

MSG No. 90.100  $P_c42_12$  [ Type IV, tetragonal ]

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

Table 2: Wyckoff site: 4b, site symmetry: 2.2'2'

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

Table 3: Wyckoff site: 4c, site symmetry: 4. .

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

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

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

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

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

Table 6: Wyckoff site: **8f**, site symmetry:  $\dots 2'$ 

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

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

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