

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: **4e**, site symmetry: $2.mm$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, 4, 7, 8]$
2	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[2, 3, 5, 6]$

continued ...

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site: **8i**, site symmetry: $\dots m$

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

Table 10: Wyckoff site: **16j**, site symmetry: 1

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