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Synthesis, Structure, and Properties of the Product Formed in the Reaction of *ortho*-Diphenylphosphinobenzaldehyde and *N*-Tosyl-1,2-phenylenediamine

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Abstract—Interaction of *ortho*-diphenylphosphinobenzaldehyde with *N*-tosyl-1,2-phenylenediamine afforded the product of intramolecular Wittig reaction, *N*-{2-[2-(Diphenylphosphoryl)benzylamino]phenyl}-4-methylbenzenesulfonamide. Its structure was established on the basis of IR, ^{1}H NMR, ^{13}C NMR, and 2D ^{1}H NMR (COSY) spectroscopy. Reaction mechanism was studied by means of quantum chemistry DFT method. Complex-forming property of the obtained diphenylphosphine oxide was investigated.

Keywords: aromatic phosphine oxide, NMR spectroscopy, quantum chemical DFT calculations, metal complexes

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The products of the reaction of *ortho*-diphenylphosphinobenzaldehyde with amines are usually Schiff's bases. A large number of analogous azomethines derived from different *N*-nucleophiles is described [1–6]. These substances are interesting first of all because of their ability to form metal complexes of various composition and structure [7–15]. These complexes are used in particular as catalysts of chemical reactions [16–26]. The aim of this work was the synthesis of a new polyfunctional ligand and the investigation of its properties. In the course of the reaction of aldehyde **I** with *N*-tosyl-1,2-phenylenediamine **II** in toluene (see Experimental) instead of the expected Schiff's base **III** product **IV** was isolated (Scheme 1). It was identified using IR, ^{1}H NMR, ^{13}C NMR, and 2D ^{1}H NMR (COSY) spectroscopy.

In the ^{1}H NMR spectrum of compound **IV** in $CDCl_3$ the signals of methyl group (2.35 ppm), of methylene group (4.21 ppm, *J* 4.5 Hz) , of the aromatic protons (6.2–7.7 ppm), a broadened triplet of $N\underline{H}CH_2$ proton (4.98 ppm), and the signal of tosylamine NH proton (7.88 ppm) were observed. After the addition of D_2O signals of both NH protons disappeared due to exchange with deuterium ions. At the same time the CH_2 group signal transformed into a singlet.

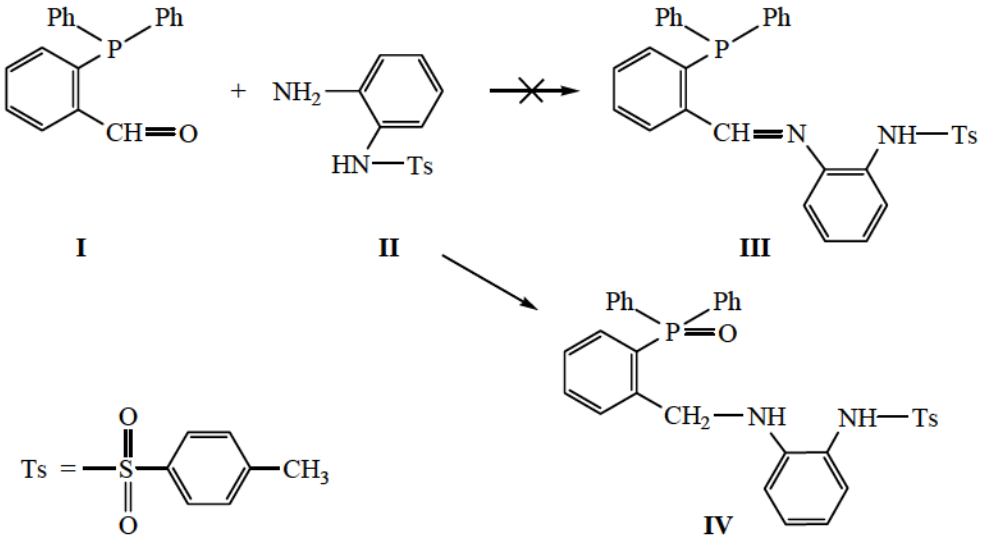
In more polar DMSO-d_6 the signal of the CH_2 group protons gave rise to a broadened doublet at 4.33 ppm, and the signal of the NH-proton shifted downfield by 0.87 ppm. Signal of the second NH proton also shifted downfield by 1.3 ppm indicating the interaction of molecules of the dissolved substance with the molecules of the solvent.

