

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $mm2$

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

continued ...

Table 5

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

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

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

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

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

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

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

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

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

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

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