

MSG No. 62.456 $P\bar{1}nma$ [Type IV, orthorhombic]

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

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: $2'/\bar{m}'..$

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: $.2'/\bar{m}$.

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: $.2'/\bar{m}$.

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: $\bar{m}'m2'$

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: $\bar{4}2m$.

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: $\bar{4}2m$.

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]