

MSG No. 195.2 $P231'$ [Type II, cubic]

Table 1: Wyckoff site: 1a, site symmetry: $23\cdot 1'$

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

Table 2: Wyckoff site: 1b, site symmetry: $23\cdot 1'$

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

Table 3: Wyckoff site: 3c, site symmetry: $222\cdot\cdot 1'$

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

Table 4: Wyckoff site: 3d, site symmetry: $222\cdot\cdot 1'$

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

Table 5: Wyckoff site: 4e, site symmetry: $\cdot 3\cdot 1'$

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

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

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

Table 7: Wyckoff site: $6g$, site symmetry: $2..1'$

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

Table 8: Wyckoff site: $6h$, site symmetry: $2..1'$

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

Table 9: Wyckoff site: $6i$, site symmetry: $2..1'$

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

Table 10: Wyckoff site: 12j, site symmetry: 11'

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