May* 1954)

Structures based on a single net of low coordination number are unlikely to occur owing to their low densities. A study has therefore been made of systems of two or more interpenetrating three-dimensional networks. Some of the possible structure types are illustrated.

1947 quinol

50. *The Structure of Molecular Compounds. Part III. Crystal Structure of Addition Complexes of Quinol with Certain Volatile Compounds.*

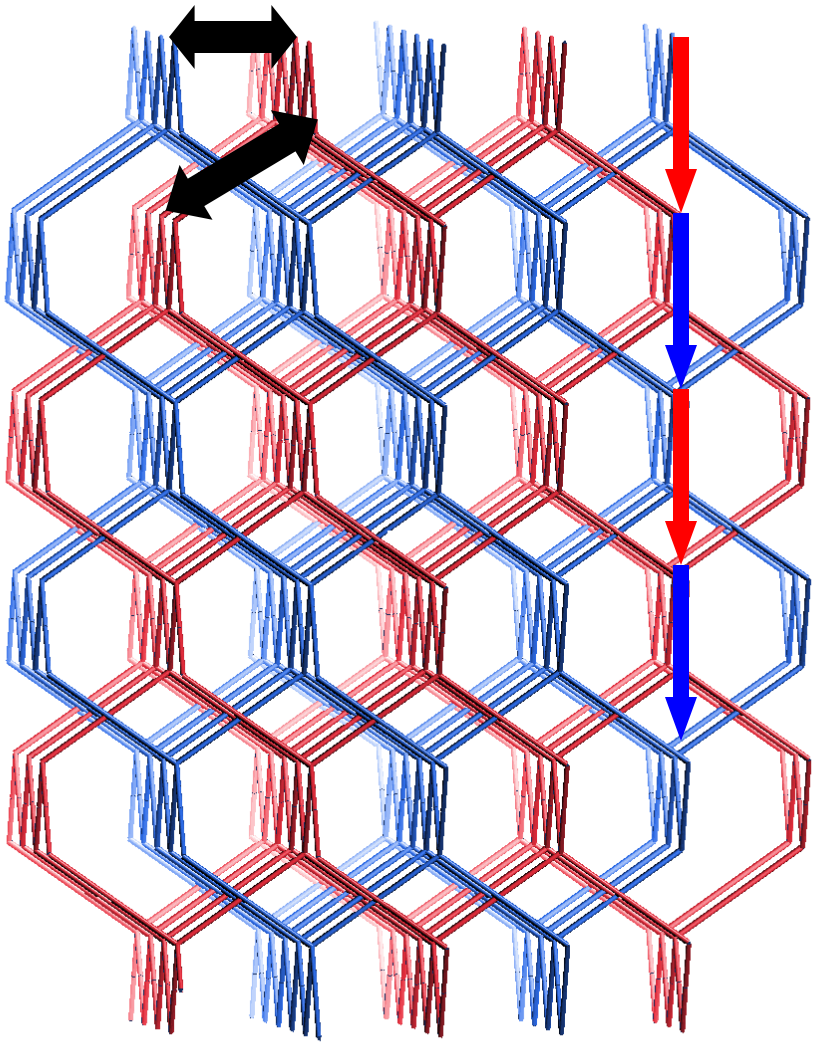
By D. E. Palin and H. M. Powell.

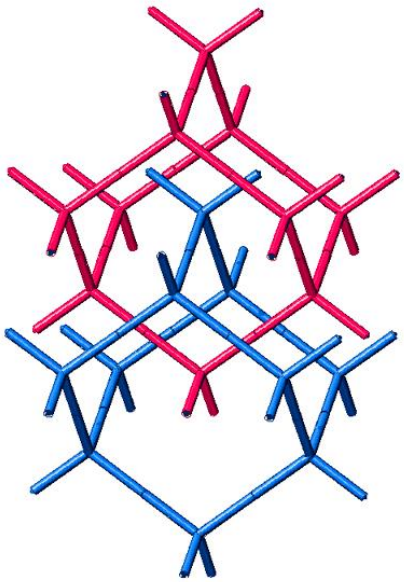


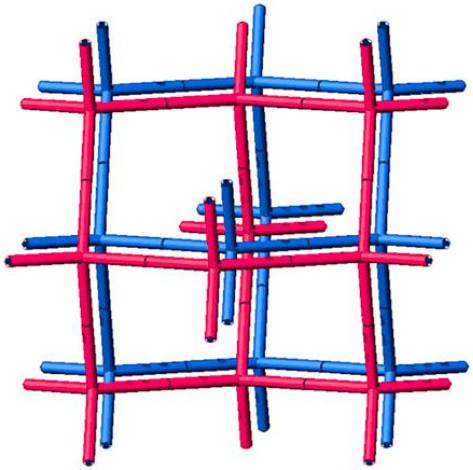
Stereoscopic representation of interpenetration of two similar hydrogen-bonded cageworks each identical with that shown in Fig. 13. Benzene rings are shown by small hexagons in the upper part of the figure but are elsewhere omitted for clarity. The larger hexagons represent the hydrogen bonds. The roughly spherical space enclosed between the two cageworks is also shown.

Cuprite
Cu_2O
Niggli
1922

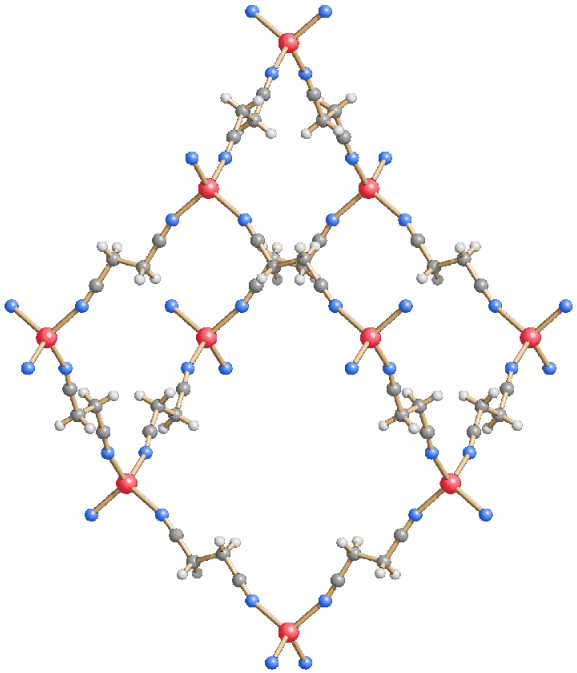
interpenetration of diamondoid nets



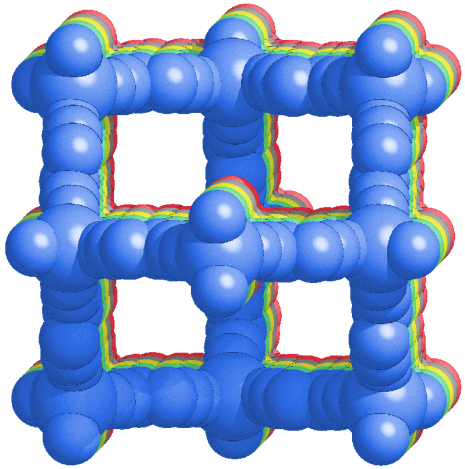


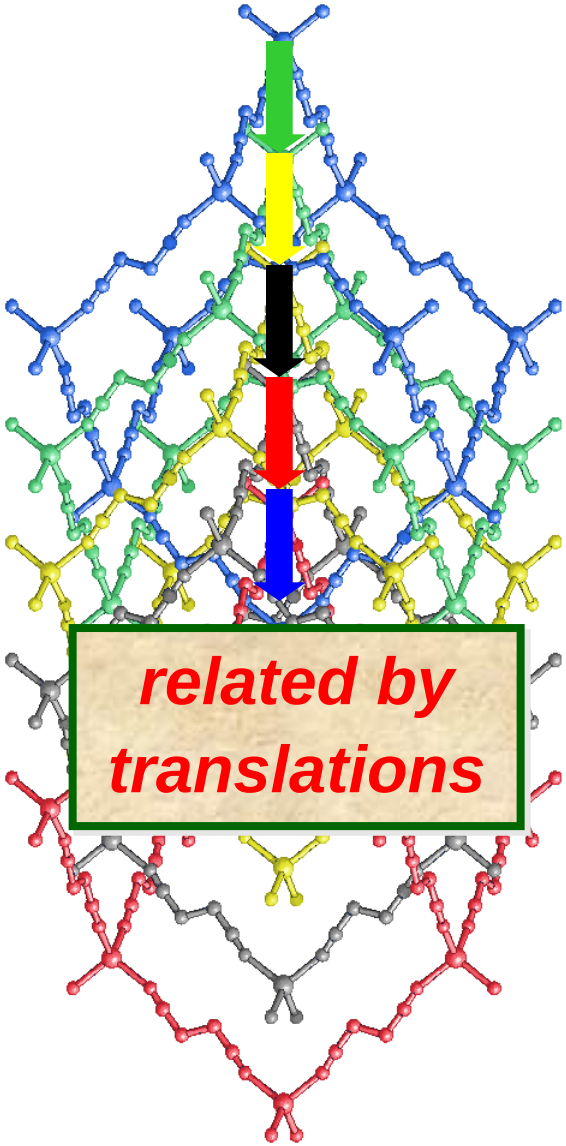


[Ag(1,4-butanedinitrile)$_2$](X) X= BF_4^-, ClO_4^-, PF_6^-, AsF_6^-, SbF_6^-



26-29
x
21-23
21-23





related by translations

Diamondoid-5f

Class I (a,b)
Nets related only by translation

Class II (a,b)
Nets related only by non-translational symmetry elements

Class III (a,b,c,d)
Nets related by translational and non-translational symmetry elements

world records of Interpenetration

2000 11-fold dia H-bond

2002 10-fold dia CNet (Ia)

2005

18-fold srs H-bond (IIIb)

2008

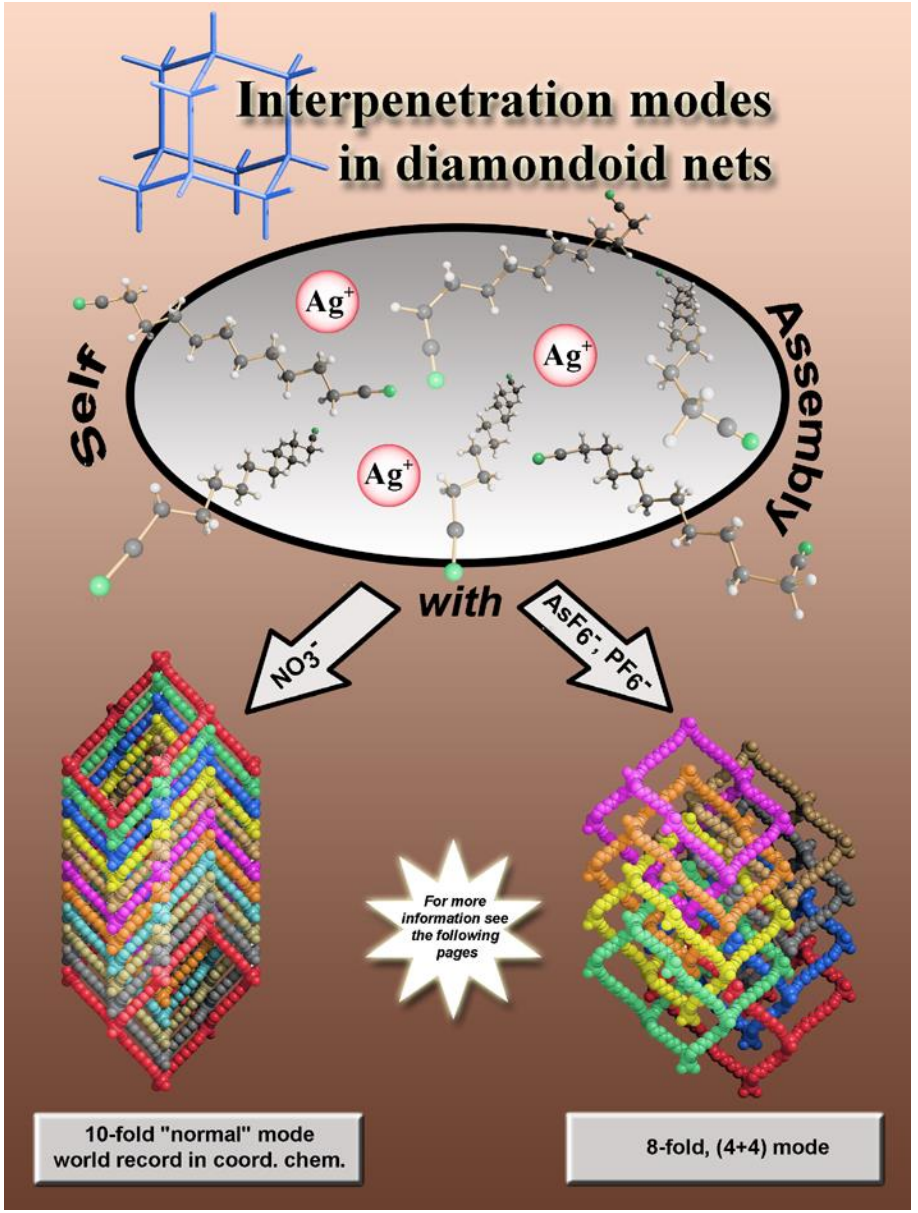
12-fold dia/ths CNet (IIIa)

2009

18-fold dia H-bond (IIIb)

2011

54-fold srs CNet (IIIb)



CRYSTAL GROWTH & DESIGN

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Article

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Applied Topological Analysis of Crystal Structures with the Program Package ToposPro

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·ogram package for multipurpose crystallochemical analysis

ToposPro

Version 5.0

PRACTICAL MANUAL 1.1.1

V.A. Blatov & D.M. Proserpio

Revision summer 2014

www.topospro.com

Samara Center

for Theoretical Materials Science

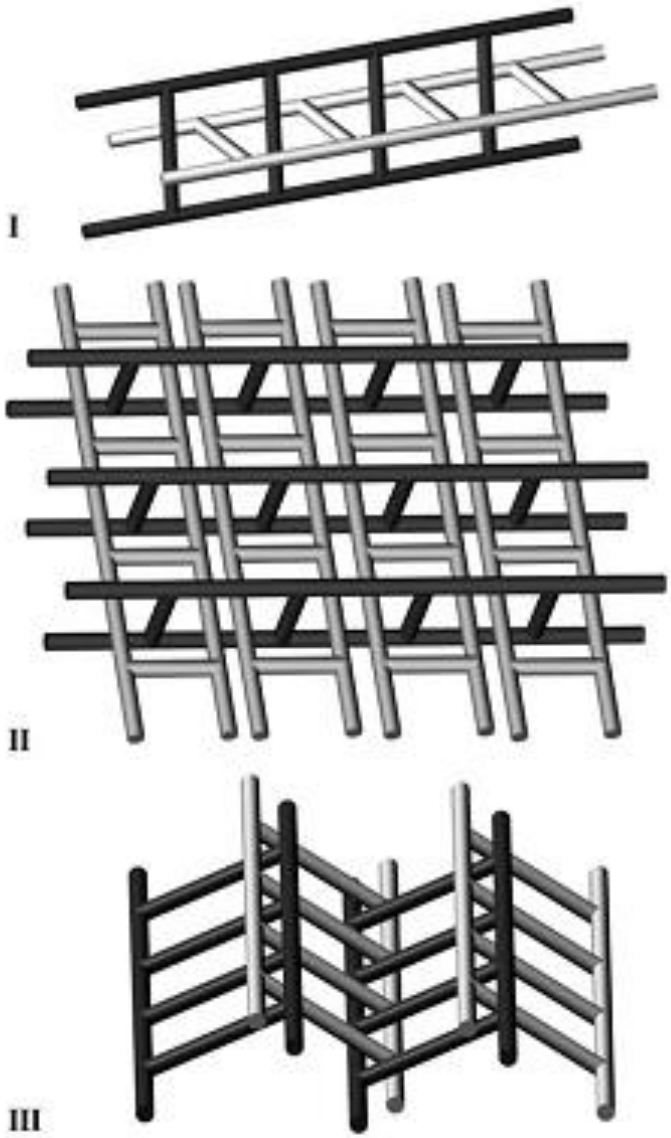
Can we entangle 1-p or 2-p nets in a different way (topological)?

Interpenetration

vs.

