

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 4, 5, 8, 10, 11, 14, 15]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, 3, 6, 7, 9, 12, 13, 16]$

Table 2: Wyckoff site: 2b, site symmetry:  $m'm'm$

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 4, 5, 8, 10, 11, 14, 15]$
2	$[0, \frac{1}{2}, 0]$	$[2, 3, 6, 7, 9, 12, 13, 16]$

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

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 4, 5, 8, 10, 11, 14, 15]$
2	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 6, 7, 9, 12, 13, 16]$

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

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 4, 5, 8, 10, 11, 14, 15]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 6, 7, 9, 12, 13, 16]$

Table 5: Wyckoff site: 4e, site symmetry:  $. . 2'/m$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 8, 12, 13]$
2	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[2, 7, 11, 14]$
3	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[3, 6, 10, 15]$
4	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[4, 5, 9, 16]$

Table 6: Wyckoff site: **4f**, site symmetry:  $\dots 2'/m$ 

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

Table 7: Wyckoff site: **4g**, site symmetry:  $2'm'm$ 

No.	position	mapping
1	$[x, 0, 0]$	$[1, 8, 10, 15]$
2	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	$[2, 7, 9, 16]$
3	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	$[3, 6, 12, 13]$
4	$[-x, 0, 0]$	$[4, 5, 11, 14]$

Table 8: Wyckoff site: **4h**, site symmetry:  $2'm'm$ 

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	$[1, 8, 10, 15]$
2	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 7, 9, 16]$
3	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	$[3, 6, 12, 13]$
4	$[-x, 0, \frac{1}{2}]$	$[4, 5, 11, 14]$

Table 9: Wyckoff site: **4i**, site symmetry:  $m'2'm$ 

No.	position	mapping
1	$[0, y, 0]$	$[1, 8, 11, 14]$
2	$[\frac{1}{2}, \frac{1}{2} - y, 0]$	$[2, 7, 12, 13]$
3	$[\frac{1}{2}, y + \frac{1}{2}, 0]$	$[3, 6, 9, 16]$
4	$[0, -y, 0]$	$[4, 5, 10, 15]$

Table 10: Wyckoff site: **4j**, site symmetry:  $m'2'm$ 

No.	position	mapping
1	$[0, y, \frac{1}{2}]$	$[1, 8, 11, 14]$
2	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	$[2, 7, 12, 13]$
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	$[3, 6, 9, 16]$
4	$[0, -y, \frac{1}{2}]$	$[4, 5, 10, 15]$

Table 11: Wyckoff site:  $4k$ , site symmetry:  $m'm'2$ 

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 14, 15]$
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[2, 3, 13, 16]$
3	$[0, 0, -z]$	$[5, 8, 10, 11]$
4	$[\frac{1}{2}, \frac{1}{2}, z]$	$[6, 7, 9, 12]$

Table 12: Wyckoff site:  $4l$ , site symmetry:  $m'm'2$ 

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4, 14, 15]$
2	$[\frac{1}{2}, 0, -z]$	$[2, 3, 13, 16]$
3	$[0, \frac{1}{2}, -z]$	$[5, 8, 10, 11]$
4	$[\frac{1}{2}, 0, z]$	$[6, 7, 9, 12]$

Table 13: Wyckoff site:  $8m$ , site symmetry:  $. . 2'$ 

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

Table 14: Wyckoff site:  $8n$ , site symmetry:  $m' . .$ 

No.	position	mapping
1	$[0, y, z]$	$[1, 14]$
2	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	$[2, 13]$
3	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	$[3, 16]$
4	$[0, -y, z]$	$[4, 15]$
5	$[0, -y, -z]$	$[5, 10]$
6	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[6, 9]$
7	$[\frac{1}{2}, \frac{1}{2} - y, z]$	$[7, 12]$
8	$[0, y, -z]$	$[8, 11]$

Table 15: Wyckoff site:  $8\mathbf{o}$ , site symmetry:  $.m'$ .

No.	position	mapping
1	$[x, 0, z]$	$[1, 15]$
2	$[x + \frac{1}{2}, \frac{1}{2}, -z]$	$[2, 16]$
3	$[\frac{1}{2} - x, \frac{1}{2}, -z]$	$[3, 13]$
4	$[-x, 0, z]$	$[4, 14]$
5	$[-x, 0, -z]$	$[5, 11]$
6	$[\frac{1}{2} - x, \frac{1}{2}, z]$	$[6, 12]$
7	$[x + \frac{1}{2}, \frac{1}{2}, z]$	$[7, 9]$
8	$[x, 0, -z]$	$[8, 10]$

Table 16: Wyckoff site:  $8\mathbf{p}$ , site symmetry:  $.m$ 

No.	position	mapping
1	$[x, y, 0]$	$[1, 8]$
2	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	$[2, 7]$
3	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	$[3, 6]$
4	$[-x, -y, 0]$	$[4, 5]$
5	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	$[9, 16]$
6	$[x, -y, 0]$	$[10, 15]$
7	$[-x, y, 0]$	$[11, 14]$
8	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	$[12, 13]$

Table 17: Wyckoff site:  $8\mathbf{q}$ , site symmetry:  $.m$ 

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

Table 18: Wyckoff site:  $16\mathbf{r}$ , site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	$[2]$
3	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	$[3]$

*continued ...*

Table 18

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