Commun.Fac.Sci.Univ.Ank.Series B
Volume 61, Number 1-2, Pages 1-14(2019)
ISSN 2687-4806
http://communications.science.ankara.edu.tr/index.php?series=B

DETERMINATION OF ABSOLUTE CONFIGURATION OF 8,8,10,10-TETRACHLORO-20,21-DIHYDRO-18H,23H-6,12-EPIAZENO-6λ5,8λ5,10λ5, 12λ5-[1,3,2]BENZOXAZAPHOSPHONINO[2 ,3 :8,9][1,3,5,7,9,2,4,6,8] PENTAAZATETRAPHOSPHACYCLOUNDSYNO[2,1-B][1,3,2] BENZOXAZAPHOSPHONINE USING X-RAY CRYSTALLOGRAPHY

GAMZE ELMAS, AYTUĞ OKUMUŞ, SATİYE SEVİM İSAOĞLU, TUNCER HÖKELEK AND ZEYNEL KILIÇ

ABSTRACT. The title compound, 8, 8, 10, 10-tetrachloro-20,21-dihydro-18H, 23H-6, 12-epiazeno-6λ5, 8λ5, 10λ5, 12λ5-[1,3,2] benzoxazaphosphonino [2',3':8,9][1,3,5,7,9,2,4,6,8] pentaazatetraphosphacyclo undsyno [2,1-b] [1,3,2] benzoxazaphosphonine; C16H16Cl4N6O2P4, a cyclotetraphosphazene, has a tetrachloro-2, 4-spiro-ansa-spiro (tetrachloro-2,4-sas) architecture in which the bicyclic structure has consisted of eight-membered tetrameric N4P4 and seven-membered ansa (N1/P1/P1′/N4′/C8′/C8/N4) rings fused with a common PNP fragment. The asymmetric unit possesses one-half of the molecule. P1 and P1′ atoms are stereogenic centres. In addition, there is a mirror plane passing through the N3 and N1 atoms in the molecule, and therefore, this compound is in meso form (RS/SR). According to the checkcif result, it is found that the absolute configuration of P1 and/or P1′ phosphorus centers is RS, displaying that in the solid-state there is only one enantiomer in the unit cell. The space group is P bnm with cell parameters of a = 6.2692(2), b = 15.8111(3), c = 22.9393(4) Å.

1. INTRODUCTION

Octachlorocyclotetraphosphazene, also known as tetrameric phosphazene, N4P4Cl8, is an important starting compound in the field of phosphazene chemistry [1,2]. It has been used in the syntheses of considerable amounts of organocyclotetraphosphazene and polymeric phosphazene derivatives with different substituents, and the composed products from these reactions display various chemical and physical properties upon the types and features of the bonded groups to the four P-atoms [1-3]. Many tetrameric phosphazene derivatives were synthesized using the mono and bidentate ligands until today [4-7], however, in the literature the Cl replacement reactions with polyfunctional ligands are limited relatively [8,9]. Tetrameric products with the bidentate ligands can produce spiro, dispiro, trispiro, tetraspiro,

Received by the editors: July 11, 2019; Accepted: August 09, 2019.
Key word and phrases: Cyclotetraphosphazene, spiro-ansa-spiro-Structure, X-ray crystallography.

ansa, spiro-ansa, bino and spiro-bino derivatives, and in addition to these products N4P4Cl8 may also give spiro-ansa-spiro, ansa-spiro-ansa and di(spiro-bino) products with the polyfunctional ligands depending on the reaction conditions [4-10].

Recently, the stereogenic properties of the cyclophosphazenes have been researched as an attractive area, and some papers have been published about this topic [11,12]. For the evaluations of the stereogenic properties of the cyclophosphazenes, were used the different methods, such as X-ray crystallography, HPLC and 31P NMR spectroscopy in the presence of (R)-(+)-2,2,2-trifluoro-1-(9'-anthryl)-ethanol (CSA) [13,14].

Organocyclophosphazenes have important and different applications in the technological and biological areas; eg. ionic liquids [15], advanced elastomers [16], Li-ion batteries [17], the anti-cancer [18] and antituberculosis [19] agents, the antibacterial and antifungal activity studies [20,21], and the oxidative cleavage of DNA [22,23].

In this paper, the tetrachloro-2,4-sas cyclotetraphosphazene was synthesized from the reaction of N4P4Cl8 with N2O2 donor-type unsymmetrical tetradentate ligand according to the published paper [24], and it was crystallized from acetonitrile. The aim of the current paper is to investigate the crystallographic and stereogenic properties of tetrachloro-2,4-sas cyclotetraphosphazene derivative. Besides, the determination of the absolute configurations of this compound is an important finding.

