

MSG No. 55.361 P_cbam [Type IV, orthorhombic]

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

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

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

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

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: $\dots 2$

No.	position	mapping
1	[0, 0, z]	[1, 4]
2	[\frac{1}{2}, \frac{1}{2}, -z]	[2, 3]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: ..2

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

Table 7: Wyckoff site: 8g, site symmetry: ..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	$[x, y, \frac{1}{2}]$	[9,16]
6	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[10,15]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[11,14]
8	$[-x, -y, \frac{1}{2}]$	[12,13]

Table 8: Wyckoff site: 8h, site symmetry: ..m'

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

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, 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]
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	$[x, y, z + \frac{1}{2}]$	[9]
10	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[-x, -y, z + \frac{1}{2}]$	[12]
13	$[-x, -y, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[14]
15	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[15]
16	$[x, y, \frac{1}{2} - z]$	[16]