In CD_3OD signals of the NH protons do not appear due to deuteration. Protons of CH_2 group give a singlet at 4.45 ppm.

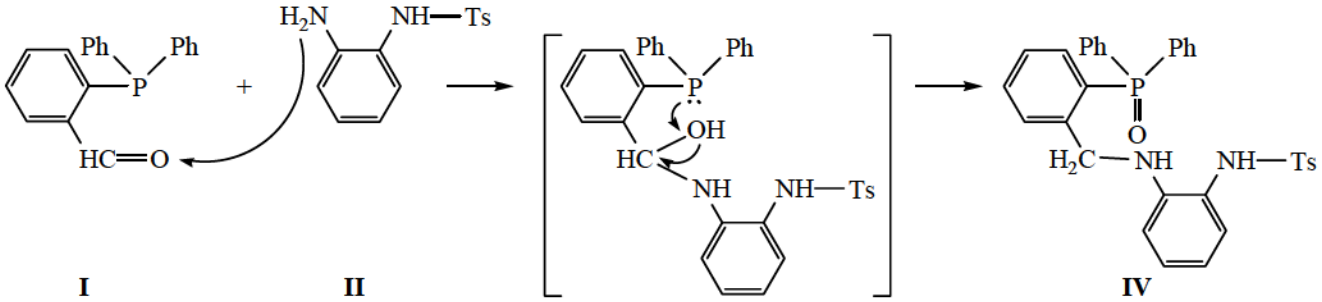
The attribution of signals in the ^{13}C NMR spectra of compound **IV** was carried out on the basis of two-dimensional COSY, NOESY, HMQC, and HMBC methods (Fig. 1). In the ^{13}C NMR spectrum the most characteristic is the doublet of the methylene group carbon atom at 45.2 ppm ($^3J_{PC}$ 3.6 Hz) and also the signals of carbon atoms directly bound with phosphorus at 130.4 and 132.8 ppm with the coupling constants $^1J_{PC}$ 100.2 and 102.1 Hz respectively. It is important to note that two phenyl substituents on phosphorus atom are magnetically equivalent and give three doublets and a singlet. Comparing ^{13}C NMR

† Deceased.

Scheme 1.



Scheme 2.

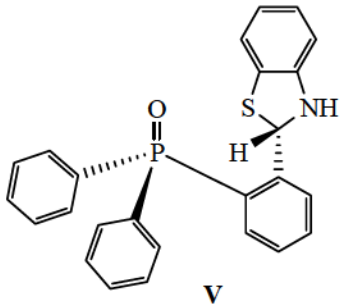


spectra of Ph_3PO and Ph_3P [27] it is possible to conclude that in the course of the reaction oxidation of phosphine to phosphine oxide takes place. This fact was confirmed also by the presence in the IR spectrum of compound **IV** of a strong absorption band of P=O group at 1165 cm^{-1}. IR spectrum also contains absorption bands of two NH groups at 3455 and 3611 cm^{-1} and the bands of asymmetric and symmetric vibrations of SO_2 group at 1331 and 1115 cm^{-1} respectively [28].

The structure of molecule provides a possibility of the formation of intramolecular as well as intermolecular H-bonds. At the dilution of compound **IV** solution in $CHCl_3$ no shift of the NH absorption band at 3453 cm^{-1} was observed. Hence, it can be stated that at least one of NH groups takes part in the formation of strong H-bonds.

The formation of compound **IV** is possible due to the intramolecular redox reaction analogous to the Wittig process (Scheme 2). In the first stage nucleophilic the oxygen atom of the aldehyde fragment is attacked. It leads to formation of an intermediate containing a hydroxy group and enamine fragment. But after that the liberation of water leading to formation of Schiff base does not occur.

Analogous reaction of *ortho*-diphenylphosphinobenzaldehyde with 2-aminothiophenol leading to benzothiazoline derivative **V** can also be regarded as intramolecular redox process [29].