2. Materials And Methods

2.1. X-ray crystal structure determination

The colourless single crystals of the title **tetrachloro-2,4-sas** compound was obtained from acetonitrile at room temperature. The crystallographic details are listed in Table 1, and the selected bond lengths and angles together with the selected torsion angles are presented in Table 2. The crystallographic data were recorded on a Bruker Kappa APEXII CCD area-detector diffractometer using Mo K_α radiation (λ=0.71073 Å) at T=100(2) K. Absorption correction by multi-scan [25] was applied. Structure was solved by direct methods and refined by full-matrix least squares against F^2 using all data [26]. All non-H atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically at distances of 0.93 Å (CH) and 0.97 Å (CH_2) from the parent C atoms; a riding model was used during the refinement process and the U_{iso}(H) values were constrained to be 1.2U_{eq}(carrier atom).

2.2. Materials used for syntheses

The starting tetradentate ligand, 2,2'-[1,2-ethanediylbis(iminomethanediyl)]diphenol, and the **tetrachloro-sas** cyclotetraphosphazene were prepared according to the published procedures [24].

TABLE 1. Crystallographic details.

Empirical Formula	$C_{16}H_{16}Cl_4N_6O_2P_4$
Fw	590.03
Crystal System	orthorhombic
Space Group	P bnm
a (Å)	6.2692(2)
b (Å)	15.8111(3)
c (Å)	22.9393(4)
α (°)	90.00
β (°)	90.00
γ (°)	90.00
V (Å^3)	2273.81(9)
Z	4
T	100(2) K
Crystal color	colourless
Crystal size	0.18x0.28x0.29 mm
μ (mm^{-1})	0.832 (Mo K_α)
ρ (calcd) (g cm^{-3})	1.724
Number of Reflections Total	12173
Number of Reflections Unique	2883
R_{int}	0.0565
$(\Delta/\sigma)_{max}$	<0.001
$(\Delta\rho)_{max}$	0.607 e Å^{-3}
$(\Delta\rho)_{min}$	−0.838 e Å^{-3}

$2\theta_{max}$ (°)	56.64
T_{min} / T_{max}	0.896/ 0.920
Number of Parameters	148
R [$F^2>2\sigma(F^2)$]	0.0466
wR	0.1226

TABLE 2. The selected bond lengths (Å) and angles (deg) with the selected torsiyon angles (°).

P1– N1	1.5605(14)	N1– P1– N4	118.86(17)	N4– P1– N1– P1′	-81.2(3)
P1– N4	1.580(3)	N5– P1– O1	103.53(16)	N4– P4– N3– P4′	-65.8(4)
P4– N3	1.5641(14)	N5– P1– N1	112.37(14)	N1– P1– N4– P4	39.4(4)
P4– N4	1.543(3)	N4– P1– O1	103.45(15)	N3– P4– N4– P1	7.0(5)
P1– N5	1.615(3)	N3– P4– N4	122.55(17)		
P4– Cl3	2.0010(10)	N5– P1– N4	111.1(2)		
P4– Cl4	2.0107(11)	P4– N3– P4′	137.8(2)		
P1– O1	1.5882(19)	P1– N1– P1′	132.6(2)		
		P1– N4– P4	133.8(2)		
		N3– P4– Cl3	105.99(12)		
		N3– P4– Cl4	109.98(13)		
		N4– P4– Cl3	107.48(13)		
		N4– P4– Cl4	107.57(16)		

3. Result And Discussion

The title cyclotetraphosphazene (Fig. 1) has consisted of a 2,4-spiro-ansa-spiro fashion with the N_2O_2 tetradentate ligand bonded to the phosphorus atoms. The asymmetric unit of the title cyclotetraphosphazene, $C_{16}H_{16}Cl_4N_6O_2P_4$, (Fig. 2) contains only one-half of the molecule. It has a tetrachloro-2,4-spiro-ansa-spiro (**tetrachloro-2,4-sas**) architecture in which the bicyclic group contains the eight-membered tetrameric, N_4P_4, ring and the seven-membered ansa, (N1/P1/P1′/N4′/C8′/C8/N4), ring fused through a common PNP fragment, and the two symmetry related benzoxazaphosphonine groups. The oxygen atoms (O1 and O1′) bonded to the phosphorus atoms (P1 and P1′) are in *cis* fashions [symmetry code: (‘) : x, y, ½ - z]. There is a mirror plane passing through the atoms N1 and N3. The **tetrachloro-2,4-sas** cyclotetraphosphazene structure has two equivalent stereogenic P centers (P1 and P1′). It was clearly determined that the absolute configuration of these P1 and P1′ atoms is

RS with respect to the checkcif data, showing that in the unit cell there is only one enantiomer in the solid-state (Figs. 1 and 2).

