

Table 1: Wyckoff site: 8a, site symmetry:  $23$ .

No.	position	mapping
1	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[1, 5, 6, 26, 34, 35, 51, 55, 60, 76, 80, 81]
2	$[\frac{1}{8}, \frac{5}{8}, \frac{5}{8}]$	[2, 10, 11, 25, 29, 30, 52, 56, 57, 75, 79, 84]
3	$[\frac{5}{8}, \frac{1}{8}, \frac{5}{8}]$	[3, 7, 12, 28, 32, 33, 49, 53, 54, 74, 82, 83]
4	$[\frac{5}{8}, \frac{5}{8}, \frac{1}{8}]$	[4, 8, 9, 27, 31, 36, 50, 58, 59, 73, 77, 78]
5	$[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}]$	[13, 17, 18, 38, 46, 47, 63, 67, 72, 88, 92, 93]
6	$[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}]$	[14, 22, 23, 37, 41, 42, 64, 68, 69, 87, 91, 96]
7	$[\frac{3}{8}, \frac{7}{8}, \frac{3}{8}]$	[15, 19, 24, 40, 44, 45, 61, 65, 66, 86, 94, 95]
8	$[\frac{3}{8}, \frac{3}{8}, \frac{7}{8}]$	[16, 20, 21, 39, 43, 48, 62, 70, 71, 85, 89, 90]

Table 2: Wyckoff site: 8b, site symmetry:  $23$ .

No.	position	mapping
1	$[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}]$	[1, 5, 6, 26, 34, 35, 51, 55, 60, 76, 80, 81]
2	$[\frac{5}{8}, \frac{1}{8}, \frac{1}{8}]$	[2, 10, 11, 25, 29, 30, 52, 56, 57, 75, 79, 84]
3	$[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}]$	[3, 7, 12, 28, 32, 33, 49, 53, 54, 74, 82, 83]
4	$[\frac{1}{8}, \frac{1}{8}, \frac{5}{8}]$	[4, 8, 9, 27, 31, 36, 50, 58, 59, 73, 77, 78]
5	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[13, 17, 18, 38, 46, 47, 63, 67, 72, 88, 92, 93]
6	$[\frac{3}{8}, \frac{7}{8}, \frac{7}{8}]$	[14, 22, 23, 37, 41, 42, 64, 68, 69, 87, 91, 96]
7	$[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}]$	[15, 19, 24, 40, 44, 45, 61, 65, 66, 86, 94, 95]
8	$[\frac{7}{8}, \frac{7}{8}, \frac{3}{8}]$	[16, 20, 21, 39, 43, 48, 62, 70, 71, 85, 89, 90]

Table 3: Wyckoff site: 16c, site symmetry:  $\bar{3}'$ .

No.	position	mapping
1	[0, 0, 0]	[1, 5, 6, 13, 17, 18]
2	$[0, \frac{3}{4}, \frac{3}{4}]$	[2, 10, 11, 38, 46, 47]
3	$[\frac{3}{4}, 0, \frac{3}{4}]$	[3, 7, 12, 63, 67, 72]
4	$[\frac{3}{4}, \frac{3}{4}, 0]$	[4, 8, 9, 88, 92, 93]
5	$[0, \frac{1}{4}, \frac{1}{4}]$	[14, 22, 23, 26, 34, 35]
6	$[\frac{1}{4}, 0, \frac{1}{4}]$	[15, 19, 24, 51, 55, 60]
7	$[\frac{1}{4}, \frac{1}{4}, 0]$	[16, 20, 21, 76, 80, 81]
8	$[0, \frac{1}{2}, \frac{1}{2}]$	[25, 29, 30, 37, 41, 42]
9	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[27, 31, 36, 87, 91, 96]
10	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[28, 32, 33, 64, 68, 69]
11	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	[39, 43, 48, 75, 79, 84]
12	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[40, 44, 45, 52, 56, 57]
13	$[\frac{1}{2}, 0, \frac{1}{2}]$	[49, 53, 54, 61, 65, 66]
14	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[50, 58, 59, 86, 94, 95]
15	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[62, 70, 71, 74, 82, 83]

*continued ...*

Table 3

No.	position	mapping
16	$[\frac{1}{2}, \frac{1}{2}, 0]$	[73,77,78,85,89,90]

Table 4: Wyckoff site: 16d, site symmetry:  $\cdot -3'$ .

