

Table 1: Wyckoff site: 2a, site symmetry: $2.2'2'$

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: $2.2'2'$

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 3: Wyckoff site: 2c, site symmetry: $-4..$

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

Table 4: Wyckoff site: 2d, site symmetry: $-4..$

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

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

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

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

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

Table 7: Wyckoff site: 4g, site symmetry: $2\dots$

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

Table 8: Wyckoff site: 4h, site symmetry: $2\dots$

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

Table 9: Wyckoff site: 4i, site symmetry: $2\dots$

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

Table 10: Wyckoff site: 8j, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[y, -x, -z]$	[3]
4	$[-y, x, -z]$	[4]

continued ...

Table 10

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