

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]