V

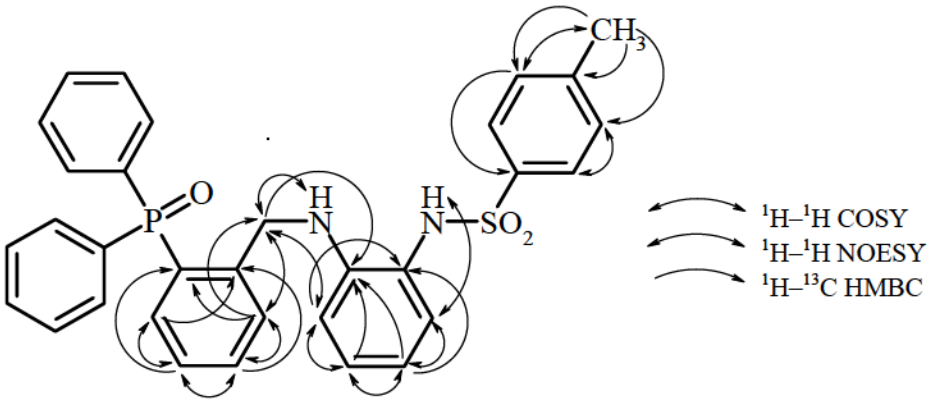


Fig. 1. $^{1}H–^{1}H$ COSY, $^{1}H–^{1}H$ NOESY, and $^{1}H–^{13}C$ HMBCX correlations in NMR spectra.

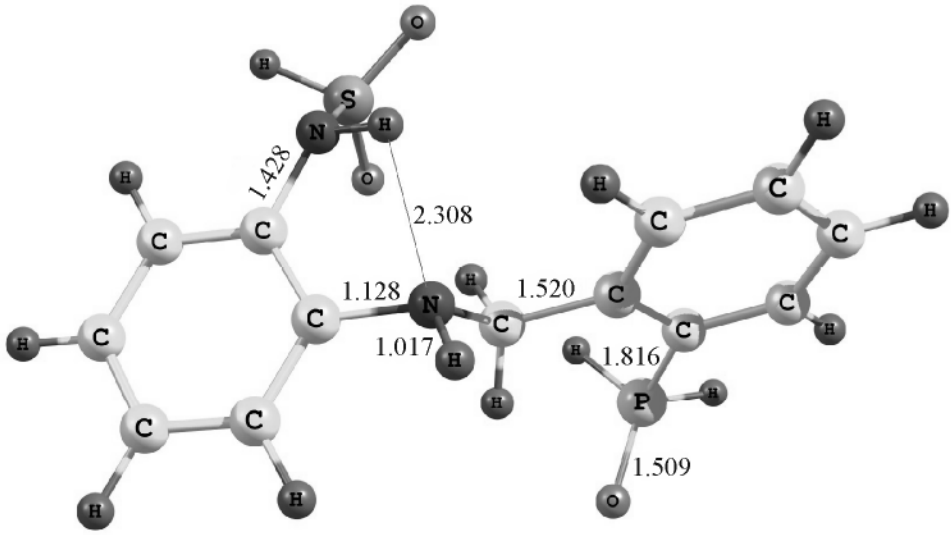


Fig. 2. General view of molecule of compound **IX** according to DFT calculations in toluene. Bond lengths are given in Å.

For the evaluation of the reaction mechanism we carried out quantum chemical DFT calculations by B3LYP method in 6-31G** basis in the gas phase, in toluene, and in ethanol using Gaussian 03 complex of programs. Solvent effects were considered according to PCM scheme [30].

We have calculated geometrical and energy characteristics of compounds **I**–**IV** using simpler models **VI**–**X** where the periphery groups which do not participate directly in the processes were substituted with hydrogen atoms (Scheme 3).

The calculations showed that in the gas phase the formation of azomethine **VIII** is preferred. Meanwhile, at the consideration of solvent effects the formation of compound **IX** becomes more favorable. Usually, the reaction of aldehydes with amines is carried out in ethanol or toluene (with the Dean–Stark trap for removing water to shift of equilibrium to the side of azomethine formation). Boiling equimolar mixture of compounds **I** and **II** in ethanol for 5 h does not cause alterations in the composition of reaction mixture. Contrary to that the reaction proceeds in toluene to give compound **IV**. According to calculations the formation of the product **VIII** in toluene is really thermodynamically unfavorable. It needs 1.0 kcal/mol. At the same time the formation of product **IX** is accompanied by the energy gain of 9.2 kcal/mol. In ethanol the formation of compound **IX** is still more favorable (Table 1). The absence of the reaction between compounds **I** and **II** observed experimentally in ethanol arises probably from the high energy barrier.

