Mn sites. Thus, there is a considerable orbital component to the magnetic moment. Bader topological analysis shows an absence of Mn-Mn bonding and the magnetic ordering is via super-exchange through the oxygen bridges. Formal electron counting suggests mixed valence Mn sites, but this is not supported by the Bader atomic charges, Mn(1)=+0.11, Mn(2)= +0.17. The topological measures show the dominant metal-ligand interactions to be electrostatic, and a simple exponential correlation is derived between Mn-O bond lengths and the values of $\nabla^2\rho$ at the bond critical points.

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Keywords: charge density, physical properties, metallorganic framework

P.14.07.17

Acta Cryst. (2005). A**61**, C429

Charge Density of 1-phenylpropane-1,2,3-triyl Trinitrate

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The organic esters of nitric acid, the nitrates, are a class of products widely used for the treatment of a number of cardiovascular diseases. The prototype of nitrates is glyceryl trinitrate (GTN, nitroglycerin) It is an oil endowed with potent vasodilating and explosive properties. The major limit in its therapeutical use as vasodilator is an early development of the tolerance. 1-Phenylpropane-1,2,3-triyl trinitrate, a phenyl substituted GTN is characterised by having a high lipophilicity and interesting *in vitro* vasodilating profiles assessed on rat aorta strips pre-exposed to GTN.

A multipole analysis has been applied to the low temperature X-ray intensities of *threo* form of 1-Phenylpropane-1,2,3-triyl trinitrate (mp 40.5-41°C); the electron density distribution obtained has been analysed using the QTAIM and the topological and energetic parameters of intra- and inter-molecular interactions have been determined. The features of experimental and *ab initio* results are in good agreement and will be discussed.

Keywords: experimental charge density, ab initio calculations, pharmaceuticals

P.14.07.18

Acta Cryst. (2005). A**61**, C429

$Ru_3(CO)_{12}$. Why D_{3h}?

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$M_3(CO)_{12}$ (M= Fe, Ru, Os) may, in theory, adopt D_3, D_{3h}, C_{2v} symmetries. Iron carbonyl has a C_{2v} structure, ruthenium and osmium carbonyls have D_{3h} structures and only their derivatives show the least hindered D_3 configuration. The D_{3h} structure of $Ru_3(CO)_{12}$ has been justified theoretically using steric or electronic parameters. Only a marginal attention was paid to the deformation of axial CO groups, and it has been attributed to steric repulsion among oxygen atoms or to a more efficient orbital superposition between Ru atoms and C atoms. X-ray intensities of a $Ru_3(CO)_{12}$ crystal have been collected at low temperature and to them a multipole analysis has been applied; the electron density distribution obtained has been studied with the QTAIM and the topological and energetic parameters of intra- and inter-molecular interactions have been determined. Significant $C_{ax}\cdots C_{ax}$ interactions have been detected. The unexpected features of experimental electron density maps will be discussed.

Keywords: experimental charge density, ab initio calculations, ruthenium cluster

P.14.07.19

Acta Cryst. (2005). A**61**, C429

On the (Non)-Planarity of 1,2,4,5-Tetramethoxybenzene

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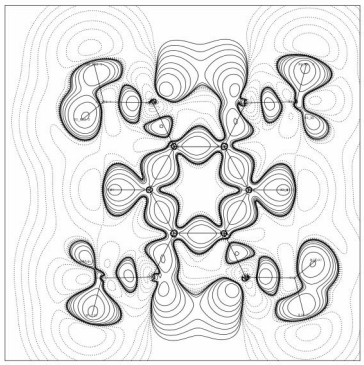
The conformation of methoxy groups on phenyl rings is a long-standing problem that has been tackled in the past with a variety of structure determination techniques and at different levels of quantum chemical calculations.

1,2,4,5-tetramethoxybenzene has two sets of *ortho*-dimethoxy moieties and displays a nearly planar structure in the crystal. We obtained a high quality data set at 150 K which was suitable for multipole refinement. The charge density maps and electronic properties in the bond critical points are compared with values from high-level quantum chemical calculations. The latter reveal a large number of energy minima on the potential energy surface.



The reason for the planarity of the molecule is not evident from the experimental structure, but the calculated bond orders in the molecule indicate that the stabilizing factor off-setting the repulsion between the free electron pairs of oxygen is the participation of the latter in the π-electron system of the ring.

Keywords: ab initio calculations, charge density, conformational studies

P.14.08.1

Acta Cryst. (2005). A**61**, C429

On the Conditions Leading to the Gaussian Distribution of the Magnetic Moments in a Spin-glass State

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The unperturbed ideal ferromagnetic system is described by a Hamiltonian of the Heisenberg type with the coupling constants J_{ij} (i and j numerate the magnetic ions). The presence of dopants (or defects) affects the values of J_{ij} for the magnetic ions surrounded by these dopants (or defects) in the random way. Thus the magnetic properties of such a system will depend on: the number of magnetic ions surrounding a j-th magnetic ion and interacting with it with the coupling constants J_{ij}, the number of dopants (or defects) surrounding a j-th ion, the coupling constants between i-th and j-th ions in the presence of dopants (or defects), and the random probability distributions of appearance of dopants (or defects) between i-th and j-th ions. These distributions correspond – after introducing so-called "global" magnetic coupling constant (which turns out to be also random) - to the conditions of the central theorem of the theory of probability (the Lyapunov theorem). Thus the distributions of magnetic moments in such systems are Gaussian. Therefore one can use the Anderson-Edwards model of the spin-glass state in order to describe the system. Several examples of the spin-glass state are described in this approach.

Keywords: spin glass, probability, central theorem of the theory of probability

P.14.08.2

Acta Cryst. (2005). A**61**, C429-C430

Spin Density and Ordered Orbital of $YTiO_3$ Observed by X-ray Magnetic Diffraction

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