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The molecular and crystal structure of the title compound, C₂₁H₁₂ClN₃O, has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the triclinic, space group *P-1* with unit cell dimensions *a*= 8.8342(9), *b*= 10.2301(8), *c*= 11.2401(9), α = 76.473(6)°, β =84.912(7)°, γ =64.419(6)°, *V*= 890.74(13)Å³, *Z*=2, *R*₁=0.045 and *wR*₂=0.130. The crystal structure of the title compound phthalonitrile derivatives, C₂₁H₁₂ClN₃O, is stabilized by π - π stacking interactions.

Calculational studies were performed by using AM1, PM3 semi-empirical and DFT methods. Geometry optimizations of compound have been carried out by using three semi-empirical methods and DFT method and bond lengths, bond and torsion angles of title compound have been determined. Atomic charge distribution have been obtained from AM1, PM3 and DFT. In order to determine conformational flexibility on the molecule, molecular energy profile of the title compound was obtained with respect to the selected torsion angle T(C21-C16-N3-C15), which is varied from -180° to +180° in every 10 via PM3 semi-empirical method.

Keywords: single crystals; crystallographic analysis; DFT

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Crystal Structures of Ferrocenyl- Phosphazene Derivatives. Asli Ozturk^a, Nuran Asmafiliz^b, Tuncer Hokelek^a, Zeynel Kilic^b. ^a*Hacettepe University, Department of Physics Engineering, 06800 Ankara, Turkey.* ^b*Ankara University, Department of Chemistry, 06100 Ankara, Turkey.*

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In this study, crystal structures of two ferrocenyl-phosphazene derivatives, C₁₅H₂₀Cl₄FeN₅P₃, (I), and C₄₂H₆₂Fe₂N₅P₃, (II), are investigated. The data have been collected with Mo K_α radiation on an Enraf-Nonius CAD-4 diffractometer.

spiro(Butane-1,4-diamino)-[N-(1-ferrocenyl-methyl)]-4,4,6,6-tetrachloro-cyclotriphosphazatriene (I) is a mono-ferrocenyl *spiro*-cyclic phosphazene derivative and it belongs to the space group *P bca* with cell parameters *a*=16.027(3), *b*=11.834(8), *c*=24.111(4) Å. It has π - π contact between cyclopentadiene rings [centroid-centroid distance = 3.278(4) Å]. The N-H...N intermolecular hydrogen bonds^[1] link the molecules, forming infinite one dimensional chains running approximately parallel to *c* axis and the intramolecular C-H...N H bonds form a dimerization.

spiro-(Butane-1,4-diamino)-[N,N'-bis(1-ferrocenyl-methyl)]-4,4,6,6-tetrakispyrrolidino-cyclotrip

hosphazatriene (II) is a bis-ferrocenyl *spiro*-cyclic phosphazene derivative including two ferrocenes and it belongs to the space group *P-1* with cell parameters *a*=11.494(4), *b*=15.259(3), *c*=15.293(3) Å and α = 60.98(1)°, β =75.49(2)°, γ =71.33(2)°. It also has π - π contact between cyclopentadiene rings and C-H... π contacts between H atoms of C13, C19, C34 and cyclopentadiene rings (C6/C7/C8/C9/C10) and (C1/C2/C3/C4/C5) and phosphazene ring (P1/N1/P2/N2/P3/N3).

[1] İltter, E. E., Asmafiliz, N., Kılıç, Z., Işıklan, M., Hökelek, T., Çaylak, N. and Şahin, E., *Inorg. Chem.*, 46, 9931-9944, 2007.

Keywords: phosphazenes; ferrocenyl-phosphazenes; hydrogen bonds

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Solid State Chemistry of Tetrabromo-and Tetrachlorosemiquinone Radical Anions. Krešimir Molčanov^a, Biserka Kojić-Prodić^a. ^a*Rudjer Bošković Institute, Zagreb, Croatia.*

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p-Tetrabromosemiquinone (bromanil) and *p*-tetrachlorosemiquinone (chloranil) radical anions are well-known for their stability. They were extensively studied by EPR, IR and Raman spectroscopies and theoretical methods; an X-ray crystallographic study was also attempted. The crystal structures, however, remained elusive.

Freshly prepared semiquinone crystals are red, but turn green in a few minutes at RT. The colour change is due to disproportionation of the radicals into a quinhydrone-like substance [1]. All previous studies of tetrachlorosemiquinone radical anion salts were done using a green compound.

For the first time, high-resolution data on geometry of semiquinone radicals not participating in charge-transfer interactions (such as coordination bonds or low-barrier hydrogen bonds) has been experimentally obtained. Geometry of the quinoid rings and C–O bond lengths (1.25 – 1.26 Å) differs slightly from the hydrogen bonded semiquinone (C–O bond lengths of 1.29–1.30 Å [1]), and these results agree well with quantum chemical models.

[1] K. Molčanov, B. Kojić-Prodić, M. Roboz, *Acta Cryst. B*, 2006, 62, 1051.

Keywords: radical salts; accurate geometry; low-temperature data collection

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Crystal Structure of 2,4,4-Tris(benzylsulfanyl)-1,1-dichloro-3-nitrobuta-1,3-diene. Cigdem Sayil^a, Goksin Aydinli^a, Cemil Ibis^a. ^a*Istanbul University, Faculty of Engineering, Department of Chemistry, 34320 Avcılar-Istanbul, Turkey.*

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The molecule of the title compound, C₂₅H₂₁Cl₂NO₂S₃, is not planar. The three phenyl rings and the butadiene group are inclined at angles of 85.9(1), 61.9(1), 81.4(1)