

Table 1: Wyckoff site: 2a, site symmetry: $4'm'm$

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

Table 2: Wyckoff site: 2b, site symmetry: $4'm'm$

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

Table 3: Wyckoff site: 4c, site symmetry: $2m'm'$

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

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

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

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

No.	position	mapping
1	$[x, 0, z]$	$[1, 14]$
2	$[0, x, z + \frac{1}{2}]$	$[2, 16]$

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: $.m'$.

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

Table 7: Wyckoff site: **16g**, site symmetry: 1

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	$[-x, y, z + \frac{1}{2}]$	[5]
6	$[x, -y, z + \frac{1}{2}]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[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	$[-x, y, z]$	[13]
14	$[x, -y, z]$	[14]
15	$[-y, -x, z + \frac{1}{2}]$	[15]
16	$[y, x, z + \frac{1}{2}]$	[16]