Polycatenation

1-p Ladders + Hopf Links



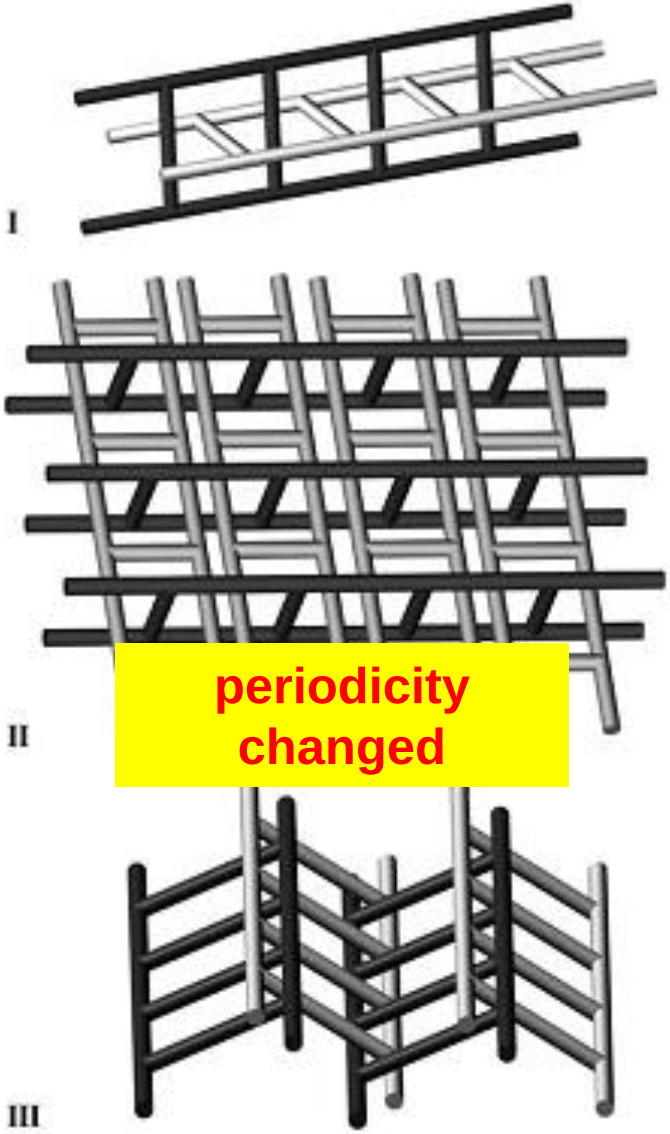
1-p ⇒ 1-p
2-fold 2007

1-p ⊥ 1-p ⇒ 2-p
2004

1-p // 1-p ⇒ 2-p
1997

periodicity unchanged

1-p Ladders + Hopf Links



periodicity changed

1-p ⇒ 1-p
2-fold 2007

1-p ⊥ 1-p ⇒ 2-p
2004

1-p // 1-p ⇒ 2-p
1997

Inextricable Entanglement via Hopf links

1-p+1-p ⇒ 2-p/3-p
2-p parallel ⇒ 2-p
2-p incline-p ⇒ 3-p
3-p ⇒ 3-p

periodicity unchanged

increase of periodicity

Interpenetration

Polycatenation

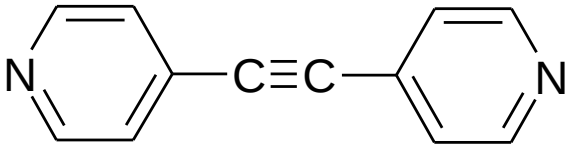
"Topological" Entanglement

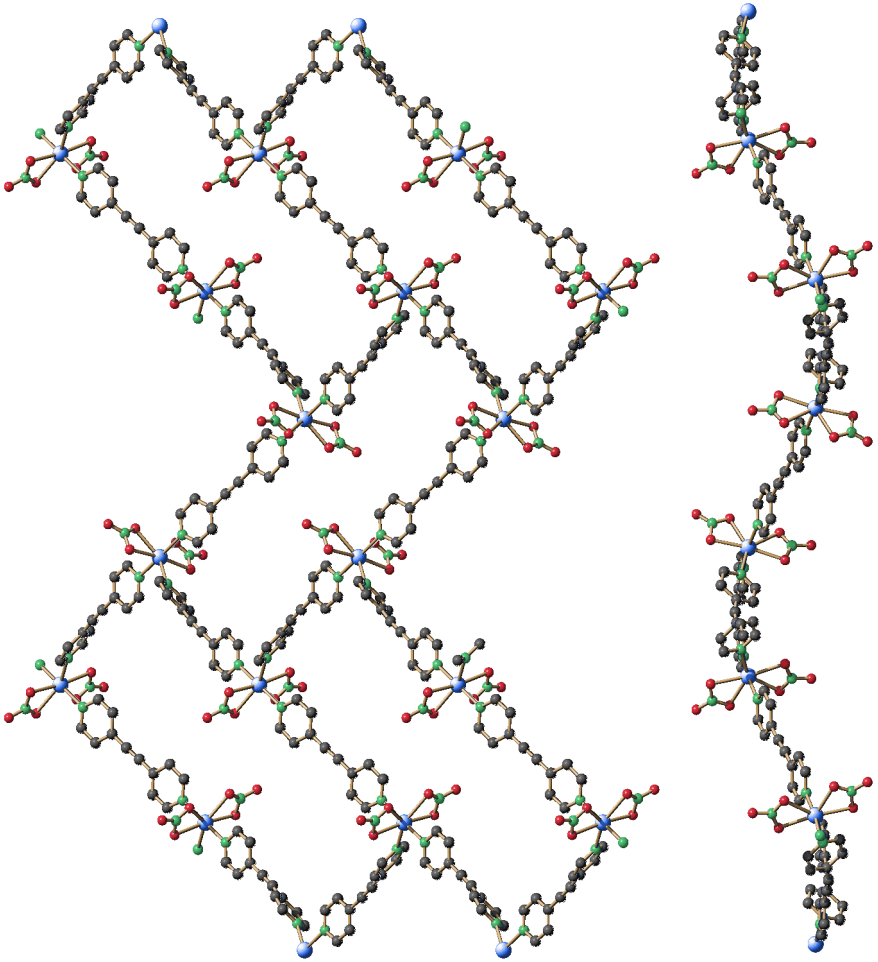
Interpenetration

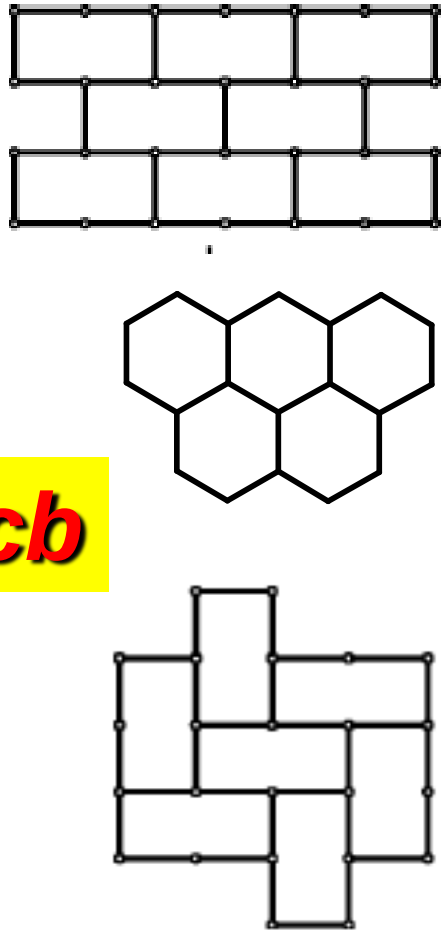
$[Cd_2(bpethy)_3](NO_3)_4$

2-p // 2-p ⇒ 2-p-3f

DEKQOZ, DEKQUZ







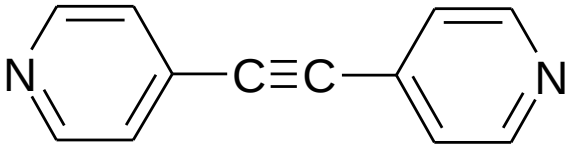
6^3-hcb

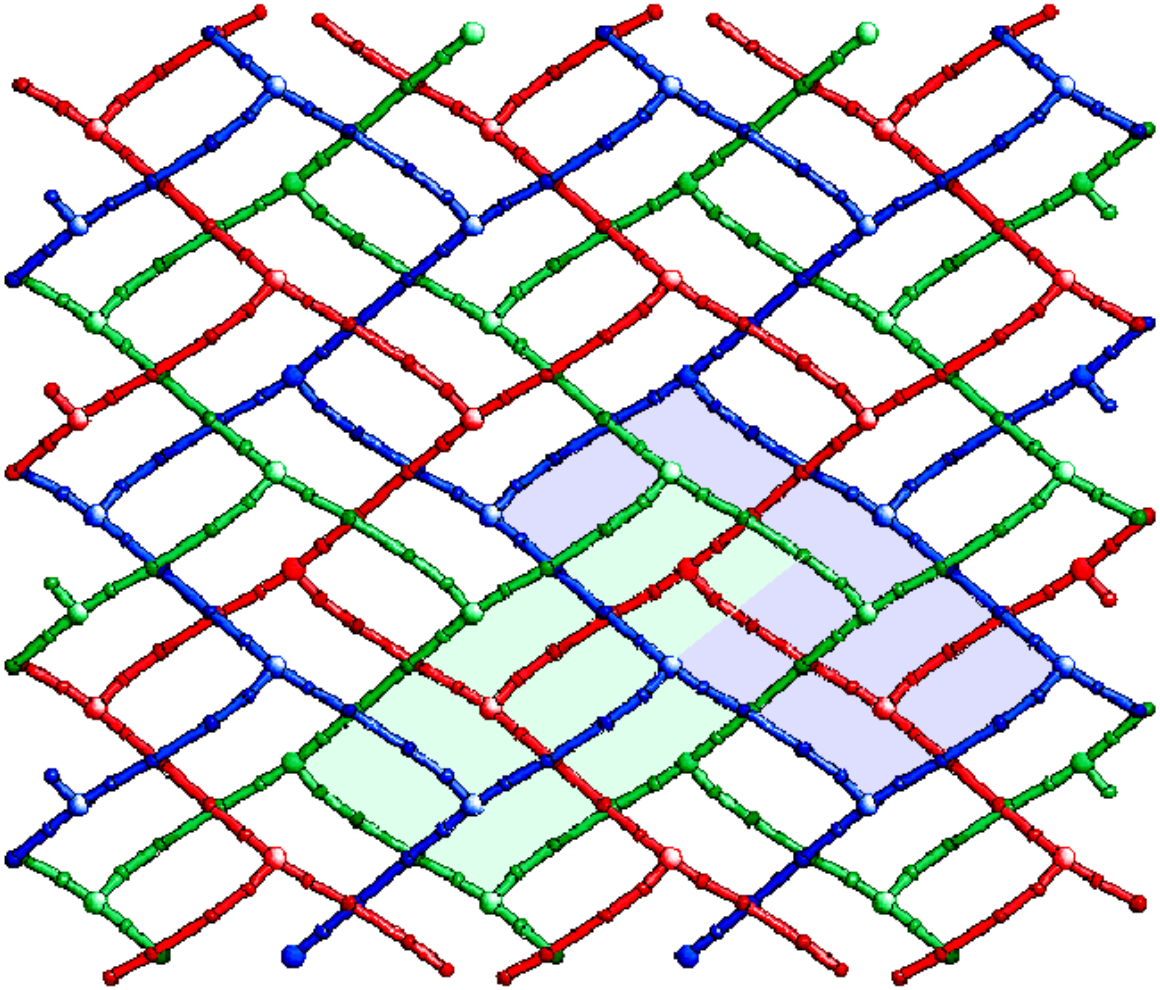
Interpenetration

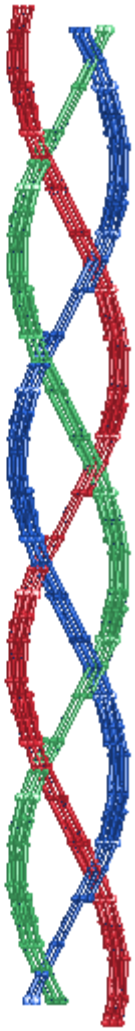
$[Cd_2(bpethy)_3](NO_3)_4$

2-p // 2-p ⇒ 2-p-3f

DEKQOZ, DEKQUZ





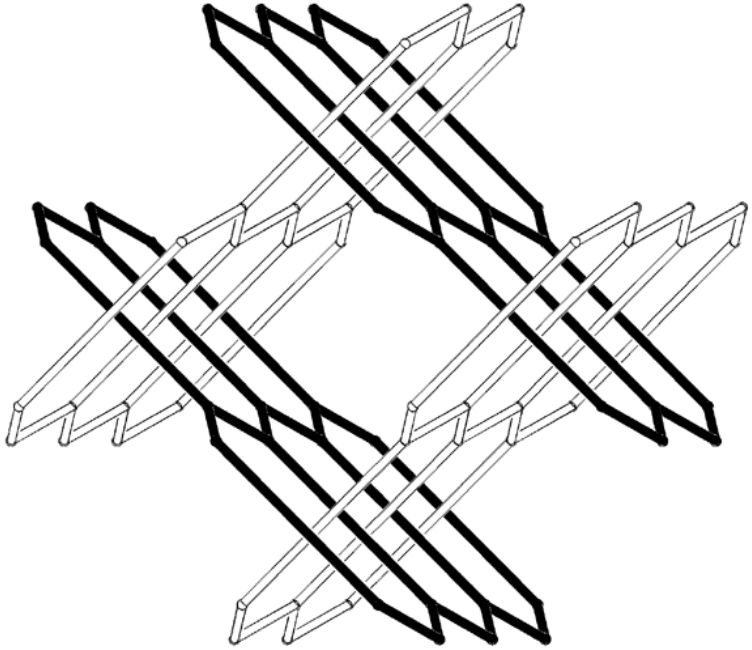


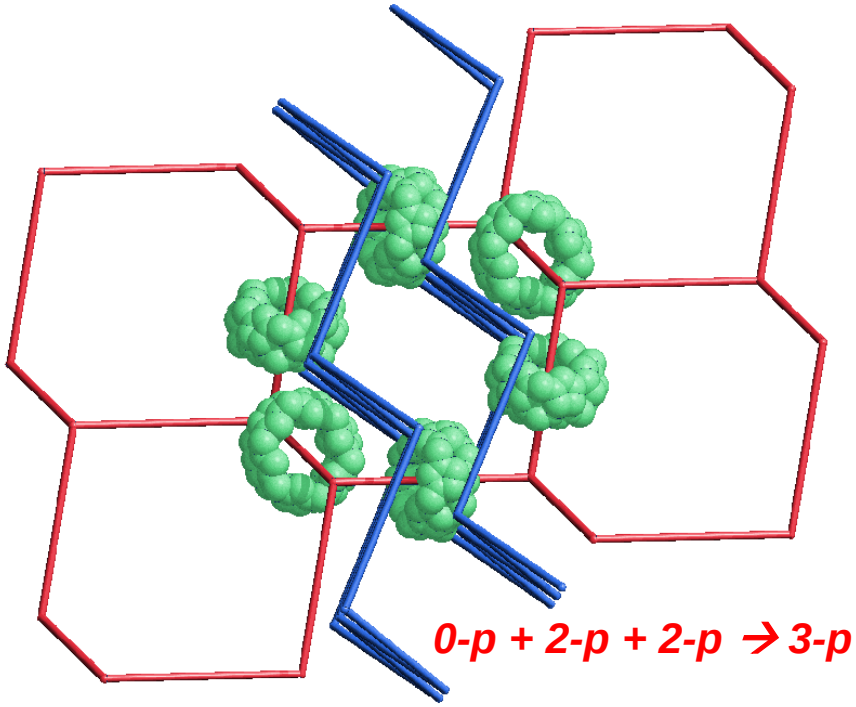
'inclined' polycatenation 2-p ⊥ 2-p ⇒ 3-p

$[Cu_2(pyz)_3](SiF_6)$
Zaworotko group, 1994

Hopf link

$[Ag_2(H_2L)_3\,(cucurbituril)_3](NO_3)_8$
K. Kim group, 1997



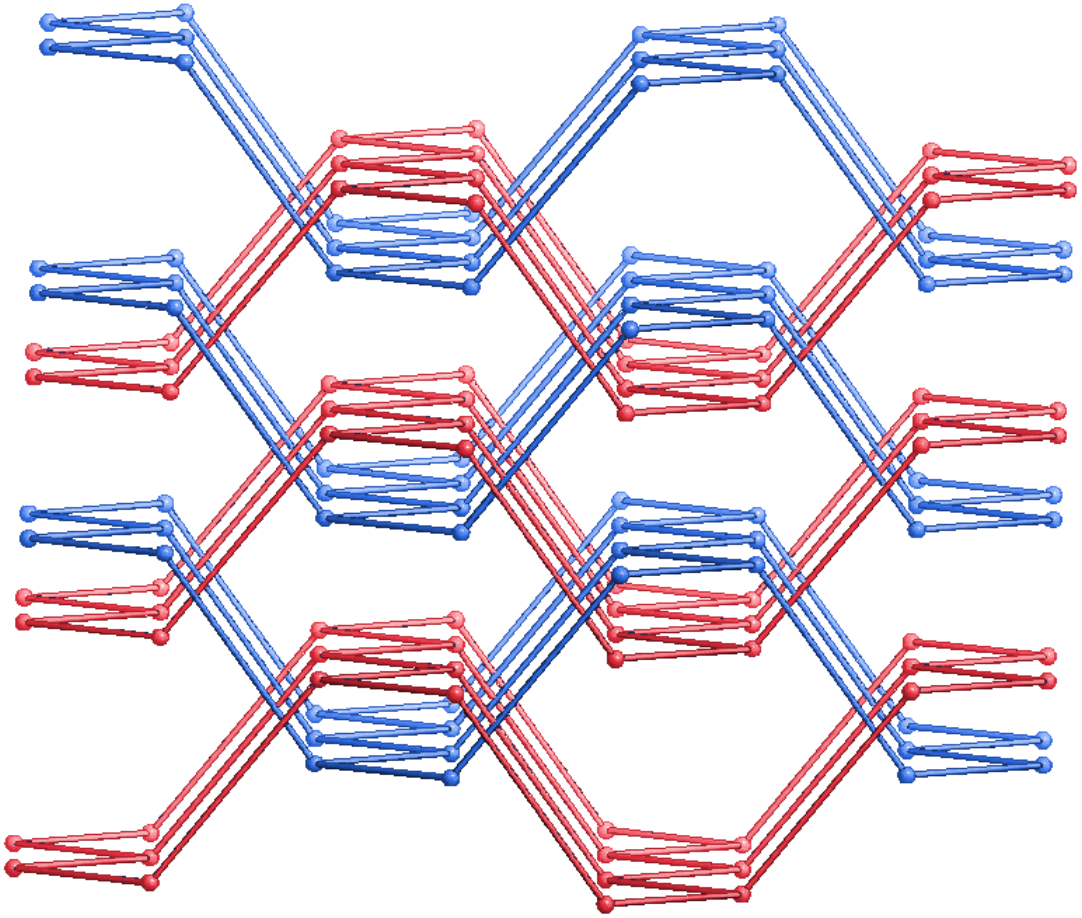


hexagonal (6^3) layers, hcb

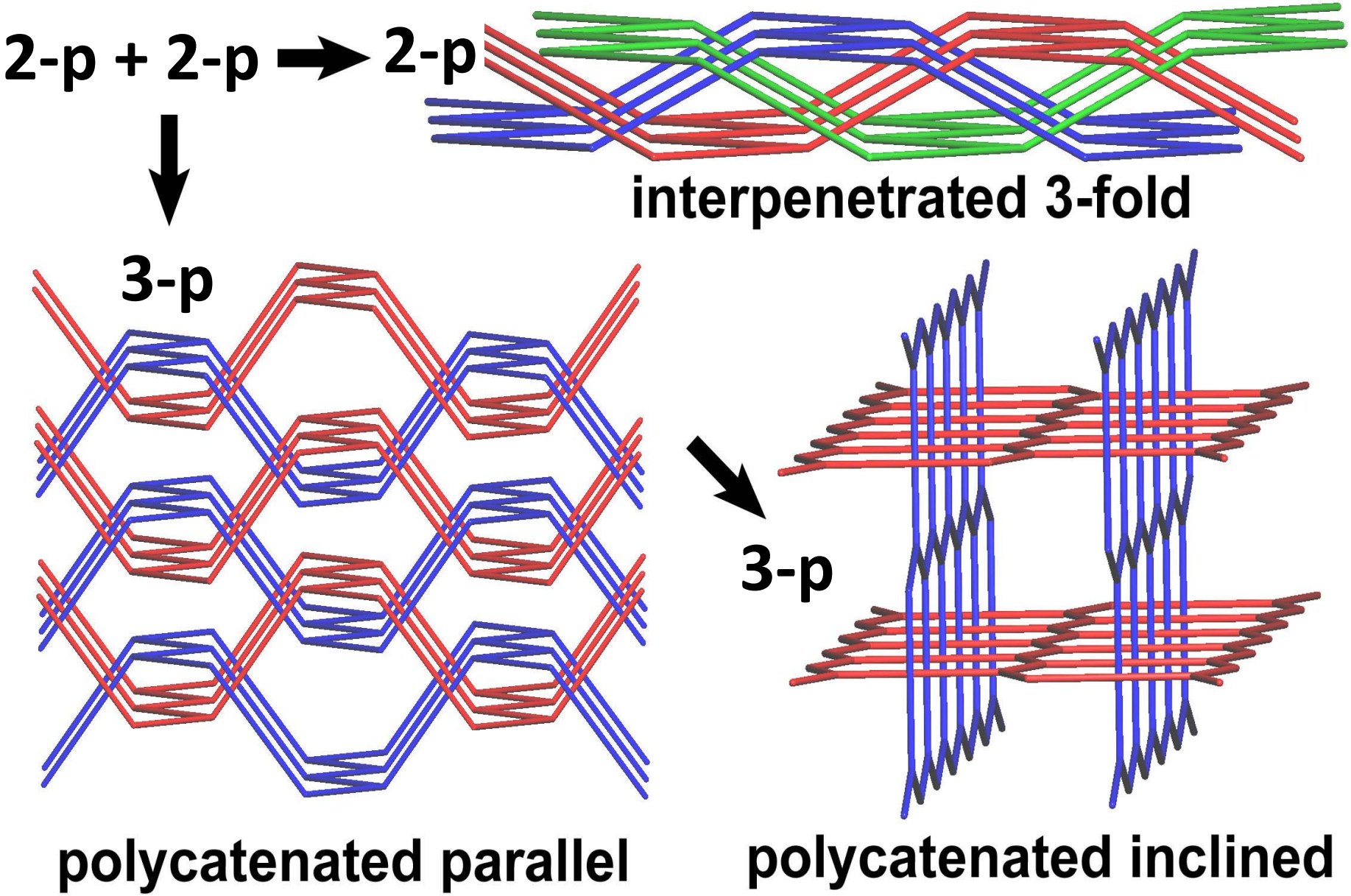
2D 'parallel' polycatenation
3-p // 3-p ⇒ 3-p

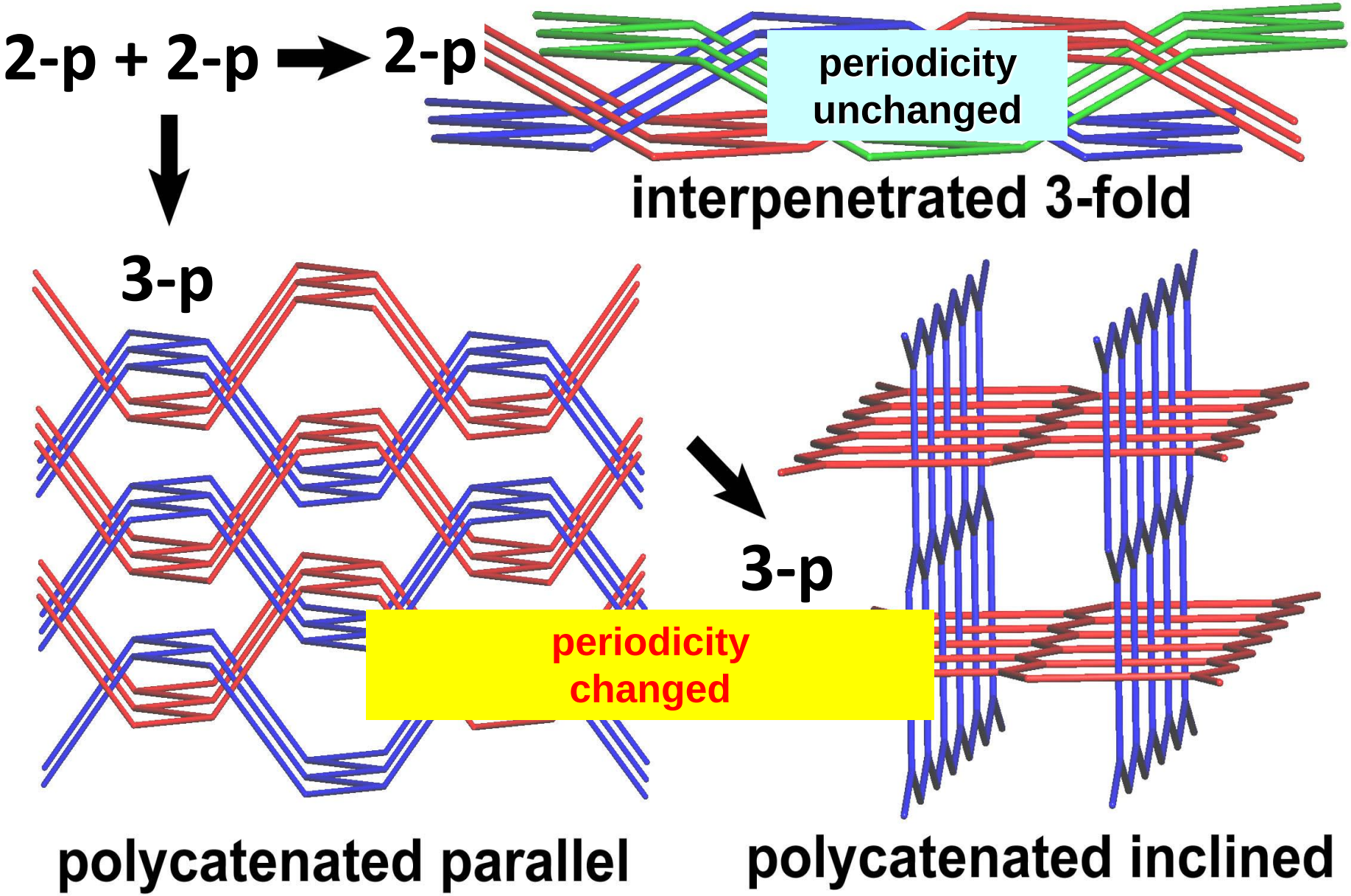
$[Cu(bpethe)_{1.5}(PPh_3)](PF_6)$

S.W. Keller group, 2001



undulated hexagonal (6^3) layers


2-p + 2-p
2-p
interpenetrated 3-fold
3-p
3-p
polycatenated parallel
polycatenated inclined

