

SG No. 220 T_d^6 $I\bar{4}3d$ [cubic]

* plus set: $+[0, 0, 0]$, $+\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

Table 1: Wyckoff site: 12a, site symmetry: -4..

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

Table 2: Wyckoff site: 12b, site symmetry: -4..

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

Table 3: Wyckoff site: 16c, site symmetry: .3.

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

Table 4: Wyckoff site: 24d, site symmetry: 2..

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	$[1, 4]$
2	$\left[\frac{1}{2} - x, 0, \frac{3}{4}\right]$	$[2, 3]$
3	$\left[\frac{1}{4}, x, 0\right]$	$[5, 8]$

continued ...

Table 4

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

Table 5: Wyckoff site: 48e, site symmetry: 1

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