

MSG No. 57.391  $P_Cbcm$  [ Type IV, orthorhombic ]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry:  $m'2'm$

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

Table 4: Wyckoff site: **8d**, 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	$[\frac{1}{2}, \frac{1}{2}, 0]$	[9, 13]
6	$[\frac{1}{2}, 0, 0]$	[10, 14]
7	$[\frac{1}{2}, 0, \frac{1}{2}]$	[11, 15]
8	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[12, 16]

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

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

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

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

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

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,8]
2	$[x, \frac{1}{2} - y, \frac{3}{4}]$	[2,7]
3	$[-x, y + \frac{1}{2}, \frac{1}{4}]$	[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	$[x + \frac{1}{2}, -y, \frac{3}{4}]$	[10,15]
7	$[\frac{1}{2} - x, y, \frac{1}{4}]$	[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	$[x, \frac{1}{2} - y, -z]$	[2]
3	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]

*continued ...*

Table 8

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