

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $m'm2'$

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	$[1, 3, 6, 8]$
2	$[0, \frac{3}{4}, -z]$	$[2, 4, 5, 7]$

*continued ...*

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site:  $8i$ , site symmetry:  $.m$ .

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

Table 10: Wyckoff site:  $16j$ , site symmetry:  $1$ 

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