

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $.2'/m.$

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

Table 4: Wyckoff site: 4d, site symmetry: $.2'/m.$

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

Table 5: Wyckoff site: 4e, site symmetry: $m'm2'$

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	$[1, 3, 6, 8]$
2	$[0, \frac{3}{4}, -z]$	$[2, 4, 5, 7]$

continued ...

Table 5

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

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

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

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

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

Table 8: Wyckoff site: **8h**, site symmetry: m'

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

Table 9: Wyckoff site: **8i**, site symmetry: $\bar{4}2m$.

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

Table 10: Wyckoff site: **16j**, site symmetry: $\bar{4}2m$.

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