

MSG No. 127.391 $P4'/mbm'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $4'..$

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

Table 6: Wyckoff site: **4f**, site symmetry: $2 \cdot m' \bar{m}'$

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

Table 7: Wyckoff site: **4g**, site symmetry: $m \cdot 2' \bar{m}'$

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

Table 8: Wyckoff site: **4h**, site symmetry: $m \cdot 2' \bar{m}'$

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

Table 9: Wyckoff site: **8i**, site symmetry: $m \cdot \cdot$

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

Table 10: Wyckoff site: 8j, site symmetry: $\mathbf{m} \cdot \cdot$

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

Table 11: Wyckoff site: 8k, site symmetry: $\cdot \cdot \mathbf{m}'$

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

Table 12: Wyckoff site: 16l, site symmetry: 1

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