

Table 1: Wyckoff site: **4a**, site symmetry: $22'2'$.

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

Table 2: Wyckoff site: **4b**, site symmetry: $22'2'$.

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

Table 3: Wyckoff site: **4c**, site symmetry: $-4'$.

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

Table 4: Wyckoff site: **4d**, site symmetry: -4 .

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

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

No.	position	mapping
1	$[\frac{1}{2}, y, \frac{1}{4}]$	[1,11]
2	$[0, \frac{1}{2} - y, \frac{1}{4}]$	[2,12]

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

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

Table 9: Wyckoff site: 8i, site symmetry: $2'..$

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

Table 10: Wyckoff site: 16j, site symmetry: 1

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