

Table 1: Wyckoff site: 4a, site symmetry: $2'/m'$. .

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

Table 2: Wyckoff site: 4b, site symmetry: $2'/m'$. .

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

Table 3: Wyckoff site: 4c, site symmetry: $m'2m'$

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

Table 4: Wyckoff site: 8d, site symmetry: $-1'$

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: m' . .

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

Table 7: Wyckoff site: 8g, site symmetry: $..m'$

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

Table 8: Wyckoff site: 16h, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[2]
3	$[-x, y, \frac{1}{2} - z]$	[3]

continued ...

Table 8

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