

Table 1: Wyckoff site: 8a, site symmetry:  $\dots 2/m$

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: 222

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

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

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

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

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{4}]$	[1, 3, 26, 28]
2	$[0, \frac{3}{4}, \frac{1}{4}]$	[2, 4, 25, 27]
3	$[0, \frac{3}{4}, \frac{3}{4}]$	[5, 7, 30, 32]

*continued ...*

Table 7

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, y, \frac{1}{4}]$	[1,19]

*continued ...*

Table 12

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,12]
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[2,11]
3	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3,10]

*continued ...*

Table 14

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, 0, z]$	[1, 20]
2	$[\frac{1}{4}, 0, \frac{1}{2} - z]$	[2, 19]
3	$[\frac{3}{4}, 0, \frac{1}{2} - z]$	[3, 18]
4	$[\frac{3}{4}, 0, z]$	[4, 17]
5	$[\frac{3}{4}, 0, -z]$	[5, 24]

*continued ...*

Table 16

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

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

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

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

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

*continued ...*

Table 18

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