

MSG No. 122.333 $I\bar{4}2d$ [Type I, tetragonal]

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

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

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

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

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

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

Table 5: Wyckoff site: **16e**, site symmetry: 1

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