

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $2.2'2'$

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

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

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

Table 6: Wyckoff site: **8f**, site symmetry: $2..$

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

Table 7: Wyckoff site: **8g**, site symmetry: $..2'$

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

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

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

Table 9: Wyckoff site: **16i**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[2]
3	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]

continued ...

Table 9

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