

Table 1: Wyckoff site: 2a, site symmetry: $42'2'$

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

Table 2: Wyckoff site: 2b, site symmetry: $42'2'$

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

Table 3: Wyckoff site: 4c, site symmetry: $22'2'$.

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

Table 4: Wyckoff site: 4d, site symmetry: 2.22

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: **8i**, site symmetry: $.2'$

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1,12]
2	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[2,15]
3	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[3,16]

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: $\dots 2$

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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