

MSG No. 63.457 *Cmcm* [Type I, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: $2/m\ldots$

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

Table 2: Wyckoff site: **4b**, site symmetry: $2/m\ldots$

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

Table 3: Wyckoff site: **4c**, site symmetry: $m\bar{2}m$

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

Table 4: Wyckoff site: **8d**, site symmetry: -1

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

Table 5: Wyckoff site: 8e, site symmetry: 2..

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

Table 6: Wyckoff site: 8f, site symmetry: m..

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

Table 7: Wyckoff site: 8g, site symmetry: ..m

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

Table 8: Wyckoff site: 16h, site symmetry: 1

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

continued ...

Table 8

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