

$F\bar{4}3c$

$T_d^5$

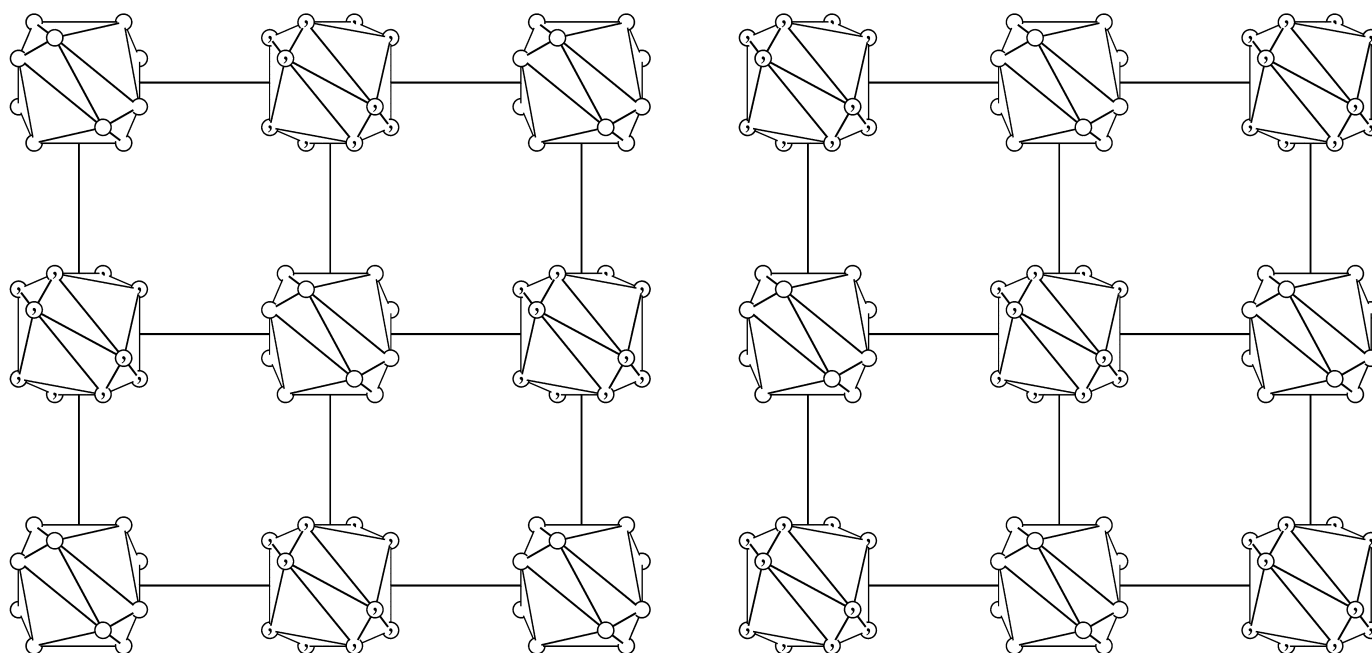
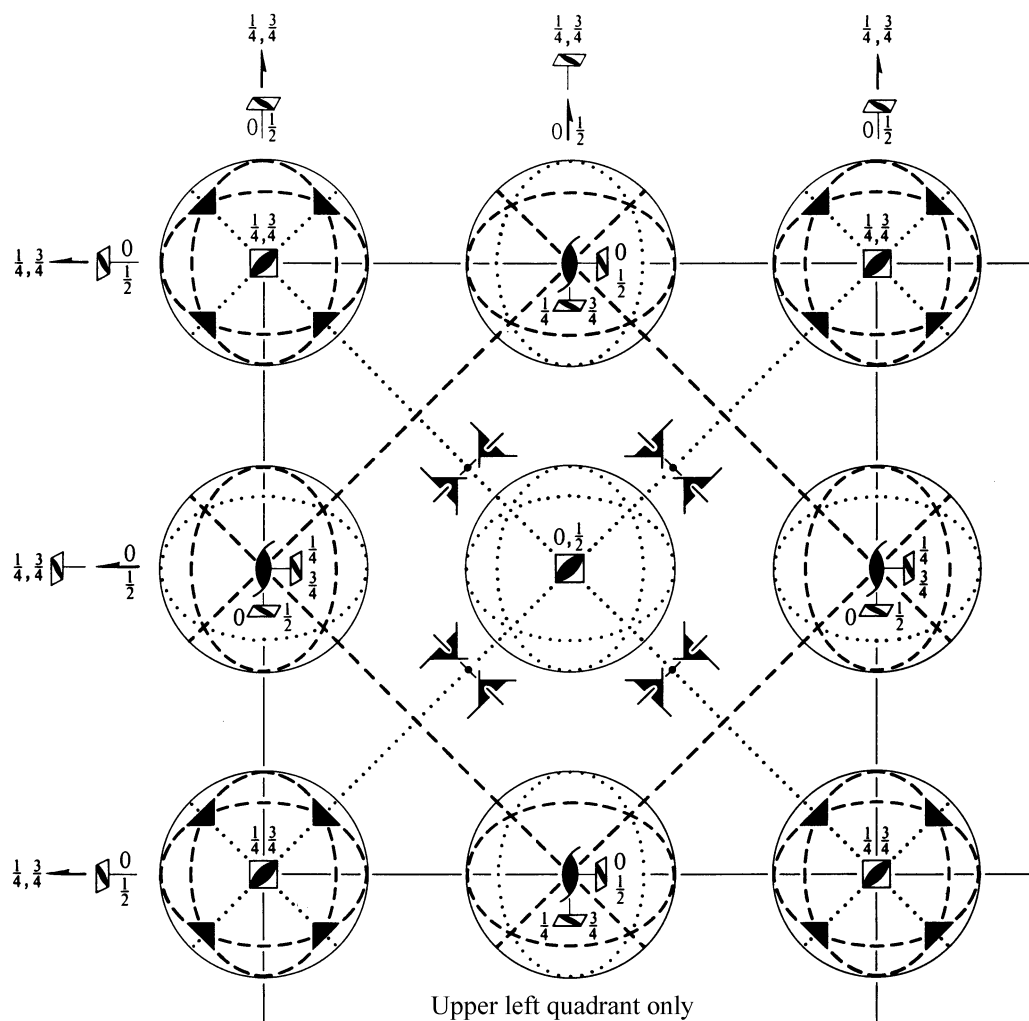
$\bar{4}3m$

