

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

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

Table 2: Wyckoff site: 4b, site symmetry:  $2'2'2$

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $2/m'..$

No.	position	mapping
1	$[0, \frac{3}{4}, \frac{1}{4}]$	[1,2,13,14]
2	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[3,4,15,16]

*continued ...*

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry:  $2/m'$  . .

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: . 2' .

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

Table 9: Wyckoff site: 8i, site symmetry:  $2'..$ 

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

Table 10: Wyckoff site: 8j, site symmetry:  $2'..$ 

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

Table 11: Wyckoff site: 8k, site symmetry:  $2..$ 

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

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

No.	position	mapping
1	$[0, y, z]$	$[1, 14]$
2	$[0, \frac{1}{2} - y, \frac{1}{2} - z]$	$[2, 13]$
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	$[3, 16]$

*continued ...*

Table 12

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

Table 13: Wyckoff site:  $16m$ , site symmetry:  $1$ 

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