

Table 1: Wyckoff site: 2a, site symmetry:  $mmm.1'$ 

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

Table 2: Wyckoff site: 2b, site symmetry:  $mmm.1'$ 

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

Table 3: Wyckoff site: 2c, site symmetry:  $mmm.1'$ 

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

Table 4: Wyckoff site: 2d, site symmetry:  $mmm.1'$ 

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

Table 5: Wyckoff site: 2e, site symmetry:  $-4m21'$ 

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

Table 6: Wyckoff site: 2f, site symmetry:  $-4m21'$ 

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

Table 7: Wyckoff site: 4g, site symmetry:  $2mm.1'$ 

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

Table 8: Wyckoff site: 4h, site symmetry:  $2mm.1'$ 

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

Table 9: Wyckoff site: 4i, site symmetry:  $2mm.1'$ 

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

Table 10: Wyckoff site: 4j, site symmetry:  $m2m.1'$ 

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

Table 11: Wyckoff site: 4k, site symmetry:  $m2m.1'$ 

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

Table 12: Wyckoff site:  $4l$ , site symmetry:  $m2m.1'$ 

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

Table 13: Wyckoff site:  $4m$ , site symmetry:  $m2m.1'$ 

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

Table 14: Wyckoff site:  $8n$ , site symmetry:  $. . 21'$ 

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

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

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

Table 16: Wyckoff site: 8p, site symmetry:  $\bar{4}m2$ 

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

Table 17: Wyckoff site: 8q, site symmetry:  $m\bar{4}2$ 

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

Table 18: Wyckoff site: 16r, site symmetry:  $4mm$ 

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