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STRUCTURAL INVESTIGATION OF THE PENTACYCLOUNDECANE

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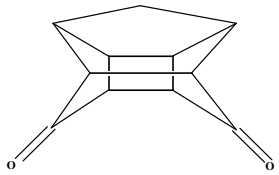
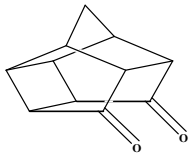
Pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]-undecane (PCU)-8,11- dione (**1**) is a polycyclic cage compound with applications ranging from pharmaceutical use, potential as a new class of energetic materials to cage annulated supramolecules for the selective binding of toxic metals from industrial waste.

PCU dione (**1**) is an unusual, rigid and strained open-ended cage compound composed of four fused five- membered rings in envelope conformations and a planar four membered ring. The molecule contains two exocyclic ketone moieties. Cage compounds have a rigid carbocyclic ring structure which results in a relatively fixed molecular geometry and special structural features, due to the deformation of the ideal carbon-carbon bond angle and their inherent ring strain. The molecular geometry of PCU dione (**1**) has been previously been studied by analogy, Dreiding stereo models and molecular orbital calculations since no single X-ray crystallography data was available. Interesting theoretical results were obtained. The difficulty of assigning the NMR of the pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]-undecane –8,11-dione and its derivatives has been commented on by researchers.

To purpose of the study is to examine the synthetic route and the unique molecular geometry of the strained PCU dione (**1**). The X-ray crystallographic data and the complete NMR elucidation of the PCU dione crystal (**1**) and a novel derivative will be reported.





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THE LIESEGANG EYES PHENOMENON

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Classical Liesegang patterns are produced in the wake of a moving reaction front. These structures are a well-known examples of spatiotemporal selforganization. In the simplest situation, an electrolyte, called outer electrolyte, diffuses into a reaction medium (in the experiments it is usually a gel) and reacts with another electrolyte (inner electrolyte) that is uniformly distributed in the reaction medium. The precipitation reaction between them produces an insoluble precipitate product, which is usually distributed quasiperiodically in the gelled medium. The importance of such studies lies that formation of complex patterns observed in chemical, biological and geochemical system can be described by the similar manner. The presence of bands or rings is related to the geometry of the experimental setup. Basic geometrical arrangement of the experiments (boundary conditions) can be divided into two categories: planar and circular (spherical). At the first case (it is a usual way), one electrolyte is placed into a test tube within a gel matrix then the outer electrolyte is placed on top of the gel column. Here the precipitation bands (1D) or parallel zones (2D, 3D) perpendicular to the diffusion front of the invading (outer) electrolyte can be expected. The second one is 2D (or 3D) radial geometrical setup, in which the inner electrolyte is placed in a gelled medium in a Petri dish and a solution of the outer electrolyte is added into its center. Reaction front will move from the center to the periphery of the dish producing separated precipitation rings behind it.

Empirical regularities (time-, spacing-, width-, and Matalon-Packter law) concerning to the pattern formation, which describe the evolution and final pattern structure, valid and have been considered in case of a planar motion of the reaction fronts.
As it is well know from the theory of chemical (BZ) waves the curvature of the waves has a great impact on the velocity of the wave (curvature effect). This effect plays an important role in a signal processing in an excitable medium and in a stability of the chemical flame balls. Although Liesegang patterning is a heterogeneous process and in this respect it differs substantially from the excitable systems, therefore that is interesting and important to see the effect of curvature of reaction front on the patten structure. The aim of the present poster is to investigate the evolution of the Liesegang pattern using a new radial geometrical setup. In this concept, we have performed the experiments in a completely new arrangement. The inner electrolyte is placed in a gel disk with a small width and the outer electrolyte diffuses from outside into a gel disk producing various type of precipitation patterns. Numerical simulations were also performed to explain experimental results applying pre-nucleation theory of the precipitation process.