

Table 1: Wyckoff site: 4a, site symmetry: 2'2'2

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

Table 2: Wyckoff site: 4b, site symmetry: 2'2'2

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1,15]
2	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[2,16]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: $2'$. .

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

Table 7: Wyckoff site: 8g, site symmetry: $.2'$.

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

Table 8: Wyckoff site: 8h, site symmetry: $. . 2$

No.	position	mapping
1	$[0, 0, z]$	[1, 2]
2	$[0, 0, z + \frac{1}{2}]$	[3, 4]
3	$[0, 0, \frac{1}{2} - z]$	[5, 6]
4	$[0, 0, -z]$	[7, 8]
5	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9, 10]

continued ...

Table 8

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

Table 9: Wyckoff site: 8i, site symmetry: $\dots 2$

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

Table 10: Wyckoff site: 8j, site symmetry: $\dots m'$

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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

continued ...

Table 11

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