

MSG No. 55.360 P_abam [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: $\dots 2/\text{m}$

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

Table 4: Wyckoff site: **4d**, site symmetry: $\dots 2/\text{m}$

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

Table 5: Wyckoff site: **4e**, site symmetry: $2'm'm$

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1, 8, 10, 15]
2	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[2, 7, 9, 16]

continued ...

Table 5

No.	position	mapping
3	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[3,6,12,13]
4	$[-x, \frac{3}{4}, 0]$	[4,5,11,14]

Table 6: Wyckoff site: 4f, site symmetry: 2'm'm

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

Table 7: Wyckoff site: 8g, site symmetry: ...2'

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

Table 8: Wyckoff site: 8h, site symmetry: ...2

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

Table 9: Wyckoff site: 8i, site symmetry: $\dots\bar{m}$

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

Table 10: Wyckoff site: 8j, site symmetry: $\dots\bar{m}$

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

Table 11: Wyckoff site: 8k, site symmetry: $.m'$.

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

Table 12: Wyckoff site: 16l, site symmetry: 1

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

continued ...

Table 12

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