

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]