

MSG No. 157.53  $P31m$  [ Type I, trigonal ]

Table 1: Wyckoff site: **1a**, site symmetry: **3.m**

No.	position	mapping
1	[0, 0, z]	[1,2,3,4,5,6]

Table 2: Wyckoff site: **2b**, site symmetry: **3..**

No.	position	mapping
1	[ $\frac{1}{3}$ , $\frac{2}{3}$ , z]	[1,2,3]
2	[ $\frac{2}{3}$ , $\frac{1}{3}$ , z]	[4,5,6]

Table 3: Wyckoff site: **3c**, site symmetry: **..m**

No.	position	mapping
1	[x, 0, z]	[1,5]
2	[0, x, z]	[2,6]
3	[-x, -x, z]	[3,4]

Table 4: Wyckoff site: **6d**, site symmetry: **1**

No.	position	mapping
1	[x, y, z]	[1]
2	[-y, x - y, z]	[2]
3	[-x + y, -x, z]	[3]
4	[-x, -x + y, z]	[4]
5	[x - y, -y, z]	[5]
6	[y, x, z]	[6]