

Структуры с анионцентрированными каркасными комплексами

Обозначаются буквой F

*На сегодняшний день известно 43 вида
каркасов.*

Условно можно разделить на 2 группы:

1. Общие каркасы

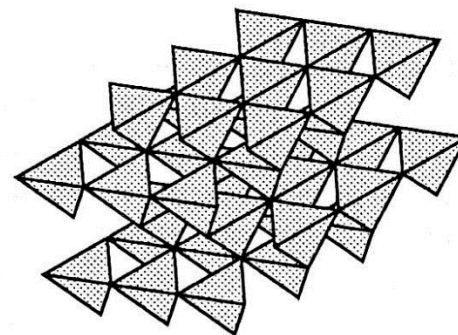
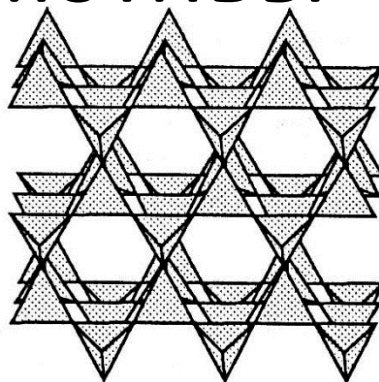
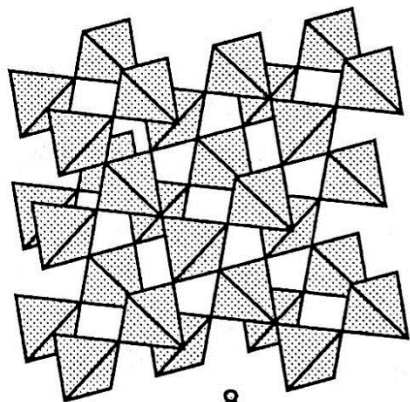
2. Флюоритоподобные каркасы:

-на основе супермодулей,

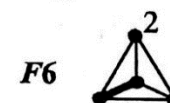
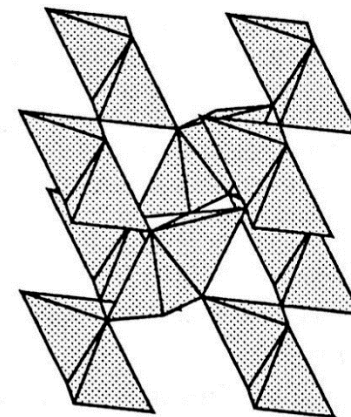
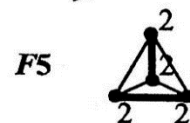
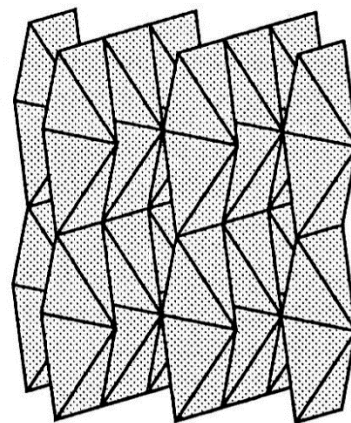
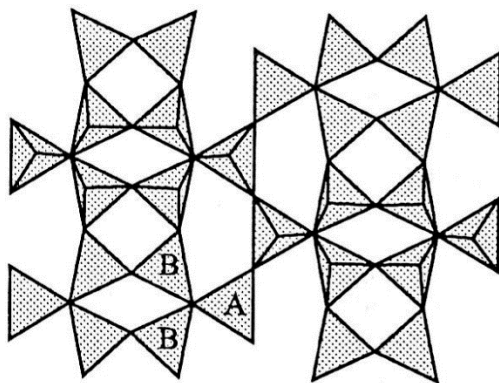
*-на основе сочленения флюоритовых
модулей по четверти грани*

Каркасные анионцентрированные

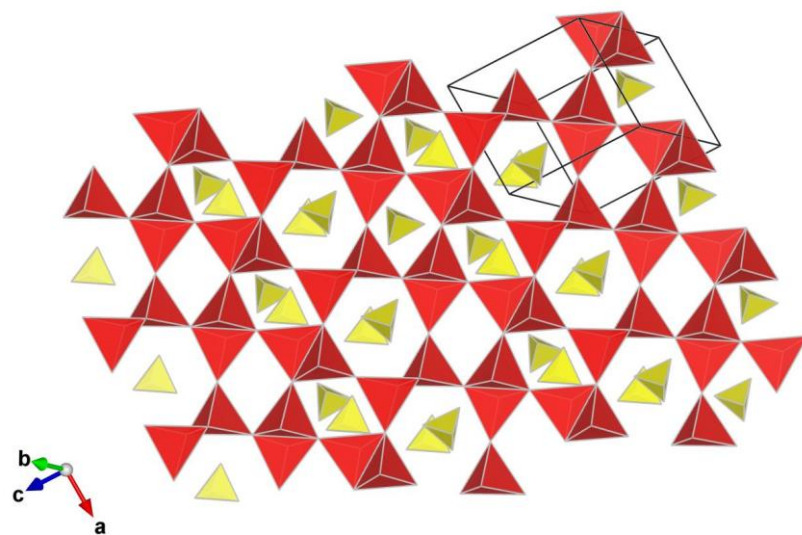
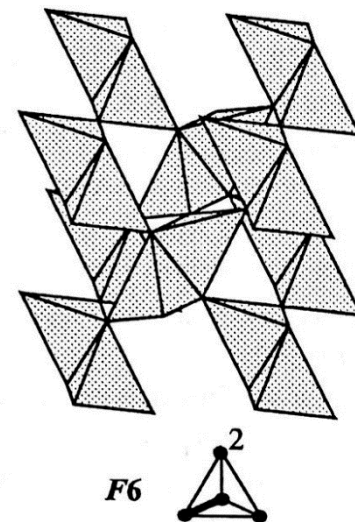
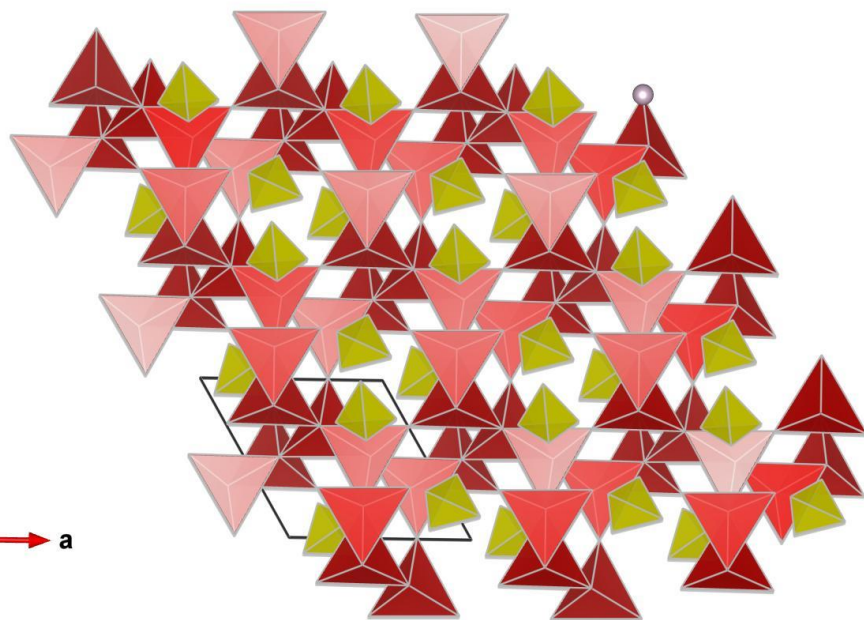
МОТИВЫ



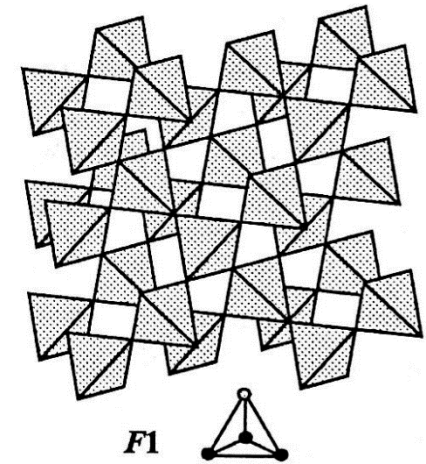
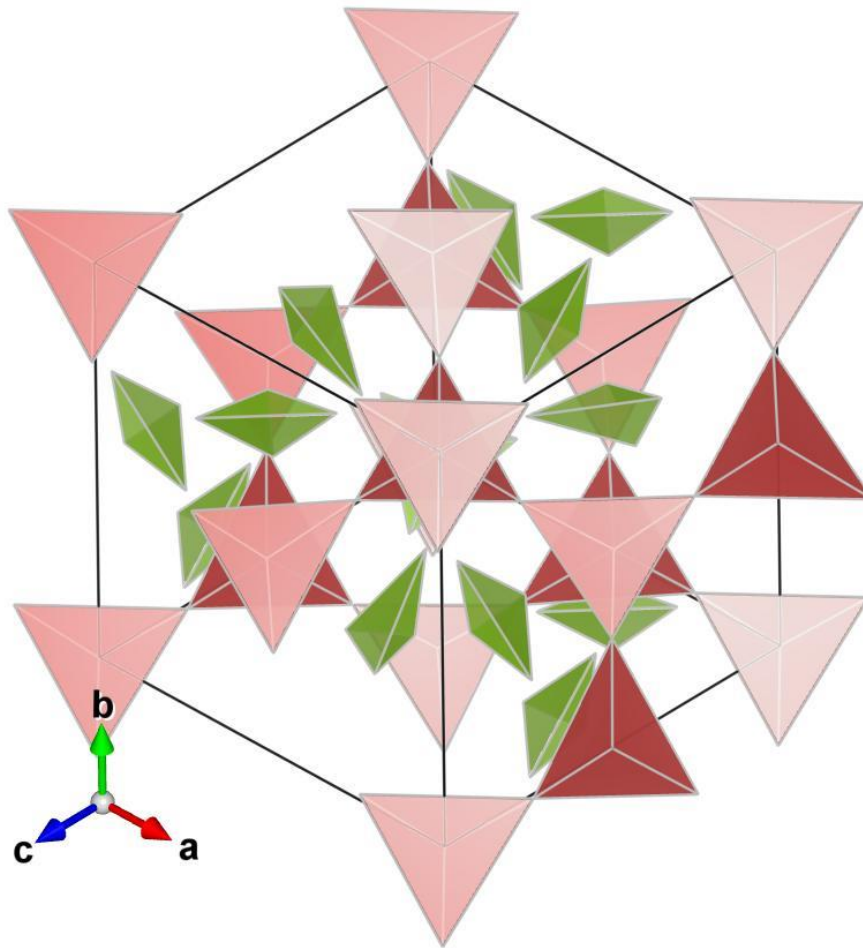
Куприт Cu₂O



