

MSG No. 57.390 P_Bbcm [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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