Midterm

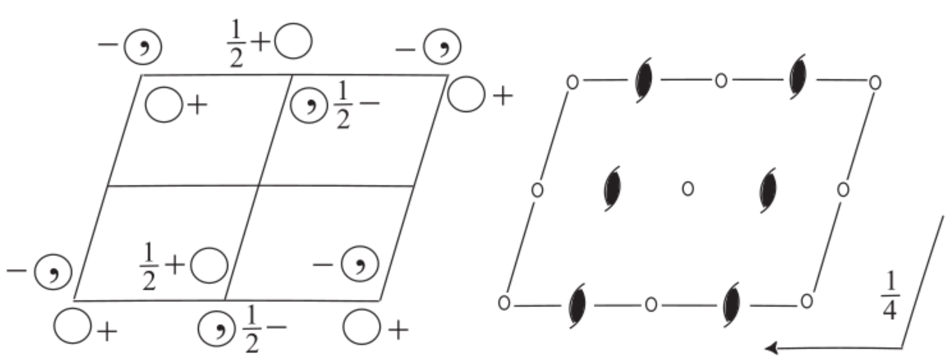
Time: 1hr 30 mins
April 7, 2026

Question 1

CuF_2 belongs to the $Fm\bar{3}m$ space group. How many branches of phonons do you expect in the first Brillouin zone? [**2 marks**]

Question 2

Of all 230 space groups there are probably more crystals that have the C_{2h}^5 ($P2_1/b$) space group than any other. Figure given below comes from the International Tables. Describe how the symmetry operations of the space group that generate the four general equivalent positions. (HINT: The symmetry operations include 2_1 screw axes, a glide plane in the plane of the paper at a height $z = 1/4$ and centers of inversion. All of these operations can be seen in the diagram.) [**8 marks**]



$C_{2h}^5(P2_1/b)$

Question 3

Consider the space group C_{2v}^5 ($Pmc2_1$).

(a) Which crystal system does this space group belong to? [**2 marks**]

(b) Three symmetry elements have been identified in the name $Pmc2_1$. What are they? What general positions do they generate? Show these positions by a projection along the $\vec{c}$−axis. [**8 marks**]

Question 4

Consider a $1D$ solid of length L, in which out of line vibrations are not allowed.

(a) Find the density of modes $g(\omega)$ and show that it is independent of ω. [**5 marks**]

(b) Find the Debye frequency ω_D and Debye temperature Θ_D. [**5 marks**]

(c) Compute the low temperature heat capacity C_v. [**5 marks**]

Some standard integrals are given below:

$$\int_0^\infty \frac{x^4 e^x}{(e^x-1)^2}dx = \frac{4\pi^4}{15},$$

$$\int_0^\infty \frac{x^3 e^x}{(e^x-1)^2}dx = 6\zeta(3) \qquad \text{where } \zeta(n) = \sum_{k=1}^{\infty} k^{-n} \text{ is the Riemann Zeta function,}$$

$$\int_0^\infty \frac{x^2 e^x}{(e^x-1)^2}dx = \frac{\pi^2}{3},$$

Question 5

Topaz is an orthorhombic crystal. The ratio of the lattice constants $a : b : c = 0.529 : 1 : 0.477$. Find the Miller indices of the faces whose intercepts are $0.264 : 1 : 0.238$. [**5 marks**]

Question 6

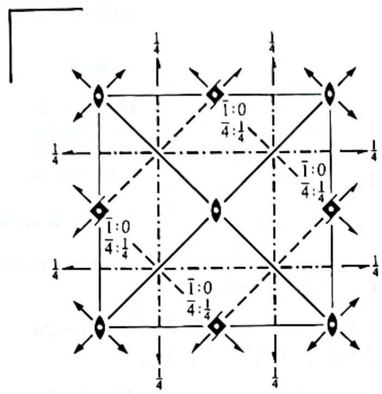
Rutile (TiO_2) crystallizes in the space group $P4_2/mnm$ with $a = 4.594$Å, $c = 2.958$Å. Ti is in $2a$ and O in $4f$ positions with $x = 0.305$. Find the coordinates of the O atoms. Draw a projection down $\vec{c}$ of the rutile structure. The space group information of atomic positions taken from the International Tables is appended. [**10 marks**]

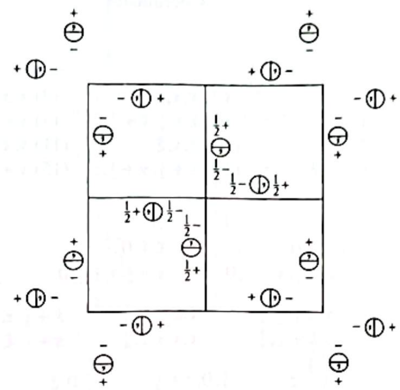
Question 7

Derive the reflection condition for the $4b$ Wyckoff positions in space group D_{2h}^{18} ($Cmce$). The space group information of atomic positions taken from the International Tables is appended. [**10 marks**]