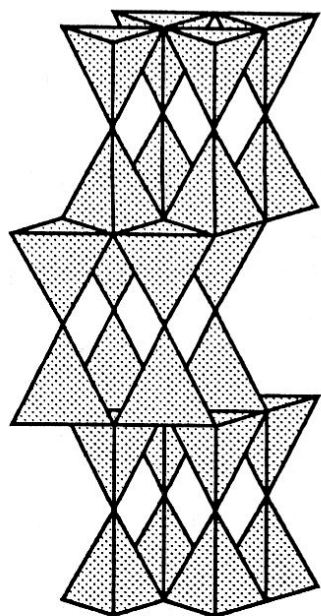
Шутеит $[O_2Hg_3]SO_4$



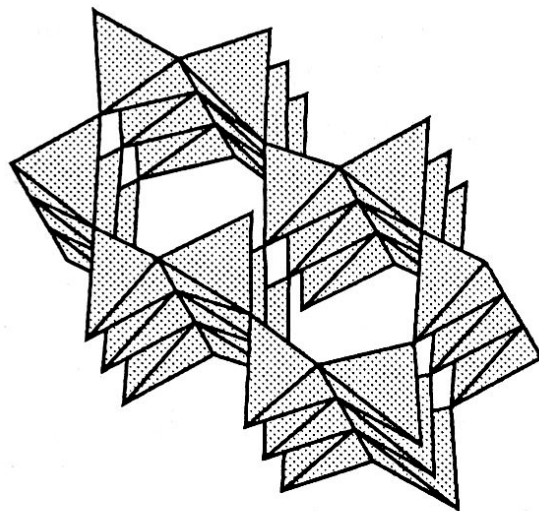
Структура Cu_2SeO_4



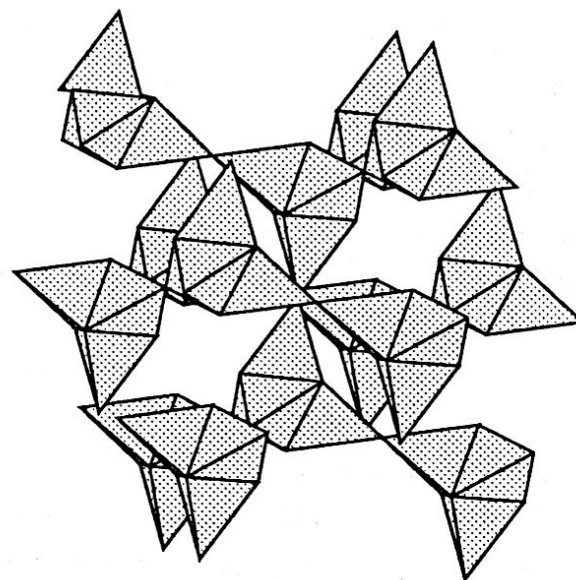
Каркасные анионцентрированные МОТИВЫ



F7



F8

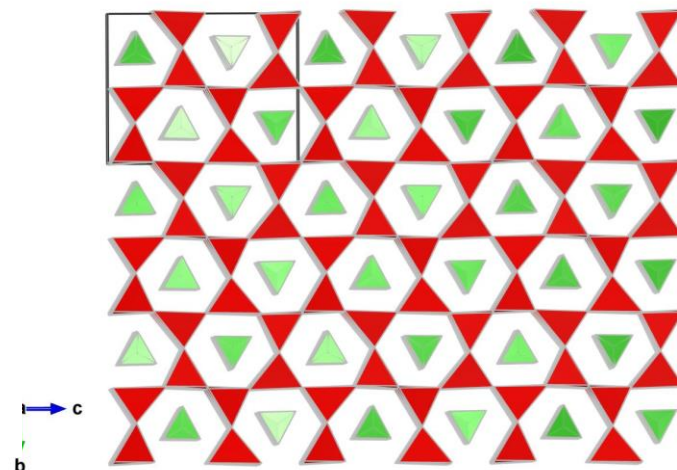
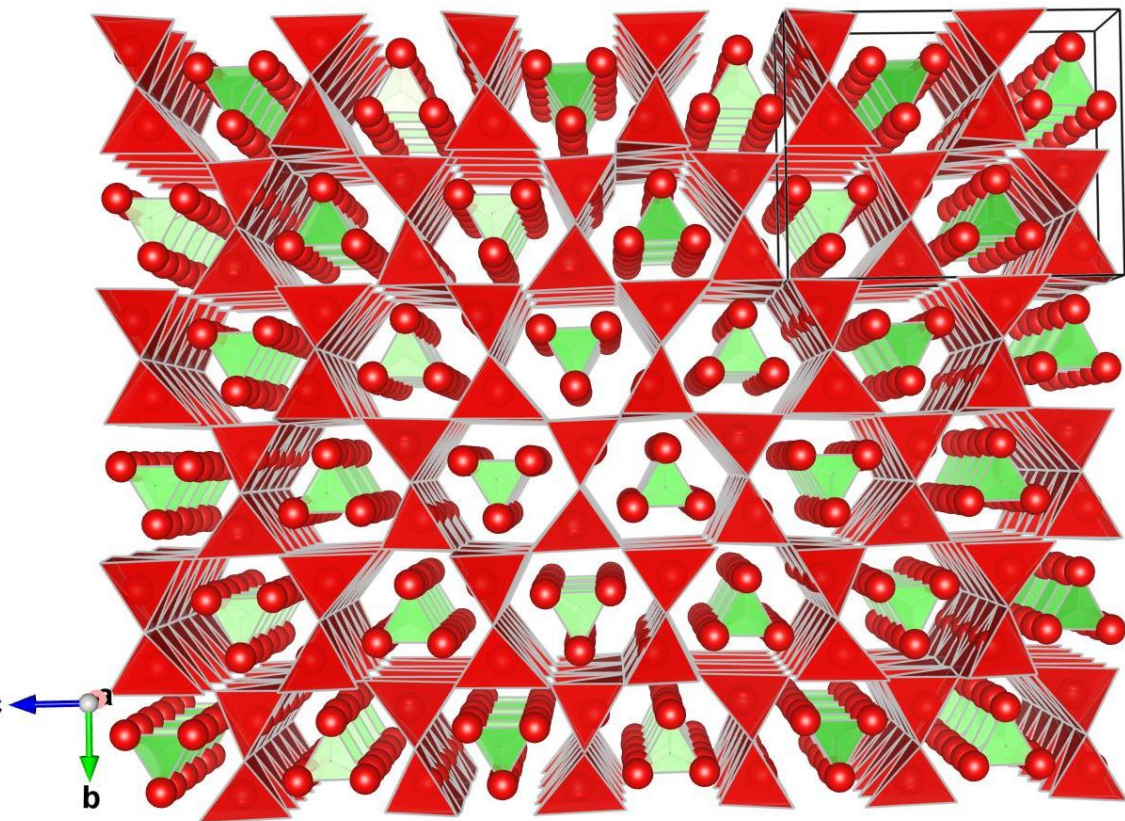
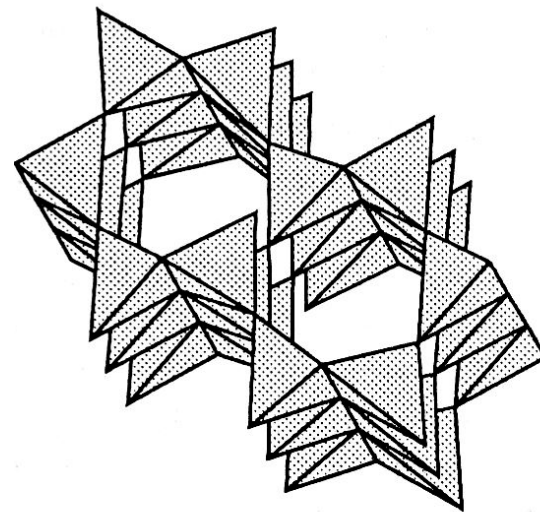


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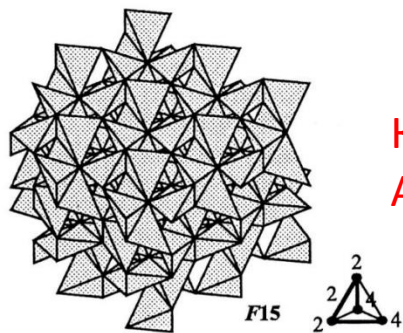
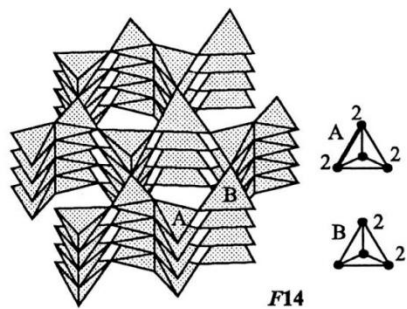


Делафосит CuFeO_2

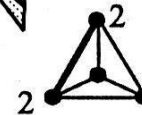
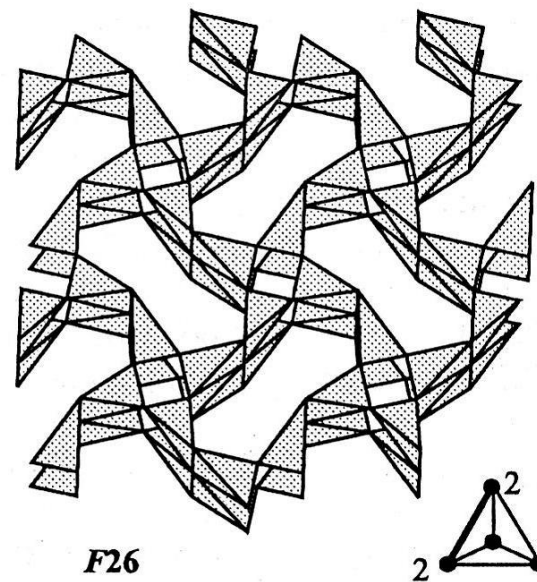
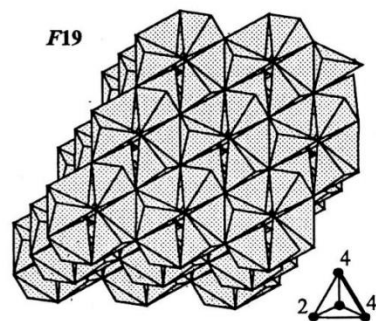
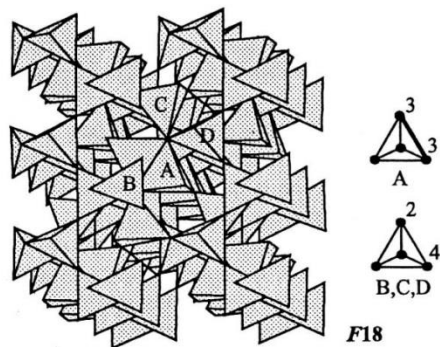
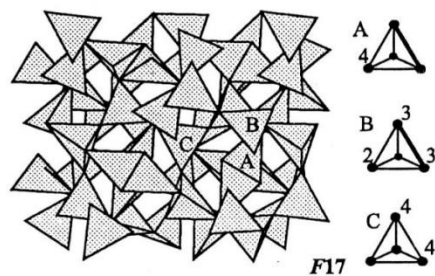
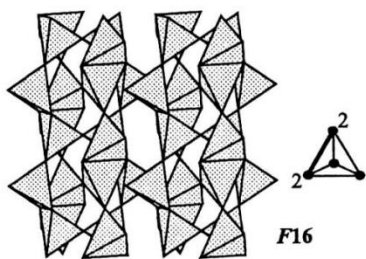
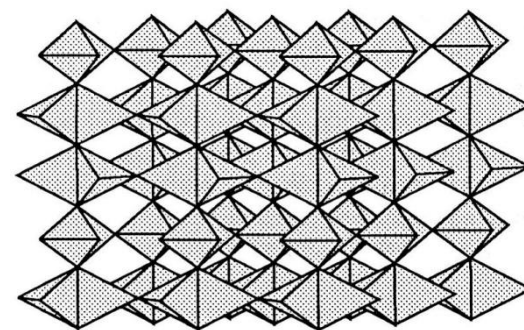
Структура $\text{Cu}_5\text{Sn}(\text{BO}_3)_2\text{O}_4$



