

# MSG No. 98.157 $I4_122$ [ Type I, tetragonal ]

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

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

Table 2: Wyckoff site: 4b, site symmetry: 2.22

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: ...2

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

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

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

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

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