

SG No. 201 T_h^2 $Pn\bar{3}$ [cubic]

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

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

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

Table 2: Wyckoff site: 4b, site symmetry: .-3.

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

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

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

Table 4: Wyckoff site: 6d, site symmetry: 222..

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

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

No.	position	mapping
1	[x, x, x]	[1,5,9]

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 12g, site symmetry: 2..

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

Table 8: Wyckoff site: 24h, site symmetry: 1

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