

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

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

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

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

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