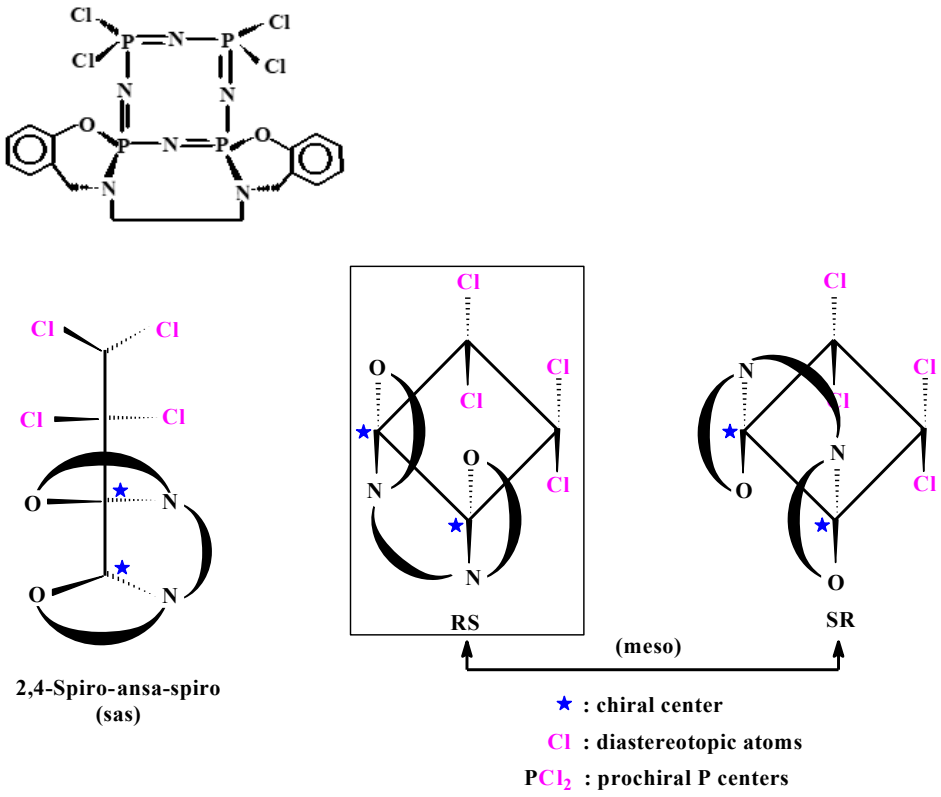


FIGURE 1. Chemical diagram and the meso forms of tetrachloro-2,4-spiro-ansa-spiro cyclotetraphosphazene.based on the ORTEP diagram *via* stick diagrams and spatial views.

The molecular and crystal structure of **tetrachloro-2,4-sas** compound along with the atom-numbering scheme is depicted in Fig. 2. The P atoms are non-coplanar and the N atoms are displaced above (+) and/or below (–) of the best least -squares plane passing through the P atoms by the following distances: N1 [–0.2957(1) Å], N3 [+0.3112(1) Å] and N4 [–0.0932(1) Å]. The conformation of the macrocyclic cyclotetraphosphazene ring is given by the torsion angles of the ring bonds (Table 2), and **tetrachloro-2,4-sas** compound comprises of a

symmetric non-planar cyclic tetrameric phosphazene ring, A (P1/N1/P1'/N4'/P4'/N3/P4/N4), in sofa conformation (Fig. 3a) with the puckering amplitude [27] Q_T of 0.5926(21) Å, while the seven-membered ansa ring, B (N1/P1/N5/C8/C8'/N5'/P1′), and the six-membered spiro ring, C (P1/O1/N5/C1/C6/C7), adopt flattened-boat (Fig. 3b) and twisted-boat (Fig. 3c) conformations with the puckering amplitudes [31] Q_T of 0.4622(32) Å and 0.5016(29) Å, respectively.