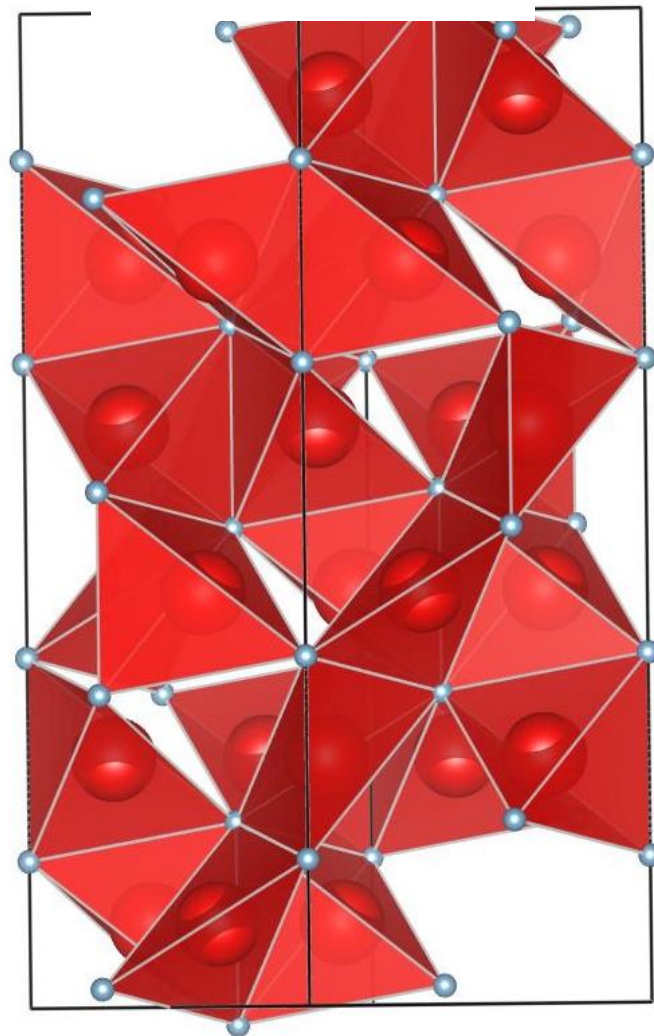
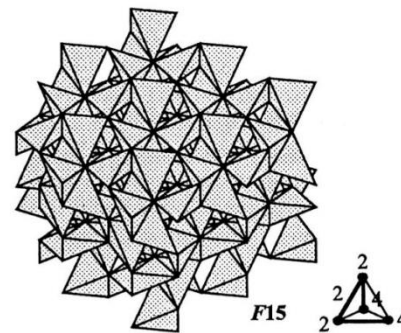
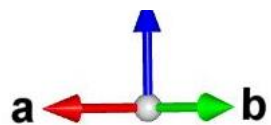
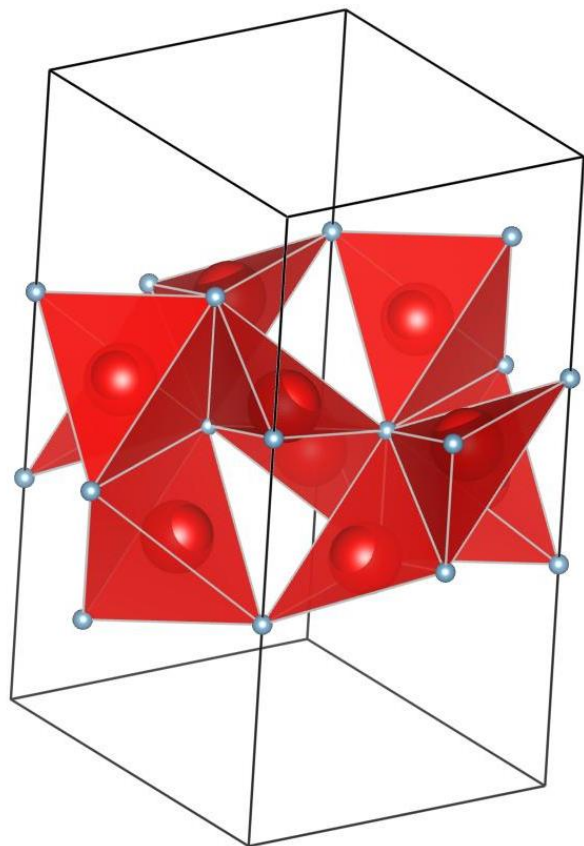
Каркасные анионцентрированные МОТИВЫ



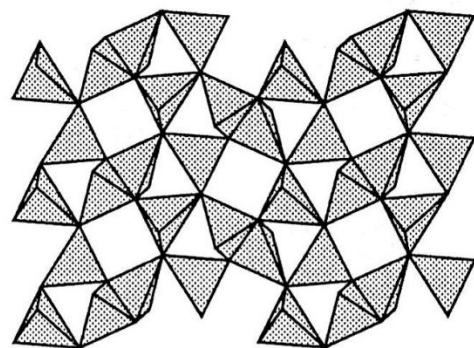
Корунд
 Al_2O_3



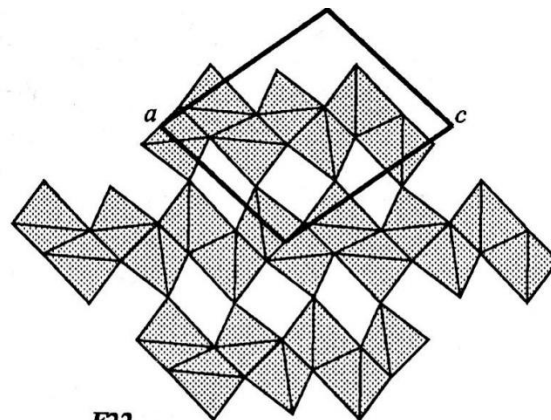
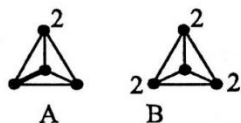
Структура корунда



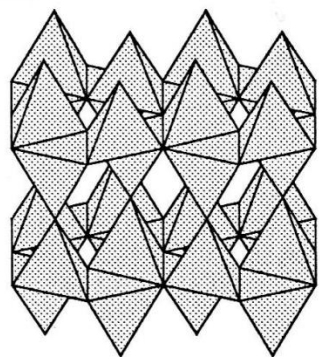
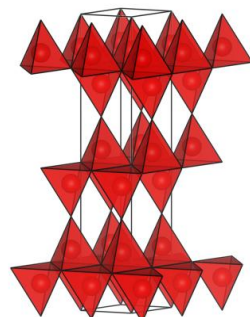
Каркасные анионцентрированные МОТИВЫ



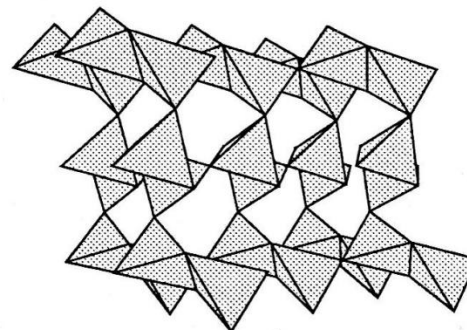
F21



F22



F23



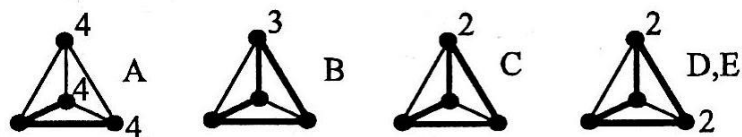
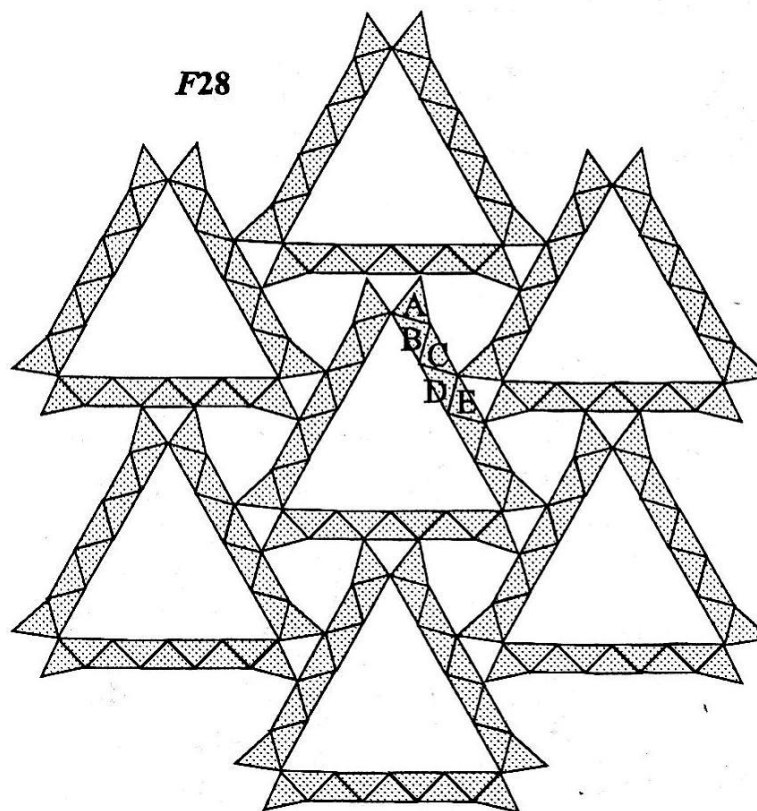
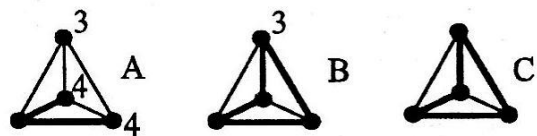
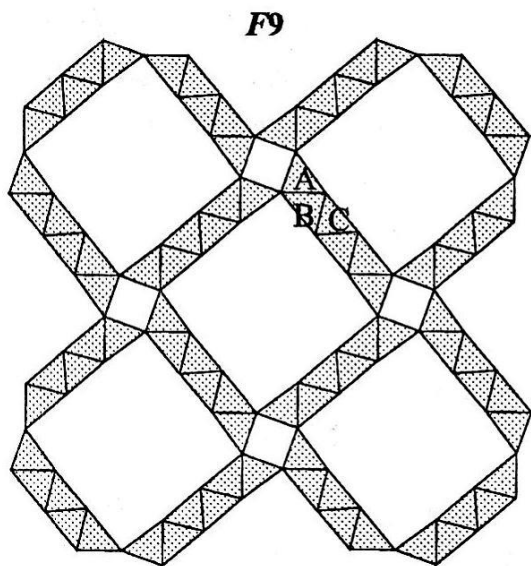
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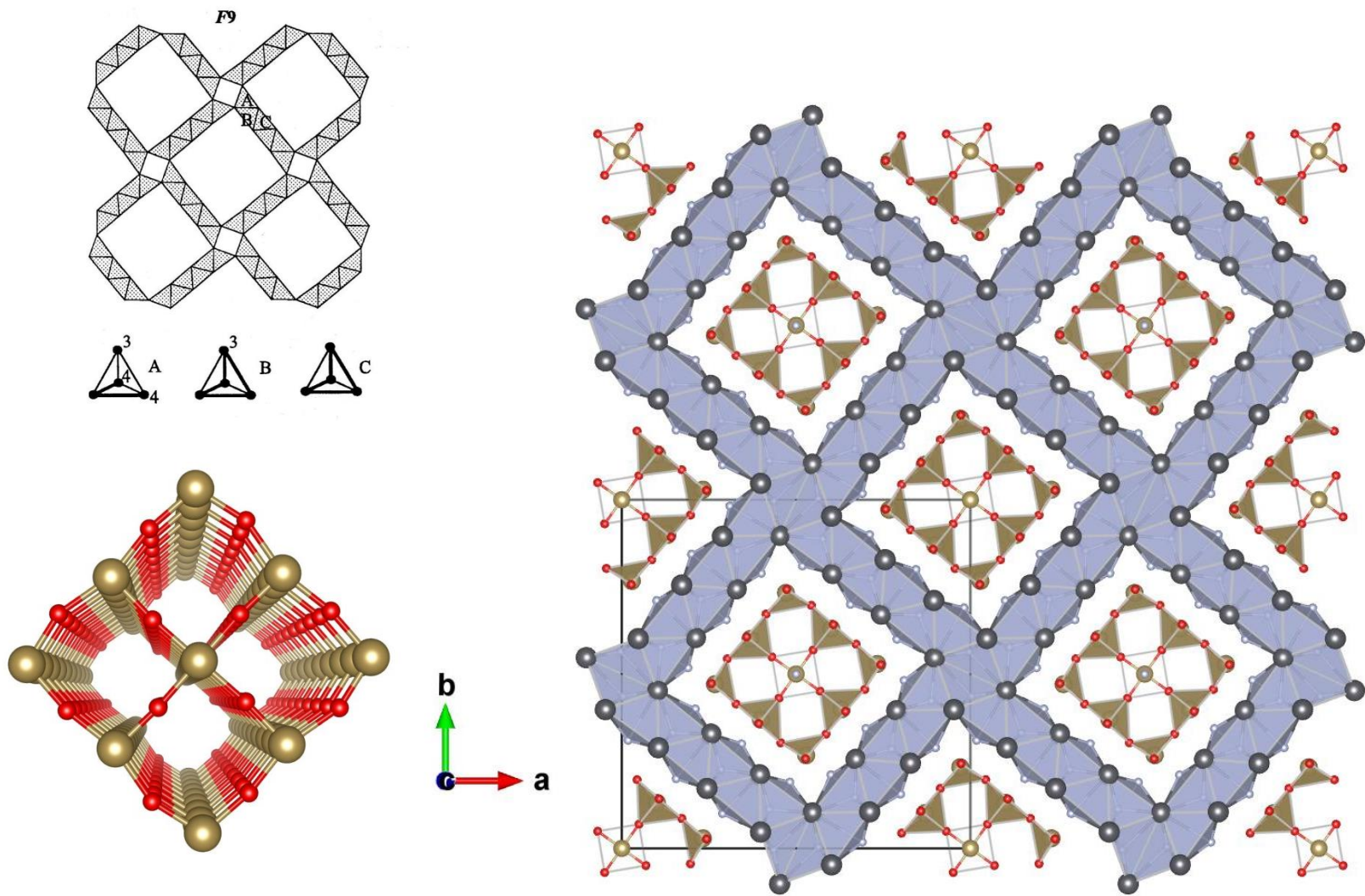
Пинчит $[\text{Hg}_5\text{O}_4]\text{Cl}_2$