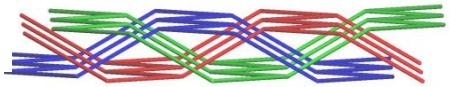

2-p + 2-p
2-p
periodicity unchanged
interpenetrated 3-fold
3-p
3-p
periodicity changed
polycatenated parallel
polycatenated inclined

Inextricable Entanglement via Hopf links

periodicity unchanged:
INTERPENETRATION

0-p + 0-p ⇒ 0-p
1-p + 1-p ⇒ 1-p
2-p + 2-p (parallel) ⇒ 2-p
3-p + 3-p ⇒ 3-p

Only 4 possibilities



components 0-p, 1-p, 2-p or 3-p

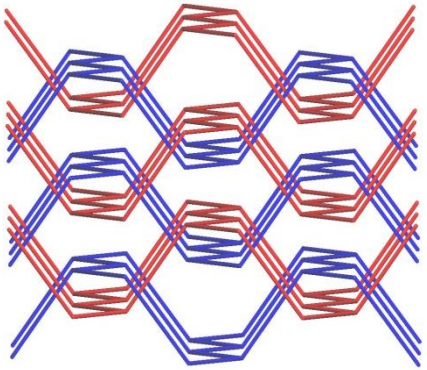
the whole has the SAME periodicity of the components

the number of entangled components is finite ***(n-fold)***

each component is interlaced with ALL the others (*)

the whole is an infinite *k*-periodic architecture

k-p + k-p ⇒ k-p
m-p + n-p ⇒ k-p
m < k; n ≤ k



increase of periodicity:
POLYCATENATION

0-p + 0-p ⇒ 1-p, 2-p or 3-p
0-p + 1-p ⇒ 1-p, 2-p or 3-p
0-p + 2-p ⇒ 2-p or 3-p
0-p + 3-p ⇒ 3-p
1-p + 1-p ⇒ 2-p or 3-p
1-p + 2-p ⇒ 2-p or 3-p
1-p + 3-p ⇒ 3-p
2-p + 2-p (inclined) ⇒ 3-p
2-p + 2-p (parallel) ⇒ 3-p
2-p + 3-p ⇒ 3-p

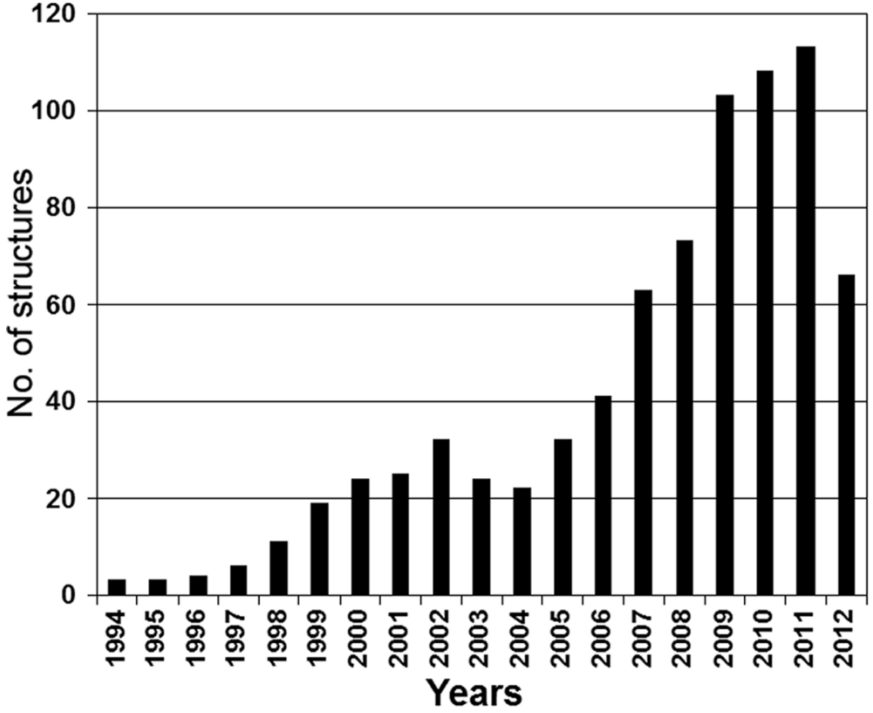
components 0-p, 1-p, 2-p or 3-p

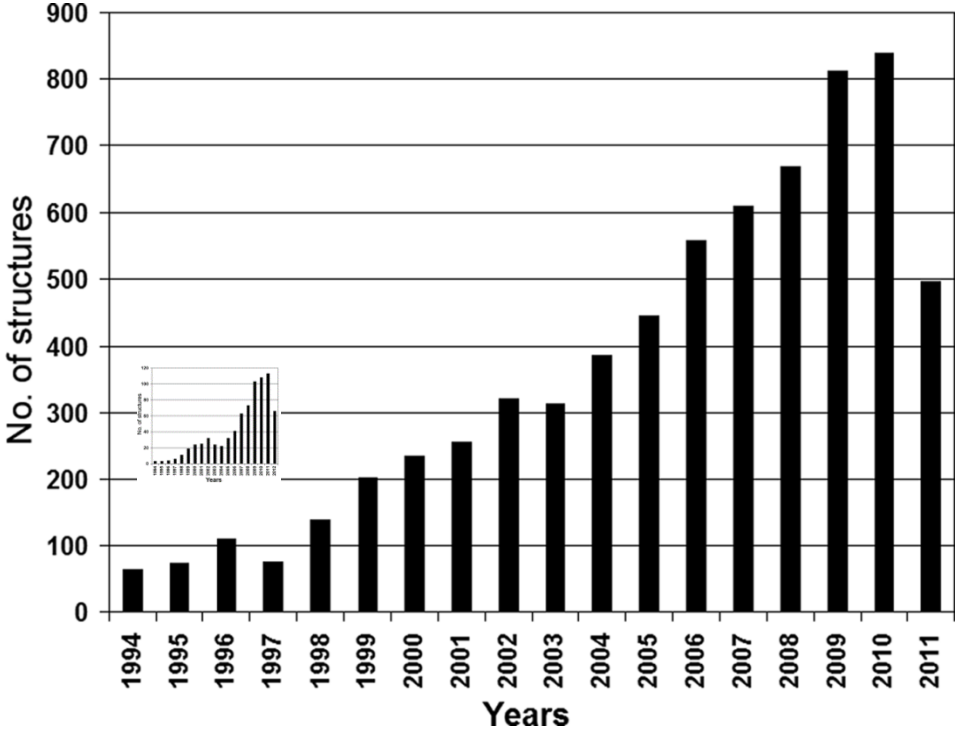
the whole has HIGHER periodicity of at least one component

the number of entangled components is infinite

at least one component is not interlaced with all the others

2-periodic coordination networks

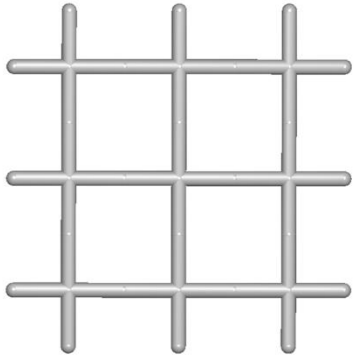




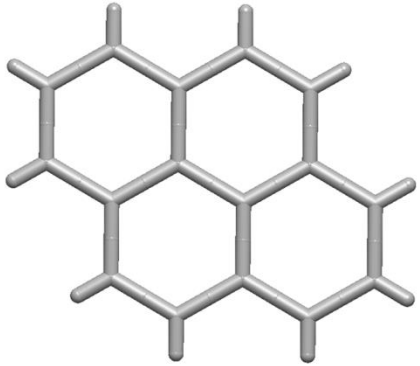
entangled **vs.** **single**

1319 **1/9**

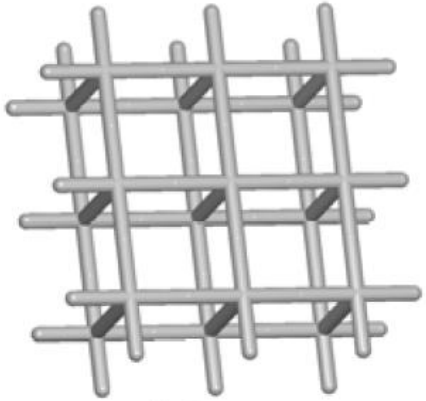
1319



(4^4) sql



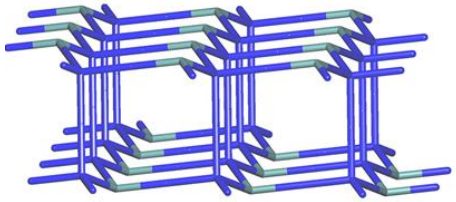
(6^3) hcb



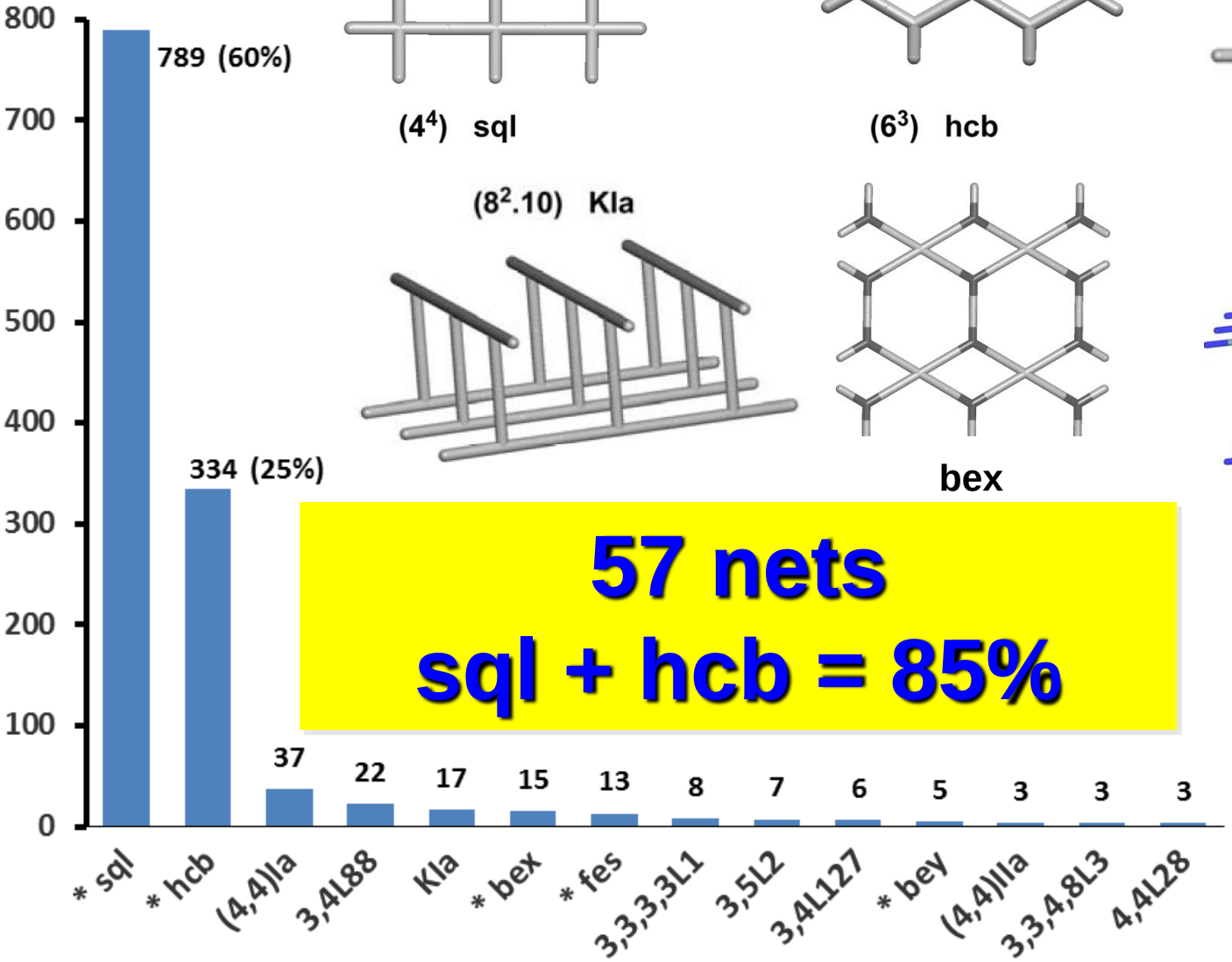
$(4^4.6^2)$ (4,4)la

$(8^2.10)$ Kla

bex

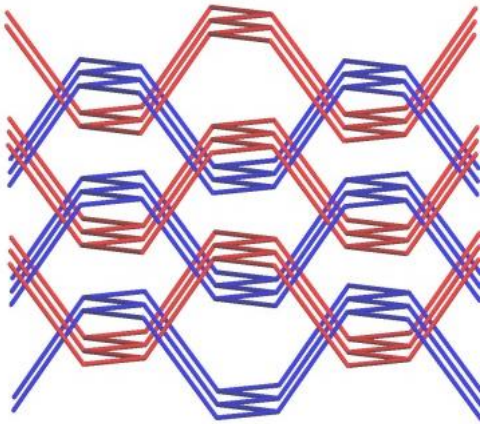


3,4L88

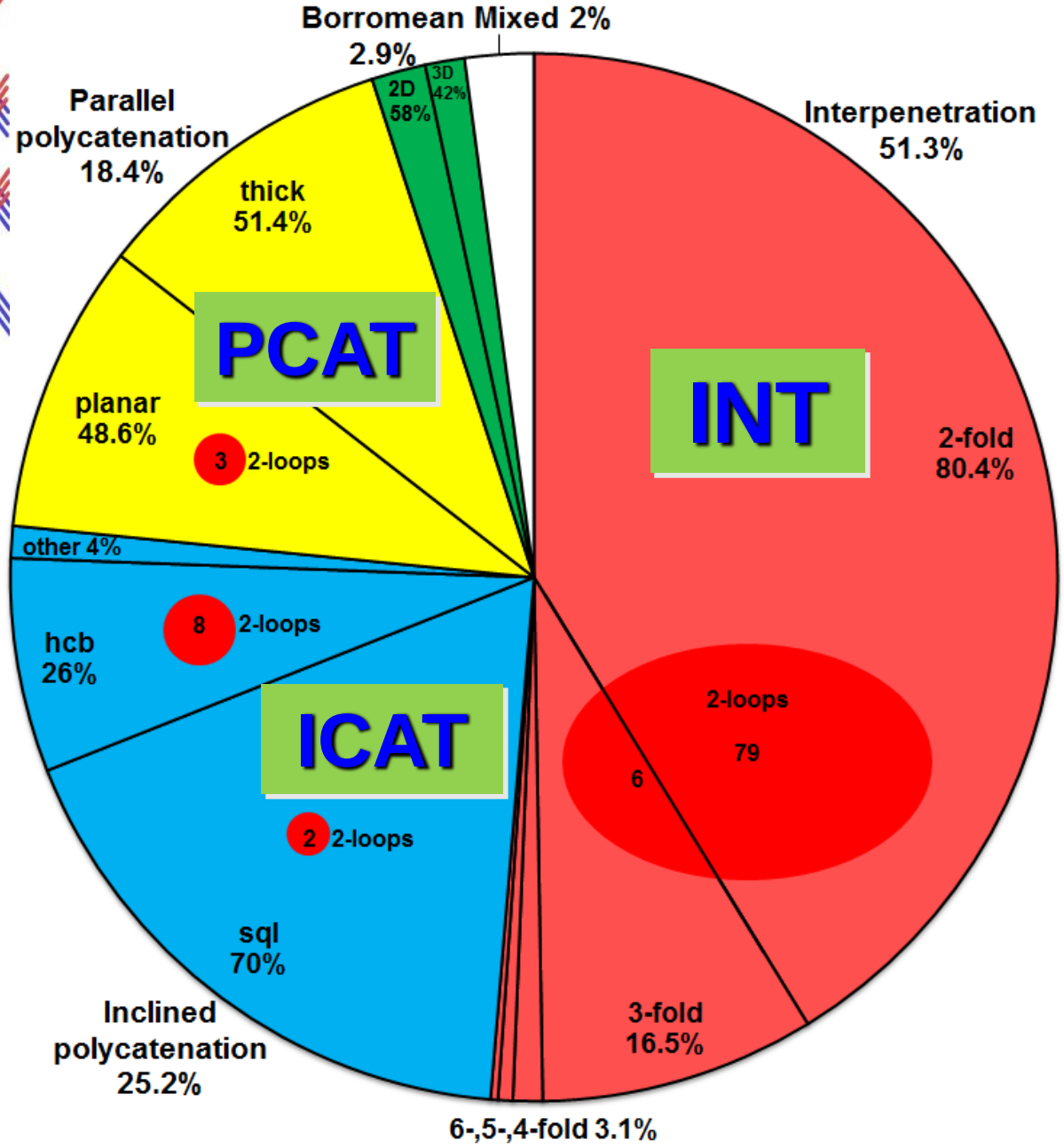


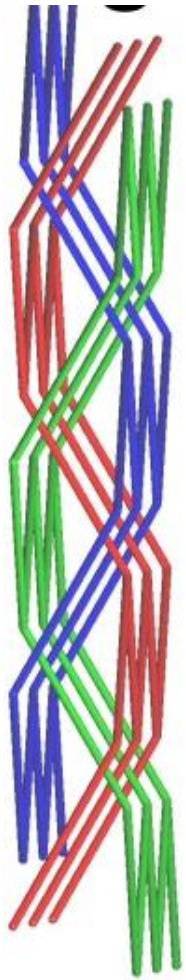
57 nets

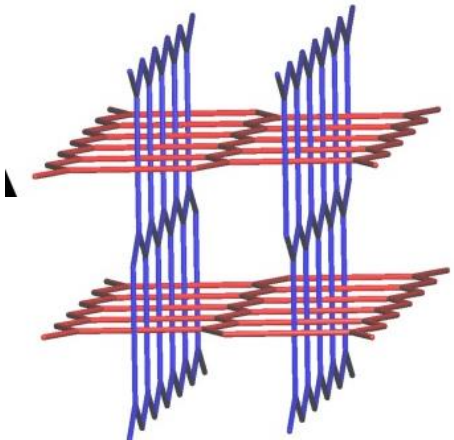
sql + hcb = 85%



1319


Borromean Mixed 2%
2.9%
2D
58%
3D
42%
Parallel
polycatenation
18.4%
thick
51.4%
PCAT
planar
48.6%
3
2-loops
Interpenetration
51.3%
INT
2-fold
80.4%
2-loops
79
6
3-fold
16.5%
6-,5-,4-fold 3.1%
other 4%
8
2-loops
hcb
26%
ICAT
2
2-loops
sql
70%
Inclined
polycatenation
25.2%





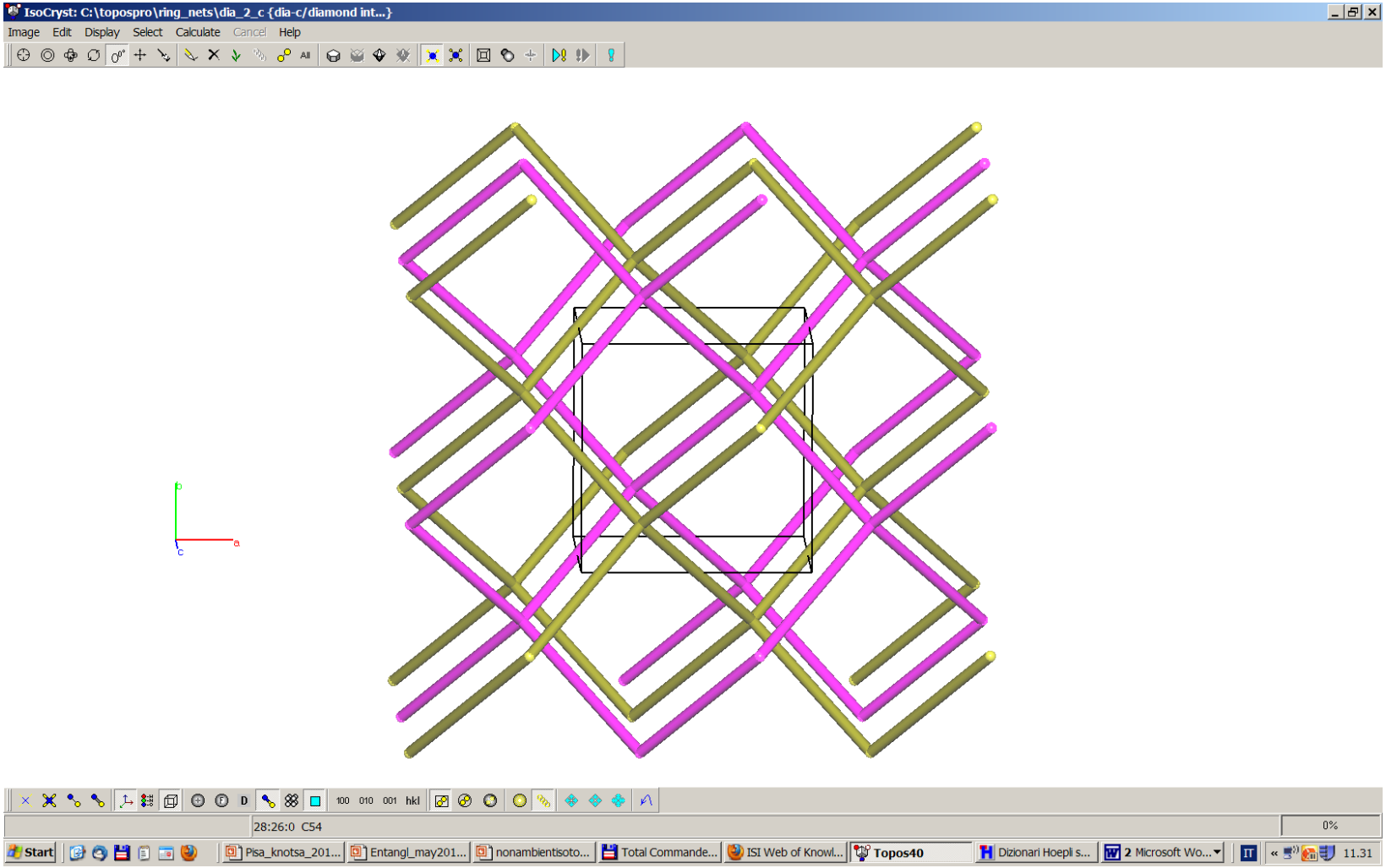
... and now a natural question:

Are these classes topologically related?

i.e. can we deform one member of a class into a member of another class?

