

MSG No. 132.454 $P4'_2/m'cm'$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: $-42'm'$

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

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

No.	position	mapping
1	[$\frac{1}{2}$, $\frac{1}{2}$, 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 4: Wyckoff site: 2d, site symmetry: $-42'm'$

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

Table 5: Wyckoff site: 4e, site symmetry: $22'2'.$

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

Table 6: Wyckoff site: **4f**, site symmetry: $2/m'..$

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

Table 7: Wyckoff site: **4g**, site symmetry: $2.m'm'$

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

Table 8: Wyckoff site: **4h**, site symmetry: $2.m'm'$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 2, 15, 16]$
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[3, 4, 13, 14]$
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 9: Wyckoff site: **4i**, site symmetry: $m'.2m'$

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

Table 10: Wyckoff site: **4j**, site symmetry: $m'.2m'$

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

Table 11: Wyckoff site: 8k, site symmetry: 2..

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

Table 12: Wyckoff site: 8l, site symmetry: .2'.

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

Table 13: Wyckoff site: 8m, site symmetry: .2'.

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

Table 14: Wyckoff site: 8n, site symmetry: m'..

No.	position	mapping
1	$[x, y, 0]$	[1,14]
2	$[-x, -y, 0]$	[2,13]
3	$[y, x, 0]$	[3,16]

continued ...

Table 14

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

Table 15: Wyckoff site: 8o, 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	$[x, -x, \frac{1}{2} - z]$	[5,11]
6	$[-x, x, \frac{1}{2} - z]$	[6,12]
7	$[-x, x, z + \frac{1}{2}]$	[7,9]
8	$[x, -x, z + \frac{1}{2}]$	[8,10]

Table 16: Wyckoff site: 16p, 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	$[y, -x, \frac{1}{2} - z]$	[5]
6	$[-y, x, \frac{1}{2} - z]$	[6]
7	$[-x, y, z + \frac{1}{2}]$	[7]
8	$[x, -y, z + \frac{1}{2}]$	[8]
9	$[-y, x, z + \frac{1}{2}]$	[9]
10	$[y, -x, z + \frac{1}{2}]$	[10]
11	$[x, -y, \frac{1}{2} - z]$	[11]
12	$[-x, y, \frac{1}{2} - z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[x, y, -z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]