

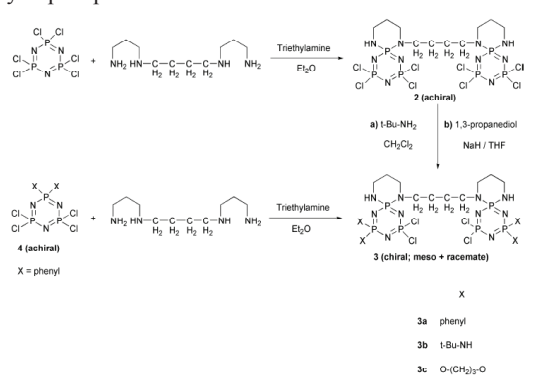
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X-Ray Crystal Structures of Chiral Spermine-Bridged Cyclophosphazenes. Yunus Zorlu^a, Gönül Yenilmez Çiftçi^a, Simon J. Coles^b, Michael B. Hursthouse^b, David B. Davies^c, Robert A. Shaw^c, Adem Kılıç^a. ^aDepartment of Chemistry, Gebze Institute of Technology, 41400 Gebze-Kocaeli, Turkey. ^bSchool of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, United Kingdom. ^cSchool of Biological and Chemical Sciences, Birkbeck College (University of London), Malet Street, London WC1E 7HX, United Kingdom.

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Tetra-coordinated phosphorus atoms in cyclophosphazenes are pentavalent and potential stereocentres. Although the possibility of optical isomerism in cyclophosphazene derivatives, [(NPXY)_n n = 3,4] was first discussed many years ago [1], chiral properties of molecules have recently been elucidated [2–5]. The spermine-bridged cyclophosphazene compound **2** has been prepared previously [6] by reaction of cyclotriphosphazene with the tetrafunctional amine, spermine. Compound **2** is achiral because the substitution pattern of each cyclophosphazene ring is the same and each cyclophosphazene ring has a plane of symmetry. However, singly-bridged analogues with gem disubstituted cyclophosphazene rings (e.g., **3**) exhibit stereoisomerism [3], because the three phosphorus atoms of each cyclophosphazene ring have different substitution patterns and those that are part of the bridge, >P(N-spiro), are stereogenic, i.e., there are R and S forms.

X-ray crystallographic studies have provided definite proof of stereogenic properties of chiral spermine-bridged cyclophosphazenes.



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Keywords: cyclophosphazene; stereogenicity; single crystal X-ray crystallography

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Synthesis, X-ray Molecular Structure, and Computational Study of (E)-2-[tris(hydroxymethyl)methyl]aminomethylen-4-methylphenol. Gonca Özdemir Tarı^a, Şamil Işık^a, Hasan Tanak^a, Ferda Erşahin^b, Erbil Ağar^c. ^aDepartment of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey. ^bGerze Sinop Vocational School, Sinop University, Sinop, Turkey. ^cDepartment of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey.

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Schiff bases can be classified by their photochromic and thermochromic properties [1]. Photo- and thermochromism arise via H-atom transfer from the hydroxy O atom to the N atom. There are two possible types of intramolecular hydrogen bonds in Schiff bases, viz. the keto-amine (N-H...O) and enol-imine (N...H-O) tautomeric forms. The present x-ray investigation shows that the title compound, prefers the enol-imine tautomeric form rather than the keto-amine tautomerism.

The crystal and molecular structure of the title compound, C₁₂H₁₇NO₄, has been synthesized and characterized by elemental analysis and x-ray single crystal determination. The compound crystallizes in the triclinic, space group P-1 with unit cell dimensions a=6.7501(6), b=8.5036(8), c=11.1290(11), M_r=239.27, V=611.91(10), Z=2, and wR₂=0.1372. The title compound C₁₂H₁₇NO₄ adopts the enol-imine tautomeric form. The structure is stabilized by intramolecular O-H...N and intermolecular O-H...O hydrogen bonds.

Geometric optimization based on x-ray diffraction technique and semi-empirical quantum mechanical calculations were performed. The calculated geometric parameters were compared to the corresponding x-ray determination results of the compound. The x-ray crystallographic data have been compared with AM1, PM3 and DFT molecular orbital methods. To inform minimum energy conformation of the title compound, selected torsion angle are varied from -180 to +180 in every 10° and then molecular energy profile is calculated by AM1 and PM3 semi-empirical method.

[1] Cohen, M. D., Schmidt, G.M.J. & Flavian, S., 1964. *J. Chem. Soc.*

Keywords: schiff base; X-ray diffraction; computational techniques

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Understanding the Oxygen Diffusion Process in Ruddlesden-Popper Phases at Room Temperature: The Special Case of La₂CoO_{4+δ}. L. Le Dréau^a, W. Paulus^a, J. Schefer^b, K. Conder^c. ^aUniversité Rennes I, Sciences Chimiques de Rennes UMR 6226, Campus Beaulieu bat 10B 35042 Rennes, France. ^bETH Zürich & Paul Scherrer Institute, Laboratory for Neutron Scattering, 5232 Villigen PSI, Switzerland. ^cPaul