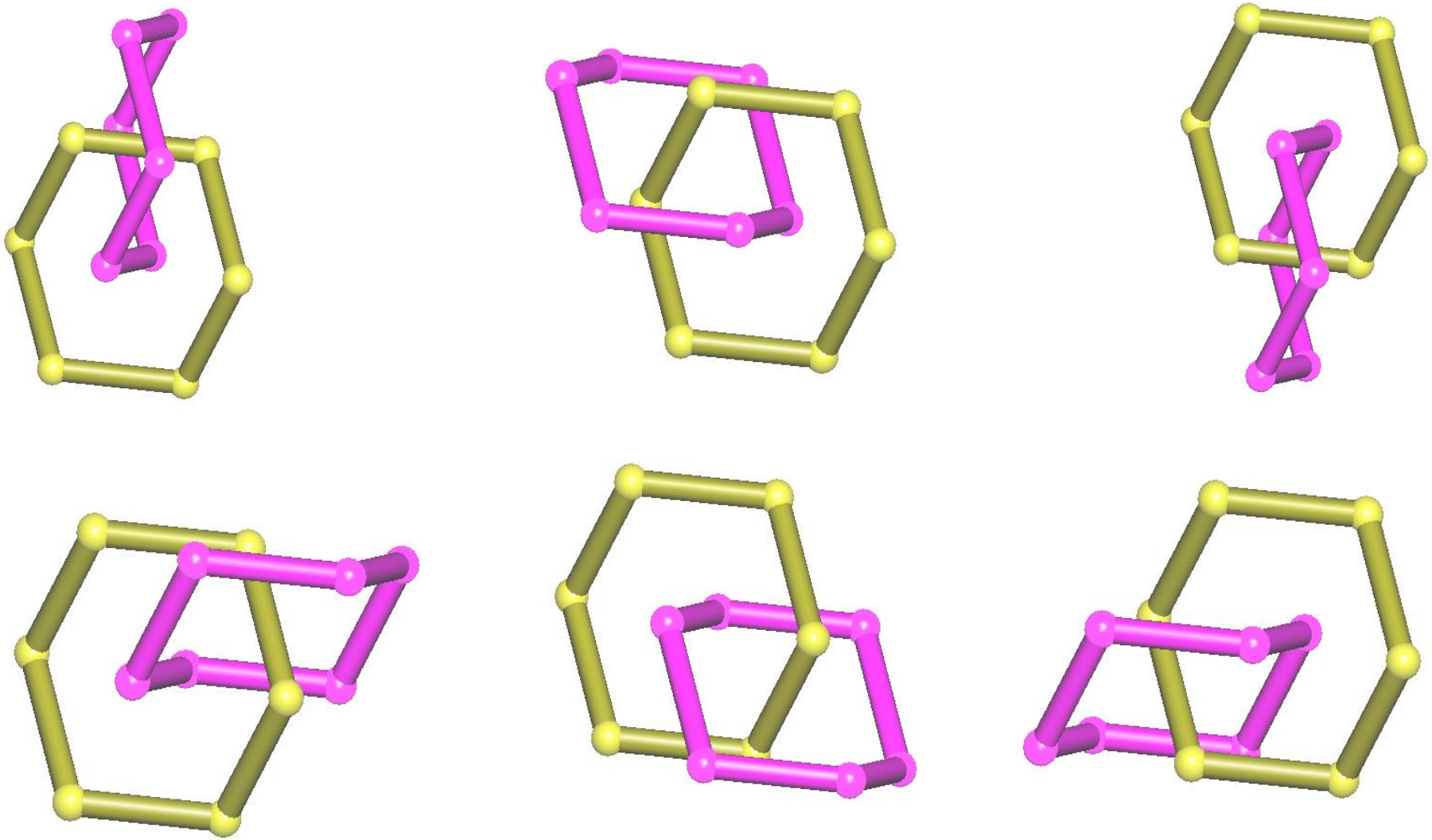
For instance we know many examples of diamondoid coordination network that are 2-fold interpenetrated....

How many are topologically distinct?


IsoCryst: C:\topospro\ring_nets\dia_2_c {dia-c/diamond int...}
Image Edit Display Select Calculate Cancel Help
28:26:0 C54
0%
Start
Pisa_knotsa_201...
Entangl_may201...
nonambientisoto...
Total Commande...
ISI Web of Knowl...
Topos40
Dizionari Hoepli s...
2 Microsoft Wo...
11.31

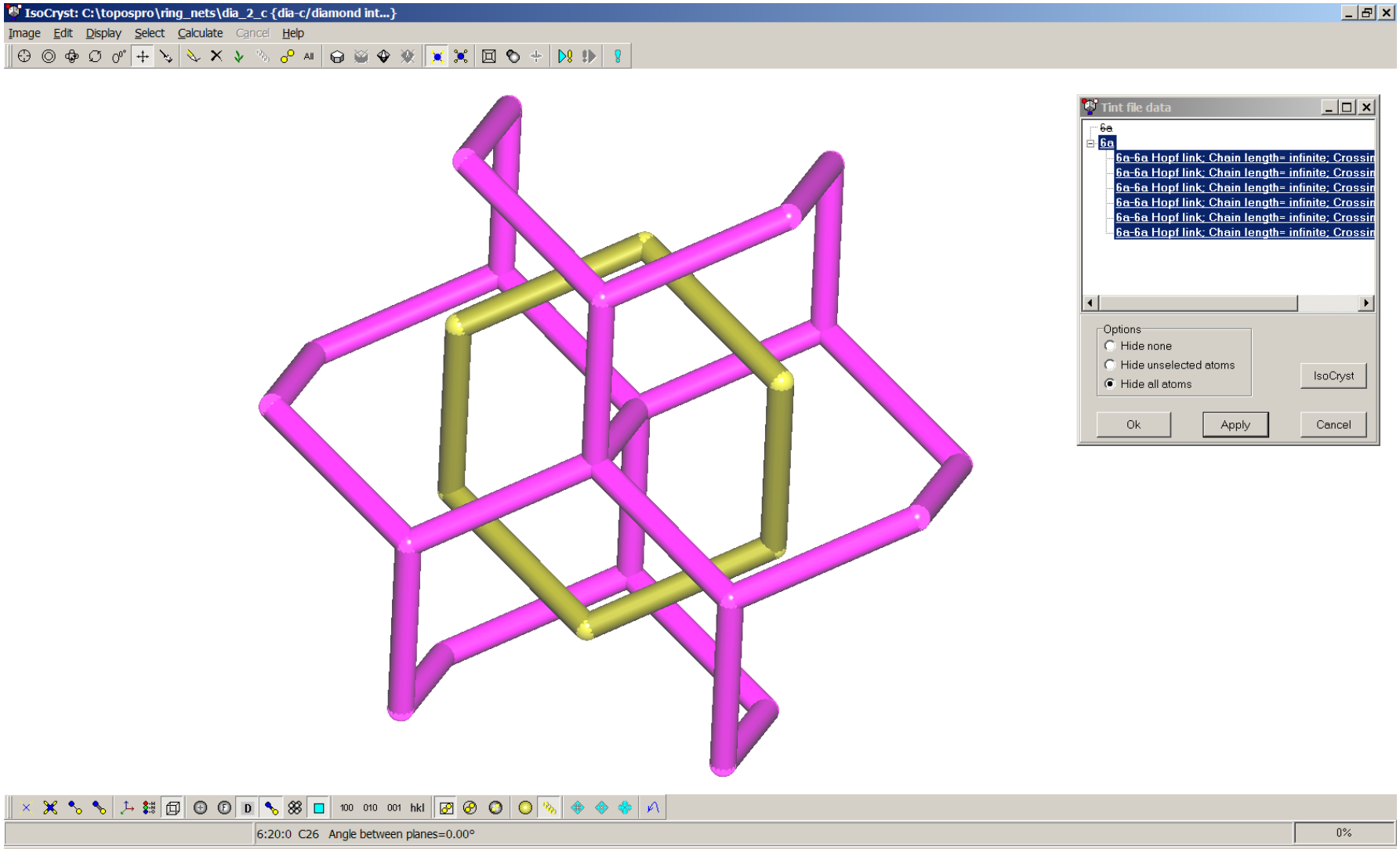
Ring links

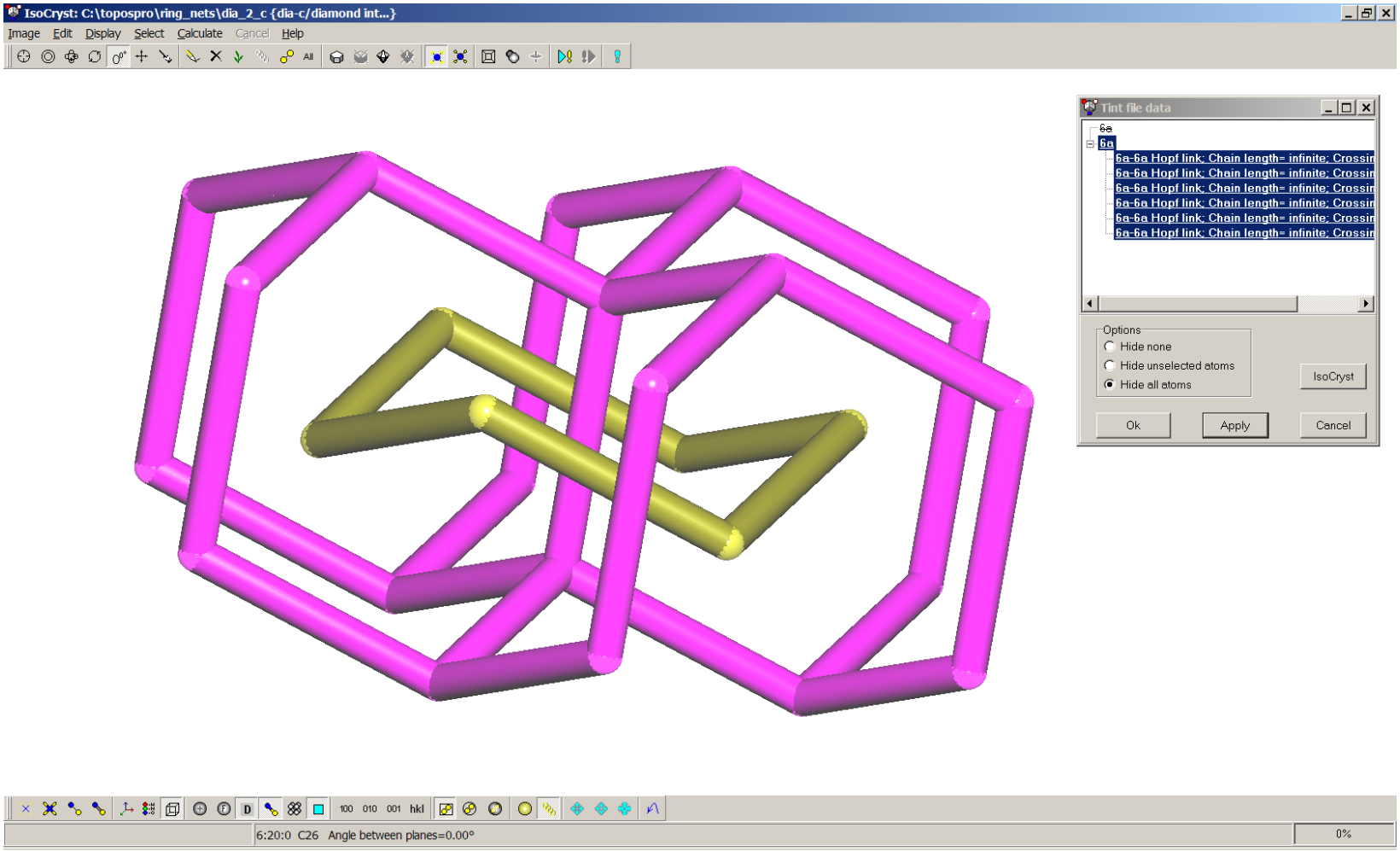
Cycle 1	Cycle 2	Chain	Cross	Link	Hopf	Mult
6a	6a	inf.	1	1	*	6



Ring links

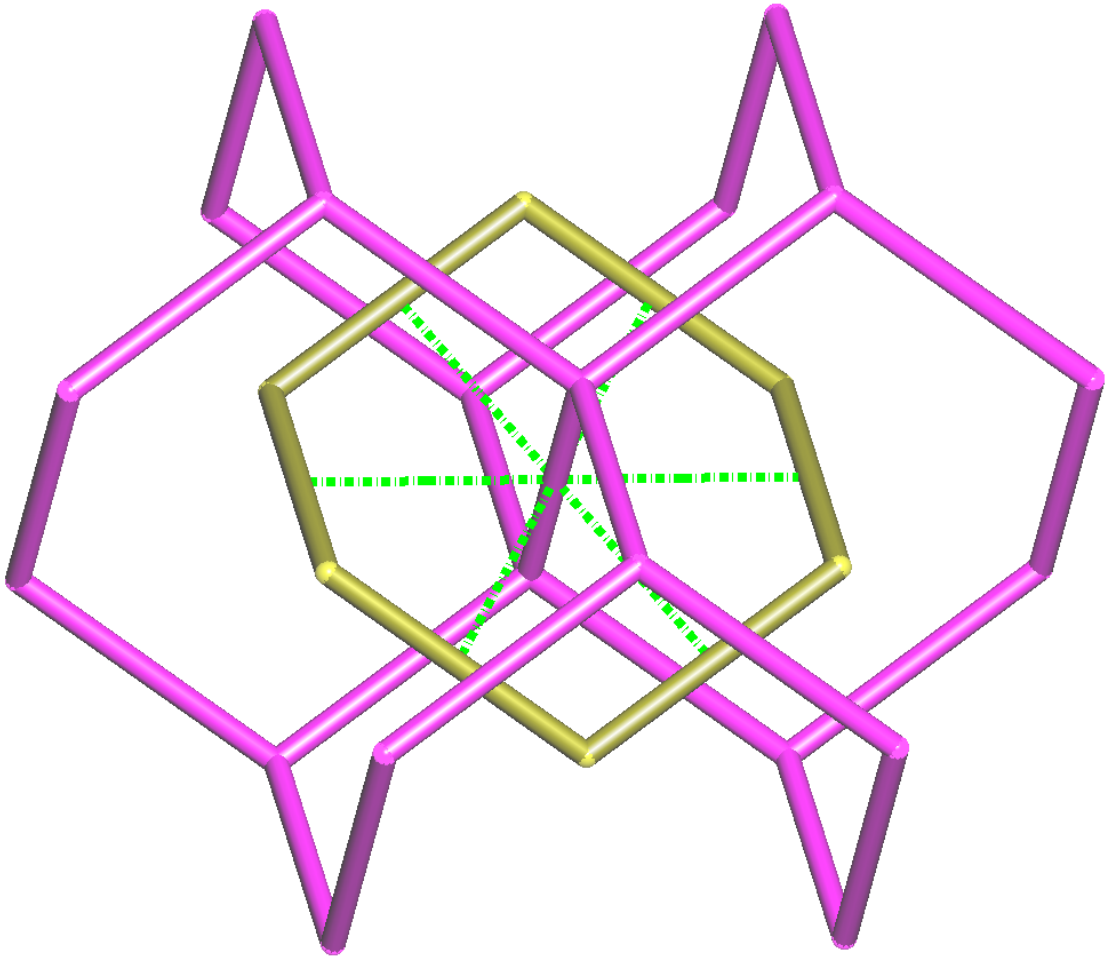
Cycle 1	Cycle 2	Chain	Cross	Link	Hopf	Mult
6a	6a	inf.	1	1	*	6




IsoCryst: C:\topospro\ring_nets\dia_2_c {dia-c/diamond int...}
Image Edit Display Select Calculate Cancel Help
Tint file data
6a
6a
6a-6a Hopf link; Chain length= infinite; Crossin
6a-6a Hopf link; Chain length= infinite; Crossin
6a-6a Hopf link; Chain length= infinite; Crossin
6a-6a Hopf link; Chain length= infinite; Crossin
6a-6a Hopf link; Chain length= infinite; Crossin
6a-6a Hopf link; Chain length= infinite; Crossin
Options
Hide none
Hide unselected atoms
Hide all atoms
IsoCryst
Ok
Apply
Cancel
100 010 001 hkl
6:20:0 C26 Angle between planes=0.00°
0%

IsoCryst: C:\topospro\ring_nets\dia_2_c_c {dia-c/diamond int...}

Image Edit Display Select Calculate Cancel Help



Tint file data

- 6a
- 6b
- 6a
  - 6a-6a Hopf link; Chain length= infinite; Crossings= 1; Links= 1
  - 6a-6a Hopf link; Chain length= infinite; Crossings= 1; Links= 1
  - 6a-6a Hopf link; Chain length= infinite; Crossings= 1; Links= 1
  - 6a-6a Hopf link; Chain length= infinite; Crossings= 1; Links= 1
  - 6a-6a Hopf link; Chain length= infinite; Crossings= 1; Links= 1
  - 6a-6a Hopf link; Chain length= infinite; Crossings= 1; Links= 1

Options
- Hide none
- Hide unselected atoms
- Hide all atoms

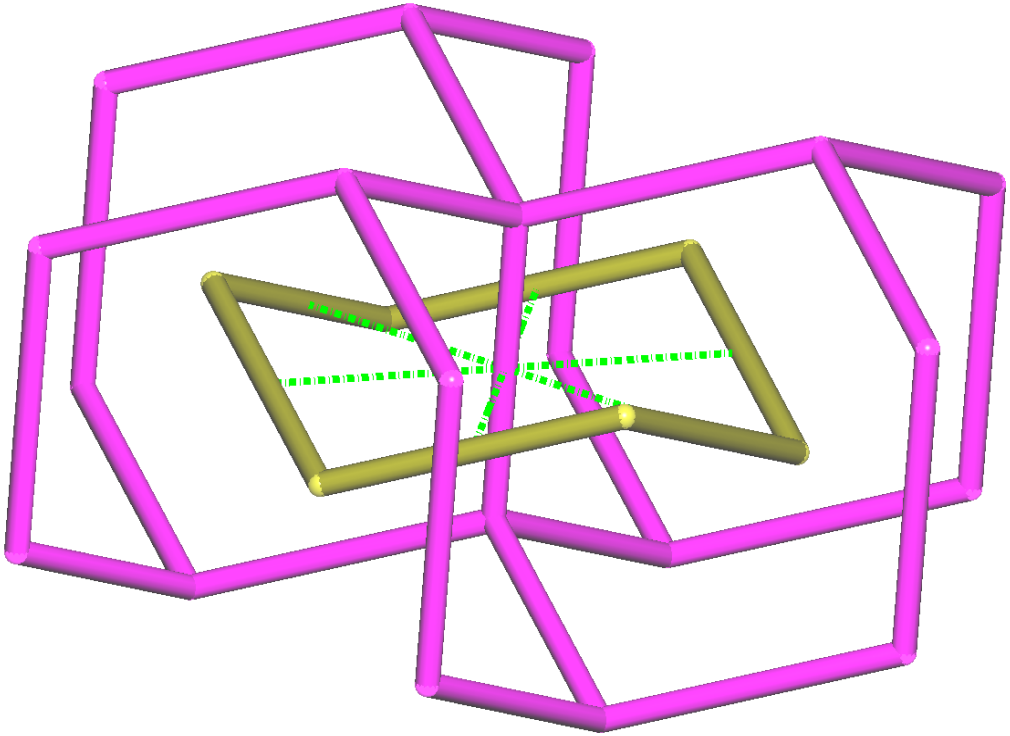
IsoCryst

Ok Apply Cancel

6:20:0 C26 Angle between planes=0.00°

0%

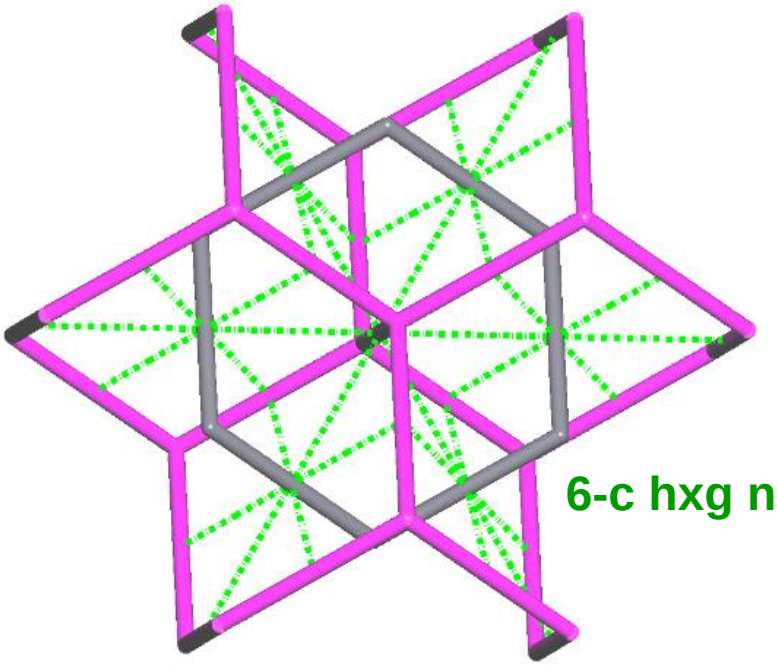
Start | Posta in arrivo -... | Composizione di... | Total Command... | Adobe Acrobat ... | dia2fold_hxg.do... | ringnets_dia-c.d... | Topos40 | putignano pisa -... | 9.45



The resulting single net (green dotted lines) represent the
"net-of-catenated-links"
Hopf Ring Net HRN
and is independent of the symmetry/space group.