The bicyclic part of the molecule contains the eight-membered tetrameric phosphazene, A (P1/N1/P1'/N4'/P4'/N3/P4/N4), ring and the seven-membered ansa, B (N1/P1/N5/C8/C8'/N5'/P1′), precursor fused through a common PNP fragment, and it resembles the stable "adamantane" structure, with a V-shaped conformation (Fig. 4a). The orientations of the A, B and C rings constituting the spiro-ansa-spiro cyclic system is shown in Fig. 4b.

In the tetrameric, N_4P_4, phosphazene ring, the endocyclic P—N bond lengths are in the ranges of 1.580(3)-1.543(3) Å, and the average endocyclic P—N bond length is 1.562(3) Å. This value is shorter than the average exocyclic P—N bond lengths of 1.602(2) Å (Table 2). In the cyclophosphazenes, the P—N single and double bonds are generally in the ranges of 1.628-1.691 Å and 1.571-1.604 Å, respectively [28], and the obtained values of **tetrachloro-2,4-sas** compound are in consistent with these values. Besides, the exocyclic P1—N5 bond lengths is 1.615 (3) Å, and is very close to the double bond length. The shortening in this bond is probably due to the electron transfer from the N5 atom to the phosphazene ring. This value can be compared with the reported value of 1.613 (5) Å in the **sas** trimeric phosphazene, $C_{16}H_{16}Cl_2N_5O_2P_3$ [29].

Additionally, while the endocyclic P—N—P bond angles are in the ranges of 132.6(2)-137.8(2)º, and the average value is 134.7(2)º, the endocyclic N—P—N bond angles are 118.86(17)º and 122.56(17)º, and the average value is 120.71(17)º. In the standard compound, $N_4P_4Cl_8$, the endocyclic P—N—P and N—P—N bond angles are 131.3º and 121.2º [30]. These variations of the endocyclic P—N—P and N—P—N angles may reflect the steric hindrances of the bulky N_2O_2 tetradentate ligand and ought to be referred to the negative hyperconjugation [31].

On the other hand, the sum of the bond angles around the N5 atom [359.8(3)°] indicates that the N5 atom is in trigonal planar geometry. Thus, although the N5 atom bonds to three different groups, it can not be a stereogenic center. Moreover, the sum of the bond angles

around the P1 atom [438.21(17)°] can be compared with the reported value [434.4(3)°] in **sas** trimeric phosphazene [29].

Fig. 5 displays the packing diagram of title compound. The molecules are elongated along the b-axis and stacked along the a-axis. Van der Waals interactions may be considered to be effective in the unit cell packing.

The crystallographic data of the compound has been deposited with the Cambridge Crystallographic Data Centre, CCDC 1953257.