Cubic

No. 219

$F\bar{4}3c$

Patterson symmetry  $Fm\bar{3}m$



Lower half of unit cell, all polyhedra at height 0

Upper half of unit cell, all polyhedra at height  $\frac{1}{2}$

Origin at 23

Asymmetric unit  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq \frac{1}{4}$ ;  $-\frac{1}{4} \leq z \leq \frac{1}{4}$ ;  $y \leq \min(x, \frac{1}{2} - x)$ ;  $-y \leq z \leq y$

Vertices  $0, 0, 0$   $\frac{1}{2}, 0, 0$   $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$   $\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

## Symmetry operations

For (0,0,0)+ set

- |   |   |   |   |
|---|---|---|---|
| (1) 1   | (2) 2 0,0,z   | (3) 2 0,y,0   | (4) 2 x,0,0   |
| (5) 3 <sup>+</sup> x,x,x                            | (6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$                    | (7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$                   | (8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x                   |
| (9) 3 <sup>-</sup> x,x,x                            | (10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$                  | (11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x                  | (12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$                   |
| (13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z | (14) c $x+\frac{1}{2},\bar{x},z$                              | (15) $\bar{4}^+$ $\frac{1}{2},0,z; \frac{1}{2},0,\frac{1}{4}$ | (16) $\bar{4}^-$ $0,\frac{1}{2},z; 0,\frac{1}{2},\frac{1}{4}$ |
| (17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y | (18) $\bar{4}^+$ $x,\frac{1}{2},0; \frac{1}{4},\frac{1}{2},0$ | (19) $\bar{4}^-$ $x,0,\frac{1}{2}; \frac{1}{4},0,\frac{1}{2}$ | (20) a $x,y+\frac{1}{2},\bar{y}$                              |
| (21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x | (22) $\bar{4}^-$ $\frac{1}{2},y,0; \frac{1}{2},\frac{1}{4},0$ | (23) b $\bar{x}+\frac{1}{2},y,x$                              | (24) $\bar{4}^+$ $0,y,\frac{1}{2}; 0,\frac{1}{4},\frac{1}{2}$ |

