

MSG No. 101.180 $P4_2cm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 2.mmm1'

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

Table 2: Wyckoff site: 2b, site symmetry: 2.mmm1'

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

Table 3: Wyckoff site: 4c, 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, $\frac{1}{2}$, $z + \frac{1}{2}$]	[5,6,13,14]
4	[$\frac{1}{2}$, 0, z]	[7,8,15,16]

Table 4: Wyckoff site: 4d, site symmetry: ..m1'

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

Table 5: Wyckoff site: 8e, 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]
5	[$-x$, y, $z + \frac{1}{2}$]	[5,13]
6	[x, $-y$, $z + \frac{1}{2}$]	[6,14]

continued ...

Table 5

No.	position	mapping
7	$[-y, -x, z]$	[7,15]
8	$[y, x, z]$	[8,16]