

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: $8e$, site symmetry: $\dots 2$

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

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

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

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