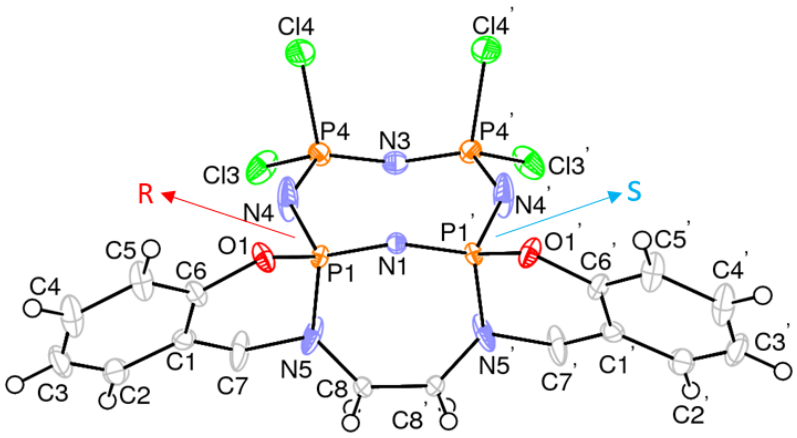
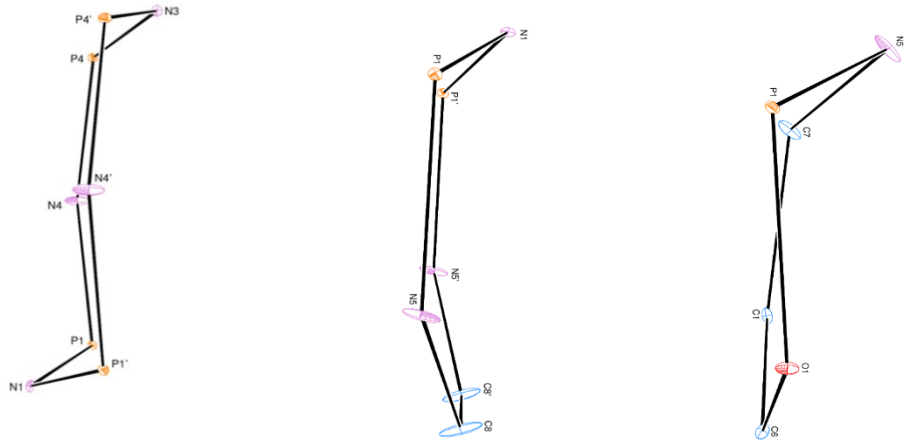
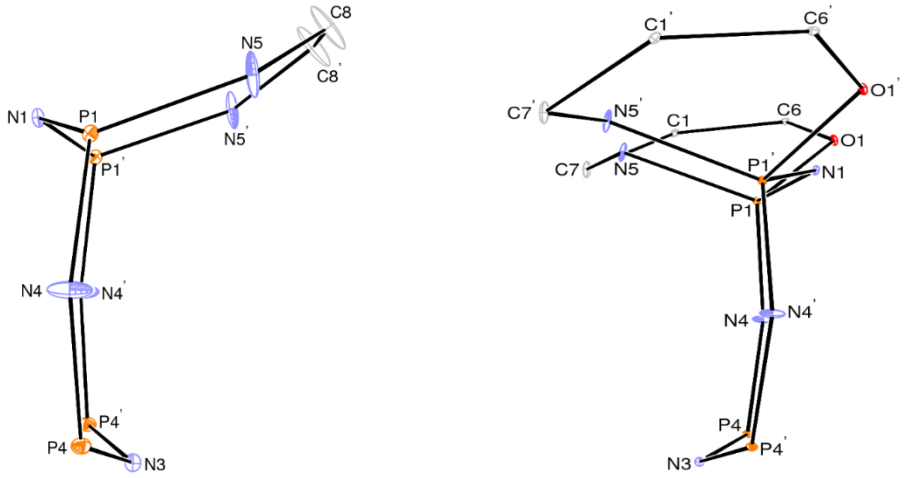


FIGURE 2. An ORTEP-3 [32] drawing of title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.



(**a**) (**b**) (**c**)

FIGURE 3. The conformations of the (**a**) cyclic tetrameric phosphazene ring, (**b**) the seven-membered ansa ring and (**c**) the six-membered spiro ring.



(**a**) (**b**)

FIGURE 4. The conformations of the (**a**) V-shaped bicyclic system containg the A and B rings, and (**b**) spiro-ansa-spiro cyclic system.

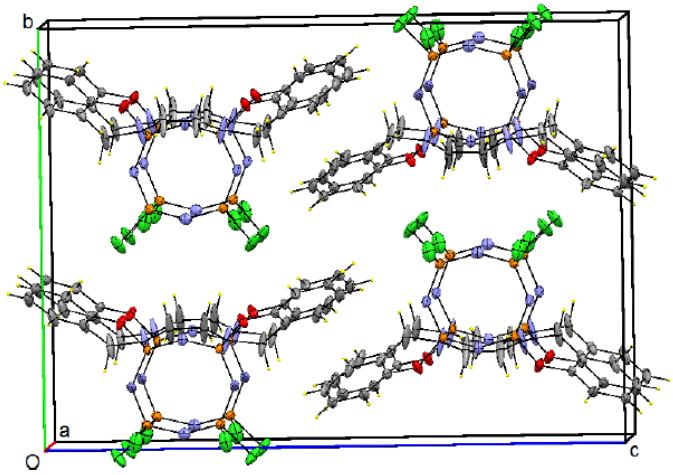


FIGURE 5. The packing diagram of tetrachloro-2,4-spiro-ansa-spiro cyclotetraphosphazene viewed down the a-axis direction.

4. Concluson

In this paper, the structure of the title **tetrachloro-2,4-sas** cyclotetraphosphazene was verified using single crystal X-ray diffraction technique. It has two equivalent chiral phosphorus (P1 and P1′) centres with respect to the X-ray structure analysis results. In addition, the molecule is a symmetric structure, and so it is in the meso form. It is undoubtedly detected that the absolute configuration of P1 and P1′ atoms is RS with checkcif data, showing that in the solid-state there is only one enantiomer in the unit cell.

