

electrical properties into the ligand and organize the compound on the surfaces for single-molecule or single-molecule layer study.

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**Keywords:** magnetism, chirality, iron

## MS66.P16

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### Crystal Structures and NLO properties of Quinoline Derivatives

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The calculation of the nonlinear optical (NLO) properties of solids using structural data has been stimulated by the increasing importance of the communications industry and the parallel need for materials having suitable properties.

The following salts have been prepared by acid-base reactions and their structures have been determined by single-crystal X-ray diffraction: 6-methoxyquinolinium trifluoroacetate, 6-methoxyquinolinium hydrogensulphate trihydrate and 6-aminoquinolinium iodide monohydrate.

Using the methodology that we have developed recently [1], we calculated the nonlinear susceptibility tensor components for these non-centrosymmetric salts. The molecular hyperpolarizabilities were calculated using Time Dependent Density Functional Theory, Hartree-Fock and Semi-empirical methods.

The second and third order nonlinear optical properties of these salts will be presented.

The theoretical predictions will be compared with such experimental results.

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**Keywords:** nonlinear optical properties, structure-physical properties relationships, organic salts

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### Distortion of the charged C<sub>60</sub> fullerene cage in the ionic complexes

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Ionic fullerene C<sub>60</sub> complexes show a variety of promising physical properties such as metallic conductivity, superconductivity and ferromagnetism. Great interest is directed to the intrinsic structural and

electronic properties of discrete fullerene C<sub>60</sub><sup>n-</sup> anions. The Jahn-Teller theorem predicts a distortion of C<sub>60</sub> from icosahedral symmetry when additional electrons are added to the degenerated t<sub>1u</sub> LUMO orbital of C<sub>60</sub>. The presence or absence of such distortion in the fullerene anions are of particular interest since the degeneracy strongly affects the electronic structure of fullerene and to a great extent defines such phenomena as superconductivity and ferromagnetism. Fullerene C<sub>60</sub> is nearly a spherical molecule and fullerene anions are disordered in most ionic complexes and salts. Precise geometry of ordered fullerene anions was determined in a few compounds only [1-3]. The new complex {Co(dppe)<sub>2</sub><sup>+</sup>·(C<sub>60</sub><sup>•-</sup>)·(C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>)<sub>2</sub>} [4] gives another crystal structure with the ordered C<sub>60</sub><sup>•-</sup> radical anions making it possible the C<sub>60</sub><sup>•-</sup> distortion to be analyzed. An elongation of the fullerene cage by 0.025 Å was found. Extended Hückel method calculations showed the 180 and 710 cm<sup>-1</sup> splitting of the C<sub>60</sub> degenerated LUMO levels. Additionally we present a comparative analysis of the C<sub>60</sub> distortion parameters for the ordered structures known and compare the t<sub>1u</sub> orbital splitting from extended Hückel method calculations and experimental data.

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**Keywords:** fullerene structure, Jahn-Teller distortion

## MS66.P18

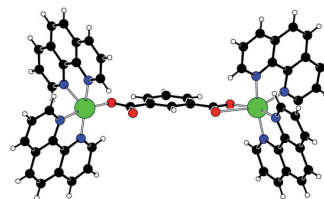
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### Low dimensional Cu(II) complexes

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Molecular based magnets capitalize on the flexibility inherent in carbon chemistry. A rational choice of ligands can be made to control the dimensionality of the system in order to enhance quantum effects. Two new copper complexes were synthesized using the solvothermal technique and their structure determined using single crystal X-ray diffraction.

In compound 1, phenanthroline-isophthalic acid-Cu(II) compound, the metal ions are assembled in dimeric complexes. Each Cu(II) ion is in a distorted octahedral environment, surrounded by four nitrogen atoms from two phenanthroline molecules and by two oxygen atoms from an isophthalate ion. The isophthalate ion bridges two metal ions (see figure). The unit cell parameters are:  $a = 13.3116(4)$ ,  $b = 13.4168(4)$ ,  $c = 22.4838(6)$  Å,  $\alpha = 83.800(2)$ ,  $\beta = 85.894(2)$ ,  $\gamma = 77.469(2)^\circ$ ,  $V = 3892.20(19)$  Å<sup>3</sup>, space group P-1.



In compound 2, there is the formation of chains of phenanthroline-2,2'-iminobenzoic acid-Cu(II) units. The metal ion is in a distorted octahedral environment, four oxygen atoms from two 2,2'-iminobenzoate units and two nitrogen atoms from one phenanthroline