

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	[0, 0, 0]	[1,5,12,16]
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	[2,6,11,15]

*continued ...*

Table 5

No.	position	mapping
3	$[0, \frac{1}{2}, \frac{1}{2}]$	[3, 7, 10, 14]
4	$[\frac{1}{2}, \frac{1}{2}, 0]$	[4, 8, 9, 13]

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

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

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

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

Table 8: Wyckoff site: 8h, site symmetry:  $\dots 2' \dots$ 

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

Table 9: Wyckoff site: 8i, site symmetry:  $\dots 2$ 

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

Table 10: Wyckoff site: 8j, site symmetry:  $\dots 2$ 

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

Table 11: Wyckoff site: 8k, site symmetry:  $\dots 2'$ 

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

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

No.	position	mapping
1	[x, y, 0]	[1,16]
2	$[x + \frac{1}{2}, -y, \frac{1}{2}]$	[2,15]
3	$[-x, y + \frac{1}{2}, \frac{1}{2}]$	[3,14]

*continued ...*

Table 12

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

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	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[6]
7	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[7]
8	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[9]
10	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[10]
11	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[11]
12	$[-x, -y, z]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[13]
14	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[14]
15	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[15]
16	$[x, y, -z]$	[16]