

Table 1: Wyckoff site: 4a, site symmetry: $-4'm2'$

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

Table 2: Wyckoff site: 4b, site symmetry: $-4'm2'$

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

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

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: **2mm**.

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

Table 6: Wyckoff site: **16f**, site symmetry: **.2'**.

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

Table 7: Wyckoff site: **16g**, site symmetry: **. . 2'**

No.	position	mapping
1	$[x, x + \frac{1}{4}, \frac{7}{8}]$	$[1, 11]$
2	$[-x, x + \frac{3}{4}, \frac{1}{8}]$	$[2, 10]$
3	$[x, \frac{3}{4} - x, \frac{1}{8}]$	$[3, 9]$
4	$[-x, \frac{1}{4} - x, \frac{7}{8}]$	$[4, 12]$
5	$[-x, x + \frac{1}{4}, \frac{7}{8}]$	$[5, 15]$
6	$[x, \frac{1}{4} - x, \frac{7}{8}]$	$[6, 14]$
7	$[-x, \frac{3}{4} - x, \frac{1}{8}]$	$[7, 13]$
8	$[x, x + \frac{3}{4}, \frac{1}{8}]$	$[8, 16]$
9	$[x + \frac{1}{2}, x + \frac{3}{4}, \frac{3}{8}]$	$[17, 27]$

continued ...

Table 7

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

Table 8: Wyckoff site: **16h**, site symmetry: $\bar{6}m$.

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

Table 9: Wyckoff site: **32i**, site symmetry: $\bar{6}m$

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

continued ...

Table 9

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