Besides, the partly substituted **tetrachloro-2,4-sas** tetrameric phosphazene may be useful as the starting compounds for the preparation of the new chiral/non-chiral multi-heterocyclic cyclotetraphosphazene derivatives. All of the obtained new products may be as biologically active compounds and/or chemotherapeutic agents.

ACKNOWLEDGEMENT

The authors thank the “Scientific and Technical Research Council of Turkey” (Grant No. 211T019).

ÖZET

Bir siklotetrafosfazen olan 8,8,10,10-tetrakloro-20,21-dihidro-18*H*,23*H*-6,12-epiazeno-6λ^5,8λ^5,10λ^5,12λ^5-[1,3,2]benzoksazafosfonino[2',3':8,9][1,3,5,7,9,2,4,6,8] pentaazatetrafosfasiklound sino [2,1-*b*][1,3,2] benzoksazafosfin; $C_{16}H_{16}Cl_4N_6O_2P_4$ bileşiği, ortak bir PNP parçası ile kaynaşmış sekiz üyeli N_4P_4 tetramerik ve yedi üyeli ansa (N1/P1/P1′/N4′/C8′/C8/N4) halkalarından oluşan bisiklik yapıdaki tetrakloro-2,4-spiro-ansa-spiro (**tetrakloro-2,4-sas**) yapısına sahiptir. Asimetrik birimde yarım molekül mevcuttur. P1 ve P1′ atomları stereojenik merkezlerdir. Ayrıca, molekül içindeki N3 ve N1 atomlarından geçen bir ayna düzlemi vardır ve bu nedenle bu bileşik mezo formundadır (RS/SR). Checkcif sonucuna göre, katı halde P1 ve/veya P1′ fosfor merkezlerinin mutlak konfigürasyonunun RS olduğu bulunmuş olup bu durum katı halde birim hücrede sadece bir enantiyomer olduğunu göstermektedir. Uzay grubu, hücre parametreleri a = 6.2692(2), b = 15.8111(3), c = 22.9393(4) Å olan P bnm'dir.

REFERENCES

[1] V. Chandrasekhar and R. S. Narayanan, Phosphazenes. Organophosphorus Chemistry, (Cambridge, UK: Royal Society of Chemistry) 45 (2016) p. 375-437.

[2] V. Chandrasekhar and R. S. Narayanan, Phosphazenes. Organophosphorus Chemistry, (Cambridge, UK: Royal Society of Chemistry) 46 (2017) p. 342-417.

[3] V. Chandrasekhar and A. Chakraborty, Phosphazenes. Organophosphorus Chemistry, (Cambridge, UK: Royal Society of Chemistry) 48 (2019) p. 400-423.

[4] X. Liu, J. P. Breon, C. Chen and H. R. Allcock, Substituent exchange reactions of trimeric and tetrameric aryloxycyclophosphazenes with sodium 2,2,2-trifluoroethoxide. Dalton Transaction, 41 (2012) 2100-2109.

[5] G. Elmas, The reactions of 2-trans-6-bis(4-fluorobenzyl)spirocyclotetraphosphazene with primary amines:spectroscopic and crystallographic characterizations. Phosphorus, Sulfur, and Silicon and the Related Elements, 192 (2017) 1224-1232.

[6] G. Elmas, A. Okumuş, Z. Kılıç, M. Çam, L. Açık and T. Hökelek, Phosphorus-nitrogen compounds. Part 40. The syntheses of (4-fluorobenzyl) pendant armed cyclotetraphosphazene derivatives: Spectroscopic, crystallographic and stereogenic properties, DNA interactions and antimicrobial activities. Inorganica Chimica Acta, 476 (2018) 110-122.

[7] G. Elmas, A. Okumuş, R. Cemaloğlu, Z. Kılıç, S. P. Çelik, L. Açık, B. Ç. Tunalı, M. Türk, N. A. Çerçi, R. Güzel and T. Hökelek, Phosphorus-nitrogen compounds. Part 38. Syntheses, characterizations,cytotoxic, antituberculosis and antimicrobial activities and DNA interactions of spirocyclotetraphosphazenes with bis-ferrocenyl pendant arms. Journal of Organometallic Chemistry, 853 (2017) 93-106.

[8] G. Mutlu, G. Elmas, Z. Kılıç, T. Hökelek, L. Y. Koç, M. Türk, L. Açık, B. Aydın and H. Dal, Phosphorus-nitrogen compounds: Part 31. Syntheses, structural and stereogenic properties, in vitro cytotoxic and antimicrobial activities, DNA interactions of novel bicyclotetraphosphazenes containing bulky side group. Inorganica Chimica Acta, 436 (2015) 69-81.