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,5,6,13,17,18]
2	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[2,10,11,38,46,47]
3	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[3,7,12,63,67,72]
4	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[4,8,9,88,92,93]
5	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[14,22,23,26,34,35]
6	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	[15,19,24,51,55,60]
7	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[16,20,21,76,80,81]
8	$[\frac{1}{2}, 0, 0]$	[25,29,30,37,41,42]
9	$[\frac{1}{4}, 0, \frac{3}{4}]$	[27,31,36,87,91,96]
10	$[\frac{1}{4}, \frac{3}{4}, 0]$	[28,32,33,64,68,69]
11	$[\frac{3}{4}, 0, \frac{1}{4}]$	[39,43,48,75,79,84]
12	$[\frac{3}{4}, \frac{1}{4}, 0]$	[40,44,45,52,56,57]
13	$[0, \frac{1}{2}, 0]$	[49,53,54,61,65,66]
14	$[0, \frac{1}{4}, \frac{3}{4}]$	[50,58,59,86,94,95]
15	$[0, \frac{3}{4}, \frac{1}{4}]$	[62,70,71,74,82,83]
16	$[0, 0, \frac{1}{2}]$	[73,77,78,85,89,90]

Table 5: Wyckoff site: 32e, site symmetry:  $\cdot 3$ .

No.	position	mapping
1	$[x, x, x]$	[1,5,6]
2	$[x, \frac{3}{4} - x, \frac{3}{4} - x]$	[2,10,11]
3	$[\frac{3}{4} - x, x, \frac{3}{4} - x]$	[3,7,12]
4	$[\frac{3}{4} - x, \frac{3}{4} - x, x]$	[4,8,9]
5	$[-x, -x, -x]$	[13,17,18]
6	$[-x, x + \frac{1}{4}, x + \frac{1}{4}]$	[14,22,23]
7	$[x + \frac{1}{4}, -x, x + \frac{1}{4}]$	[15,19,24]
8	$[x + \frac{1}{4}, x + \frac{1}{4}, -x]$	[16,20,21]
9	$[x, x + \frac{1}{2}, x + \frac{1}{2}]$	[25,29,30]
10	$[x, \frac{1}{4} - x, \frac{1}{4} - x]$	[26,34,35]
11	$[\frac{3}{4} - x, x + \frac{1}{2}, \frac{1}{4} - x]$	[27,31,36]
12	$[\frac{3}{4} - x, \frac{1}{4} - x, x + \frac{1}{2}]$	[28,32,33]
13	$[-x, \frac{1}{2} - x, \frac{1}{2} - x]$	[37,41,42]
14	$[-x, x + \frac{3}{4}, x + \frac{3}{4}]$	[38,46,47]
15	$[x + \frac{1}{4}, \frac{1}{2} - x, x + \frac{3}{4}]$	[39,43,48]
16	$[x + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - x]$	[40,44,45]
17	$[x + \frac{1}{2}, x, x + \frac{1}{2}]$	[49,53,54]

continued ...

Table 5

No.	position	mapping
18	$[x + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - x]$	[50, 58, 59]
19	$[\frac{1}{4} - x, x, \frac{1}{4} - x]$	[51, 55, 60]
20	$[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{1}{2}]$	[52, 56, 57]
21	$[\frac{1}{2} - x, -x, \frac{1}{2} - x]$	[61, 65, 66]
22	$[\frac{1}{2} - x, x + \frac{1}{4}, x + \frac{3}{4}]$	[62, 70, 71]
23	$[x + \frac{3}{4}, -x, x + \frac{3}{4}]$	[63, 67, 72]
24	$[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - x]$	[64, 68, 69]
25	$[x + \frac{1}{2}, x + \frac{1}{2}, x]$	[73, 77, 78]
26	$[x + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - x]$	[74, 82, 83]
27	$[\frac{1}{4} - x, x + \frac{1}{2}, \frac{3}{4} - x]$	[75, 79, 84]
28	$[\frac{1}{4} - x, \frac{1}{4} - x, x]$	[76, 80, 81]
29	$[\frac{1}{2} - x, \frac{1}{2} - x, -x]$	[85, 89, 90]
30	$[\frac{1}{2} - x, x + \frac{3}{4}, x + \frac{1}{4}]$	[86, 94, 95]
31	$[x + \frac{3}{4}, \frac{1}{2} - x, x + \frac{1}{4}]$	[87, 91, 96]
32	$[x + \frac{3}{4}, x + \frac{3}{4}, -x]$	[88, 92, 93]

