

Table 31A-6-001. $\text{TiH}_3(\text{SeO}_3)_2$. Crystal structure of phase I [83Shu]. $T = \text{RT}$. Fractional coordinates and temperature parameters [\AA]. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B
Tl	0.0302(1)	0.0194(1)	0.16353(4)	2.75(4)
Se(1)	0.4935(4)	0.0866(3)	0.01030(8)	1.67(7)
Se(2)	0.0239(3)	0.4512(2)	0.64279(8)	1.76(7)
O(1)	0.027(2)	0.436(2)	0.0819(5)	2.1(6)
O(2)	0.229(2)	0.068(3)	0.5261(9)	2.2(5)
O(3)	0.283(2)	0.426(3)	0.4575(8)	2.8(8)
O(4)	0.153(2)	0.312(2)	0.7062(7)	2.1(6)
O(5)	0.444(2)	0.279(2)	0.1731(7)	1.8(7)
O(6)	0.249(2)	0.084(2)	0.3248(7)	2.4(4)

Table 31A-6-002. $\text{TiH}_3(\text{SeO}_3)_2$. Crystal structure of phase I [83Shu]. Interatomic distances [\AA].

Tl–O(1)	2.95(1)	Se(2)–O(4)	1.62(1)
–O(2)	2.91(2)	–O(5)	1.76(1)
–O(3)	2.92(1)	–O(6)	1.75(1)
–O(4)	2.88(1)	O(1)–O(2)	2.60(2)
–O(4)	3.40(1)	O(1)–O(3)	2.65(2)
–O(5)	2.94(1)	O(2)–O(3)	2.67(2)
–O(6)	3.16(1)	O(4)–O(5)	2.65(2)
–O(6)	3.20(1)	O(4)–O(6)	2.55(2)
Se(1)–O(1)	1.673(9)	O(5)–O(6)	2.62(2)
–O(2)	1.66(2)	O(2)–O(3)	2.54(2)
–O(3)	1.76(2)	O(4)–O(5)	2.56(2)
		O(1)–O(6)	2.52(2)