

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: 4f, site symmetry:  $mmm$ .

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

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

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

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

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

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

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

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

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

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

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

Table 12: Wyckoff site: 8l, site symmetry:  $m2m$ .

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

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

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	$[1, 13, 20, 30]$
2	$[0, x, \frac{3}{4}]$	$[2, 16, 23, 27]$
3	$[0, -x, \frac{3}{4}]$	$[3, 15, 24, 26]$

*continued ...*

Table 13

No.	position	mapping
4	$[x, 0, \frac{3}{4}]$	[4, 14, 17, 29]
5	$[-x, 0, \frac{3}{4}]$	[5, 9, 22, 28]
6	$[-x, 0, \frac{1}{4}]$	[6, 12, 21, 25]
7	$[0, x, \frac{1}{4}]$	[7, 11, 18, 32]
8	$[0, -x, \frac{1}{4}]$	[8, 10, 19, 31]

Table 14: Wyckoff site: 8n, site symmetry: m2m.

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

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

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

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

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

*continued ...*

Table 16

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

Table 17: Wyckoff site: 16q, site symmetry:  $m'..$ 

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

Table 18: Wyckoff site: 16r, site symmetry:  $..m'$ 

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

*continued ...*

Table 18

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

Table 19: Wyckoff site:  $16s$ , site symmetry:  $.m$ .

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

Table 20: Wyckoff site:  $16t$ , site symmetry:  $.m$ .

No.	position	mapping
1	$[x, \frac{1}{2}, z]$	[1,13]
2	$[\frac{1}{2}, x, z + \frac{1}{2}]$	[2,16]
3	$[\frac{1}{2}, -x, z + \frac{1}{2}]$	[3,15]
4	$[x, \frac{1}{2}, -z]$	[4,14]
5	$[-x, \frac{1}{2}, -z]$	[5,9]
6	$[-x, \frac{1}{2}, z]$	[6,12]
7	$[\frac{1}{2}, x, \frac{1}{2} - z]$	[7,11]
8	$[\frac{1}{2}, -x, \frac{1}{2} - z]$	[8,10]
9	$[x, \frac{1}{2}, z + \frac{1}{2}]$	[17,29]
10	$[\frac{1}{2}, x, z]$	[18,32]

*continued ...*

Table 20

No.	position	mapping
11	$[\frac{1}{2}, -x, z]$	[19, 31]
12	$[x, \frac{1}{2}, \frac{1}{2} - z]$	[20, 30]
13	$[-x, \frac{1}{2}, \frac{1}{2} - z]$	[21, 25]
14	$[-x, \frac{1}{2}, z + \frac{1}{2}]$	[22, 28]
15	$[\frac{1}{2}, x, -z]$	[23, 27]
16	$[\frac{1}{2}, -x, -z]$	[24, 26]

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

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