

Table 1: Wyckoff site: 2a, site symmetry: $mmm1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 17, 18, 19, 20, 21, 22, 23, 24]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, 11, 12, 13, 14, 15, 16, 25, 26, 27, 28, 29, 30, 31, 32]$

Table 2: Wyckoff site: 2b, site symmetry: $mmm1'$

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 17, 18, 19, 20, 21, 22, 23, 24]$
2	$[0, \frac{1}{2}, 0]$	$[9, 10, 11, 12, 13, 14, 15, 16, 25, 26, 27, 28, 29, 30, 31, 32]$

Table 3: Wyckoff site: 2c, site symmetry: $mmm1'$

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 17, 18, 19, 20, 21, 22, 23, 24]$
2	$[0, \frac{1}{2}, \frac{1}{2}]$	$[9, 10, 11, 12, 13, 14, 15, 16, 25, 26, 27, 28, 29, 30, 31, 32]$

Table 4: Wyckoff site: 2d, site symmetry: $mmm1'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 17, 18, 19, 20, 21, 22, 23, 24]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9, 10, 11, 12, 13, 14, 15, 16, 25, 26, 27, 28, 29, 30, 31, 32]$

Table 5: Wyckoff site: 4e, site symmetry: $..2/m1'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 8, 12, 13, 17, 24, 28, 29]$
2	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[2, 7, 11, 14, 18, 23, 27, 30]$
3	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[3, 6, 10, 15, 19, 22, 26, 31]$
4	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[4, 5, 9, 16, 20, 21, 25, 32]$

Table 6: Wyckoff site: 4f, site symmetry: $\dots 2/m1'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[1, 8, 12, 13, 17, 24, 28, 29]
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[2, 7, 11, 14, 18, 23, 27, 30]
3	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[3, 6, 10, 15, 19, 22, 26, 31]
4	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[4, 5, 9, 16, 20, 21, 25, 32]

Table 7: Wyckoff site: 4g, site symmetry: $2mm1'$

No.	position	mapping
1	$[x, 0, 0]$	[1, 2, 7, 8, 17, 18, 23, 24]
2	$[-x, 0, 0]$	[3, 4, 5, 6, 19, 20, 21, 22]
3	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[9, 10, 15, 16, 25, 26, 31, 32]
4	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[11, 12, 13, 14, 27, 28, 29, 30]

Table 8: Wyckoff site: 4h, site symmetry: $2mm1'$

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1, 2, 7, 8, 17, 18, 23, 24]
2	$[-x, 0, \frac{1}{2}]$	[3, 4, 5, 6, 19, 20, 21, 22]
3	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9, 10, 15, 16, 25, 26, 31, 32]
4	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[11, 12, 13, 14, 27, 28, 29, 30]

Table 9: Wyckoff site: 4i, site symmetry: $m2m1'$

No.	position	mapping
1	$[0, y, 0]$	[1, 3, 6, 8, 17, 19, 22, 24]
2	$[0, -y, 0]$	[2, 4, 5, 7, 18, 20, 21, 23]
3	$[\frac{1}{2}, y + \frac{1}{2}, 0]$	[9, 11, 14, 16, 25, 27, 30, 32]
4	$[\frac{1}{2}, \frac{1}{2} - y, 0]$	[10, 12, 13, 15, 26, 28, 29, 31]

Table 10: Wyckoff site: 4j, site symmetry: $m2m1'$

No.	position	mapping
1	$[0, y, \frac{1}{2}]$	[1, 3, 6, 8, 17, 19, 22, 24]
2	$[0, -y, \frac{1}{2}]$	[2, 4, 5, 7, 18, 20, 21, 23]
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[9, 11, 14, 16, 25, 27, 30, 32]
4	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[10, 12, 13, 15, 26, 28, 29, 31]

Table 11: Wyckoff site: 4k, site symmetry: $\text{mm}21'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 6, 7, 17, 20, 22, 23]$
2	$[0, 0, -z]$	$[2, 3, 5, 8, 18, 19, 21, 24]$
3	$[\frac{1}{2}, \frac{1}{2}, z]$	$[9, 12, 14, 15, 25, 28, 30, 31]$
4	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[10, 11, 13, 16, 26, 27, 29, 32]$

Table 12: Wyckoff site: 4l, site symmetry: $\text{mm}21'$

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4, 6, 7, 17, 20, 22, 23]$
2	$[0, \frac{1}{2}, -z]$	$[2, 3, 5, 8, 18, 19, 21, 24]$
3	$[\frac{1}{2}, 0, z]$	$[9, 12, 14, 15, 25, 28, 30, 31]$
4	$[\frac{1}{2}, 0, -z]$	$[10, 11, 13, 16, 26, 27, 29, 32]$

