Сложность кристаллических структур минералов и неорганических соединений

С. Кривовичев   СПбГУ, Санкт-Петербург

Angewandte Reviews

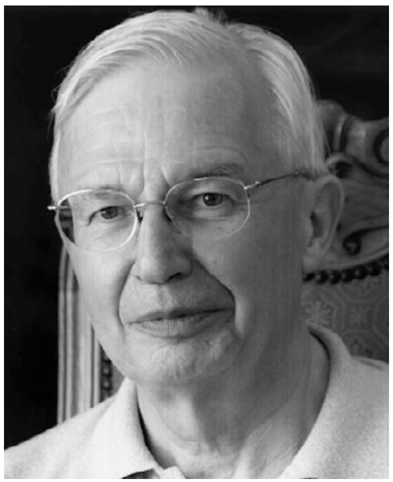
Angew. Chem. Int. Ed. **2013**, 52, 2836 – 2850

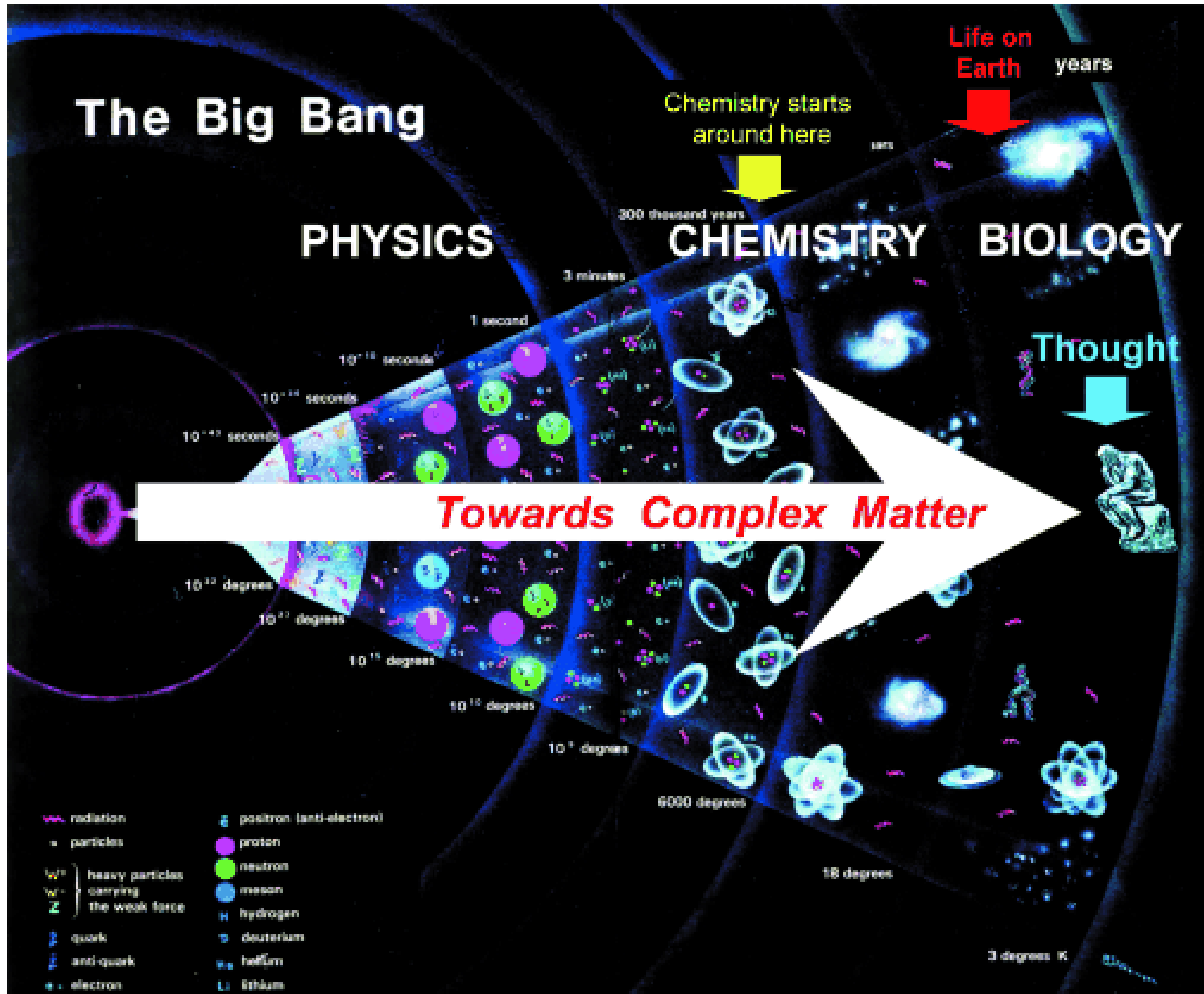
Towards Complex Matter

DOI: 10.1002/anie.201208397

Perspectives in Chemistry—Steps towards Complex Matter

*Jean-Marie Lehn**





Chemistry is to Physics what a Beethoven quartet is to the laws of acoustics!

Content

1. Crystal structures as complex systems
2. Which system is more complex? Intuitive feelings
3. Static complexity of spatial structures: quantitative approach
4. Dynamic complexity: cellular automata and design
5. When complexity matters: metastable crystallization
6. Conclusions

Crystal structures as complex systems

Charles H. Bennett
IBM Research, Yorktown Heights NY 10598, USA

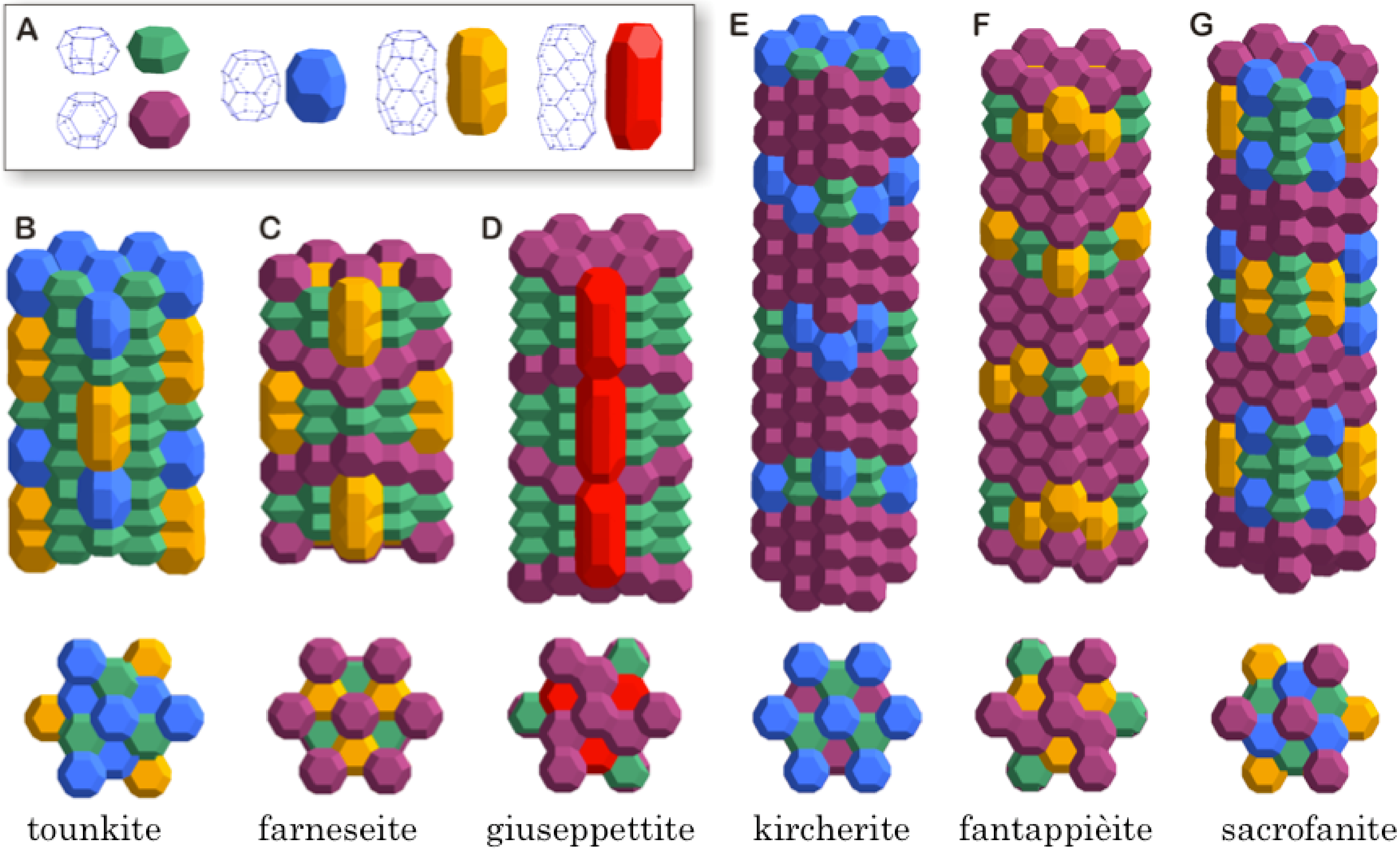
How to Define Complexity in Physics, and Why

Long-Range Order, the existence of statistical correlations between arbitrarily remote parts of a body, is an unsatisfactory complexity measure, because it is present in such intuitively simple objects such as perfect crystals.

Bennet, C.H. (1990) How to define complexity in physics, and why. In: Zurek, W.H. (ed.) *Complexity, Entropy, and the Physics of Information. Santa Fe Institute Studies in the Sciences of Complexity*. Vol. VIII. Addison-Wesley, pp. 137-148.

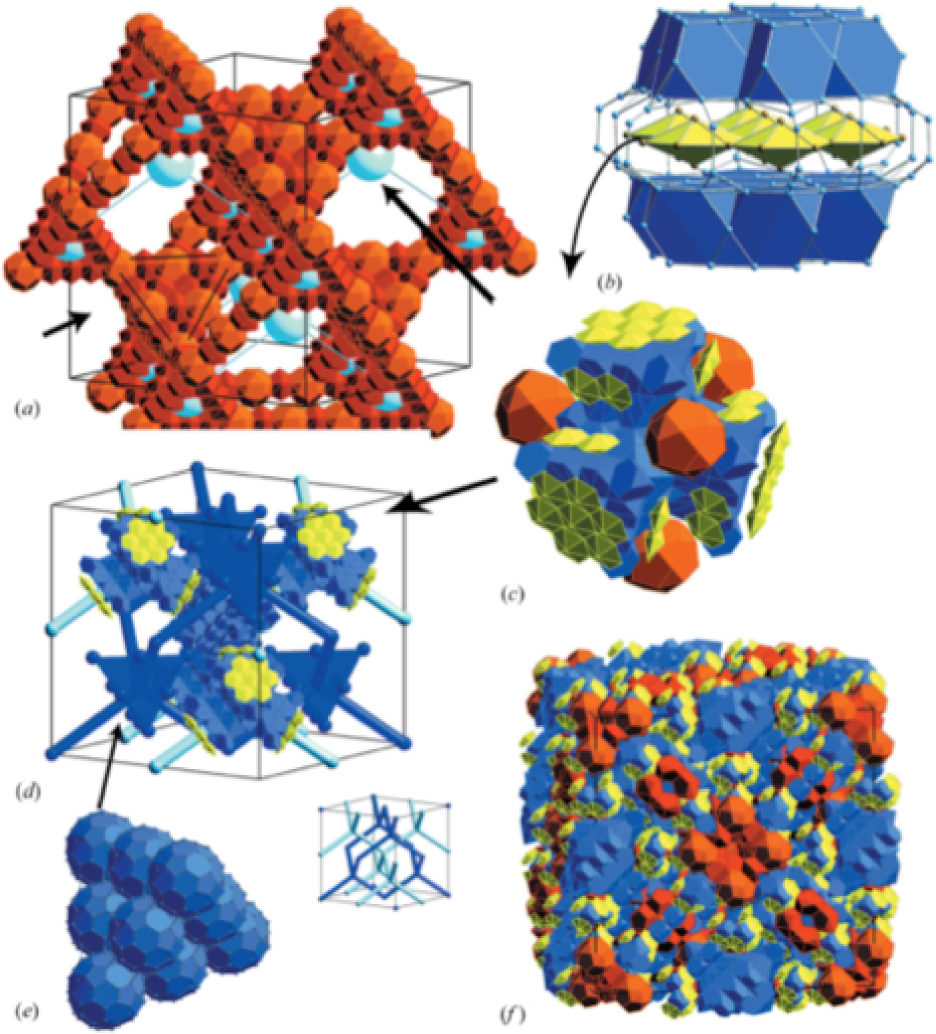
Complex Mineral Structures

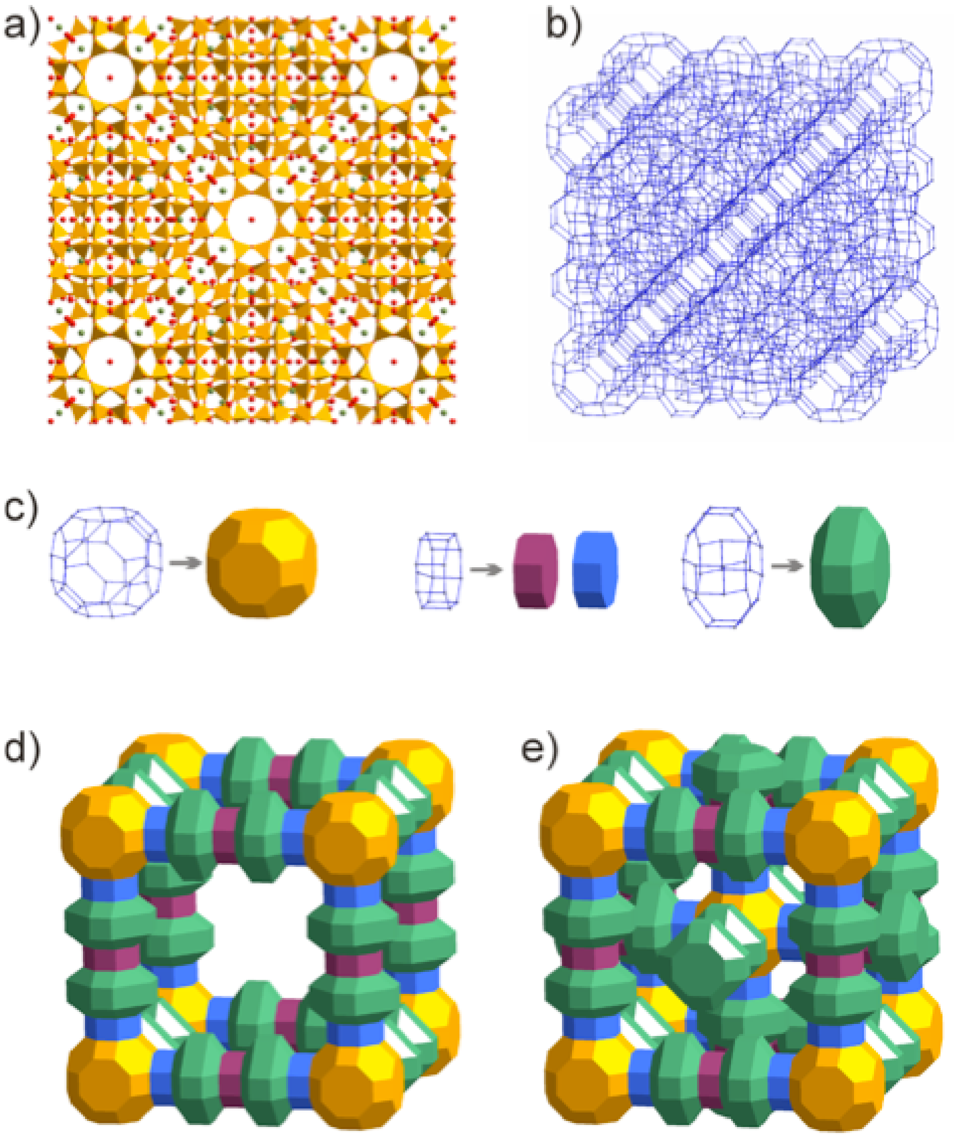
Minerals of the Cancrinite-Sodalite Supergroup



Cámara *et al.*, 2005, 2010, 2012; Bonaccorsi, 2004; Bonaccorsi *et al.*, 2012; Rozenberg *et al.*, 2004

Complex Inorganic Structures





Complexity

Static Complexity

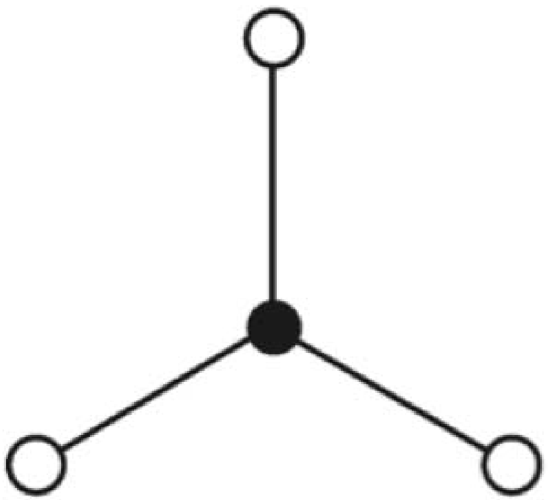
addresses purely structural informational aspects and is independent of the processes by which information is encoded and decoded

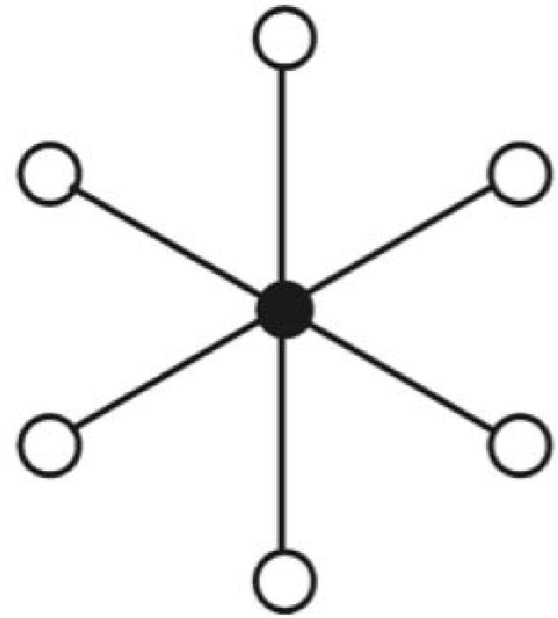
Dynamic Complexity

addresses the question of how much dynamical or computational effort is required to build a system

Which system is more complex?

Intuitive feelings



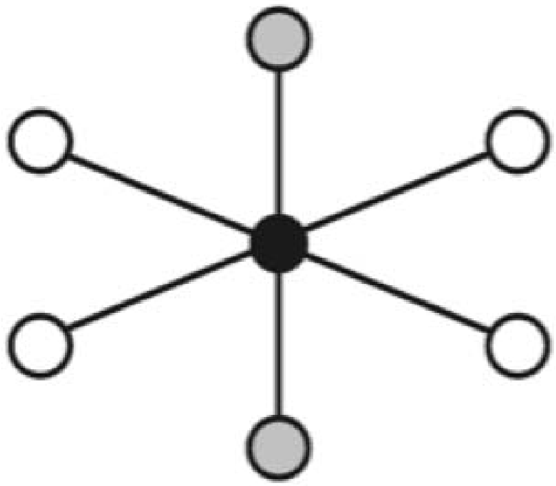


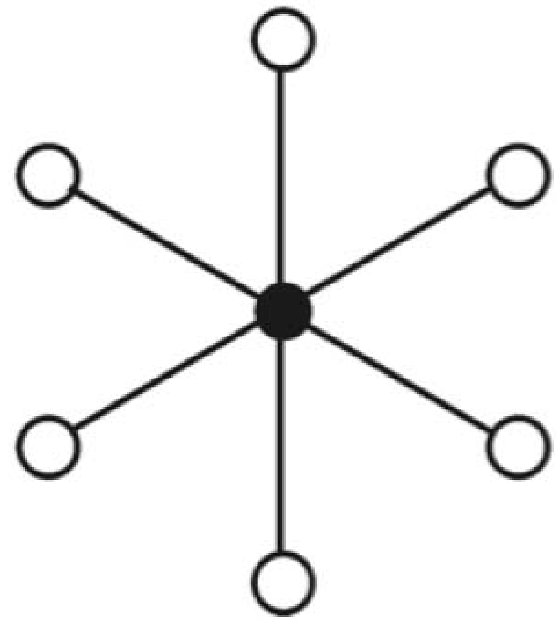
FIRST CONSIDERATION

The more parts the system has, the more complex it is

Which system is more complex?

Intuitive feelings



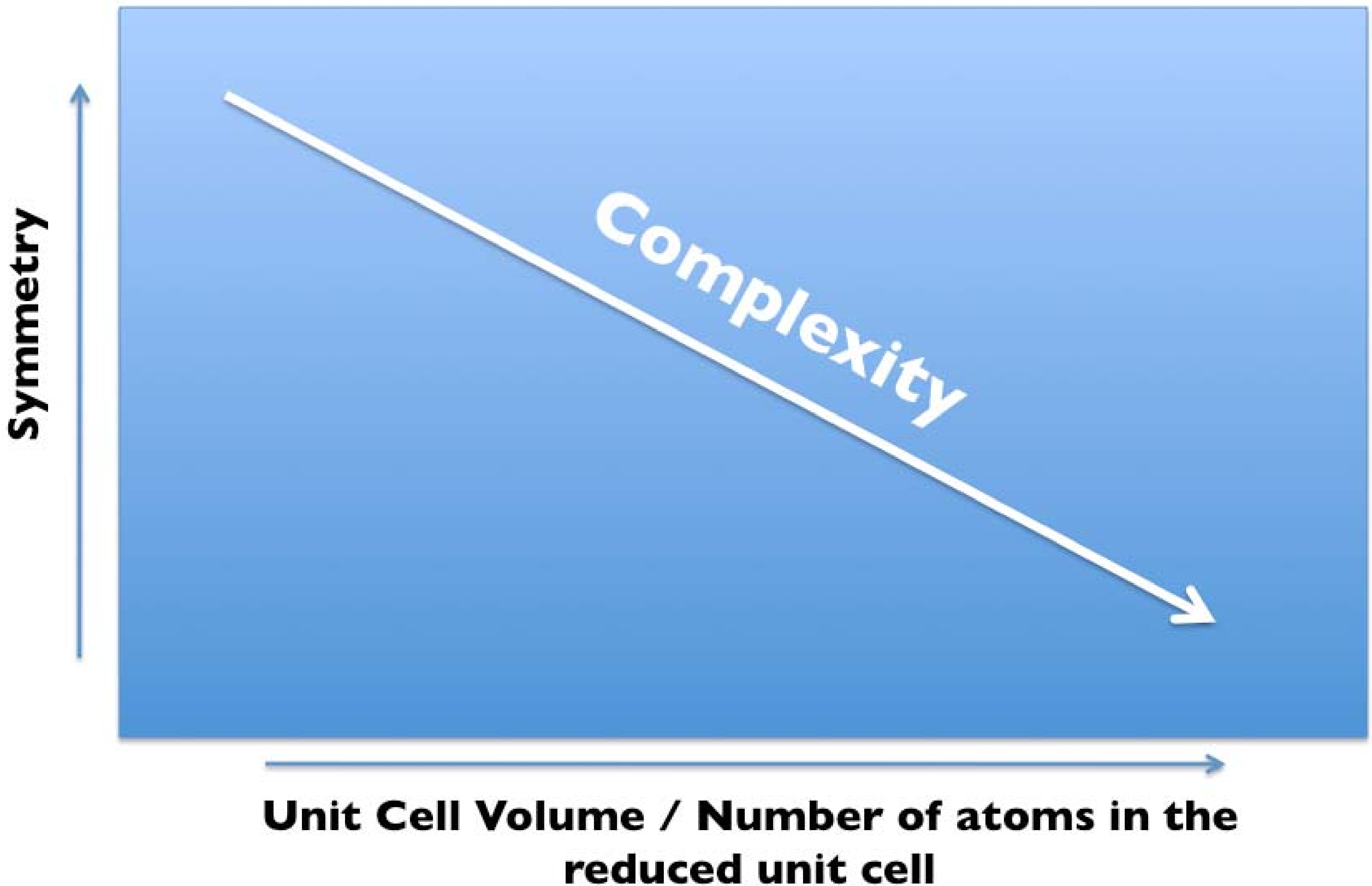


SECOND CONSIDERATION

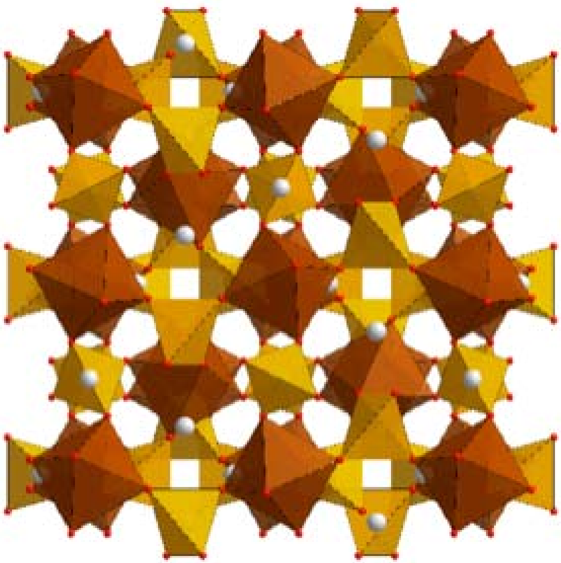
The lower the symmetry of the system, the more complex it is

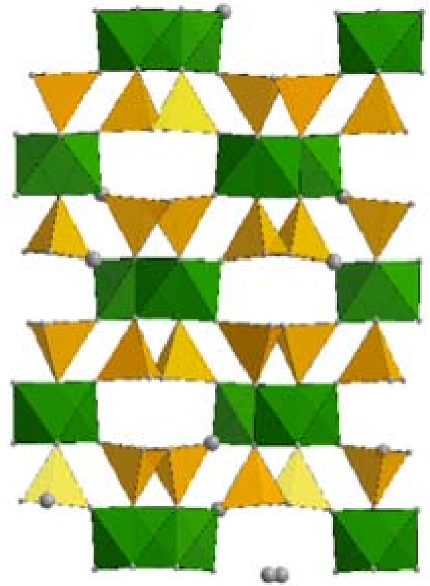
Which structure is complex?

