

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $mm2$

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

Table 4: Wyckoff site: 8d, site symmetry: $-1'$

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

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

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

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

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

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

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

Table 8: Wyckoff site: $16h$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[x + \frac{1}{2}, -y, -z]$	$[2]$
3	$[-x, y, -z]$	$[3]$

continued ...

Table 8

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