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Reactions of C-halogen Bond Activation Mediated by a Rhodium POP Complex

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The reactions of C-halogen bond activation are fundamental steps in organic transformations mediated by transition metal complexes, such as cross-coupling reactions,1as well as in the chemical destruction of halogen-containing organic pollutants, among other processes.

Recently we have shown that the complex RhH{xant(PiPr2)2} (xant(PiPr2)2= 9,9-dimethyl-4,5-bis(diisopropylphosphino)xanthene) reacts with fluoroarenes to give products resulting from processes of C-H bond activations,2 while in the case of chloroarenes the C-Cl bond activation takes place (Figure 1).3 In the present contribution, we will show the preliminary results of the reactivity of the related complex RhCl{xant(PiPr2)2} towards halogenated hydrocarbons. The X-ray diffraction analysis of the products obtained have helped us confirm its reactivity.

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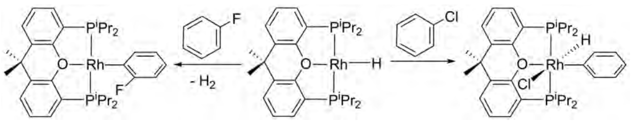

References:

[1] See for example: Biffis, A.; Centomo, P.; Del Zotto, A.; Zecca, M. Chem. Rev. 2018, 118, 2249-2295.

[2] Esteruelas, M. A.; Oliván, M.; Vélez, A. Organometallics 2015, 34, 1911-1924.

[3] Curto, S. G.; Esteruelas, M. A.; Oliván, M.; Oñate, E.; Vélez, A. Organometallics 2017, 36, 114-128

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Solid State Thermochromism in an Octahedral Co(ii) Complex Studied by X-Ray Powder Diffraction

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Thermochromism is the phenomenom known as the reversible change in the colour of a compound when it is heated or cooled [1]. This process can take place over a wide (continuous thermochromism) or a narrow (discontinuous thermochromism) range of temperature. The latter, typical of inorganic substances, may be associated to a structural phase transition [2].

In the present work, we have studied the colour change in the pink octahedral cobalt (II) complex [CoCl2(PyTn)]·2H2O [PyTn: 2-(pyrazol-1-yl)-2-thiazoline] [3] in the solid phase over a temperature range from 30ºC to 160ºC by means of powder X-ray diffraction. This compound, previously studied in solution, transforms into the blue dinuclear asymmetrical complex [CoCl2(μ-Cl)2Co(PyTn)2]. The thermochromic transition temperature is considerably higher in the solid state than in solution, as it was expected.

Colour transformation was monitored by means of in-situ X-ray powder thermodiffraction with the aim of discovering reaction intermediates. The X-ray experiment was carried out on a Bruker D8 Advance powder diffractometer equipped with a temperature chamber, using CuKα1 radiation. Measurements were made in the 10-30º2θ range and collected at temperature intervals of 5ºC.

Reaction product was identified by comparing the measured patterns to the simulated one for known single crystal structure using Mercury CSD software. In additon, TG-DTG curves were obtained in a dynamic air atmosphere in the same temperature range, as well as a DSC curve. From these, it can be concluded that only the two crystallization water molecules are released, keeping the compound its integrity

References:

[1] Day, J. H. (1968). Chem. Rev., 68, 649-657

[2] Van Ooort, M. J. M. (1988). J. Chem. Ed., 65, 84.

[3] Bernalte-García, A., Lozano-Vila, A. M., Luna-Giles, F. & Pedrero-Marín, R. (2006). Polyhedron, 25, 1399-1407.

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