

MSG No. 57.385 $Pb'c'm'$ [Type III, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: **-1'**

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

Table 2: Wyckoff site: **4b**, site symmetry: **-1'**

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

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

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

Table 4: Wyckoff site: **4d**, site symmetry: **..m'**

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

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

No.	position	mapping
1	[x , y , z]	[1]
2	[x , $\frac{1}{2} - y$, $-z$]	[2]

continued ...

Table 5

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