

MSG No. 52.307 *Pn'na* [ Type III, orthorhombic ]

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 5

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