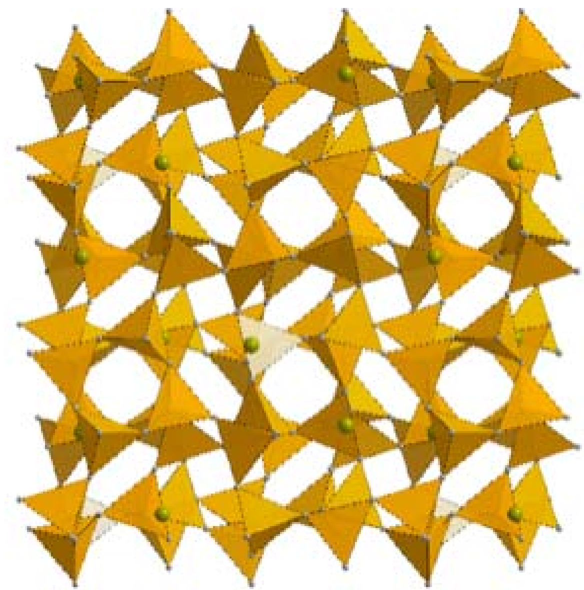
Intuitive feelings



Which structure is more complex?

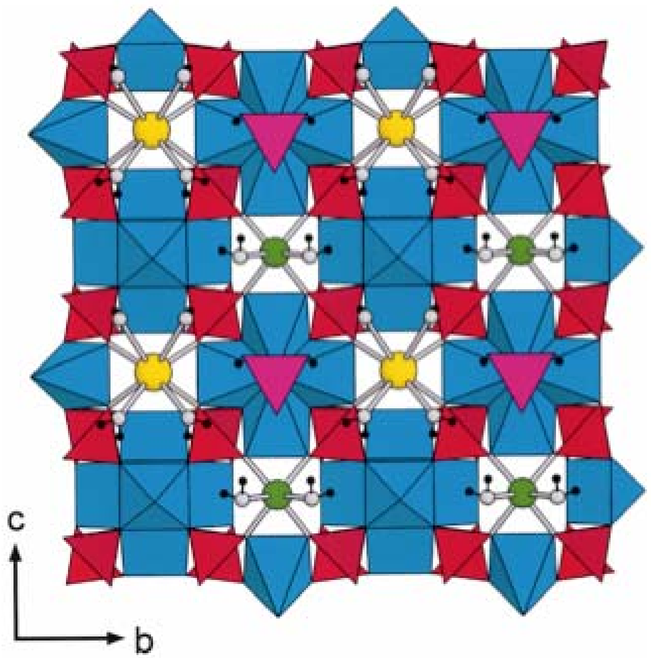


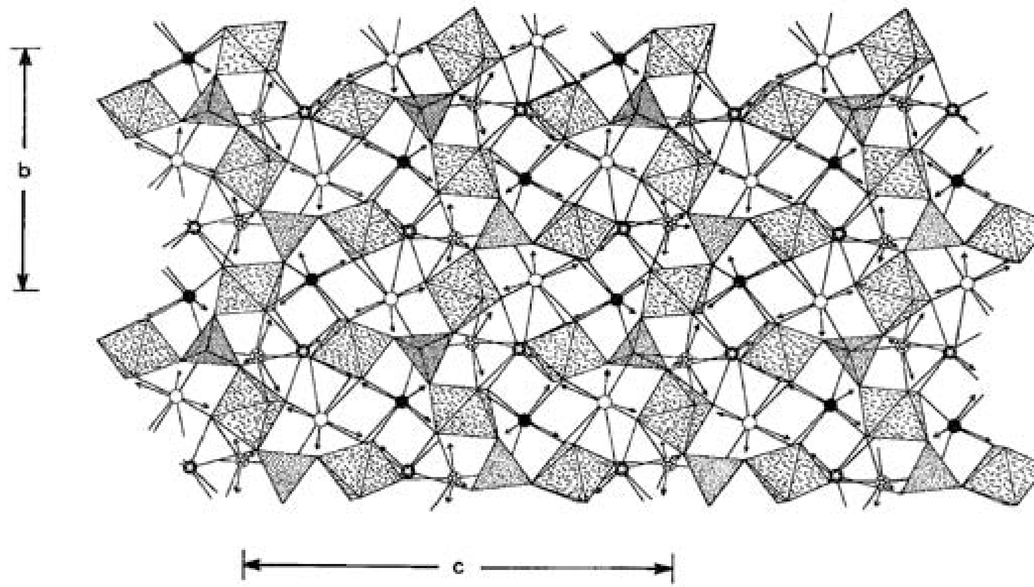




Andradite $Ca_3Fe_2(SiO_4)_3$	Orthoenstatite $Mg_2Si_2O_6$	Leucite (high) $KAlSiO_4$
Ia-3*d*	*Pbca*	*Ia*-3*d*
	80 atoms in the reduced unit cell	
V = 876.59 Å^3	V = 836.85 Å^3	V = 1179.90 Å^3

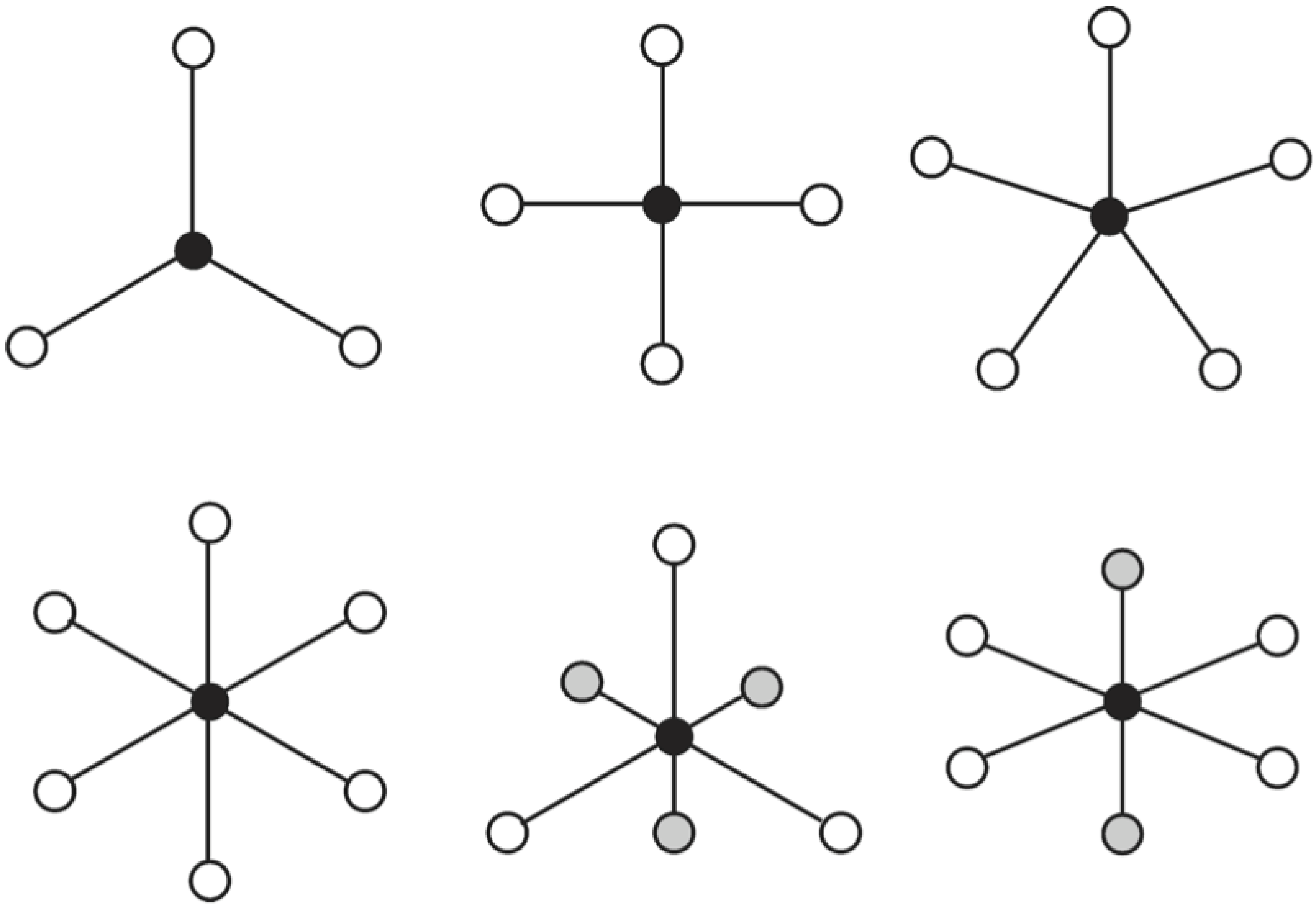
Which structure is more complex?



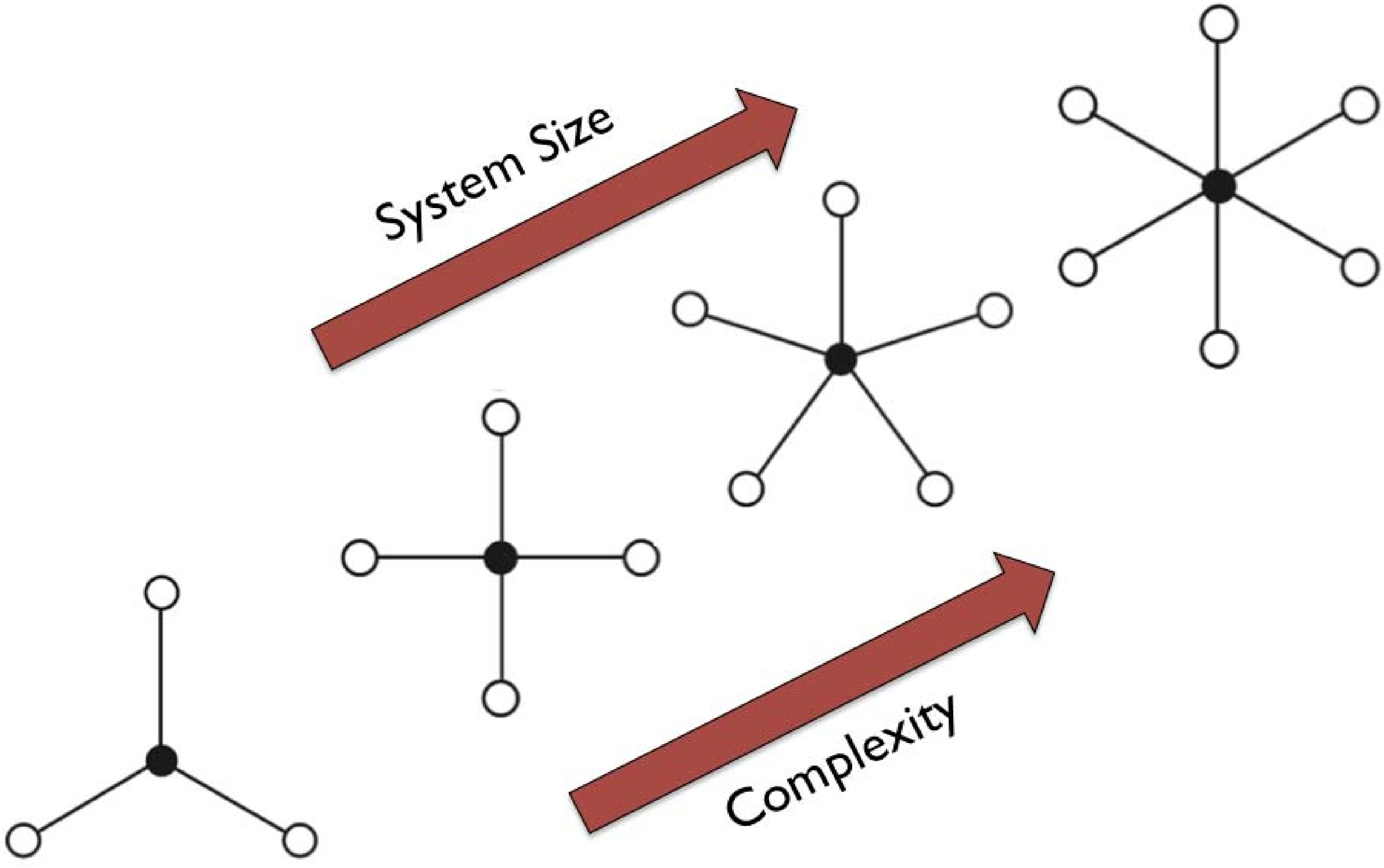


Andyrobertsite $KCdCu_5(AsO_4)_4(AsO_2(OH)_2)(H_2O)_2$	Bøggildite $Na_2Sr_2Al_2(PO_4)F_9$
$P2_1/m$	$P2_1/c$
80 atoms in the reduced unit cell	
V = 962.71 Å^3	V = 973.34 Å^3

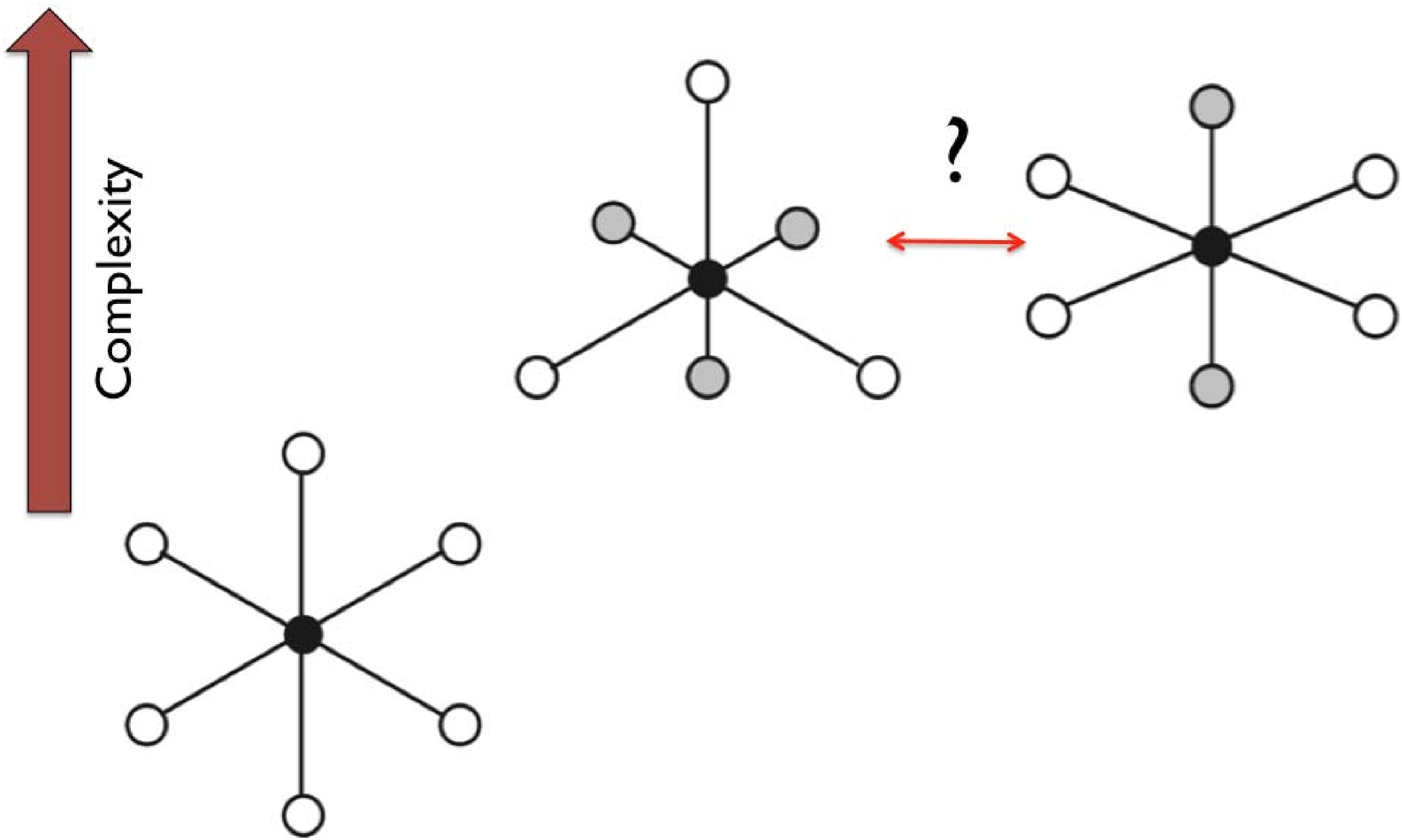
Which object is more complex?



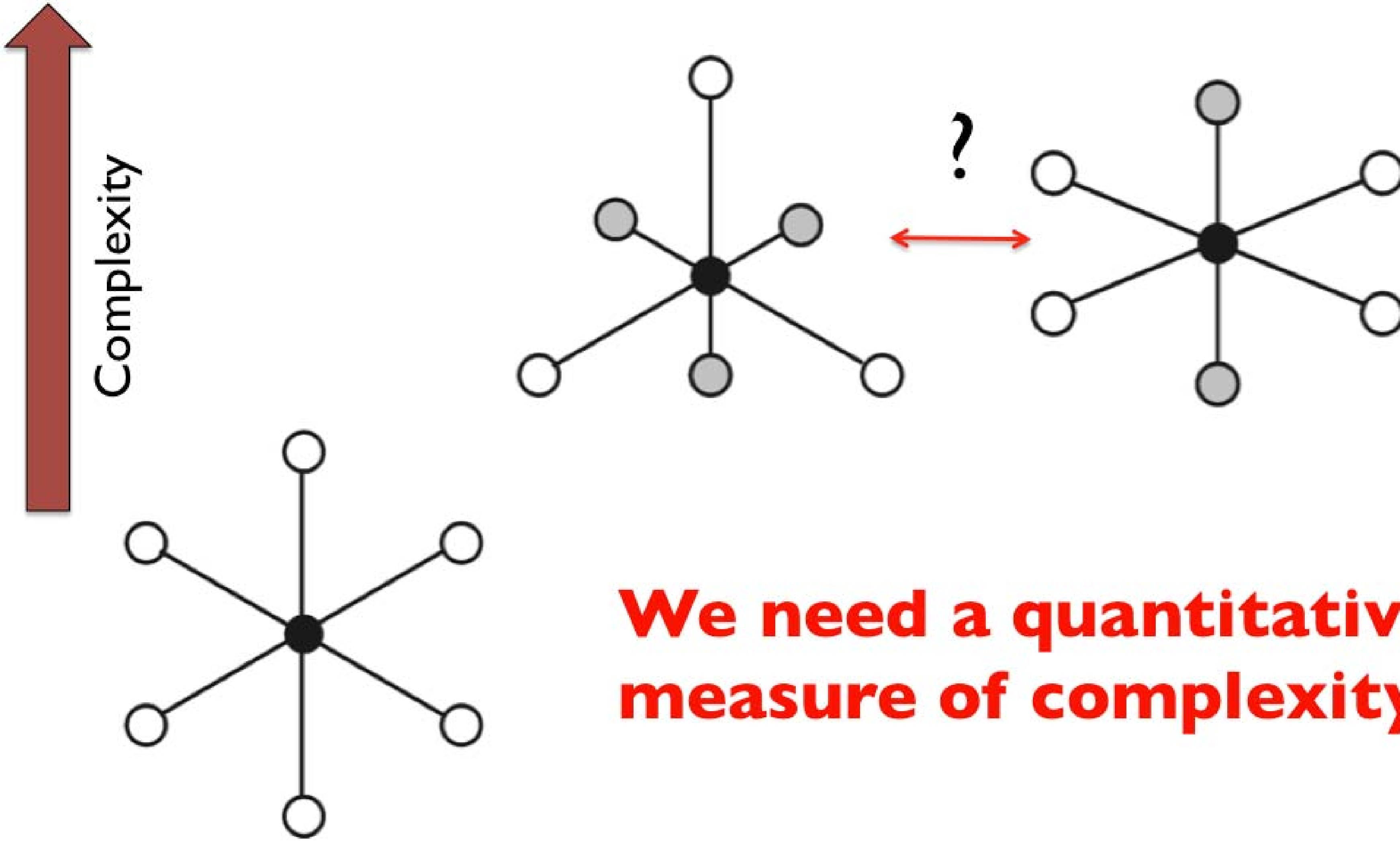
Which object is more complex?



Which object is more complex?

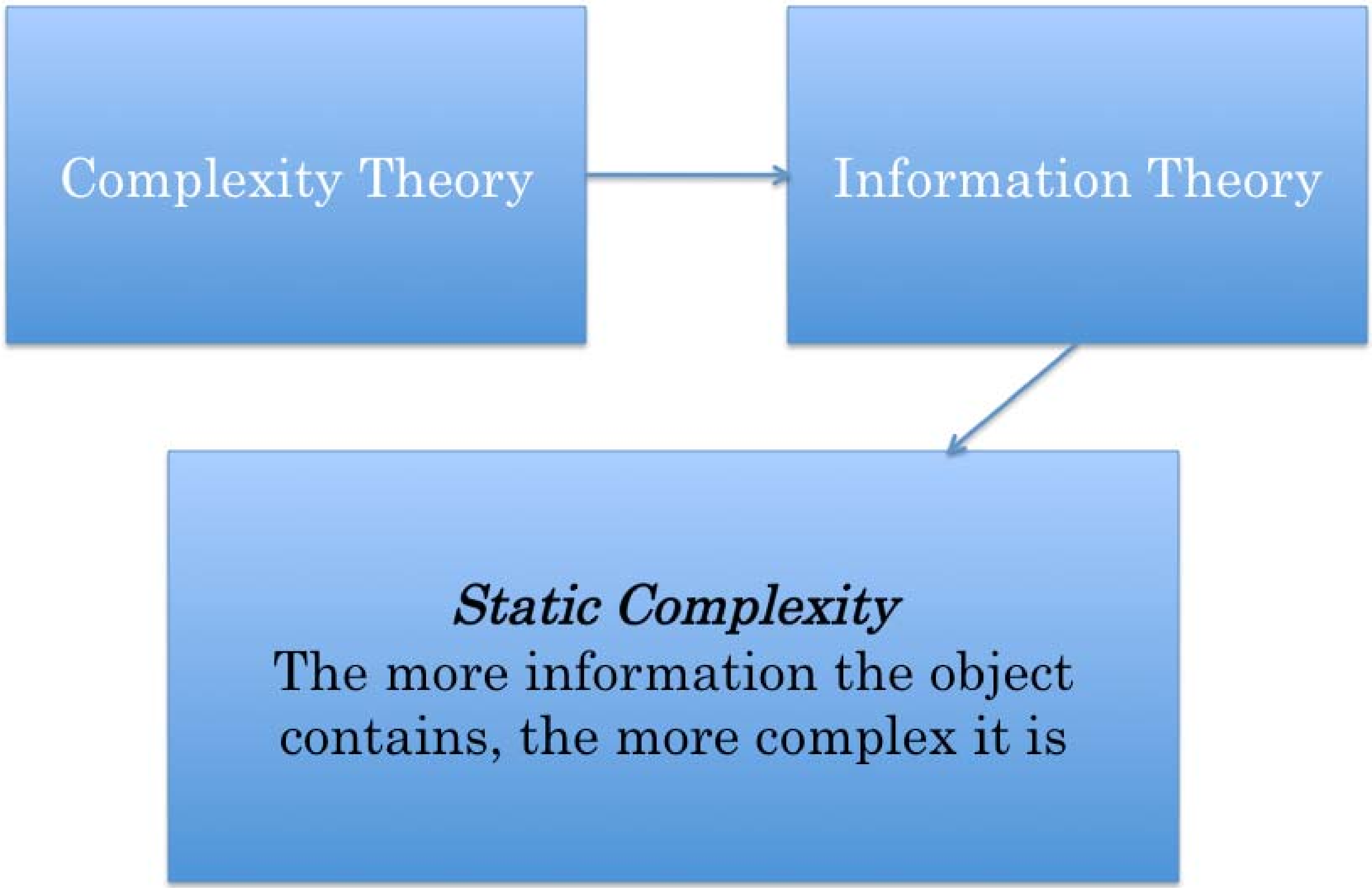


Which object is more complex?

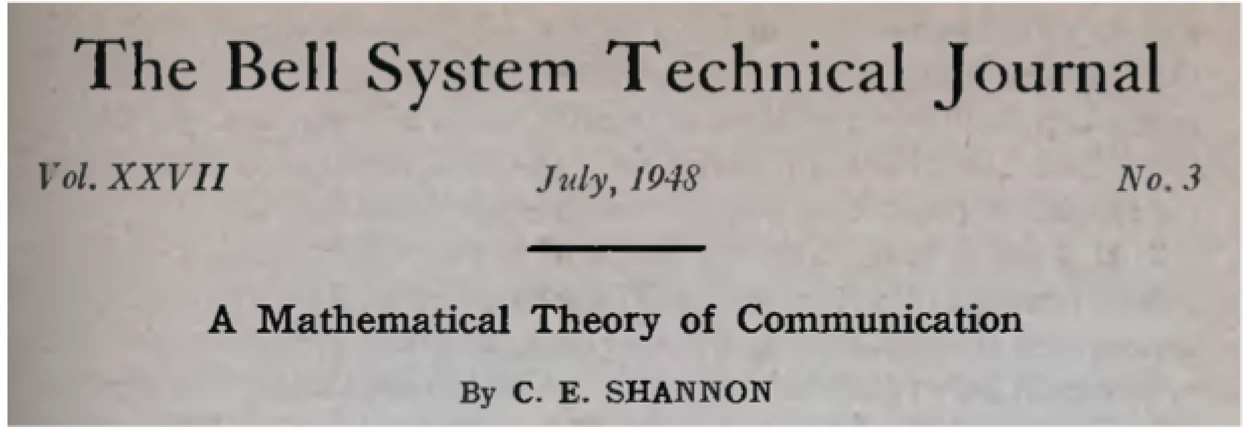


We need a quantitative measure of complexity

Which object is more complex?