[..\Пинчит Hg5 O4 Cl2 024593.vesta](#)

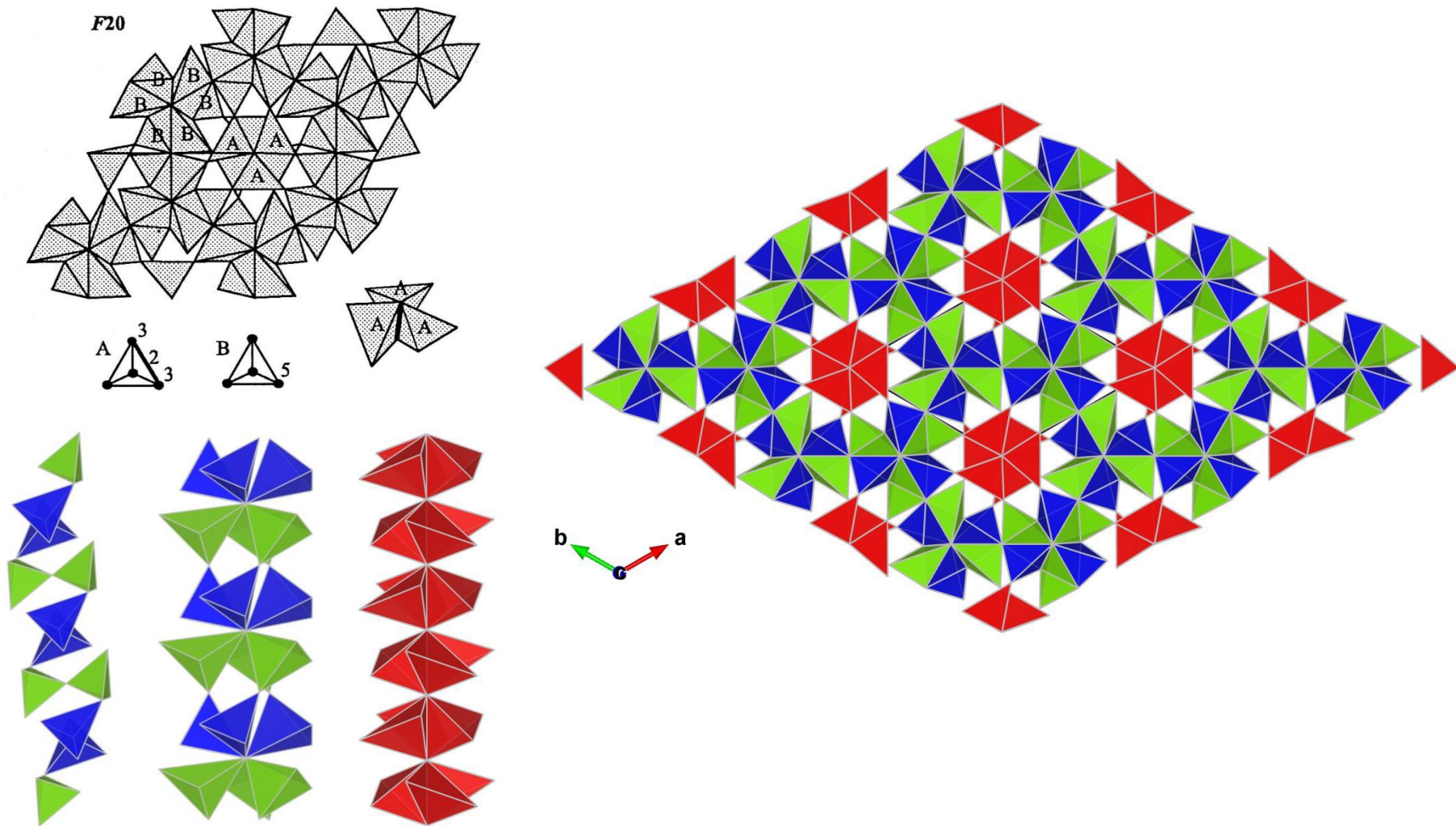
Каркасные анионцентрированные МОТИВЫ



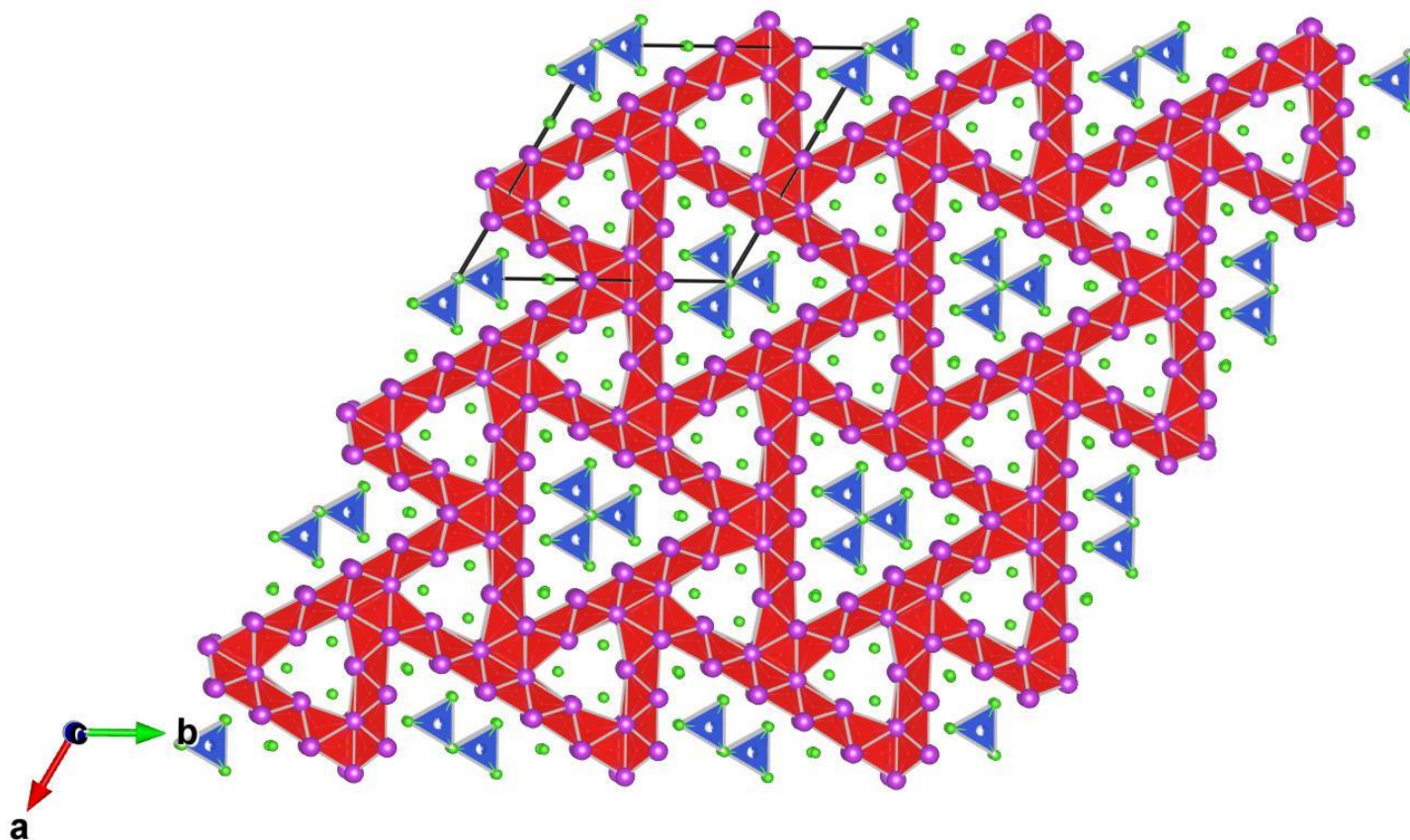
Структура $[\text{Pb}_{12}\text{O}_{12}]\text{F}_4[\text{Ta}_9\text{F}_{13}\text{O}_{20}]$



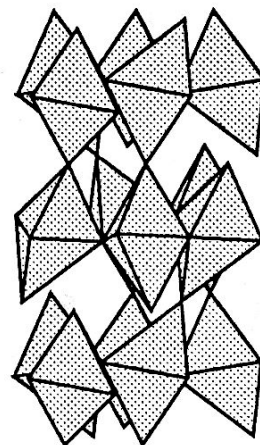
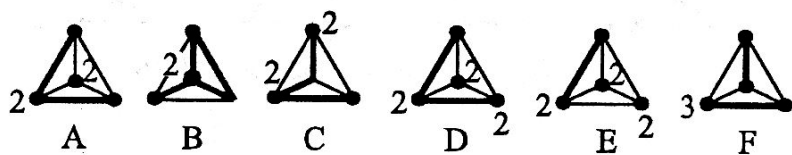
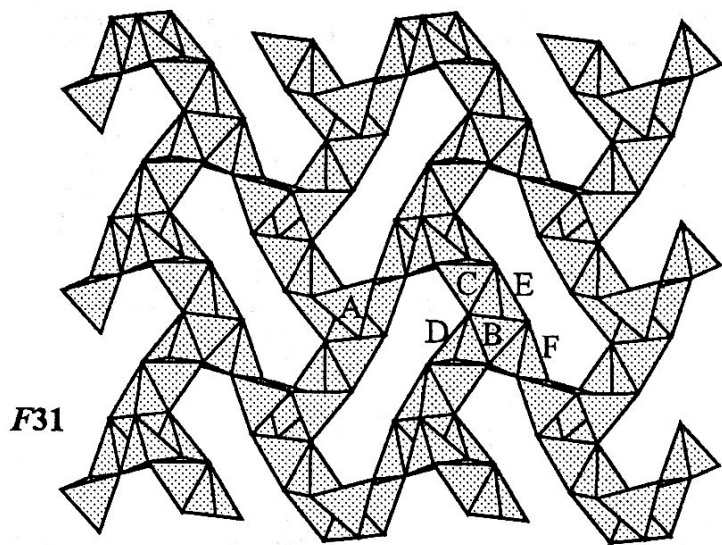
Структура $\text{Ag}_{25}\text{Bi}_3\text{O}_{18}$



Структура $(\text{Cu}_5\text{Cl})[\text{Bi}_8\text{O}_9]_6\text{O}_5\text{Cl}_{30}$



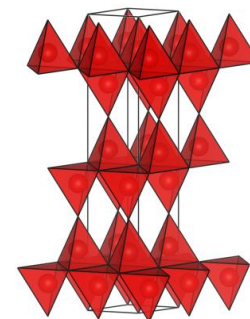
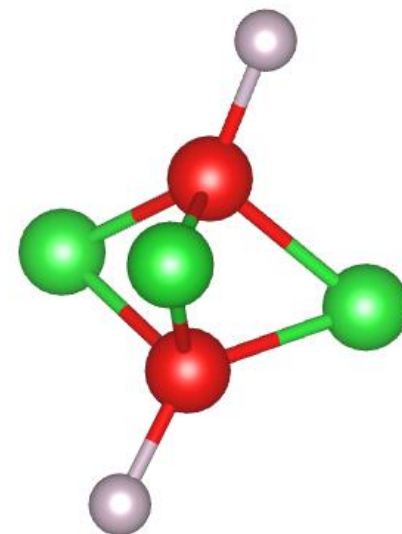
Каркасные анионцентрированные МОТИВЫ



