

MSG No. 66.493 $Cc'm$ [Type III, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $22'2'$

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

Table 2: Wyckoff site: 4b, site symmetry: $22'2'$

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $\dots 2'/m$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 4, 14, 15]$
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	$[2, 3, 13, 16]$

continued ...

Table 5

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

Table 6: Wyckoff site: $4f$, site symmetry: $\dots 2'/m$

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

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

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: $\dots 2'$

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

Table 10: Wyckoff site: 8j, site symmetry: $\dots 2'$

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

Table 11: Wyckoff site: 8k, site symmetry: $\dots 2'$

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

Table 12: Wyckoff site: 8l, site symmetry: $\dots m$

No.	position	mapping
1	$[x, y, 0]$	$[1, 4]$
2	$[x, -y, \frac{1}{2}]$	$[2, 3]$
3	$[-x, y, \frac{1}{2}]$	$[5, 8]$

continued ...

Table 12

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

Table 13: Wyckoff site: $16m$, site symmetry: 1

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