Crystal Molecule Structure of Tetraphenoxytitanium(IV) Monophenolate, $Ti(OPh)_4$,HOPh

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Summary An *X*-ray diffraction study of tetraphenoxytitanium(IV) monophenolate has shown the structure to be dimer of octahedrally co-ordinated alkoxytitanium molecules.

STRUCTURES of alkyloxy-titanates have received considerable attention in recent years.[1-5] We report on the structure of tetraphenoxytitanium(IV) monophenolate, an alkoxy-dimer with octahedrally co-ordinated titanium.

The title compound was prepared by the addition of phenol to tetraisopropoxytitanium(IV) and isopropyl alcohol was removed under reduced pressure. The orange-red product was recrystallized from toluene.

Tetraphenoxytitanium(IV) monophenolate, $Ti(OPh)_4$, HOPh, $M = 514{\cdot}44$, monoclinic, $a = 10{\cdot}491$, $b = 18{\cdot}406$, $c = 13{\cdot}858$ Å, $\beta = 101{\cdot}54°$, $D_m = 1{\cdot}31$ (by flotation), $Z = 4$, $D_c = 1{\cdot}30$. Space group, $P2_1/n$. Cu-K_α radiation. Intensity data were collected by multiple film equi-inclination Weissenberg methods. 1485 Reflections were investigated on layers $0kl$ to $6kl$ with 1076 observed and 409 treated as unobserved. The structure was determined by Patterson and heavy-atom Fourier methods. Block-diagonal least-squares refinement reduced the conventional reliability factor R to 0·139. Full-matrix least-squares refinement with anisotropic temperature factors over all non-hydrogen atoms reduced R to 0·081. Hydrogen atoms were included in their computed positions.

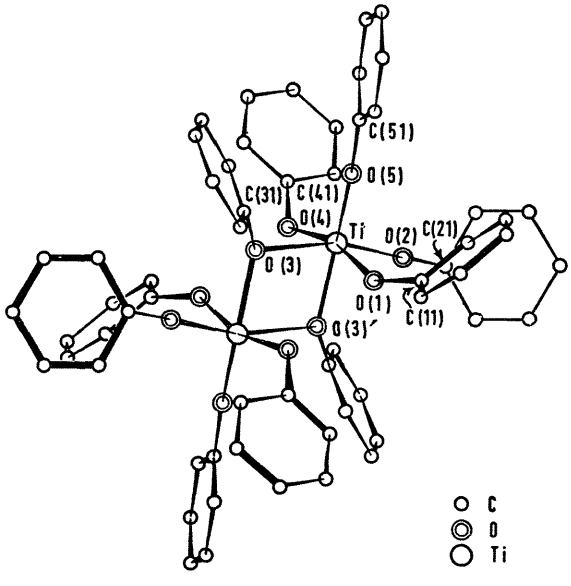

FIGURE. *A view of the dimer projected along the* a*-axis.*

The structure shown in the Figure consists of dimers bridged by phenoxy oxygen atoms so that the co-ordination about the titanium is a distorted octahedron. The five titanium–oxygen bond lengths are in agreement with other reported results.[1-5] Pertinent bond distances are Ti–O(1) = 2·200, Ti–O(2) = 1·842, Ti–O(3) = 2·045, Ti–O(4) = 1·884, Ti–O(5) = 1·789, and Ti–O(3)′ = 2·027 Å. The Ti–Ti distance is 3·309 Å and the Ti–O–Ti angle is 109°.

The Ti–O–C bond angles at O(1), O(3), and O(4), are 132, 126, and 127°, respectively. The Ti–O–C bond angle for O(2) is 169°, and for O(5) is 175°. Almost linear Ti–O–C bond angles have been observed in dichlorodiphenoxy-,[3] and dichlorodiethoxy-titanates.[5]

The shortest O–C distance is 1·268 Å between O(2) and C(21). The O–C distance of the bridging oxygen O(3)–C(31) is 1·418 Å. The remaining O–C distances are equal at 1·36 Å.

The C–C bond distances are normal.

(*Received, March 18th*, 1971; *Com.* 347.)

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