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

- |  |  |   |   |
|--|--|---|---|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$   | (2) 2(0,0, $\frac{1}{2}$ ) 0, $\frac{1}{4},z$  | (3) 2(0, $\frac{1}{2},0$ ) 0,y, $\frac{1}{4}$   | (4) 2 $x,\frac{1}{4},\frac{1}{4}$                                       |
| (5) 3 <sup>+</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x-\frac{1}{3},x-\frac{1}{6},x$ | (6) 3 <sup>+</sup> $\bar{x},x+\frac{1}{2},\bar{x}$   | (7) 3 <sup>+</sup> ( $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ | (8) 3 <sup>+</sup> $\bar{x},\bar{x}+\frac{1}{2},x$                      |
| (9) 3 <sup>-</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x-\frac{1}{6},x+\frac{1}{6},x$ | (10) 3 <sup>-</sup> ( $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) 3 <sup>-</sup> $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$   | (12) 3 <sup>-</sup> $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$         |
| (13) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$                                      | (14) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$   | (15) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z; \frac{1}{4},-\frac{1}{4},0$                                 | (16) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},0$ |
| (17) a x,y,y   | (18) $\bar{4}^+$ $x,0,0; \frac{1}{4},0,0$  | (19) $\bar{4}^-$ $x,0,0; \frac{1}{4},0,0$   | (20) a x,y, $\bar{y}$   |
| (21) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$                                      | (22) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}; \frac{1}{4},0,-\frac{1}{4}$                                  | (23) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$  | (24) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}; \frac{1}{4},0,\frac{1}{4}$ |

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

- |  |   |   |  |
|--|---|---|--|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$   | (2) 2(0,0, $\frac{1}{2}$ ) $\frac{1}{4},0,z$  | (3) 2 $\frac{1}{4},y,\frac{1}{4}$                                       | (4) 2( $\frac{1}{2},0,0$ ) x,0, $\frac{1}{4}$  |
| (5) 3 <sup>+</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x+\frac{1}{6},x-\frac{1}{6},x$ | (6) 3 <sup>+</sup> ( $\frac{1}{3},-\frac{1}{3},\frac{1}{3}$ ) $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ | (7) 3 <sup>+</sup> $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$          | (8) 3 <sup>+</sup> $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$   |
| (9) 3 <sup>-</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x-\frac{1}{6},x-\frac{1}{3},x$ | (10) 3 <sup>-</sup> $x+\frac{1}{2},\bar{x},\bar{x}$   | (11) 3 <sup>-</sup> $\bar{x}+\frac{1}{2},\bar{x},x$                     | (12) 3 <sup>-</sup> ( $\frac{1}{3},-\frac{1}{3},\frac{1}{3}$ ) $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$                                      | (14) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$  | (15) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},0$ | (16) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z; -\frac{1}{4},\frac{1}{4},0$                                  |
| (17) $g(0,\frac{1}{4},\frac{1}{4})$ x,y, $\frac{1}{4},y$                                     | (18) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}; 0,\frac{1}{4},-\frac{1}{4}$                                 | (19) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}; 0,\frac{1}{4},\frac{1}{4}$ | (20) $g(0,\frac{1}{4},-\frac{1}{4})$ x,y, $\frac{1}{4},\bar{y}$  |
| (21) b x,y,x   | (22) $\bar{4}^-$ 0,y,0; 0, $\frac{1}{4},0$  | (23) b $\bar{x},y,x$  | (24) $\bar{4}^+$ 0,y,0; 0, $\frac{1}{4},0$   |

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

- |  |   |   |   |
|--|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$   | (2) 2 $\frac{1}{4},\frac{1}{4},z$                                       | (3) 2(0, $\frac{1}{2},0$ ) $\frac{1}{4},y,0$  | (4) 2( $\frac{1}{2},0,0$ ) x, $\frac{1}{4},0$   |
| (5) 3 <sup>+</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x+\frac{1}{6},x+\frac{1}{3},x$ | (6) 3 <sup>+</sup> $\bar{x}+\frac{1}{2},x,\bar{x}$                      | (7) 3 <sup>+</sup> $x+\frac{1}{2},\bar{x},\bar{x}$  | (8) 3 <sup>+</sup> ( $\frac{1}{3},\frac{1}{3},-\frac{1}{3}$ ) $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$ |
| (9) 3 <sup>-</sup> ( $\frac{1}{3},\frac{1}{3},\frac{1}{3}$ ) $x+\frac{1}{3},x+\frac{1}{6},x$ | (10) 3 <sup>-</sup> x, $\bar{x}+\frac{1}{2},\bar{x}$                    | (11) 3 <sup>-</sup> ( $-\frac{1}{3},\frac{1}{3},-\frac{1}{3}$ ) $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) 3 <sup>-</sup> $\bar{x},x+\frac{1}{2},\bar{x}$   |
| (13) c x,x,z   | (14) c x, $\bar{x},z$   | (15) $\bar{4}^+$ 0,0,z; 0,0, $\frac{1}{4}$  | (16) $\bar{4}^-$ 0,0,z; 0,0, $\frac{1}{4}$  |
| (17) $g(0,\frac{1}{4},\frac{1}{4})$ x,y, $-\frac{1}{4},y$                                    | (18) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}; 0,\frac{1}{4},\frac{1}{4}$ | (19) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}; 0,-\frac{1}{4},\frac{1}{4}$                                   | (20) $g(0,-\frac{1}{4},\frac{1}{4})$ x,y, $\frac{1}{4},\bar{y}$   |
| (21) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$                                      | (22) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}; \frac{1}{4},0,\frac{1}{4}$ | (23) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$  | (24) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}; -\frac{1}{4},0,\frac{1}{4}$                                 |

