

Table 1: Wyckoff site: **4a**, site symmetry: $2.2'2'$

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

Table 2: Wyckoff site: **4b**, site symmetry: $-4..$

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

Table 3: Wyckoff site: **4c**, site symmetry: $-4..$

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: $..2'$

No.	position	mapping
1	$[x, x, \frac{1}{4}]$	[1,5]
2	$[-x, -x, \frac{1}{4}]$	[2,6]

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, 0]$	[1,13]
2	$[-x, \frac{1}{2} - x, 0]$	[2,14]
3	$[x + \frac{1}{2}, -x, 0]$	[3,16]
4	$[\frac{1}{2} - x, x, 0]$	[4,15]
5	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[5,9]

continued ...

Table 8

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

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

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