Table 6: Wyckoff site: **48f**, site symmetry:  $2..$ 

No.	position	mapping
1	$[x, \frac{1}{8}, \frac{1}{8}]$	[1, 26]
2	$[x, \frac{5}{8}, \frac{5}{8}]$	[2, 25]
3	$[\frac{3}{4} - x, \frac{1}{8}, \frac{5}{8}]$	[3, 28]
4	$[\frac{3}{4} - x, \frac{5}{8}, \frac{1}{8}]$	[4, 27]
5	$[\frac{1}{8}, x, \frac{1}{8}]$	[5, 60]
6	$[\frac{1}{8}, \frac{1}{8}, x]$	[6, 81]
7	$[\frac{5}{8}, \frac{1}{8}, \frac{3}{4} - x]$	[7, 83]
8	$[\frac{5}{8}, \frac{3}{4} - x, \frac{1}{8}]$	[8, 58]
9	$[\frac{5}{8}, \frac{5}{8}, x]$	[9, 78]
10	$[\frac{1}{8}, \frac{3}{4} - x, \frac{5}{8}]$	[10, 56]
11	$[\frac{1}{8}, \frac{5}{8}, \frac{3}{4} - x]$	[11, 79]
12	$[\frac{5}{8}, x, \frac{5}{8}]$	[12, 53]
13	$[-x, \frac{7}{8}, \frac{7}{8}]$	[13, 38]
14	$[-x, \frac{3}{8}, \frac{3}{8}]$	[14, 37]
15	$[x + \frac{1}{4}, \frac{7}{8}, \frac{3}{8}]$	[15, 40]
16	$[x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}]$	[16, 39]
17	$[\frac{7}{8}, -x, \frac{7}{8}]$	[17, 72]
18	$[\frac{7}{8}, \frac{7}{8}, -x]$	[18, 93]
19	$[\frac{3}{8}, \frac{7}{8}, x + \frac{1}{4}]$	[19, 95]
20	$[\frac{3}{8}, x + \frac{1}{4}, \frac{7}{8}]$	[20, 70]
21	$[\frac{3}{8}, \frac{3}{8}, -x]$	[21, 90]
22	$[\frac{7}{8}, x + \frac{1}{4}, \frac{3}{8}]$	[22, 68]
23	$[\frac{7}{8}, \frac{3}{8}, x + \frac{1}{4}]$	[23, 91]
24	$[\frac{3}{8}, -x, \frac{3}{8}]$	[24, 65]
25	$[\frac{1}{8}, x + \frac{1}{2}, \frac{5}{8}]$	[29, 84]

continued ...

