

Table 1: Wyckoff site: 8a, site symmetry: $2'22'$

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

Table 2: Wyckoff site: 8b, site symmetry: $22'2'$

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

Table 3: Wyckoff site: 8c, site symmetry: $.2/m'$

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

Table 4: Wyckoff site: **8d**, site symmetry: $.2'/m'$.

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

Table 5: Wyckoff site: **8e**, site symmetry: $2'/m$.

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

Table 6: Wyckoff site: **8f**, site symmetry: $2/m$.

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

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

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

continued ...

Table 7

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

Table 8: Wyckoff site: 16h, site symmetry: .2.

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

Table 9: Wyckoff site: 16i, site symmetry: .2'.

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

continued ...

Table 9

No.	position	mapping
14	$[\frac{3}{4}, y + \frac{1}{2}, 0]$	[14, 32]
15	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[15, 29]
16	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[16, 30]

Table 10: Wyckoff site: 16j, site symmetry: $2'..$

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

Table 11: Wyckoff site: 16k, site symmetry: $2..$

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

continued ...

Table 11

No.	position	mapping
16	$[x, \frac{1}{2}, 0]$	[31,32]

Table 12: Wyckoff site: $16\bar{1}$, site symmetry: $\bar{3}2'$

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

Table 13: Wyckoff site: $16\bar{m}$, site symmetry: $\bar{3}m'$

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

Table 14: Wyckoff site: **16n**, site symmetry: **m**.

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

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

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

continued ...

Table 15

No.	position	mapping
24	$[x + \frac{1}{2}, y, -z]$	[24]
25	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[25]
26	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[26]
27	$[-x, y + \frac{1}{2}, -z]$	[27]
28	$[-x, \frac{1}{2} - y, z]$	[28]
29	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[29]
30	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[30]
31	$[x, \frac{1}{2} - y, z]$	[31]
32	$[x, y + \frac{1}{2}, -z]$	[32]