

Table 1: Wyckoff site: 4a, site symmetry: $2/m..1'$

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

Table 2: Wyckoff site: 4b, site symmetry: $2/m..1'$

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

Table 3: Wyckoff site: 4c, site symmetry: $.2/m.1'$

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

Table 4: Wyckoff site: 4d, site symmetry: $.2/m.1'$

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

Table 5: Wyckoff site: 4e, site symmetry: $mm21'$

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	$[1, 4, 6, 7, 17, 20, 22, 23]$
2	$[0, \frac{3}{4}, -z]$	$[2, 3, 5, 8, 18, 19, 21, 24]$

continued ...

Table 5

No.	position	mapping
3	$[\frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	$[9, 12, 14, 15, 25, 28, 30, 31]$
4	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	$[10, 11, 13, 16, 26, 27, 29, 32]$

Table 6: Wyckoff site: $8f$, site symmetry: $2..1'$

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

Table 7: Wyckoff site: $8g$, site symmetry: $.2.1'$

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

Table 8: Wyckoff site: $8h$, site symmetry: $m..1'$

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

Table 9: Wyckoff site: $8i$, site symmetry: $.m.1'$

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

Table 10: Wyckoff site: $16j$, site symmetry: $11'$

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