Information Theory



The Bell System Technical Journal

Vol. XXVII *July, 1948* *No. 3*

A Mathematical Theory of Communication

By C. E. SHANNON

Information amount H of the message X,
consisting from n
symbols, subdivided into k equivalence classes
that contain n_1, n_2, ... n_k symbols can be
calculated according to the Shannon formula:

$$H(X) = - \Sigma\, p_i \log_2 p_i \quad \text{(bits/symbol)}$$

(amount of information per 1 symbol),

where $p_i = n_i/n$

Information Theory

GTKTTGKTGGK

11 symbols : $n = 11$

Information Theory

GTKTTGKTGGK

11 symbols : $n = 11$

3 classes : $n_1 = 4$, $n_2 = 4$, $n_3 = 3$

Information Theory

GTKTTGKTGGK

11 symbols : $n = 11$

3 classes : $n_1 = 4$, $n_2 = 4$, $n_3 = 3$

$p_1 = 4/11$, $p_2 = 4/11$, $p_3 = 3/11$

Information Theory

GTKTTGKTGGK

$$H = -\left[4/11 \log_2 (4/11) + 4/11 \log_2 (4/11) + 3/11 \log_2 (3/11)\right] =$$

$$= 1.573 \text{ bits/symbol}$$

Total information content = 11*1.573 = 17.303 bits

BULLETIN OF
MATHEMATICAL BIOPHYSICS
VOLUME 17, 1955

Information Theory Applied to Graphs

LIFE, INFORMATION THEORY, AND TOPOLOGY

N. RASHEVSKY
COMMITTEE ON MATHEMATICAL BIOLOGY
THE UNIVERSITY OF CHICAGO

The topological information content, or entropy per symbol, of the graph (due to its points) was defined by N. Rashevsky as

$$I = -\sum_{k=1}^{m} w_k \lg w_k \,, \qquad (1)$$

where lg denotes the logarithm to the base 2, and

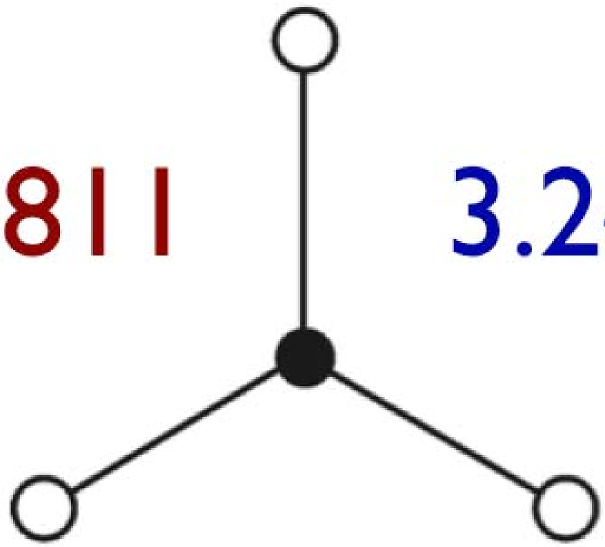
$$w_k = \frac{n_k}{n} \,; \qquad (2)$$

m is the number of sets of topologically equivalent points in the graph, and n_k the number of points belonging to the kth set. The

Information Theory Applied to Graphs

Information per vertex (bits/vertex)

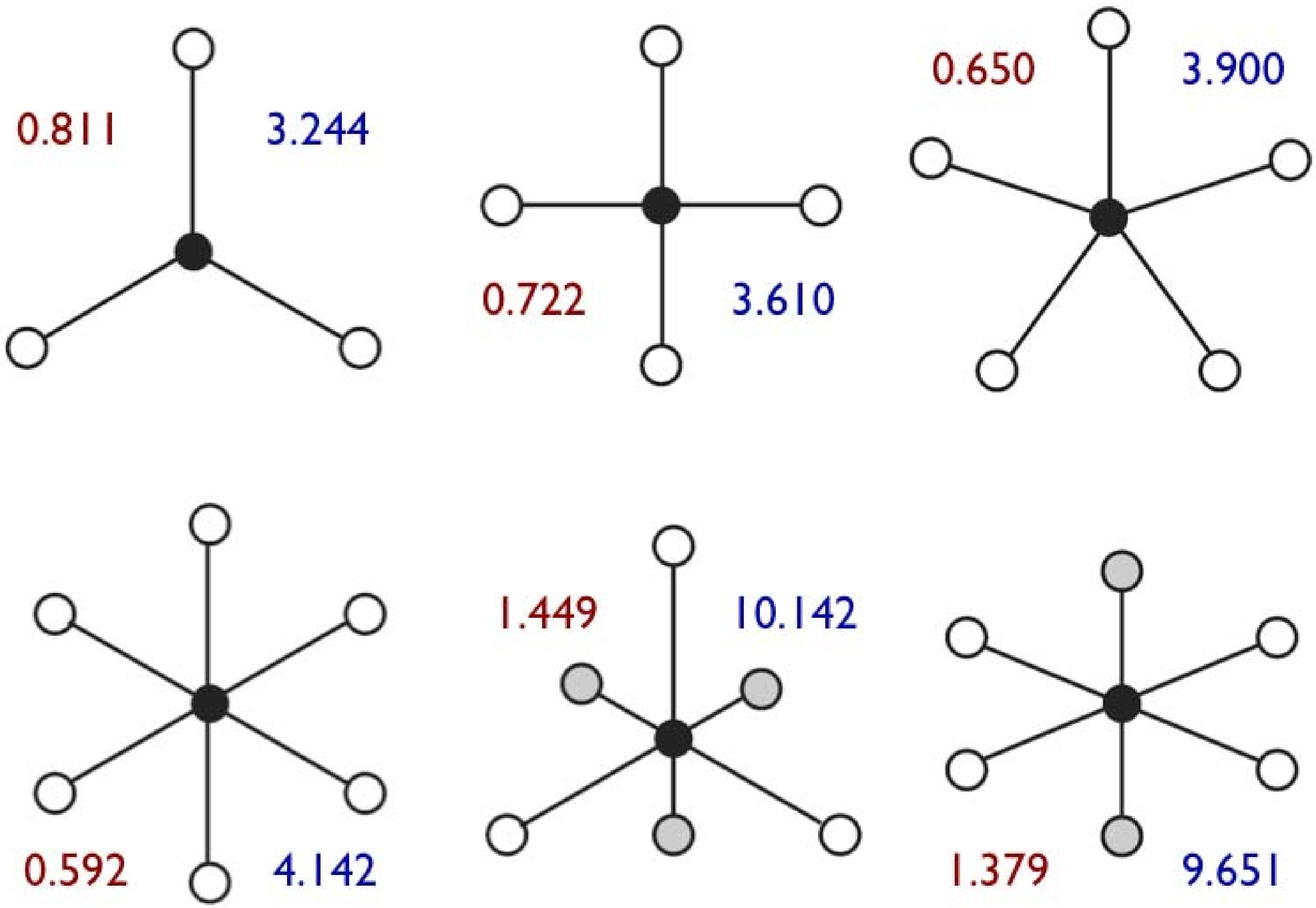
0.811



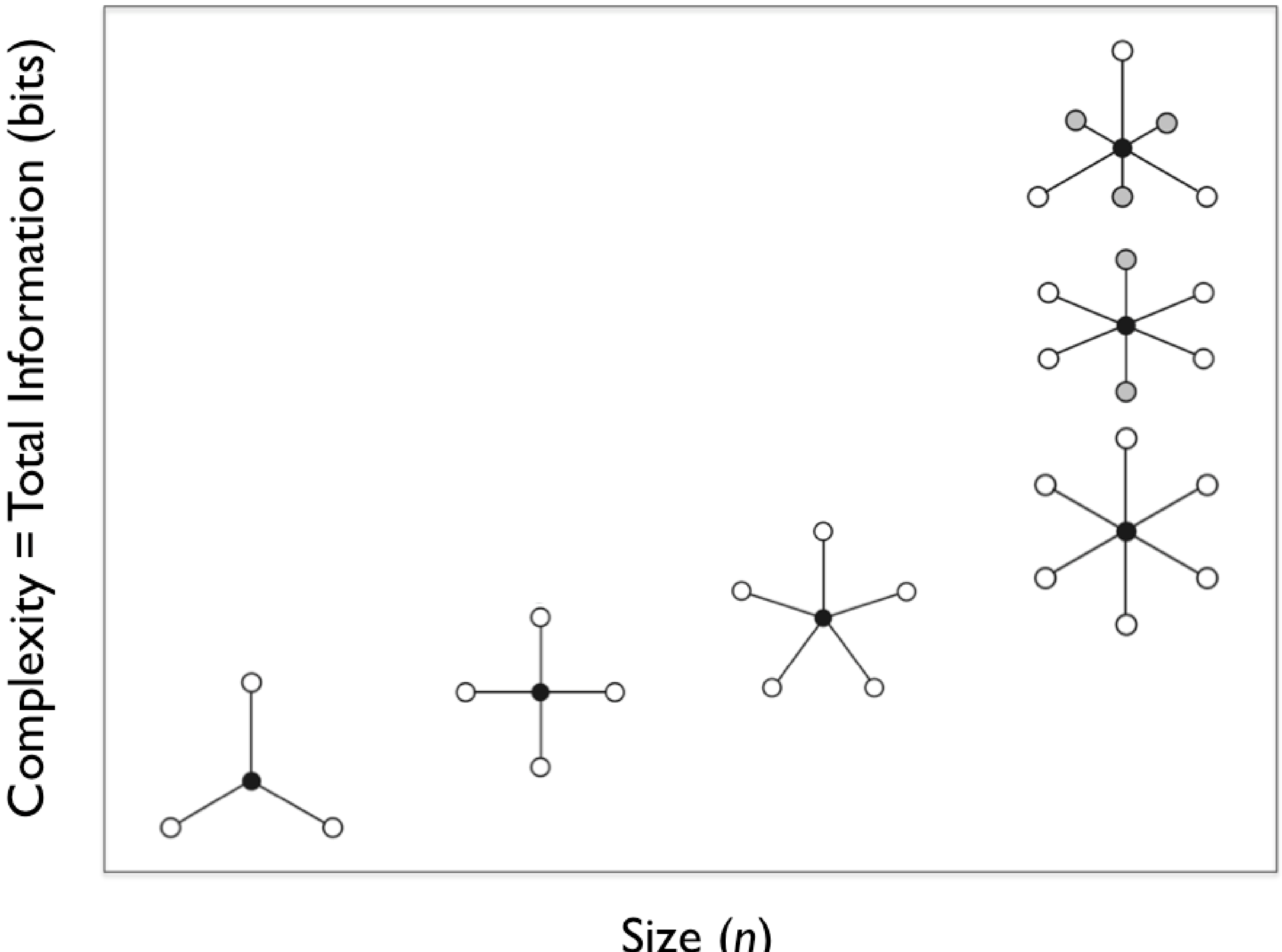
3.244

Information per graph (bits)

Information Theory Applied to Graphs



Which object is more complex?



Information Theory Applied to Crystals

$$I_{G,total} = -v \sum_{i=1}^{v} p_i \log_2 p_i$$

where $p_i = m_i / v$

v : number of atoms in the reduced unit cell

m_i : multiplicity of the crystallographic orbit occupied by the ith atom

Complexity of a Crystal Structure

$$I_{G,total} = -v \sum_{i=1}^{v} p_i \log_2 p_i$$

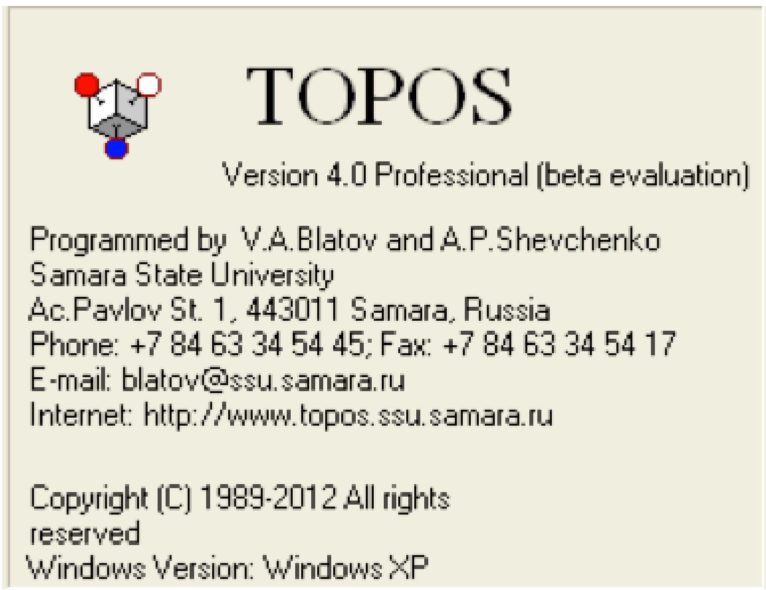
size-sensitive
(symbolic complexity)

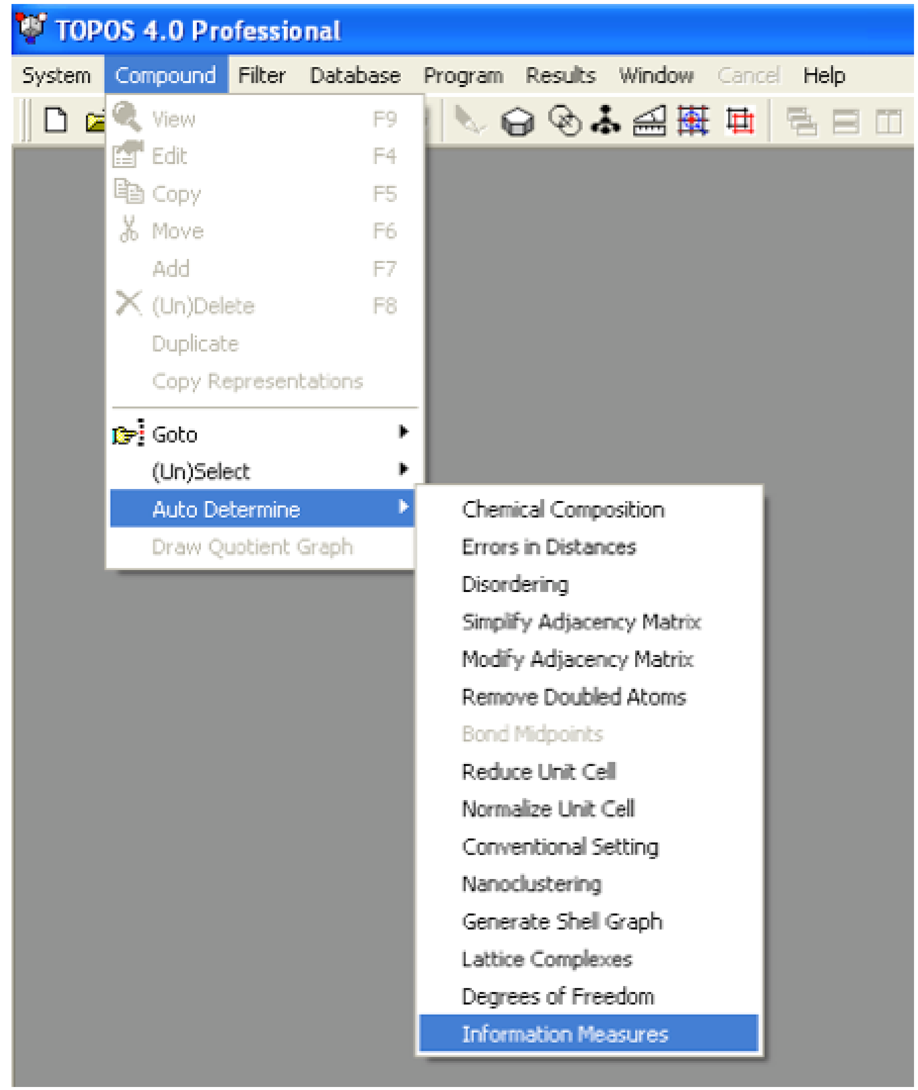
symmetry-sensitive
(combinatorial complexity)

Acta Crystallographica A68 (2012) 393-398; Structural Chemistry 23 (2012) 1045-1052; Mineralogical Magazine 77 (2013) 275-326; Angewandte Chemie 2013, in press

Complexity of Inorganic Structures

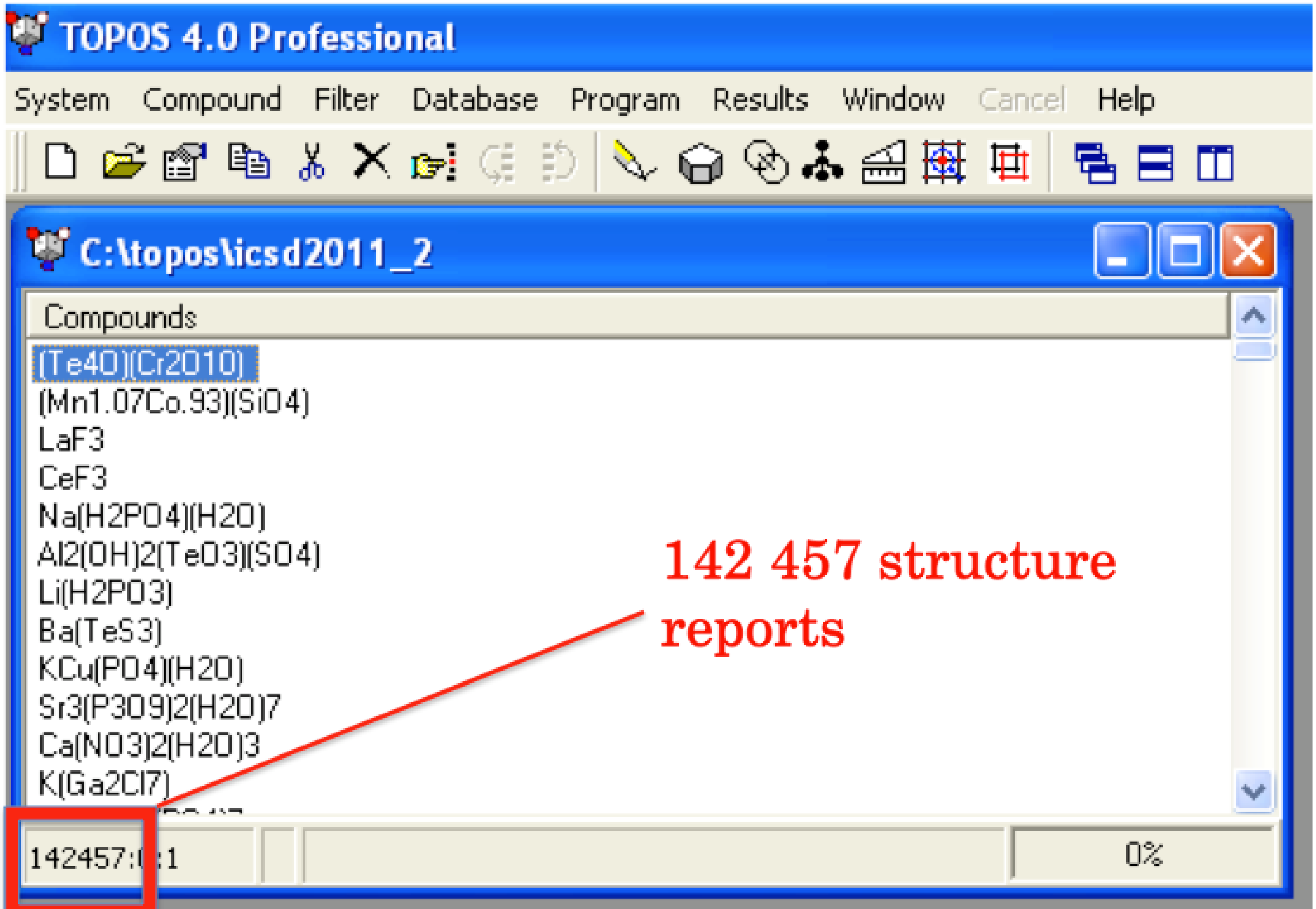
Inorganic Crystal Structure Database analysis



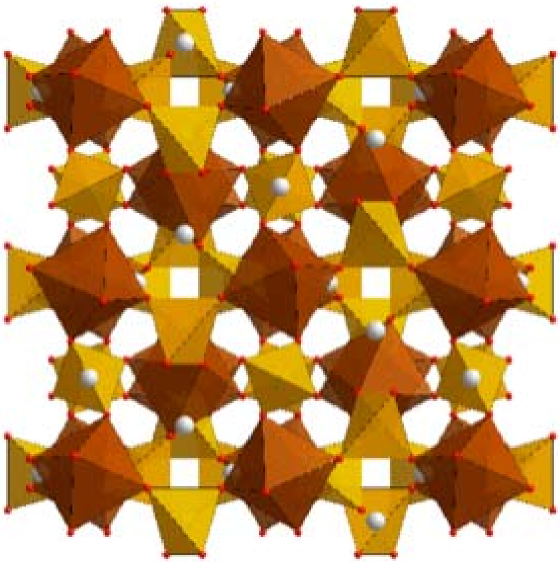


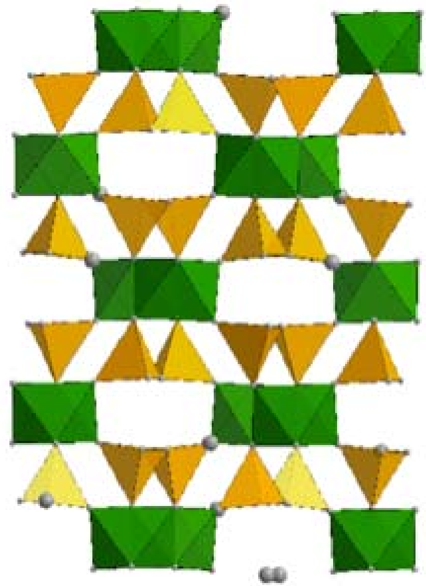
Complexity of Inorganic Structures

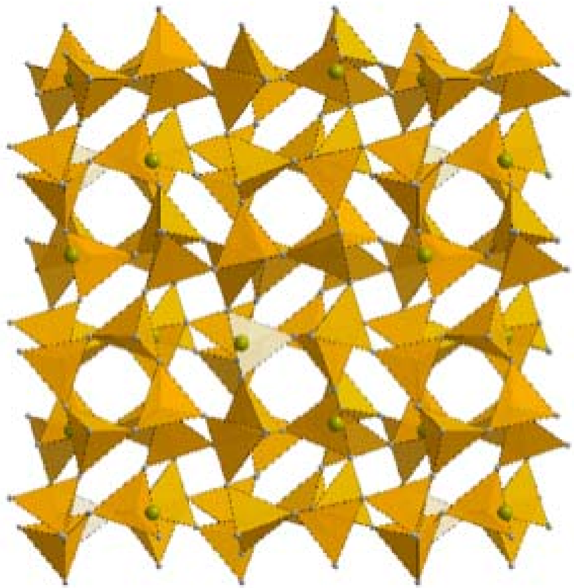
Inorganic Crystal Structure Database analysis



Which structure is more complex?

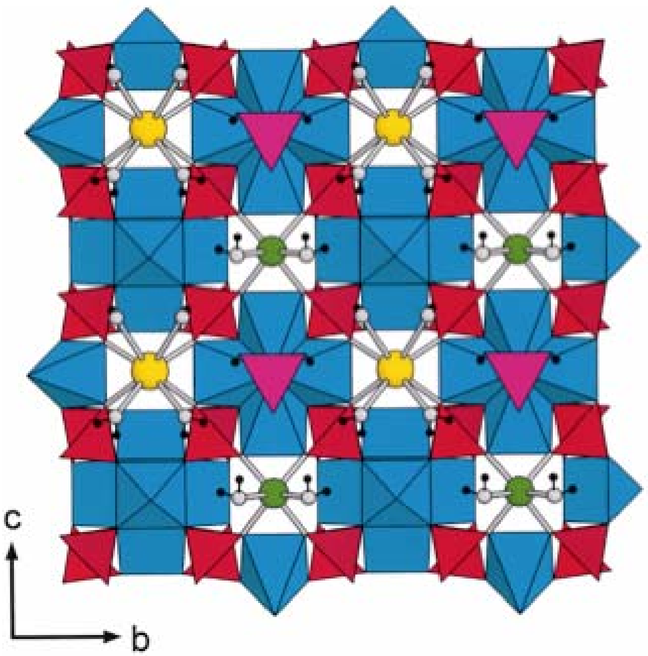


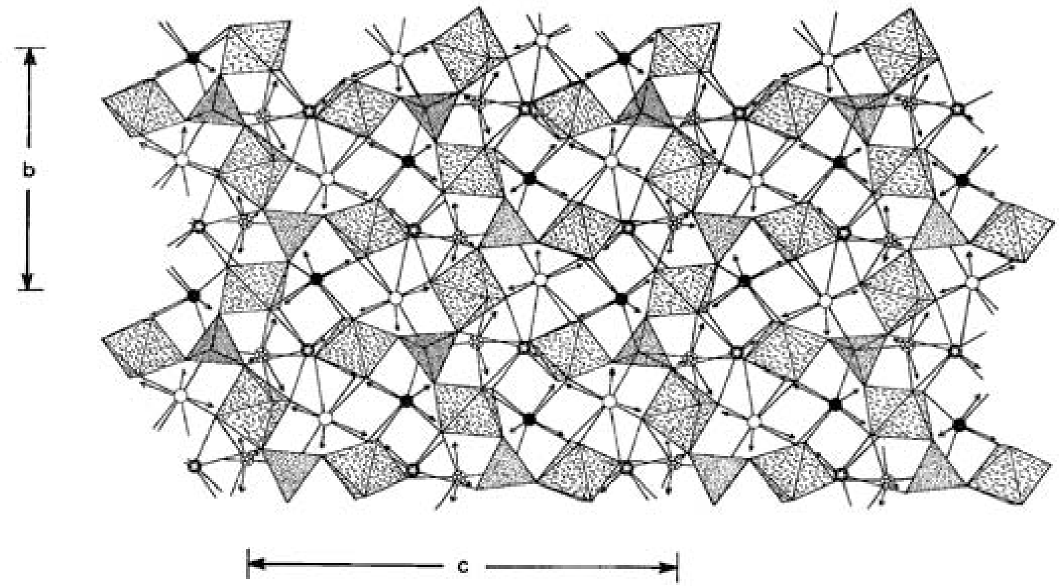




Andradite $Ca_3Fe_2(SiO_4)_3$	Orthoenstatite $Mg_2Si_2O_6$	Leucite (high) $KAlSiO_4$
Ia-3*d*	*Pbca*	*Ia*-3*d*
80 atoms in the reduced unit cell		
V = 876.59 Å^3	V = 836.85 Å^3	V = 1179.90 Å^3
127.637 bits	265.754 bits	103.637 bits

Which structure is more complex?

