

Table 1: Wyckoff site: 4a, site symmetry: $2'22'$

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

Table 2: Wyckoff site: 4b, site symmetry: $2'22'$

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

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

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

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

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

Table 5: Wyckoff site: 4e, 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]

continued ...

Table 5

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

Table 6: Wyckoff site: $4f$, 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	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9, 11, 13, 15]
4	$[0, \frac{1}{2}, \frac{1}{2}]$	[10, 12, 14, 16]

Table 7: Wyckoff site: $4g$, site symmetry: $mm2$

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

Table 8: Wyckoff site: $8h$, site symmetry: $2'..$

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

Table 9: Wyckoff site: $8i$, site symmetry: $2'..$

No.	position	mapping
1	$[x, \frac{3}{4}, \frac{1}{2}]$	[1, 10]
2	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[2, 9]
3	$[-x, \frac{3}{4}, \frac{1}{2}]$	[3, 12]

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, 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	$[\frac{1}{2}, y + \frac{1}{2}, 0]$	[9, 11]
6	$[0, \frac{1}{2} - y, 0]$	[10, 12]
7	$[\frac{1}{2}, \frac{1}{2} - y, 0]$	[13, 15]
8	$[0, y + \frac{1}{2}, 0]$	[14, 16]

Table 11: Wyckoff site: 8k, site symmetry: .2.

No.	position	mapping
1	$[0, y, \frac{1}{2}]$	[1, 3]
2	$[\frac{1}{2}, -y, \frac{1}{2}]$	[2, 4]
3	$[0, -y, \frac{1}{2}]$	[5, 7]
4	$[\frac{1}{2}, y, \frac{1}{2}]$	[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 12: Wyckoff site: 8l, site symmetry: .2'

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

continued ...

Table 12

No.	position	mapping
7	$[0, \frac{1}{4}, z]$	[7,14]
8	$[\frac{1}{2}, \frac{3}{4}, -z]$	[8,13]

Table 13: Wyckoff site: $8m$, site symmetry: m .

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

Table 14: Wyckoff site: $8n$, 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	$[x + \frac{1}{2}, \frac{1}{2}, z]$	[9,15]
6	$[x, \frac{1}{2}, -z]$	[10,16]
7	$[\frac{1}{2} - x, \frac{1}{2}, -z]$	[11,13]
8	$[-x, \frac{1}{2}, z]$	[12,14]

Table 15: Wyckoff site: $16o$, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[9]

continued ...

Table 15

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