

Table 1: Wyckoff site: 2a, site symmetry:  $-4'm2'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $-4'm2'$

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

Table 3: Wyckoff site: 4c, site symmetry:  $2mm$ .

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

Table 4: Wyckoff site: 4d, site symmetry:  $2mm$ .

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

Table 5: Wyckoff site: 8e, site symmetry:  $-1$

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

*continued ...*

Table 5

No.	position	mapping
7	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[11,15]
8	$[0, 0, \frac{1}{2}]$	[12,16]

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

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

Table 7: Wyckoff site: **8g**, site symmetry:  $\dots m$ .

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

Table 8: Wyckoff site: **16h**, site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, -y, -z]$	[2]
3	$[-x, y + \frac{1}{2}, -z]$	[3]
4	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[\frac{1}{2} - x, y, z]$	[6]
7	$[x, \frac{1}{2} - y, z]$	[7]
8	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[8]
9	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[9]

*continued ...*

Table 8

No.	position	mapping
10	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[-y, -x, \frac{1}{2} - z]$	[12]
13	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[13]
14	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[15]
16	$[y, x, z + \frac{1}{2}]$	[16]