

Table 1: Wyckoff site: 8a, site symmetry: $..2/m'$

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

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

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: $\dots 2'/m'$

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

Table 5: Wyckoff site: 8e, site symmetry: $2'2'2$

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

Table 6: Wyckoff site: 8f, site symmetry: $2'22'$

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

Table 7: Wyckoff site: 8g, site symmetry: $22'2'$

No.	position	mapping
1	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, 2, 19, 20]$
2	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[3, 4, 17, 18]$
3	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[5, 6, 23, 24]$

continued ...

Table 7

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

Table 8: Wyckoff site: 8h, site symmetry: 222

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

Table 9: Wyckoff site: 16i, site symmetry: $2^2 \dots$

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

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

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

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

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

Table 12: Wyckoff site: 16l, site symmetry: $.2$

No.	position	mapping
1	$[0, y, \frac{1}{4}]$	[1, 3]

continued ...

Table 12

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

Table 13: Wyckoff site: 16m, site symmetry: $\dots 2$

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

Table 14: Wyckoff site: 16n, site symmetry: $\dots 2$

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	[1, 4]
2	$[0, \frac{1}{4}, \frac{1}{2} - z]$	[2, 3]
3	$[\frac{1}{2}, \frac{1}{4}, -z]$	[5, 8]

continued ...

Table 14

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

Table 15: Wyckoff site: 16o, site symmetry: $\dots 2'$

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

Table 16: Wyckoff site: 16p, site symmetry: $\dots 2'$

No.	position	mapping
1	$[0, 0, z]$	[1,28]
2	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[2,27]
3	$[0, 0, \frac{1}{2} - z]$	[3,26]
4	$[0, \frac{1}{2}, z]$	[4,25]
5	$[\frac{1}{2}, \frac{1}{2}, -z]$	[5,32]

continued ...

Table 16

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[2]
3	$[-x, y, \frac{1}{2} - z]$	[3]
4	$[-x, \frac{1}{2} - y, z]$	[4]
5	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[5]
6	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[6]
7	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[7]

continued ...

Table 18

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