

MSG No. 159.61 *P31c* [ Type I, trigonal ]

Table 1: Wyckoff site: **2a**, site symmetry: 3..

No.	position	mapping
1	[0, 0, $z$ ]	[1,2,3]
2	[0, 0, $z + \frac{1}{2}$ ]	[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	[ $\frac{2}{3}$ , $\frac{1}{3}$ , $z + \frac{1}{2}$ ]	[4,5,6]

Table 3: Wyckoff site: **6c**, site symmetry: 1

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