

Table 1: Wyckoff site: 4a, site symmetry: $22'2'$

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

Table 2: Wyckoff site: 4b, site symmetry: $22'2'$

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

Table 3: Wyckoff site: 8c, site symmetry: $-1'$

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{2}, z]$	[1,4]
2	$[\frac{1}{4}, 0, \frac{1}{2} - z]$	[2,3]
3	$[\frac{3}{4}, \frac{1}{2}, -z]$	[5,8]

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: 1

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