

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

Table 1: Wyckoff site: 1a, site symmetry: 23.1'

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: 23.1'

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..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..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: .3.1'

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]