

MSG No. 57.378 *Pbcm1'* [Type II, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: **-11'**

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

Table 2: Wyckoff site: **4b**, site symmetry: **-11'**

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

Table 3: Wyckoff site: **4c**, site symmetry: **2..1'**

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: **11'**

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

continued ...

Table 5

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