

Table 1: Wyckoff site: 4a, site symmetry:  $2.22$

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,6,15,16]
2	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[2,3,12,13]

*continued ...*

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site: 8i, site symmetry:  $\bar{3}m'$ 

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

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

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