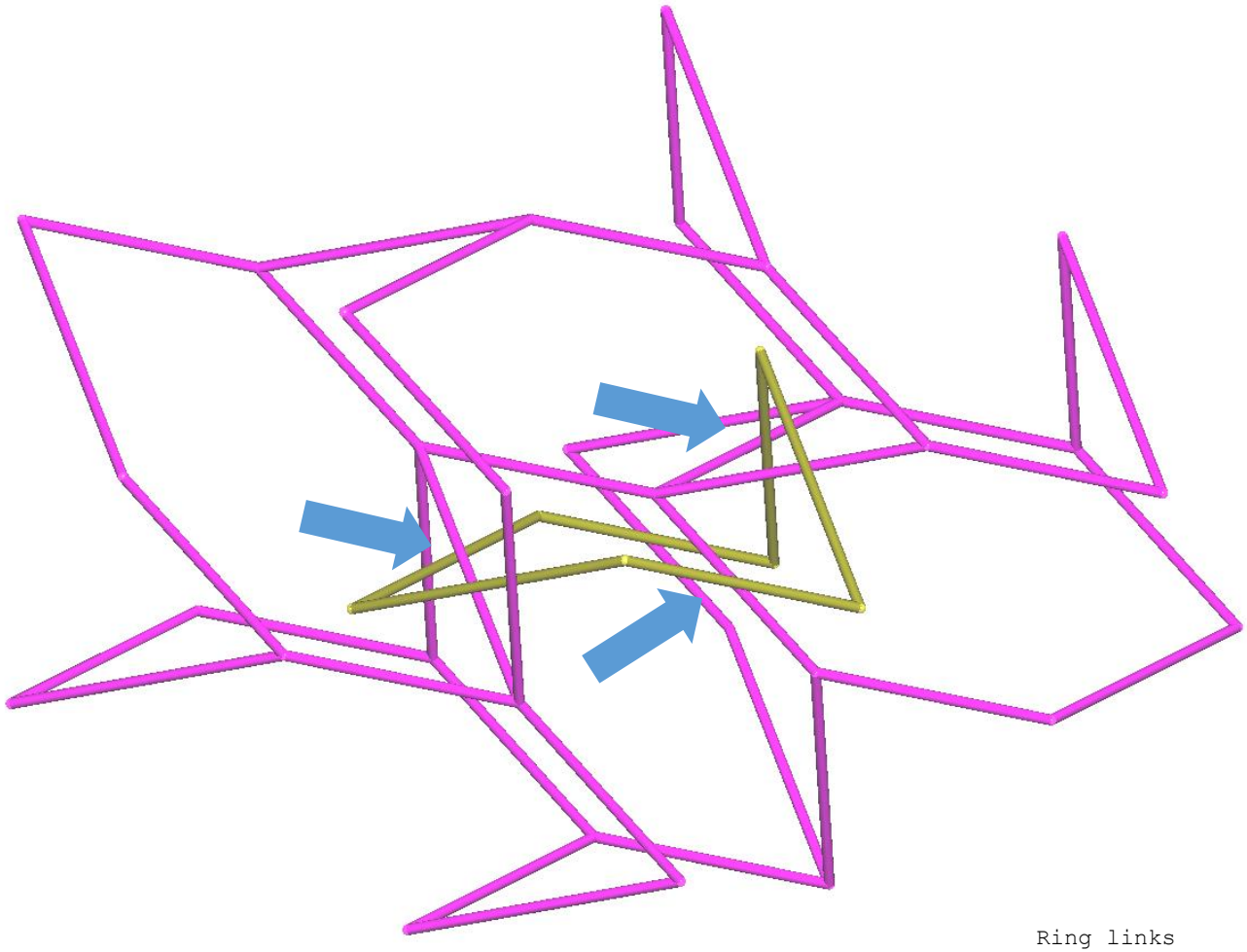
Q: dia 2fold class Ia can be transformed to class IIa ??

A: YES, for all known cases! only one example is different



6-c hxg net

… and the difference for is due to extra crossings : 3 vs. 1



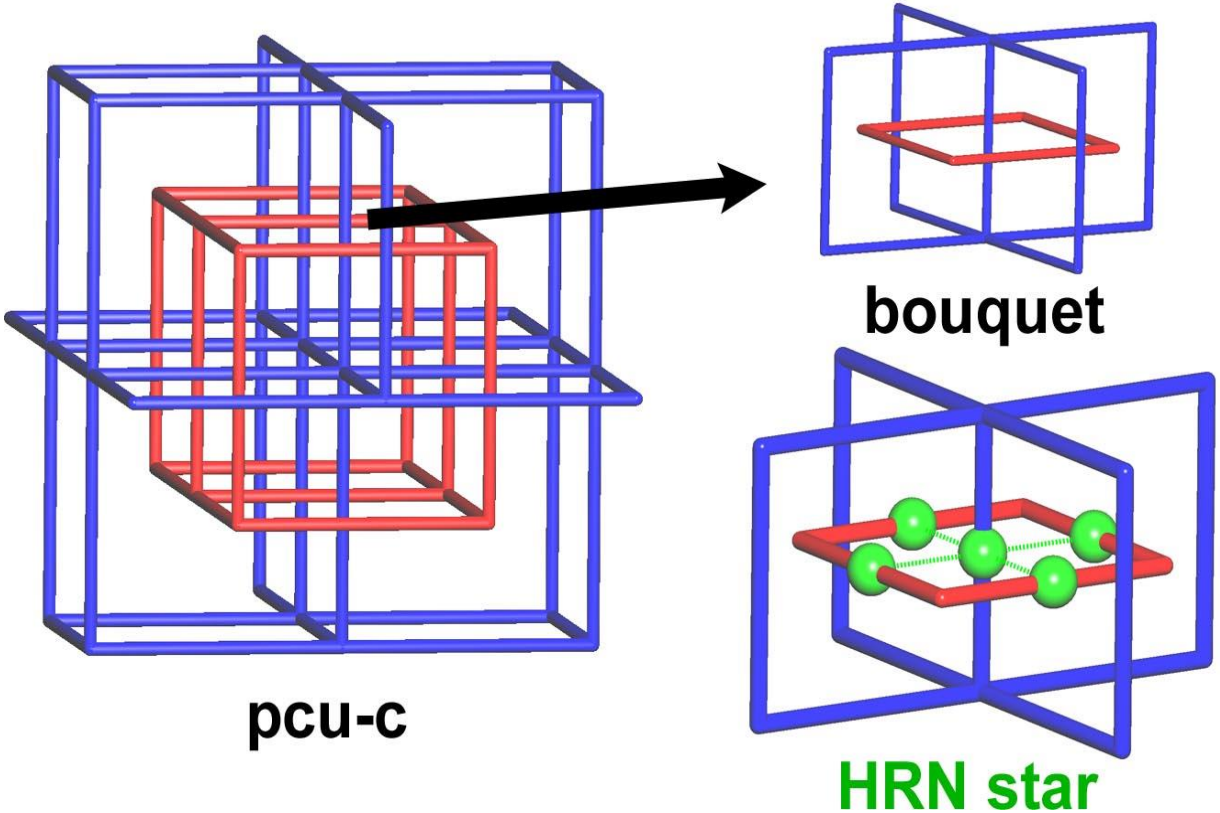
Ring links

Cycle 1	Cycle 2	Chain	Cross	Link	Hopf	Mult
6a	6a	inf.	1	1	*	2
6a	6b	inf.	1	1	*	4
6b	6a	inf.	1	1	*	4
6b	6b	inf.	1	1	*	6

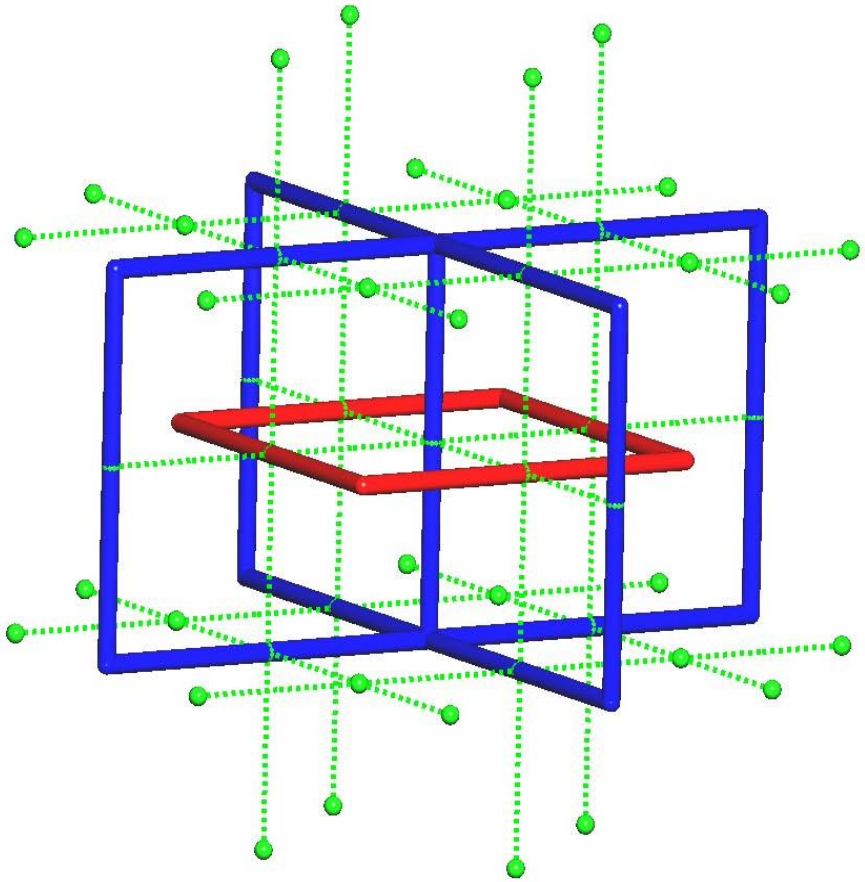
Acta Crystallographica Section A
Foundations of Crystallography
2012
3

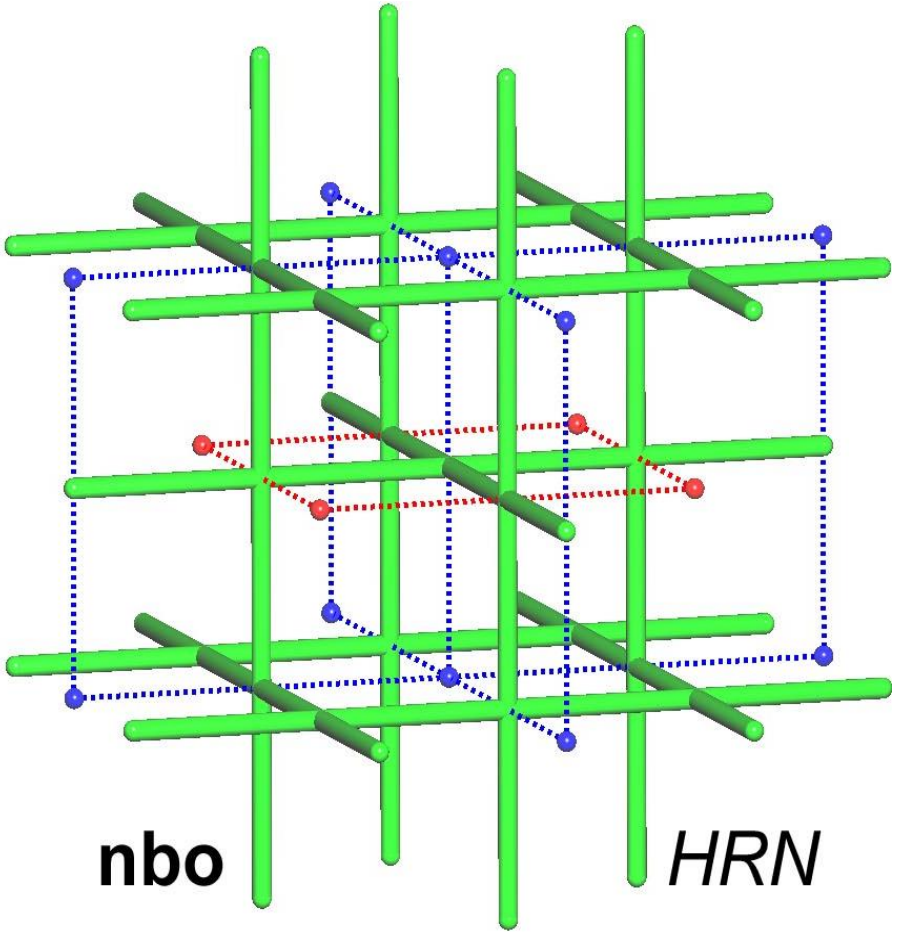
A topological method for the classification of entanglements in crystal networks[1]

Eugeny V. Alexandrov,[a] Vladislav A. Blatov[a]* and Davide M. Proserpio[b]*

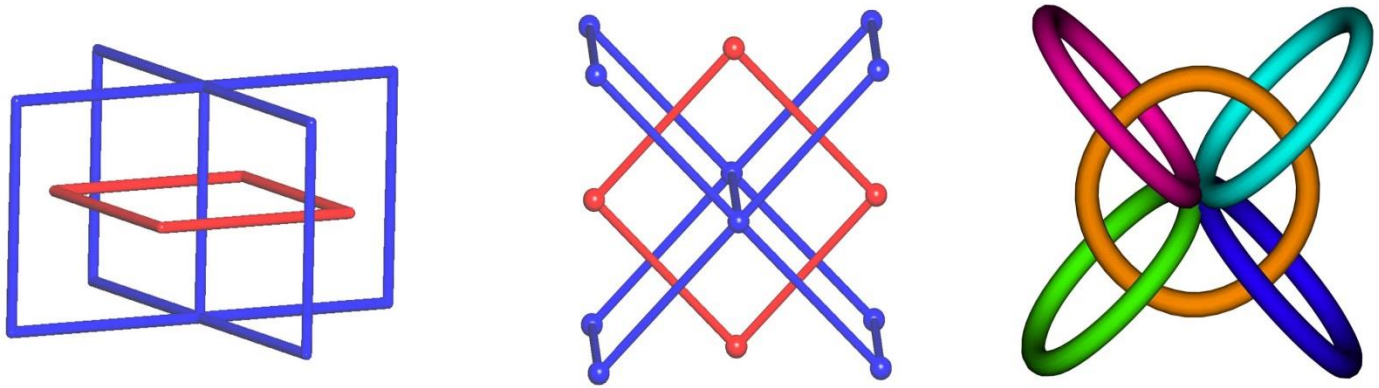


Pattern of catenation = HRN = Hopf ring net…



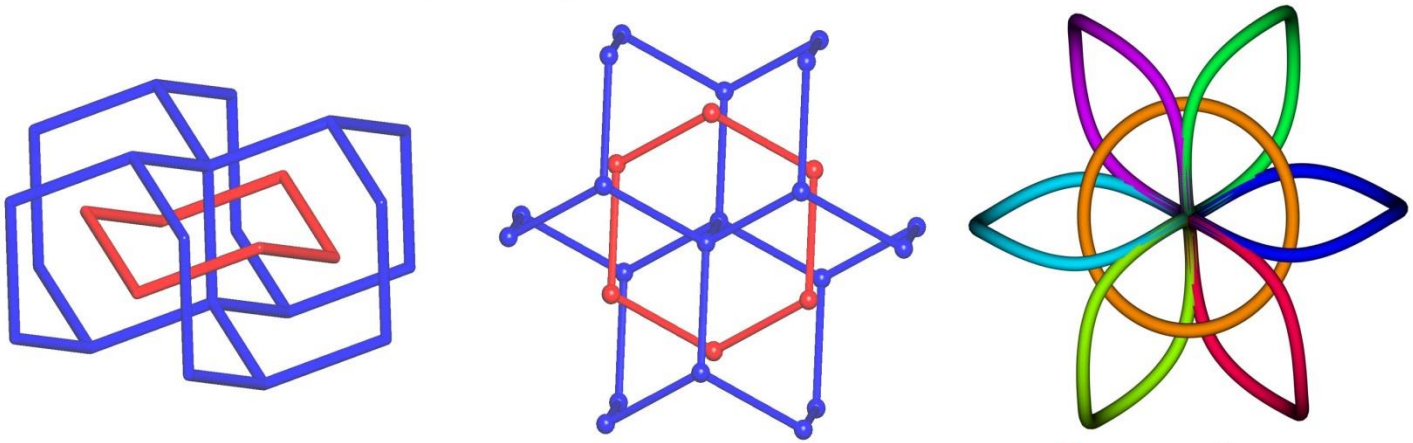


... that is the nbo net.



2 fold pcu = pcu-c

4-coor nbo

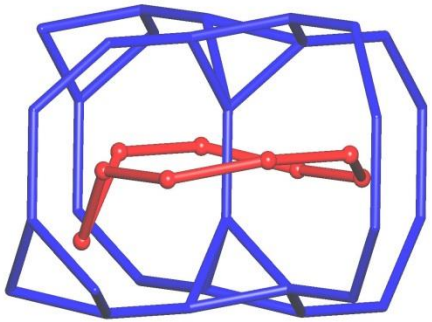


2 fold dia = dia-c

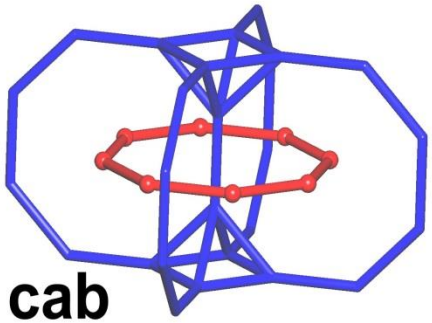
6-coor hxg

... but are these patterns observed in other 2-fold interpenetrated nets?

