

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $4..$

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

Table 4: Wyckoff site: 8d, site symmetry:  $-1$

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

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

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

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

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

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

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