

構造化学

晶系とBravais格子

第9回 6月11日

河野淳也

前回の復習

対称要素と点群について述べました。

○対称要素

p 回回転軸、 p 回反軸、対称心、鏡面

○特定の対称要素の組み合わせが群をなす

○結晶に表れる点群は32種類

本日の目標

Bravais格子について理解しよう

内容

- 平面格子
- 空間格子
- 7つの晶系
- Bravais格子

対称性

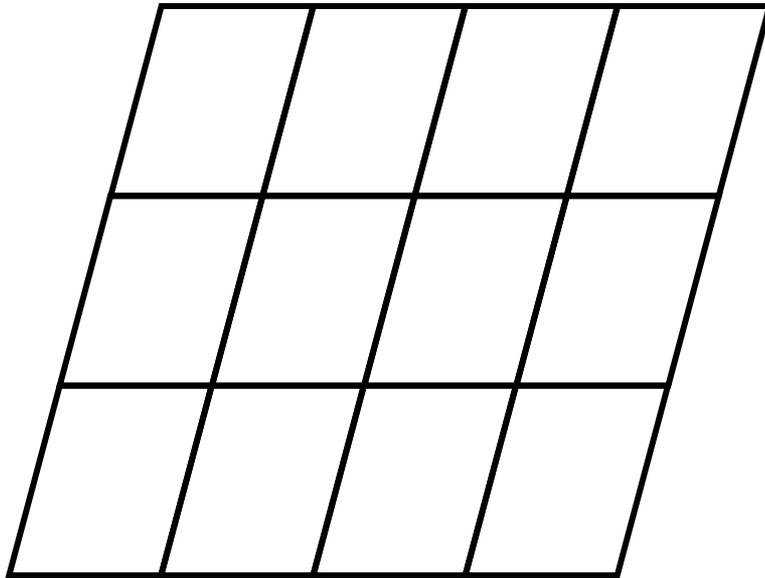
点の回りの対称(1次元): 32種類の点群

平面格子の単位胞の対称(2次元): 5種類

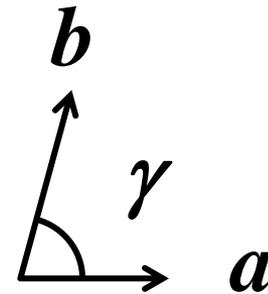
空間格子の単位胞の対称(3次元): 7種類(7晶系)

7晶系 + 複合格子 = 格子

平面格子

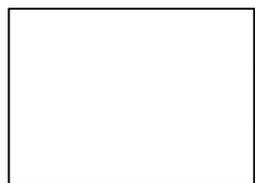


パラメータ



2回軸以上の対称性をもつ
平面格子を考える

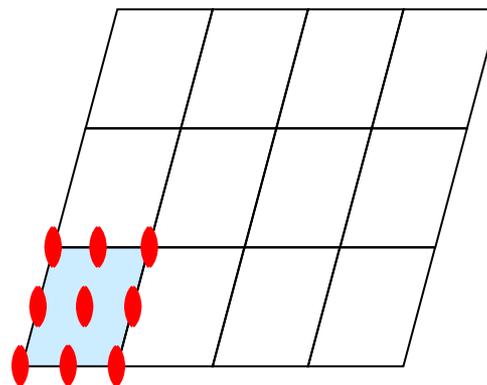
平面格子(1)



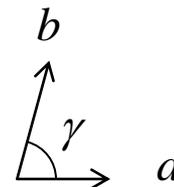
格子(oblique net)

$$a \neq b$$

γ 任意



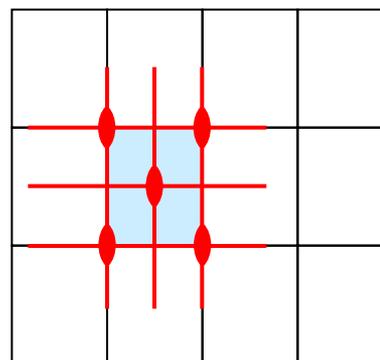
2



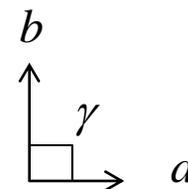
格子(rectangular net)

$$a \neq b$$

$$\gamma = 90^\circ$$



m



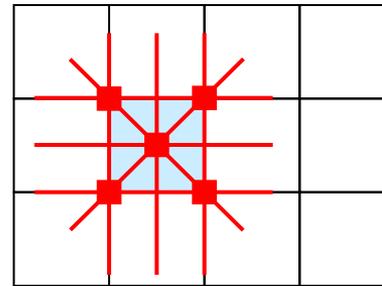
平面格子(2)



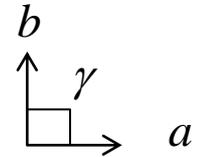
格子(square net)

$$a = b$$

$$\gamma = 90^\circ$$



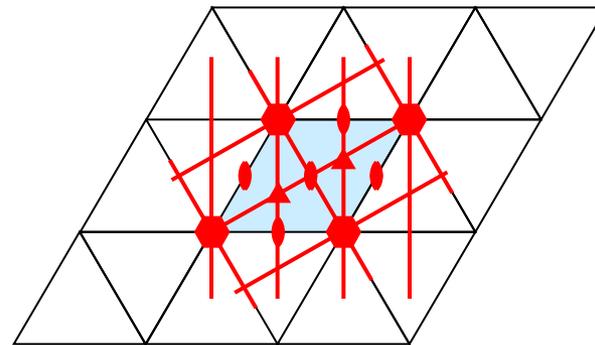
4



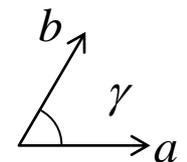
格子(hexagonal net)

$$a = b$$

$$\gamma = 60^\circ, 120^\circ$$



6



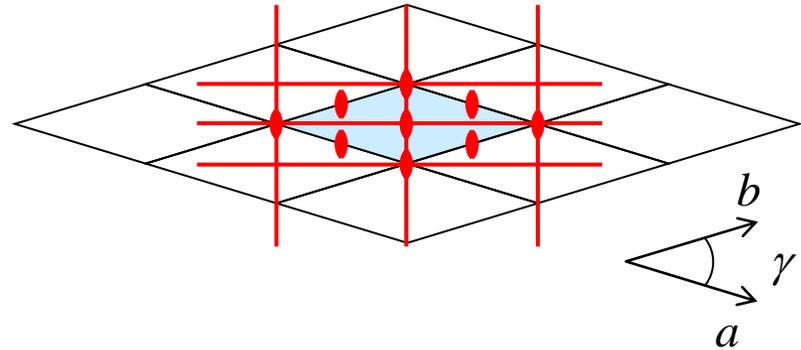
平面格子(3)



格子(rhombic net)