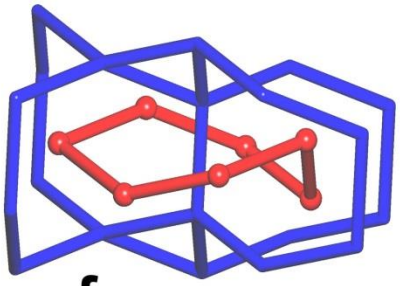
***YES*, the same HRN may be found for different nets.**
same "bouquet"



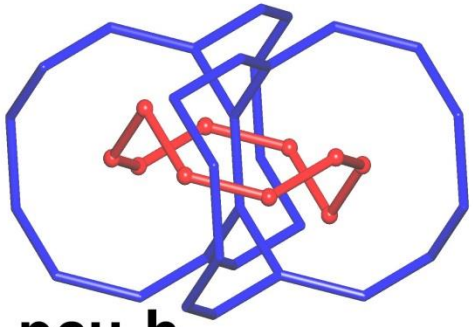
unp



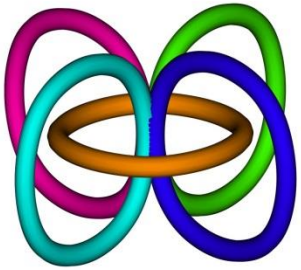
cab



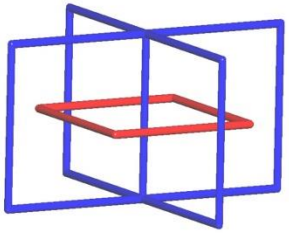
afw

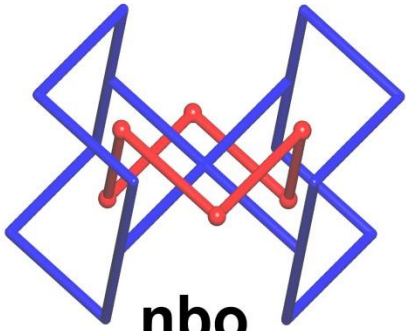


pcu-h

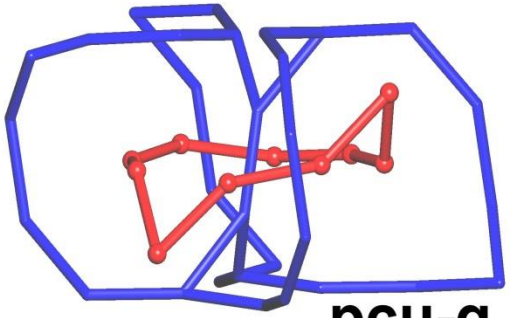


pcu

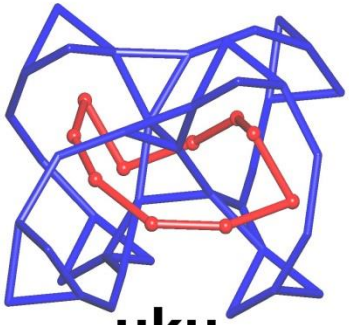




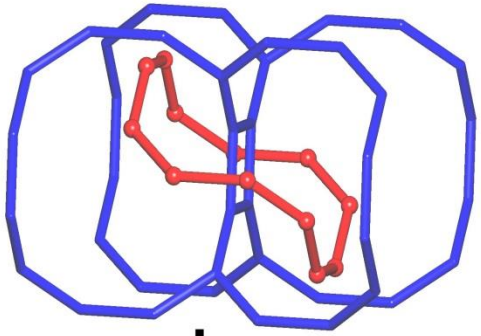
nbo



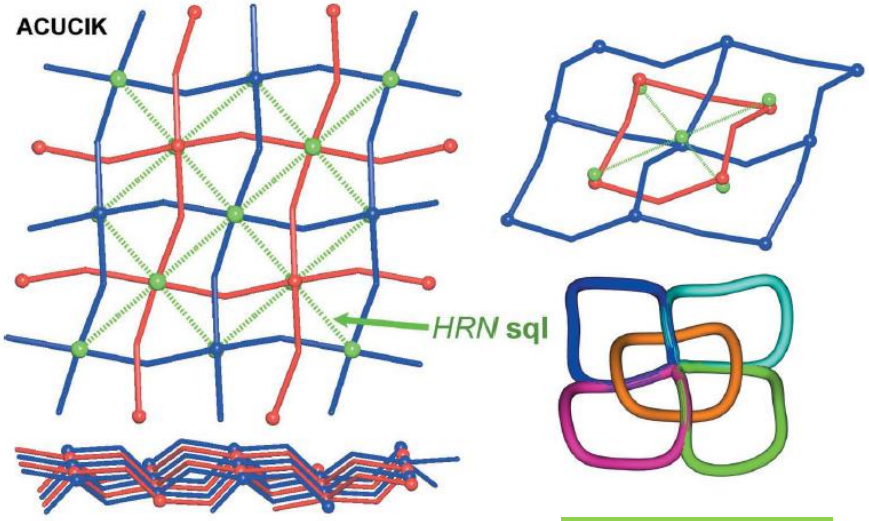
pcu-g



uku

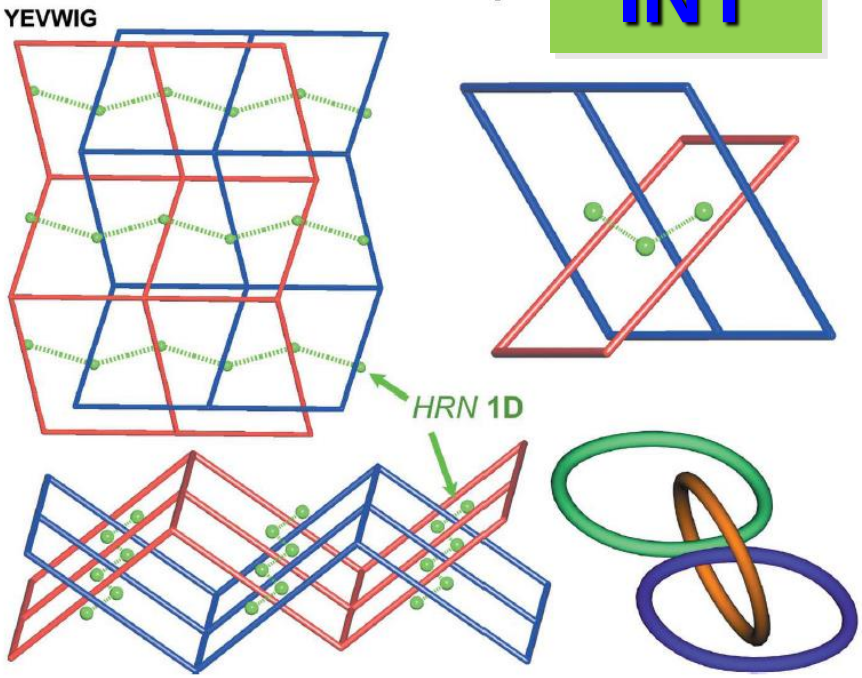


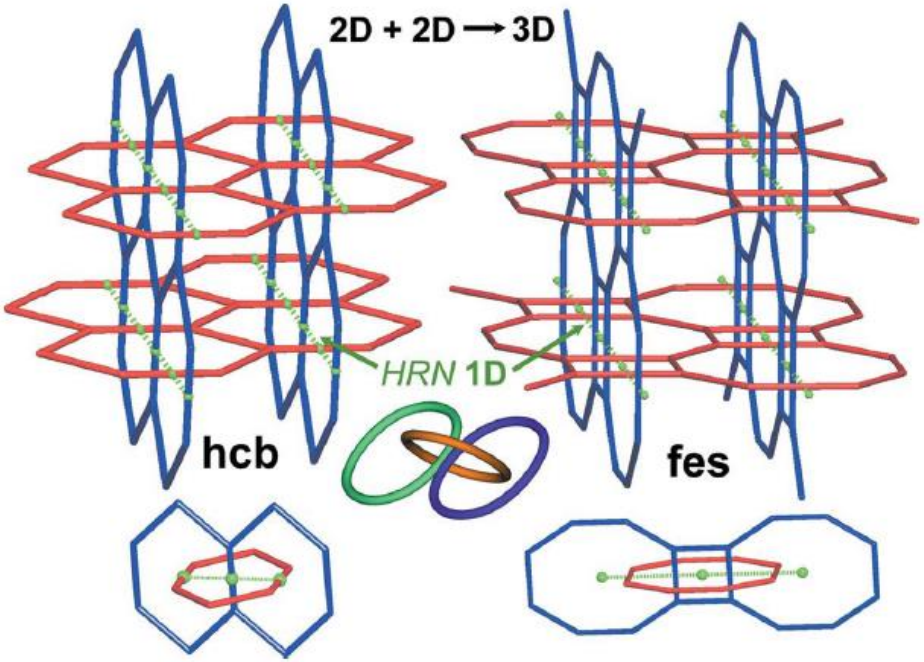
nbo-a



2-fold **sql**

INT

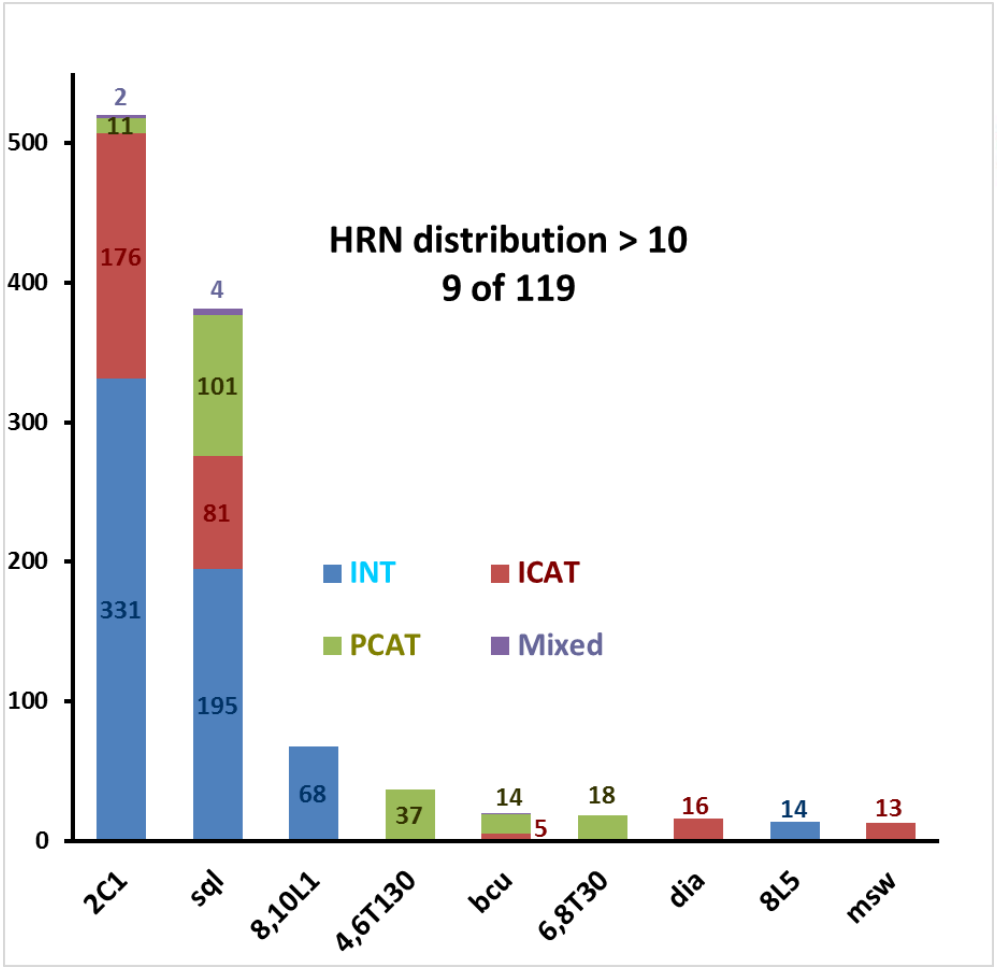


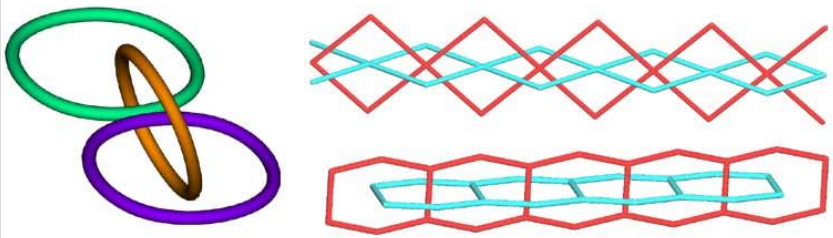


ICAT

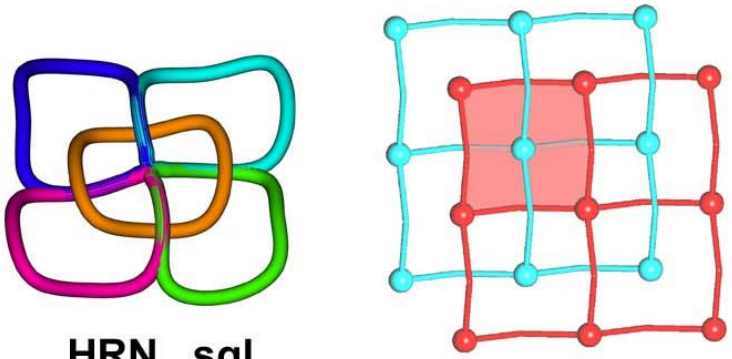
Some HRN in 2-periodic entanglements:
sql and simple chain (2C1)

119 HRN in 2-periodic entanglements: 70% are simple chain (2C1) and sql





HRN 2C1

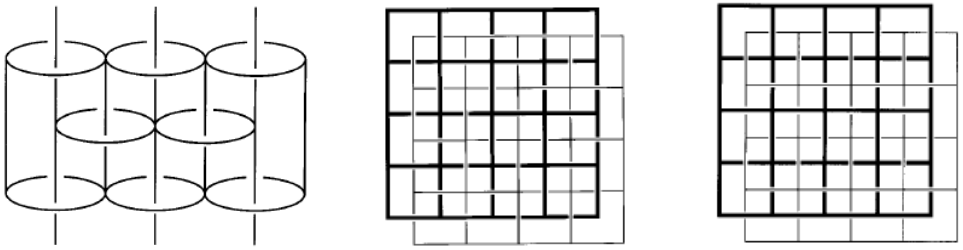


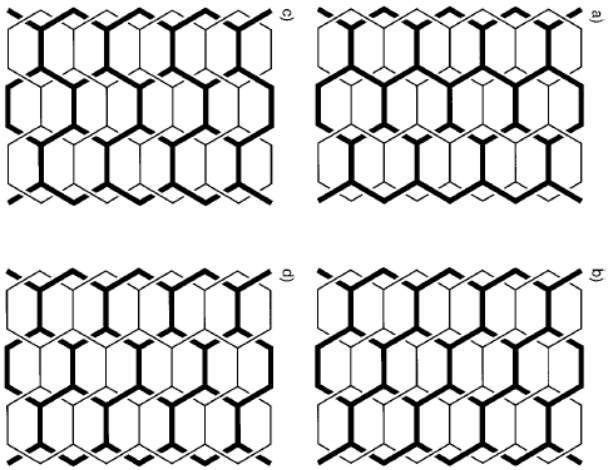
HRN sql

Interpenetrating Nets: Ordered, Periodic Entanglement

Stuart R. Batten and Richard Robson*

Angew. Chem. Int. Ed. **1998**, *37*, 1460 – 1494

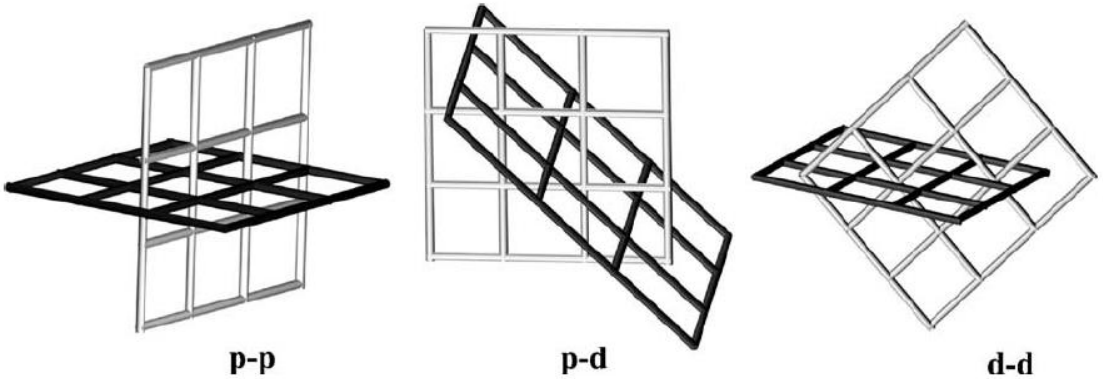




Chem. Rev. **2001**, *101*, 1629–1658

From Molecules to Crystal Engineering: Supramolecular Isomerism and Polymorphism in Network Solids

Brian Moulton and Michael J. Zaworotko*



Underlying net topology

sql, hcb, Kla…

Ring nets

FRN + HRN = ERN

Pattern of catenation

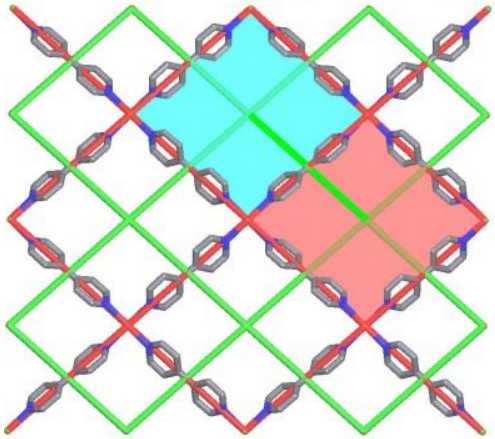
Hopf ring net HRN

Entanglement

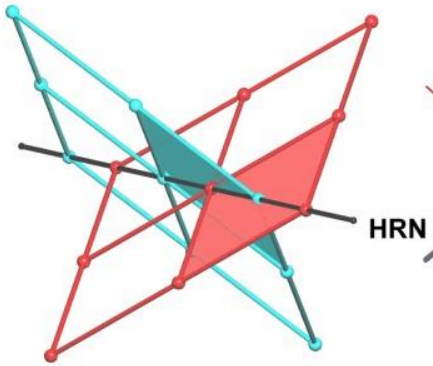
INT, ICAT, PCAT…

... and from HRN + FRN = ERN

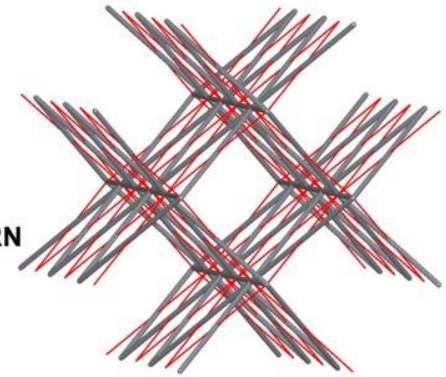
JEZRUB $[Zn(H_2O)_2(4,4'\text{-bipy})_2]^{2+}$



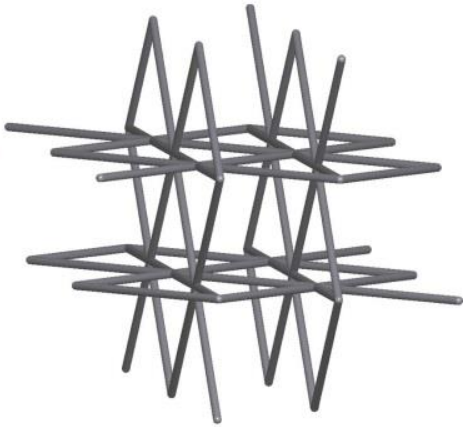
underlying net (red) **sql +**
fused ring net (green) FRN **sql**



inclined catenation of two **sql** +
Hopf ring net (HRN) 2-c linear chain

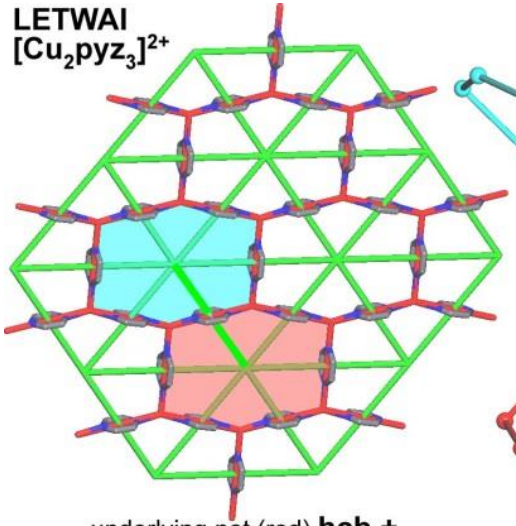


inclined catenation of **sql** (red) +
6-c *extended ring net* (grey) ERN

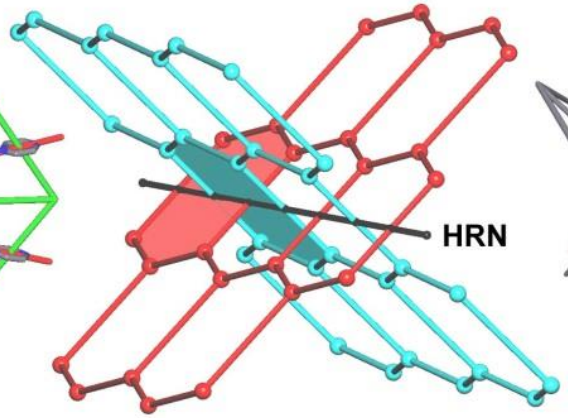


single 6-c *extended ring net*
ERN = FRN+HRN = $(4^9.6^6)$-6T13

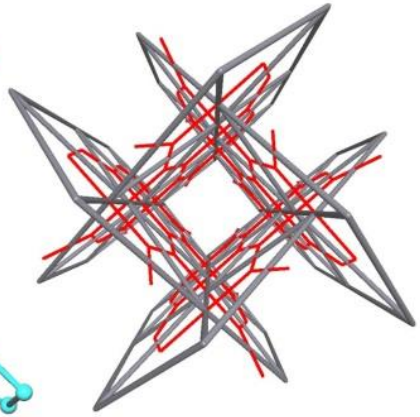
LETWAI
$[Cu_2pyz_3]^{2+}$



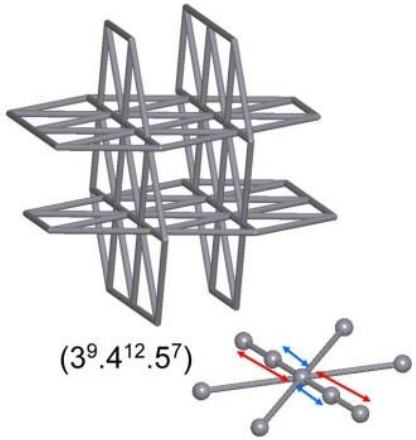
underlying net (red) **hcb +**
fused ring net (green) FRN **hxl**



inclined catenation of two **hcb** +
Hopf ring net (HRN) 2-c linear chain



inclined catenation of **hcb** (red) +
8-c *extended ring net (grey) ERN*



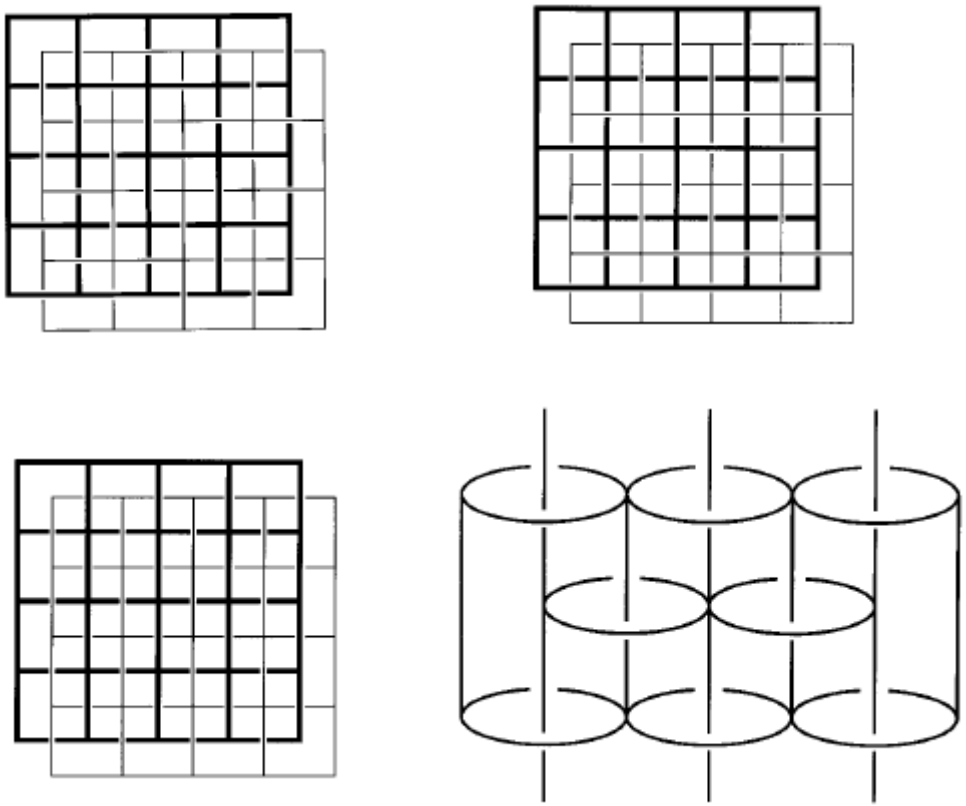
single 8-c *extended ring net*
with some coincident edges

