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**Keywords:** molecular recognition, selectivity, weak interactions

### P.06.07.13

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#### Inclusion of Molecular Iodine into Channels of the Organic Zeolite Gossypol

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Gossypol, a phenolic pigment extracted from cotton seeds, demonstrates unique ability as a host compound and its polymorphism [1] makes gossypol an interesting object of solid supramolecular chemistry.

Channel-type zeolite has been obtained by desolvation of the unstable clathrate of gossypol with dichloromethane. Removal of the solvent molecules does not affect the crystal structure of the host: channels are retained, although they show a slight contraction (4%). Sorption experiments performed in the gas phase or in water showed that the zeolitic form of gossypol can take up molecular iodine. The crystal structure of the gained complex is isomorphic with the structure of the dichloromethane clathrate where hydrogen-bonded columns of gossypol molecules are packed by means of Van der Waals forces into a porous architecture. In the complex, iodine molecules enter the extended cavities of the channels within the zeolitic structure, occupying 1/8 of the possible sites. The host-guest ratio of the obtained product depends on the size of crystallites of the initial zeolite and the absorption temperature. The higher sorption temperature the higher amount of absorbed molecules but the lesser crystallinity of the product. However, the iodine molecules can be removed with the help of vacuum giving back to the initial zeolite.

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**Keywords:** gossypol, inclusion compound, organic zeolite

### P.06.10.1

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#### Crystal Structure and Properties of a Tetrakis(tert-butylthio) Butatriene Compound

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1,2,3-butatrienes have long attracted organometallic chemists because of their highly unsaturated structure [1]. Since the butatrienes obtained here keep some energy in their skeletons, they must be reactive molecules, and thus their applications to further organic transformations will be interesting subject [2].

The aim of this work is to synthesis [3] and to determine the crystal structure of Tetrakis(tert-butylthio)butatriene compound. Crystal of Tetrakis(tert-butylthio)butatriene was mounted on a Rigaku R-Axis Rapid-S Diffractometer with a graphite monochromatized MoK $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). The structure was solved by direct method with SIR92 [4] and refined with Crystals.

Crystal data: C<sub>20</sub>H<sub>36</sub>S<sub>4</sub>, the compound is monoclinic, space group P2<sub>1</sub>/n,  $a = 11.061(6)$ ,  $b = 10.850(4)$ ,  $c = 11.271(6) \text{ \AA}$ ,  $\beta = 116.427(12)^\circ$ ,  $V = 1211.51(10) \text{ \AA}^3$ ,  $Z = 4$ ,  $D_{\text{calc}} = 2.219 \text{ g/cm}^3$ ,  $F(000) = 880.00$ ,  $\mu(\text{MoK}\alpha) = 7.86$ .

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**Keywords:** small organic molecules, sulfur compounds, structures of organic compounds

### P.06.10.2

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#### Crystal Structure of a Tetrakis(4-chlorophenylthio) Butatriene Compound

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Compounds with cumulated double bonds, such as allene or ketene, are fairly reactive because of their strained structures, thus, effective synthesis of these compounds is still challenging in organic chemistry. Construction of three cumulated carbon-carbon double bonds is more difficult problem, and the effective synthetic methods of butatrienes are still very few [1].

The aim of this work is to synthesis [2] and to determine the crystal structure of Tetrakis(4-chlorophenylthio)butatriene compound. Crystal of Tetrakis(4-chlorophenylthio)butatriene was mounted on a Rigaku R-Axis Rapid-S Diffractometer with a graphite monochromatized MoK $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). The structure was solved by direct method with SIR92 [3] and refined with Crystals.

Crystal data: C<sub>28</sub>H<sub>16</sub>Cl<sub>4</sub>S<sub>4</sub>. The compound is monoclinic, space group P2<sub>1</sub>/c,  $a = 6.9785(8)$ ,  $b = 8.6803(9)$ ,  $c = 22.884(2) \text{ \AA}$ ,  $\beta = 93.887(6)^\circ$ ,  $V = 1383.0(3) \text{ \AA}^3$ ,  $Z = 2$ ,  $D_{\text{calc}} = 1.495 \text{ g/cm}^3$ ,  $F(000) = 632.00$ ,  $\mu(\text{MoK}\alpha) = 7.47$ .

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**Keywords:** sulfur compounds, small organic molecules, structures of organic compounds

### P.06.10.3

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#### Structural Insights of a Potential Inhibition Against Leishmania Major

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Leishmaniasis is a tropical disease caused by a protozoal parasite of the order Kinetoplastid. According to the World Health Organization reports, 88 countries are affected, with 12 million infected people and approximately 350 million people at risk. The need for new drugs for the treatment of leishmaniasis infections comes from a lack of safe drugs and the serious secondary effects observed in available chemotherapy. Looking for new bioactive substances [1], potentially useful against leishmaniasis, we used both PRTase adenine phosphoribosyltransferase from *L. tarentolae* and parasite *L. major* as a model system to screen the inhibitory capacity of one small molecule compound from Brazilian plant. The data collection was performed using Enraf Nonius KappaCCD at room temperature. The structure was analyzed from 1425 reflections with  $I > 2\sigma(I)$  and refined to R1-values of 0.033 [1]. The molecules are joined in crystal structure through five twice classical O-H...O hydrogen bonds linking the atoms O4-H4...O5<sup>i</sup> [ $i = -x+3, 0.5+y, -z+1$ ], O5-H5...O2<sup>ii</sup> [ $ii = x, y, 1+z$ ], O2-H2...O4<sup>iii</sup> [ $iii = x+2, y-0.5, -z$ ], O1-H1...O3<sup>iv</sup> [ $iv = x-1, y, z$ ] and O3-H3...O1<sup>v</sup> [ $v = -x+2, 0.5+y, -z$ ] with distances between donor and acceptor of 2.707(1), 2.808(1), 2.780(1), 2.736(1) and 2.843(2) Å, respectively. The theoretical analysis of occupancy factor for the hydrogen atoms of two last ones is consistent to crystallographic model.

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**Keywords:** leishmaniasis, inhibition, phosphoribosyltransferase

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#### Crystal Structures of trans- and cis-octenes

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