According to the quantum chemistry calculations the proton of the NH group bound with CH_2 does not take part in the formation of intramolecular H-bond either with P=O group or the adjacent NH group (Fig. 2) what agrees completely with the ^{1}H NMR

Table 1. Full and relative energies of the systems **VI**–**IX** (considering the corrections for the zero vibrations energies) according to the DFT calculations data[a]

Compound	Gas phase		Toluene		Ethanol	
	E_{tot}, a.u.	E_{rel}, kcal/mol	E_{tot}, a.u.	E_{rel}, kcal/mol	E_{tot}, a.u.	E_{rel}, kcal/mol
VI + **VII**	–1578.78611	0.0	–1578.79583	0.0	–1579.06847	0.0
XI	–1578.78611	0.0	–1578.79284	1.9	–1579.06698	0.9
IX	–1578.79747	–7.1	–1578.80763	–9.2	–1579.08637	–11.2
VIII + H_2O	–1578.80131	–9.5	–1578.79428	1.0	–1579.06468	2.4

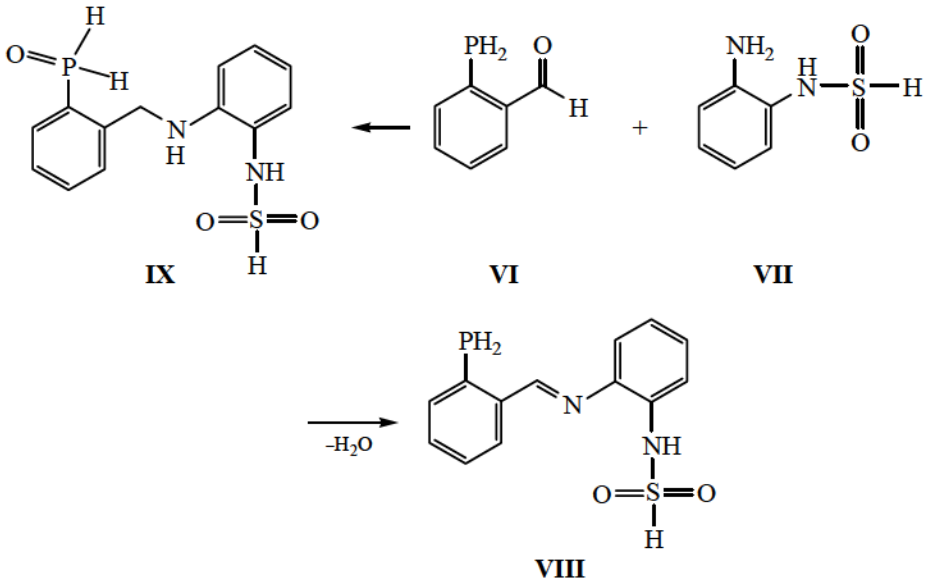
[a] Total energy of the infinitely separated reagents **VI** and **VII** was assumed to be zero.

spectral data of compound **IV** where the location of its signal depends on the concentration of solution.

The reaction pathway, that is, the formation of phosphine oxide and not the Schiff's base, is characteristic not only of the aromatic phosphinoaldehydes, but of the conjugated systems as well (Scheme 4).

The reaction of amines with 3-phosphinopropen-1-al **X** leading to the formation of aminoalcohol **XI** as a matter of fact develops not as the bimolecular nucleophilic reaction, but as a three-molecular process with the participation of two molecules of amine and one of the carbonyl compound. Analogous reaction mechanism for the reaction of amines with aldehydes

Scheme 3.



Scheme 4.