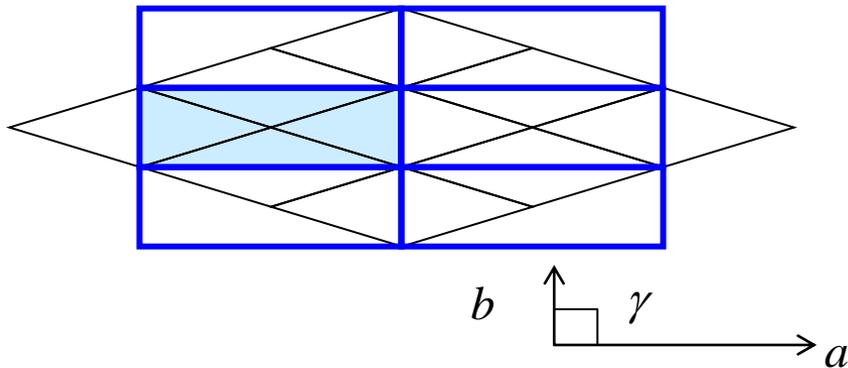
$$a = b$$

γ 任意



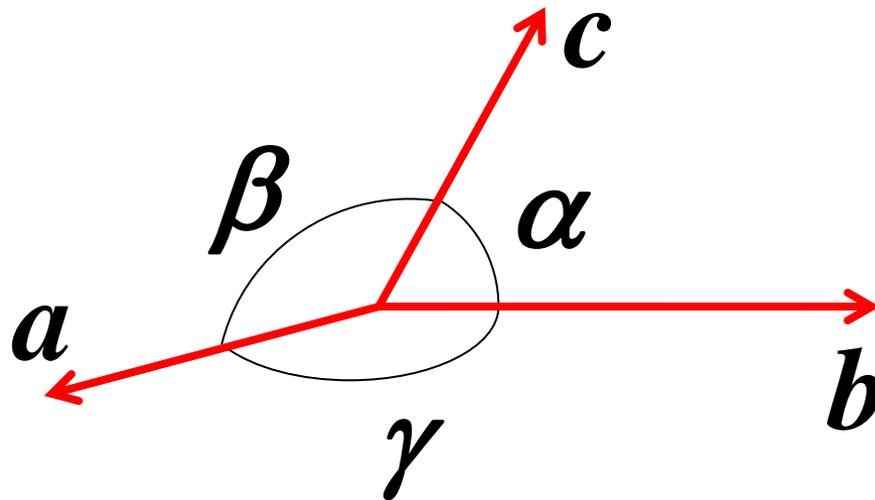
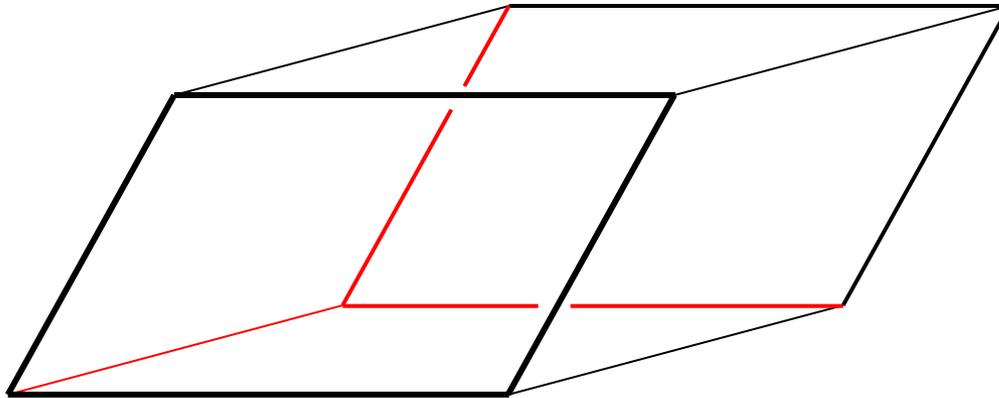
2

面心長方格子ともいえる



基本単位格子ではないが、
対称性をよく表している。
→Bravais格子の考え方

空間格子のパラメータ



7晶系

晶系	必須の対称要素	単位胞の形状
三斜	なし	$a \neq b \neq c, \alpha \neq \beta \neq \gamma$ ($c < a < b$)
単斜	1本の2回軸	$a \neq b \neq c, \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$ ($c < a$)
斜方	3本の2回軸	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$ ($c < a < b$)
正方	1本の4回軸	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$
三方 六方 菱面	1本の3回軸	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$ $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$
六方	1本の6回軸	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$
立方	4本の3回軸	$a = b = c, \alpha = \beta = \gamma = 90^\circ$

7つの晶系



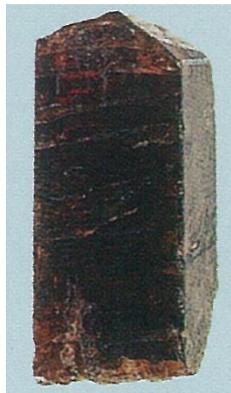
三斜



単斜



斜方



正方



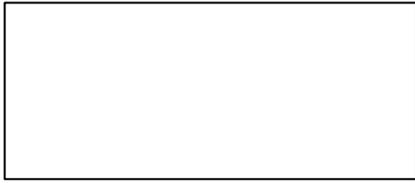
三方



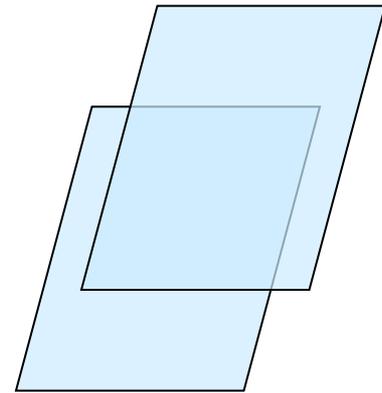
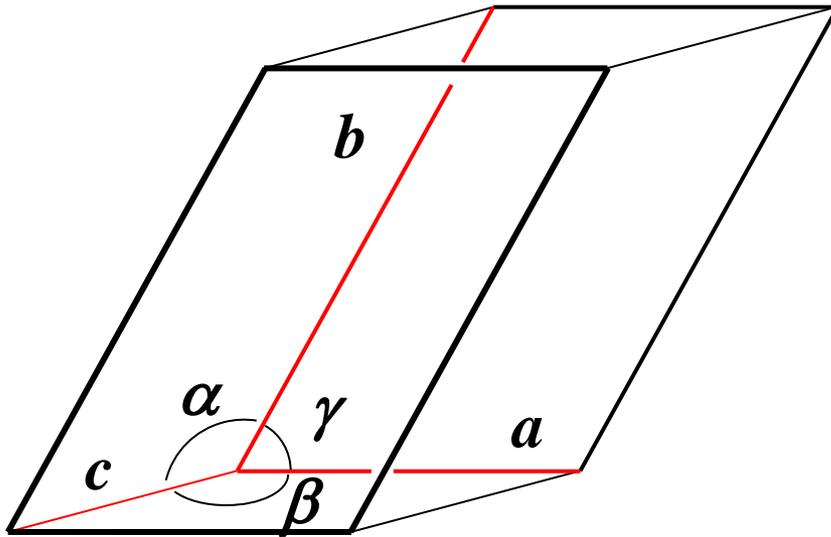
六方



立方



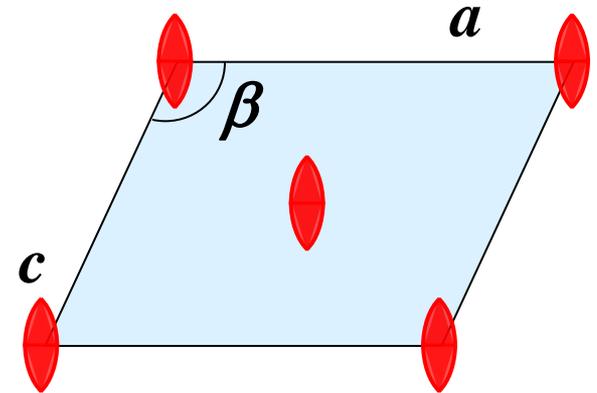
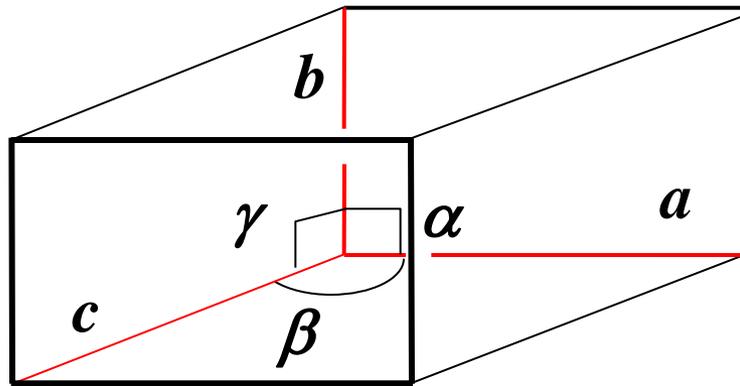
晶系 Triclinic