$P4_2/mnm$ $\quad D_{4h}^{14}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 136 $\quad P\ 4_2/m\ 2_1/n\ 2/m$ $\quad$ Patterson symmetry $P4/mmm$





Origin at centre (mmm) at $2/m12/m$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},\frac{1}{4}$	(7) $2\ \ x,x,0$	(8) $2\ \ x,\bar{x},0$
(9) $\bar{1}\ \ 0,0,0$	(10) $m\ \ x,y,0$	(11) $\bar{4}^+\ \ \frac{1}{2},0,z;\ \ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-\ \ 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,z$	(15) $m\ \ x,\bar{x},z$	(16) $m\ \ x,x,z$

CONTINUED No. 136 $P4_2/mnm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
16	k	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $y,x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$ (15) $\bar{y},\bar{x},z$ (16) y,x,z	$0kl$: $k+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
				Special: as above, plus
8	j	$..m$	x,x,z $\bar{x},\bar{x},z$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ $x,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
8	i	$m..$	$x,y,0$ $\bar{x},\bar{y},0$ $\bar{y}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $y+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$ $y,x,0$ $\bar{y},\bar{x},0$	no extra conditions
8	h	$2..$	$0,\frac{1}{2},z$ $0,\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}$ $0,\frac{1}{2},\bar{z}$ $0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,z+\frac{1}{2}$ $\frac{1}{2},0,z$	hkl: $h+k,l=2n$
4	g	$m.2m$	$x,\bar{x},0$ $\bar{x},x,0$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	f	$m.2m$	$x,x,0$ $\bar{x},\bar{x},0$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	e	$2.mm$	$0,0,z$ $\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,0,\bar{z}$	hkl: $h+k+l=2n$
4	d	$\bar{4}..$	$0,\frac{1}{2},\frac{1}{4}$ $0,\frac{1}{2},\frac{3}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k,l=2n$
4	c	$2/m..$	$0,\frac{1}{2},0$ $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},0,0$	hkl: $h+k,l=2n$
2	b	$m.mm$	$0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$	hkl: $h+k+l=2n$
2	a	$m.mm$	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$

Symmetry of special projections

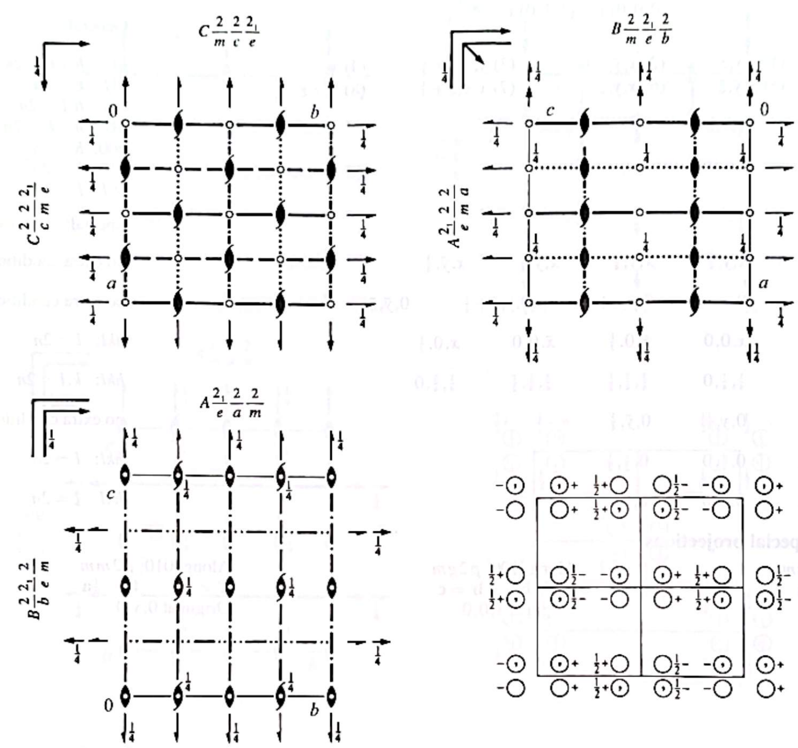
Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$Cmce$	D_{2h}^{18}	mmm	Orthorhombic
No. 64	$C\ 2/m\ 2/c\ 2_1/e$		Patterson symmetry $Cmmm$

Former space-group symbol $Cmca$; *cf.* Section 2.1.2



Origin at centre $(2/m)$ at $2/mn1$

Asymmetric unit $0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $b\quad x,y,\frac{1}{4}$	(7) $c\quad x,\frac{1}{4},z$	(8) $m\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(8) $b\quad \frac{1}{4},y,z$

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CONTINUED No. 64 *Cmce*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	g	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	f	m . .	$0,y,z$	$0,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8	e	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{4}$	hkl: $h=2n$
8	d	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$	$x,\frac{1}{2},\frac{1}{2}$	hkl: $k+l=2n$
8	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	hkl: $k,l=2n$
4	b	$2/m$ . .	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
4	a	$2/m$ . .	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$