

MSG No. 74.557 *Imma'* [Type III, orthorhombic]

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

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

Table 2: Wyckoff site: **4b**, site symmetry: $2'/\text{m..}$

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

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

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

Table 4: Wyckoff site: **4d**, site symmetry: $.2'/\text{m.}$

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

Table 5: Wyckoff site: **4e**, site symmetry: **mm2**

No.	position	mapping
1	[0, $\frac{1}{4}$, z]	[1,2,3,4]
2	[0, $\frac{3}{4}$, $-z$]	[5,6,7,8]

continued ...

Table 5

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: 16j, site symmetry: 1

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