$$a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma$$
$$(c < a < b)$$

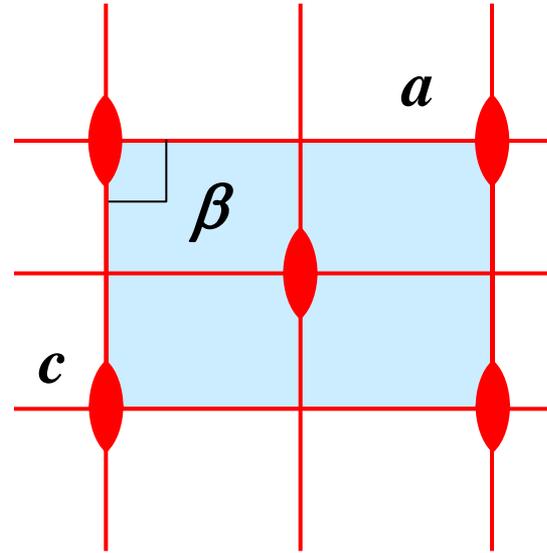
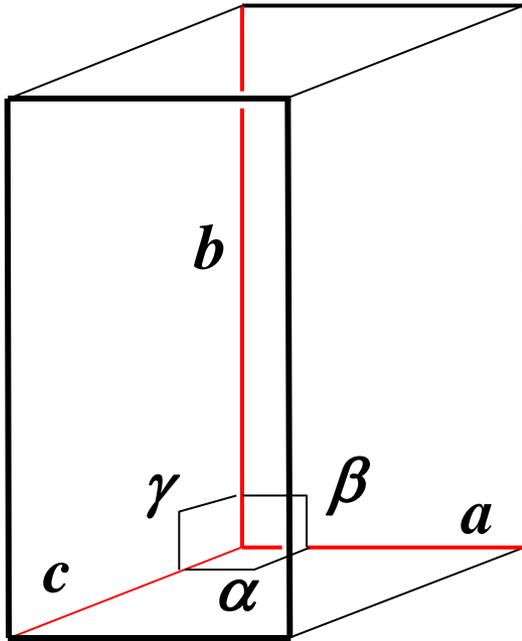


晶系 Monoclinic



$$a \neq b \neq c, \quad \alpha = \gamma = 90^\circ, \quad \beta \neq 90^\circ$$
$$(c < a)$$

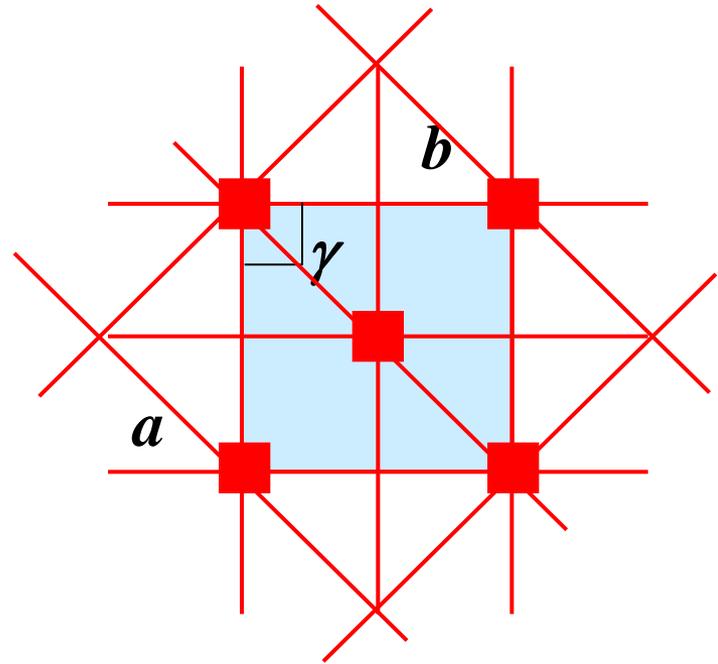
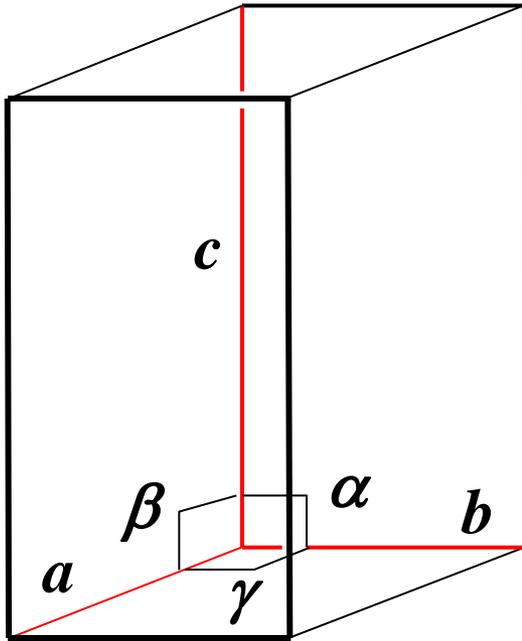
晶系 Orthorhombic



$$a \neq b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$$

$$(c < a < b)$$

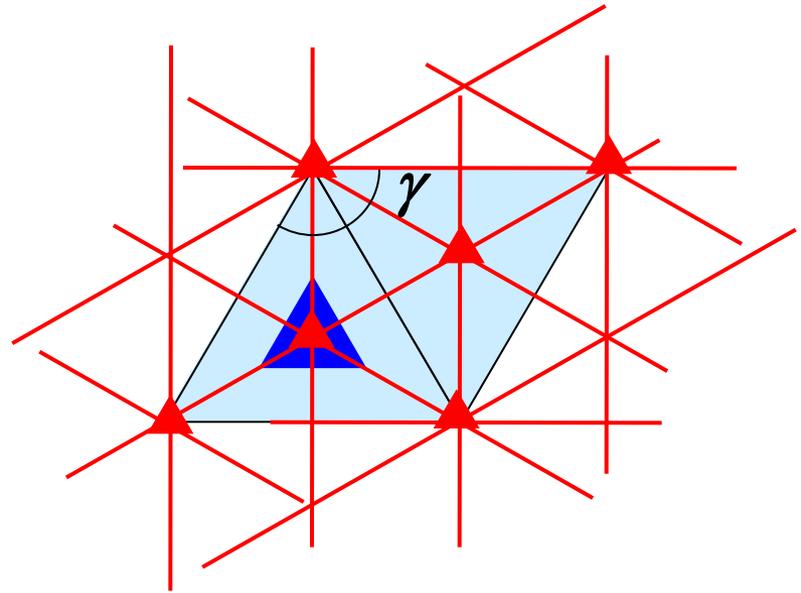
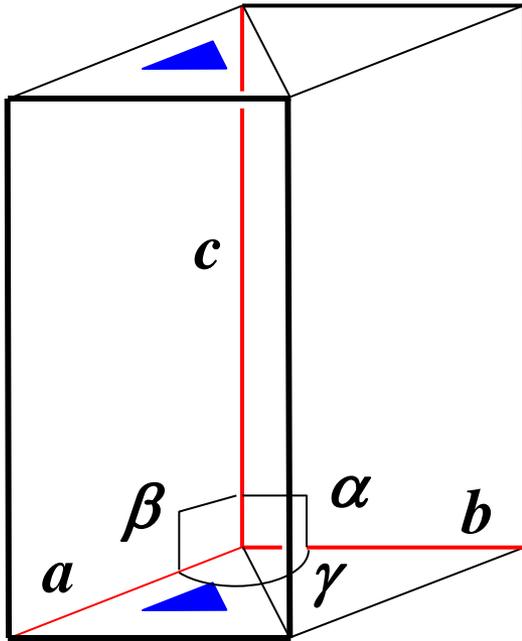
晶系 Tetragonal



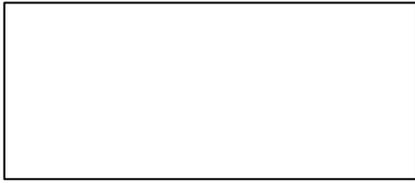
$$a = b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$$



