

Table 1: Wyckoff site: 4a, site symmetry:  $\dots 2'/m$

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

Table 2: Wyckoff site: 4b, site symmetry:  $\dots 2'/m$

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

Table 3: Wyckoff site: 4c, site symmetry:  $\dots 2/m$

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

Table 4: Wyckoff site: 4d, site symmetry:  $\dots 2/m$

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

Table 5: Wyckoff site: 4e, site symmetry:  $2'm'm$

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1,8,10,15]
2	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[2,7,9,16]

*continued ...*

Table 5

No.	position	mapping
3	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	$[3, 6, 12, 13]$
4	$[-x, \frac{3}{4}, 0]$	$[4, 5, 11, 14]$

Table 6: Wyckoff site:  $4\mathbf{f}$ , site symmetry:  $2'm'm$ 

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

Table 7: Wyckoff site:  $8\mathbf{g}$ , site symmetry:  $..2'$ 

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

Table 8: Wyckoff site:  $8\mathbf{h}$ , site symmetry:  $..2$ 

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

Table 9: Wyckoff site: **8i**, site symmetry:  $\bar{3}m$ 

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

Table 10: Wyckoff site: **8j**, site symmetry:  $\bar{3}m$ 

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

Table 11: Wyckoff site: **8k**, site symmetry:  $\bar{3}m'$ 

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

Table 12: Wyckoff site: **16l**, site symmetry:  $\bar{1}$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	$[2]$
3	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	$[3]$

*continued ...*

Table 12

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