

Table 1: Wyckoff site: 2a, site symmetry: $4'\text{mm}'$

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

Table 2: Wyckoff site: 2b, site symmetry: $4'\text{mm}'$

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

Table 3: Wyckoff site: 4c, site symmetry: 2mm .

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

Table 4: Wyckoff site: 8d, site symmetry: $..m'$

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

Table 5: Wyckoff site: 8e, site symmetry: $..m$.

No.	position	mapping
1	$[x, 0, z]$	$[1, 6]$
2	$[0, x, z + \frac{1}{2}]$	$[2, 8]$

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: $\bar{4}2m$.

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

Table 7: Wyckoff site: **16g**, site symmetry: $\bar{4}2m$.

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