

Table 1: Wyckoff site: 2a, site symmetry: $2221'$

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

Table 2: Wyckoff site: 2b, site symmetry: $2221'$

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

Table 3: Wyckoff site: 2c, site symmetry: $2221'$

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

Table 4: Wyckoff site: 2d, site symmetry: $2221'$

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

Table 5: Wyckoff site: 4e, site symmetry: $-11'$

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

Table 6: Wyckoff site: 4f, site symmetry: $-11'$

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

Table 7: Wyckoff site: 4g, site symmetry: $2..1'$

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

Table 8: Wyckoff site: 4h, site symmetry: $2..1'$

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

Table 9: Wyckoff site: 4i, site symmetry: $.2.1'$

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

Table 10: Wyckoff site: 4j, site symmetry: $.2.1'$

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

Table 11: Wyckoff site: 4k, site symmetry: $\dots 21'$

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

Table 12: Wyckoff site: 4l, site symmetry: $\dots 21'$

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

Table 13: Wyckoff site: 8m, site symmetry: $11'$

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