

MSG No. 12.59 $C2/m1'$ [Type II, monoclinic]

Table 1: Wyckoff site: 2a, site symmetry: $2/m1'$

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

Table 2: Wyckoff site: 2b, site symmetry: $2/m1'$

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

Table 3: Wyckoff site: 2c, site symmetry: $2/m1'$

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

Table 4: Wyckoff site: 2d, site symmetry: $2/m1'$

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

Table 5: Wyckoff site: 4e, 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}, 0]	[2, 8, 10, 16]
3	[\frac{3}{4}, \frac{3}{4}, 0]	[3, 5, 11, 13]
4	[\frac{1}{4}, \frac{3}{4}, 0]	[4, 6, 12, 14]

Table 6: Wyckoff site: 4f, site symmetry: -11'

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

Table 7: Wyckoff site: 4g, site symmetry: 21'

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

Table 8: Wyckoff site: 4h, site symmetry: 21'

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

Table 9: Wyckoff site: 4i, site symmetry: m1'

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

Table 10: Wyckoff site: 8j, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1, 9]
2	$[-x, y, -z]$	[2, 10]
3	$[-x, -y, -z]$	[3, 11]
4	$[x, -y, z]$	[4, 12]

continued ...

Table 10

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