

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

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

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

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

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

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

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

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

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

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

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

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

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