

SG No. 205  $T_h^6$   $Pa\bar{3}$  [ cubic ]

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

Table 1: Wyckoff site: 4a, site symmetry: .-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: 4b, site symmetry: .-3.

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

Table 3: Wyckoff site: 8c, site symmetry: .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: 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]

*continued ...*

Table 4

No.	position	mapping
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]