



XXI ICICU

BOOK OF ABSTRACTS

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The Book of abstracts contains the materials of invited, plenary and poster presentations reports on XXI International Conference on Inorganic Chemistry Ukraine (XXI ICICU) which take place in Uzhhorod June 3-6, 2024. At the conference were considered issues of solid state chemistry, solid inorganic materials, crystal chemistry, synthesis of new compounds for modern medicine and pharmaceutical chemistry, chemistry and physics of materials, atomic and electronic structure of solid inorganic materials, materials for "green" chemistry. The conference will cover issues on solid state chemistry, solid-state inorganic materials, crystal chemistry, synthesis of new compounds for modern medicine and pharmaceutical chemistry, materials chemistry and physics, atomic and electronic structure of solid inorganic materials, materials for "green" chemistry, etc. The reports contain the latest scientific results and advanced research methods in the field: 1. Chemistry of inorganic and coordination compounds, including medicinal and pharmaceutical chemistry; 2. Characterization and properties of new inorganic substances, crystal chemistry; 3. Physical inorganic chemistry, nanochemistry; 4. Dual-use materials, alternative energy sources, environmental chemistry.

REACTIVITY IN THE SULFUR DIOXIDE – ALKANOL – TRIS(HYDROXYMETHYL)AMINOMETHANE SYSTEMS

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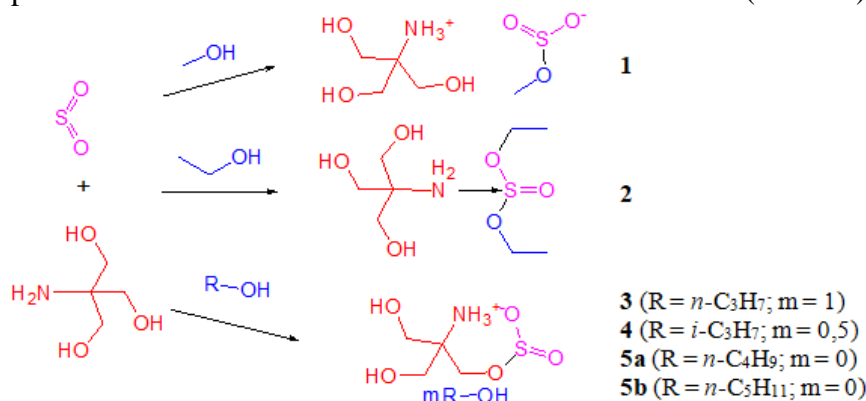
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Data comparison of the OH-acidity of alkanols in the gas phase [1, 2] and their lipophilicity [3]. With a decrease in hydrophilicity in the series of alkanols CH_3OH (-0.77) > $\text{C}_2\text{H}_5\text{OH}$ (-0.31) > *i*- $\text{C}_3\text{H}_7\text{OH}$ (0.05) > *n*- $\text{C}_3\text{H}_7\text{OH}$ (0.25) > *n*- $\text{C}_4\text{H}_9\text{OH}$ (0.88) > *n*- $\text{C}_5\text{H}_{11}\text{OH}$ (1.56) (experimental values $\log P_{\text{ow}}$ are indicated in parentheses according to [3]) their OH-acidity decreases. Due to the fact that there are no data on OH-acidity of Tris in the literature ($\log P_{\text{ow}}(\text{Tris}) = -2.31$ [3]), and $\log P_{\text{ow}}$ is additive value [4], then the average lipophilicity value per functional group (three -OH and one -NH₂) equals to $\frac{1}{4}\log P_{\text{ow}}(\text{Tris}) = -2.31/4 = -0.58$.

In reaction mixture $\text{SO}_2 - \text{ROH} - (\text{HOCH}_2)_3\text{CNH}_2$ [5] the formation of *O*-alkyl sulfites occurs through the nucleophilic addition of RO-anions to sulfur dioxide molecules (Scheme).



Scheme. Synthesis of sulfite esters **1** – **5** [5].

There are hydrophilic *O*-methyl sulfite methanol and ethanol forms (**1**) and diethyl sulfite (**2**) by S-N binding, respectively. Ethanol neutralizes the effect of the stronger OH-acid Tris due to the concentration factor. In solutions of lipophilic alkanols hydrophilic Tris enters into a competitive reaction forming *O*-alkyl sulfite (polymorphic forms **5a**, **5b**) and its solvates (**3**, **4**). Interesting to note that the most hydrophilic CH_3OH and Tris being the strongest OH-acids in the studied reaction medium form SO_2 addition products: $\text{ROH} = 1 : 1$ whereas the weaker OH acid $\text{C}_2\text{H}_5\text{OH}$ forms the $\text{SO}_2 : \text{ROH} = 1 : 2$ addition product. This will be the subject of our future research.

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