Table 6

No.	position	mapping
26	$[\frac{1}{8}, \frac{5}{8}, x + \frac{1}{2}]$	[30, 57]
27	$[\frac{5}{8}, \frac{5}{8}, \frac{1}{4} - x]$	[31, 59]
28	$[\frac{5}{8}, \frac{1}{4} - x, \frac{5}{8}]$	[32, 82]
29	$[\frac{5}{8}, \frac{1}{8}, x + \frac{1}{2}]$	[33, 54]
30	$[\frac{1}{8}, \frac{1}{4} - x, \frac{1}{8}]$	[34, 80]
31	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{4} - x]$	[35, 55]
32	$[\frac{5}{8}, x + \frac{1}{2}, \frac{1}{8}]$	[36, 77]
33	$[\frac{7}{8}, \frac{1}{2} - x, \frac{3}{8}]$	[41, 96]
34	$[\frac{7}{8}, \frac{3}{8}, \frac{1}{2} - x]$	[42, 69]
35	$[\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}]$	[43, 71]
36	$[\frac{3}{8}, x + \frac{3}{4}, \frac{3}{8}]$	[44, 94]
37	$[\frac{3}{8}, \frac{7}{8}, \frac{1}{2} - x]$	[45, 66]
38	$[\frac{7}{8}, x + \frac{3}{4}, \frac{7}{8}]$	[46, 92]
39	$[\frac{7}{8}, \frac{7}{8}, x + \frac{3}{4}]$	[47, 67]
40	$[\frac{3}{8}, \frac{1}{2} - x, \frac{7}{8}]$	[48, 89]
41	$[x + \frac{1}{2}, \frac{1}{8}, \frac{5}{8}]$	[49, 74]
42	$[x + \frac{1}{2}, \frac{5}{8}, \frac{1}{8}]$	[50, 73]
43	$[\frac{1}{4} - x, \frac{1}{8}, \frac{1}{8}]$	[51, 76]
44	$[\frac{1}{4} - x, \frac{5}{8}, \frac{5}{8}]$	[52, 75]
45	$[\frac{1}{2} - x, \frac{7}{8}, \frac{3}{8}]$	[61, 86]
46	$[\frac{1}{2} - x, \frac{3}{8}, \frac{7}{8}]$	[62, 85]
47	$[x + \frac{3}{4}, \frac{7}{8}, \frac{7}{8}]$	[63, 88]
48	$[x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}]$	[64, 87]

Table 7: Wyckoff site: **96g**, site symmetry: 1

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

continued ...

Table 7

No.	position	mapping
18	$[-y, -z, -x]$	[18]
19	$[y + \frac{1}{4}, -z, x + \frac{1}{4}]$	[19]
20	$[z + \frac{1}{4}, x + \frac{1}{4}, -y]$	[20]
21	$[y + \frac{1}{4}, z + \frac{1}{4}, -x]$	[21]
22	$[-z, x + \frac{1}{4}, y + \frac{1}{4}]$	[22]
23	$[-y, z + \frac{1}{4}, x + \frac{1}{4}]$	[23]
24	$[z + \frac{1}{4}, -x, y + \frac{1}{4}]$	[24]
25	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[25]
26	$[x, \frac{1}{4} - y, \frac{1}{4} - z]$	[26]
27	$[\frac{3}{4} - x, y + \frac{1}{2}, \frac{1}{4} - z]$	[27]
28	$[\frac{3}{4} - x, \frac{1}{4} - y, z + \frac{1}{2}]$	[28]
29	$[z, x + \frac{1}{2}, y + \frac{1}{2}]$	[29]
30	$[y, z + \frac{1}{2}, x + \frac{1}{2}]$	[30]
31	$[\frac{3}{4} - y, z + \frac{1}{2}, \frac{1}{4} - x]$	[31]
32	$[\frac{3}{4} - z, \frac{1}{4} - x, y + \frac{1}{2}]$	[32]
33	$[\frac{3}{4} - y, \frac{1}{4} - z, x + \frac{1}{2}]$	[33]
34	$[z, \frac{1}{4} - x, \frac{1}{4} - y]$	[34]
35	$[y, \frac{1}{4} - z, \frac{1}{4} - x]$	[35]
36	$[\frac{3}{4} - z, x + \frac{1}{2}, \frac{1}{4} - y]$	[36]
37	$[-x, \frac{1}{2} - y, \frac{1}{2} - z]$	[37]
38	$[-x, y + \frac{3}{4}, z + \frac{3}{4}]$	[38]
39	$[x + \frac{1}{4}, \frac{1}{2} - y, z + \frac{3}{4}]$	[39]
40	$[x + \frac{1}{4}, y + \frac{3}{4}, \frac{1}{2} - z]$	[40]
41	$[-z, \frac{1}{2} - x, \frac{1}{2} - y]$	[41]
42	$[-y, \frac{1}{2} - z, \frac{1}{2} - x]$	[42]
43	$[y + \frac{1}{4}, \frac{1}{2} - z, x + \frac{3}{4}]$	[43]
44	$[z + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - y]$	[44]
45	$[y + \frac{1}{4}, z + \frac{3}{4}, \frac{1}{2} - x]$	[45]
46	$[-z, x + \frac{3}{4}, y + \frac{3}{4}]$	[46]
47	$[-y, z + \frac{3}{4}, x + \frac{3}{4}]$	[47]
48	$[z + \frac{1}{4}, \frac{1}{2} - x, y + \frac{3}{4}]$	[48]
49	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[49]
50	$[x + \frac{1}{2}, \frac{3}{4} - y, \frac{1}{4} - z]$	[50]
51	$[\frac{1}{4} - x, y, \frac{1}{4} - z]$	[51]
52	$[\frac{1}{4} - x, \frac{3}{4} - y, z + \frac{1}{2}]$	[52]
53	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[53]
54	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[54]
55	$[\frac{1}{4} - y, z, \frac{1}{4} - x]$	[55]
56	$[\frac{1}{4} - z, \frac{3}{4} - x, y + \frac{1}{2}]$	[56]
57	$[\frac{1}{4} - y, \frac{3}{4} - z, x + \frac{1}{2}]$	[57]
58	$[z + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - y]$	[58]
59	$[y + \frac{1}{2}, \frac{3}{4} - z, \frac{1}{4} - x]$	[59]
60	$[\frac{1}{4} - z, x, \frac{1}{4} - y]$	[60]
61	$[\frac{1}{2} - x, -y, \frac{1}{2} - z]$	[61]
62	$[\frac{1}{2} - x, y + \frac{1}{4}, z + \frac{3}{4}]$	[62]
63	$[x + \frac{3}{4}, -y, z + \frac{3}{4}]$	[63]
64	$[x + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2} - z]$	[64]

