

MSG No. 136.502 $P4'_2/m'nm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $m' \cdot m'm'$

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

Table 2: Wyckoff site: 2b, site symmetry: $m' \cdot m'm'$

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $-4 \dots$

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

Table 5: Wyckoff site: 4e, site symmetry: $2 \cdot m'm'$

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

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

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

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

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

Table 8: Wyckoff site: **8h**, site symmetry: $2..$

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

Table 9: Wyckoff site: **8i**, site symmetry: $\text{m'}..$

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

Table 10: Wyckoff site: 8j, site symmetry: . .m'

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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