

SG No. 206  $T_h^7$   $Ia\bar{3}$  [ cubic ]

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

Table 1: Wyckoff site: 8a, site symmetry:  $\bar{3}$ .

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

Table 2: Wyckoff site: 8b, site symmetry:  $\bar{3}$ .

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

Table 3: Wyckoff site: 16c, site symmetry:  $\bar{3}$ .

No.	position	mapping
1	$[x, x, x]$	$[1, 5, 9]$
2	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	$[2, 7, 12]$
3	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	$[3, 8, 10]$
4	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	$[4, 6, 11]$
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	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	$[16, 18, 23]$

Table 4: Wyckoff site: 24d, site symmetry:  $2\bar{3}$ .

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	$[1, 4]$
2	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	$[2, 3]$
3	$[\frac{1}{4}, x, 0]$	$[5, 8]$
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	$[-x, 0, \frac{3}{4}]$	$[13, 16]$

*continued ...*

Table 4

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