

MSG No. 13.70 P_a2/c [Type IV, monoclinic]

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

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

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

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

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

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

Table 5: Wyckoff site: **4e**, site symmetry: **2**

No.	position	mapping
1	[0, y , $\frac{1}{4}$]	[1,2]
2	[0, $-y$, $\frac{3}{4}$]	[3,4]

continued ...

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry: 2²

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

Table 7: Wyckoff site: 8g, 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	$[x, -y, z + \frac{1}{2}]$	[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	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[8]