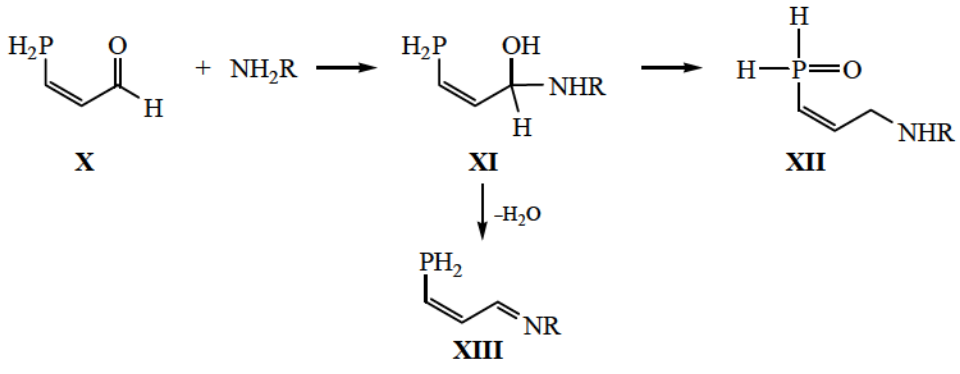
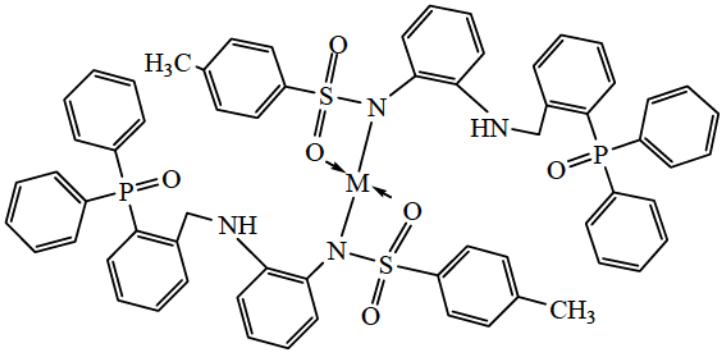


Table 2. Full and relative energies of the compounds **X**-**XIII** (considering the corrections for the zero vibrations energies) according to the DFT calculations data for the gas phase and ethanol[a]

Compound	Gas phase		Ethanol	
	E_{tot}, a.u.	E_{rel}, kcal/mol	E_{tot}, a.u.	E_{rel}, kcal/mol
X + NRH_2	–590.31936	0.0	–590.43611	0.0
XI	–590.31570	2.3	–590.43402	1.3
XII	–590.32481	–3.5	–590.45210	–10.0
XIII + H_2O	–590.30404	9.6	–590.42040	9.9

[a] Total energy of the infinitely separated compounds **X** and NH_2R for R=H was assumed to be zero.

Scheme 5.



XIV

M = Pd, Cd, Ni.

was considered in [31]. Our calculations show that the elimination of water molecule from aminoalcohol **XI** and the formation of Schiff's base **XIII** requires 7.3 kcal/mol in the gas phase. At the same time the conversion of compound **X** to phosphine oxide **XII** proceeds with the energy gain of 5.8 kcal/mol (Table 2).

It may be suggested that the reason of the formation of phosphine oxide is evidently the short distance between the hydroxy and phosphine groups in the aminoalcohol. At the same time the calculations showed that ionic mechanism including heterolysis of C–OH bond in the intermediate of the type **X** leading to the formation of ion pairs required the consumption of more than 129 kcal/mol in the gas phase and in the solution.

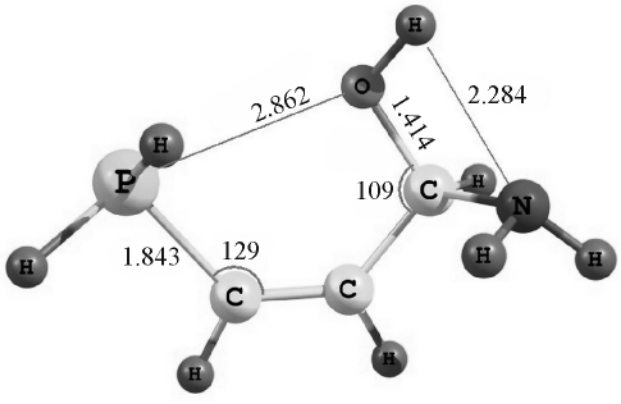


Fig. 3. General view of molecule of compound **XI** according to DFT calculations in toluene. Bond lengths are given in Å, bond angles, in degrees. M = Pd, Cd, Ni.