continued ...

Table 7

No.	position	mapping
65	$[\frac{1}{2} - z, -x, \frac{1}{2} - y]$	[65]
66	$[\frac{1}{2} - y, -z, \frac{1}{2} - x]$	[66]
67	$[y + \frac{3}{4}, -z, x + \frac{3}{4}]$	[67]
68	$[z + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - y]$	[68]
69	$[y + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - x]$	[69]
70	$[\frac{1}{2} - z, x + \frac{1}{4}, y + \frac{3}{4}]$	[70]
71	$[\frac{1}{2} - y, z + \frac{1}{4}, x + \frac{3}{4}]$	[71]
72	$[z + \frac{3}{4}, -x, y + \frac{3}{4}]$	[72]
73	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[73]
74	$[x + \frac{1}{2}, \frac{1}{4} - y, \frac{3}{4} - z]$	[74]
75	$[\frac{1}{4} - x, y + \frac{1}{2}, \frac{3}{4} - z]$	[75]
76	$[\frac{1}{4} - x, \frac{1}{4} - y, z]$	[76]
77	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[77]
78	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[78]
79	$[\frac{1}{4} - y, z + \frac{1}{2}, \frac{3}{4} - x]$	[79]
80	$[\frac{1}{4} - z, \frac{1}{4} - x, y]$	[80]
81	$[\frac{1}{4} - y, \frac{1}{4} - z, x]$	[81]
82	$[z + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - y]$	[82]
83	$[y + \frac{1}{2}, \frac{1}{4} - z, \frac{3}{4} - x]$	[83]
84	$[\frac{1}{4} - z, x + \frac{1}{2}, \frac{3}{4} - y]$	[84]
85	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[85]
86	$[\frac{1}{2} - x, y + \frac{3}{4}, z + \frac{1}{4}]$	[86]
87	$[x + \frac{3}{4}, \frac{1}{2} - y, z + \frac{1}{4}]$	[87]
88	$[x + \frac{3}{4}, y + \frac{3}{4}, -z]$	[88]
89	$[\frac{1}{2} - z, \frac{1}{2} - x, -y]$	[89]
90	$[\frac{1}{2} - y, \frac{1}{2} - z, -x]$	[90]
91	$[y + \frac{3}{4}, \frac{1}{2} - z, x + \frac{1}{4}]$	[91]
92	$[z + \frac{3}{4}, x + \frac{3}{4}, -y]$	[92]
93	$[y + \frac{3}{4}, z + \frac{3}{4}, -x]$	[93]
94	$[\frac{1}{2} - z, x + \frac{3}{4}, y + \frac{1}{4}]$	[94]
95	$[\frac{1}{2} - y, z + \frac{3}{4}, x + \frac{1}{4}]$	[95]
96	$[z + \frac{3}{4}, \frac{1}{2} - x, y + \frac{1}{4}]$	[96]