

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: $-1'$

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

Table 4: Wyckoff site: 8d, site symmetry: $2..$

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

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

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

Table 6: Wyckoff site: $8f$, site symmetry: m' .

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

Table 7: Wyckoff site: $16g$, site symmetry: 1

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