

Table 1: Wyckoff site: 4a, site symmetry: $mm2$

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $mm2$

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

Table 4: Wyckoff site: 4d, site symmetry: $mm'2'$

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

Table 5: Wyckoff site: 8e, site symmetry: $.m.$

No.	position	mapping
1	$[x, 0, z]$	$[1, 4]$
2	$[-x, 0, z]$	$[2, 3]$

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, y, z]$	[1,3]
2	$[\frac{1}{2}, -y, z]$	[2,4]
3	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[5,7]
4	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[6,8]
5	$[\frac{1}{2}, y, z + \frac{1}{2}]$	[9,11]

continued ...

Table 8

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

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

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