

MSG No. 52.311 $Pnn'a'$ [Type III, orthorhombic]

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

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

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

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

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	[$\frac{3}{4}$, 0, $-z$]	[3,8]
4	[$\frac{3}{4}$, $\frac{1}{2}$, $z + \frac{1}{2}$]	[4,7]

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

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