

MSG No. 147.14 $P\bar{3}1'$ [Type II, trigonal]

Table 1: Wyckoff site: 1a, site symmetry: -3..1'

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: -3..1'

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

Table 3: Wyckoff site: 2c, site symmetry: 3..1'

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

Table 4: Wyckoff site: 2d, site symmetry: 3..1'

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

Table 5: Wyckoff site: 3e, site symmetry: -11'

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

Table 6: Wyckoff site: 3f, site symmetry: -11'

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

Table 7: Wyckoff site: 6g, site symmetry: 11'

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