

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $-4m2$ 

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

Table 5: Wyckoff site: 4e, site symmetry:  $4mm$ 

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

Table 6: Wyckoff site:  $8f$ , site symmetry:  $\dots 2/m$ 

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

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

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

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

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

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

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

*continued ...*

Table 9

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

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

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

Table 11: Wyckoff site: 16k, site symmetry:  $\dots 2$ 

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

Table 12: Wyckoff site: 16l, site symmetry:  $m'\bar{1}$ .

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

Table 13: Wyckoff site: 16m, site symmetry:  $\bar{1}m$ .

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

Table 14: Wyckoff site: 16n, site symmetry:  $\bar{1}m$ .

No.	position	mapping
1	$[\frac{1}{4}, y, z]$	[1,12]

*continued ...*

Table 14

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

Table 15: Wyckoff site: **32o**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{2} - y, x, z]$	[2]
3	$[y, \frac{1}{2} - x, z]$	[3]
4	$[x + \frac{1}{2}, -y, -z]$	[4]
5	$[-x, y + \frac{1}{2}, -z]$	[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	$[y + \frac{1}{2}, -x, -z]$	[10]
11	$[-y, x + \frac{1}{2}, -z]$	[11]
12	$[\frac{1}{2} - x, y, z]$	[12]
13	$[x, \frac{1}{2} - y, z]$	[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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[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	$[-x, -y, z + \frac{1}{2}]$	[22]
23	$[y, x, \frac{1}{2} - z]$	[23]
24	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[24]
25	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[25]

continued ...

Table 15

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	$[x, y, \frac{1}{2} - z]$	[30]
31	$[-y, -x, z + \frac{1}{2}]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[32]