

Table 1: Wyckoff site: 4a, site symmetry: $\dots 2/m$

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $\dots 2/m'$

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

Table 5: Wyckoff site: 8e, site symmetry: $\dots 2$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4]$
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[2, 3]$

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: 1

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