

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry:  $4'2'2$

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

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

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

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

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

Table 6: Wyckoff site:  $4f$ , site symmetry:  $22'2'$ .

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

Table 7: Wyckoff site:  $4g$ , site symmetry:  $4'$ .

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

Table 8: Wyckoff site:  $4h$ , site symmetry:  $4'$ .

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

Table 9: Wyckoff site:  $8i$ , site symmetry:  $2$ .

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

Table 10: Wyckoff site: 8j, site symmetry:  $\dots 2$ 

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

Table 11: Wyckoff site: 8k, site symmetry:  $\dots 2'$ 

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

Table 12: Wyckoff site: 8l, site symmetry:  $\dots 2'$ 

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

Table 13: Wyckoff site: 8m, site symmetry:  $m' \dots$ 

No.	position	mapping
1	$[x, y, 0]$	$[1, 14]$
2	$[-x, -y, 0]$	$[2, 13]$
3	$[y, x, \frac{1}{2}]$	$[3, 16]$

*continued ...*

Table 13

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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