[9] G. Elmas, A. Okumuş, L.Y. Koç, H. Soltanzade, Z. Kılıç, T. Hökelek, H. Dal, L. Açık, Z. Üstündağ, D. Dündar and M. Yavuz, Phosphorus-nitrogen compounds. Part 29. Syntheses, crystal structures, spectroscopic and stereogenic properties, electrochemical investigations, antituberculosis, antimicrobial and cytotoxic activities and DNA interactions of ansa-spiro-ansa cyclotetraphosphazenes. Europane Journal of Medicinal Chemistry, 87 (2014) 662-676.

[10] T. S. Cameron, A. Linden, G. Guerch, J. P. Bonnet and J. Labarre, Crystal and molecular structure of the spiransa and dispiransa cyclophosphazenic derivatives from spermidine and spermine. Journal of Molecular Structure, 212 (1989) 295-304.

[11] A. Uslu and S. Yeşilot, Chiral configurations in cyclophosphazene chemistry. Coordination Chemistry Reviews, 291 (2015) 28-67.

[12] K. Kajiyama, Y. Setone, K. Aoyagi and H. Yuge, Chiral HPLC Separation, Absolute Structural Elucidation, and Determination of Stereochemical Stability of trans- Bis[2-(2- pyridinyl)aminophenolato] Cyclotriphosphazene. Chirality, 28 (2016) 556-561.

[13] G. Elmas, Syntheses and structural characterizations of 2-pyridyl(N/O)spirocyclotriphosphazene derivatives. Phosphorus, Sulfur, and Silicon and the Related Elements,194/1-2 (2019) 13-24.

[14] A. Binici, A. Okumuş, G. Elmas, Z. Kılıç, N. Ramazanoğlu, L. Açık, H. Şimşek, B.Ç. Tunalı, M. Türk, R. Güzel and T. Hökelek. Phosphorus–nitrogen compounds. Part 42. The comparative syntheses of 2-cis-4-ansa(N/O) and spiro(N/O) cyclotetraphosphazene

derivatives: spectroscopic and crystallographic characterization, antituberculosis and cytotoxic activity studies. New Journal of Chemistry, 43 (2019) 6856-6873.

[15] T. L. Greaves and C. J. Drummond, Protic Ionic Liquids: Properties and Applications. Chemical Reviews, 108 (2008) 206-237.

[16] H. R. Allcock, Recent developments in polyphosphazene materials science. Current Opinion in Solid State and Materials Science, 10 (2006) 231-240.

[17] M. K. Harrup, K. L. Gering, H. W. Rollins, S. V. Sazhin, M. T. Benson, D. K. Jamison, C. J. Michelbacher and T. A. Luther, Phosphazene based additives for ımprovement of safety and battery lifetimes in lithium-ıon batteries. ESC Transaction, 41 (2012) 13-25.

[18] G. Elmas, A. Okumuş, P. Sevinç, Z. Kılıç, L. Açık, M. Atalan, M. Türk, G. Deniz and T. Hökelek, Phosphorus-nitrogen compounds. Part 37. Syntheses and structural characterizations, biological activities of mono and bis(4-fluorobenzyl)spirocyclotetraphosphazenes. New Journal of Chemistry, 41 (2017) 5818-5835.

[19] A. Okumuş, G. Elmas, R. Cemaloğlu, B. Aydın, A. Binici, H. Şimşek, L. Açık, M. Türk, R. Güzel, Z. Kılıç and T. Hökelek, Phosphorus–nitrogen compounds. Part 35. Syntheses, spectroscopic and electrochemical properties, and antituberculosis, antimicrobial and cytotoxic activities of mono-ferrocenyl-spirocyclotetraphosphazenes. New Journal of Chemistry, 40 (2016) 5588-5603.

[20] G. Elmas, A. Okumuş, Z. Kılıç, S.P. Çelik and L. Açık, The spectroscopic and thermal properties, antibacterial and antifungal Activity and DNA interactions of 4-(fluorobenzyl)spiro(N/O)cyclotri phosphazenium salts. Journal of the Turkish Chemical Society, Section A: Chemistry, 4/3 (2017) 993-1016.

