

Table 1: Wyckoff site: 2a, site symmetry: $-4m2$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4m2$

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

Table 3: Wyckoff site: 4c, site symmetry: $2mm$.

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

Table 4: Wyckoff site: 4d, site symmetry: $2mm$.

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

Table 5: Wyckoff site: 8e, site symmetry: $-1'$

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

continued ...

Table 5

No.	position	mapping
7	$[\frac{1}{2}, 0, 0]$	[7, 11]
8	$[0, \frac{1}{2}, 0]$	[8, 12]

Table 6: Wyckoff site: 8f, site symmetry: $\dots 2$

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[2]
3	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[-y, -x, \frac{1}{2} - z]$	[4]
5	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[5]
6	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[6]
7	$[\frac{1}{2} - x, y, z]$	[7]
8	$[x, \frac{1}{2} - y, z]$	[8]
9	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[9]

continued ...

Table 8

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