

MSG No. 64.473 *Cmca'* [Type III, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $2'/\text{m..}$

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

Table 2: Wyckoff site: 4b, site symmetry: $2'/\text{m..}$

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

Table 3: Wyckoff site: 8c, site symmetry: $-1'$

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

Table 4: Wyckoff site: 8d, site symmetry: $2'..$

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

Table 5: Wyckoff site: 8e, site symmetry: .2¹.

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

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

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

Table 7: Wyckoff site: 16g, site symmetry: 1

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