

Table 1: Wyckoff site: 2a, site symmetry:  $4'32'$

No.	position	mapping
1	$[0, 0, 0]$	[1, 8, 9, 10, 17, 18, 19, 20, 21, 22, 23, 24, 26, 27, 28, 29, 30, 31, 35, 36, 37, 38, 39, 40]
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[2, 3, 4, 5, 6, 7, 11, 12, 13, 14, 15, 16, 25, 32, 33, 34, 41, 42, 43, 44, 45, 46, 47, 48]

Table 2: Wyckoff site: 6b, site symmetry:  $4'2.2'$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	[1, 8, 9, 10, 26, 27, 37, 38]
2	$[\frac{1}{2}, 0, 0]$	[2, 3, 13, 14, 25, 32, 33, 34]
3	$[0, 0, \frac{1}{2}]$	[4, 5, 15, 16, 42, 43, 45, 47]
4	$[0, \frac{1}{2}, 0]$	[6, 7, 11, 12, 41, 44, 46, 48]
5	$[\frac{1}{2}, 0, \frac{1}{2}]$	[17, 20, 22, 24, 30, 31, 35, 36]
6	$[\frac{1}{2}, \frac{1}{2}, 0]$	[18, 19, 21, 23, 28, 29, 39, 40]

Table 3: Wyckoff site: 8c, site symmetry:  $.32$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1, 12, 14, 16, 17, 18]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[2, 7, 9, 15, 19, 24]
3	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[3, 4, 10, 11, 20, 21]
4	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[5, 6, 8, 13, 22, 23]
5	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25, 36, 38, 40, 41, 42]
6	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[26, 31, 33, 39, 43, 48]
7	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[27, 28, 34, 35, 44, 45]
8	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[29, 30, 32, 37, 46, 47]

Table 4: Wyckoff site: 12d, site symmetry:  $2.22$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{2}, 0]$	[1, 8, 13, 14]
2	$[\frac{3}{4}, \frac{1}{2}, 0]$	[2, 3, 9, 10]
3	$[\frac{1}{2}, 0, \frac{1}{4}]$	[4, 16, 18, 21]
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	[5, 15, 19, 23]
5	$[0, \frac{3}{4}, \frac{1}{2}]$	[6, 11, 20, 22]
6	$[0, \frac{1}{4}, \frac{1}{2}]$	[7, 12, 17, 24]
7	$[\frac{3}{4}, 0, \frac{1}{2}]$	[25, 32, 37, 38]
8	$[\frac{1}{4}, 0, \frac{1}{2}]$	[26, 27, 33, 34]
9	$[0, \frac{1}{2}, \frac{3}{4}]$	[28, 40, 42, 45]

*continued ...*

Table 4

No.	position	mapping
10	$[0, \frac{1}{2}, \frac{1}{4}]$	[29, 39, 43, 47]
11	$[\frac{1}{2}, \frac{1}{4}, 0]$	[30, 35, 44, 46]
12	$[\frac{1}{2}, \frac{3}{4}, 0]$	[31, 36, 41, 48]

Table 5: Wyckoff site:  $12e$ , site symmetry:  $4'$  . .

No.	position	mapping
1	$[x, 0, 0]$	[1, 8, 26, 27]
2	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[2, 3, 25, 32]
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[4, 16, 43, 47]
4	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[5, 15, 42, 45]
5	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[6, 11, 41, 48]
6	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[7, 12, 44, 46]
7	$[-x, 0, 0]$	[9, 10, 37, 38]
8	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[13, 14, 33, 34]
9	$[0, x, 0]$	[17, 24, 30, 35]
10	$[0, 0, x]$	[18, 21, 29, 39]
11	$[0, 0, -x]$	[19, 23, 28, 40]
12	$[0, -x, 0]$	[20, 22, 31, 36]

Table 6: Wyckoff site:  $16f$ , site symmetry:  $.3$ .

No.	position	mapping
1	$[x, x, x]$	[1, 17, 18]
2	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[2, 7, 15]
3	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[3, 4, 11]
4	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[5, 6, 13]
5	$[x, -x, -x]$	[8, 22, 23]
6	$[-x, x, -x]$	[9, 19, 24]
7	$[-x, -x, x]$	[10, 20, 21]
8	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[12, 14, 16]
9	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[25, 41, 42]
10	$[x, -x, x]$	[26, 31, 39]
11	$[x, x, -x]$	[27, 28, 35]
12	$[-x, x, x]$	[29, 30, 37]
13	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[32, 46, 47]
14	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[33, 43, 48]
15	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[34, 44, 45]
16	$[-x, -x, -x]$	[36, 38, 40]

Table 7: Wyckoff site: 24g, site symmetry: 2 . .

