

MSG No. 84.52 $P4_2/m1'$ [Type II, tetragonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: 2/m..1'

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

Table 3: Wyckoff site: 2c, site symmetry: 2/m..1'

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

Table 4: Wyckoff site: 2d, site symmetry: 2/m..1'

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

Table 5: Wyckoff site: 2e, site symmetry: -4..1'

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

Table 6: Wyckoff site: 2f, site symmetry: -4..1'

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

Table 7: Wyckoff site: 4g, site symmetry: 2..1'

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

Table 8: Wyckoff site: 4h, site symmetry: 2..1'

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

Table 9: Wyckoff site: 4i, site symmetry: 2..1'

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

Table 10: Wyckoff site: 4j, site symmetry: m..1'

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

Table 11: Wyckoff site: 8k, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1,9]
2	[-y, x, $z + \frac{1}{2}$]	[2,10]
3	[y, -x, $z + \frac{1}{2}$]	[3,11]
4	[-x, -y, z]	[4,12]

continued ...

Table 11

No.	position	mapping
5	$[-x, -y, -z]$	[5,13]
6	$[y, -x, \frac{1}{2} - z]$	[6,14]
7	$[-y, x, \frac{1}{2} - z]$	[7,15]
8	$[x, y, -z]$	[8,16]