MS32-P11

Altering the solid-state photochromic behavior of N-salicylideneanilines molecular switches by co-crystallization

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N-salicylideneaniline derivatives are among the most studied man-made thermo- and photo-switchable systems. These systems can switch between three different colored forms: an enol colorless form, a yellow *cis*-keto form and a red *trans*-keto form. A thermal tautomeric equilibrium between the enol and *cis*-keto form accounts for their thermochromism, whereas a *cis-trans* photoisomerization between the *cis*-keto form and the *trans*-keto form is the mechanism behind their photochromism. Photochromism can lead to a broad range of applications, *i.e.* in information storage and electronic display systems or in optical switching devices like ophthalmic glasses. However, due to the volume requirements of the *cis-trans* photoisomerization, photochromism is not easily encountered in the solid state. For this reason, we have used co-crystallization with the aim to induce photochromism in a non-photochromic *N*-salicylideneaniline chromophore. Our results (single-crystal structures and UV-vis diffusion reflectance) reveal how co-crystallization can be successfully employed for this purpose due to the fact that it changes both the free available volume of each molecule in the crystal and the intermolecular interactions.[1,2]

References:

[1] Carletta, A, et al. (2017). Chem. - A Eur. J., 23, 5317–5329.
[2] Carletta, A, et al. (2016) J. Phys. Chem. C, 120, 10001–10008.

Keywords: Co-crystals, photochromism, N-salicylideneanilines

MS32-P12

X-Ray study of new titanium (III) complexes derived from salicylic acid derivatives and N,N-bidentate ligands or monodentate O, N,-ligands

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The Titanium complexes stand for a new category of potential anticancer compound. The first studies of titanium complexes copied square-planar arrangement of cis-platin complexes. These complexes show a significant anticancer activity for a wide range of cell lines of cancer [1]. We synthesized new titanium complexes derived from salicylic acid derivatives (as 3-methoxysalicylic acid) and N,N-bidentate ligands (as 1,10-phenanthroline) or monodentate O, N,-ligands (as imidazole) [2]. These complexes were prepared in monocrystal form and suitable crystals were selected for X-ray experiment. All experiments were performed by Stoe STADIVARI diffractometer with a Dectris Pilatus 300 K detector and with an Genix3D Cu HF source (Cu-Kα, λ = 1.54186 Å) at 100 K using a nitrogen gas open-flow cooler Cobra Oxford Cryosystems. Data reduction was performed using X-Area (Stoe, 2017) software package [3]. The crystal structures for measured compounds were solved in OLEX2 software using SHELXT-2015 program via Intrinsic Phasing and refined with SHELXL-2014 by least-squares procedure on F2. Since few efforts have been made towards the synthesis and use of titanium complexes as chemotherapeutic agents, this is an important area of our research.

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References:

[1] Kaushal, R. et al. (2014). Bioinorganic Chemistry and Applications. 2014, 1-12.
[2] Kucková, L., et al. (2015). Molecules. 20, 2115-2137.
[3] STOE & Cie GmbH (2016). X-Area 1.76, software package for collecting single-crystal data on STOE area-detector diffractometers, for image processing, scaling reflection intensities and for outlier rejection; Darmstadt, Germany.

Keywords: anticancer activity, titanium complex, salicylic acid.