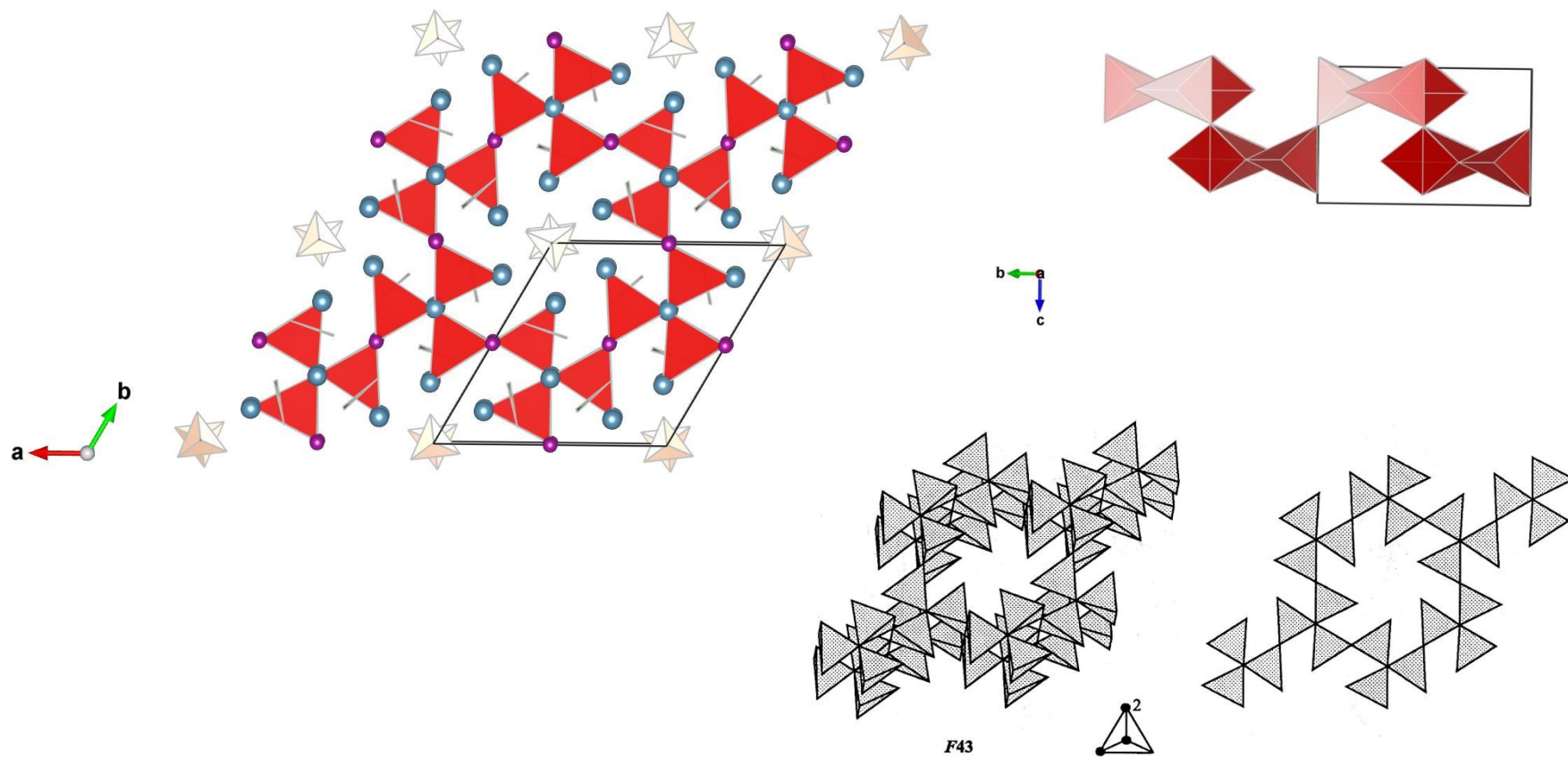
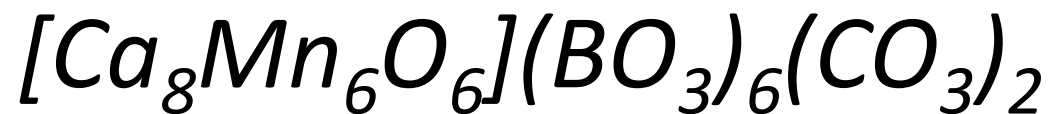
F32



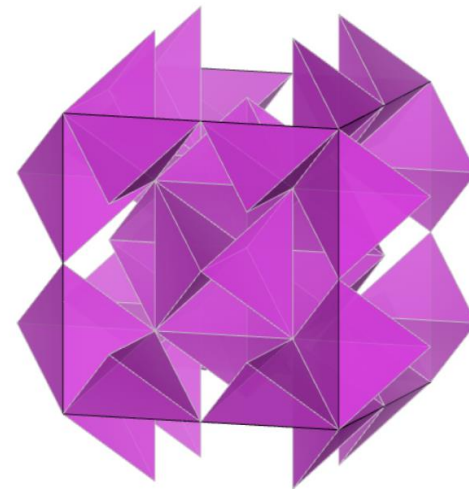
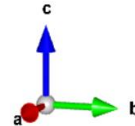
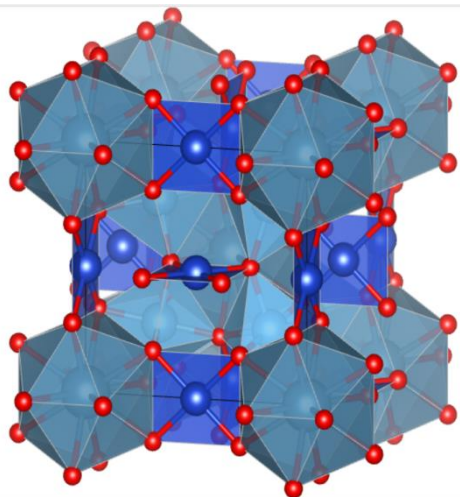
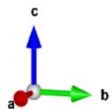
BaHgO₂



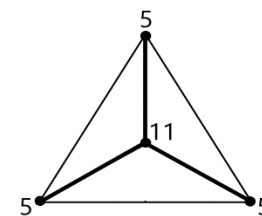
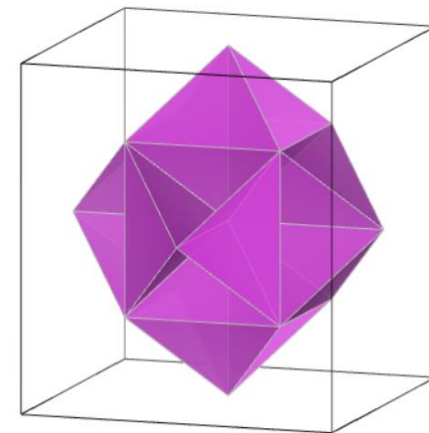
Структура годефруита



CaCu₃(TiO₃)₄



Характеристика	Обозначение	-
Размерность	D	3
Тип объединения тетраэдров в комплексе	ML	1,2
Тип объединения тетраэдра	L	1,2
Формула связности	-	(26:1-26;2-3)
Диаграмма связности	-	
Отношение количества катионов к анионам	X:A	12:15
Число классов топологической эквивалентности	e ^t	1
Число классов конфигурационной эквивалентности	e ^c	1
Соотношение мощности классов конфигурационной эквивалентности	A:B:C	1

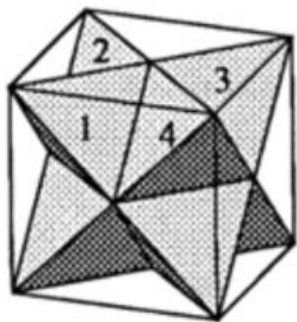


Флюоритоподобные каркасы

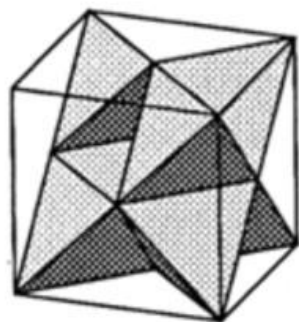
Формула	Тип	Соединение	Литература
$\frac{3}{\infty} [X_2A]$	F10	[CeO ₂], церианит [ThO ₂], торинанит [UO ₂], уранинит	Wolcyrz, Kepinski, 1992 Morss et al., 1989 Wasserstein, 1951
$\frac{3}{\infty} [X_3A_2]$	F11	[(Mn,Fe) ₂ O ₃], биксбиит	Dachs, 1956; Geller, 1971
$\frac{3}{\infty} [XA]$	F12	[A ₆ O ₆](A'O ₆), A = In, Y, Eu, La; A' = W, U	Beaury et al., 1978; Michel, Kahn, 1982; Hinatsu et al., 1988; Fujino et al., 1990
$\frac{3}{\infty} [X_4A_5]$	F35	[CdY ₄ O ₄](MoO ₄) ₃ [Nd ₅ O ₄](MoO ₄) ₃	Bourdet et al., 1982 Hubert et al., 1973
$\frac{3}{\infty} [X_8A_7]$	F36	[Mn ₇ O ₈](SiO ₄), браунит [CaMn ₆ O ₈](SiO ₄), нельтнерит [CuMn ₆ O ₈](SiO ₄), абсвурмбахит [Mn ₇ O ₈](GeO ₄) [HgAg ₆ O ₈](NO ₃)	Ohmann et al., 1998; Palvadeau et al., 1991; Miletich et al., 1998 Damon et al., 1966 Reinecke et al., 1991 Gueho et al., 1993
$\frac{3}{\infty} [X_2A_3]$	F37	[A ₃ O ₂][A'O ₅], A = Y, REE; A' = Nb, Sb, Ta, Ir, Mo	Jansen, Bilow, 1992 Rossell, 1979a, b, c; Groen et al., 1987; Vente, Ijdo, 1991; Klimenko et al., 1992; Vente et al., 1994; Kahn-Harari et al., 1995; Greedan et al., 1997; Khalifah et al., 2000
$\frac{3}{\infty} [XA]$	F38	[A ₁₀ O ₁₀][W ₂ O ₁₁], A = Y, Er	Bevan et al., 1982
$\frac{3}{\infty} [X_{59}A_{52}]$	F39	Tb ₂ ³⁺ Tb ⁴⁺ [Tb ₅₂ ³⁺ O ₅₉](GeO ₄) ₁₂	Илюхин, Джурицкий, 1994
$\frac{3}{\infty} [X_{27}A_{18}]$	F40	[Bi ₈ La ₁₀ O ₂₇]	Michel et al., 1991
$\frac{3}{\infty} [X_{10}A_7]$	F41	[Bi ₁₄ O ₂₀](SO ₄) [Bi ₁₄ O ₂₀](A'O ₄), A' = W, Mo	Francesconi et al., 1998 Ling et al., 1999b
$\frac{3}{\infty} [X_{10}A_{11}]$	F42	[A ₁₁ O ₁₀](GeO ₄)(PO ₄) ₃ , A = Pr, Nd [Pr ₁₁ O ₁₀](V ⁴⁺ O ₄)(V ⁵⁺ O ₄) ₃ [A ₁₁ O ₁₀](GeO ₄)(VO ₄) ₃ , A = La-Eu	Палкина и др., 1997; Целебровская и др., 1994 Müller-Buschbaum, Werner, 1994 Джурицкий и др., 1997

Флюоритоподобные каркасы

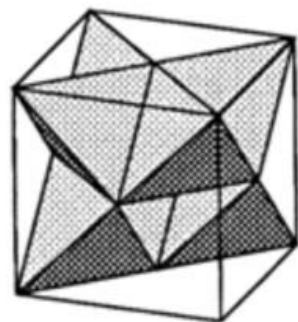
Канг и Эйринг предложили элегантный метод описания оксидов лантаноидов с переменной валентностью, основанный на использовании флюоритоподобных модулей с разным количеством вакансий.



