

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]