

MSG No. 195.1 *P*23 [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]