

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	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, 13, 14]$
4	$[0, \frac{1}{2}, \frac{1}{2}]$	$[11, 12, 15, 16]$

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

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

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

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

Table 4: Wyckoff site: 8d, 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	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10]$
6	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[11, 12]$
7	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	$[13, 14]$
8	$[x, \frac{1}{2}, \frac{1}{2}]$	$[15, 16]$

Table 5: Wyckoff site: $8e$, 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	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{4}]$	[9, 11]
6	$[\frac{3}{4}, \frac{1}{2} - y, \frac{3}{4}]$	[10, 12]
7	$[\frac{1}{4}, \frac{1}{2} - y, \frac{3}{4}]$	[13, 15]
8	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{4}]$	[14, 16]

Table 6: Wyckoff site: $8f$, 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	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[9, 14]
6	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[10, 13]
7	$[0, y + \frac{1}{2}, \frac{1}{2} - z]$	[11, 16]
8	$[0, \frac{1}{2} - y, z + \frac{1}{2}]$	[12, 15]

Table 7: Wyckoff site: $16g$, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[9]
10	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[10]
11	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14]
15	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[15]
16	$[x, y + \frac{1}{2}, \frac{1}{2} - z]$	[16]