

MSG No. 59.413  $P_cmmn$  [ Type IV, orthorhombic ]

Table 1: Wyckoff site: 4a, site symmetry:  $mm2$

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

Table 2: Wyckoff site: 4b, site symmetry:  $mm2$

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

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

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

Table 4: Wyckoff site: 8d, site symmetry:  $-1'$

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

Table 5: Wyckoff site: **8e**, site symmetry:  $\bar{m}$ .

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

Table 6: Wyckoff site: **8f**, site symmetry:  $\bar{m}$ .

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

Table 7: Wyckoff site: **16g**, site symmetry:  $\bar{1}$ 

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