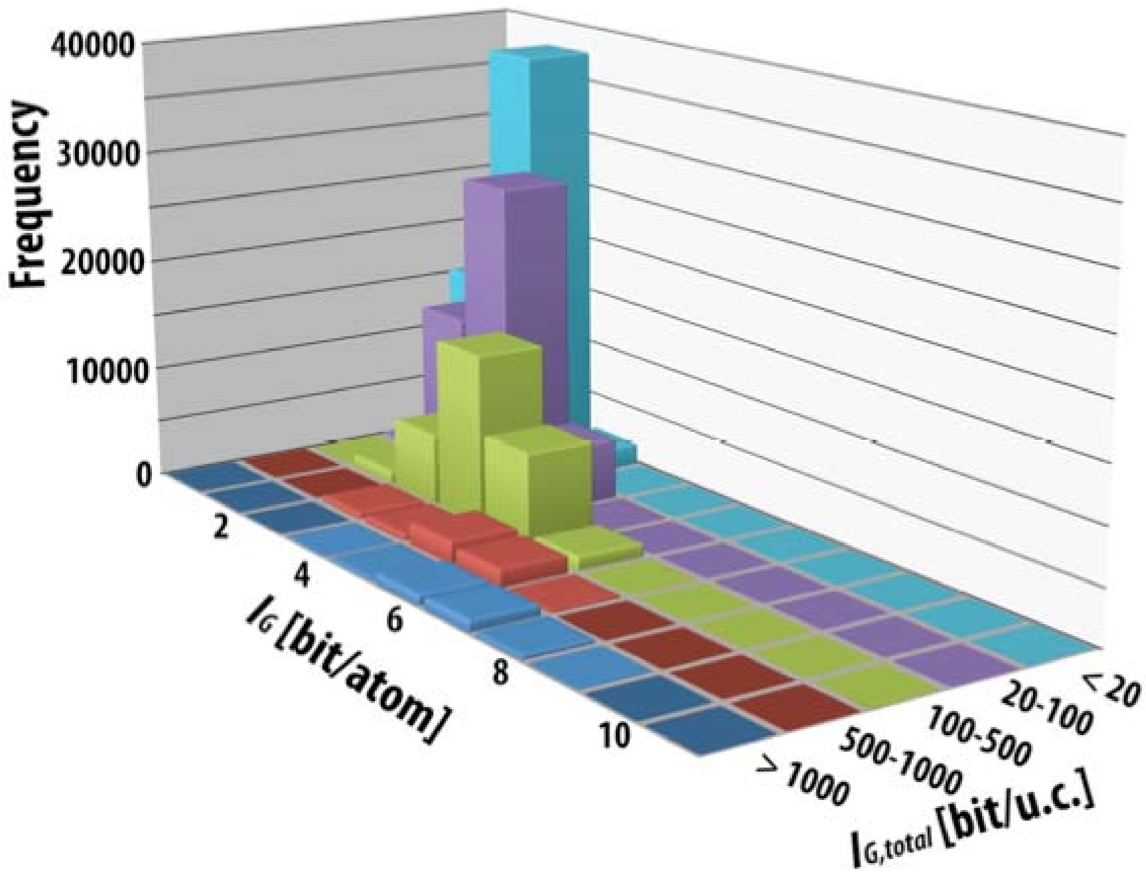




Andyrobertsite $KCdCu_5(AsO_4)_4(AsO_2(OH)_2)(H_2O)_2$	Bøggildite $Na_2Sr_2Al_2(PO_4)F_9$
$P2_1/m$	$P2_1/c$
80 atoms in the reduced unit cell	
V = 962.71 Å^3	V = 973.34 Å^3
361.754 bits	349.754 bits

Most Complex Inorganic Compounds

Inorganic Crystal Structure Database Analysis



Angew. Chem. Int. Ed. **2014**, 53, 654 – 661

Most Complex Inorganic Compounds

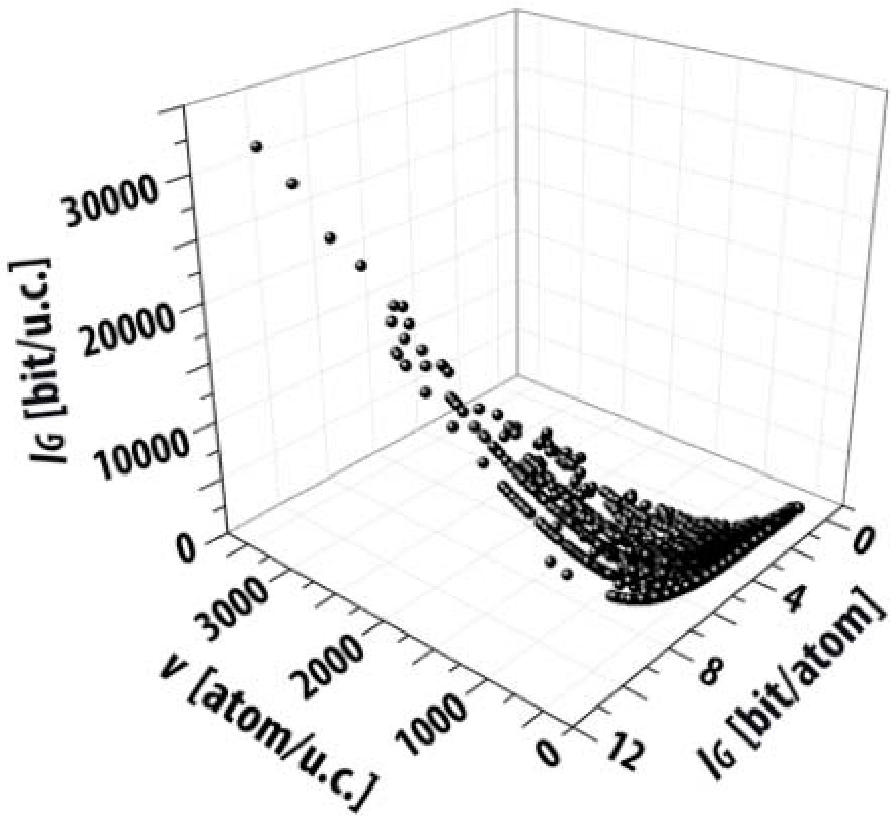
Classification of Inorganic Structures by Complexity

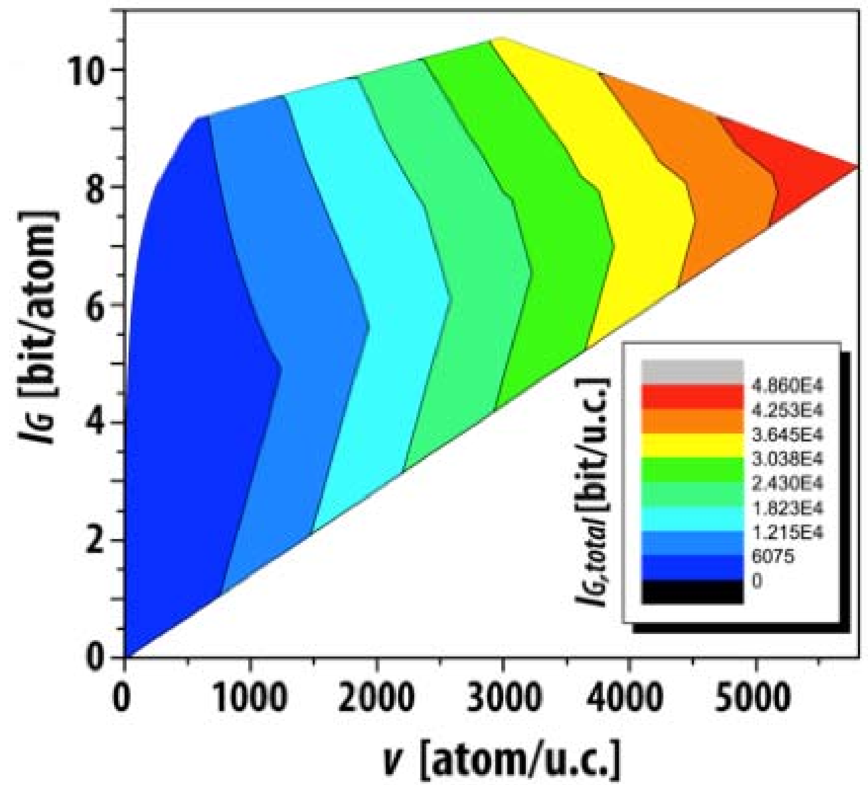
Category	$I_{G,total}$ [bits/u.c.]	Number of ICSD entries
very simple	< 20	~ 55 000
simple	20-100	~ 50 000
intermediate	100-500	~ 33 000
complex	500-1000	~ 5 000
very complex	> 1000	~ 3 000

Angew. Chem. Int. Ed. **2014**, *53*, 654 – 661

Most Complex Inorganic Compounds

Inorganic Crystal Structure Database Analysis



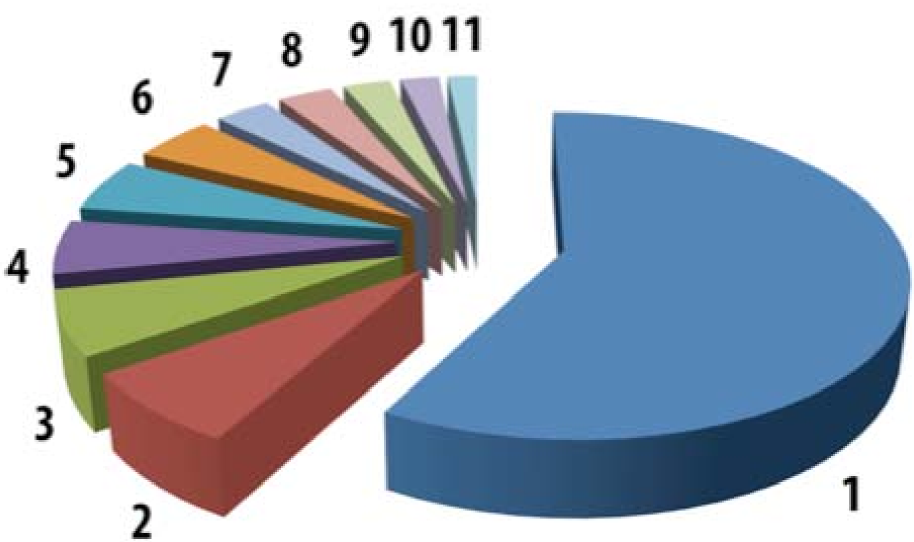


Angew. Chem. Int. Ed. **2014**, *53*, 654–661

Most Complex Inorganic Compounds

Inorganic Crystal Structure Database Analysis

2000 most complex inorganic structures according to their chemical identity:



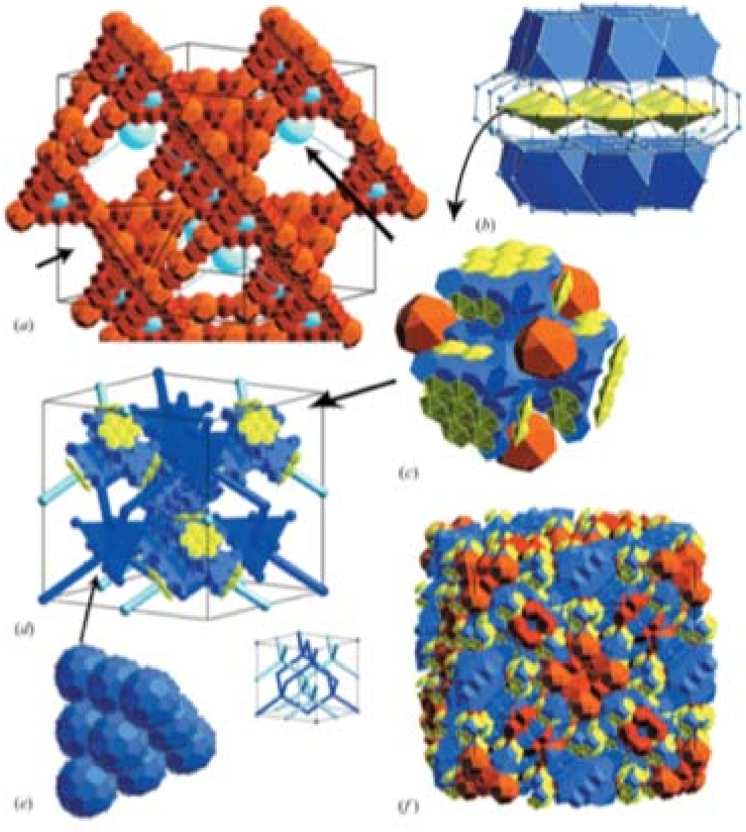
1 – Mo-W-V-based polyoxometallates;
2 – oxides and oxysalts;
3 – structures containing (nano)clusters;
4 – zeolites and microporous framework compounds;
5 – intermetallic compounds;
6 – fullerene-based structures;
7 – uranyl peroxide nanospheres;
8 – superstructures;
9 – Nb-Ti-based polyoxometallates;
10 – sulphides and selenides;
11 – halogenides.

Angew. Chem. Int. Ed. **2014**, 53, 654 – 661

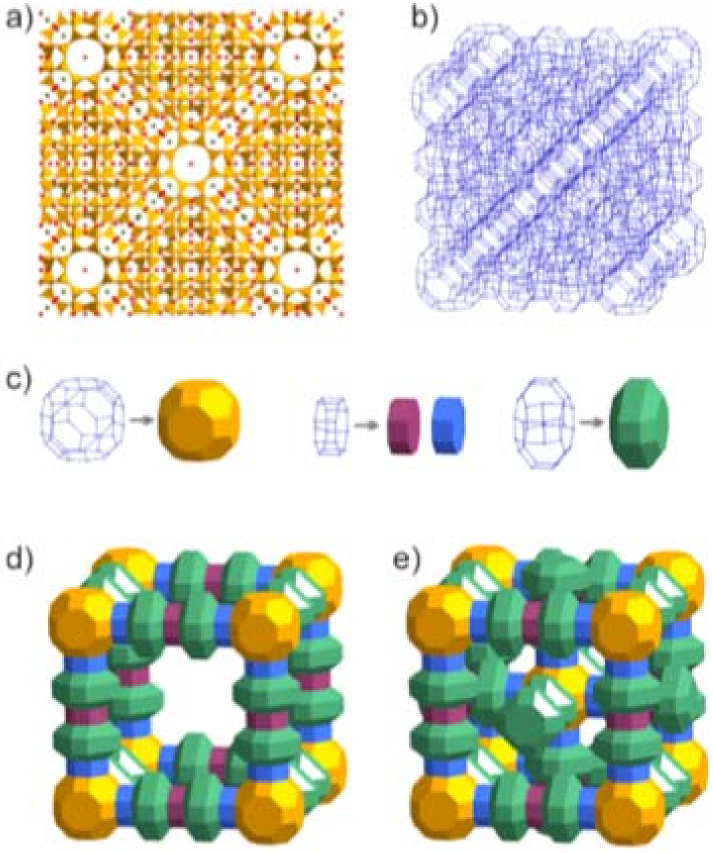
Complexity of Inorganic Structures

Inorganic Crystal Structure Database analysis

The most complex inorganic structure:
$Al_{55.4}Cu_{5.4}Ta_{39.1}$
$I_{G,total}$ = 48538.637 bits

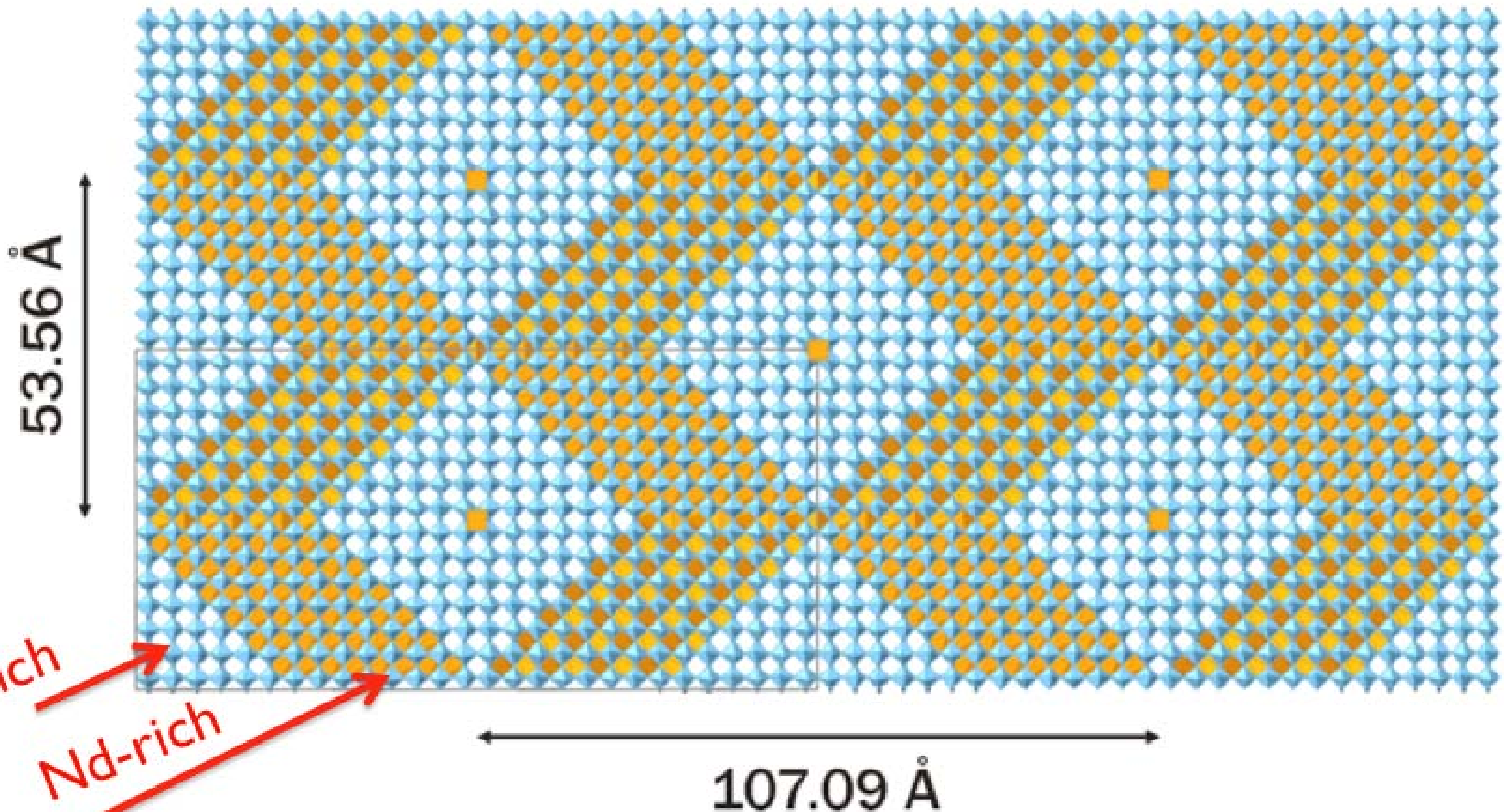


The most complex mineral structure:
Paulingite
$I_{G,total}$ = 6766.998 bits



Most Complex Rare Earth Compounds

$Nd_{7/12}Li_{1/4}TiO_3$

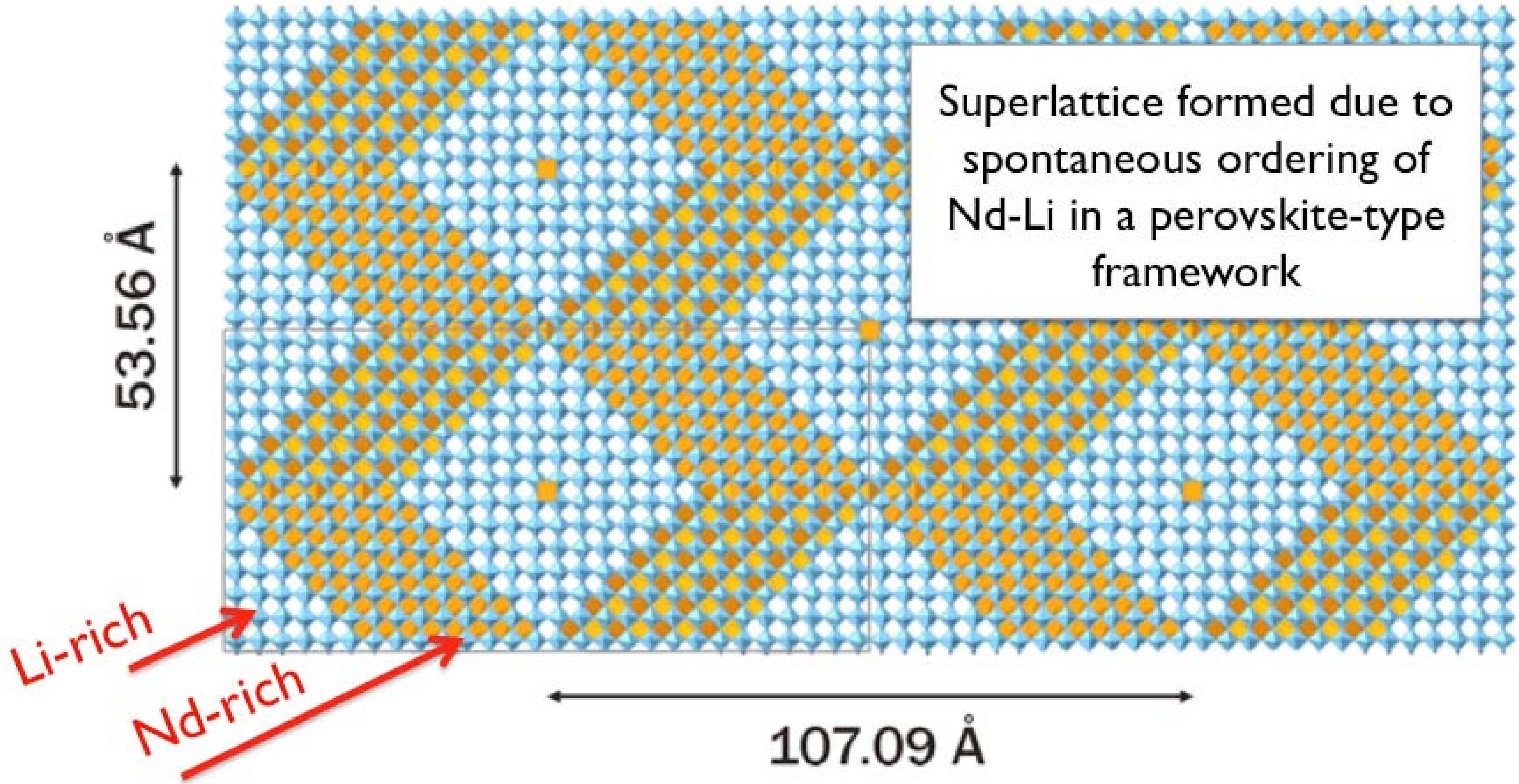


v = 1973 ; I_G = 8.431 bit/atom ; $I_{G,total}$ = 16634.804 bit/u.c.

B. S. Guiton, H. Wu, P. K. Davies, *Chem. Mater.* **2008**, *20*, 2860-2862.

Most Complex Rare Earth Compounds

$Nd_{7/12}Li_{1/4}TiO_3$



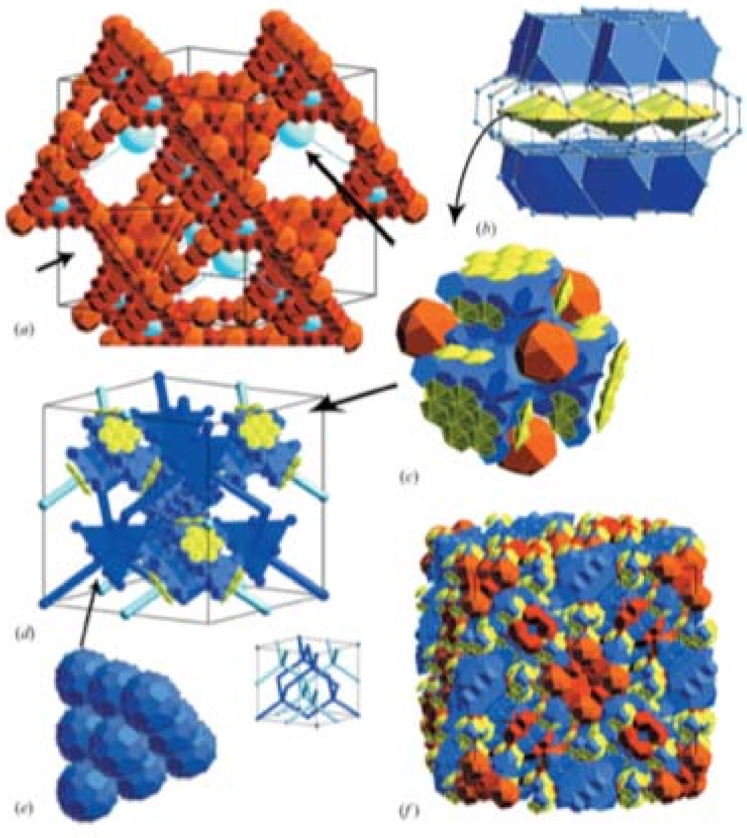
v = 1973 ; I_G = 8.431 bit/atom ; $I_{G,total}$ = 16634.804 bit/u.c.