According to the calculations the equilibrium O–P distance in compound **XI** is 2.862 Å (Fig. 3). Therefore another mechanism of the reaction is the most probable proceeding in the intermolecular associate. Examples of such associates are presented in [31].

The presence of several donor centers and labile hydrogen atoms in the molecule of compound **IV** makes possible the the formation of metal complexes on its basis. The reaction of compound **IV** with nickel(II), palladium(II), and cadmium(II) acetates leads to the formation of complex compound of the composition $[M(HL)_2)]$ where HL is monodeprotonated form of compound **IV**. The presumable structure of these complexes is presented in Scheme 5.

The composition and structure of the obtained complexes was established on the basis of the

elemental analysis data, and the IR and ^{1}H NMR spectra. Magnetochemical measurements showed that nickel(II) complex is diamagnetic what permitted to study it by means of NMR spectroscopy. But due to low solubility of Ni(II) and Pd(II) compounds it was impossible to use this method.

In the ^{1}H NMR spectra of cadmium(II) in DMSO-d_6 as compared to the spectrum of the ligand **IV** the disappearance of NH proton of tosylamine fragment was observed. The multiplicity and chemical shift of the signal of NH proton bound with CH_2 group practically does not alter. It is a broadened triplet at 5.6 ppm. Besides, in the ^{1}H NMR spectrum of cadmium(II) complex the signals of methyl group (2.28 ppm), of methylene group (4.2 ppm), and of aromatic fragments (6.3–7.7 ppm) are observed.

Character of the coordination of ligand **IV** in the obtained metal chelates is confirmed by the absence of the absorption bands one of the NH group in the IR spectra of complexes. The absorption band of another NH group is shifted to the low frequency range. Besides, the absorption band of SO_2 group is also shifted to the low frequency area by 40–50 cm^{-1} showing its coordination by the metal ion. Hence, the obtained results confirm the above-suggested structure of complexes **XIV**.

EXPERIMENTAL

Elemental analysis was carried out on a Perkin-Elmer 240C analyzer. NMR spectra were taken on a Varian Unity (300 MHz) spectrometer at 20°C. IR spectra were registered on a Varian Scimitar 1000 FT-IR spectrophotometer in the range 400–4000 cm^{-1}. Specific magnetic susceptibility of nickel(II) complex was evaluated by the relative Faraday method at 298 K. $Hg[Co(CNS)_4]$ was used as a reference substance for calibration.

***N*-{2-[2-(Diphenylphosphoryl)benzylamino]phenyl}-4-methylbenzenesulfonamide IV**. To a hot solution of 1 mmol of aldehyde **I** in 5 mL of toluene 1 mmol of amine **II** in 5 mL of toluene and the catalytic amount of *p*-toluenesulfonic acid were added. The obtained solution was refluxed for 6 h. After that toluene was distilled off and 5 mL of *n*-heptane was added. The precipitate formed was filtered off and crystallized from 9 : 1 ethyl acetate–methanol mixture. White amorphous substance. Yield 76%, mp 206–207°C. IR spectrum, ν, cm^{-1}: 437, 467, 509, 555, 697, 722, 751, 776, 816, 1115, 1165, 1244, 1277, 1331, 1520, 1606, 3455, 3611. ^{1}H NMR spectrum (DMSO-d_6), δ, ppm (*J*, Hz): 2.42 s (3H, CH_3), 4.38 d (2H, CH_2, ^3J 3.6), 5.79 d (1H, H$^{3'}$, ^3J 7.7), 5.85 br.t (1H, NHCH$_2$, ^3J 3.6), 6.34 d.d (1H, H$^{5'}$, ^3J 7.5, ^3J 7.8), 6.65 d (1H, H$^{6'}$, ^3J 7.8), 6.71 d.d (1H, H$^{4'}$, ^3J 7.5, ^3J 7.7), 7.01 d.d (1H, H$^{3''}$, ^3J 7.6, $^3J_{PH}$ 13.8), 7.23–7.32 m (2H, H$^{4'',6''}$), 7.34 d (2H, H^{3,5}, ^3J 8.0), 7.45 d.d (1H, ^3J 7.5, ^3J 7.6), 7.57–7.74 m (12H, H^{2,6}, Ph), 9.18 br.s (1H, $NHSO_2$). ^{13}C NMR spectrum (DMSO-d_6), δ_C, ppm (J_{PC}, Hz): 21.6 (CH_3), 45.2 d (CH_2, ^3J 8.0), 111.1 (C$^{3'}$), 115.8 (C$^{5'}$), 121.4 (C$^{1'}$), 126.6 d (C$^{4''}$, ^3J 13.2), 127.5 (C^{2,6}), 127.7 d (C$^{6''}$, ^3J 9.8), 127.8 (C$^{4'}$), 128.0 (C$^{6'}$), 129.2 d (C$^{3''',5'''}$, ^3J 11.8), 129.7 (C^{3,5}), 130.4 d (C$^{2''}$, ^1J 100.2), 131.9 d (C$^{2''',6'''}$, ^3J 9.7), 132.5 (C$^{4'''}$), 132.8 d (C$^{1'''}$, ^1J 102.1), 133.0 d (C$^{3''}$, ^2J 12.5), 138.0 (C^1), 143.2 (C^4), 144.1 (C$^{2'}$), 144.9 d (C$^{1''}$, ^2J 7.8). Found, %: C 69.23; H 5.38; N 5.15. $C_{32}H_{29}N_2O_3PS$. Calculated, %: C 69.55: H 5.29; N 5.07.