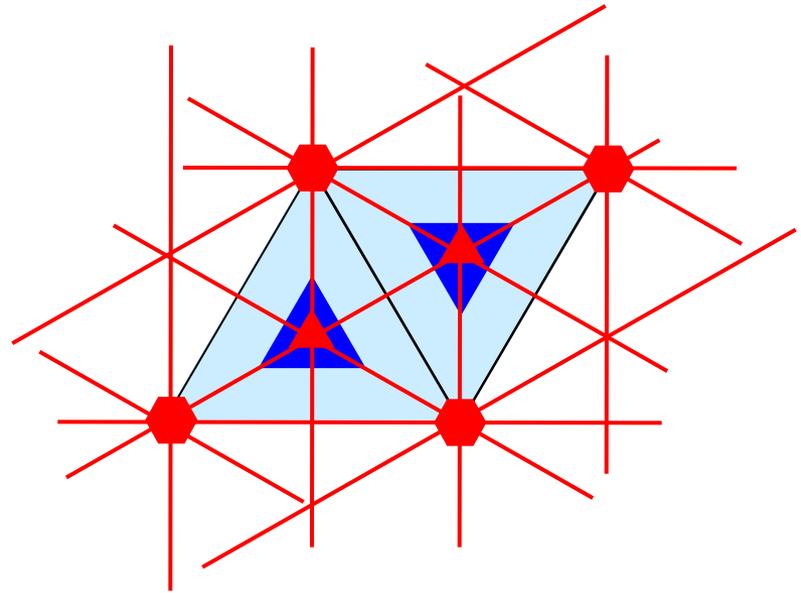
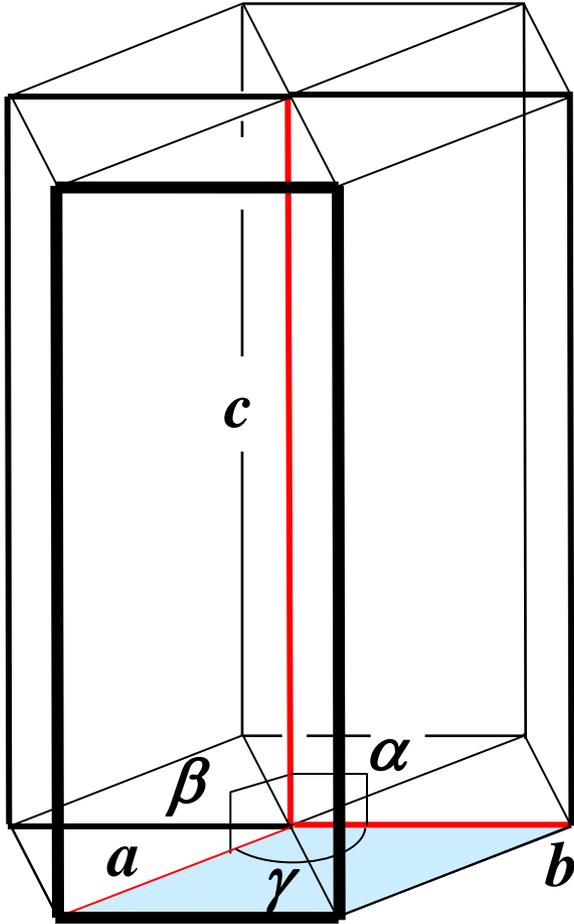
晶系 Trigonal



