

Table 1: Wyckoff site: 2a, site symmetry: 222

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

Table 2: Wyckoff site: 2b, site symmetry: 222

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

Table 3: Wyckoff site: 2c, site symmetry: 222

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

Table 4: Wyckoff site: 2d, site symmetry: 222

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

Table 5: Wyckoff site: 4e, site symmetry:  $-1$

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

Table 6: Wyckoff site:  $4\mathbf{f}$ , site symmetry:  $-1$ 

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

Table 7: Wyckoff site:  $4\mathbf{g}$ , site symmetry:  $2. .$ 

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

Table 8: Wyckoff site:  $4\mathbf{h}$ , site symmetry:  $2. .$ 

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

Table 9: Wyckoff site:  $4\mathbf{i}$ , site symmetry:  $.2.$ 

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

Table 10: Wyckoff site:  $4\mathbf{j}$ , site symmetry:  $.2.$ 

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

Table 11: Wyckoff site:  $4\mathbf{k}$ , site symmetry:  $\dots 2$ 

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

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

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

Table 13: Wyckoff site:  $8\mathbf{m}$ , site symmetry:  $1$ 

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