

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	$[x - y, x, -z]$	$[6, 12]$