

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

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

Table 2: Wyckoff site: 4b, site symmetry: 2.22

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

Table 3: Wyckoff site: 8c, site symmetry: 2'..

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

Table 4: Wyckoff site: 8d, site symmetry: 2'..

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

Table 5: Wyckoff site: **8e**, site symmetry:  $\dots 2'$ 

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

Table 6: Wyckoff site: **8f**, site symmetry:  $\dots 2$ 

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

Table 7: Wyckoff site: **16g**, site symmetry:  $1$ 

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