

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	$[1, 6, 12, 15]$
2	$[0, \frac{3}{4}, -z]$	$[2, 5, 11, 16]$

continued ...

Table 5

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

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

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

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

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

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

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

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

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

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

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