

MSG No. 122.335 $I\bar{4}'2'd$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: $-4' \dots$

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

Table 2: Wyckoff site: 4b, site symmetry: $-4' \dots$

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

Table 3: Wyckoff site: 8c, site symmetry: $2 \dots$

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

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

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