

MSG No. 62.452 $P_c nma$ [Type IV, orthorhombic]

Table 1: Wyckoff site: 8a, site symmetry: $-1'$

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

Table 2: Wyckoff site: 8b, site symmetry: -1

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

Table 3: Wyckoff site: 8c, site symmetry: $..2'$

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

Table 4: Wyckoff site: **8d**, site symmetry: $\bar{4}m$.

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

Table 5: Wyckoff site: **16e**, site symmetry: $\bar{4}m$.

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