

MSG No. 97.155  $I4'2'2$  [ Type III, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $4'2'2$

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $22'2'$ .

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

Table 4: Wyckoff site: 4d, site symmetry:  $2.22$

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

Table 5: Wyckoff site: 4e, site symmetry:  $4'..$

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

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

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

Table 7: Wyckoff site: **8g**, site symmetry:  $..2$ 

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

Table 8: Wyckoff site: **8h**, site symmetry:  $.2'$ 

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

Table 9: Wyckoff site: **8i**, site symmetry:  $.2'$ 

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	$[1, 7]$
2	$[-x, 0, \frac{1}{2}]$	$[2, 8]$
3	$[0, x, \frac{1}{2}]$	$[3, 5]$

*continued ...*

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry:  $\cdot \cdot 2$ 

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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