

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $4'..$

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

Table 6: Wyckoff site: 4f, site symmetry: 2.mm

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

Table 7: Wyckoff site: 4g, site symmetry: m.2m

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

Table 8: Wyckoff site: 4h, site symmetry: m.2m

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

Table 9: Wyckoff site: 8i, site symmetry: m..

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

Table 10: Wyckoff site: 8j, site symmetry: $m..$

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

Table 11: Wyckoff site: 8k, site symmetry: $..m$

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

Table 12: Wyckoff site: 16l, site symmetry: 1

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