

Table 1: Wyckoff site: 4a, site symmetry: $4'22'$

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

Table 2: Wyckoff site: 4b, site symmetry: $-42m$

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

Table 3: Wyckoff site: 4c, site symmetry: $4'/m'..$

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

Table 4: Wyckoff site: 4d, site symmetry: $m'.mm$

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

Table 5: Wyckoff site: 8e, site symmetry: $..2'/m$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1, 11, 23, 29]
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[2, 10, 22, 30]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 4' . .

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

Table 7: Wyckoff site: 8g, site symmetry: 2.mm

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, 0]$	[1, 16, 24, 27]
2	$[x, \frac{1}{2} - x, \frac{1}{2}]$	[2, 15, 21, 26]
3	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[3, 14, 22, 25]
4	$[-x, \frac{1}{2} - x, 0]$	[4, 13, 23, 28]
5	$[x + \frac{1}{2}, -x, 0]$	[5, 10, 18, 31]

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{2} - x, x, 0]$	[6, 9, 19, 30]
7	$[\frac{1}{2} - x, -x, \frac{1}{2}]$	[7, 12, 20, 29]
8	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[8, 11, 17, 32]

Table 9: Wyckoff site: 16i, site symmetry: $\cdot\cdot 2'$

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

Table 10: Wyckoff site: 16j, site symmetry: $\cdot 2$.

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

continued ...

Table 10

No.	position	mapping
16	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[31,32]

Table 11: Wyckoff site: 16k, site symmetry: $m'\dots$

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

Table 12: Wyckoff site: 16l, site symmetry: $\dots m$

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

Table 13: Wyckoff site: $32m$, site symmetry: 1

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