

Table 1: Wyckoff site: 2a, site symmetry: 32 .

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

Table 2: Wyckoff site: 2b, site symmetry: 3.2

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

Table 3: Wyckoff site: 2c, site symmetry: 3.2

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

Table 4: Wyckoff site: 2d, site symmetry: 3.2

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

Table 5: Wyckoff site: 4e, site symmetry: $3..$

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

Table 6: Wyckoff site: 4f, site symmetry: 3..

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

Table 7: Wyckoff site: 6g, site symmetry: .2.

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

Table 8: Wyckoff site: 6h, site symmetry: .2

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

Table 9: Wyckoff site: 12i, site symmetry: 1

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

continued ...

Table 9

No.	position	mapping
12	$[-y, -x, \frac{1}{2} - z]$	[12]