

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	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[1,4,5,6]
2	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[2,3,7,8]
3	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[9,10,13,16]
4	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[11,12,14,15]

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	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[2,3,5,6]

continued ...

Table 5

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