## CRYSTAL STRUCTURE OF A $\pi$ COMPLEX OF AgBF<sub>4</sub> WITH 2-ALLYL-5-PHENYL-2*H*-TETRAZOLE OF THE COMPOSITION [Ag(C<sub>10</sub>H<sub>10</sub>N<sub>4</sub>)(BF<sub>4</sub>)]

## Yu. I. Slyvka

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By the interaction of AgBF<sub>4</sub> with 2-allyl-5-phenyl-2*H*-tetrazole (2*aphet*) in the ethanol solution, a  $\pi$  complex of [Ag(2*aphet*)(BF<sub>4</sub>)] is obtained which is studied using single crystal X-ray diffraction.

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Coordination compounds of tetrazole derivatives have found a sufficiently wide application in the organic synthesis as the precursors and catalysts for producing biologically active substances, corrosion inhibitors, luminophores, and as efficient tools in crystal engineering of metal complexes [1]. Among the  $\pi$  coordinated compounds of *d* metals of Ib group with allyl derivatives of tetrazoles only three crystalline  $\pi$  complexes of Ag(I) have been studied [2, 3], so in the continuation of the investigation of the behavior of other substituted tetrazoles as compared with Ag<sup>+</sup>, this work reports the results of the synthesis and X-ray diffraction analysis of a new  $\pi$  complex of AgBF<sub>4</sub> with 2-allyl-5-phenyl-2*H*-tetrazole (2*aphet*) of the composition [Ag(2*aphet*)BF<sub>4</sub>] (1).

**Experimental. Synthesis.** 5-Phenyltetrazole was obtained according to the known technique [4] from benzonitrile and sodium azide. 5-Phenyltetrazole was alkylated with allyl chloride in the presence of an equivalent amount of NaHCO<sub>3</sub> in the ethanol solution resulting in a product of N-allyl-5-phenyltetrazole (*aphet*). Yield was 94 %.

The crystals of the  $[Ag(2aphet)BF_4]$  compound (1) were synthesized by the interaction of silver(I) tetrafluoroborate (formed *in situ* from Ag<sub>2</sub>CO<sub>3</sub> and HBF<sub>4</sub>) with 2-*aphet* in the ethanol solution. To the solution of 0.27 mmol (0.05 g) of 2-*aphet* in 0.7 ml of ethanol, at room temperature, 0.36 mmol (0.1 g) of freshly prepared Ag<sub>2</sub>CO<sub>3</sub> was added. The suspension was acidified with concentrated HBF<sub>4</sub> to pH ~ 4, and a newly formed white, slightly rose suspension was left in the dark at room temperature. In 52 h, on the surface of the precipitate from the solution, the colorless prismatic crystals of compound 1 formed.

Single crystal X-ray diffraction study. The array of the integrated reflection intensities for the crystals of compound 1 was recorded on a single crystal Rigaku AFC7 diffractometer equipped with a coordinate Mercury CCD detector (Mo $K_{\alpha}$  radiation, graphite monochromator). The structure was solved and refined using the SHELXS-97 and SHELXL-97 software [5]. The details of the single crystal X-ray diffraction study and the main crystal structural data for 1 are as follows: composition C<sub>10</sub>H<sub>10</sub>N<sub>4</sub>AgBF<sub>4</sub>, M= 380.9 g/mol, triclinic crystals, space group  $P\overline{1}$ , a = 6.3063(12) Å, b = 7.0074(12) Å, c = 14.394(3) Å,  $\alpha = 80.179(8)^{\circ}$ ,  $\beta = 88.241(7)^{\circ}$ ,  $\gamma = 78.732(6)^{\circ}$ , V = 614.7(2) Å<sup>3</sup>, Z = 2,  $\rho_{calc} = 2.06$  g/cm<sup>3</sup>,  $\mu(MoK_{\alpha}) = 1.683$  mm<sup>-1</sup>, S = 1.077, R(F) = 0.0544 for 2389 reflections with  $I \ge 2\sigma(I)$ ,  $R_w = 0.1475$  for all 2534 independent

Franko National University of Lviv, Lviv, Ukraine; y\_slyvka@franko.lviv.ua. Translated from *Zhurnal Strukturnoi Khimii*, Vol. 56, No. 1, pp. 187-188, January-February, 2015. Original article submitted December 16, 2013.



**Fig. 1.** Fragment of the structure of  $\{Ag(2aphet)BF_4\}_n$  (1).

reflections. Three of four F atoms of the tetrafluoroborate anion are disordered over three sites. The positions of these F atoms were refined in the isotropic approximation. Atomic coordinates and other parameters of compound **1** were deposited with the Cambridge Structural Database (No. CCDC 976329) at the address of www.ccdc.cam.ac.uk/data\_request/cif.

**Results and discussion.** In the structure of **1**, the 2*aphet* molecule serves as a bridge-chelate  $\pi,\sigma$ -ligand and is coordinated to the Ag(I) atom through the olefinic C=C bond of the allyl group and two N1 and N3 atoms of the tetrazole core (Fig. 1). Therefore, the linear organometallic cationic chains of the composition  $\{Ag(2aphet)\}_n^{n+}$  are formed in the structure. The phenyl ring in 2*aphet* is turned at 10.4° relative to the plane of the tetrazole core. A distorted trigonal-bipyramidal environment of the silver atom consists of three mentioned active centers of 2*aphet* and two F atoms. The respective Ag-*m*<sup>*i*</sup> (where *m* is the middle of the C=C bond, *i* = *x*-1, *y*, *z*), Ag-N1<sup>*i*</sup>, Ag-N3, Ag-F1<sup>*i*</sup> (*ii* = 1–*x*, 1–*y*, 1–*z*), and Ag-F42 distances are 2.330(4) Å, 2.420(4) Å, 2.231(4) Å, 3.05(1) Å, and 2.53(1) Å respectively. As a whole, the topology of compound **1** is similar to that of the previously studied  $\pi$ -complexes of Cu(I) with 2-allylbenzotriazole [6].

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