

Table 1: Wyckoff site: 4a, site symmetry: $m'\overline{.mm}$

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

Table 2: Wyckoff site: 4b, site symmetry: $m'\overline{.m'm'}$

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

Table 3: Wyckoff site: 4c, site symmetry: $m'\overline{.mm'}$

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

Table 4: Wyckoff site: 4d, site symmetry: $m'\overline{.mm'}$

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

Table 5: Wyckoff site: 4e, site symmetry: $\overline{4'}2'm$

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[1, 6, 15, 16, 20, 21, 26, 27]
2	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[2, 3, 12, 13, 23, 24, 25, 30]

continued ...

Table 5

No.	position	mapping
3	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[4, 5, 10, 11, 17, 22, 31, 32]$
4	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[7, 8, 9, 14, 18, 19, 28, 29]$

Table 6: Wyckoff site: 4f, site symmetry: $-42'm'$

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, x, 0]$	$[1, 16, 23, 30]$
2	$[\frac{1}{2} - x, x, \frac{1}{2}]$	$[2, 12, 21, 27]$
3	$[x, \frac{1}{2} - x, \frac{1}{2}]$	$[3, 13, 20, 26]$

continued ...

Table 12

No.	position	mapping
4	$[x + \frac{1}{2}, -x, \frac{1}{2}]$	[4, 10, 19, 29]
5	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[5, 11, 18, 28]
6	$[\frac{1}{2} - x, \frac{1}{2} - x, 0]$	[6, 15, 24, 25]
7	$[x + \frac{1}{2}, x + \frac{1}{2}, 0]$	[7, 14, 17, 32]
8	$[-x, -x, 0]$	[8, 9, 22, 31]

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

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

Table 14: Wyckoff site: $16n$, site symmetry: $.2'.$

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

Table 15: Wyckoff site: **16o**, site symmetry: $\bar{3}m$

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

Table 16: Wyckoff site: **16p**, site symmetry: $\bar{3}m'$

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

Table 17: Wyckoff site: **16q**, site symmetry: $m'\bar{3}$

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1,30]

continued ...

Table 17

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

Table 18: Wyckoff site: **32r**, site symmetry: 1

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

continued ...

Table 18

No.	position	mapping
26	$[y, \frac{1}{2} - x, \frac{1}{2} - z]$	[26]
27	$[\frac{1}{2} - y, x, \frac{1}{2} - z]$	[27]
28	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[28]
29	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[29]
30	$[x, y, -z]$	[30]
31	$[-y, -x, z]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[32]