[21] A. Okumuş, G. Elmas, Z. Kılıç, N. Ramazanoğlu, L. Açık, M. Türk and G. Akça, The reactions of N3P3Cl6 with monodentate and bidentate ligands: The syntheses and structural characterizations, In vitro antimicrobial activities and DNA interactions of 4-fluorobenzyl(N/O)spirocylotriphosphazenes. Turkish Journal of Chemistry, 41 (2017) 525-547.

[22] G. Elmas, A. Okumuş, Z. Kılıç, L. Y. Gönder, L. Açık and T. Hökelek, The Syntheses and Structural Characterizations, Antimicrobial Activity and In vitro DNA Binding of 4-fluorobenzylspıro(N/O)cyclotriphosphazenes and Their Phosphazenium salts. Journal of the Turkish Chemical Society, Section A: Chemistry, 3 (2016) 25-46.

[23]G. Elmas, Syntheses and spectroscopic investigations of 2-pyridyl(N/N)spirocyclotriphosphazenes. Journal of the Turkish Chemical Society, Section A: Chemistry, 5/2 (2018) 621-634.

[24] G. Elmas (nee Egemen), A. Okumuş, Z. Kılıç, T. Hökelek, L. Açık, H. Dal, N. Ramazanoğlu and L. Y. Koç, Phosphorus−nitrogen compounds. Part 24. Syntheses, crystal structures, spectroscopic and stereogenic properties, biological activities, and DNA interactions of novel spiro-ansa-spiro- and ansaspiro-ansa-cyclotetraphosphazenes. Inorganic Chemistry, 51 (2012) 12841-12856.

[25] Bruker SADABS, Bruker AXS Inc. Madison, Wisconsin, USA (2005).

[26] G. M. Sheldrick, SHELXS-97, SHELXL-97 University of Gottingen, Gottingen, Germany (1997).

[27] D. Cremer and J. A. Pople, General definition of ring puckering coordinates. Journal of American Chemical Society, 97 (1975) 1354-1358.

[28] F. H. Allen, O. Kennard, D. G. Watson, L. Brammer, G. Orpen and R. Taylor, Tables of bond lengths determined by X-ray and neutron diffraction. Part 1. Bond lengths in organic compounds. Journal of the Chemical Society, Perkin Transactions 2. 12 (1987) 1-19.

[29] S. Safran, T. Hökelek, S. Bilge, Ş. Demiriz, A. Natsagdorj, and Z. Kılıç, Crystal Structure of 8,8-dichloro-1,2,10,11,13,14-hexahydro-6λ5,8λ5,10λ5-6,10-nitrilo[1,3,5,7,2,4,6]tetrazatriphosphoninobis [1,3,2]oxazaphosphorine. Analytical Sciences X-ray Structure Analysis Online, 21 (2005) x77-x78.

[30] A. J. Wagner, A. Vos, The crystal structure of compounds with (N-P)n rings. IV. The stable modification (T form) of tetrameric phosphonitrilic chloride, N4P4Cl8. Acta Crystallograhica Section B. B24 (1968) 707-713.

[31] A. B. Chaplin, J. A. Harrison and P. J. Dyson, Revisiting the electronic structure of phosphazenes. Inorganic Chemistry, 44 (2005) 8407-8417.

[32] L. J. Farrugia, ORTEP-3 for Windows- a version of ORTEP-III with a Graphical User Interface (GUI). Journal of Applied Crystallography, 30 (1997) 565-566.

Current Address: GAMZE ELMAS Department of Chemistry, Ankara University, 06100 Ankara, TURKEY
E-mail Address: gegemen@ankara.edu.tr
ORCID: https://orcid.org/0000-0003-4877-3697

Current Address: AYTUĞ OKUMUŞ: Department of Chemistry, Ankara University, 06100 Ankara, TURKEY
E-mail Address: okumus@science.ankara.edu.tr
ORCID: https://orcid.org/0000-0002-2169-5695

Current Address: SATİYE SEVİM İSAOĞLU: Cebrail Neighborhood, Kuleli Street No.14A/2 Kastamonu, TURKEY
E-mail Address: satiyesevim@gmail.com

Current Address: TUNCER HÖKELEK: Department of Physics, Hacettepe University, 06800 Ankara, TURKEY
E-mail Address: merzifon@hacettepe.edu.tr
ORCID: https://orcid.org/0000-0002-8602-4382

Current Address: ZEYNEL KILIÇ (Corresponding author): Department of Chemistry, Ankara University, 06100 Ankara, TURKEY
E-mail Address: zkilic@science.ankara.edu.tr
ORCID: https://orcid.org/0000-0003-1061-8122