

SG No. 218  $T_d^4$   $P\bar{4}3n$  [ cubic ]

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

Table 1: Wyckoff site: 2a, site symmetry: 23.

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

Table 2: Wyckoff site: 6b, site symmetry: 222..

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

Table 3: Wyckoff site: 6c, site symmetry: -4..

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

Table 4: Wyckoff site: 6d, site symmetry: -4..

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

Table 5: Wyckoff site: 8e, site symmetry: .3.

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

Table 6: Wyckoff site: 12f, site symmetry: 2..

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

Table 7: Wyckoff site: 12g, 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	[0, x + $\frac{1}{2}$ , $\frac{1}{2}$ ]	[13,16]
8	[0, $\frac{1}{2}$ - x, $\frac{1}{2}$ ]	[14,15]
9	[x + $\frac{1}{2}$ , $\frac{1}{2}$ , 0]	[17,20]
10	[ $\frac{1}{2}$ - x, $\frac{1}{2}$ , 0]	[18,19]
11	[ $\frac{1}{2}$ , 0, x + $\frac{1}{2}$ ]	[21,24]
12	[ $\frac{1}{2}$ , 0, $\frac{1}{2}$ - x]	[22,23]

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

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

Table 9: Wyckoff site: 24i, 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	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[14]
15	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[15]
16	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[16]
17	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[17]
18	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[18]
19	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[19]
20	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[20]
21	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[21]
22	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[22]
23	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[23]
24	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[24]