

Table 1: Wyckoff site: **3a**, site symmetry: $2221'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 4, 7, 11, 13, 16, 19, 23]$
2	$[0, 0, \frac{2}{3}]$	$[2, 5, 9, 10, 14, 17, 21, 22]$
3	$[0, 0, \frac{1}{3}]$	$[3, 6, 8, 12, 15, 18, 20, 24]$

Table 2: Wyckoff site: **3b**, site symmetry: $2221'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 4, 7, 11, 13, 16, 19, 23]$
2	$[0, 0, \frac{1}{6}]$	$[2, 5, 9, 10, 14, 17, 21, 22]$
3	$[0, 0, \frac{5}{6}]$	$[3, 6, 8, 12, 15, 18, 20, 24]$

Table 3: Wyckoff site: **3c**, site symmetry: $2221'$

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 4, 7, 11, 13, 16, 19, 23]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{2}{3}]$	$[2, 5, 9, 10, 14, 17, 21, 22]$
3	$[0, \frac{1}{2}, \frac{1}{3}]$	$[3, 6, 8, 12, 15, 18, 20, 24]$

Table 4: Wyckoff site: **3d**, site symmetry: $2221'$

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 4, 7, 11, 13, 16, 19, 23]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{6}]$	$[2, 5, 9, 10, 14, 17, 21, 22]$
3	$[0, \frac{1}{2}, \frac{5}{6}]$	$[3, 6, 8, 12, 15, 18, 20, 24]$

Table 5: Wyckoff site: **6e**, site symmetry: $2..1'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 13, 16]$
2	$[0, 0, z + \frac{2}{3}]$	$[2, 5, 14, 17]$
3	$[0, 0, z + \frac{1}{3}]$	$[3, 6, 15, 18]$
4	$[0, 0, -z]$	$[7, 11, 19, 23]$
5	$[0, 0, \frac{1}{3} - z]$	$[8, 12, 20, 24]$
6	$[0, 0, \frac{2}{3} - z]$	$[9, 10, 21, 22]$

Table 6: Wyckoff site: **6f**, site symmetry: $2..1'$

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1,4,13,16]
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{2}{3}]$	[2,5,14,17]
3	$[0, \frac{1}{2}, z + \frac{1}{3}]$	[3,6,15,18]
4	$[\frac{1}{2}, 0, -z]$	[7,11,19,23]
5	$[0, \frac{1}{2}, \frac{1}{3} - z]$	[8,12,20,24]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{2}{3} - z]$	[9,10,21,22]

Table 7: Wyckoff site: **6g**, site symmetry: $.2.1'$

No.	position	mapping
1	$[x, 0, 0]$	[1,7,13,19]
2	$[x, x, \frac{2}{3}]$	[2,10,14,22]
3	$[0, x, \frac{1}{3}]$	[3,8,15,20]
4	$[-x, 0, 0]$	[4,11,16,23]
5	$[-x, -x, \frac{2}{3}]$	[5,9,17,21]
6	$[0, -x, \frac{1}{3}]$	[6,12,18,24]

Table 8: Wyckoff site: **6h**, site symmetry: $.2.1'$

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1,7,13,19]
2	$[x, x, \frac{1}{6}]$	[2,10,14,22]
3	$[0, x, \frac{5}{6}]$	[3,8,15,20]
4	$[-x, 0, \frac{1}{2}]$	[4,11,16,23]
5	$[-x, -x, \frac{1}{6}]$	[5,9,17,21]
6	$[0, -x, \frac{5}{6}]$	[6,12,18,24]

Table 9: Wyckoff site: **6i**, site symmetry: $..21'$

No.	position	mapping
1	$[x, 2x, 0]$	[1,11,13,23]
2	$[-x, x, \frac{2}{3}]$	[2,9,14,21]
3	$[-2x, -x, \frac{1}{3}]$	[3,12,15,24]
4	$[-x, -2x, 0]$	[4,7,16,19]
5	$[x, -x, \frac{2}{3}]$	[5,10,17,22]
6	$[2x, x, \frac{1}{3}]$	[6,8,18,20]

Table 10: Wyckoff site: 6j, site symmetry: $\bar{3}21'$

No.	position	mapping
1	$[x, 2x, \frac{1}{2}]$	$[1, 11, 13, 23]$
2	$[-x, x, \frac{1}{6}]$	$[2, 9, 14, 21]$
3	$[-2x, -x, \frac{5}{6}]$	$[3, 12, 15, 24]$
4	$[-x, -2x, \frac{1}{2}]$	$[4, 7, 16, 19]$
5	$[x, -x, \frac{1}{6}]$	$[5, 10, 17, 22]$
6	$[2x, x, \frac{5}{6}]$	$[6, 8, 18, 20]$

Table 11: Wyckoff site: 12k, site symmetry: $\bar{4}32'$

No.	position	mapping
1	$[x, y, z]$	$[1, 13]$
2	$[x - y, x, z + \frac{2}{3}]$	$[2, 14]$
3	$[-y, x - y, z + \frac{1}{3}]$	$[3, 15]$
4	$[-x, -y, z]$	$[4, 16]$
5	$[-x + y, -x, z + \frac{2}{3}]$	$[5, 17]$
6	$[y, -x + y, z + \frac{1}{3}]$	$[6, 18]$
7	$[x - y, -y, -z]$	$[7, 19]$
8	$[y, x, \frac{1}{3} - z]$	$[8, 20]$
9	$[-x, -x + y, \frac{2}{3} - z]$	$[9, 21]$
10	$[x, x - y, \frac{2}{3} - z]$	$[10, 22]$
11	$[-x + y, y, -z]$	$[11, 23]$
12	$[-y, -x, \frac{1}{3} - z]$	$[12, 24]$