

On the monocrystal, rutile has a sharp texture of topotactic type, with the (110) plane remaining nevertheless parallel to the monocrystal face.

The macroscopic geometry of the metal seems to play as important a part as its crystal orientations.

Results are given in the table below. The values obtained from (I) and (II) agree to within 3σ in all but three cases. More interesting, but not surprising, the standard distances to oxygen obtained here mainly from organic molecular compounds with mixed coordinative environments agree with those obtained by Brown and Shannon from oxides and inorganic oxyacid salts.

Table: Standard bond lengths d_{iO} ($CN_O = 4$); values for other CN's may be obtained from (I), (II), c and N.

	Mg	Al	Si	P	
C		2.032(3)	1.872(1)	1.788(1)	a)
		2.032(3)	1.872(1)	1.786(1)	b)
N		1.851(10)	1.721(5)	1.616(1)	a)
		1.850(9)	1.718(4)	1.615(1)	b)
O	1.885(14)	1.701(7)	1.610(4)	1.534(1)	a)
	1.898(11)	1.715(6)	1.613(4)	1.534(1)	b)
F			1.500(6)	1.402(3)	a)
			1.520(5)	1.418(3)	b)
Si(-Si)			2.391(11)	2.168(22)	a)
P(-P)			2.391(15)	2.145(26)	b)
Cl	2.297(17)	2.131(3)	2.026(8)	1.935(5)	a)
	2.281(17)	2.131(3)	2.022(8)	1.913(5)	b)
c	0.501(37)	0.466(19)	0.455(13)	0.484(6)	a)
N	4.31(30)	4.25(16)	4.01(11)	3.41(4)	b)
σ^2	0.0858	0.0195	0.0099	0.0067	a) c)
	0.0785	0.0182	0.0099	0.0065	b) c)
m	504	522	826	1878	c)
N _{obs}	89	117	189	441	c)

a) (I); b) (II); c) m=number of distances used in refinement; N_{obs}=number of structures in data set; p=number of standard bond lengths refined $\sigma^2 = (\sum N_{obs} - \sum N_{calc})^2 / N_{obs} - (p + 1)$

04.1-7 STANDARD BOND LENGTHS IN MOLECULAR COMPOUNDS FROM EMPIRICAL BOND LENGTH-BOND STRENGTH RELATIONSHIPS (Mg,Al,Si,P-C,N,O,F,Cl) By G. Klebe, H.B. Bürgli, Laboratorium für Chemische und Mineralogische Kristallographie, Universität Bern, Freiestr. 3, CH-3012 Bern, Switzerland

Standard bond lengths are a prerequisite for interpretations and comparisons of interatomic distances. Such distances (d_O) are given here for bonds from Mg,Al,Si,P to C,N,O,F,Cl. They are based on least squares analysis using two empirical bond strength (n)-bond length(d) relationships: (I) $n_i/n_O = \exp[-(d_i/d_{iO})/c]$ (L. Pauling, The Nature of the Chemical Bond, Cornell University Press, Ithaca, (1940)); (II) $n_i/n_O = (d_i/d_{iO})^{-N}$ (G. Donnay and R. Allmann, Amer. Min. (1970), 55, 1003; I.D. Brown and R.D. Shannon, Acta Cryst. (1973), A29,266). The data for Al,Si,P with coordination numbers (CN) 4,5,6 were taken from the Cambridge Structural Data Base and supplemented with gas phase electron diffraction data; the data for Mg were taken from J.C.J. Bart and P. Vitarelli (Inorg. Chim. Acta (1983), 73, 215). The data include molecules with up to 4 different ligand atoms around the central atom. Details will be given in a future, full account of the work. Values of d_{iO} , c and N, respectively, were determined by minimizing the expression

$$(CN_O - \sum_{i=1}^{CN} n_i)^2$$

for Mg,Al,Si,P separately, but considering all coordination numbers simultaneously; CN_O is a reference coordination number, n_O is taken as 1.

04.1-8 CONTRIBUTION TO THE CRYSTAL CHEMISTRY OF SODIUM HEXACHLOROANTIMONATE, -NIOBATE, AND -TANTALATE. By Henning Henke, Institut für Anorg. Chemie der Universität Karlsruhe (TH), D 7500 Karlsruhe, Bundesrepublik Deutschland.

From single-crystal X-ray data collected at room temperature the individual structures of three sodium salts can be established:

	a [Å]	b [Å]	c [Å]	β [°]
NaSbCl ₆	6.393(2)	6.393	10.717(4)	--
NaNbCl ₆	6.398(2)	6.850(2)	19.012(4)	90.72(2)
NaTaCl ₆	6.449(2)	6.880(2)	18.989(6)	90.87(2)

While NaSbCl₆ is tetragonal with space group $P4_2/m$ and $Z=2$, the niobium and tantalum analogues crystallize both in the monoclinic space group $P2_1/c$; since there is a doubling of the c-axis the unit cell has $Z=4$. Parameter refinement includes absorption and extinction corrections; the final R-values are 0.018 (NaSbCl₆, 611 obs.refl.), 0.018 (NaNbCl₆, 2214 obs.refl.), and 0.024 (NaTaCl₆, 2341 obs.refl.). All three compounds contain discrete MCl_6^- ions arranged with their centres like $PtCl_6^{2-}$ in cubic K_2PtCl_6 . The same applies to the cations