

MSG No. 62.453  $P_{Anma}$  [ Type IV, orthorhombic ]

Table 1: Wyckoff site: 4a, site symmetry:  $.2'/m$ .

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $m'm2'$

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

Table 4: Wyckoff site: 8d, site symmetry:  $-1$

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

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

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

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

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

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

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

Table 8: Wyckoff site: **16h**, site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	$[2]$
3	$[-x, y + \frac{1}{2}, -z]$	$[3]$

*continued ...*

Table 8

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