Table 13: Wyckoff site: 8m, site symmetry: $\dots 21'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, 12, 17, 28]$
2	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[2, 11, 18, 27]$
3	$[\frac{3}{4}, \frac{1}{4}, -z]$	$[3, 10, 19, 26]$
4	$[\frac{3}{4}, \frac{3}{4}, z]$	$[4, 9, 20, 25]$
5	$[\frac{3}{4}, \frac{3}{4}, -z]$	$[5, 16, 21, 32]$
6	$[\frac{3}{4}, \frac{1}{4}, z]$	$[6, 15, 22, 31]$
7	$[\frac{1}{4}, \frac{3}{4}, z]$	$[7, 14, 23, 30]$
8	$[\frac{1}{4}, \frac{1}{4}, -z]$	$[8, 13, 24, 29]$

Table 14: Wyckoff site: 8n, site symmetry: $\text{m} \dots 1'$

No.	position	mapping
1	$[0, y, z]$	$[1, 6, 17, 22]$
2	$[0, -y, -z]$	$[2, 5, 18, 21]$
3	$[0, y, -z]$	$[3, 8, 19, 24]$
4	$[0, -y, z]$	$[4, 7, 20, 23]$
5	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[9, 14, 25, 30]$
6	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	$[10, 13, 26, 29]$
7	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	$[11, 16, 27, 32]$
8	$[\frac{1}{2}, \frac{1}{2} - y, z]$	$[12, 15, 28, 31]$

Table 15: Wyckoff site: 8o, site symmetry: $\cdot m \cdot 1'$

No.	position	mapping
1	$[x, 0, z]$	$[1, 7, 17, 23]$
2	$[x, 0, -z]$	$[2, 8, 18, 24]$
3	$[-x, 0, -z]$	$[3, 5, 19, 21]$
4	$[-x, 0, z]$	$[4, 6, 20, 22]$
5	$[x + \frac{1}{2}, \frac{1}{2}, z]$	$[9, 15, 25, 31]$
6	$[x + \frac{1}{2}, \frac{1}{2}, -z]$	$[10, 16, 26, 32]$
7	$[\frac{1}{2} - x, \frac{1}{2}, -z]$	$[11, 13, 27, 29]$
8	$[\frac{1}{2} - x, \frac{1}{2}, z]$	$[12, 14, 28, 30]$

Table 16: Wyckoff site: 8p, site symmetry: $\cdot \cdot m 1'$

No.	position	mapping
1	$[x, y, 0]$	$[1, 8, 17, 24]$
2	$[x, -y, 0]$	$[2, 7, 18, 23]$
3	$[-x, y, 0]$	$[3, 6, 19, 22]$
4	$[-x, -y, 0]$	$[4, 5, 20, 21]$
5	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	$[9, 16, 25, 32]$
6	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	$[10, 15, 26, 31]$
7	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	$[11, 14, 27, 30]$
8	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	$[12, 13, 28, 29]$

Table 17: Wyckoff site: 8q, site symmetry: $\cdot \cdot m 1'$

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	$[1, 8, 17, 24]$
2	$[x, -y, \frac{1}{2}]$	$[2, 7, 18, 23]$
3	$[-x, y, \frac{1}{2}]$	$[3, 6, 19, 22]$
4	$[-x, -y, \frac{1}{2}]$	$[4, 5, 20, 21]$
5	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	$[9, 16, 25, 32]$
6	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	$[10, 15, 26, 31]$
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	$[11, 14, 27, 30]$
8	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	$[12, 13, 28, 29]$

Table 18: Wyckoff site: 16r, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[x, -y, -z]$	$[2, 18]$
3	$[-x, y, -z]$	$[3, 19]$

continued ...

Table 18

No.	position	mapping
4	$[-x, -y, z]$	$[4, 20]$
5	$[-x, -y, -z]$	$[5, 21]$
6	$[-x, y, z]$	$[6, 22]$
7	$[x, -y, z]$	$[7, 23]$
8	$[x, y, -z]$	$[8, 24]$
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	$[9, 25]$
10	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	$[10, 26]$
11	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	$[11, 27]$
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	$[12, 28]$
13	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	$[13, 29]$
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	$[14, 30]$
15	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	$[15, 31]$
16	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	$[16, 32]$