

MSG No. 52.306 *Pnna1'* [Type II, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: **. . 21'**

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

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

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

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

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

continued ...

Table 5

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