

Table 1: Wyckoff site: 8a, site symmetry: $..-3'$.

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

Table 2: Wyckoff site: 8b, site symmetry: $..-3'$.

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

Table 3: Wyckoff site: 16c, site symmetry: $..3$.

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

continued ...

Table 3

No.	position	mapping
16	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	[40, 44, 45]

Table 4: Wyckoff site: 24d, site symmetry: 2 . .

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

Table 5: Wyckoff site: 48e, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, \frac{1}{2} - z]$	[2]
3	$[\frac{1}{2} - x, y, -z]$	[3]
4	$[-x, \frac{1}{2} - y, z]$	[4]
5	$[z, x, y]$	[5]
6	$[y, z, x]$	[6]
7	$[\frac{1}{2} - y, z, -x]$	[7]
8	$[-z, \frac{1}{2} - x, y]$	[8]
9	$[-y, \frac{1}{2} - z, x]$	[9]

continued ...

Table 5

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