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Double Deprotonation of functionalized aryl amines leading to new Ti (IV) imido derivates

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The π -donor imido functional group gives rise to a chemistry that is generally dominated by medium to high metal oxidation states; also showing a variety of coordination modes such as terminal metal-nitrogen multiple bond or bridging disposition. This chemistry is interesting not only because of their structural features, and their remarkable reactivity, as well, nowadays it is well recognized the importance of imido compounds in industrial processes, organic synthesis and catalysis. [1]

The most reactive of imido compounds occur within group 4. As an example, titanium imides react with many organic substrates including alkenes, allenes, alkynes, heterocumulenes, nitriles, isocitriles, isocyanates, and phosphaalkynes, and in many cases these reactions result in the formation of both novel organic products and metal-containing species. [2]

Our studies are focused on species containing imido ligands which possess functionalized substituents as we are interested in analysing the effect of the additional functionality on the coordination behaviour of these derivatives and on their reactivity. As well the presence of an additional donor atom in the ligand would enhance the capacity of the species synthesized to behave as metalloligands for the construction of ordered supramolecular structures.

The treatment of the complexes $[Ti(NR_2)_4]$, $[Ti(C_5Me_5)Cl_3]$ and $[Ti(C_5Me_5)(NR_2)_3]$ with functionalized aromatic amines leads to the formation of new amido complexes. To achieve the double deprotonation it is necessary to introduce in the reaction an additional base such as alkyl lithium or magnesium derivates. In these conditions it is possible to attain the formation of imido species as the one show *Organometallics* 2005, 24, 5084. (f) P. Mountford, *Chem. Commun.* 1997, 2127. [2] (a) P. Mountford, N. Hazari, *Acc. Chem. Res.* 2005, 38, 839-849. (b) S. Dunn, N. Hazari, A.R. Cowley, J.C. Green, P. Mountford, *Organometallics* 2006, 25, 1755. [3] (a) C.T. Vroegop, J.H. Teuben, F. van Bolhuis, J.G.M. van der Linden *Chem.Commun.* 1983, 550. (b) W.J. Grigsby, M.M. Olmstead, P.P. Power, *J. Organomet. Chem.* 1996, 513, 173. (c) A. Abarca, P. Gomez-Sal, A. Martin, M. Mena, J.M. Poblet, C.Yelamos, *Inorg.Chem.* 2000, 39, 642. (d) K. Hughes, S.M.B. Marsh, J.A.K. Howard, P.S. Ford *J. Organomet. Chem.* 1997, 528, 195.

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X-Ray Diffraction Studies of Monocyclopentadienyl Cyclometalated Aryl Tantalum(V) Compounds

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Mono- and bis(cyclopentadienyl) complexes of early transition metals have received an increased attention stimulated by their use in understanding the chemistry of important catalytic processes, in particular those related to olefin and ring-opening polimerization metathesis.[1] Many aryl tantalum compounds are labile and tend to decompose via β-H elimination reactions forming benzyne complexes, for example, TaCp*Me₃Ph.[2] However, ancillary ligands capable of π -bonding have a stabilizing influence on σ -bonded aryl ligands in high oxidation state early transition metal chemistry. For it, a possible approach to overcome complications caused by β -H elimination is to prepare derivatives by employing an aryl ligand that has an ortho-substituted C,N-chelating arylamine ligands form an additional coordinative bond (σ-donor N) to the metal center and thereby enhance the kinetic stability of the organometallic complex formed.[3] These bidentated ligands possess a hard anionic carbon (C_i) atom and a neutral tertiary N donor atom as ligating sites; moreover, such ligands form cyclometalated complexes which contain a five-membered chelate ring.

As part our interest in the structure-reactivity relationship analysis in Group 5 metal monocyclopentadienyl compounds, we will describe the results obtained by using the 2-{(dimethylamino)methyl}phe nyl ligand in the synthesis of new tantalum(V) complexes and their structural study by spectroscopic, X-ray diffraction and DFT methods.

in figure 1. This compound crystallizes as a triclinic in the space group P-1; only half of the molecule is found in the asymmetric unit, through an inversion centre is generated the titanium (IV) dinuclear species. Interestingly not many titanocenes with bridging imido arene ligands have been described. [3]



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	1	2	3
Ta(1)-N	2.467(9)	2.524(4)	2.529(9)
Ta(1)-Cp	2.120	2.147	2.211
C(17)-N	1.482(14)	1.494(7)	1.512(14)
Cp-Ta(1)-N	175.6	176.0	174.7

^aCp is the centroid of C(1)-C(2)-C(3)-C(4)-C(5) ring.