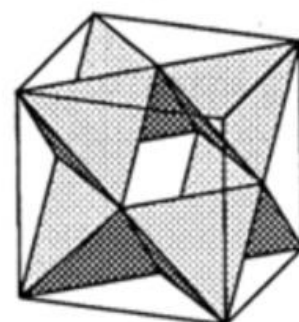
F



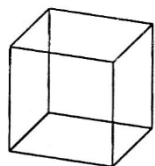
U^1



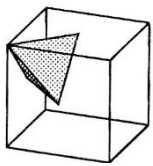
D_4



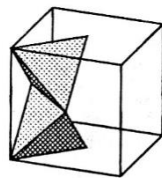
W_2^4



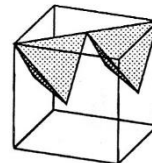
O



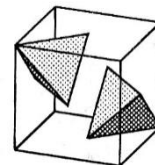
$3_W^{2,3,4}$
4



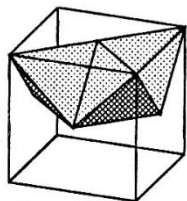
$3_W^{2,3,4}$
 $3_{2,3,4}$



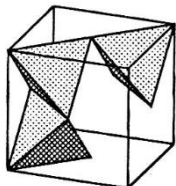
$2_W^{2,4}$
4



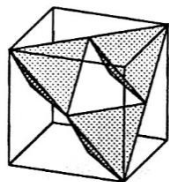
$3_W^{2,3,4}$
 $3_{2,3,4}$



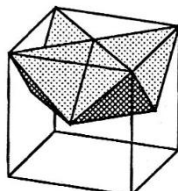
1_W^3
4



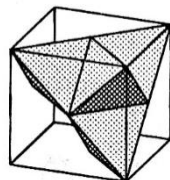
$2_W^{2,3,4}$
3



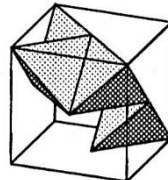
$2_W^{2,4}$
 $3_{1,2,3}$



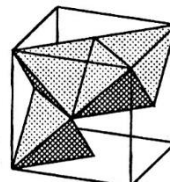
0_W
4



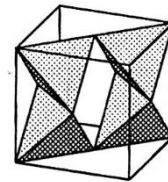
1_W^2
 $3_{1,2,3}$



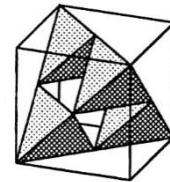
1_W^3
 $3_{1,2,4}$



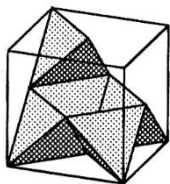
1_W^2
 $3_{2,3,4}$



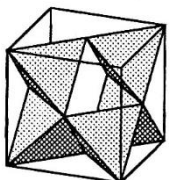
$2_W^{2,4}$
 $2_{2,4}$



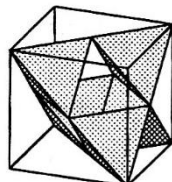
$2_W^{1,3}$
 $2_{2,4}$



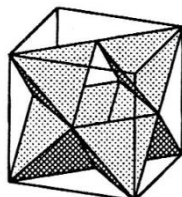
$3_W^{1,3,4}$
0



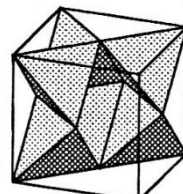
$2_W^{2,4}$
1 2



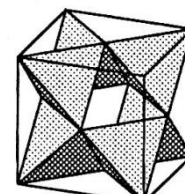
$2_W^{2,4}$
1 1



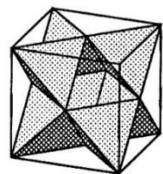
$2_W^{2,4}$
0



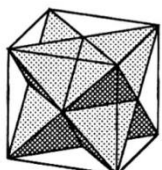
1_W^4
1 4



1_W^4
1 2














U^4














F

Типы флюоритоподобных модулей

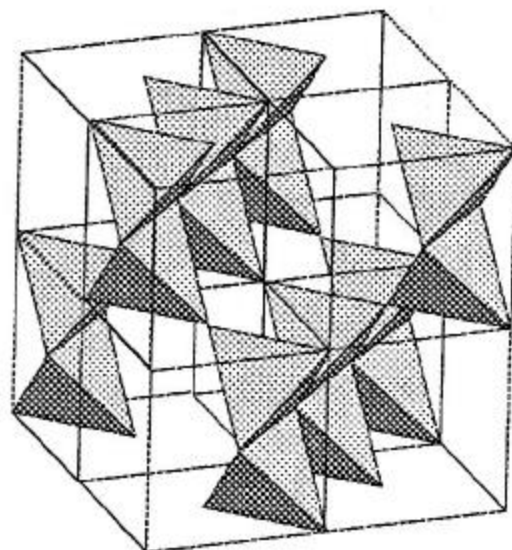
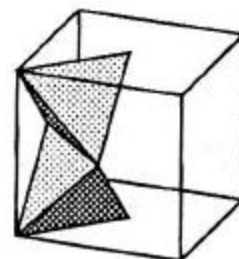
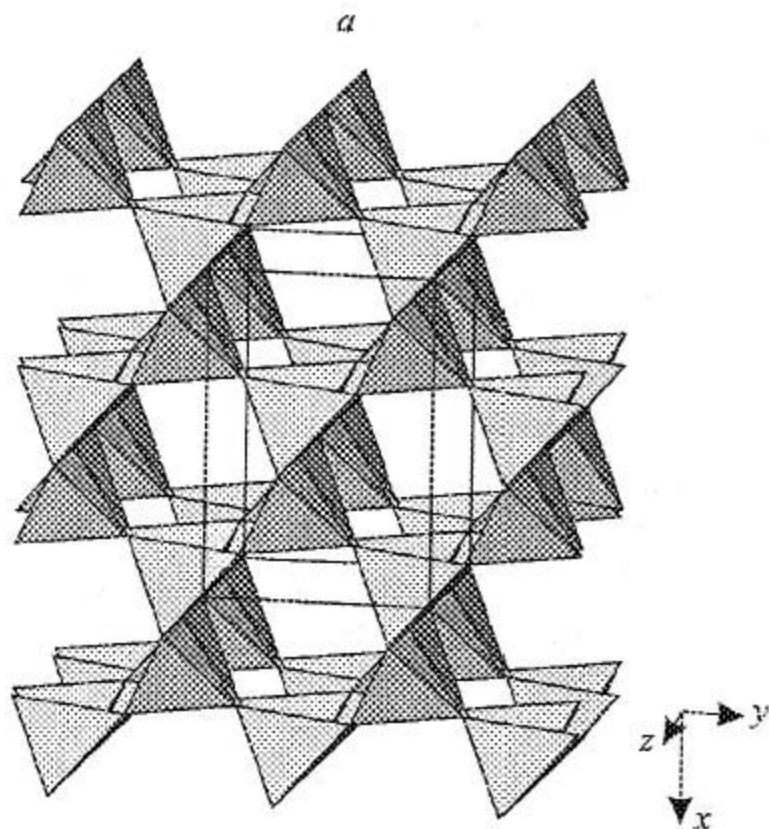
Характеристики некоторых типов модулей

№	Число вакансий	Симметрия	Формула	Тип	Вид
1	8	$m\bar{3}$	O	a	
2	7	3m	$\begin{matrix} 3 \\ 4 \end{matrix} W_{2,3,4}$	b	
3	6	mm2	$\begin{matrix} 2 \\ 4 \end{matrix} W_{2,4}$	c	
4	6	mm2	$\begin{matrix} 3 \\ 3 \end{matrix} W_{2,3,4}$	d	
5	6	3m	$\begin{matrix} 3 \\ 3 \end{matrix} W_{2,3,4} \\ 1,2,4$	e	
6	5	m	$\begin{matrix} 1 \\ 4 \end{matrix} W^3$	f	
7	5	m	$\begin{matrix} 2 \\ 3 \end{matrix} W_{2,4} \\ 2,3,4$	g	
8	5	3m	$\begin{matrix} 2 \\ 3 \end{matrix} W_{2,4} \\ 1,2,3$	h	
9	4	4mm	$\begin{matrix} 0 \\ 4 \end{matrix} W$	i	
10	4	3m	$\begin{matrix} 1 \\ 3 \end{matrix} W^2 \\ 1,2,3$	j	
11	4	m	$\begin{matrix} 1 \\ 3 \end{matrix} W^3 \\ 1,2,4$	k	

22 типа неэквивалентных модулей

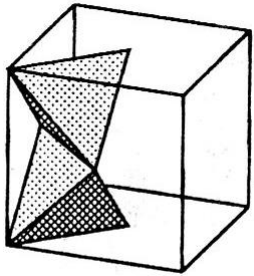
Число вакан сий	Симметрия	Формула	Тип	Вид
4	1	${}^1_3W^{2,3,4}$	l	
4	mmm	${}^2_2W^{2,4}$	m	
4	$\bar{4}3m$	${}^2_2W^{1,3,2,4}$	n	
3	1	${}^3_0W^{1,3,4}$	o	
3	m	${}^2_1W^{2,4}$	p	
3	1	${}^2_1W^{2,4}$	q	
2	mm2	${}^2_0W^{2,4}$	r	
2	mm2	${}^1_1W^4$	s	
2	3m	${}^1_1W^4$	t	
1	3m	U^4	u	
0	$m\bar{3}m$	F	v	

Флюоритоподобный каркас, построенный на
 супермодуле ${}^3_{3}W^{2,3,4}_{2,3,4}$ в структурах
 соединений $[A_2O_7] BO_5$, $A=Y, Sc, REE$, $B=Nb, Sb, Ta, Ir, Mo$

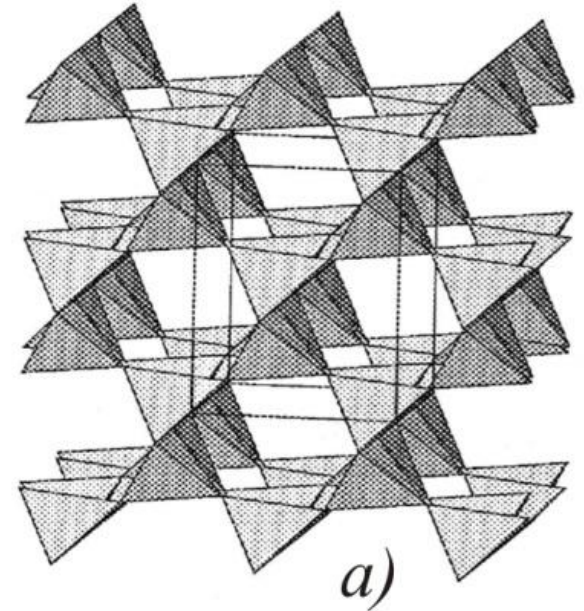


Представление структуры $[\text{Nd}_5\text{O}_4](\text{MoO}_4)_3$ в формульном и модульном виде

