

The structure of complex cation $[Cu_2(L)_2(H_2O)_2]^{4+}$

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Keywords: pyridoxal, thiosemicarbazone, copper

MS61.P12

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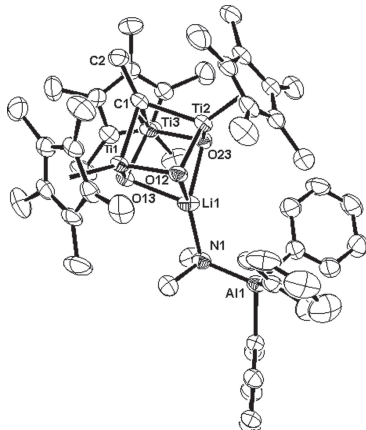
Incorporation of different lithium aluminates to titanium oxide organometallic ligands

Alberto Hernán-Gómez, Avelino Martín, Miguel Mena and Cristina Santamaría. *Departamento de Química Inorgánica. Universidad de Alcalá. Campus Universitario. 28871-Alcalá de Henares-Madrid (Spain)*. E-mail: alberto.hernan@uah.es

During the last years our research group has investigated the coordination of the organometallic oxides $[Ti(\eta^5-C_5Me_5)(\mu-O)]_3(\mu_3-CR)$ [R = H(1), Me(2)] to different inorganic fragments of groups 1 and 13 elements. Reactions with group 1 derivatives lead to dehydrogenation processes of the alkylidyne moiety to give $[M(\mu_3-O)_3\{Ti_3(\eta^5-C_5Me_5)_3(\mu_3-C)\}]_2$ (M = Li, Na, K) complexes [1].

On the other hand, the novel adducts $[E_3M\{\mu_3-O\}(\mu-O)_2\{Ti(\eta^5-C_5Me_5)_3(\mu_3-CR)\}]$ (R = H, Me; M = B, Al, Ga; E = alkyl, haloalkyl, halide) are obtained when group 13 derivatives react with 1 and 2 [2]. These species exhibit coordination of 1 or 2 through one of the three oxygen atoms of the Ti_3O_3 ring to the metal center. Now, we are studying the chemical reactivity of this family of compounds with different alkyl, amide or alkoxyde lithium derivatives in order to isolate the theoretical possible intermediate species in the reactions between 1 and 2 with the group 1 derivatives. We will show how dimethylamide and 2,6-dimethylphenoxyde lithium derivatives coordinate to the organometallic oxides in a chelate tridentate fashion. Now, this bonding system is stabilized by the alkyl aluminum fragment, which avoids that the amide or alkoxyde fragments react with the alkylidyne moiety (see figure).

However, when the same reaction is carried out with *p*-tolyl lithium and the triphenylgallium adduct, abstraction and redistribution reactions are observed. The lithium atom is then encapsulated by two units of 1 and the new gallate species stabilizes a phenyllithium unit.



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Keywords: aluminate, gallium, titanium

MS61.P13

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Discrete role of chlorine substitutions in the conformation and supramolecular architecture of isostructural arylsulfonamides

William B. Fernandes,^a Angelo Q. Aragão,^a Felipe T. Martins,^b Caridad Noda-Perez,^b Carlito Lariucci,^c Hamilton B. Napolitano,^a ^aScience and Technology Center, State University of Goiás, Anápolis, (Brazil). ^bInstitute of Chemistry, Federal University of Goiás, Goiânia, (Brazil). ^cInstitute of Physics, Federal University of Goiás, Goiânia, (Brazil). E-mail: willfernandes@iqsc.usp.br

Compounds containing sulfonamide groups SO_2NH occur in many biologically active molecules, including antimicrobial, antithyroid, antitumor and antimalarial drugs [1,2,3,4]. In this study, two arylsulfonamide derivatives differing for two chlorine substitutions at one of their two phenyl rings were synthesised and characterized by X-ray diffraction technique in order to establish structural relationships and the chlorine role in the conformation and crystal assembly. The compounds (4-N(phenyl-sulphonyl-amide-acetophenone)) (I) and 4-N [(2, 5-dichlorophenyl)sulfonyl-amide] acetophenone (II) were obtained by the equimolar coupling between benzene sulfonyl chloride or 2,5-dichlorobenzene sulfonyl chloride and 4-amineacetophenone in dichloromethane or acetone as solvent at 343K for until six hours. The precipitate was re-crystallized in suitable solvents to obtain the single crystals. Crystallographic data for compounds (I) and (II) were collected using a Enraf Nonius diffractometer at room temperature. All crystal structures were solved by Direct Methods, and refined by full matrix least square method on F^2 . The non hydrogen atoms were refined anisotropically. All C-H hydrogens were placed geometrically and refined using riding model. The hydrogen H1 bonded to nitrogen was found from the difference Fourier map and its positional parameters were refined freely. The tables, geometrical calculations, molecular packing and drawings were done with the WinGX [5,6]. program package, obtaining the following results: **(I)** Molecular Formula: $C_{14}H_{13}NO_3S$. Unit Cell Parameters: $a = 13.0007(5) \text{ \AA}$, $b = 8.3615(4) \text{ \AA}$, $c = 12.5179(6) \text{ \AA}$, $\beta = 98.118(3)^\circ$, monoclinic, space group $P2_1/c$, $Z = 4$, $V = 1347.13(1) \text{ \AA}^3$. 5393 measured reflections with 3009 unique and 2214 observed. Final indices $R_1 = 0.0483$ for 177 refined parameters. **(II)** Molecular formula: $C_{14}H_{11}NO_3SCl_2$. Structure: $a = 13.3622(2) \text{ \AA}$, $b = 8.1542(2) \text{ \AA}$, $c = 15.6845(3) \text{ \AA}$, $\beta = 120.180(1)^\circ$, monoclinic, space group $P2_1/c$, $Z = 4$, $1477.24(5) \text{ \AA}^3$. 5653 measured reflections with 2972 unique and 2463 observed. Final indices $R_1 = 0.049$ for 195 refined parameters. There are several classical and non-classical hydrogen bonds and $\pi-\pi$ stacking interactions contributing to stabilize the crystal packing of the compounds.