ERN fully characterize the entanglement

Interpenetrating Nets: Ordered, Periodic Entanglement

Stuart R. Batten and Richard Robson*

Angew. Chem. Int. Ed. **1998**, *37*, 1460 – 1494



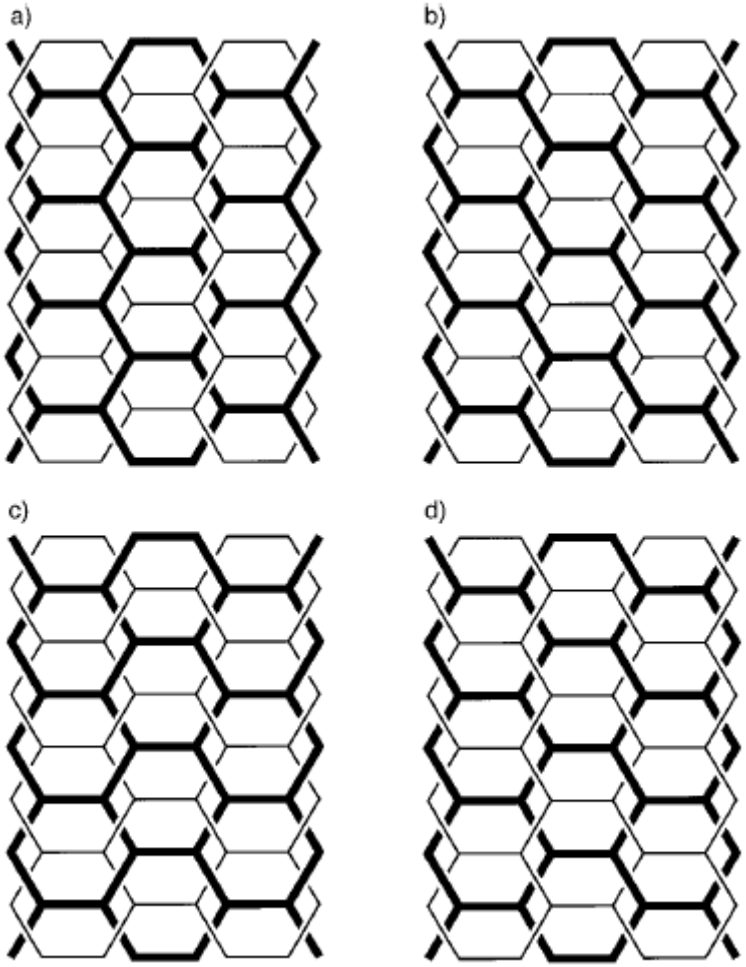
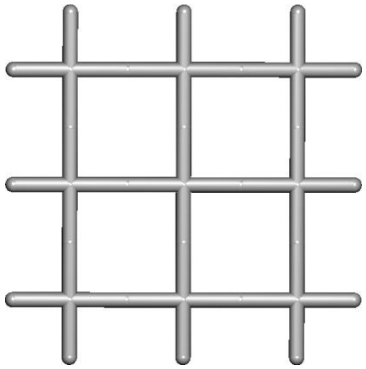


Figure 11. a) – d) Four topologically different modes of parallel interpenetration of (6,3) nets.

2-fold Interpenetration sql

11 Extended ring nets ERN

330 sql 2-fold



4 HRN

216 2C1
1-periodic

8

- **108 structures** (4,4)IIa (B17)
- **101 structures** (4,4)IIb
- YEGRAD (B16)
- BUBPAR, CISSUU
- OWUFOC
- IBUDIT
- ETEVAC
- GIKREZ

6 different patterns

104 sql
2-periodic

- **104 structures** (B18)

5 4^4-(0,2)
1-periodic

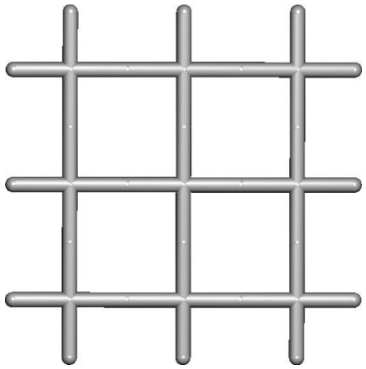
- **5 Solomon link A**

5 Kla
2-periodic

- **5 Solomon link B**

2-fold Interpenetration sql

330 sql 2-fold



4 HRN

216 2C1
1-periodic

8

11 Extended ring nets ERN

108 structures (4,4)IIa (B17) **32.7%**

101 structures (4,4)IIb **30.5%**

YEGRAD (B16) | BUBPAR, CISSUU
OWUFOC | IBUDIT
ETEVAC | GIKREZ

6 different patterns

104 sql
2-periodic

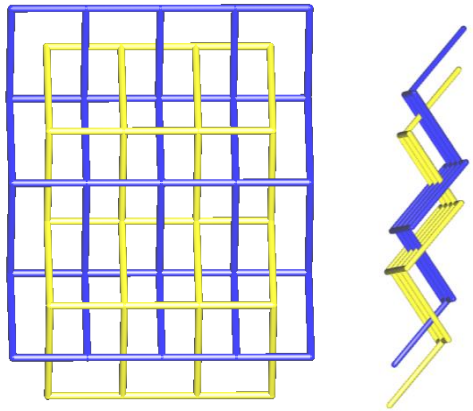
104 structures (B18) **31.5%**

5 4^4-(0,2)
1-periodic

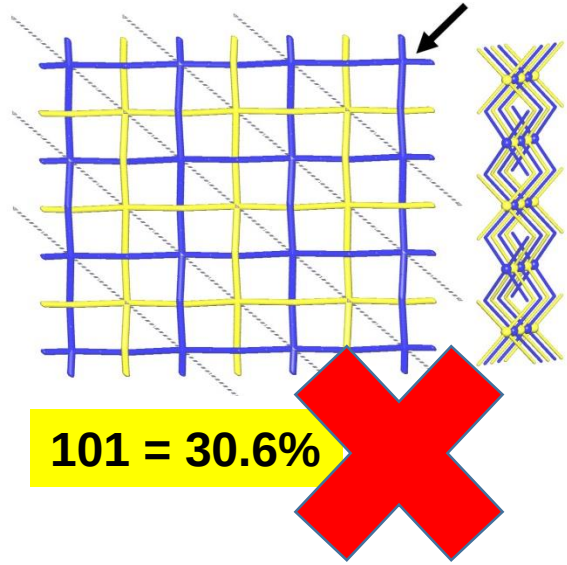
5 Solomon link A

5 Kla
2-periodic

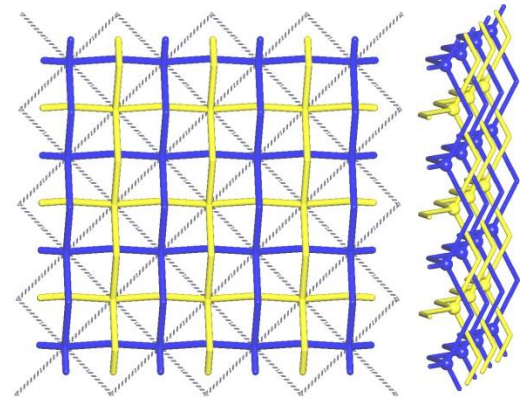
5 Solomon link B



108 = 32.7%



101 = 30.6%



104 = 31.5%

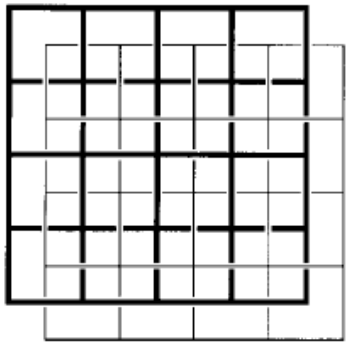


Figure 17. a) Two parallel interpenetrating (4,4) nets in the structure of [Cu(tcm)(bipy)]. The large circles represent Cu atoms, and the small circles C and N atoms. b) Schematic representation of the mode of interpenetration.

Interpenetrating Nets: Ordered, Periodic Entanglement

Stuart R. Batten and Richard Robson*

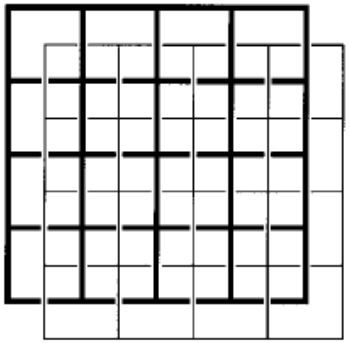


Figure 18. Schematic representation of the two parallel interpenetrating hydrogen-bonded (4,4) nets in the structure of $[Re_4(CO)_{12}(OH)_4] \cdot 2\,bipy \cdot 2\,MeOH$. The four-connected nodes shown represent the centers of the Re_4 clusters.

2-fold interpenetration sql

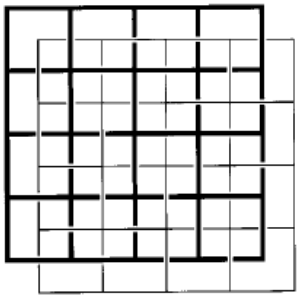
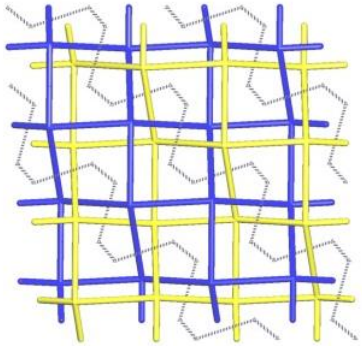


Figure 16. a) Parallel interpenetrating (4,4) nets in the structure of $[Cd(4\text{-pic})_2[Ag(CN)_2]_2](4\text{-pic})$ (4-pic = 4-methylpyridine). The pendant 4-pic

YEGRAD



YEGRAD

YEGRAD (B16)

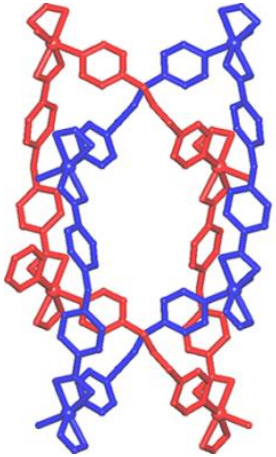
BUBPAR CISSUU

OWUFOC

IBUDIT

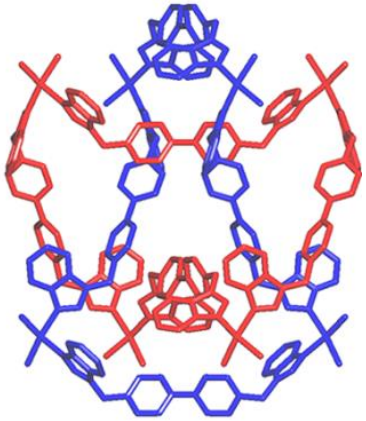
ETEVAC

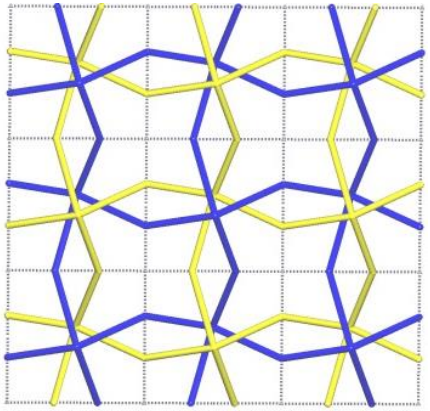
GIKREZ



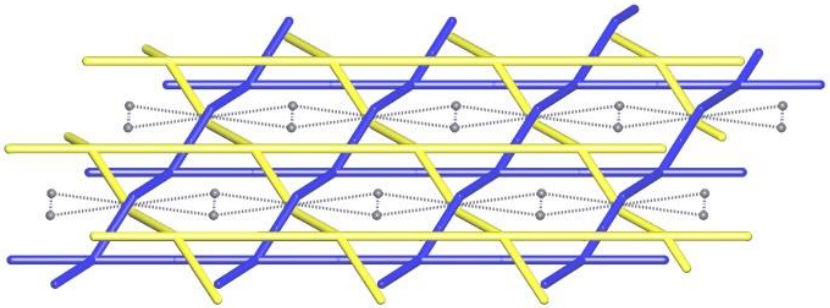
Solomon link

4-crossings
[2]-catenane





5 Solomon link A

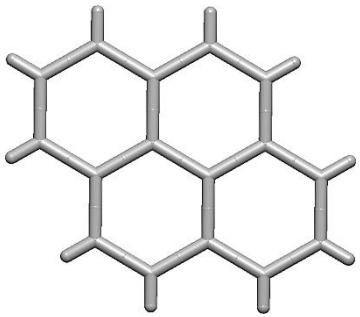


5 Solomon link B

2-fold interpenetration sql

2-fold Interpenetration hcb

90 hcb 2-fold



2 HRN

86 2C1
1-periodic

4 sql
2-periodic

4 ERN

82 structures (3,6)II (B11a)

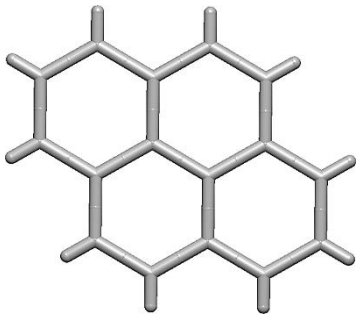
IQEHUI, IQEJAQ, IQEJEU, MOYYAB (B11c)

NUHMEJ, OPESIM

NALQAU, TUCQEO (B11b)

2-fold Interpenetration hcb

90 hcb 2-fold



2 HRN

86 2C1
1-periodic

4 sql
2-periodic

4 ERN

82 structures (B11a) **91%**

IQEHUI, IQEJAQ, IQEJEU, MOYYAB (B11c)

NUHMEJ, OPESIM

NALQAU, TUCQEO (B11b)

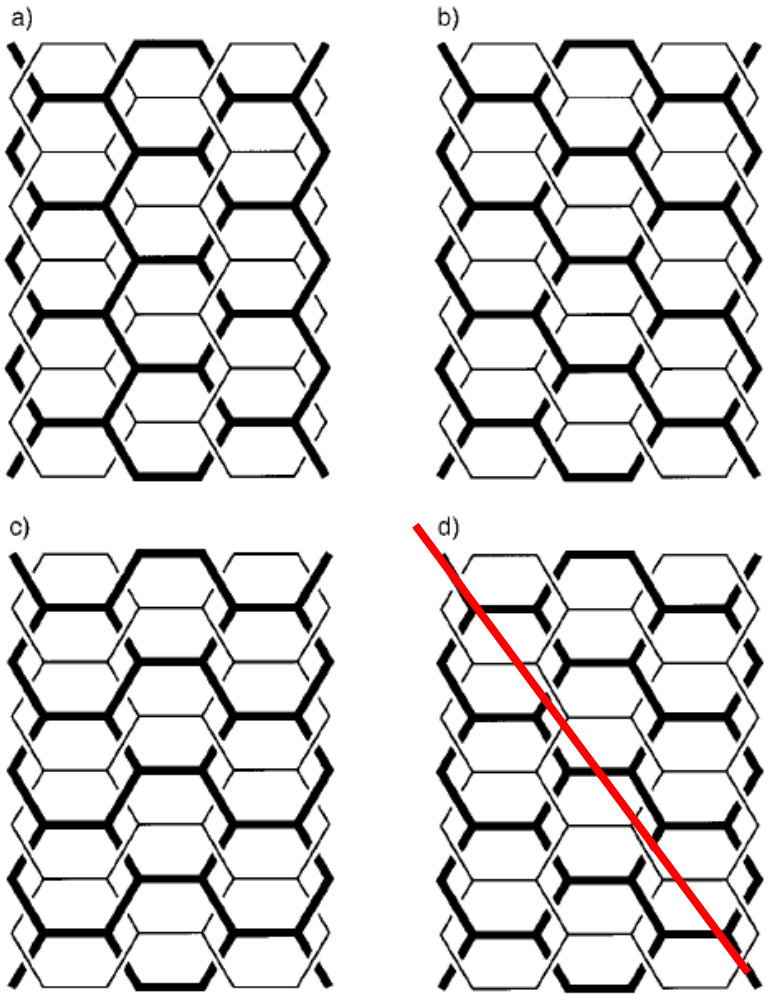
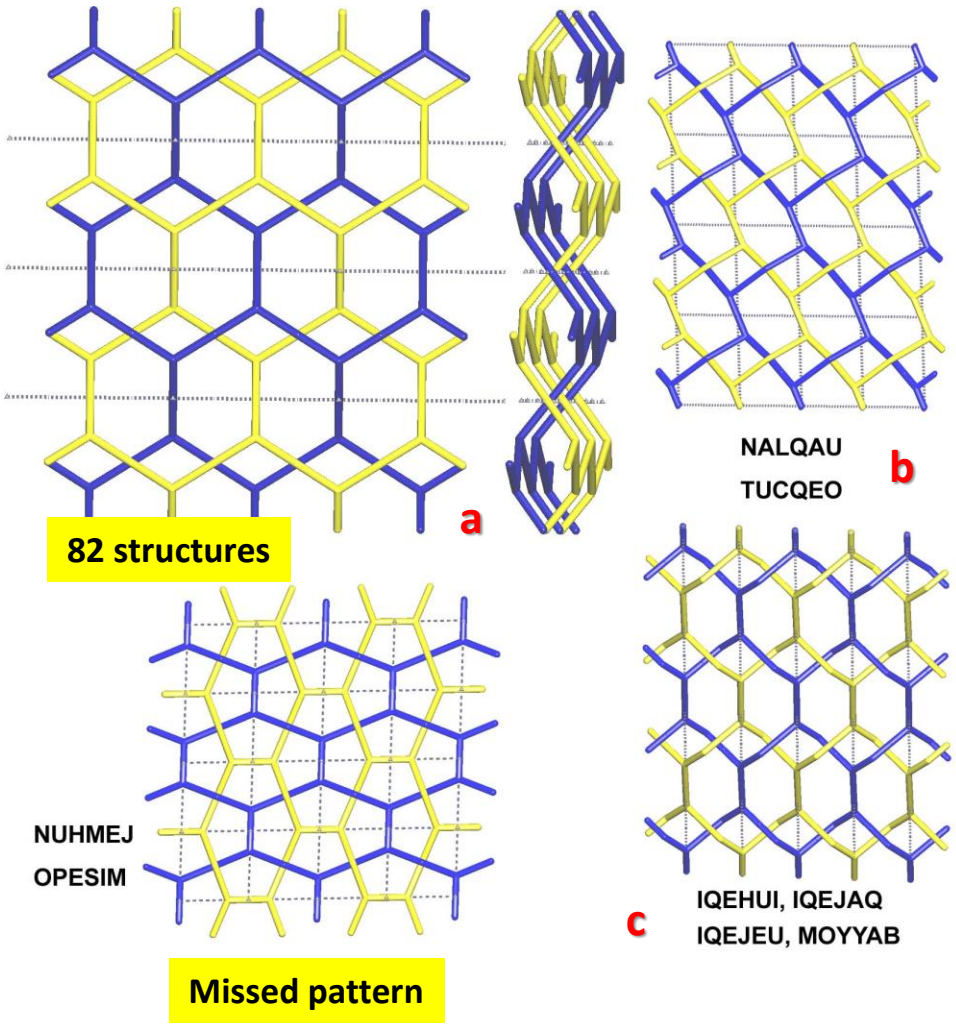
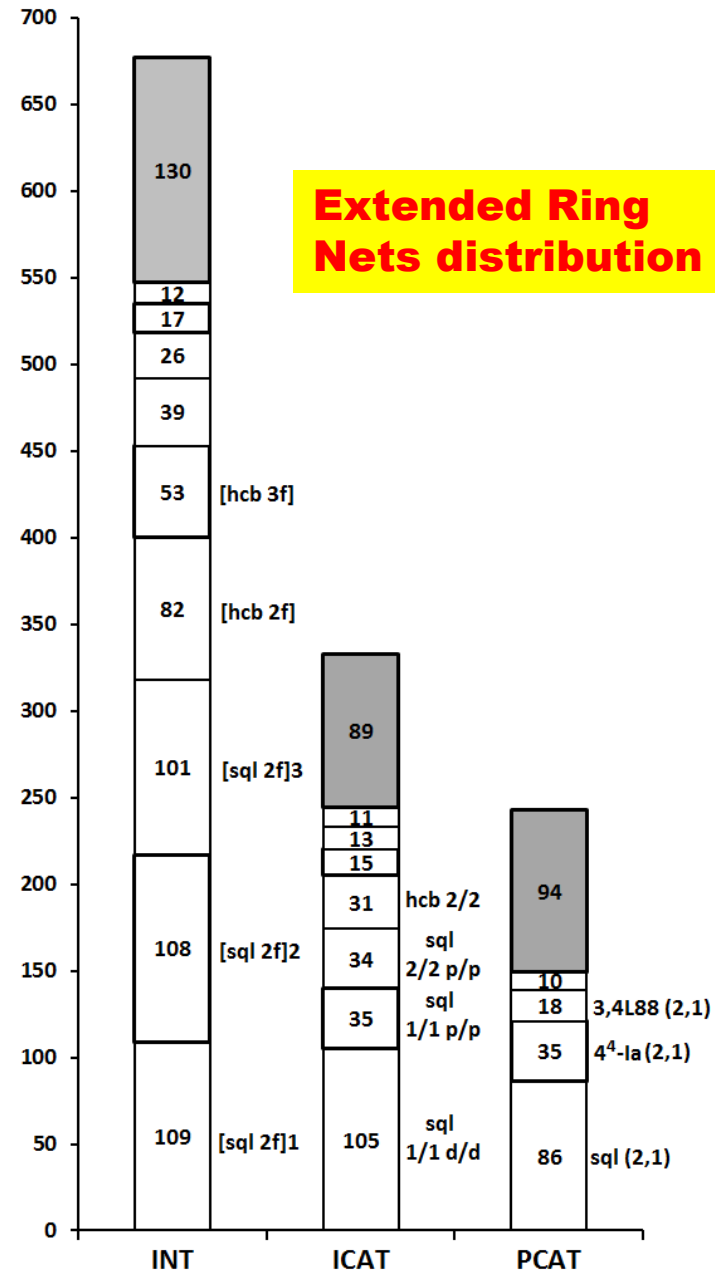