$$a = b \neq c, \quad \alpha = \beta = 90^\circ, \quad \gamma = 120^\circ$$



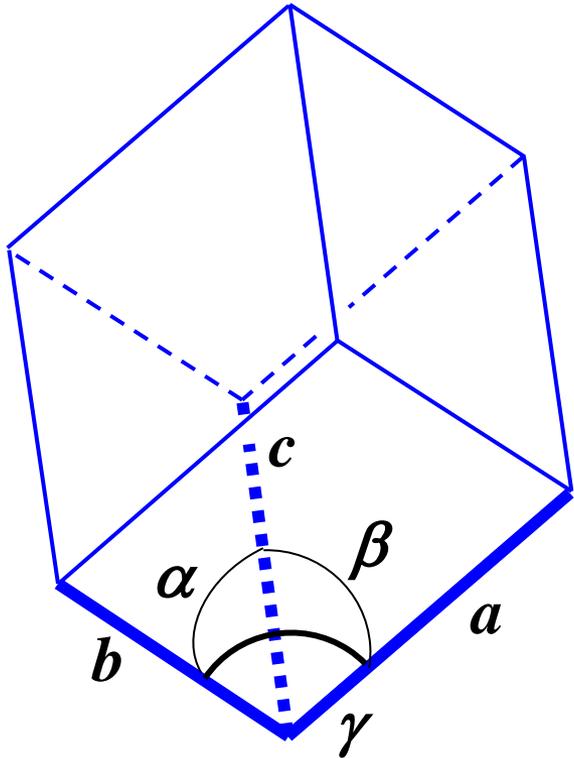
晶系 Hexagonal



$$a = b \neq c,$$

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$

晶系 Rhombohedral

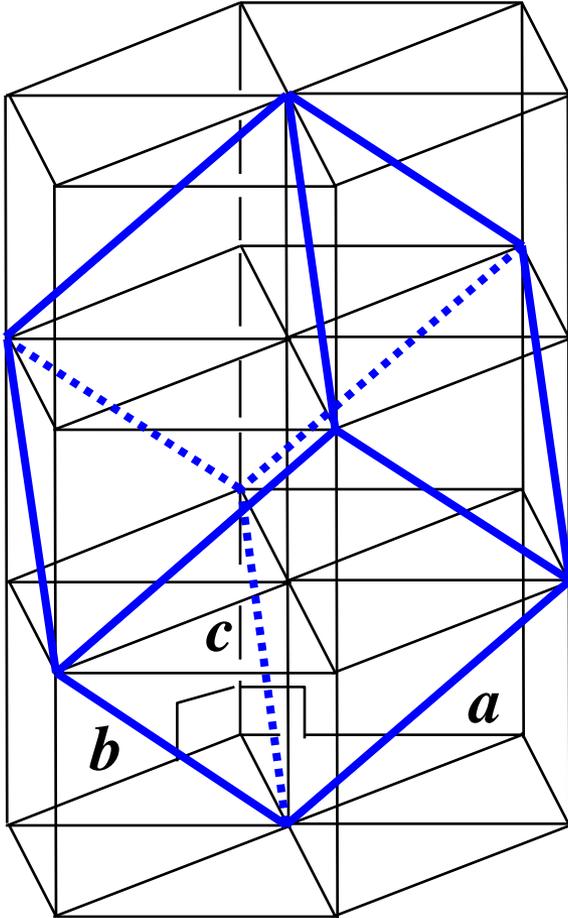


$$a = b = c,$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

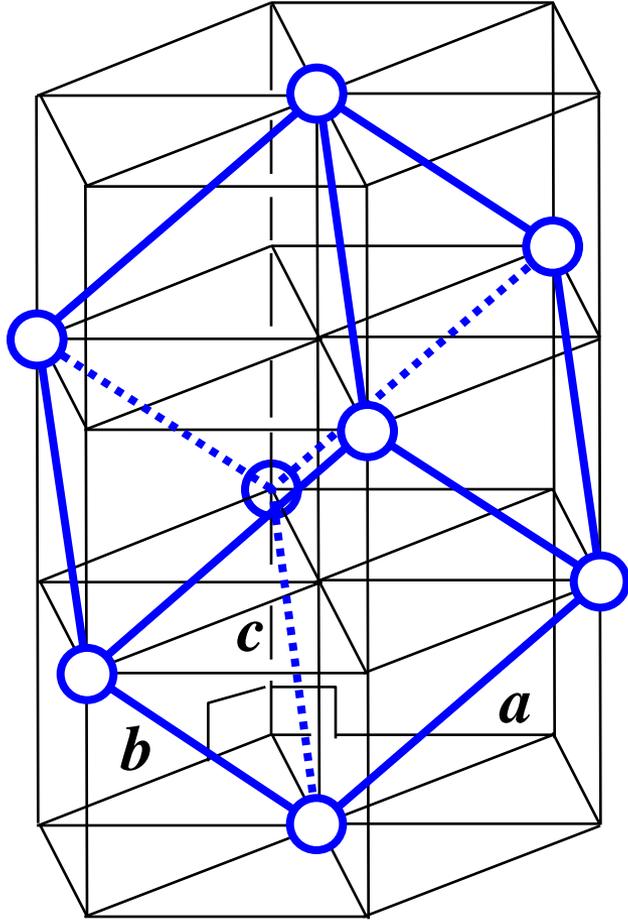


晶系 Rhombohedral

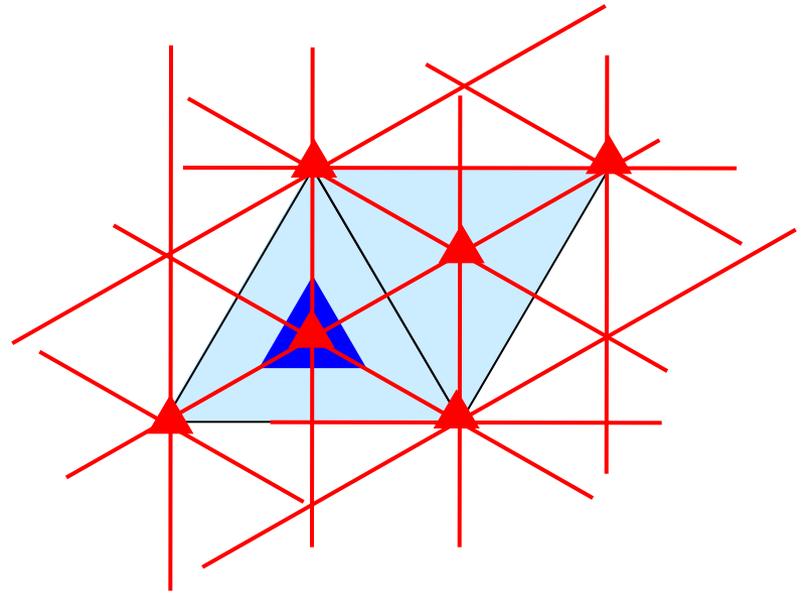
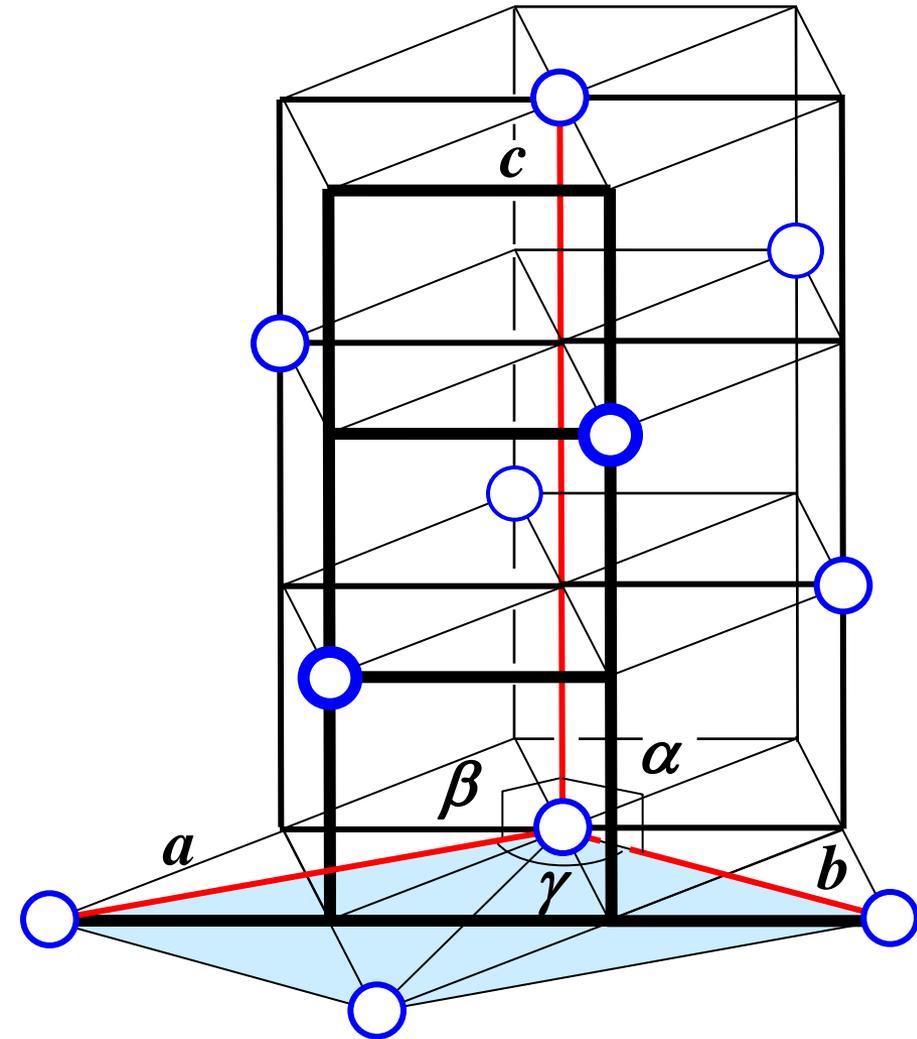




晶系 Rhombohedral



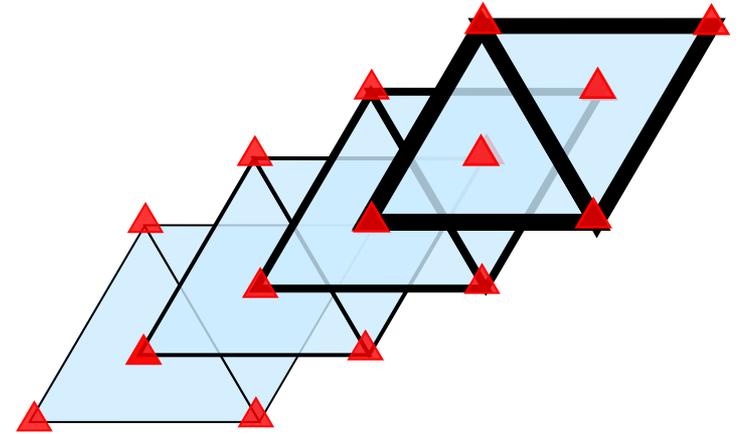
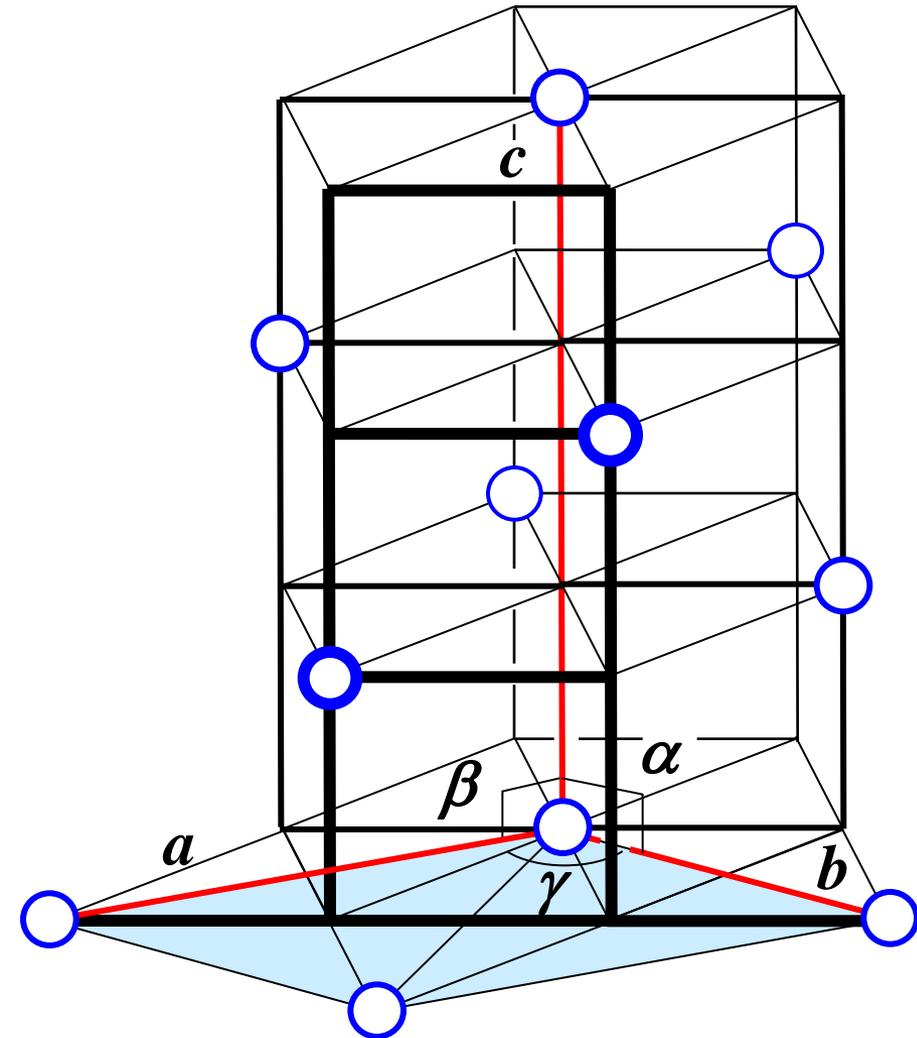
晶系 Rhombohedral