B. S. Guiton, H. Wu, P. K. Davies, *Chem. Mater.* **2008**, *20*, 2860-2862.

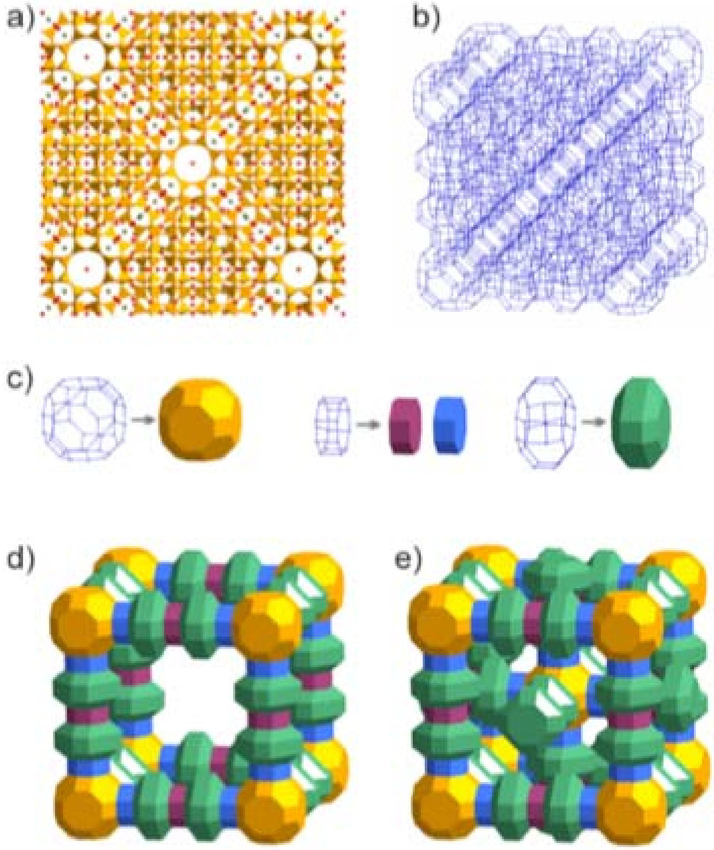
Complexity of Inorganic Structures

Inorganic Crystal Structure Database analysis

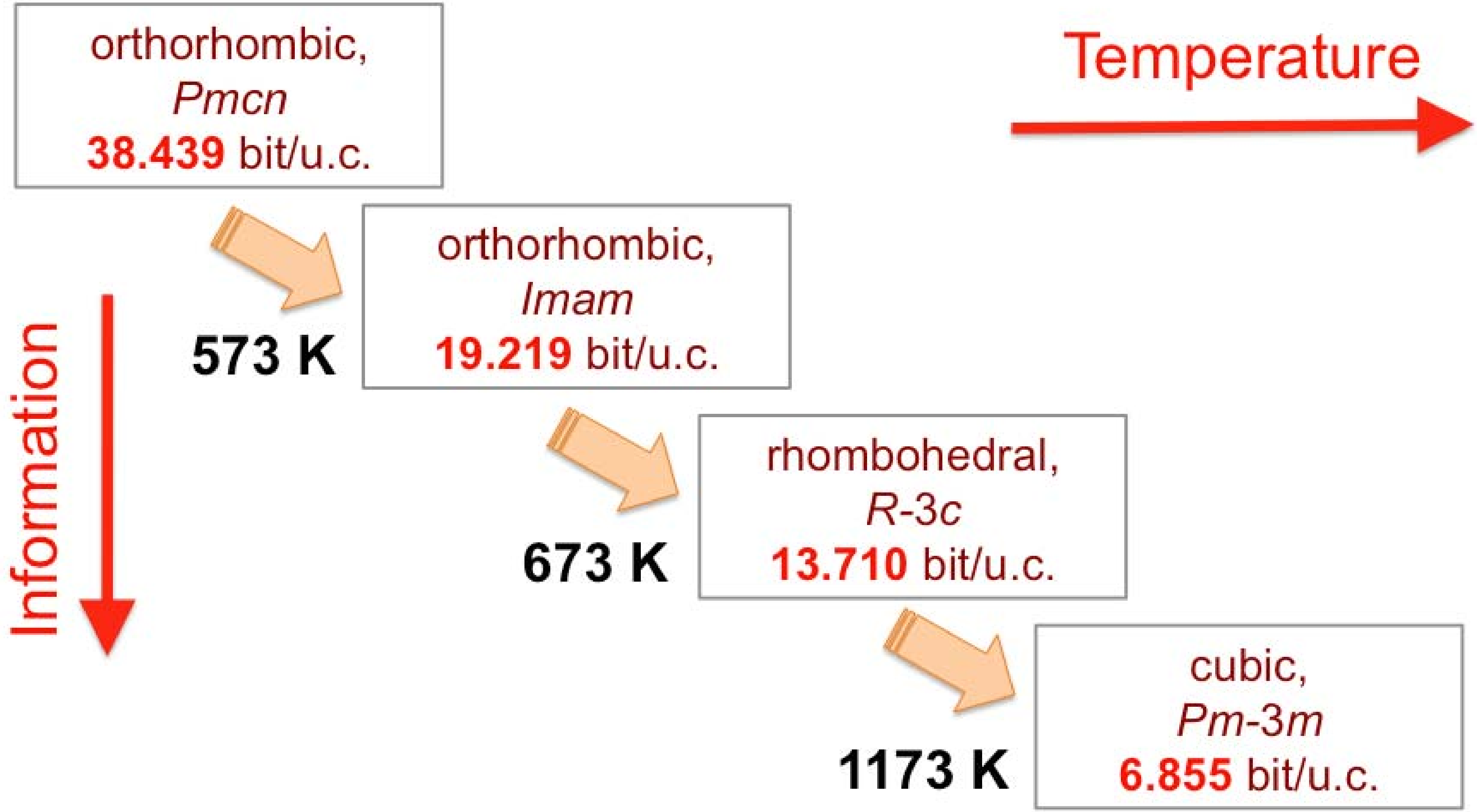
The most complex inorganic structure:
$Al_{55.4}Cu_{5.4}Ta_{39.1}$
$I_{G,total}$ = 48538.637 bits



The most complex mineral structure:
Paulingite
$I_{G,total}$ = 6766.998 bits

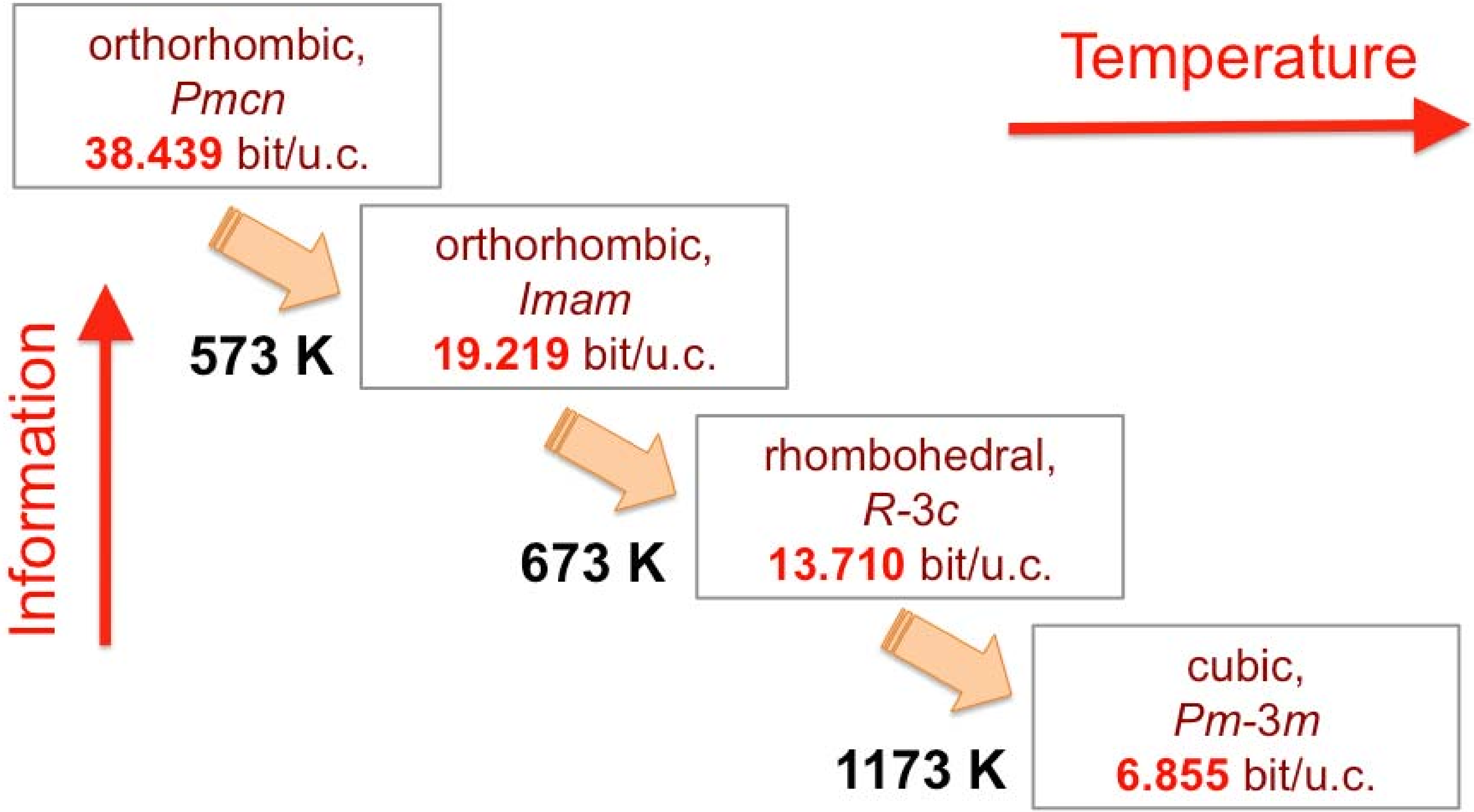


Complexity vs. Temperature
$BaCeO_3$



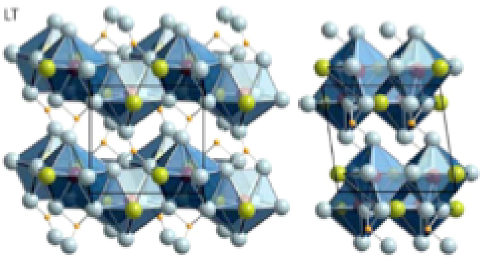
Medvedev et al. *Progr. Mater. Sci.*, **2014**, *60*, 72-129

Complexity vs. Temperature
$BaCeO_3$



Medvedev et al. *Progr. Mater. Sci.*, **2014**, *60*, 72-129

Complexity vs. Temperature
LuF(SeO_3)

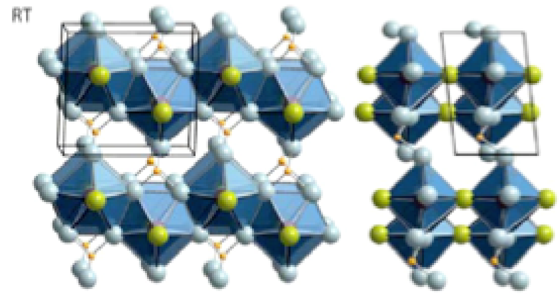


monoclinic, $P2_1/c$
62.039 bit/u.c.

Temperature →

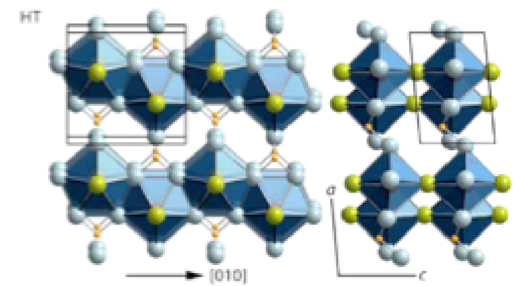
Information ↑

233 K



triclinic, *P*-1
31.020 bit/u.c.

383 K



monoclinic, $P2_1/m$
27.020 bit/u.c.

C. Lipp, T. Schleid, *Z. Anorg. Allg. Chem.*, **2007**, *633*, 1429-1434.
C. Lipp, R. Dinnebier, T. Schleid, *Inorg. Chem.*, **2013**, *52*, 10788-10794.

Polymorphism of REE_2O_3 oxides vs. Temperature

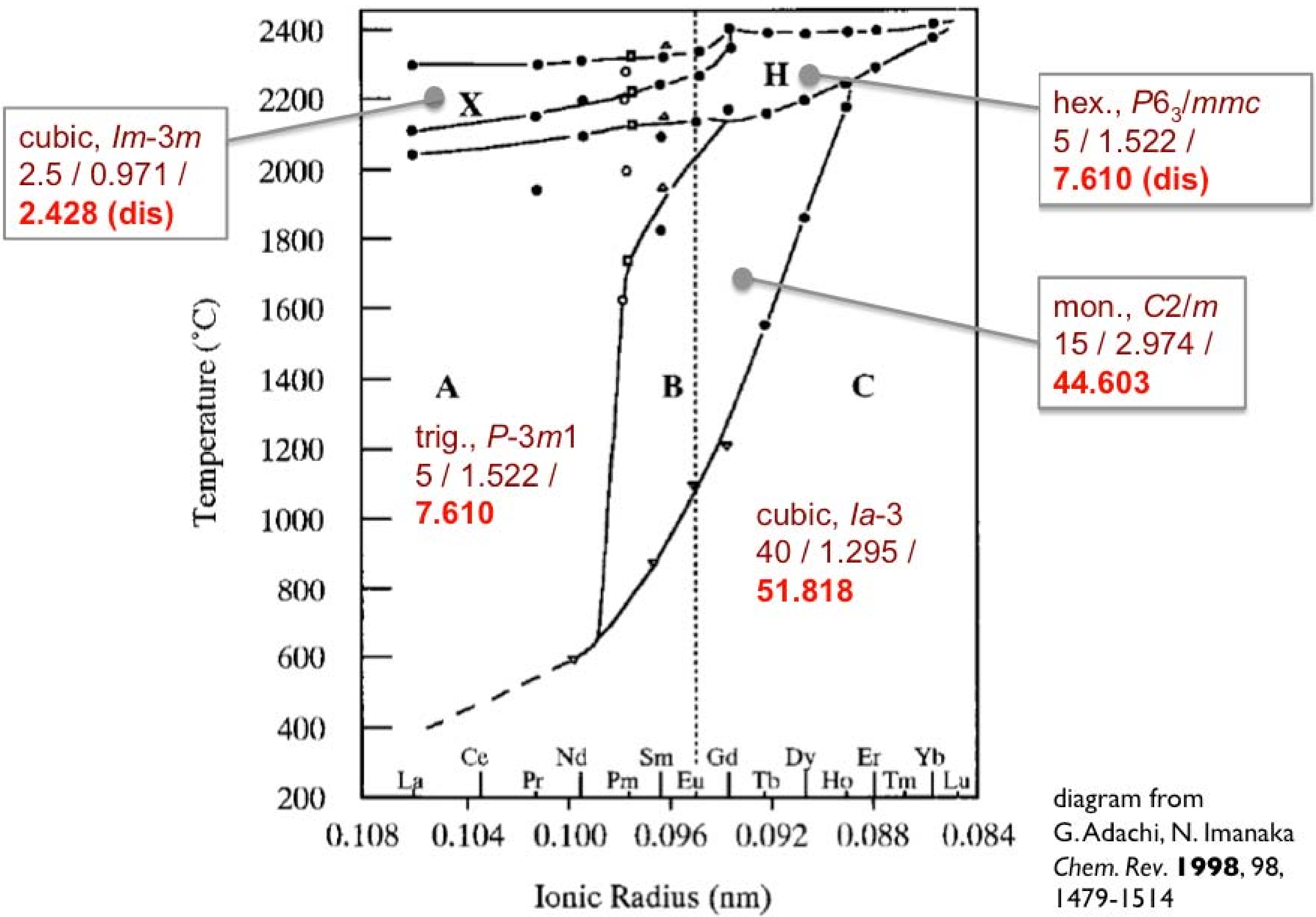
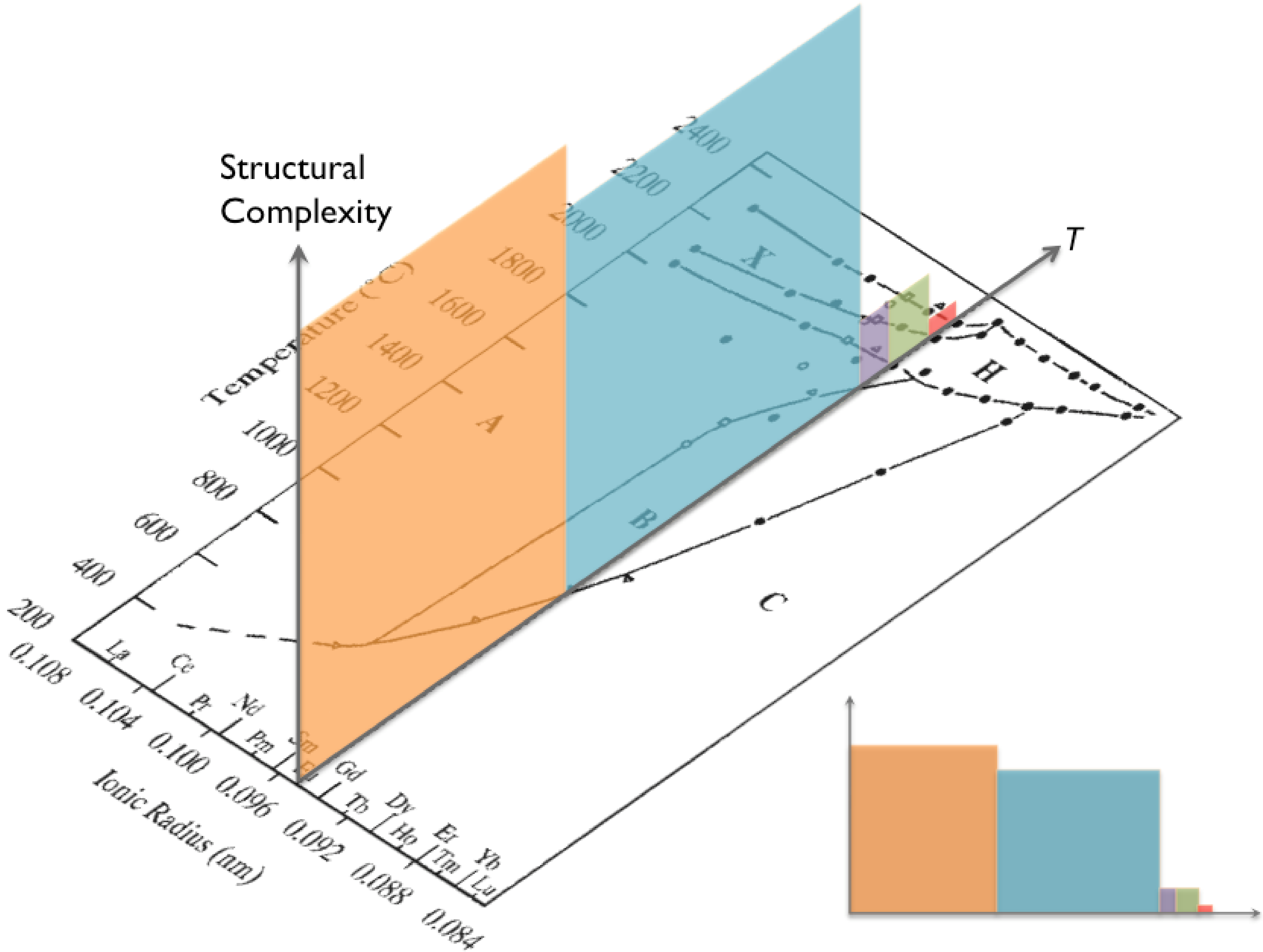


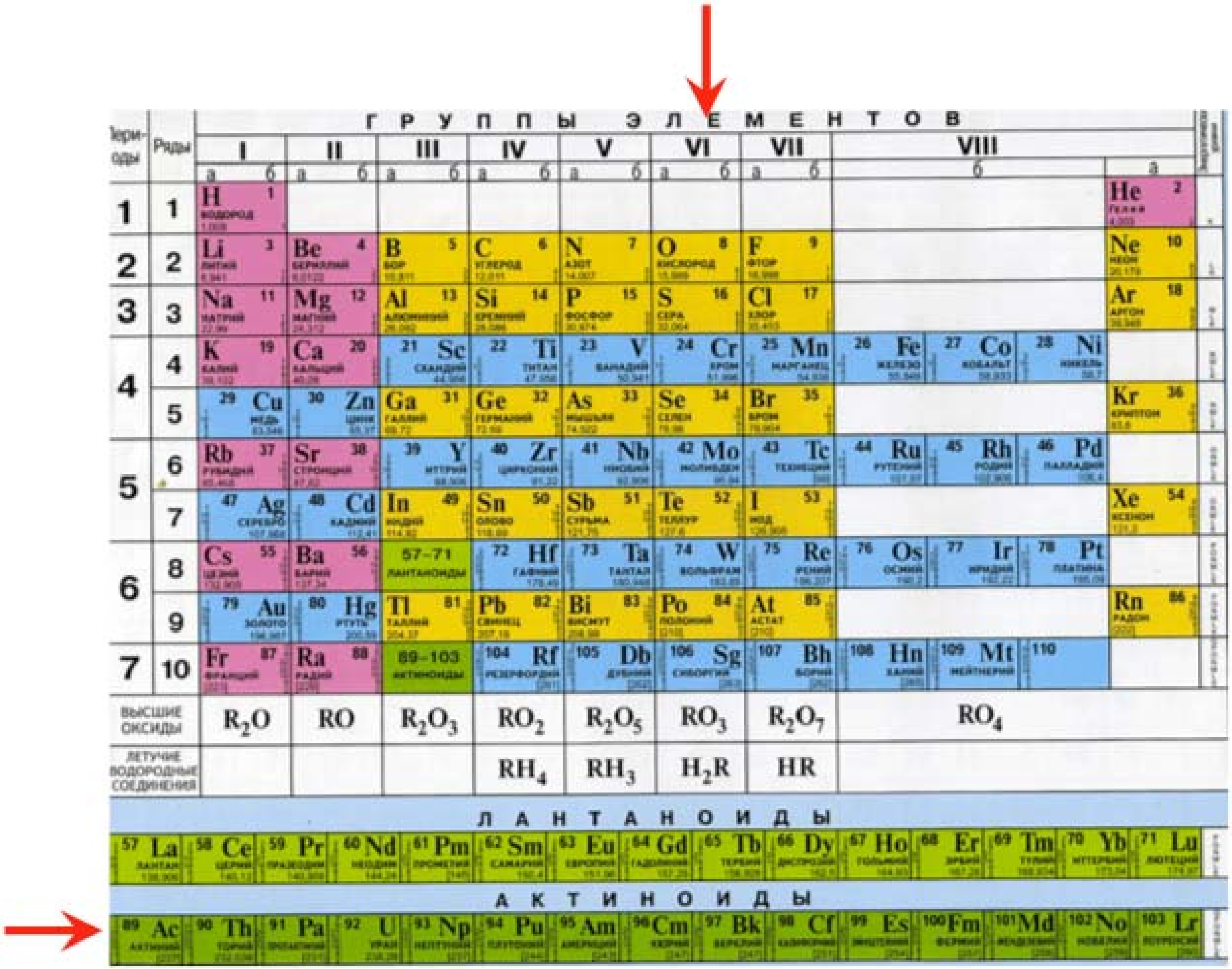
diagram from
G. Adachi, N. Imanaka
Chem. Rev. **1998**, 98,
1479-1514

Polymorphism of REE_2O_3 oxides vs. Temperature



Dynamic Complexity: Cellular Automata and Design

Actinyl oxysalt compounds with VIth-group elements



S 16
sulfur

24 Cr
chromium

Se 34
selenium

42 Mo
molybdenum

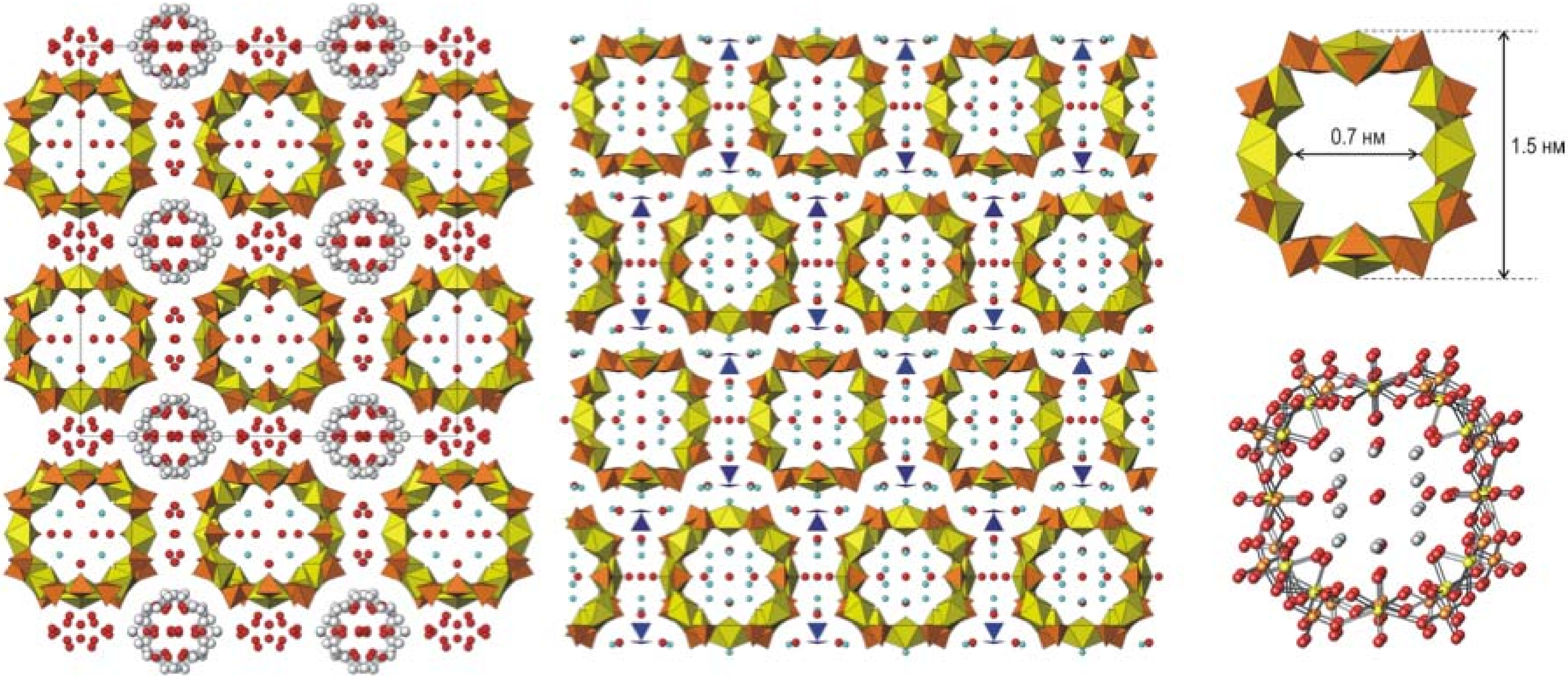
74 W
tungsten

92 U
uranium

93 Np
neptunium

94 Pu
plutonium

Nanotubules $[(UO_2)_3(SeO_4)_5]^{2-}$

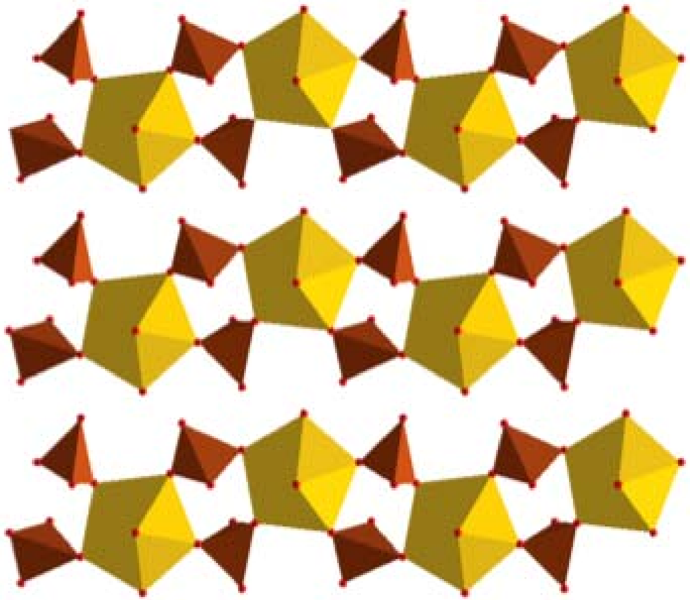


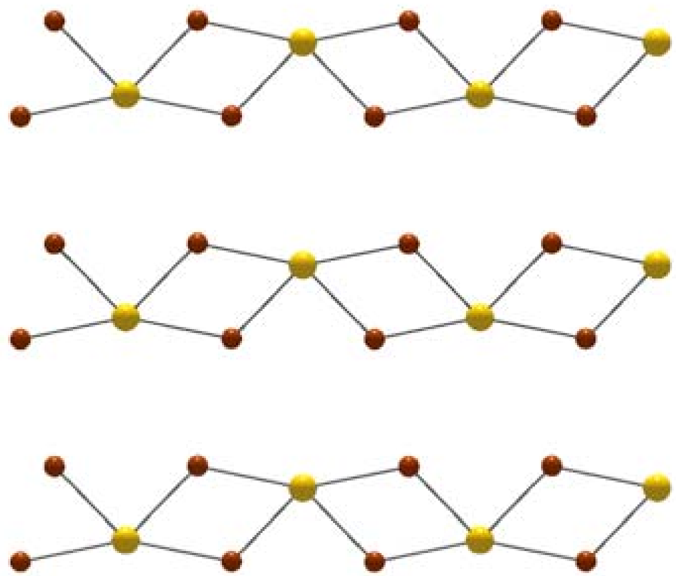
Angew. Chem. Int. Ed. 44 (2005) 1134-1136; Radiochemistry 47 (2005) 481-491; J. Amer. Chem. Soc. 127 (2005) 1072-1073; J. Alloys and Compounds. 444-445 (2007) 457-463; Angew. Chem. Int. Ed. 47 (2008) 549-551