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	[1, 8]
2	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[2, 3]
3	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[4, 16]
4	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[5, 15]
5	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[6, 11]
6	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[7, 12]
7	$[-x, \frac{1}{2}, 0]$	[9, 10]
8	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[13, 14]
9	$[0, x, \frac{1}{2}]$	[17, 24]
10	$[\frac{1}{2}, 0, x]$	[18, 21]
11	$[\frac{1}{2}, 0, -x]$	[19, 23]
12	$[0, -x, \frac{1}{2}]$	[20, 22]
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[25, 32]
14	$[x, 0, \frac{1}{2}]$	[26, 27]
15	$[0, \frac{1}{2}, -x]$	[28, 40]
16	$[0, \frac{1}{2}, x]$	[29, 39]
17	$[\frac{1}{2}, x, 0]$	[30, 35]
18	$[\frac{1}{2}, -x, 0]$	[31, 36]
19	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[33, 34]
20	$[-x, 0, \frac{1}{2}]$	[37, 38]
21	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[41, 48]
22	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[42, 45]
23	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[43, 47]
24	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[44, 46]

Table 8: Wyckoff site: 24h, site symmetry: . . 2'

No.	position	mapping
1	$[0, y, y]$	[1, 37]
2	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[2, 34]
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[3, 33]
4	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[4, 42]
5	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[5, 43]
6	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[6, 44]
7	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[7, 41]
8	$[0, -y, -y]$	[8, 38]
9	$[0, y, -y]$	[9, 27]
10	$[0, -y, y]$	[10, 26]
11	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[11, 46]
12	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[12, 48]
13	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[13, 25]
14	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[14, 32]
15	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[15, 47]

*continued ...*

Table 8

No.	position	mapping
16	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[16,45]
17	$[y, 0, y]$	[17,31]
18	$[y, y, 0]$	[18,28]
19	$[-y, y, 0]$	[19,29]
20	$[-y, 0, y]$	[20,30]
21	$[-y, -y, 0]$	[21,40]
22	$[y, 0, -y]$	[22,35]
23	$[y, -y, 0]$	[23,39]
24	$[-y, 0, -y]$	[24,36]

Table 9: Wyckoff site: 24i, site symmetry: . . 2

No.	position	mapping
1	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[1,14]
2	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[2,9]
3	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[3,10]
4	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[4,21]
5	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[5,23]
6	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[6,22]
7	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[7,24]
8	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[8,13]
9	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[11,20]
10	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[12,17]
11	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[15,19]
12	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[16,18]
13	$[\frac{3}{4}, y + \frac{1}{2}, -y]$	[25,38]
14	$[\frac{1}{4}, y + \frac{1}{2}, y]$	[26,33]
15	$[\frac{1}{4}, \frac{1}{2} - y, -y]$	[27,34]
16	$[\frac{1}{2} - y, y, \frac{3}{4}]$	[28,45]
17	$[y + \frac{1}{2}, y, \frac{1}{4}]$	[29,47]
18	$[-y, \frac{1}{4}, \frac{1}{2} - y]$	[30,46]
19	$[y, \frac{3}{4}, \frac{1}{2} - y]$	[31,48]
20	$[\frac{3}{4}, \frac{1}{2} - y, y]$	[32,37]
21	$[y, \frac{1}{4}, y + \frac{1}{2}]$	[35,44]
22	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[36,41]
23	$[\frac{1}{2} - y, -y, \frac{1}{4}]$	[39,43]
24	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[40,42]

Table 10: Wyckoff site: 48j, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[2]
3	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[3]
4	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[4]
5	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[14]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[15]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[16]
17	$[z, x, y]$	[17]
18	$[y, z, x]$	[18]
19	$[-y, z, -x]$	[19]
20	$[-z, -x, y]$	[20]
21	$[-y, -z, x]$	[21]
22	$[z, -x, -y]$	[22]
23	$[y, -z, -x]$	[23]
24	$[-z, x, -y]$	[24]
25	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[25]
26	$[x, -z, y]$	[26]
27	$[x, z, -y]$	[27]
28	$[z, y, -x]$	[28]
29	$[-z, y, x]$	[29]
30	$[-y, x, z]$	[30]
31	$[y, -x, z]$	[31]
32	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[32]
33	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[33]
34	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[34]
35	$[y, x, -z]$	[35]
36	$[-y, -x, -z]$	[36]
37	$[-x, z, y]$	[37]
38	$[-x, -z, -y]$	[38]
39	$[z, -y, x]$	[39]
40	$[-z, -y, -x]$	[40]
41	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[41]
42	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[42]
43	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[43]
44	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[44]
45	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[45]
46	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[46]

*continued ...*

Table 10

No.	position	mapping
47	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[47]
48	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[48]