

MSG No. 157.54 $P31m1'$ [Type II, trigonal]

Table 1: Wyckoff site: 1a, site symmetry: 3..m1'

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

Table 2: Wyckoff site: 2b, 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 3: Wyckoff site: 3c, site symmetry: ..m1'

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

Table 4: Wyckoff site: 6d, 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, -x + y, z]	[4,10]
5	[x - y, -y, z]	[5,11]
6	[y, x, z]	[6,12]