Phase formation in the system
(UO2)(NO3)2 - H2SeO4 - H2O - CH3NH2 (methylamine)

U:Se = 1:2

$(CH_3NH_3)_2[(UO_2)(SeO_4)_2(H_2O)](H_2O)$





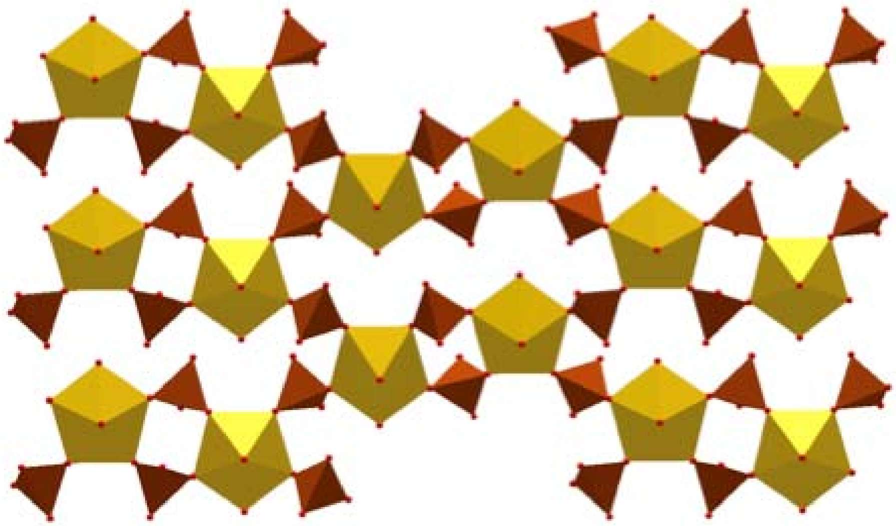
Pna2_1, *a* = 7.550, *b* = 15.836, *c* = 12.014 Å, *V* = 1436.34 Å^3,
$2\Theta_{max}$ = 53.66°, R_1 = 0.046, wR_2 = 0.106, #refl = 1429

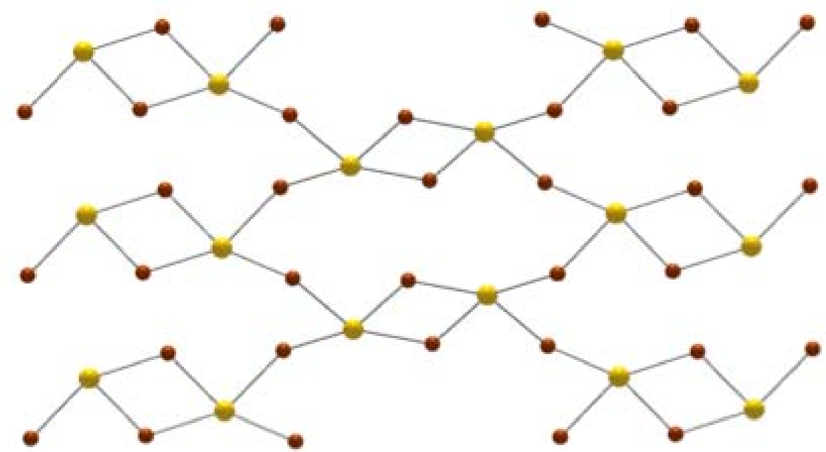
Phase formation in the system

(UO2)(NO3)2 - H2SeO4 - H2O - CH3NH2 (methylamine)

U:Se = 1:2

$(CH_3NH_3)_2[(UO_2)(SeO_4)_2(H_2O)]$





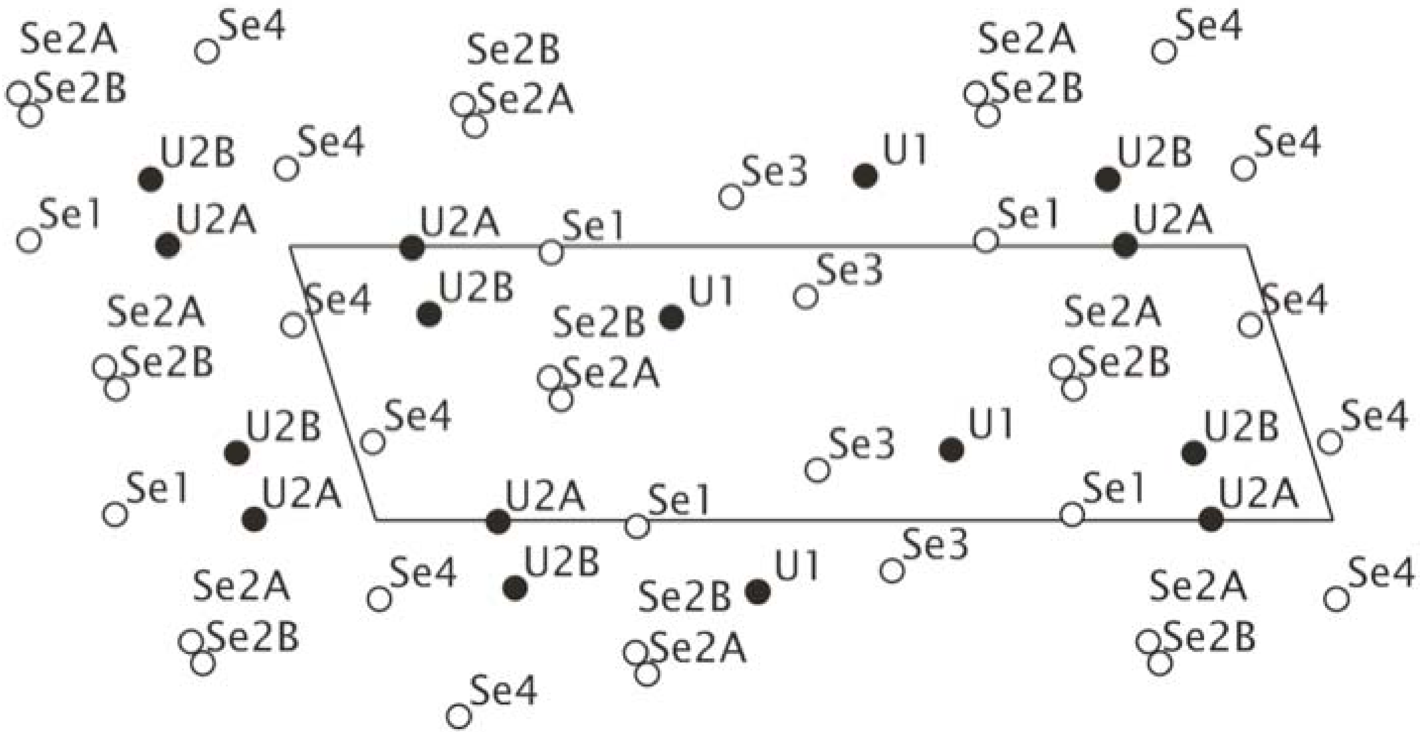
$P2_1/c$, a = 8.237, b = 7.589, c = 22.260 Å, β = 104.57°, V = 1346.7 $Å^3$

$R1$ = 0.047, #refl = 2661

Phase formation in the system
(UO2)(NO3)2 - H2SeO4 - H2O - CH3NH2 (methylamine)

U:Se = 1:2

$(CH_3NH_3)_2[(UO_2)(SeO_4)_2(H_2O)](H_2O)_n$

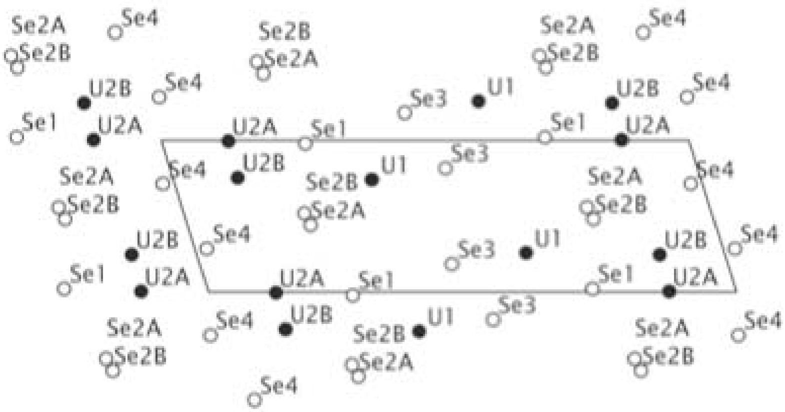


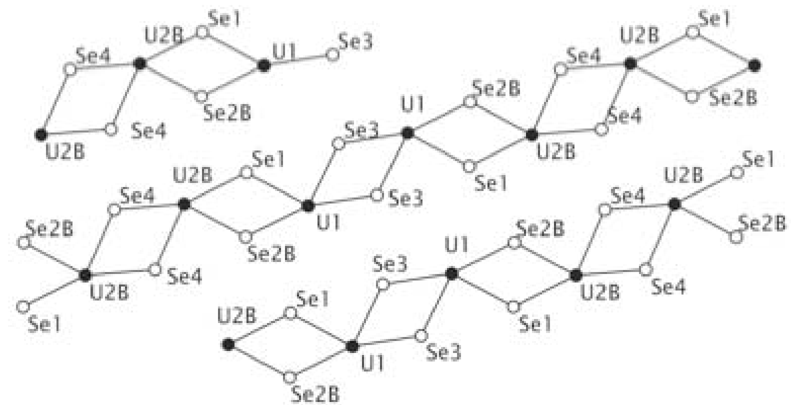
$P2_1/a$, a = 7.563, b = 15.344, c = 25.204 Å, beta = 107.46°, V = 2790.0 Å^3,
R_1 = 0.072, wR_2 = 0.184, #refl = 3820

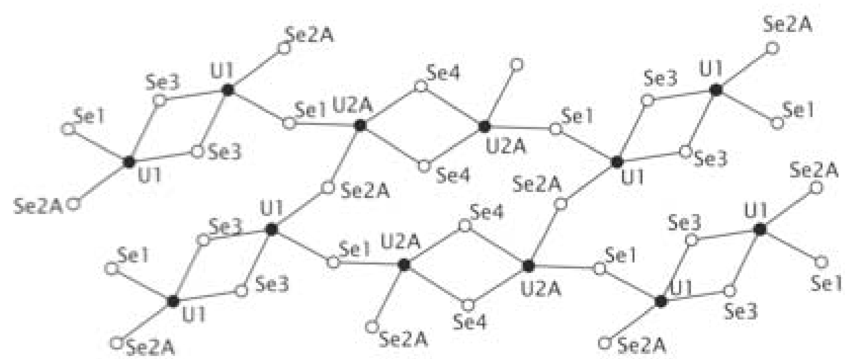
Phase formation in the system
$(UO_2)(NO_3)_2$ - H_2SeO_4 - H_2O - CH_3NH_2 (methylamine)

U:Se = 1:2

$(CH_3NH_3)_2[(UO_2)(SeO_4)_2(H_2O)](H_2O)_n$

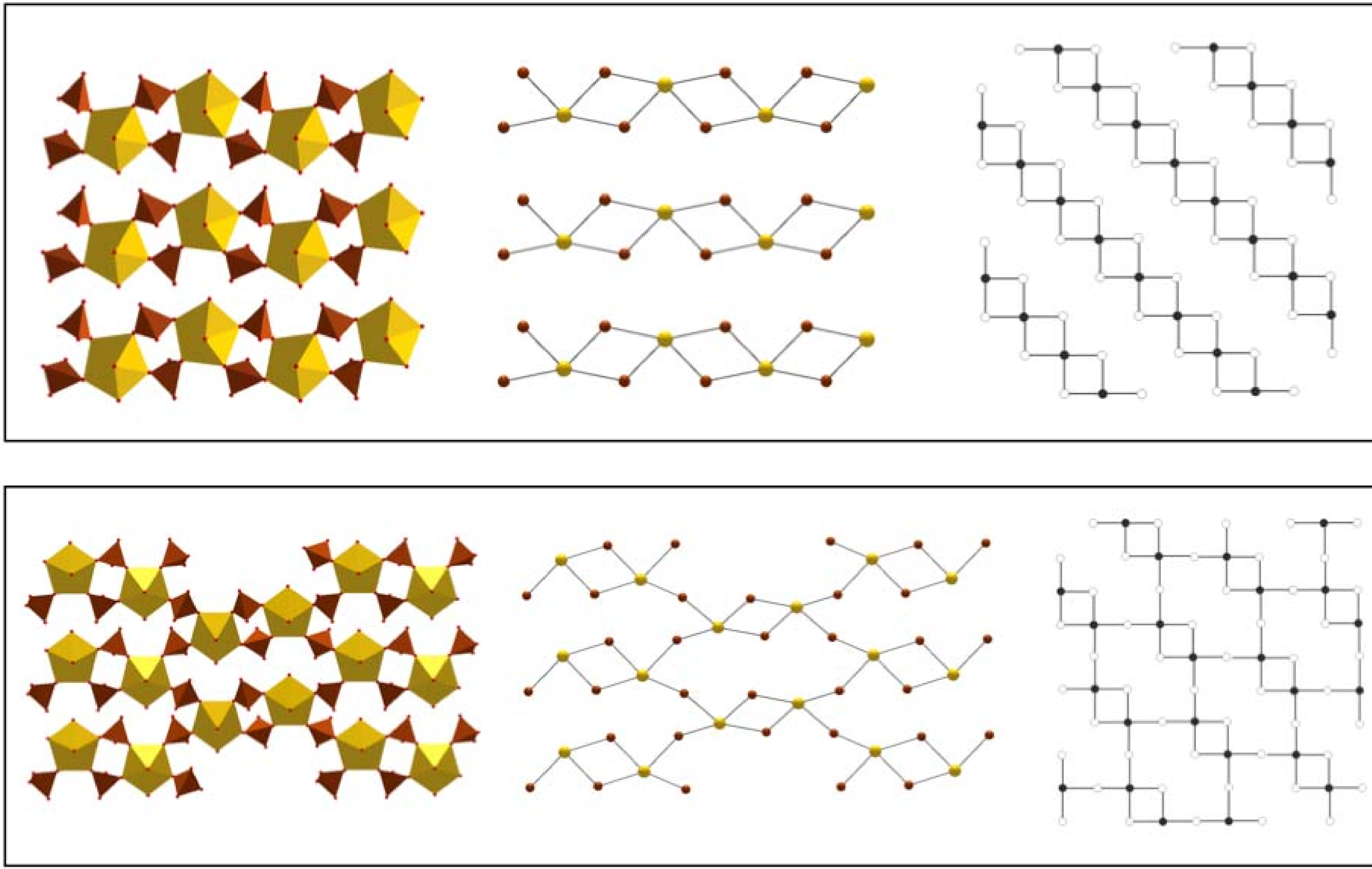


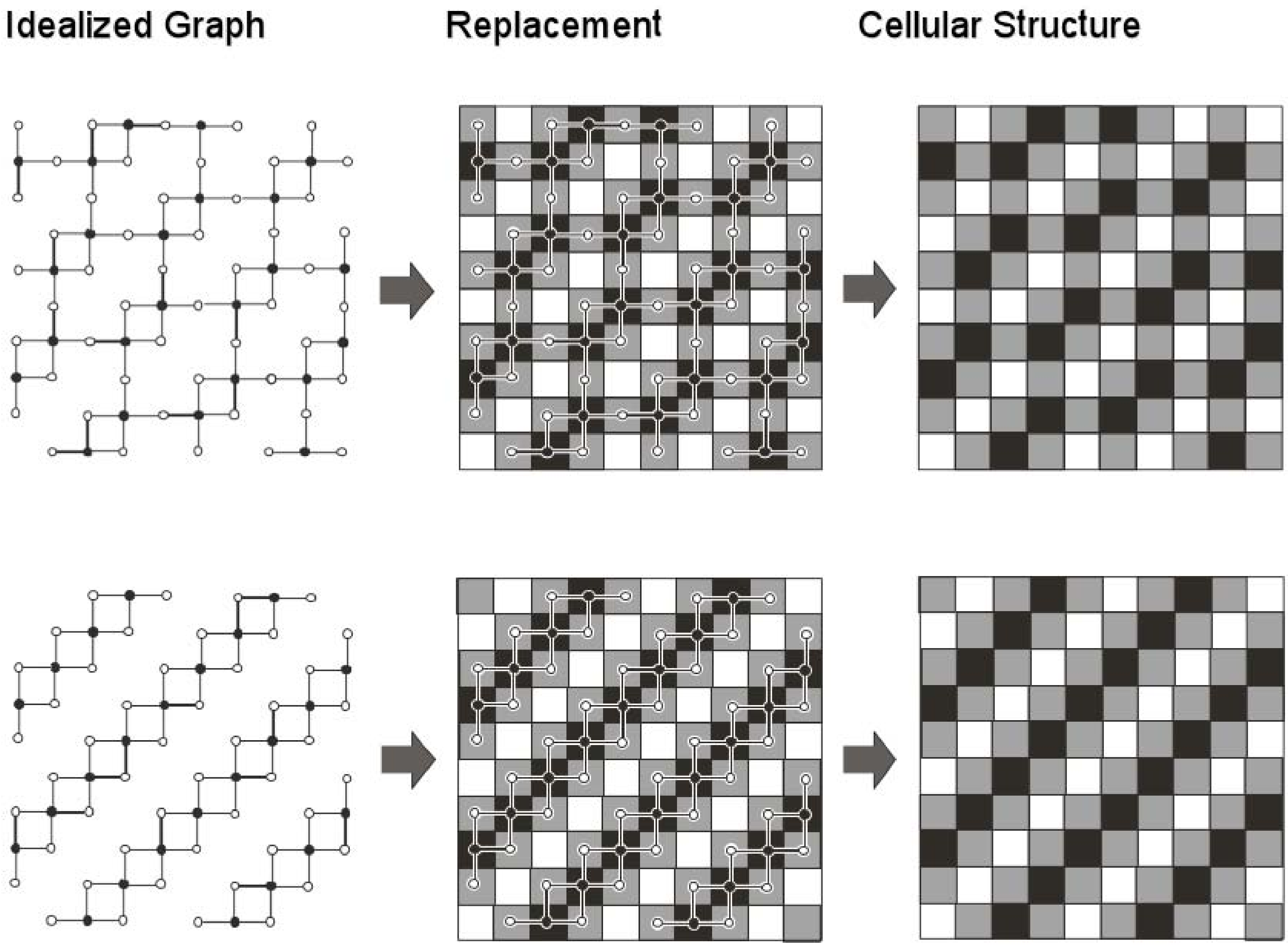




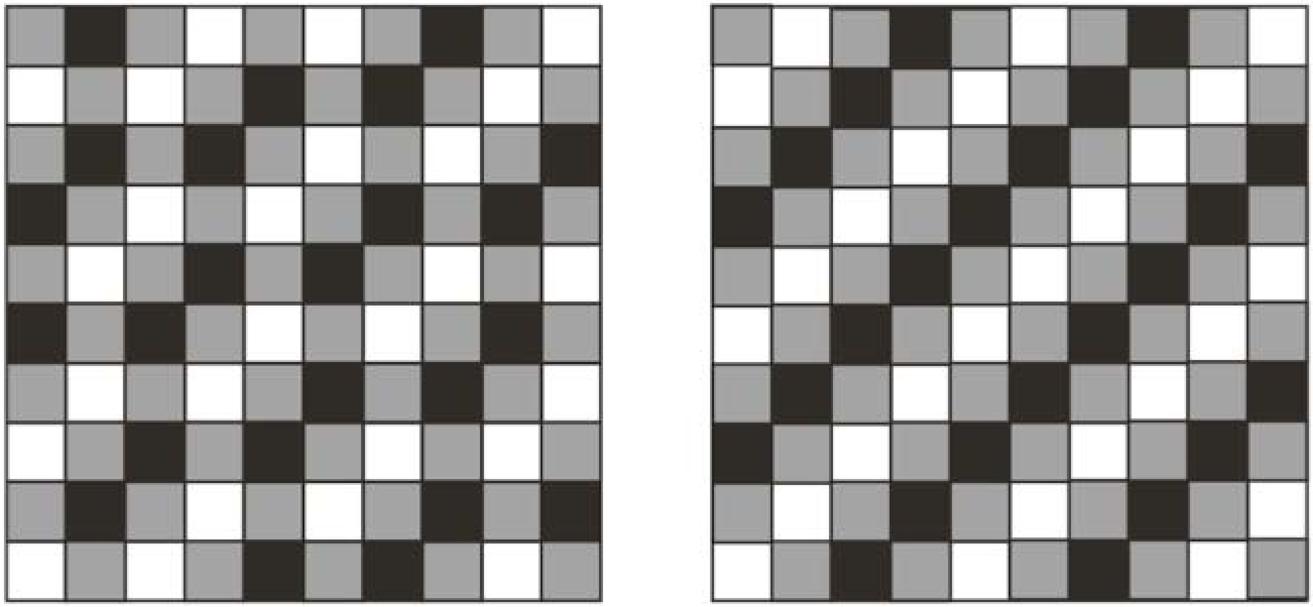
The overall structure is a superposition of chain (1D) and layered (2D) structures

