

MSG No. 94.132 $P_c4_22_12$ [Type IV, tetragonal]

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

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

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

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

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

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

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

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