Слой 1

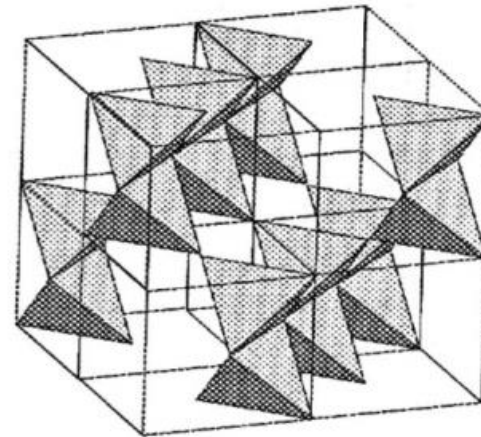


$3^W_{3^W} 1,2,3$ $3^W 1,2,3$	$2^W_{3^W} 1,3,4$ $3^W 1,3,4$
$2^W_{3^W} 1,3,4$ $3^W 1,3,4$	$3^W_{3^W} 1,2,3$ $3^W 1,2,3$



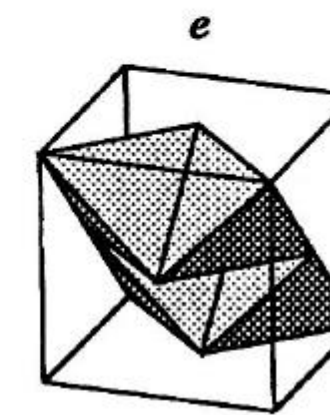
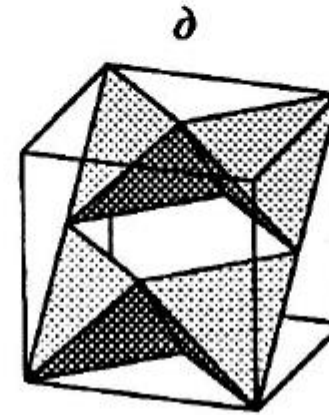
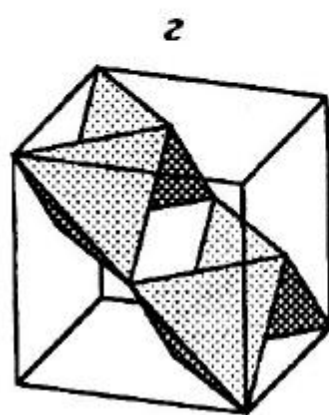
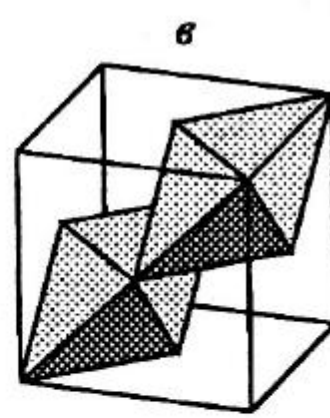
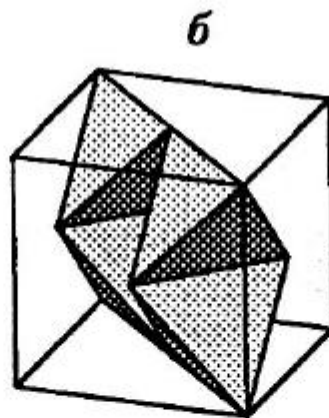
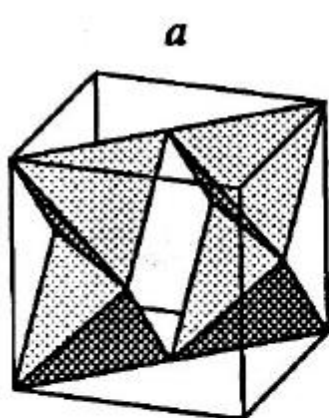
$2^W_{3^W} 1,3,4$ $3^W 1,3,4$	$3^W_{3^W} 1,2,3$ $3^W 1,2,3$
$3^W_{3^W} 1,2,3$ $3^W 1,2,3$	$2^W_{3^W} 1,3,4$ $3^W 1,3,4$

Слой 2



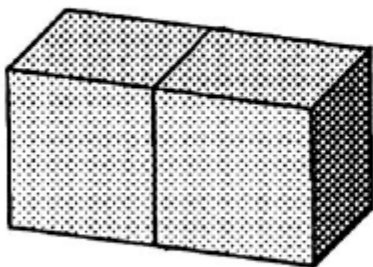
b)

Неэквивалентные положения комплекса t

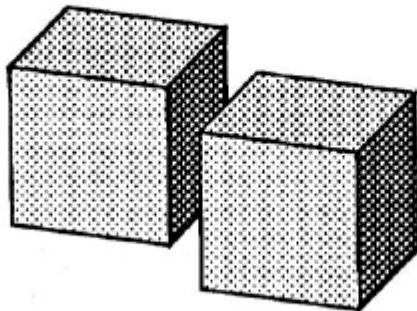


Способы сочленения флюоритоподобных модулей

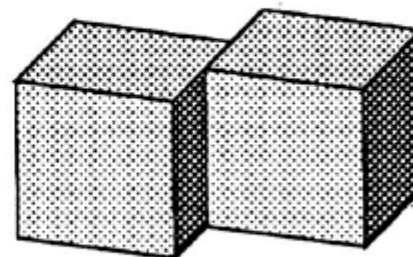
a



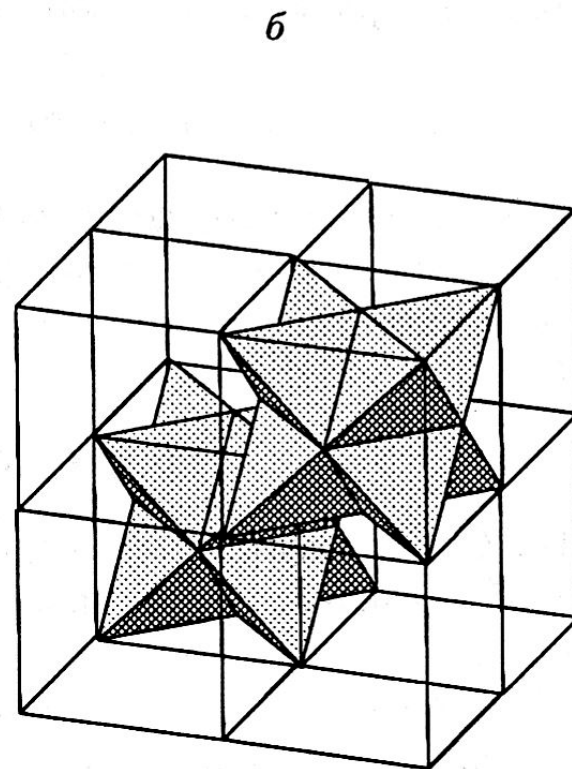
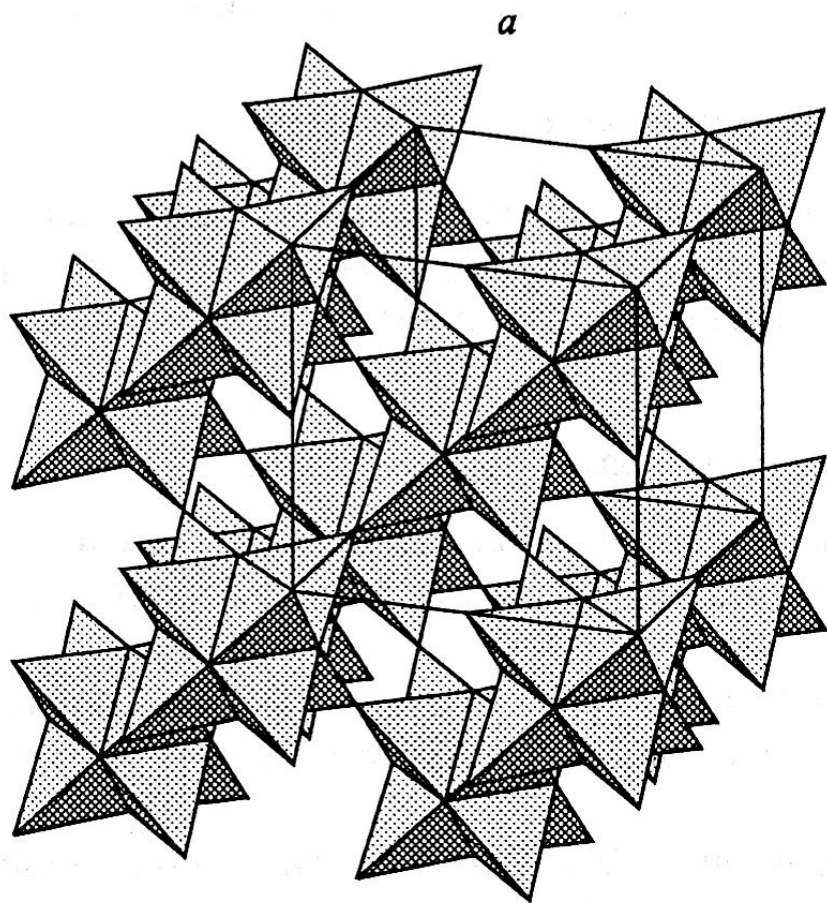
б



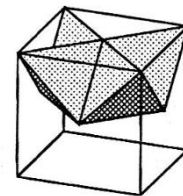
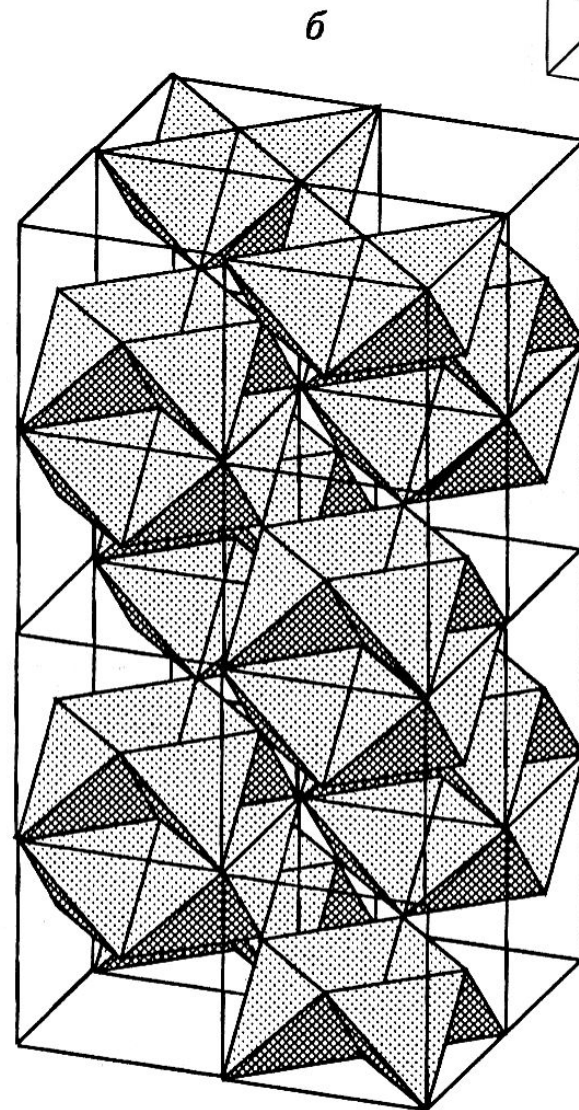
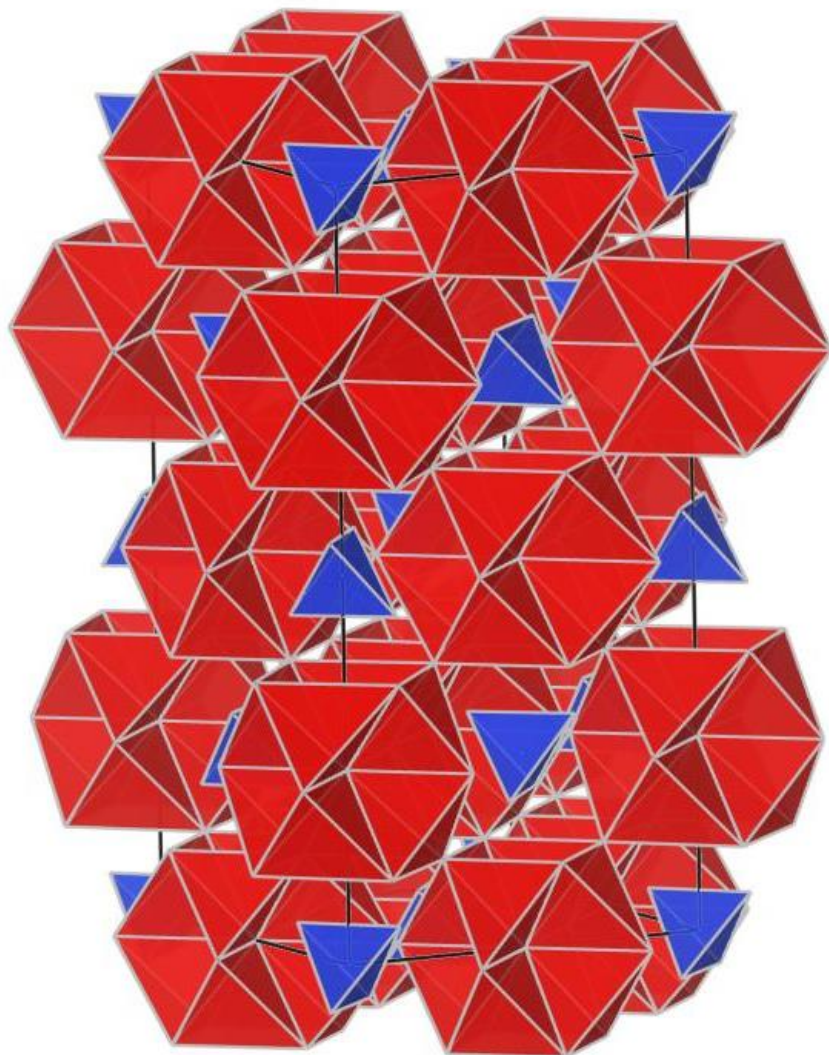
в