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,\frac{1}{2},\frac{1}{2})$ ;  $t(\frac{1}{2},0,\frac{1}{2})$ ; (2); (3); (5); (13)

## Positions

| Multiplicity,<br>Wyckoff letter,<br>Site symmetry | Coordinates   |   |   |   | Reflection conditions   |  |           |
|---|---|---|---|---|---|--|-----------|
|   | (0,0,0)+  | (0, $\frac{1}{2},\frac{1}{2}$ )+  | ( $\frac{1}{2},0,\frac{1}{2}$ )+  | ( $\frac{1}{2},\frac{1}{2},0$ )+  | h,k,l permutable<br>General:  |  |           |
| 96 h 1  | (1) x,y,z<br>(5) z,x,y<br>(9) y,z,x<br>(13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$<br>(17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$<br>(21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$ | (2) $\bar{x},\bar{y},z$<br>(6) z, $\bar{x},\bar{y}$<br>(10) $\bar{y},z,\bar{x}$<br>(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$<br>(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$<br>(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$ | (3) $\bar{x},y,\bar{z}$<br>(7) $\bar{z},\bar{x},y$<br>(11) y, $\bar{z},\bar{x}$<br>(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$<br>(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$<br>(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ | (4) x, $\bar{y},\bar{z}$<br>(8) $\bar{z},x,\bar{y}$<br>(12) $\bar{y},\bar{z},x$<br>(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$<br>(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$<br>(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$ | hkl: h+k=2n and<br>h+l,k+l=2n<br>Ok: k,l=2n<br>hhl: h,l=2n<br>h00: h=2n |  |           |
| 48 g 2..  | $x,\frac{1}{4},\frac{1}{4}$<br>$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$  | $\bar{x},\frac{3}{4},\frac{1}{4}$<br>$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$  | $\frac{1}{4},x,\frac{1}{4}$<br>$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$  | $\frac{1}{4},\bar{x},\frac{3}{4}$<br>$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$  | $\frac{1}{4},\frac{1}{4},x$<br>$\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$  | $\frac{3}{4},\frac{1}{4},\bar{x}$<br>$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$ | hkl: h=2n |
| 48 f 2..  | x,0,0<br>$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$  | $\bar{x},0,0$<br>$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$  | 0,x,0<br>$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$  | 0, $\bar{x},0$<br>$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$   | 0,0,x<br>$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$                        | 0,0, $\bar{x}$<br>$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$                    | hkl: h=2n |
| 32 e .3.  | x,x,x<br>$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$  | $\bar{x},\bar{x},x$<br>$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$  | $\bar{x},x,\bar{x}$<br>$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$  | x, $\bar{x},\bar{x}$<br>$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$   | hkl: h=2n   |  |           |
| 24 d $\bar{4}$ ..                                 | $\frac{1}{4},0,0$   | $\frac{3}{4},0,0$   | 0, $\frac{1}{4},0$  | 0, $\frac{3}{4},0$  | 0,0, $\frac{1}{4}$  | 0,0, $\frac{3}{4}$   | hkl: h=2n |
| 24 c $\bar{4}$ ..                                 | 0, $\frac{1}{4},\frac{1}{4}$  | 0, $\frac{3}{4},\frac{1}{4}$  | $\frac{1}{4},0,\frac{1}{4}$   | $\frac{1}{4},0,\frac{3}{4}$   | $\frac{1}{4},\frac{1}{4},0$   | $\frac{3}{4},\frac{1}{4},0$  | hkl: h=2n |
| 8 b 23.   | $\frac{1}{4},\frac{1}{4},\frac{1}{4}$   | $\frac{3}{4},\frac{3}{4},\frac{3}{4}$   |   |   |   | hkl: h=2n  |           |
| 8 a 23.   | 0,0,0   | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$   |   |   |   | hkl: h=2n  |           |

## Symmetry of special projections

Along [001]  $p4mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$   $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   
 Origin at 0,0,z

Along [111]  $p31m$   
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$   $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$   
 Origin at x,x,x

Along [110]  $p1m1$   
 $\mathbf{a}' = \frac{1}{4}(-\mathbf{a} + \mathbf{b})$   $\mathbf{b}' = \frac{1}{2}\mathbf{c}$   
 Origin at x,x,0