$$a = b \neq c,$$

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$

晶系 Rhombohedral



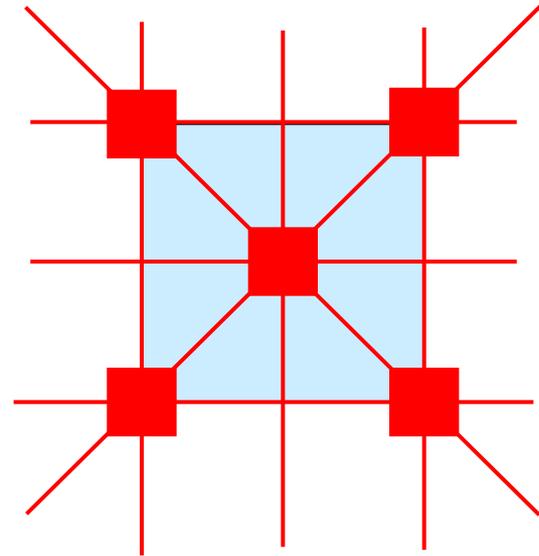
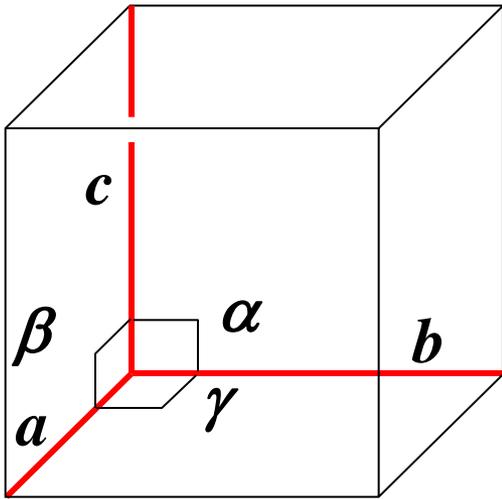
$$a = b \neq c,$$

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$

菱面体 \in 三方



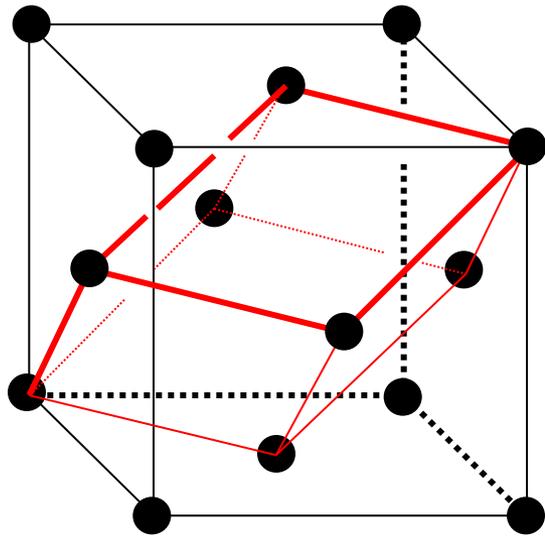
晶系 Cubic



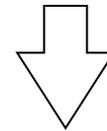
$$a = b = c,$$

$$\alpha = \beta = \gamma = 90^\circ$$

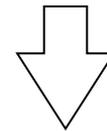
複合格子 complex lattice



単純単位胞(赤)は
結晶の対称性を
表していない

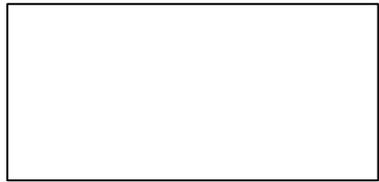
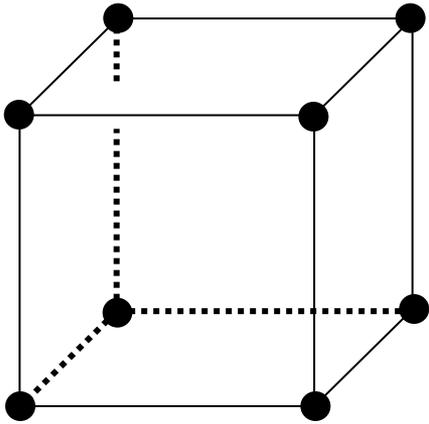


複合格子



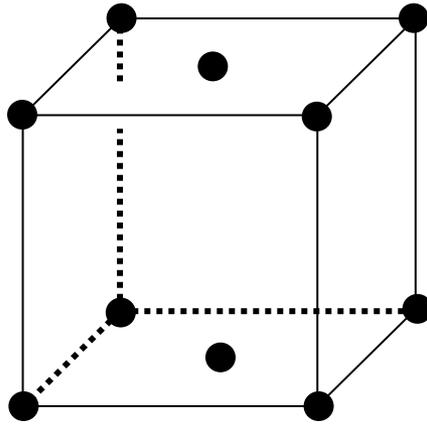
Bravais格子

複合格子の種類



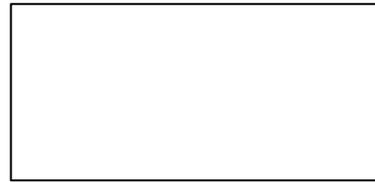
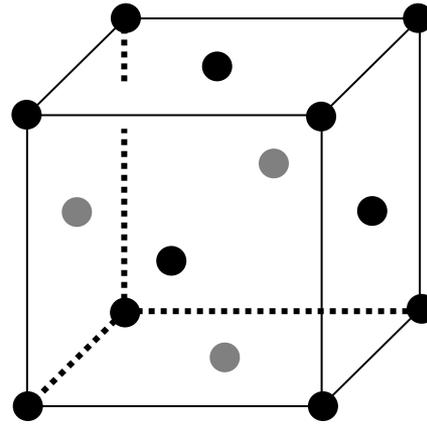
P

