

MSG No. 122.334 $I\bar{4}2d1'$ [Type II, tetragonal]

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 4, 5, 6, 17, 20, 21, 22]$
2	$[0, \frac{1}{2}, \frac{1}{4}]$	$[2, 3, 7, 8, 18, 19, 23, 24]$
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9, 12, 13, 14, 25, 28, 29, 30]$
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[10, 11, 15, 16, 26, 27, 31, 32]$

Table 2: Wyckoff site: 4b, site symmetry: $-4..1'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 4, 5, 6, 17, 20, 21, 22]$
2	$[0, \frac{1}{2}, \frac{3}{4}]$	$[2, 3, 7, 8, 18, 19, 23, 24]$
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 12, 13, 14, 25, 28, 29, 30]$
4	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[10, 11, 15, 16, 26, 27, 31, 32]$

Table 3: Wyckoff site: 8c, site symmetry: $2..1'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 17, 20]$
2	$[0, \frac{1}{2}, \frac{1}{4} - z]$	$[2, 3, 18, 19]$
3	$[0, 0, -z]$	$[5, 6, 21, 22]$
4	$[0, \frac{1}{2}, z + \frac{1}{4}]$	$[7, 8, 23, 24]$
5	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[9, 12, 25, 28]$
6	$[\frac{1}{2}, 0, \frac{3}{4} - z]$	$[10, 11, 26, 27]$
7	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[13, 14, 29, 30]$
8	$[\frac{1}{2}, 0, z + \frac{3}{4}]$	$[15, 16, 31, 32]$

Table 4: Wyckoff site: 8d, site symmetry: $.2.1'$

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{8}]$	$[1, 2, 17, 18]$
2	$[-x, \frac{3}{4}, \frac{1}{8}]$	$[3, 4, 19, 20]$
3	$[\frac{1}{4}, -x, \frac{7}{8}]$	$[5, 15, 21, 31]$
4	$[\frac{3}{4}, x, \frac{7}{8}]$	$[6, 16, 22, 32]$
5	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{8}]$	$[7, 13, 23, 29]$
6	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{8}]$	$[8, 14, 24, 30]$
7	$[x + \frac{1}{2}, \frac{3}{4}, \frac{5}{8}]$	$[9, 10, 25, 26]$
8	$[\frac{1}{2} - x, \frac{1}{4}, \frac{5}{8}]$	$[11, 12, 27, 28]$

Table 5: Wyckoff site: $16\mathbf{e}$, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[x, \frac{1}{2} - y, \frac{1}{4} - z]$	$[2, 18]$
3	$[-x, y + \frac{1}{2}, \frac{1}{4} - z]$	$[3, 19]$
4	$[-x, -y, z]$	$[4, 20]$
5	$[y, -x, -z]$	$[5, 21]$
6	$[-y, x, -z]$	$[6, 22]$
7	$[-y, \frac{1}{2} - x, z + \frac{1}{4}]$	$[7, 23]$
8	$[y, x + \frac{1}{2}, z + \frac{1}{4}]$	$[8, 24]$
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 25]$
10	$[x + \frac{1}{2}, -y, \frac{3}{4} - z]$	$[10, 26]$
11	$[\frac{1}{2} - x, y, \frac{3}{4} - z]$	$[11, 27]$
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[12, 28]$
13	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	$[13, 29]$
14	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	$[14, 30]$
15	$[\frac{1}{2} - y, -x, z + \frac{3}{4}]$	$[15, 31]$
16	$[y + \frac{1}{2}, x, z + \frac{3}{4}]$	$[16, 32]$