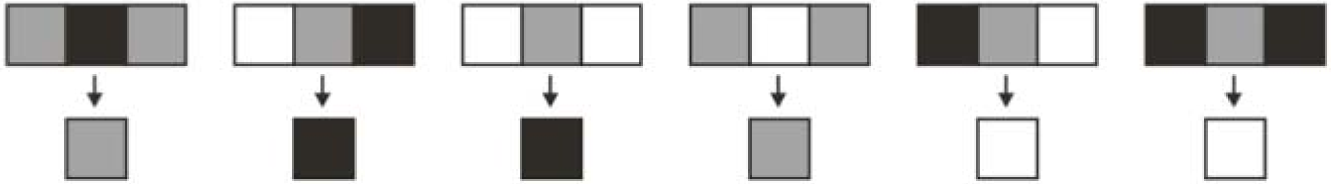
2D Layer → Graph → Idealized Graph

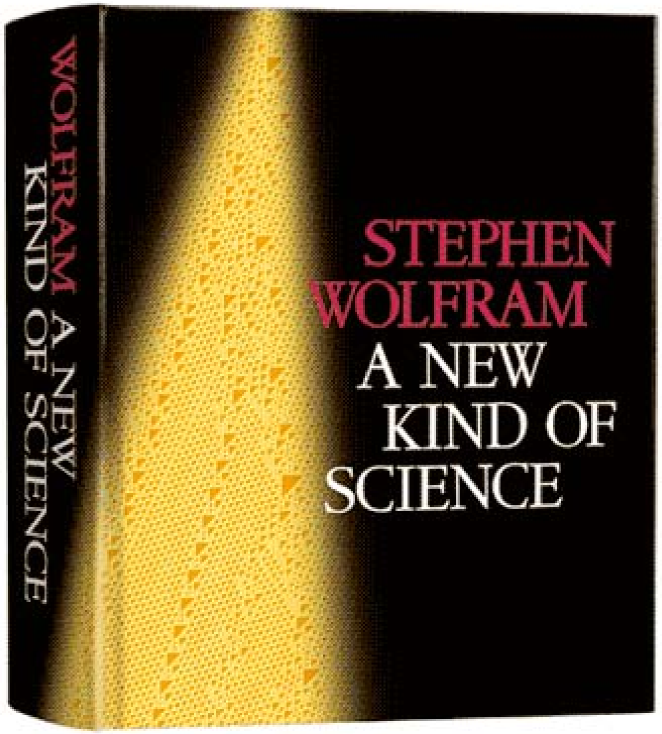



Idealized Graph
Replacement
Cellular Structure

From Cellular Structure to Cellular Automaton







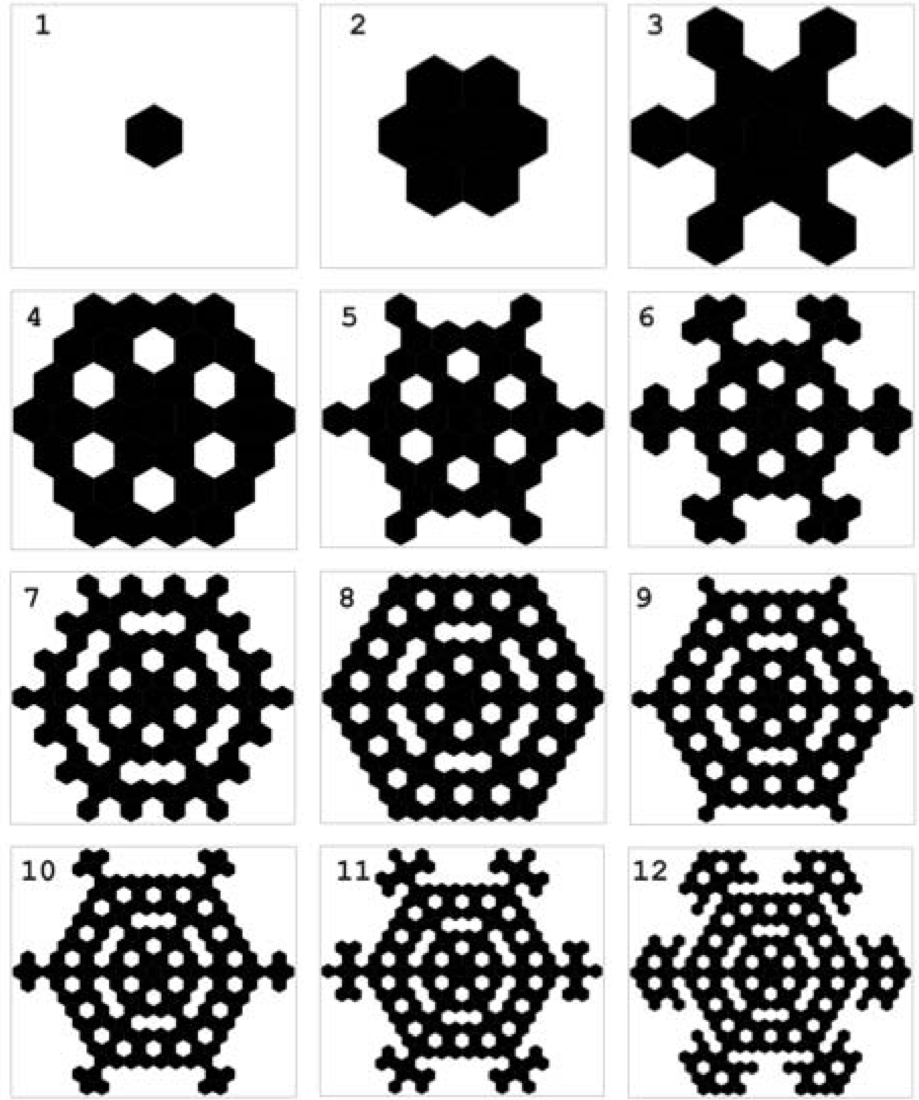
John von Neumann
1903 - 1957

Theory of Self-
Reproducing
Automata

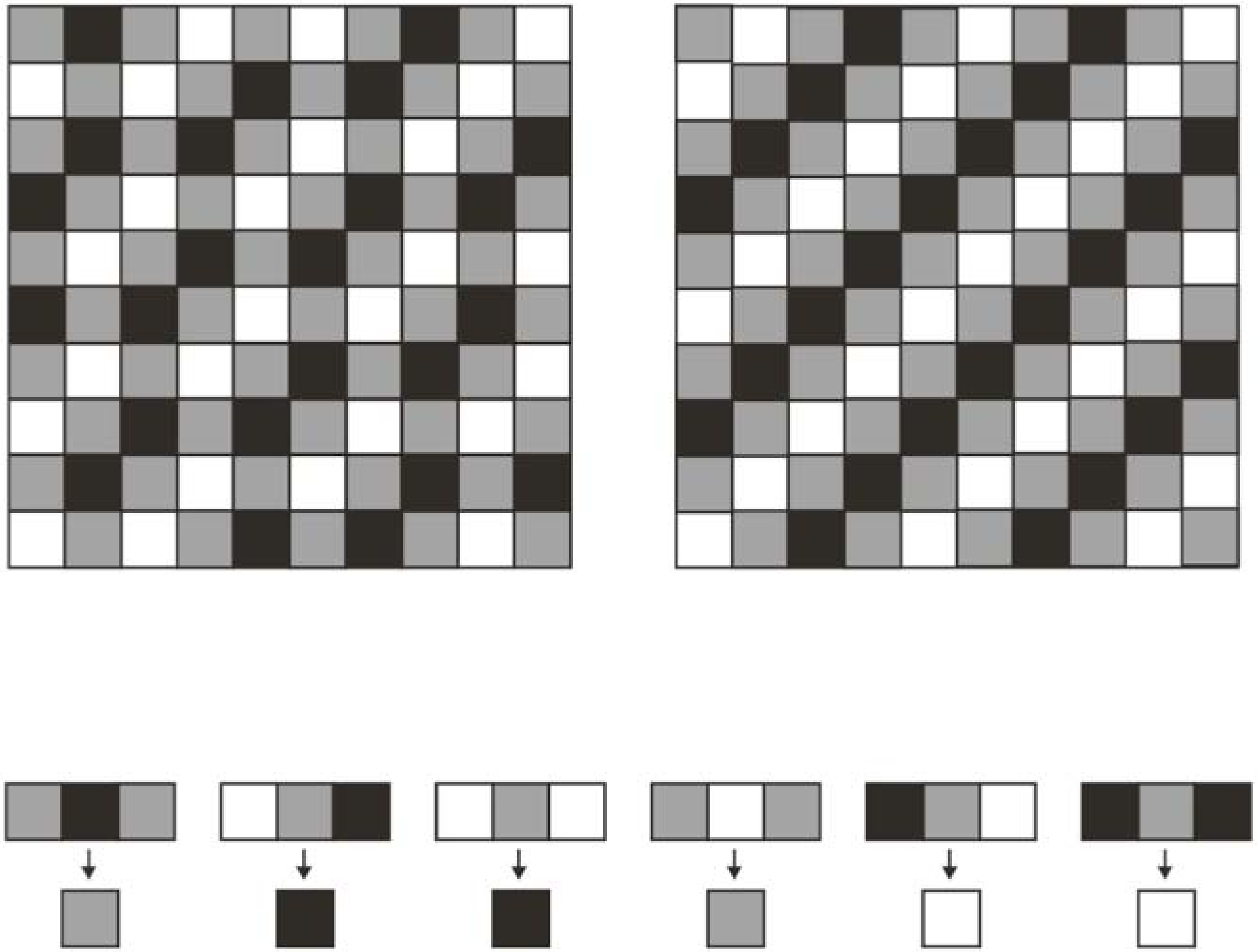
Stephen Wolfram

'New Kind of Science'
cellular automata as universal
models of physical and chemical
dynamic systems

Cellular Automata as Models of Crystals

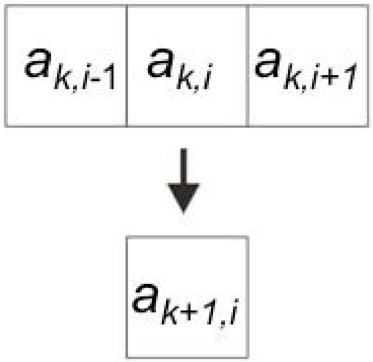


From Cellular Structure to Cellular Automaton



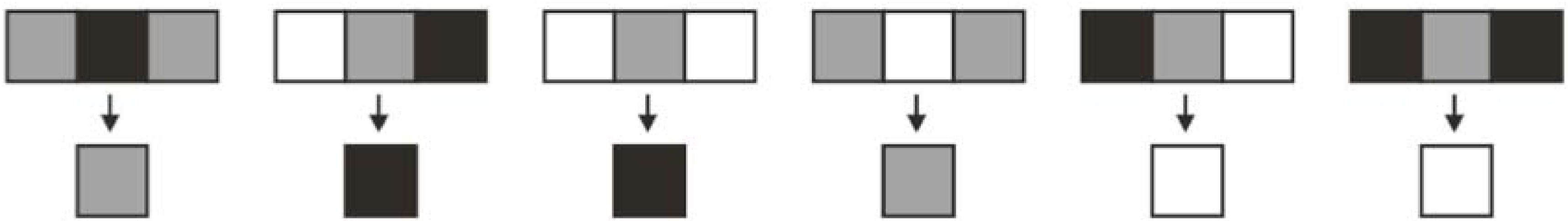
Eur. J. Inorg. Chem. 2010, 2594-2603 (2010).

Cellular Atomaton : structure

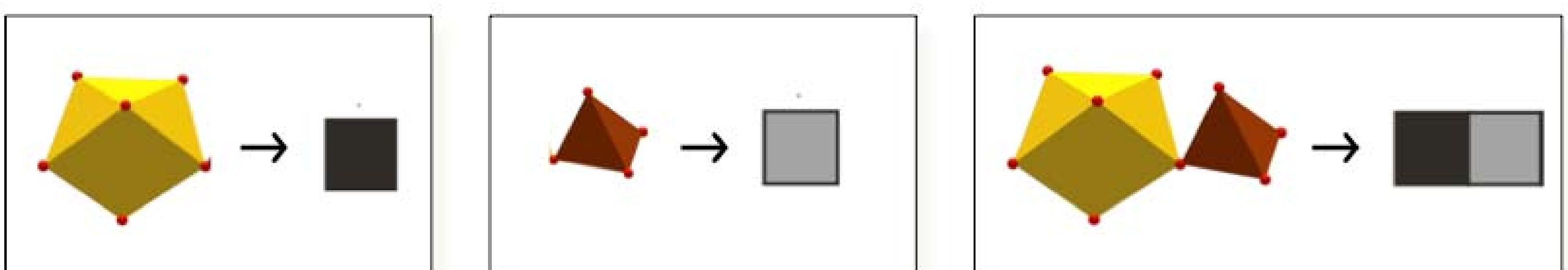


Transition Rules

$$\{a_{k,i-1}, a_{k,i}, a_{k,i+1}\} \longrightarrow a_{k+1,i}$$



$\{1,2,1\} \rightarrow 1$ $\{0,1,2\} \rightarrow 2$ $\{0,1,0\} \rightarrow 2$ $\{1,0,1\} \rightarrow 1$ $\{2,1,0\} \rightarrow 0$ $\{2,1,2\} \rightarrow 0$



Evolution of Cellular Structure

Modeling growing topologies

Wolfram *Mathematica* 7
COMPUTE DEVELOP DEPLOY

Transition Functions

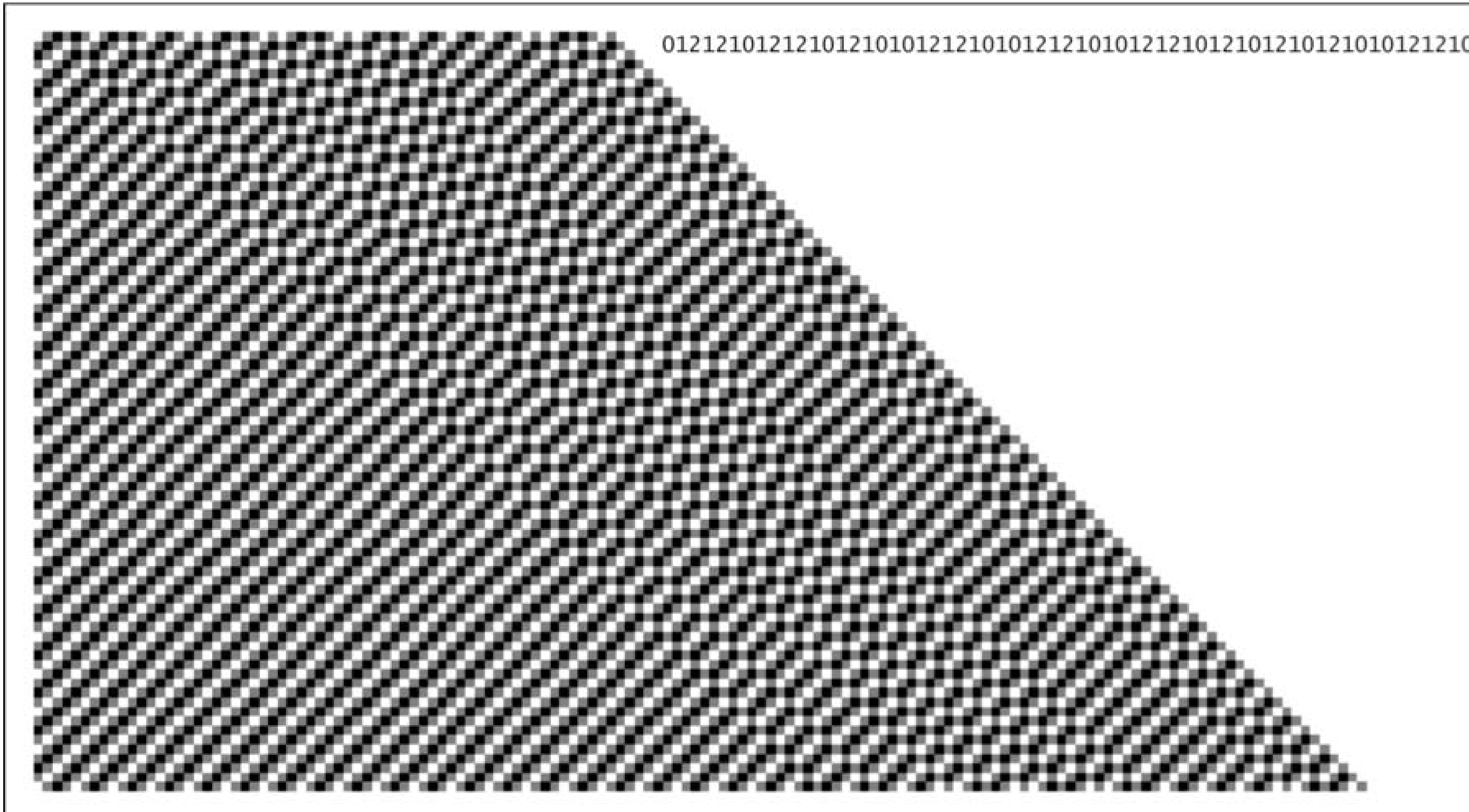
```
Tuples[{0, 1, 2}, 3]

ArrayPlot[
 CellularAutomaton[{{0, 0, 0} → 0, {0, 0, 1} → 1, {0, 0, 2} → 0, {0, 1, 0} → 2, {0, 1, 1} → 0,
   {0, 1, 2} → 2, {0, 2, 0} → 1, {0, 2, 1} → 1, {0, 2, 2} → 0, {1, 0, 0} → 1, {1, 0, 1} → 1,
   {1, 0, 2} → 1, {1, 1, 0} → 0, {1, 1, 1} → 1, {1, 1, 2} → 1, {1, 2, 0} → 1, {1, 2, 1} → 1,
   {1, 2, 2} → 1, {2, 0, 0} → 1, {2, 0, 1} → 1, {2, 0, 2} → 1, {2, 1, 0} → 0, {2, 1, 1} → 1,
   {2, 1, 2} → 0, {2, 2, 0} → 1, {2, 2, 1} → 1, {2, 2, 2} → 1},
  {{0, 1, 2, 1, 2, 1, 0, 1, 2, 1, 2, 1, 0, 1, 2, 1, 0, 1, 0, 1, 2, 1, 2, 1, 0, 1, 0, 1, 2, 1,
    2, 1, 0, 1, 0, 1, 2, 1, 2, 1, 0, 1, 2, 1, 0, 1, 2, 1, 0, 1, 2, 1, 0, 1, 0, 1, 2, 1, 2, 1, 0, 1}, 0
  {80, {0, 150}}]]
```

Initial Conditions

Eur. J. Inorg. Chem. 2010, 2594-2603 (2010).

Evolution of Cellular Structure

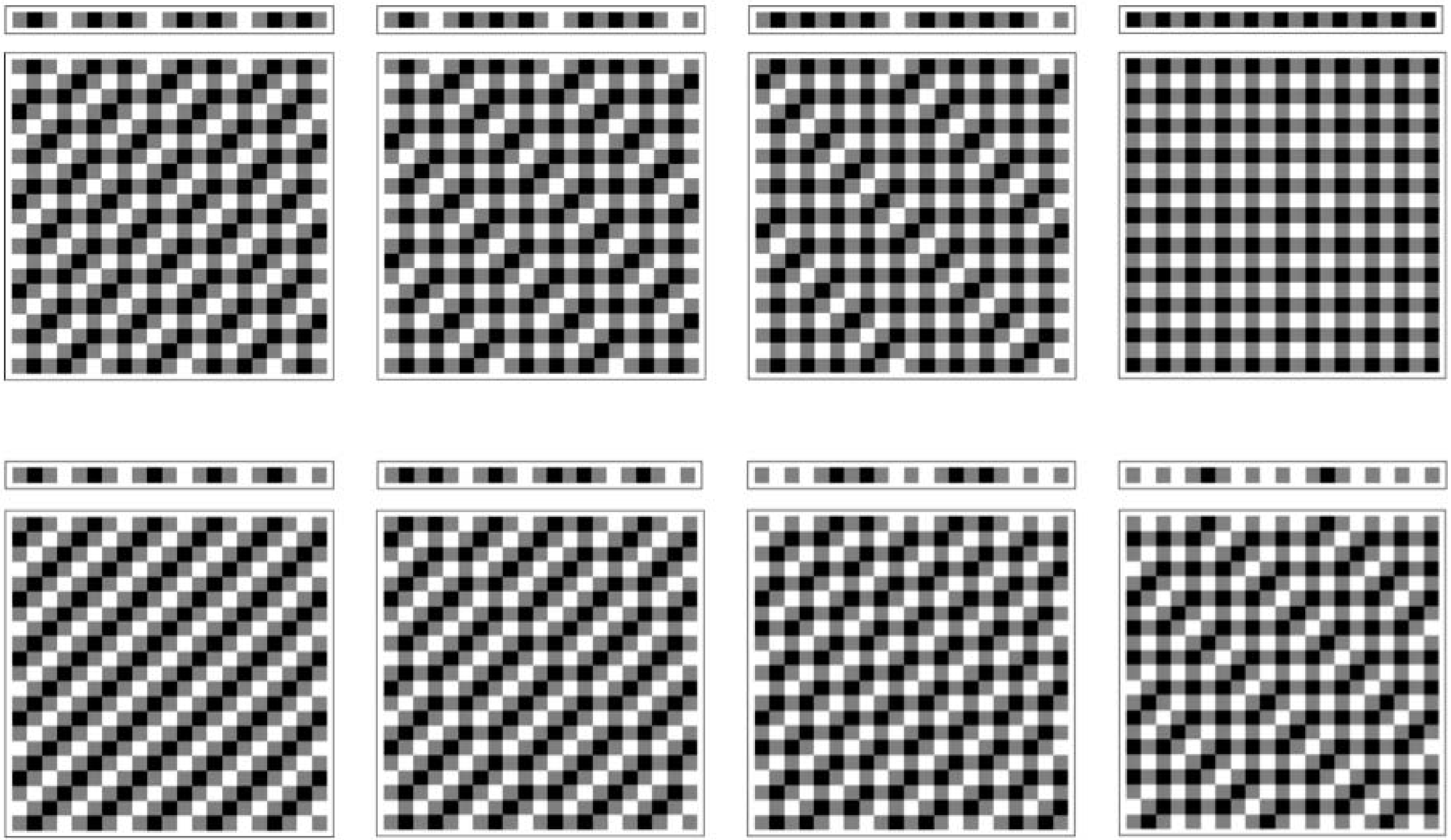
Modeling growing topologies



Eur. J. Inorg. Chem. 2010, 2594-2603 (2010).

Evolution of Cellular Structure

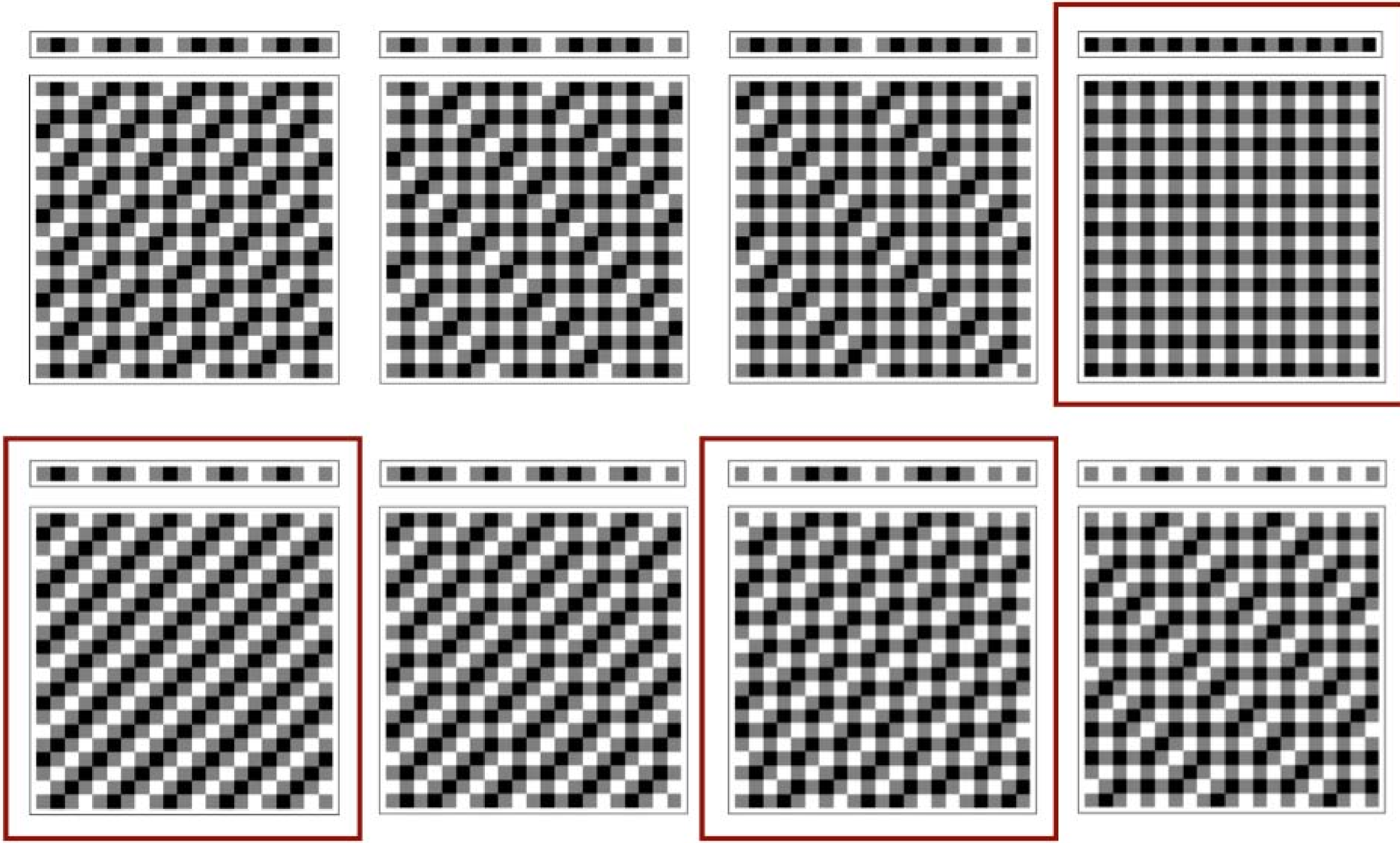
Modeling growing topologies



Eur. J. Inorg. Chem. 2010, 2594-2603 (2010).

Evolution of Cellular Structure

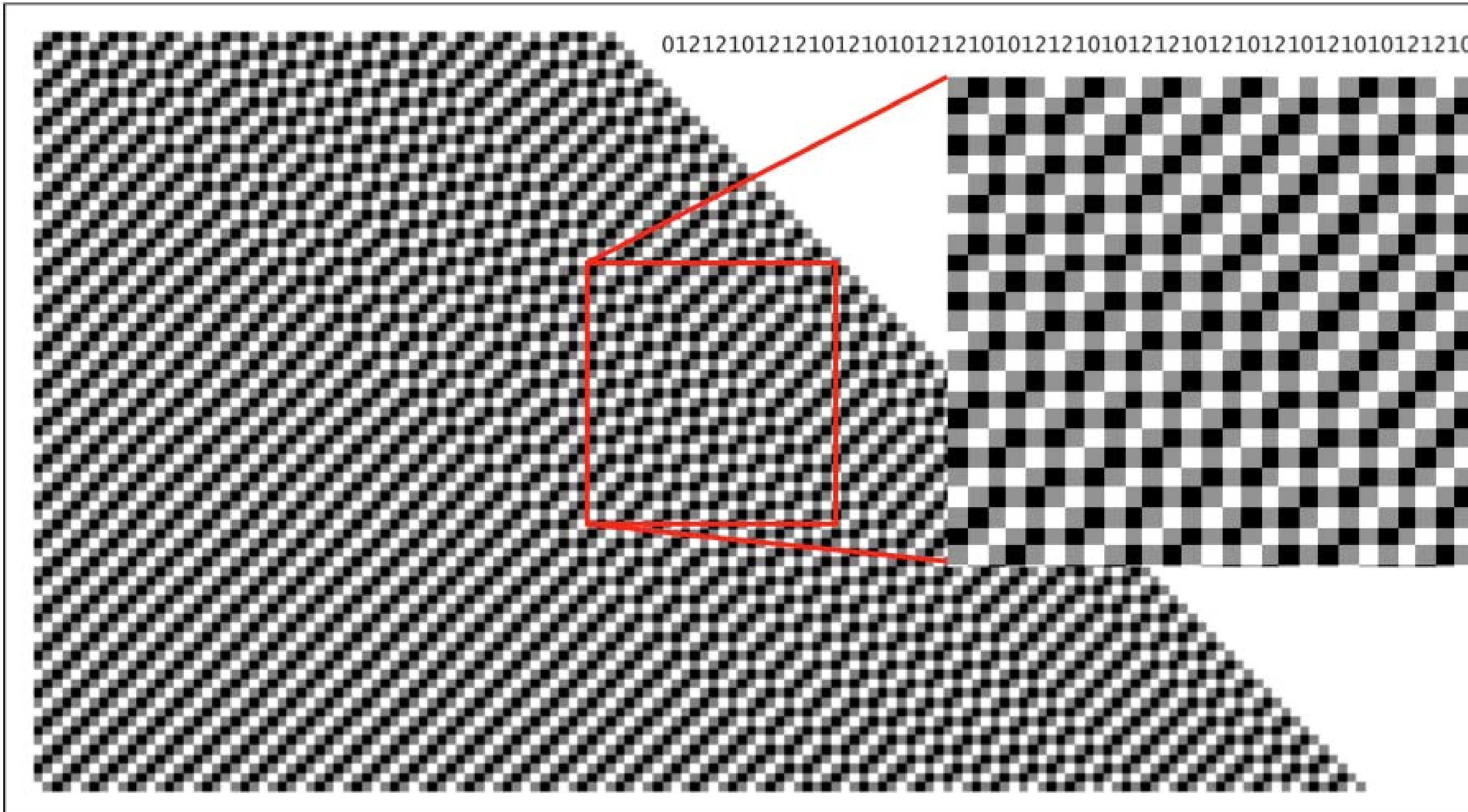
Modeling growing topologies



Eur. J. Inorg. Chem. 2010, 2594-2603 (2010).