Complexes of *N*-{2-[2-diphenylphosphoryl)benzylamino]phenyl}-4-methylbenzenesulfonamide with metals *(general procedure)*. To a solution of 0.002 mol of ligand **IV** in 5 mL of methanol a solution of 0.001 mol of the corresponding metal acetate in 3 mL of methanol was added. The obtained solution was boiled until the complete formation of precipitate.

Complex of *N*-{2-[2-diphenylphosphoryl)benzylamino]phenyl}-4-methylbenzenesulfonamide with Ni(II). Grey amorphous powder. Yield 48.2%, mp 320°C. IR spectrum, ν, cm^{-1}: 476, 498, 519, 545, 572, 592, 657, 695, 709, 723, 753, 770, 822, 885, 934, 956, 977, 1061, 1089, 1127, 1144, 1194, 1248, 1290, 1489, 1594, 1711, 3054, 3244, 3401. Found, %: C 66.09; H 4.97; N 4.68; Ni 5.27. $C_{64}H_{56}N_4O_6P_2S_2Ni$. Calculated, %: C 66.16; H 4.86; N 4.82; Ni 5.05.

Complex of *N*-{2-[2-diphenylphosphoryl)benzylamino]phenyl}-4-methylbenzenesulfonamide with Cd(II). Light yellow amorphous powder. Yield 41.5%, mp > 350°C. IR spectrum, ν, cm^{-1}: 454, 494,522, 544, 570, 658, 694, 708, 725, 745, 767, 817, 884, 927, 939, 1021, 1089, 1126, 1191, 1245, 1260, 1290, 1485, 1593, 3285, 3400. Found, %: C 63.31; H 4.58; N 4.47; Cd 9.14. $C_{64}H_{56}N_4O_6P_2S_2Cd$. Calculated, %: C 63.23; H 4.64; N 4.61; Cd 9.25.

Complex of *N*-{2-[2-diphenylphosphoryl)benzylamino]phenyl}-4-methylbenzenesulfonamide with Pd(II). Light yellow amorphous powder. Yield 47.2%, mp > 350°C. IR spectrum, ν, cm^{-1}: 514, 544, 569, 613, 645, 675, 697, 708, 720, 758, 770, 813, 841, 889, 966, 1033, 1059, 1090, 1109, 1145, 1193, 1249, 1272,

1311, 1489, 1569, 1595, 1714, 3052, 3190, 3435. Found, %: C 63.58; H 4.73; N 4.73; Pd 9.07. $C_{64}H_{56}N_4O_6P_2S_2Pd$. Calculated, %: C 63.55; H 4.67; N 4.63; Pd 8.80.

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