

MSG No. 88.82 $I4_1/a1'$ [Type II, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: $-11'$

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

Table 4: Wyckoff site: 8d, site symmetry: $-11'$

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

Table 5: Wyckoff site: **8e**, site symmetry: $2..1'$

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

Table 6: Wyckoff site: **16f**, site symmetry: $11'$

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