

MSG No. 135.486  $P4'_2/mb'c$  [ Type III, tetragonal ]

Table 1: Wyckoff site: 4a, site symmetry:  $2/\mathfrak{m}..$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 5, 6]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, 4, 7, 8]$
3	$[0, 0, \frac{1}{2}]$	$[9, 10, 13, 14]$
4	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11, 12, 15, 16]$

Table 2: Wyckoff site: 4b, site symmetry:  $-4'..$

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 2, 13, 14]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[3, 4, 15, 16]$
3	$[0, 0, \frac{3}{4}]$	$[5, 6, 9, 10]$
4	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[7, 8, 11, 12]$

Table 3: Wyckoff site: 4c, site symmetry:  $2/\mathfrak{m}..$

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 2, 5, 6]$
2	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 4, 7, 8]$
3	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[9, 10, 13, 14]$
4	$[\frac{1}{2}, 0, 0]$	$[11, 12, 15, 16]$

Table 4: Wyckoff site: 4d, site symmetry:  $2.22$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 2, 3, 4]$
2	$[0, \frac{1}{2}, \frac{3}{4}]$	$[5, 6, 7, 8]$
3	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[9, 10, 11, 12]$
4	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[13, 14, 15, 16]$

Table 5: Wyckoff site: 8e, site symmetry:  $2..$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[3, 4]$

*continued ...*

Table 5

No.	position	mapping
3	$[0, 0, -z]$	$[5, 6]$
4	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 8]$
5	$[0, 0, z + \frac{1}{2}]$	$[9, 10]$
6	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[11, 12]$
7	$[0, 0, \frac{1}{2} - z]$	$[13, 14]$
8	$[\frac{1}{2}, \frac{1}{2}, z]$	$[15, 16]$

Table 6: Wyckoff site: **8f**, site symmetry:  $2..$ 

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 2]$
2	$[0, \frac{1}{2}, \frac{1}{2} - z]$	$[3, 4]$
3	$[0, \frac{1}{2}, -z]$	$[5, 6]$
4	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 8]$
5	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[9, 10]$
6	$[\frac{1}{2}, 0, -z]$	$[11, 12]$
7	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[13, 14]$
8	$[\frac{1}{2}, 0, z]$	$[15, 16]$

Table 7: Wyckoff site: **8g**, site symmetry:  $..2$ 

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{4}]$	$[1, 3]$
2	$[-x, \frac{1}{2} - x, \frac{1}{4}]$	$[2, 4]$
3	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	$[5, 7]$
4	$[x, x + \frac{1}{2}, \frac{3}{4}]$	$[6, 8]$
5	$[\frac{1}{2} - x, x, \frac{3}{4}]$	$[9, 12]$
6	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	$[10, 11]$
7	$[x + \frac{1}{2}, -x, \frac{1}{4}]$	$[13, 16]$
8	$[\frac{1}{2} - x, x, \frac{1}{4}]$	$[14, 15]$

Table 8: Wyckoff site: **8h**, site symmetry:  $m..$ 

No.	position	mapping
1	$[x, y, 0]$	$[1, 6]$
2	$[-x, -y, 0]$	$[2, 5]$
3	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[3, 8]$
4	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2}]$	$[4, 7]$
5	$[-y, x, \frac{1}{2}]$	$[9, 14]$

*continued ...*

Table 8

No.	position	mapping
6	$[y, -x, \frac{1}{2}]$	[10, 13]
7	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[11, 16]
8	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[12, 15]

Table 9: Wyckoff site: 16i, site symmetry: 1

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