

Table 1: Wyckoff site: 2a, site symmetry:  $22'2'$ .

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 2, 5, 6]$
2	$[0, 0, \frac{3}{4}]$	$[3, 4, 7, 8]$

Table 2: Wyckoff site: 2b, site symmetry:  $22'2'$ .

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[1, 2, 5, 6]$
2	$[0, \frac{1}{2}, \frac{3}{4}]$	$[3, 4, 7, 8]$

Table 3: Wyckoff site: 2c, site symmetry:  $22'2'$ .

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[1, 2, 5, 6]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[3, 4, 7, 8]$

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

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 2, 5, 6]$
2	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[3, 4, 7, 8]$

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 7, 8]$
2	$[0, 0, \frac{1}{2}]$	$[3, 4, 5, 6]$

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, 2, 7, 8]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, 4, 5, 6]$

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

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1, 5]
2	$[-x, 0, \frac{1}{4}]$	[2, 6]
3	$[0, -x, \frac{3}{4}]$	[3, 7]
4	$[0, x, \frac{3}{4}]$	[4, 8]

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

No.	position	mapping
1	$[\frac{1}{2}, y, \frac{1}{4}]$	[1, 6]
2	$[\frac{1}{2}, -y, \frac{1}{4}]$	[2, 5]
3	$[-y, \frac{1}{2}, \frac{3}{4}]$	[3, 8]
4	$[y, \frac{1}{2}, \frac{3}{4}]$	[4, 7]

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

No.	position	mapping
1	$[x, \frac{1}{2}, \frac{1}{4}]$	[1, 5]
2	$[-x, \frac{1}{2}, \frac{1}{4}]$	[2, 6]
3	$[\frac{1}{2}, -x, \frac{3}{4}]$	[3, 7]
4	$[\frac{1}{2}, x, \frac{3}{4}]$	[4, 8]

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

No.	position	mapping
1	$[0, y, \frac{1}{4}]$	[1, 6]
2	$[0, -y, \frac{1}{4}]$	[2, 5]
3	$[-y, 0, \frac{3}{4}]$	[3, 8]
4	$[y, 0, \frac{3}{4}]$	[4, 7]

Table 11: Wyckoff site: 4k, site symmetry:  $2..$ 

No.	position	mapping
1	$[0, 0, z]$	[1, 2]
2	$[0, 0, z + \frac{1}{2}]$	[3, 4]
3	$[0, 0, \frac{1}{2} - z]$	[5, 6]
4	$[0, 0, -z]$	[7, 8]

Table 12: Wyckoff site:  $4\mathbf{l}$ , site symmetry:  $2..$ 

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

Table 13: Wyckoff site:  $4\mathbf{m}$ , site symmetry:  $2..$ 

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 2]$
2	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[3, 4]$
3	$[0, \frac{1}{2}, \frac{1}{2} - z]$	$[5, 6]$
4	$[\frac{1}{2}, 0, -z]$	$[7, 8]$

Table 14: Wyckoff site:  $8\mathbf{n}$ , site symmetry:  $1$ 

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