

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, y, \frac{3}{4}]$	$[1, 3]$
2	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	$[2, 4]$

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{2} - x, \frac{1}{2}, z]$	[6,12]
7	$[x, 0, z + \frac{1}{2}]$	[7,9]
8	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[8,10]

Table 9: Wyckoff site: 16i, site symmetry: 1

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