New methods to capture insoluble, unstable titanium (IV) species in single-crystal form.

M Roy¹, M Olmstead², A Balch¹

¹University of California, Davis, Davis, CA, ²Dept of Chemistry, Univ of California Davis mriroy@ucdavis.edu

The coordination of titanium (IV) halides to neutral L-type ligands and L-L type chelates results in fascinating geometries, brilliant colors unusual for a d0 species, and unusual changes in Ti-X bond lengths. In spite of being a small, hard, highly lewis-acidic metal center, Ti (IV) can surprisingly form eight-coordinate complexes with such ligands. However, TiX4(L)2 or TiX4(L-L) species are typically unstable in solution when soluble, and more often than not, intractable solids that do not dissolve in common organic solvents. A methodology has been created for small-scale TiX4-ligand reactions that result in direct formation of high-quality single crystals. The method has been utilized in elucidating the structures of several insoluble titanium complexes that have evaded crystallographic characterization for generations.

