

MSG No. 101.179 $P4_2cm$ [Type I, tetragonal]

Table 1: Wyckoff site: **2a**, site symmetry: **2.m̄m**

No.	position	mapping
1	[0, 0, z]	[1, 4, 7, 8]
2	[0, 0, $z + \frac{1}{2}$]	[2, 3, 5, 6]

Table 2: Wyckoff site: **2b**, site symmetry: **2.m̄m**

No.	position	mapping
1	[$\frac{1}{2}$, $\frac{1}{2}$, z]	[1, 4, 7, 8]
2	[$\frac{1}{2}$, $\frac{1}{2}$, $z + \frac{1}{2}$]	[2, 3, 5, 6]

Table 3: Wyckoff site: **4c**, site symmetry: **2..**

No.	position	mapping
1	[0, $\frac{1}{2}$, z]	[1, 4]
2	[$\frac{1}{2}$, 0, $z + \frac{1}{2}$]	[2, 3]
3	[0, $\frac{1}{2}$, $z + \frac{1}{2}$]	[5, 6]
4	[$\frac{1}{2}$, 0, z]	[7, 8]

Table 4: Wyckoff site: **4d**, site symmetry: **..m̄**

No.	position	mapping
1	[x, x, z]	[1, 8]
2	[$-x$, x, $z + \frac{1}{2}$]	[2, 5]
3	[x, $-x$, $z + \frac{1}{2}$]	[3, 6]
4	[$-x$, $-x$, z]	[4, 7]

Table 5: Wyckoff site: **8e**, site symmetry: **1**

No.	position	mapping
1	[x, y, z]	[1]
2	[$-y$, x, $z + \frac{1}{2}$]	[2]
3	[y, $-x$, $z + \frac{1}{2}$]	[3]
4	[$-x$, $-y$, z]	[4]
5	[$-x$, y, $z + \frac{1}{2}$]	[5]
6	[x, $-y$, $z + \frac{1}{2}$]	[6]

continued ...

Table 5

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