

MSG No. 15.86 $C2/c1'$ [Type II, monoclinic]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: -11'

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

Table 4: Wyckoff site: 4d, site symmetry: -11'

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

Table 5: Wyckoff site: 4e, site symmetry: 21'

No.	position	mapping
1	[0, y , $\frac{1}{4}$]	[1, 2, 9, 10]
2	[0, $-y$, $\frac{3}{4}$]	[3, 4, 11, 12]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 11'

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