

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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