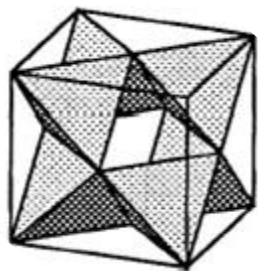


Флюоритоподобный каркас,
построенный на основе модуля F в
структуре $[\text{CdY}_4\text{O}_4](\text{MoO}_4)$

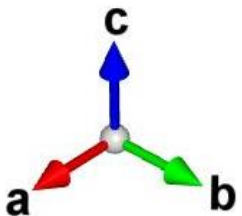
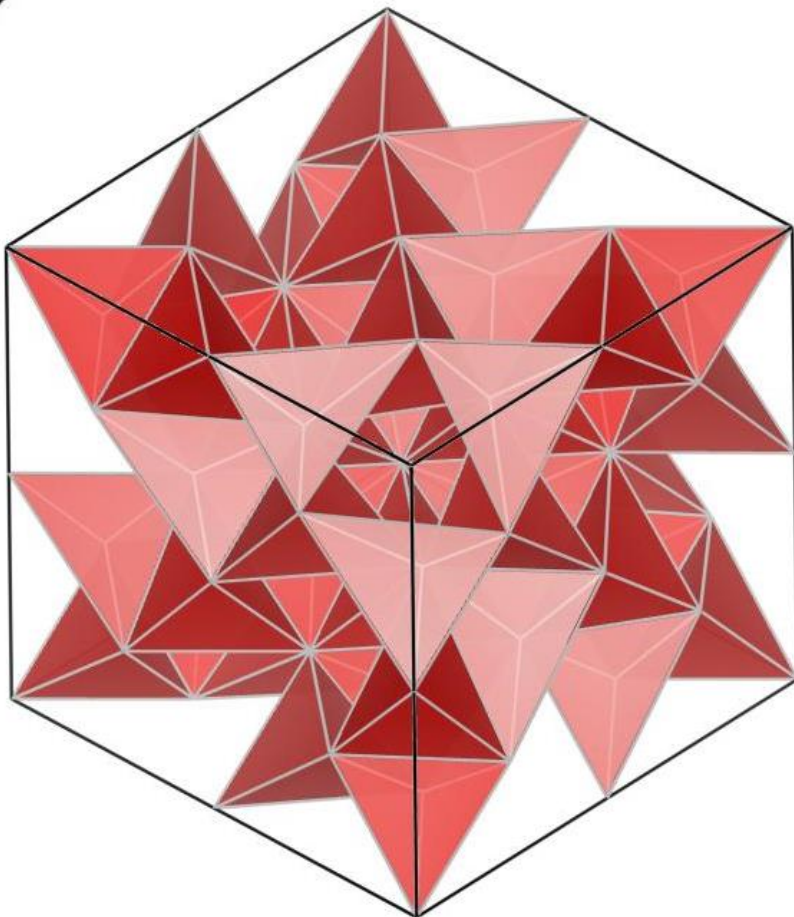


Флюоритоподобный каркас браунита $Mn_7O_8(SiO_4)$ и его супермодуль

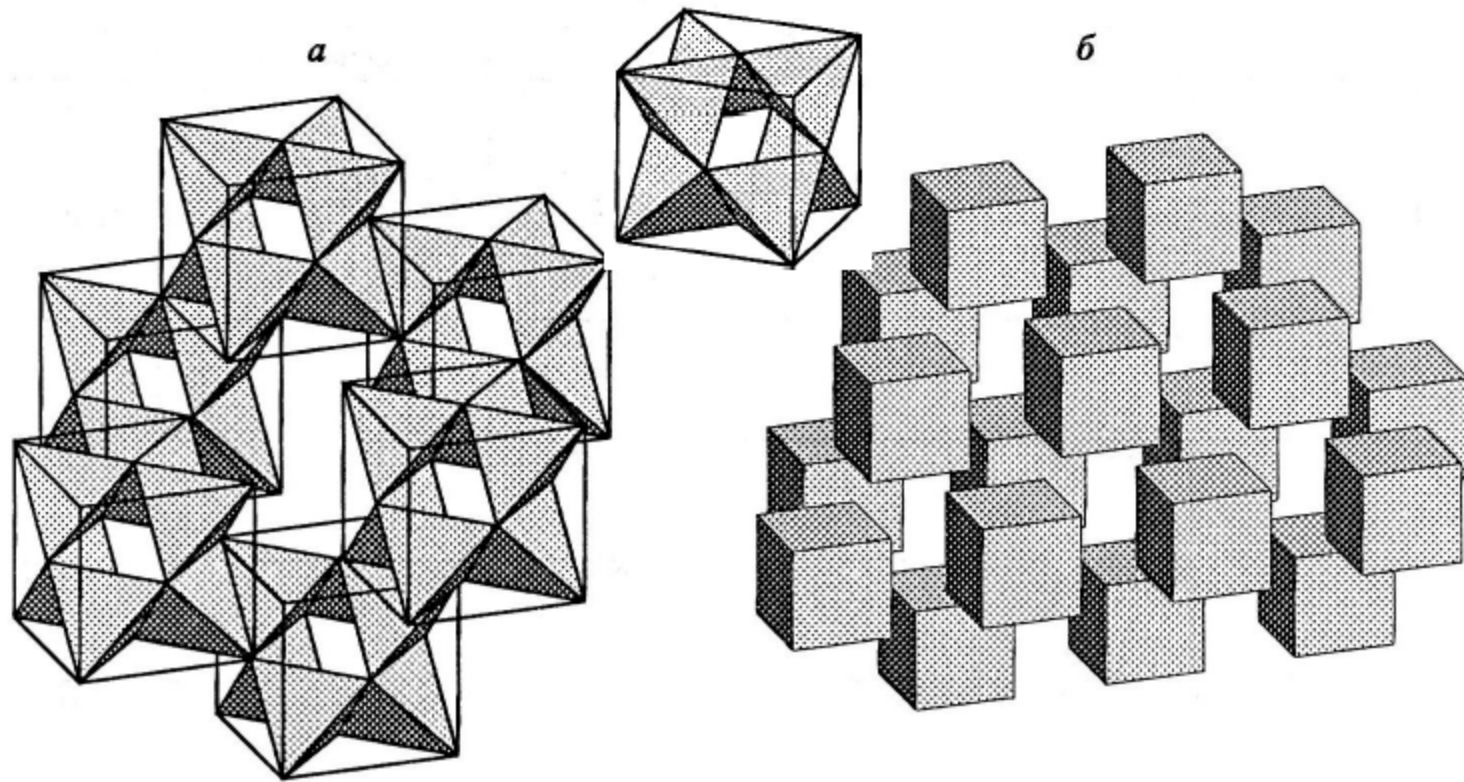




Биксбиит Mn_2O_3

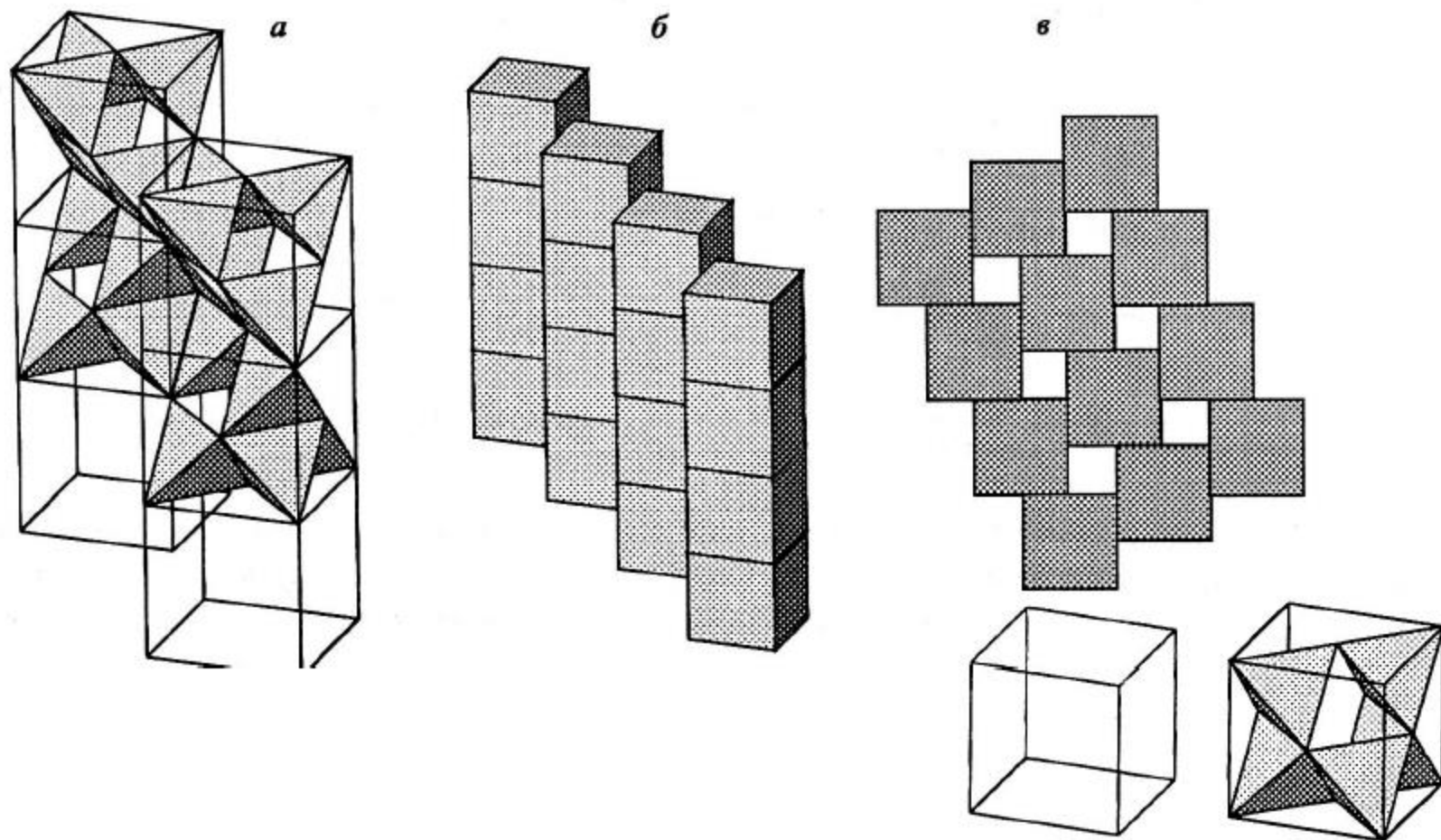


Каркасы с флюоритоподобными модулями, объединенными через четверть грани



*Структура $[Ti_6O_6](TeO_6)$, : каркас биксбитовых модулей,
объединенных по четверти грани.*

Каркас из пустых и трех-вакансионных модулей,
сочлененных по четверти грани в соединении
 $[A_{11}O_{10}](GeO_4)(PO_4)_3$, $A=Pr, Nd$



Домашняя работа

Вариант1	2	3
Клейнит $[\text{Hg}_2\text{N}](\text{Cl}, \text{H}_2\text{O}, \text{SO}_4)$	Меланоталлит $[\text{Cu}_2\text{O}]\text{Cl}_2$	Мозезит $[\text{HgN}_2] (\text{SO}_4) \text{H}_2\text{O}$
Терлингуаит $\text{Hg}_4\text{O}_2\text{Cl}_2$	Делафосит CuFeO_2	Тенорит CuO
$[\text{Pr}_3\text{O}_2](\text{NbO}_5)$, 1992, 1995 гг	Абсурмбахит $[\text{CuMn}_6\text{O}_8](\text{SiO}_4)$	$\text{Bi}_8\text{La}_{10}\text{O}_{27}$, 1991г
Грандидьерит $[\text{MgAl}_3\text{O}_2](\text{SiO}_4)(\text{BO}_3)$	Креднерит CuMnO_2	нелътнерит $[\text{CaMn}_6\text{O}_8](\text{SiO}_4)$