

Table 1: Wyckoff site: 2a, site symmetry:  $mmm'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $mmm'$

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

Table 3: Wyckoff site: 2c, site symmetry:  $mmm'$

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

Table 4: Wyckoff site: 2d, site symmetry:  $mmm'$

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

Table 5: Wyckoff site: 4e, site symmetry:  $mm2$

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

Table 6: Wyckoff site: **4f**, site symmetry: **mm2**

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

Table 7: Wyckoff site: **4g**, site symmetry: **2'mm'**

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

Table 8: Wyckoff site: **4h**, site symmetry: **2'mm'**

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

Table 9: Wyckoff site: **4i**, site symmetry: **m2'm'**

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

Table 10: Wyckoff site: **4j**, site symmetry: **m2'm'**

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

Table 11: Wyckoff site:  $8k$ , site symmetry:  $-1$ 

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

Table 12: Wyckoff site:  $8l$ , site symmetry:  $. . m'$ 

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

Table 13: Wyckoff site:  $8m$ , site symmetry:  $m . .$ 

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

Table 14: Wyckoff site:  $8n$ , site symmetry:  $. . m$ .

No.	position	mapping
1	$[x, \frac{1}{4}, z]$	$[1, 7]$
2	$[x + \frac{1}{2}, \frac{3}{4}, -z]$	$[2, 8]$
3	$[-x, \frac{3}{4}, -z]$	$[3, 5]$

*continued ...*

Table 14

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

Table 15: Wyckoff site: 16o, site symmetry: 1

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