primitive



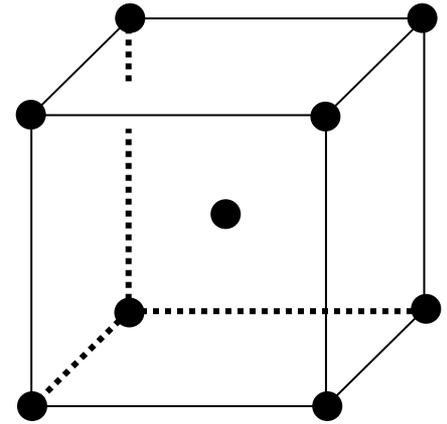
A, B, C

base-centered



F

face-centered



I

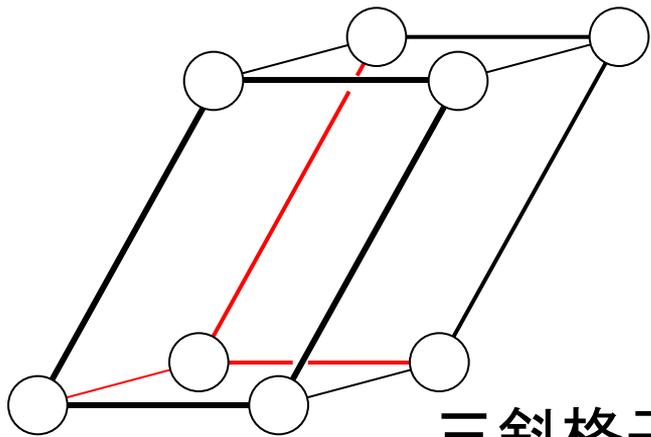
body-centered

Bravais格子

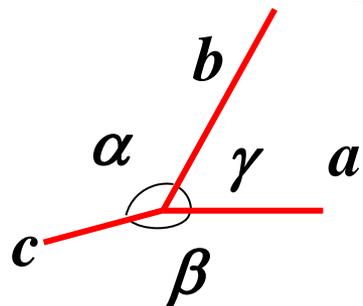
晶系	必須の対称要素	単位胞の形状	Bravais格子
三斜	なし	$a \neq b \neq c, \alpha \neq \beta \neq \gamma$ ($c < a < b$)	P
単斜	1本の2回軸	$a \neq b \neq c, \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$ ($c < a$)	$P, (C, A)$
斜方	3本の2回軸	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$ ($c < a < b$)	$P, (C, A, B), I, F$
正方	1本の4回軸	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$	P, I
三方 六方菱面	1本の3回軸	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$ $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	P
六方	1本の6回軸	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	P
立方	4本の3回軸	$a = b = c, \alpha = \beta = \gamma = 90^\circ$	P, I, F

Bravais格子

三斜晶系



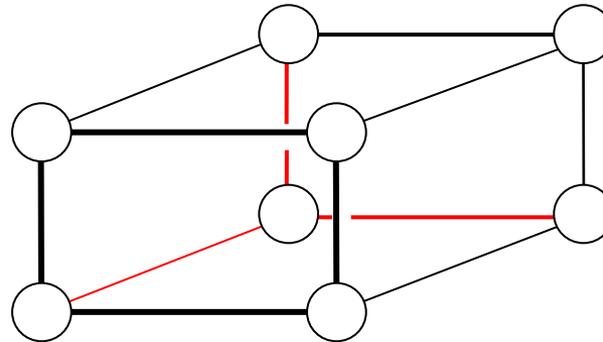
三斜格子



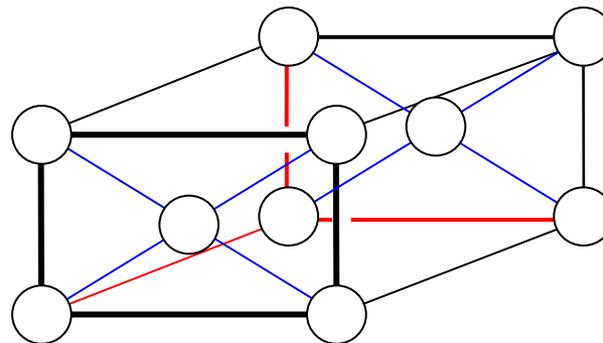
$$a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma$$

$$(c < a < b)$$

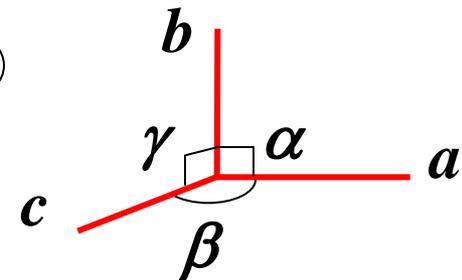
单斜晶系



单纯单斜格子



C底心单斜格子
(A)

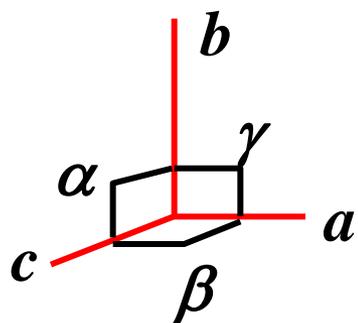


$$a \neq b \neq c, \quad \alpha = \gamma = 90^\circ, \quad \beta \neq 90^\circ$$

$$(c < a)$$

Bravais格子

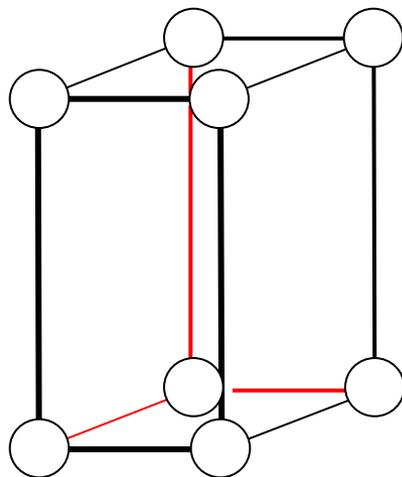
斜方晶系



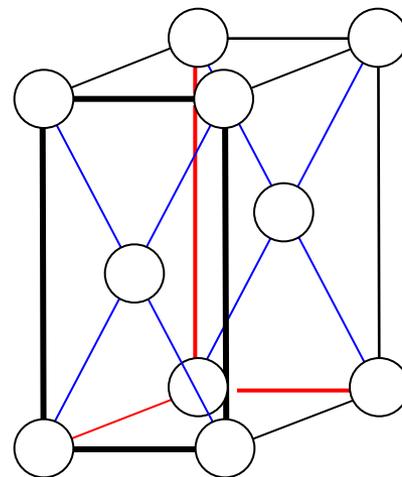
$$a \neq b \neq c,$$

$$\alpha = \beta = \gamma = 90^\circ$$

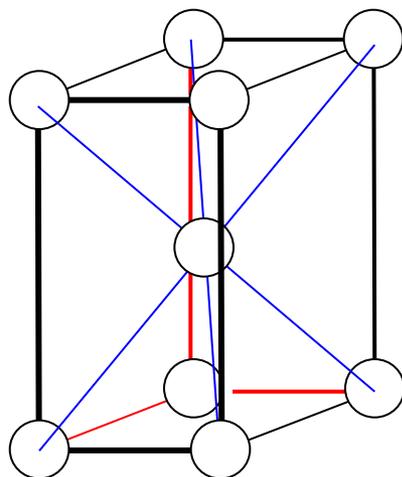
$$(c < a < b)$$



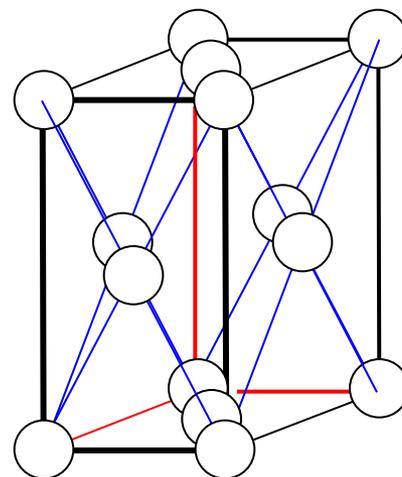
单纯斜方格子



C底心斜方格子(A,B)



