

MSG No. 54.349 *P_{Acca}* [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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