

SG No. 215  $T_d^1$   $P\bar{4}3m$  [ cubic ]

\* plus set: + [0, 0, 0]

Table 1: Wyckoff site: 1a, site symmetry: -43m

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

Table 2: Wyckoff site: 1b, site symmetry: -43m

No.	position	mapping
1	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

Table 3: Wyckoff site: 3c, site symmetry: -42.m

No.	position	mapping
1	[0, \frac{1}{2}, \frac{1}{2}]	[1,2,3,4,17,18,19,20]
2	[\frac{1}{2}, 0, \frac{1}{2}]	[5,6,7,8,13,14,15,16]
3	[\frac{1}{2}, \frac{1}{2}, 0]	[9,10,11,12,21,22,23,24]

Table 4: Wyckoff site: 3d, site symmetry: -42.m

No.	position	mapping
1	[\frac{1}{2}, 0, 0]	[1,2,3,4,17,18,19,20]
2	[0, \frac{1}{2}, 0]	[5,6,7,8,13,14,15,16]
3	[0, 0, \frac{1}{2}]	[9,10,11,12,21,22,23,24]

Table 5: Wyckoff site: 4e, site symmetry: .3m

No.	position	mapping
1	[x, x, x]	[1,5,9,13,17,21]
2	[-x, -x, x]	[2,7,12,14,19,24]
3	[-x, x, -x]	[3,8,10,16,18,23]
4	[x, -x, -x]	[4,6,11,15,20,22]

Table 6: Wyckoff site: 6f, site symmetry: 2..mm

No.	position	mapping
1	$[x, 0, 0]$	[1, 4, 17, 20]
2	$[-x, 0, 0]$	[2, 3, 18, 19]
3	$[0, x, 0]$	[5, 8, 13, 16]
4	$[0, -x, 0]$	[6, 7, 14, 15]
5	$[0, 0, x]$	[9, 12, 21, 24]
6	$[0, 0, -x]$	[10, 11, 22, 23]

Table 7: Wyckoff site: 6g, site symmetry: 2..mm

No.	position	mapping
1	$[x, \frac{1}{2}, \frac{1}{2}]$	[1, 4, 17, 20]
2	$[-x, \frac{1}{2}, \frac{1}{2}]$	[2, 3, 18, 19]
3	$[\frac{1}{2}, x, \frac{1}{2}]$	[5, 8, 13, 16]
4	$[\frac{1}{2}, -x, \frac{1}{2}]$	[6, 7, 14, 15]
5	$[\frac{1}{2}, \frac{1}{2}, x]$	[9, 12, 21, 24]
6	$[\frac{1}{2}, \frac{1}{2}, -x]$	[10, 11, 22, 23]

Table 8: Wyckoff site: 12h, site symmetry: 2..

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	[1, 4]
2	$[-x, \frac{1}{2}, 0]$	[2, 3]
3	$[0, x, \frac{1}{2}]$	[5, 8]
4	$[0, -x, \frac{1}{2}]$	[6, 7]
5	$[\frac{1}{2}, 0, x]$	[9, 12]
6	$[\frac{1}{2}, 0, -x]$	[10, 11]
7	$[\frac{1}{2}, x, 0]$	[13, 16]
8	$[\frac{1}{2}, -x, 0]$	[14, 15]
9	$[x, 0, \frac{1}{2}]$	[17, 20]
10	$[-x, 0, \frac{1}{2}]$	[18, 19]
11	$[0, \frac{1}{2}, x]$	[21, 24]
12	$[0, \frac{1}{2}, -x]$	[22, 23]

Table 9: Wyckoff site: 12i, site symmetry: ...m

No.	position	mapping
1	$[x, x, z]$	[1, 13]
2	$[-x, -x, z]$	[2, 14]
3	$[-x, x, -z]$	[3, 16]

*continued ...*

Table 9

No.	position	mapping
4	$[x, -x, -z]$	[4,15]
5	$[z, x, x]$	[5,21]
6	$[z, -x, -x]$	[6,22]
7	$[-z, -x, x]$	[7,24]
8	$[-z, x, -x]$	[8,23]
9	$[x, z, x]$	[9,17]
10	$[-x, z, -x]$	[10,18]
11	$[x, -z, -x]$	[11,20]
12	$[-x, -z, x]$	[12,19]

Table 10: Wyckoff site: 24j, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[-x, y, -z]$	[3]
4	$[x, -y, -z]$	[4]
5	$[z, x, y]$	[5]
6	$[z, -x, -y]$	[6]
7	$[-z, -x, y]$	[7]
8	$[-z, x, -y]$	[8]
9	$[y, z, x]$	[9]
10	$[-y, z, -x]$	[10]
11	$[y, -z, -x]$	[11]
12	$[-y, -z, x]$	[12]
13	$[y, x, z]$	[13]
14	$[-y, -x, z]$	[14]
15	$[y, -x, -z]$	[15]
16	$[-y, x, -z]$	[16]
17	$[x, z, y]$	[17]
18	$[-x, z, -y]$	[18]
19	$[-x, -z, y]$	[19]
20	$[x, -z, -y]$	[20]
21	$[z, y, x]$	[21]
22	$[z, -y, -x]$	[22]
23	$[-z, y, -x]$	[23]
24	$[-z, -y, x]$	[24]