

MSG No. 11.55 P_a2_1/m [Type IV, monoclinic]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: **-1**

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

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

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

Table 5: Wyckoff site: **4e**, site symmetry: **m**

No.	position	mapping
1	[x , $\frac{1}{4}$, z]	[1,4]
2	[$-x$, $\frac{3}{4}$, $-z$]	[2,3]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 1

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