

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $m.mm'$

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

Table 6: Wyckoff site:  $4f$ , site symmetry:  $m.mm'$ 

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

Table 7: Wyckoff site:  $4g$ , site symmetry:  $4'm'm$ 

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

Table 8: Wyckoff site:  $4h$ , site symmetry:  $4m'm'$ 

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

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

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

Table 10: Wyckoff site:  $8j$ , site symmetry:  $mm'2'$ .

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

Table 11: Wyckoff site:  $8k$ , site symmetry:  $mm'2'$ .

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

Table 12: Wyckoff site:  $8l$ , site symmetry:  $m.2m$ 

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

Table 13: Wyckoff site:  $8m$ , site symmetry:  $m.2m$ 

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

*continued ...*

Table 13

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

Table 14: Wyckoff site: 8n, site symmetry:  $m.2'm'$ 

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

Table 15: Wyckoff site: 8o, site symmetry:  $m.2'm'$ 

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

Table 16: Wyckoff site: 16p, site symmetry:  $m..$ 

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

*continued ...*

Table 16

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

Table 17: Wyckoff site: 16q, site symmetry:  $\bar{m}$ .

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

Table 18: Wyckoff site: 16r, site symmetry:  $\bar{m}'$ .

No.	position	mapping
1	$[0, y, z]$	[1, 28]
2	$[-y, 0, z]$	[2, 31]
3	$[y, 0, z]$	[3, 32]
4	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[4, 25]
5	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[5, 30]
6	$[0, -y, z]$	[6, 29]
7	$[y + \frac{1}{2}, \frac{1}{2}, -z]$	[7, 26]
8	$[\frac{1}{2} - y, \frac{1}{2}, -z]$	[8, 27]

*continued ...*

Table 18

No.	position	mapping
9	$[0, -y, -z]$	$[9, 20]$
10	$[y, 0, -z]$	$[10, 23]$
11	$[-y, 0, -z]$	$[11, 24]$
12	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[12, 17]$
13	$[\frac{1}{2}, \frac{1}{2} - y, z]$	$[13, 22]$
14	$[0, y, -z]$	$[14, 21]$
15	$[\frac{1}{2} - y, \frac{1}{2}, z]$	$[15, 18]$
16	$[y + \frac{1}{2}, \frac{1}{2}, z]$	$[16, 19]$

Table 19: Wyckoff site:  $16s$ , site symmetry:  $\bar{3}m$ 

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

Table 20: Wyckoff site:  $16t$ , site symmetry:  $\bar{3}m'$ 

No.	position	mapping
1	$[x, x, z]$	$[1, 32]$
2	$[-x, x, z]$	$[2, 28]$
3	$[x, -x, z]$	$[3, 29]$
4	$[x + \frac{1}{2}, \frac{1}{2} - x, -z]$	$[4, 26]$
5	$[\frac{1}{2} - x, x + \frac{1}{2}, -z]$	$[5, 27]$
6	$[-x, -x, z]$	$[6, 31]$
7	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	$[7, 30]$
8	$[\frac{1}{2} - x, \frac{1}{2} - x, -z]$	$[8, 25]$
9	$[-x, -x, -z]$	$[9, 24]$
10	$[x, -x, -z]$	$[10, 20]$

*continued ...*

Table 20

No.	position	mapping
11	$[-x, x, -z]$	[11,21]
12	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[12,18]
13	$[x + \frac{1}{2}, \frac{1}{2} - x, z]$	[13,19]
14	$[x, x, -z]$	[14,23]
15	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[15,22]
16	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[16,17]

Table 21: Wyckoff site: 32u, site symmetry: 1

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