Figure 11. a) – d) Four topologically different modes of parallel interpenetration of (6,3) nets.



2-fold interpenetration hcb

Layer	Entang type	DOC, IS, Z	HRN	ERN	hits
sql	INT	Z 2	2C1	6-c 4^4-IIb	101
sql	INT	Z 2	2C1	6-c 4^4-IIa	109
sql	INT	Z 2	sql	8-c 4^4-IV	108
sql	INT	Z 3	sql	8-c^1	17
sql	INT	Z 3	8L5	12-c^1	12
hcb	INT	Z 2	2C1	8-c 3^6-II	82
hcb	INT	Z 3	sql	10-c^1	53
hcb	INT	Z 2, 2-loop	8,10L1	16,35-c	26
sql	INT	Z 2, 2-loop	8,10L1	16,27,27-c	39
sql	ICAT	DOC 1/1 d/d	2C1	6T13	105
sql	ICAT	DOC 1/1 p/p	2C1	6-c sqc23	35
sql	ICAT	DOC 2/2 p/p	sql	8-c^2	34
sql	ICAT	DOC 2/2 d/d	sql	8T4	15
hcb	ICAT	DOC 1/1	2C1	8-c^3	13
hcb	ICAT	DOC 2/2	sql	10-c^2	31
hcb	ICAT	DOC 3/3	msw	12-c^2	11
sql	PCAT	DOC 2, IS 1	sql	8-c hex	86
4^4-Ia	PCAT	DOC 2, IS 1	4,6T130	12,16-c	35
3,4L88	PCAT	DOC 2, IS 1	6,8T30	21,24-c	18
hcb	PCAT	DOC 2, IS 1	sql	10-c bct	10



The 20 most frequent patterns of entanglement (of 224)- ERN

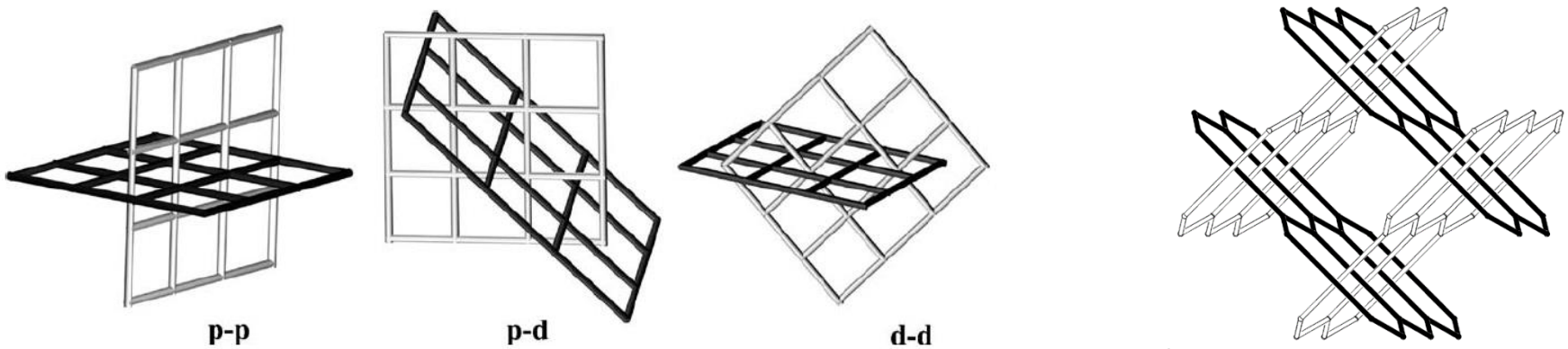
ICAT

Layer	Entang .type	DOC, IS, Z	HRN	ERN	hits
sql	ICAT	DOC 1/1 d/d	2C1	6T13	105
sql	ICAT	DOC 1/1 p/p	2C1	6-c sqc23	35
sql	ICAT	DOC 2/2 p/p	sql	8-c^2	34
sql	ICAT	DOC 2/2 d/d	sql	8T4	15
hcb	ICAT	DOC 1/1	2C1	8-c^3	13
hcb	ICAT	DOC 2/2	sql	10-c^2	31
hcb	ICAT	DOC 3/3	msw	12-c^2	11

Chem. Rev. **2001**, *101*, 1629–1658

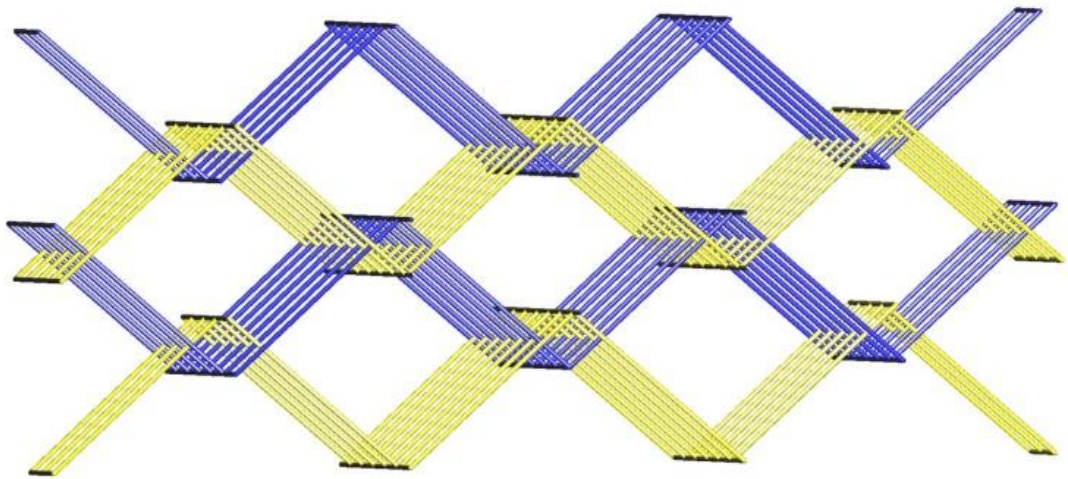
From Molecules to Crystal Engineering: Supramolecular Isomerism and Polymorphism in Network Solids

Brian Moulton and Michael J. Zaworotko*

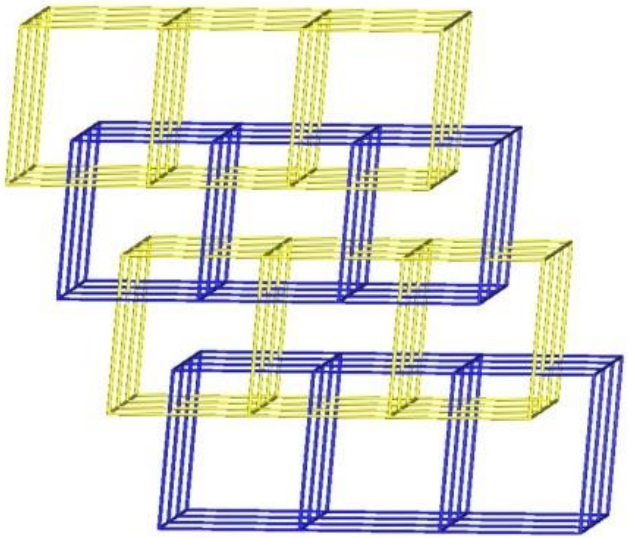


PCAT

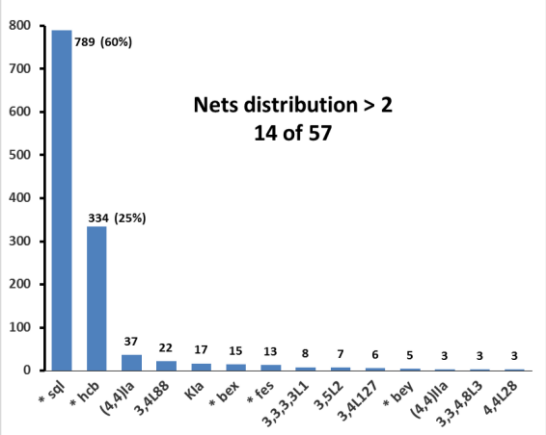
Layer	Entang type	DOC, IS, Z	HRN	ERN	hits
sql	PCAT	DOC 2, IS 1	sql	8-c hex	86
4^4-Ia	PCAT	DOC 2, IS 1	4,6T130	12,16-c	35
3,4L88	PCAT	DOC 2, IS 1	6,8T30	21,24-c	18
hcb	PCAT	DOC 2, IS 1	sql	10-c bct	10



86 PCAT of undulated sql



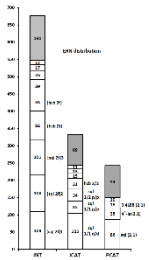
24 PCAT of double sql 4^4-Ia

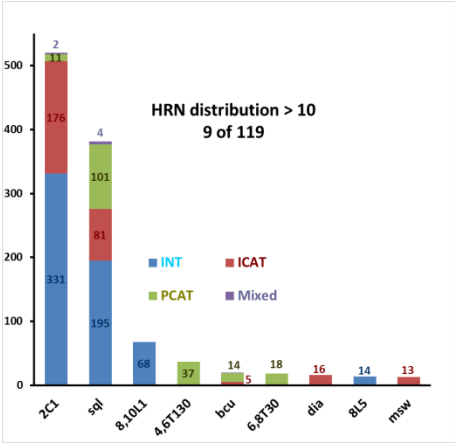


57 Underlying net topology

sql, hcb 85%

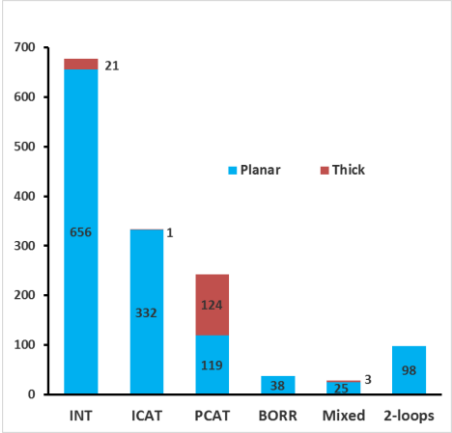
1319 structures





224 ERN

20 for 73%



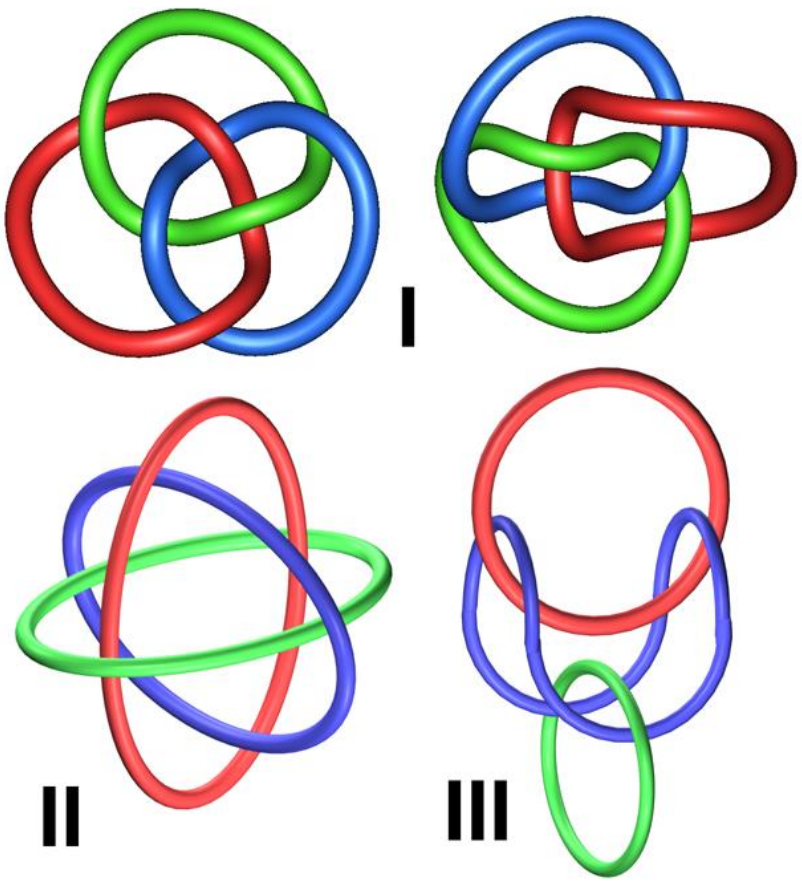
119 Pattern of catenation HRN

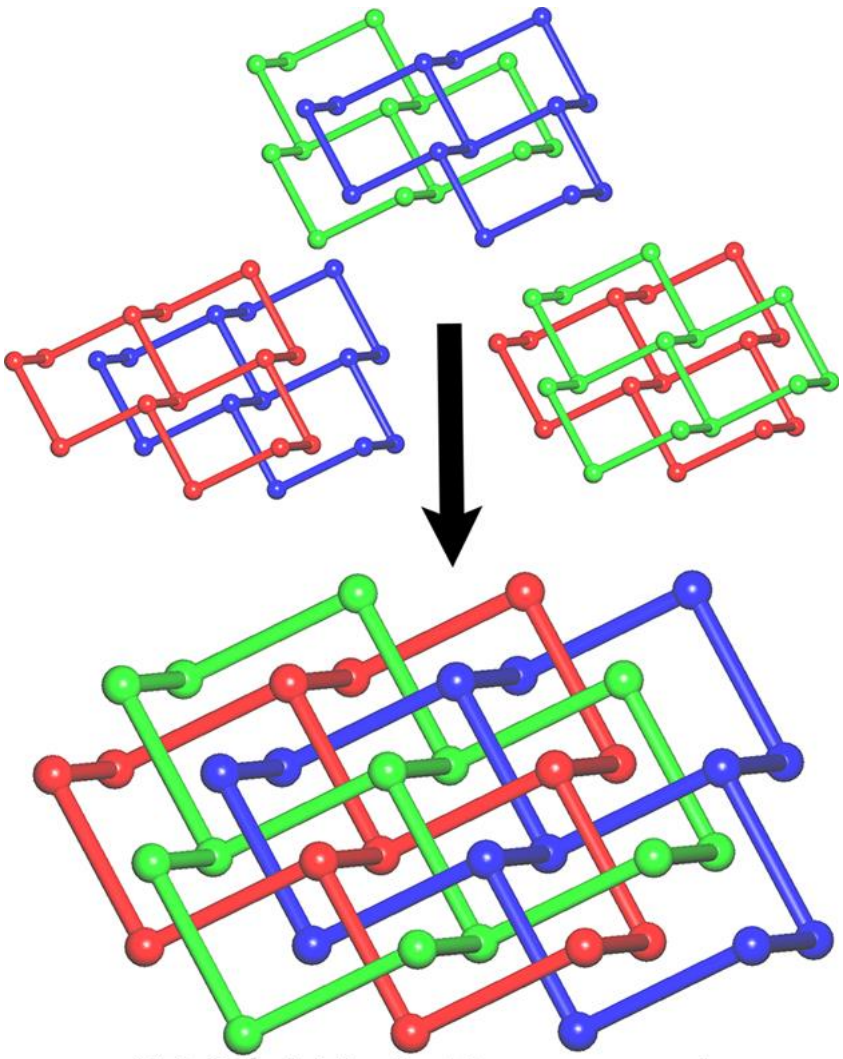
sql, 2C1 70%

Entanglement

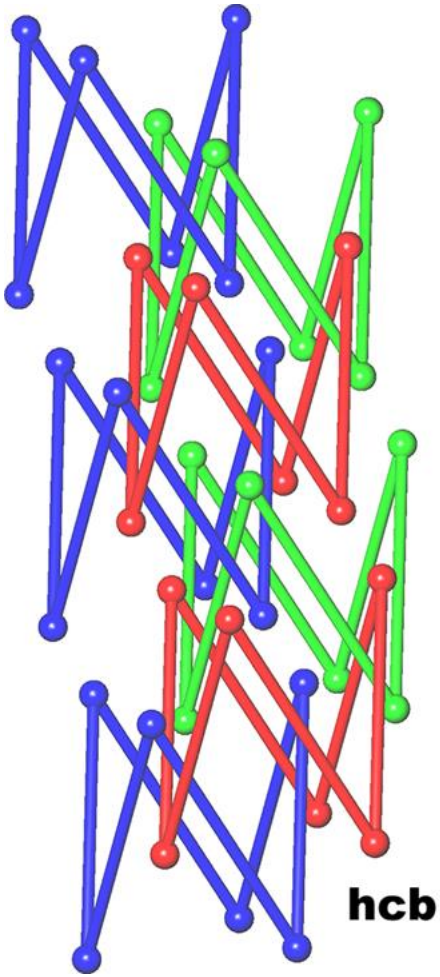
INT, ICAT, PCAT, **BORR**

Borromean links

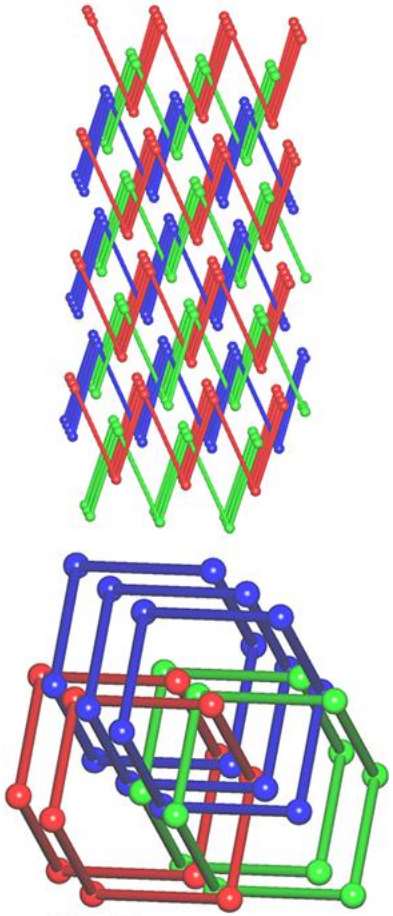




2D 3-fold **hcb** Borromean layer



hcb



3D Borromean

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Applied Topological Analysis of Crystal Structures with the Program Package ToposPro

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program package for multipurpose crystallochemical analysis

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PRACTICAL MANUAL 1.1.1

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