

MSG No. 62.456 $P1nma$ [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $.2'/m.$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $m'm2'$

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	$[1, 7, 12, 14]$
2	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	$[2, 8, 11, 13]$

continued ...

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site: $8i$, site symmetry: $.m$.

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

Table 10: Wyckoff site: $16j$, 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]
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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[x, -y, -z]$	[10]
11	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[11]
12	$[-x, \frac{1}{2} - y, z]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[13]
14	$[-x, y, z]$	[14]
15	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[15]
16	$[x, y + \frac{1}{2}, -z]$	[16]