

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:  $\dots 2$ 

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:  $\dots m'$ 

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	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	$[16]$