

SG No. 219  $T_d^5$   $F\bar{4}3c$  [ cubic ]

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

Table 1: Wyckoff site: 8a, site symmetry: 23.

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

Table 2: Wyckoff site: 8b, 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 3: Wyckoff site: 24c, site symmetry:  $-4..$

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

Table 4: Wyckoff site: 24d, site symmetry:  $-4..$

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

Table 5: Wyckoff site: 32e, site symmetry:  $.3.$

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

*continued ...*

Table 5

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

Table 6: Wyckoff site: 48f, site symmetry: 2 . .

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

Table 7: Wyckoff site: 48g, site symmetry: 2 . .

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

Table 8: Wyckoff site: **96h**, site symmetry: 1

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