Evolution of Cellular Structure

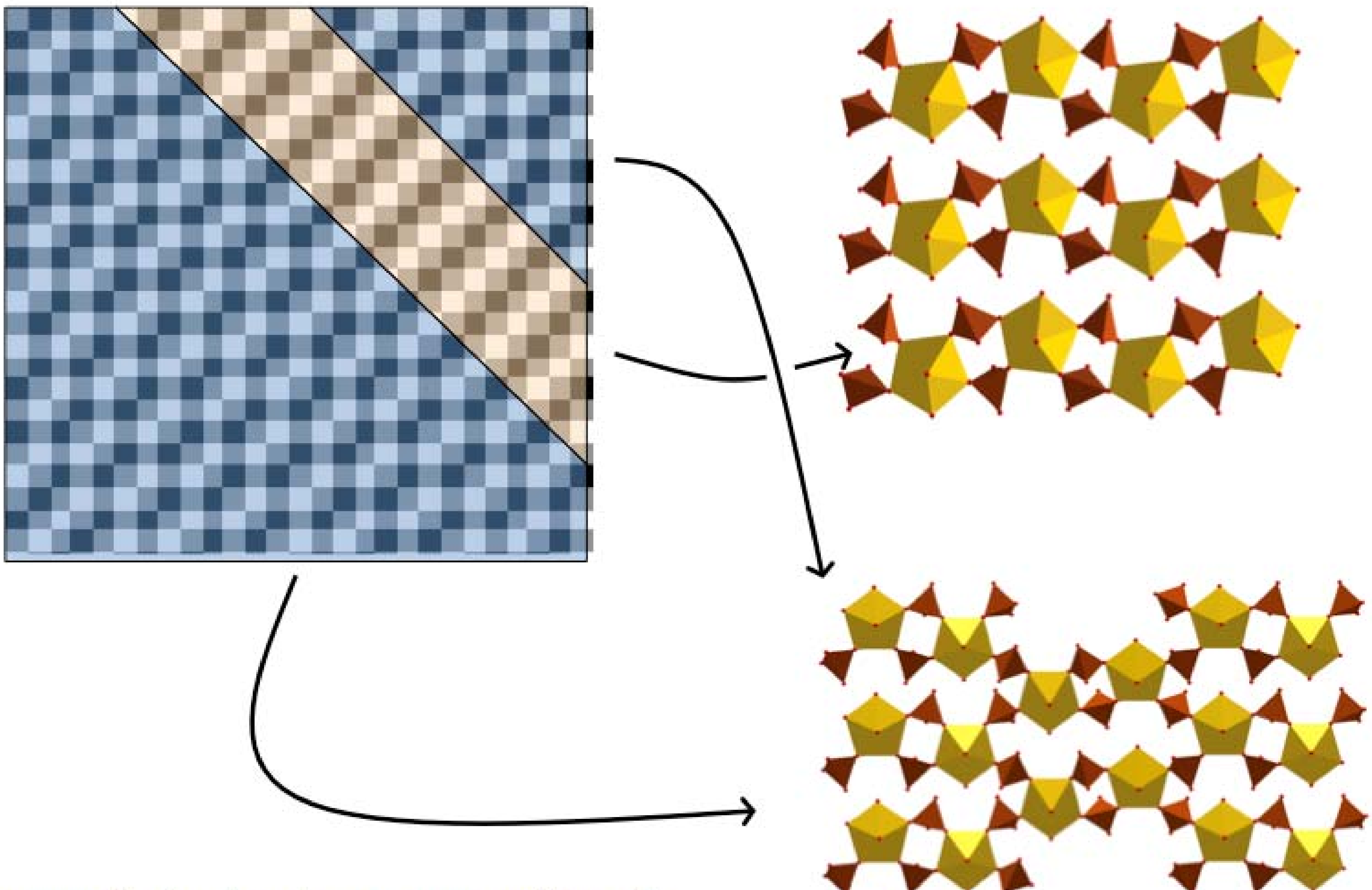
Modeling growing topologies



Eur. J. Inorg. Chem. 2010, 2594-2603 (2010).

Evolution of Cellular Structure

Modeling growing topologies



The overall structure is a superposition of chain (1D) and layered (2D) structures

Eur. J. Inorg. Chem. 2010, 2594-2603 (2010).

CRYSTALLOGRAPHY	COMPUTER SCIENCE
CRYSTAL	AUTOMATON
BUILDING BLOCK (CLUSTER, PARTICLE)	CELL
SPACE	LATTICE
CRYSTAL GROWTH	COMPUTATION
CHEMICALLY PROHIBITED CONFIGURATION (CPC)	ORPHAN-CONFIGURATION OF CELLS
STRUCTURE WITH CPC	GARDEN-OF-EDEN

When Complexity Matters: Metastable Crystallization

When Complexity Matters:
Structural Information and the Ostwald Rule

… I would like to summarize all the experience on the subject up to now in the general statement that, if a system leaves its state to head for a more stable one, it does not go to the most stable one, but to the energetically nearest one.

W. Ostwald. Studien ueber die Bildung und Umwandlung fester Koerper.
Z. Phys. Chem. 22 (1897) 289.

When Complexity Matters:
Structural Information and the Ostwald Rule

Crystallization is viewed as a kinetic process, the relative "ease" of which is influenced by details of the structures involved. The word "simplexity" is used as a measure of structural complexity. In general, high "simplexity" is synonymous with disorder, or structural simplicity, or high entropy. Nucleation and growth of phases with high simplexity are favored - in many cases over more stable compounds of lower simplexity.

Goldsmith, J.R. (1953) A "simplexity principle" and its relation to "ease" of crystallization. *Journal of Geology*, **61**, 439-451.

When Complexity Matters:
Structural Information and the Ostwald Rule

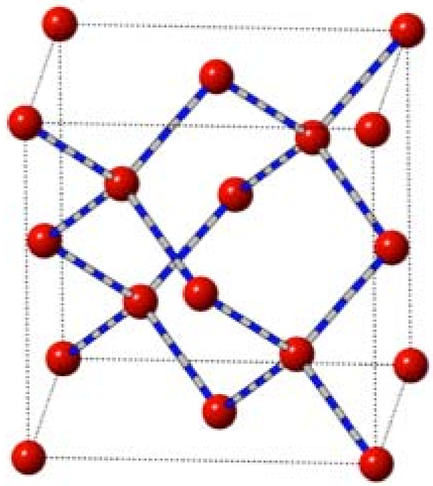
Crystallization of cubic ice I_c from supercooled water

- The metastable cubic phase I_c is thought to persist in the coldest regions of Earth's atmosphere where temperatures fall below 200 K
- In the atmosphere, the transient presence of the metastable phase is thought to modify the shape of snowflakes and may lead to substantial changes in ice-particle concentrations in cold cirrus clouds.

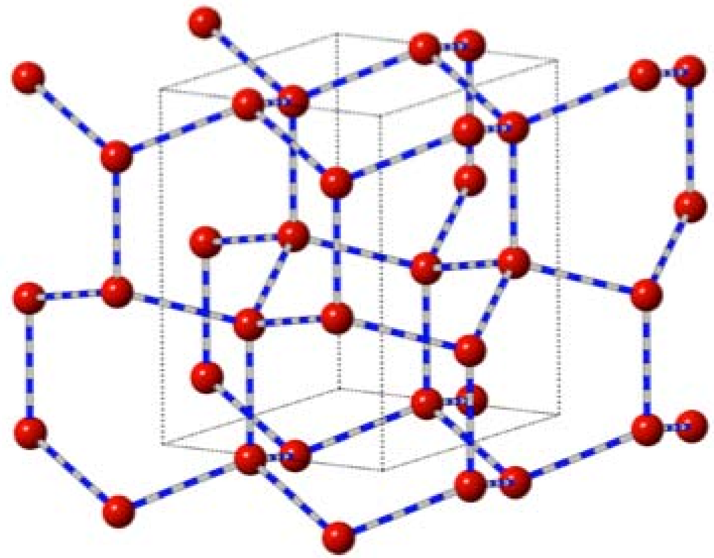
Malkin et al. *Proc Natl Acad Sci USA* **109**:1041–1045 (2012)

When Complexity Matters:
Structural Information and the Ostwald Rule

Crystallization of cubic ice I_c from supercooled water



cubic ice I_c
(metastable)
5.510 bits/u.c.



hexagonal ice I_h
(stable)
17.510 bits/u.c.

Metastable phase has the lower information content compared to the stable phase in the system

When Complexity Matters:
Structural Information and the Ostwald Rule

Hydrothermal flow-through experiments of silica precipitation responsible for quartz vein formation showed the following sequence of metastable transformations:

opal-A (amorphous) (**0 bits/u.c.**) →

low-ordered opal-C (**5.510 bits/u.c.**) →

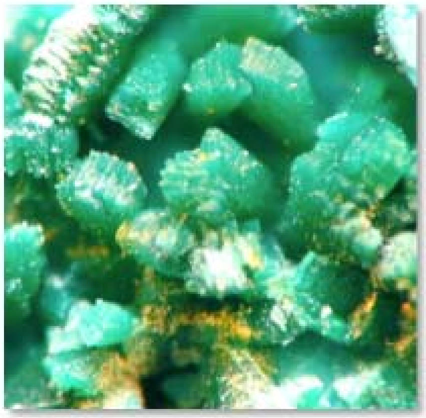
high-ordered opal-C (**5.510 bits/u.c.**) →

quartz (**8.265 bits/u.c.**)

Okamoto, A., Saishu, H., Hirano, N. and Tsuchiya, N. (2010) Mineralogical and textural variation of silica minerals in hydrothermal flow-through experiments: implications for quartz vein formation. *Geochimica et Cosmochimica Acta*, 74, 3692-3706

When Complexity Matters:
The Ostwald Rule and Structural Complexity

Ostwald cascade of phases in the $Cu_2(OH)_3Cl$ system




botallackite ⟶ atacamite ⟶ clinoatacamite - - - -> anatacamite

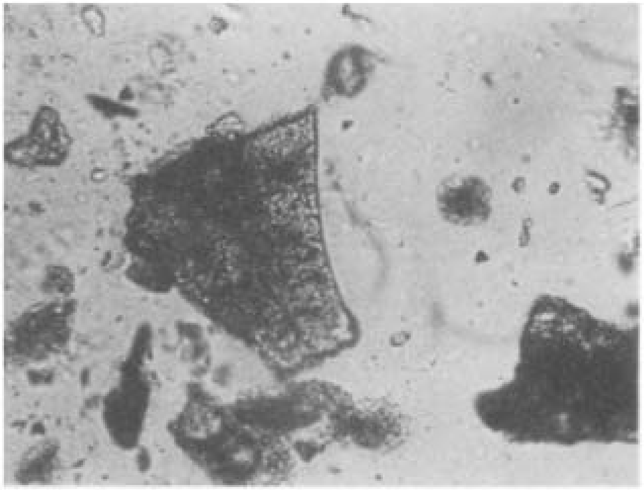
Alteration zones of Cu sulfide mineral deposits;
Patina on the surface of copper and bronze monuments;
Ancient pigments;
Magnetic materials with kagomé nets

When Complexity Matters:
The Ostwald Rule and Structural Complexity

Formation of brochantite and atacamite on the Statue of Liberty as the result of attack by acid rains.

Livingston, R.A. (1991) Influence of the environment on the patina of the Statue of Liberty. Environmental Science and Technology, 25, 1400–1408.

When Complexity Matters:
The Ostwald Rule and Structural Complexity

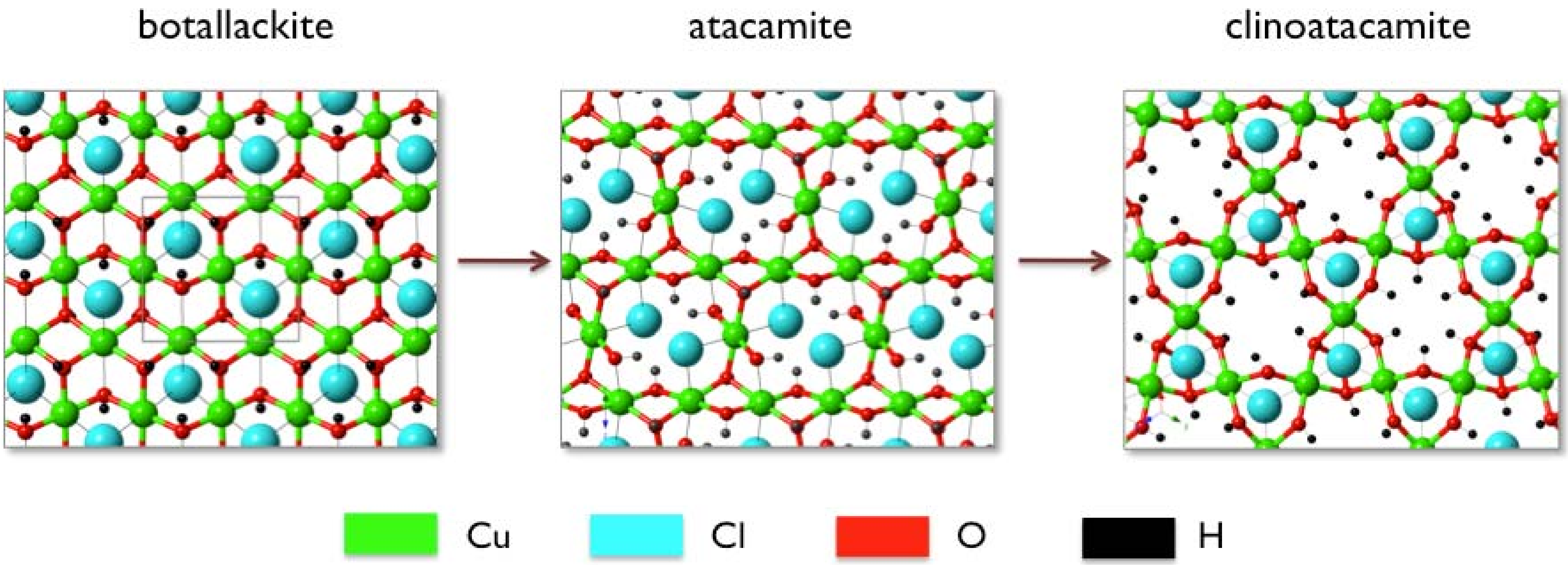


Atacamite plates

Copper oxysalts in ancient paintings:
Dionisius frescos in Ferapontov monastery (Vologda area)

M. M. Naumova, S. A. Pisareva and G. O. Nechiporenko, Green Copper Pigments of Old Russian Frescoes. Studies in Conservation, 35 (1990) 81-88

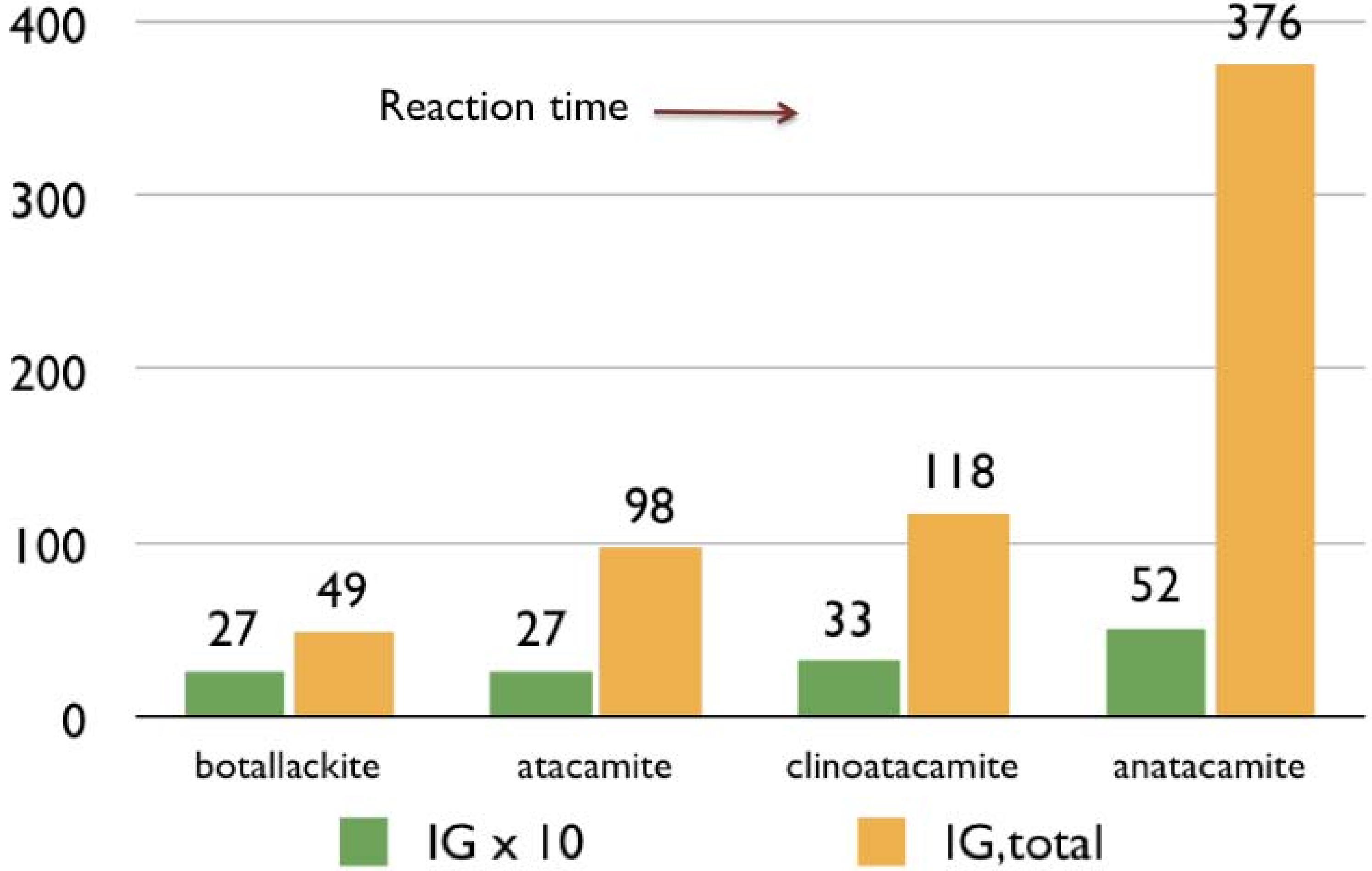
When Complexity Matters:
The Ostwald Rule and Structural Complexity



Layer-SubLayer Transformation in $Cu_2(OH)_3Cl$ polymorphs

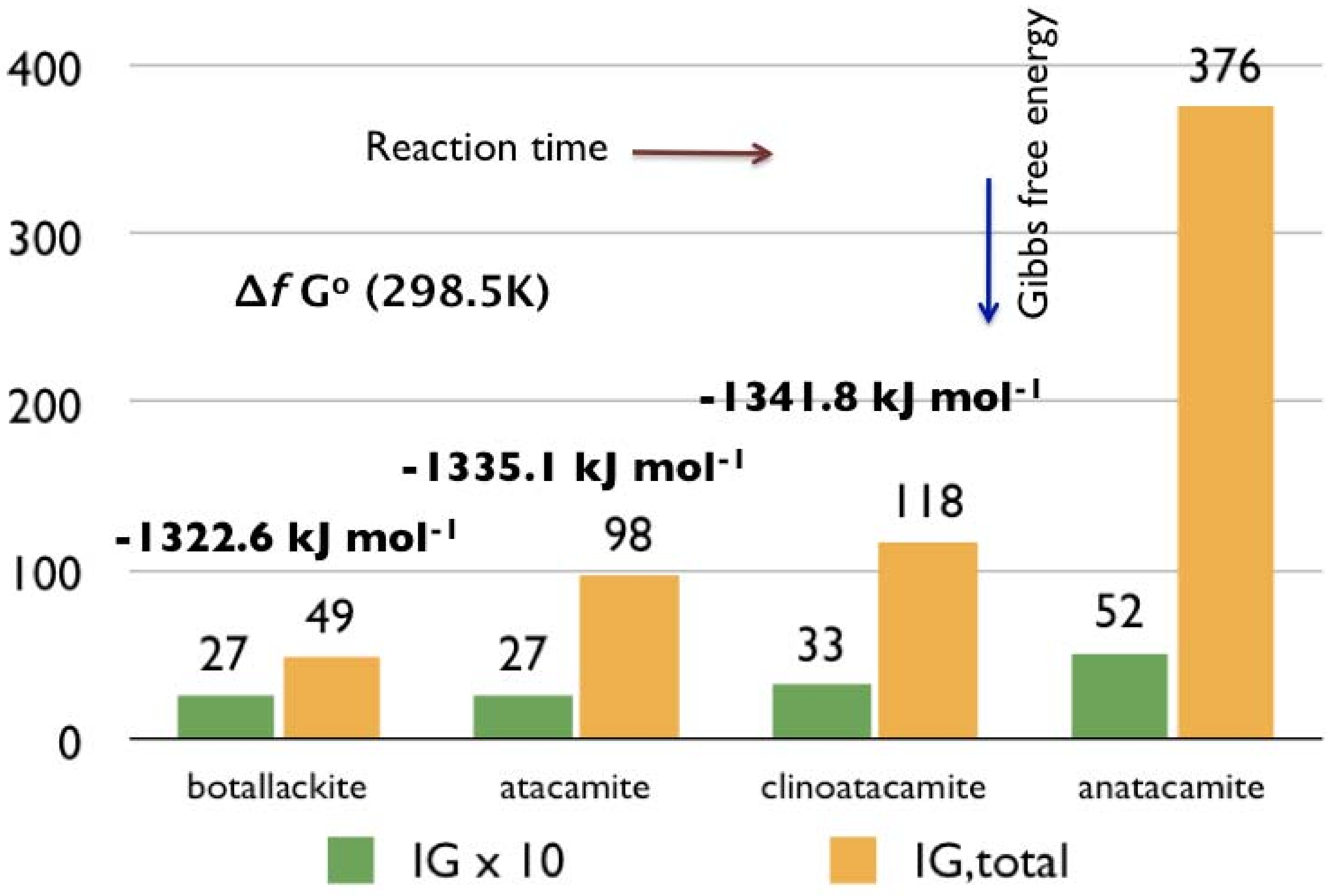
Krivovichev, Hawthorne, Williams, in preparation

When Complexity Matters:
The Ostwald Rule and Structural Complexity



Krivovichev, Hawthorne, Williams, in preparation

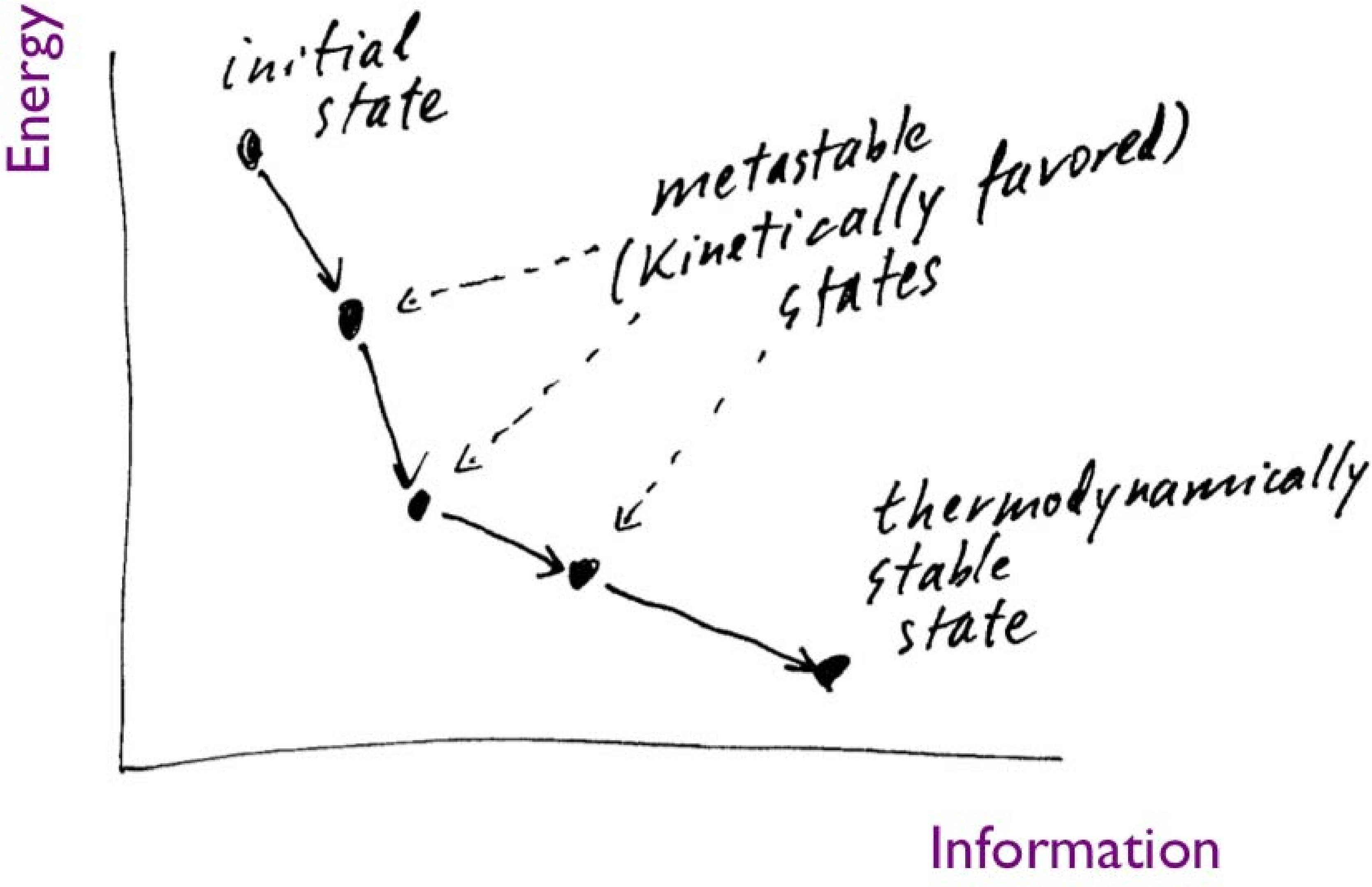
When Complexity Matters:
The Ostwald Rule and Structural Complexity



Krivovichev, Hawthorne, Williams, in preparation

When Complexity Matters:

Trajectory of Structural Evolution in the Energy-Information Coordinates



Energy and Complexity

Energy-to-Information Conversion and the Landauer's Principle

erasure of 1 bit of information at constant temperature T is associated with the release of energy not less than $k_B T \ln 2$, where k_B is a Boltzmann constant

Information has a physical nature and represents a negative contribution to the free energy of the system

Landauer, R. (1961) Dissipation and heat generation in the computing process. *IBM Journal of Research and Development*, **5**, 183–191; Landauer R. (1996) The physical nature of information. *Physics Letters A*, **217**, 188-193.

LETTERS
PUBLISHED ONLINE: 14 NOVEMBER 2010 | DOI:10.1038/NPHYS1821
nature physics

Experimental demonstration of information-to-energy conversion and validation of the generalized Jarzynski equality

Shoichi Toyabe[1], Takahiro Sagawa[2], Masahito Ueda[2,3], Eiro Muneyuki[1]★ and Masaki Sano[2]★

LETTER
doi:10.1038/nature10872

Experimental verification of Landauer's principle linking information and thermodynamics

Antoine Bérut[1], Artak Arakelyan[1], Artyom Petrosyan[1], Sergio Ciliberto[1], Raoul Dillenschneider[2] & Eric Lutz[3]†

Minds & Machines (2013) 23:473–487
DOI 10.1007/s11023-013-9302-x

The Thermodynamic Cost of Fast Thought

Alexandre de Castro

Conclusions

1. Complexity (Structural Information) is an important parameter that influences crystallization processes and stability of crystalline solids.

2. Construction of dynamic complexity models in terms of finite automata provides a new tool for interpretation of crystal growth and modeling new topologies in old systems.

3. Both static and dynamic complexity arguments are important for the design of novel complex materials and prediction and interpretation of experimental results.

4. Relations between information and energy as applied to crystalline materials remain unclear.

Thank you for your attention