

MSG No. 64.469 *Cmca* [Type I, orthorhombic]

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

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

Table 2: Wyckoff site: 4b, site symmetry: 2/m..

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

Table 3: Wyckoff site: 8c, 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{1}{4}, \frac{1}{4}, \frac{1}{2}]	[3,15]
4	[\frac{1}{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{3}{4}, \frac{3}{4}, \frac{1}{2}]	[7,11]
8	[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]	[8,12]

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

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

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

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

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

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

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

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