Titanium alkoxide complexes as molecular models for surface interaction between drug and sol-gel derived titania nanoparticles for drug delivery

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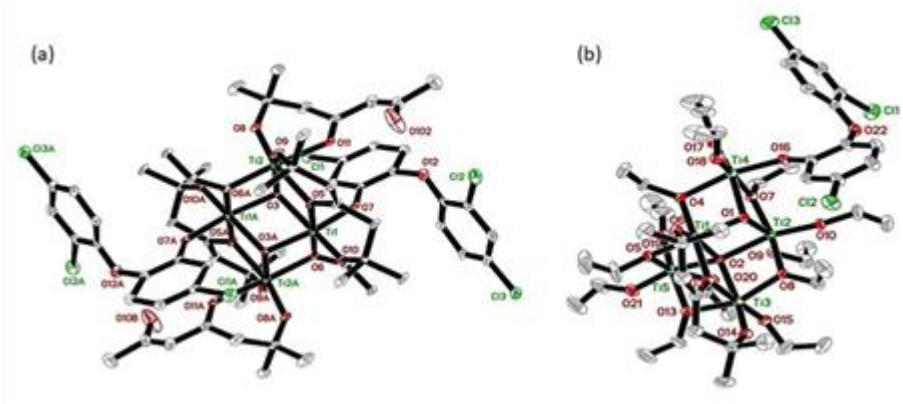
Titania nanoparticles are attractive mediators for drug delivery[1,2] and can be produced with fine control via sol-gel synthesis. The surface interaction between titania nanoparticles and different medical agents can be studied via complexes of pharmaceuticals. Surface chemistry can be revealed by structural studies. Here[3,4], two new coordination complexes $[Ti_4(\mu_3\text{-}O)_2(\mu_2\text{-}OEt)_2(C_9H_{16}O_3)_2(C_8H_{12}O_3)_2(C_{12}H_6Cl_3O_2)_2 \bullet 4\ C_3H_6O]$, **1**, and $[Ti_5(\mu_3\text{-}O)_2(\mu_2\text{-}OEt)_5(\mu\text{-}OEt)_8(C_9H_{16}O_3)(C_{12}H_6Cl_3O_2)]$, **2** (Figure 1) were synthesized and their structures were determined by single crystal X-ray diffraction. Triclosan coordinate to titanium atoms via phenoxide bonding. Hydrolysed compound **1** was tested against *Staphylococcus aureus* and was found to have an inhibitory effect. Thermolysis and hydrolysis of compound **1** were studied. High thermal stability of phenoxide ligands causes topotactic transformation upon calcining. The phenoxide ligands does not stabilize compound **1** against water, but hydrolyses to titania (anatase) nanoparticles with primary size of about 5 nm, as determined by transmission electron microscopy.



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