

Table 1: Wyckoff site: 8a, site symmetry: $.32$

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

Table 2: Wyckoff site: 8b, site symmetry: $.32'$

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

Table 3: Wyckoff site: 12c, site symmetry: $2' .2'2$

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

Table 4: Wyckoff site: 12d, site symmetry: $2' . 2' 2$

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

Table 5: Wyckoff site: 16e, site symmetry: $. 3.$

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

Table 6: Wyckoff site: 24f, site symmetry: $2' . .$

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1, 32]
2	$[x + \frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[2, 27]
3	$[x + \frac{1}{4}, 0, \frac{3}{4}]$	[3, 26]
4	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4} - x]$	[4, 40]
5	$[\frac{1}{2}, \frac{1}{4}, x + \frac{3}{4}]$	[5, 39]

continued ...

Table 6

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

Table 7: Wyckoff site: 24g, site symmetry: $\dots 2'$

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

continued ...

Table 7

No.	position	mapping
22	$[y + \frac{3}{4}, \frac{3}{8}, -y]$	[22,35]
23	$[y + \frac{1}{2}, \frac{1}{4} - y, \frac{7}{8}]$	[23,39]
24	$[\frac{3}{4} - y, \frac{5}{8}, \frac{1}{2} - y]$	[24,36]

Table 8: Wyckoff site: 24h, site symmetry: $\dots 2$

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

Table 9: Wyckoff site: 48i, site symmetry: 1

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

continued ...

Table 9

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