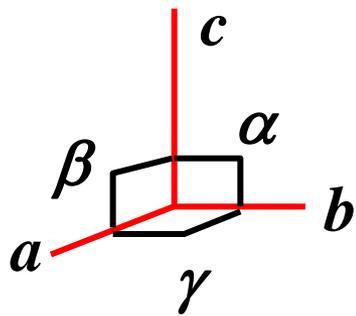
体心斜方格子



面心斜方格子

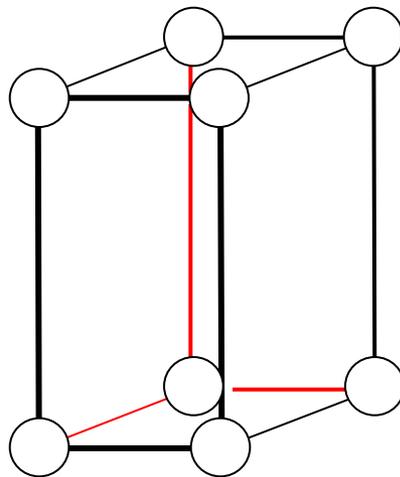
Bravais格子

正方晶系

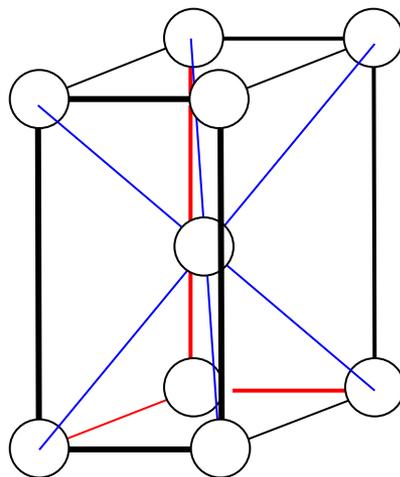


$$a = b \neq c,$$

$$\alpha = \beta = \gamma = 90^\circ$$



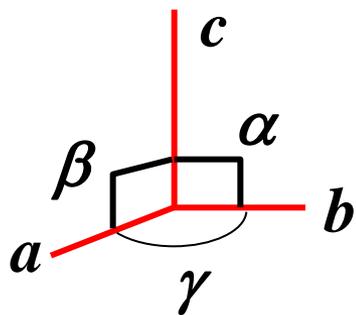
单纯正方格子



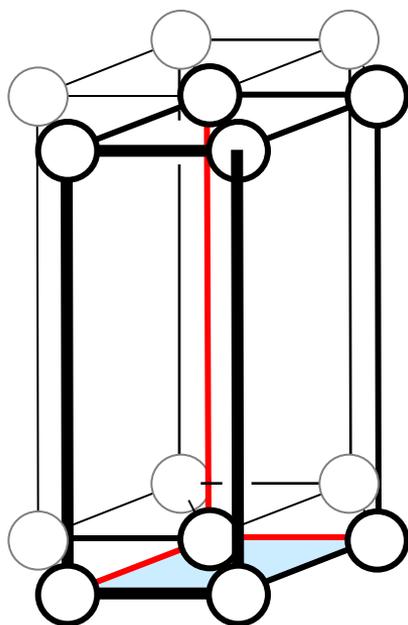
体心正方格子

Bravais格子

六方晶系
三方晶系

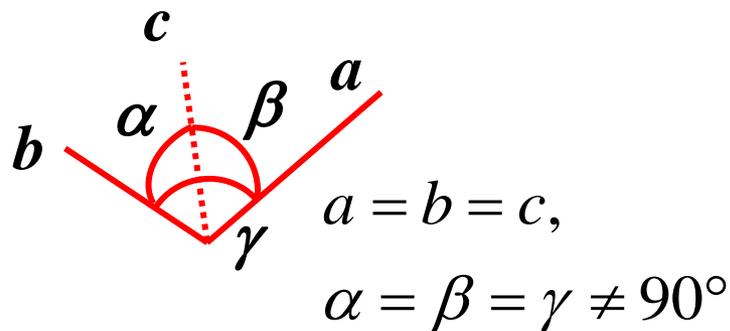


$$a = b \neq c,$$
$$\alpha = \beta = 90^\circ$$
$$\gamma = 120^\circ$$

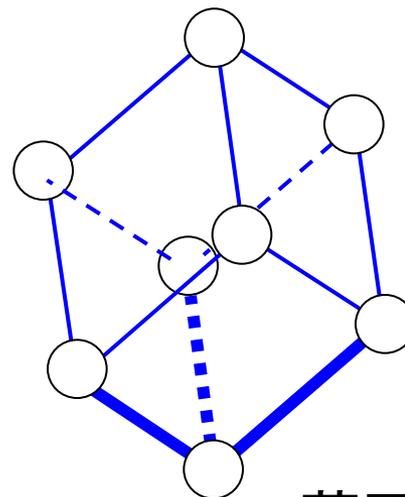


六方格子
三方格子

菱面体晶系



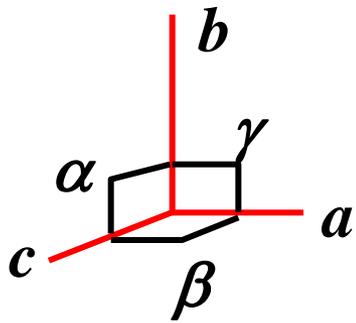
$$a = b = c,$$
$$\alpha = \beta = \gamma \neq 90^\circ$$



菱面体格子

Bravais格子

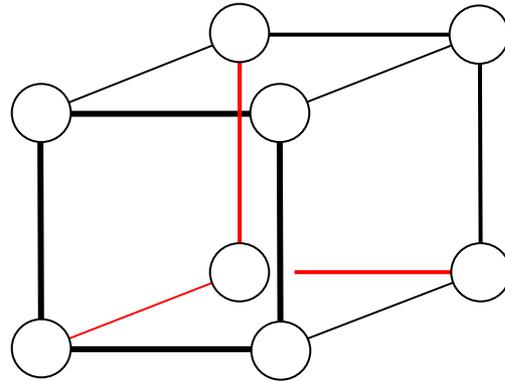
立方晶系



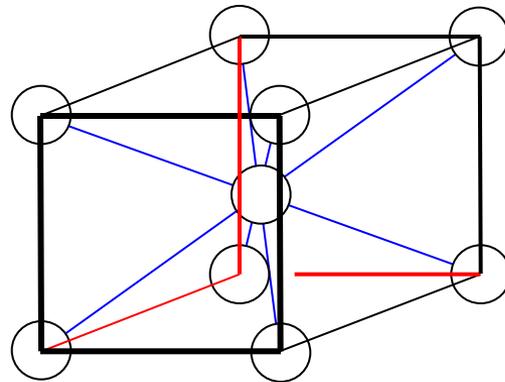
$$a \neq b \neq c,$$

$$\alpha = \beta = \gamma = 90^\circ$$

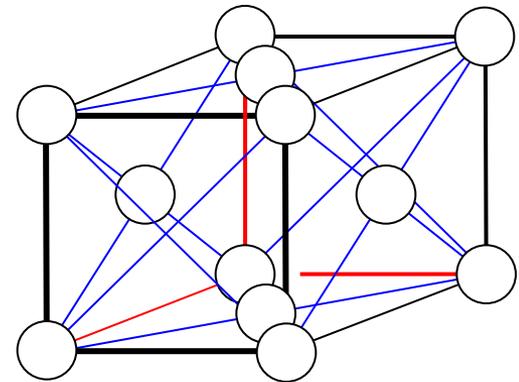
$$(c < a < b)$$



单纯立方格子



体心立方格子



面心立方格子

まとめ

○7つの晶系

三斜、単斜、斜方、正方、三方(菱面体)、
六方、立方

○14種のBravais格子

三斜、単斜(P, C)、斜方(P, C, I, F)、
正方(P, I)、三方(菱面体)、六方、
立方(P, I, F)

