

MSG No. 195.1 $P23$ [Type I, cubic]

Table 1: Wyckoff site: $1a$, site symmetry: 23 .

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$

Table 2: Wyckoff site: $1b$, site symmetry: 23 .

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

Table 3: Wyckoff site: $3c$, site symmetry: 222 .

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

Table 4: Wyckoff site: $3d$, site symmetry: 222 .

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

Table 5: Wyckoff site: $4e$, site symmetry: $.3$.

No.	position	mapping
1	$[x, x, x]$	$[1, 5, 6]$
2	$[x, -x, -x]$	$[2, 10, 11]$
3	$[-x, x, -x]$	$[3, 7, 12]$
4	$[-x, -x, x]$	$[4, 8, 9]$

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2]$
2	$[-x, 0, 0]$	$[3, 4]$
3	$[0, x, 0]$	$[5, 12]$
4	$[0, 0, x]$	$[6, 9]$
5	$[0, 0, -x]$	$[7, 11]$
6	$[0, -x, 0]$	$[8, 10]$

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

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

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

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

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

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

Table 10: Wyckoff site: 12j, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, -z]$	[2]
3	$[-x, y, -z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[z, x, y]$	[5]
6	$[y, z, x]$	[6]
7	$[-y, z, -x]$	[7]
8	$[-z, -x, y]$	[8]
9	$[-y, -z, x]$	[9]
10	$[z, -x, -y]$	[10]
11	$[y, -z, -x]$	[11]
12	$[-z, x, -y]$	[12]