

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

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

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

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

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

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

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

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

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

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

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

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

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

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