

MSG No. 15.90 C_2/c [Type IV, monoclinic]

Table 1: Wyckoff site: 4a, site symmetry: $2/m'$

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

Table 2: Wyckoff site: 4b, site symmetry: $2/m'$

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

Table 3: Wyckoff site: 4c, site symmetry: $2'/m'$

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $-1'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1, 15]$
2	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[2, 16]$

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: $8g$, site symmetry: 2

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

Table 8: Wyckoff site: $8h$, site symmetry: $2'$

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

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[6,13]
7	$[\frac{1}{2}, \frac{1}{2} - y, 0]$	[7,16]
8	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[8,15]

Table 9: Wyckoff site: 8i, site symmetry: m'

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

Table 10: Wyckoff site: 16j, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[5]
6	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[6]
7	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[7]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[8]
9	$[x, y, z + \frac{1}{2}]$	[9]
10	$[-x, y, -z]$	[10]
11	$[-x, -y, \frac{1}{2} - z]$	[11]
12	$[x, -y, z]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[14]
15	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[16]