

***I*4**

***C*<sub>4</sub><sup>5</sup>**

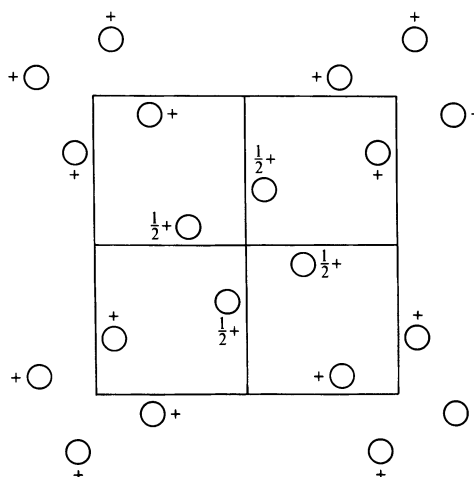
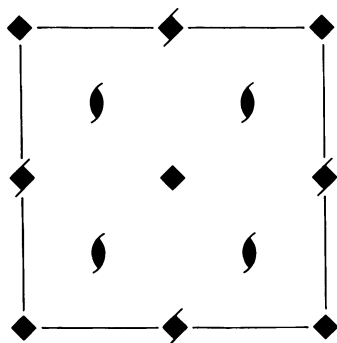
**4**

**Tetragonal**

No. 79

***I*4**

Patterson symmetry *I*4/*m*



**Origin** on 4

**Asymmetric unit**  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

**Symmetry operations**

For (0,0,0)+ set

- (1) 1                      (2) 2 0,0,z                      (3) 4<sup>+</sup> 0,0,z                      (4) 4<sup>-</sup> 0,0,z

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

- (1)  $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$                       (2)  $2(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$                       (3)  $4^+(0, 0, \frac{1}{2}) 0, \frac{1}{2}, z$                       (4)  $4^-(0, 0, \frac{1}{2}) \frac{1}{2}, 0, z$

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

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

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

8 *c* 1                      (1) *x,y,z*                      (2)  $\bar{x}, \bar{y}, z$                       (3)  $\bar{y}, x, z$                       (4) *y, \bar{x}, z*

Reflection conditions

General:

- hkl*:  $h + k + l = 2n$   
*hk0*:  $h + k = 2n$   
*0kl*:  $k + l = 2n$   
*hhl*:  $l = 2n$   
*00l*:  $l = 2n$   
*h00*:  $h = 2n$

Special: as above, plus

*hkl*:  $l = 2n$

no extra conditions

4 *b* 2..                       $0, \frac{1}{2}, z$                        $\frac{1}{2}, 0, z$

2 *a* 4..                       $0, 0, z$

**Symmetry of special projections**

Along [001] *p*4

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$                        $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$

Origin at 0,0,z

Along [100] *c*1*m*1

$\mathbf{a}' = \mathbf{b}$                        $\mathbf{b}' = \mathbf{c}$

Origin at *x*,0,0

Along [110] *p*1*m*1

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$                        $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at *x,x*,0