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, pharmaceutical