**Origin** on 3 [1 1 1] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel $2_1$ axes

**Positions**

Multiplicity, Wyckoff letter, Site symmetry, Coordinates

**Patterson peaks (U, V, W (Multiplicity))**

| | | | | |
|---|---|---|---|---|
| 24 | c 1 | x,y,z; 1/2-x,-y,1/2+z; etc. | | |
| | | ***0, 0, 0 (24)*** | ***1/2+2x, 2y, 1/2 (2)*** | ***2x, 1/2, 1/2+2z (2)*** |
| | | ***1/2, 1/2+2y, 2z (2)*** | ***x-z, -x+y, -y+z (2)*** | ***1/2+x-z, 1/2+x+y, y+z (2)*** |
| | | ***1/2+x+z, x+y, 1/2-y+z (2)*** | ***x+z, 1/2-x+y, 1/2+y+z (2)*** | |
| 12 | b 2 . . | x,0,1/4; 1/2-x,0,3/4; etc. | | |
| | | ***0, 0, 0 (12)*** | ***1/2+2x, 0, 1/2 (2)*** | ***3/4+x, -x, 1/4 (2)*** |
| 8 | a . 3 . | x,x,x; 1/2-x,-x,1/2+x; etc. | | |
| | | ***0, 0, 0 (8)*** | ***1/2+2x, 2x, 1/2 (2)*** | |

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**Vectors between two sets of unique atoms**

| Wyckoff letters | |
|---|---|
| c, c | ***x1-x2, y1-y2, z1-z2 (2)*** |
| | ***1/2+x1+x2, y1+y2, 1/2+z1-z2 (2)*** |
| | ***x1+x2, 1/2+y1-y2, 1/2+z1+z2 (2)*** |
| | ***1/2+x1-x2, 1/2+y1+y2, z1+z2 (2)*** |
| | ***x1-z2, y1-x2, z1-y2 (2)*** |
| | ***1/2+x1-z2, 1/2+y1+x2, z1+y2 (2)*** |
| | ***1/2+x1+z2, y1+x2, 1/2+z1-y2 (2)*** |
| | ***x1+z2, 1/2+y1-x2, 1/2+z1+y2 (2)*** |
| | ***x1-y2, y1-z2, z1-x2 (2)*** |
| | ***x1+y2, 1/2+y1-z2, 1/2+z1+x2 (2)*** |
| | ***1/2+x1-y2, 1/2+y1+z2, z1+x2 (2)*** |
| | ***1/2+x1+y2, y1+z2, 1/2+z1-x2 (2)*** |
| c, b | ***x1-x2, y1, 3/4+z1 (2)*** |
| | ***1/2+x1+x2, y1, 1/4+z1 (2)*** |
| | ***3/4+x1, y1-x2, z1 (2)*** |
| | ***1/4+x1, 1/2+y1+x2, z1 (2)*** |
| | ***x1, 3/4+y1, z1-x2 (2)*** |
| | ***x1, 1/4+y1, 1/2+z1+x2 (2)*** |
| | ***-x1+x2, -y1, 3/4-z1 (2)*** |
| | ***1/2-x1-x2, -y1, 1/4-z1 (2)*** |
| | ***3/4-x1, -y1+x2, -z1 (2)*** |
| | ***1/4-x1, 1/2-y1-x2, -z1 (2)*** |
| | ***-x1, 3/4-y1, -z1+x2 (2)*** |
| | ***-x1, 1/4-y1, 1/2-z1-x2 (2)*** |
| c, a | ***x1-x2, y1-x2, z1-x2 (2)*** |
| | ***1/2+x1+x2, y1+x2, 1/2+z1-x2 (2)*** |
| | ***x1+x2, 1/2+y1-x2, 1/2+z1+x2 (2)*** |
| | ***1/2+x1-x2, 1/2+y1+x2, z1+x2 (2)*** |
| b, b | ***x1-x2, 0, 0 (4)*** |
| | ***1/2+x1+x2, 0, 1/2 (4)*** |
| | ***3/4+x1, -x2, 1/4 (2)*** |
| | ***x1, 3/4, 1/4-x2 (2)*** |
| | ***3/4-x1, x2, 1/4 (2)*** |
| | ***-x1, 3/4, 1/4+x2 (2)*** |
| b, a | ***x1-x2, -x2, 1/4-x2 (2)*** |
| | ***1/2+x1+x2, x2, 3/4-x2 (2)*** |
| | ***-x1+x2, x2, 1/4+x2 (2)*** |
| | ***1/2-x1-x2, -x2, 3/4+x2 (2)*** |
| a, a | ***x1-x2, x1-x2, x1-x2 (2)*** |
| | ***1/2+x1+x2, x1+x2, 1/2+x1-x2 (2)*** |