

MSG No. 122.337 $I\bar{4}2'd'$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: $-4..$

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

Table 2: Wyckoff site: 4b, site symmetry: $-4..$

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

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

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

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

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

Table 5: Wyckoff site: **16e**, 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	$[x, \frac{1}{2} - y, \frac{1}{4} - z]$	[5]
6	$[-x, y + \frac{1}{2}, \frac{1}{4} - z]$	[6]
7	$[-y, \frac{1}{2} - x, z + \frac{1}{4}]$	[7]
8	$[y, x + \frac{1}{2}, z + \frac{1}{4}]$	[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	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[12]
13	$[x + \frac{1}{2}, -y, \frac{3}{4} - z]$	[13]
14	$[\frac{1}{2} - x, y, \frac{3}{4} - z]$	[14]
15	$[\frac{1}{2} - y, -x, z + \frac{3}{4}]$	[15]
16	$[y + \frac{1}{2}, x, z + \frac{3}{4}]$	[16]