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SC_P24

Stereochemical aspect of influence of [Cu(*diethylenetriamine*)(H_2O)]$SO_4 \cdot H_2O$ chelate compound onto combustibility decrease of epoxy-amine composite materials

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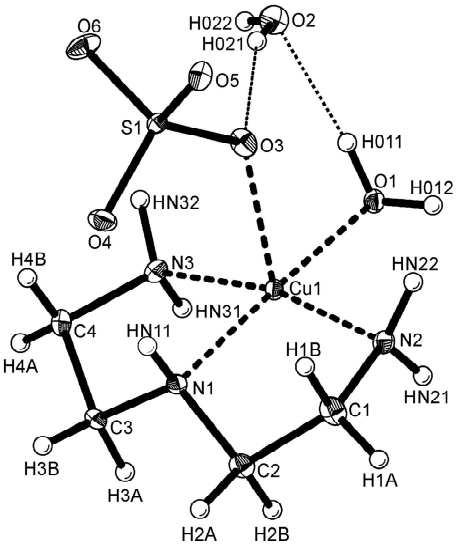
It is known that copper(II) salts can be used for effective suppression of the inflammation of amines and nitriles [1]. In this flame retardant process, the decisive role belongs the chemical interaction (Cu–N donor-acceptor bonding), which causes the formation of practically incombustible copper(II) complex. It opens up new vistas of using the transition metals salts in production of self-extinguishing epoxy-amine composites. Recently there has been a tendency to use, as a hardener of epoxy resins, the chemically bonded amines with salts of transition metals instead of the pure amines. Therefore, we undertook an attempt to study interaction of *diethylenetriamine* (hardener) with copper(II) sulfate whose anhydrous salt in solid state has been employed as retarder in the prototype of epoxy-amine polymeric materials with the depressed combustibility. The chelate complex of [Cu(*diethylenetriamine*)(H_2O)]$SO_4 \cdot H_2O$ (see Figure) have been determined by X-ray diffraction methods (Sp.gr. $P\bar{1}$, a = 7.2819(4), b = 8.4669(4), c = 8.7020(3) Å, α = 83.590(3), β = 89.620(4), γ = 84.946(4)°, V = 531.09(4) Å^3, Z = 2). The crystals of this chelate consist of discrete [Cu(*diethylenetriamine*)H_2O]$^{2+}$ complex cations and hydrated $[H_2O \cdot SO_4]^{2-}$ anions. The environment of the Cu(II) atom is elongated square pyramid which consists of three N atoms of the *diethylenetriamine* and O atom of the water molecule in the basal plane of the square pyramid. The apical position of the coordination polyhedron is occupied by complementary O atom of the sulfate anion. The average lengths of the in-plane Cu–N and Cu–O bonds are 2.00 Å whereas the length of the axial Cu–O bond is 2.421(1) Å. The crystal packing is governed by strong hydrogen bonds of O–H···O and N–H···O types. Thus, the strong coordination bonds that arise between metal atoms of incombustible $CuSO_4$ and nitrogen atoms of the amine hardener are responsible for the flammability suppression of the epoxy-amine compositions. The high stability of this compound in solid state is a determining factor at producing of the self-extinguishing epoxy-amine composites modified by $CuSO_4$.



Literature:

[1] Godovanets, N.M.; Mykhalitchko, B.M.; Shcherbyna, O.M.; Vyniavska, G.F., Influence of the complexation process on combustibility decrease of aniline into hydrochloric aqueous solution of copper(I) chloride. *Fire Safety* **2010,** 4, 70-76.

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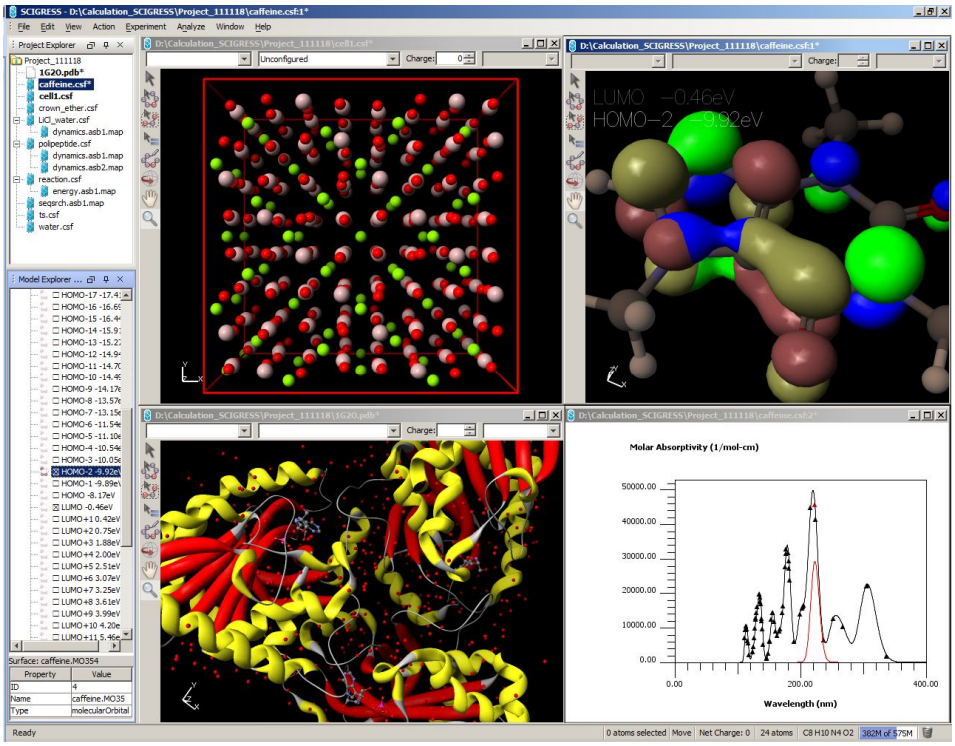

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