

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 2.mm

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

continued ...

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site: **8i**, site symmetry: $\bar{3}m$

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

Table 10: Wyckoff site: **16j**, site symmetry: $\bar{1}$

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