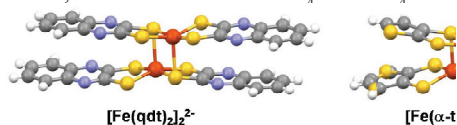


to the formation of dimeric arrangements through two Fe-S bonds between distorted square based $[\text{Fe}(\text{S}_2\text{L})_2]^-$ units, $[\text{Fe}(\text{S}_2\text{L})_2]_2^{2-}$. The first, and so far unique, exception to this rule was the *n*-Bu₄N $[\text{Fe}(\text{qdt})_2]$ complex [1], displaying a perfectly square planar coordination geometry and a $S = 1/2$ spin state.

The crystal structure of the new $(\text{BrBzPy})_2[\text{Fe}(\text{qdt})_2]_2$ complex shows a rare weak Fe^{III} bisdithiolene dimerisation with unusual molecular planarity and long apical S-Fe distances, in an anion configuration intermediate between the only monomeric Fe bisdithiolene reported so far, and the common strong dimeric geometry also observed in other $[\text{Fe}(\text{qdt})_2]$ salts. The standard strong dimeric situation is also observed in the new $[\text{Fe}(\alpha\text{-tpdt})_2]_2$ salt with the same cation, as well as with the *n*-Bu₄N and Et₃N Cations.



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Keywords: molecular compounds; Fe-bisdithiolene complexes; crystal engineering

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pH Indicators – Molecular Structure and Proton Distribution. Zofia Urbanczyk-Lipkowska^a, Przemysław Kalicki^a. ^a*Institute of Organic Chemistry, Polish Academy of Sciences. 01-224 Warsaw, Poland*
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A pH indicators are usually weak bases or weak acids that recognize selectively hydronium ions. In common organic solvents they exist as equilibrium of variously protonated forms and/or open/cyclic structures. Apart of common use in chemical laboratories, medical diagnostics and industry, solid state structural data on pH indicators are scarce [1-3]. Here we present X-ray structures of bromocresol purple, bromothymol blue, 4',5'-dibromofluorescein, and Congo red crystallized in different crystallization conditions and at different pH. Such problems like proton distribution and electronic structure of the molecules will be addressed.

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Keywords: pH indicators; lactones; electronic structure

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Enclathration by a Xanthenol Host via Solid-solid Reactions: Structures and Kinetics. Ayesha Jacobs^a, Luigi R. Nassimbeni^a, Kanyisa L. Nohako^a, Gaëlle Ramon^a, Jana H. Taljaard^b. ^a*Department of*

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The compound, 9-(4-methoxyphenol)-9H-xanthen-9-ol (H) has proved to be a versatile host and has included a variety of small organic guests [1,2]. Solid-solid reactions with this host and a series of polycyclic unsaturated hydrocarbons have also been reported [3]. In this study the host compound, H, has successfully included the solid guests 1-naphthylamine(NAPA), 8-hydroxyquinoline(HQ), triethylenediamine(TEDA) and acridine(ACR). The structures for all four inclusion compounds were solved in the space group P-1. Similar packing motifs were found for the NAPA and HQ inclusion compounds where neighbouring host molecules form dimers of the type (Host)-OH...O(Host). The TEDA and ACR guests hydrogen bond to the host molecule. In addition the compounds were also formed by direct grinding of the host with each of the guests and the kinetics of the solid-solid reactions determined using powder x-ray diffraction. The kinetics for all four reactions were modelled using the first order rate law: $f(\alpha) = \ln(1-\alpha) = -kt$ where α is the extent of the reaction.

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Keywords: solid-solid reactions; inclusion compounds; kinetics

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Existence Region of Type-I Clathrates in the System Ba-Ni-Ge. Umut Aydemir^a, Horst Borrmann^a, Cécile Hébert^b, Nguyễn Thị Kim Liên^a, Ulrich Burkhardt^a, Michael Baitinger^a, Yuri Grin^a. ^a*Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.* ^b*Ecole Polytechnique Fédérale de Lausanne, Lausanne, France.*

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The formation of voids in the framework of Ge clathrates has a strong impact on their crystallographic and physical properties. In the binary system Ba – Ge, the composition of a hypothetical clathrate-I compound without defects is Ba₈Ge₄₆. Since a four-bonded framework Ge₄₆ can be already formed with uncharged Ge atoms, the additional valence electrons of the Ba atoms would occupy antibonding states. However, the formation of defects is more favorable for Ge clathrates. Each defect □ in a framework Ge_{46-x}□_x is surrounded by four three-bonded Ge atoms (3b)Ge¹⁻. Hence, the 16 valence electrons from 8 Ba atoms would be completely compensated by four defects surrounded by 16 (3b)Ge¹⁻. Actually, instead of the expected composition Ba₈Ge₄₂□₄, the binary clathrate was found to be Ba₈Ge₄₃□₃ with 4 conduction electrons per formula unit [1]. Ternary type-I clathrates Ba – TM – Ge can be obtained with