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The Synthesis and Structure of Palladium 2,4-dimethyl-8-hydroselenoquinolinate

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Abstract. **The internal complex palladium 2,4-dimethyl-8-hydroselenoquinolinate Pd[$C_9H_4(CH_3)_2NSe]_2$ (I) has been synthesized in the course of study of the complexing activity of 8-hydroselenoquinoline and investigation of the nature of chemical bond metal-selenium in the five-membered metal-containing ring. X-ray diffraction data for I: Monoclinic, space group $P2_1/n$, a = 9.0092(4), b = 16.3290(7), c = 14.1073(6) Å, β = 106.710(2)°, V = 1987.7(2) Å^3, Z = 4, R1=0.0477, wR2=0.1182 for 4499 reflections (diffractometer Bruker-Nonius KappaCCD, λMoK_α).**

The crystal structure of the complex I is formed by neutral asymmetric molecules Pd[$C_9H_4(CH_3)_2NSe]_2$ in which the central atom palladium is connected bidentically (Se,N) with two 2,4-dimethyl-8-hydroselenoquinoline ligands. The structure of palladium coordination polyhedron is *cis*-square (2Se+2N) somewhat tetrahedrally distorted. Dihedral angle between the SePdN / SePdN coordination planes is 20.15(1)°.

The Pd–Se and Pd–N bonds are covalent. The transition of *trans-* (complex Pd($C_9H_6NSe)_2$ (II) to *cis*-coordination (complex I) causes the weakening of the Pd–N bonds (compare 2.162(5) and 2.159(5) Å (I) , 2.065(3) Å (II)).

Keywords: **palladium 2,4-dimethyl-8-hydroselenoquinolinate, palladium coordination compounds, synthesis of 8-hydroselenoquinolinates, X-ray diffraction analysis**

INTRODUCTION

In the course of studies concerning the metal–sulphur bond in the internal complexes of transition and non-transition elements, at the Laboratory of Internal Complexes of INC of RTU a plenty of 8-mercaptoquinoline and its derivatives complexes have been synthesized and structurally investigated earlier [1]. The obtained results have been compared with the structures of the corresponding 8-hydroxyquinolinate.

The synthesis and X-ray structural investigations of the internal complexes of 8-hydroselenoquinoline and its derivatives have been continued in order to elucidate the character of the bonds M-Se(O,S) and their dynamics in the mutually similar five-membered metal-containing cyclic compounds belonging to one and the same VI group. The similar systematic structural investigations of the internal complex compounds are not known in the literature up to now. Therefore, the issue concerning the coordination abilities of the selenium (II) atom as a ligand atom, as well as the experimental determination of the length of the valence bonds M-Se in the internal complexes is a matter of principle. Up to now, we have established the molecular and crystal structure of 8-hydroselenoquinoline complexes with platinum [2], palladium [3], cadmium [2], zinc [4], mercury [5], antimony [6] and bismuth [7] as well as platinum, cadmium, zinc, mercury, antimony and bismuth 2-methyl-8-hydroselenoquinolinates [8–13] and zinc and cadmium 2-phenyl-8-hydroselenoquinolinates [14-15]. In the crystal structures containing the 2-methyl- and 2-phenylsubstituted ligands, the effect of position and nature of the substituent on the molecular structure of the complex has been observed. The changes in the molecular structure, mainly, in the coordination environment of the central atom are different in the complexes of the transition and non-transition metals. The determined structure of palladium 2,4-dimethyl-8-hydroselenol-quinolinates Pd[$C_9H_4(2\text{-}CH_3,4\text{-}CH_3)NSe]_2$ (I) being considered in the present research will be able to exert the effect of the summary action of the two electron–donor substituents in the 8-hydroselenoquinoline ligand on the coordination environment of the complexing palladium atom.

EXPERIMENTAL SECTION

Synthesis

Dissolve 0.1 g (0.00056 mmol) of $PdCl_2$ in 1 ml of half-concentrated hydrochloric acid and add 10ml of water. Dissolve 0.3 g (0.00064 mmol) of 2,2’,4,4’-tetramethyl-8,8’-diquinolyl diselenide in 2 ml of half-concentrated hydrochloric acid, add 1ml of 50% H_3PO_2 and allow to stand for 10 min. Then add 10 ml of ethanol, 1 ml of saturated sodium acetate solution and, finally, add the palladium solution that was prepared earlier. The deposited red deposit filter wash with water and dry in the air. Yield 0.27 g (83 %).

Found, %: C 46.25; H 3.58; N 4.75. $C_{22}H_{20}N_2Se_2Pd$.

Calculated, %: C 45.84; H 3.49; N 4.85.

The single crystals were grown up from the chloroform solution.

X-ray Diffraction Analysis

X-ray diffraction data were collected from a dark red single crystal (imperfect form). The Bruker-Nonius KappaCCD automatic diffractometer was used. The structure was solved by the direct method with a subsequent Fourier synthesis and refined by the least squares matrix analysis using SHELXL package in the full-matrix anisotropic approximation for non-hydrogen atoms, taking into account the coordinates of the hydrogen atoms. Hydrogen atoms were located both from the differential synthesis and from idealized position and refined using a riding model [16, 17]. Calculations were performed using the software [18].

The crystallographic characteristics and the results of the structure refinement are listed in Table 1; the final coordinates and thermal parameters of the basic atoms of structure I – in Table 2; the selected geometric characteristics of complex I – in Table 3 and 4.

TABLE 1

CRYSTALLOGRAPHIC PARAMETERS, EXPERIMENTAL AND STRUCTURE REFINEMENT DETAILS FOR STRUCTURE I

Parameter	Value
Empirical formula	$C_{22}H_{20}N_2Se_2Pd$
Molecular mass	576.72
Temperature, K	293(2)
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell parameters:	
a, Å	9.0092(4)
b, Å	16.3290(7)
c, Å	14.1073(6)
α, deg	90
β, deg	106.710(2)
γ, deg	90
V, Å^3	1987.7(2)
Z	4
$\rho_{calc,}$ g/cm^3	1.927
μ, mm-1	4.605
F(000)	1120
Crystal dimensions, mm	0.17 x 0.13 x 0.12
Crystal colour	Dark red
Data collection	KappaCCD
Scan mode	θ / 2θ
$2\theta_{max.}$, deg	55.0
Radiation type	MoK_α
Wavelength, Å	0.71073
Reflection index range	-11< =h<=11,-19<=k<=21, -18< =l<=18
Absorption correction	None
Reflections collected	8004
Independent reflections, [R(int) = 0.0439]	4499
Refinement method	Full-matrix least-squares calculation on F^2
Parameters refined	244
Final R for I > $2\sigma(I_{obs.})$	R1 = 0.0477, wR2 = 0.1128
R for all reflections	R1 = 0.0914, wR2 = 0.1375
Largest diff. peak and hole, e/Å^3	0.609 and –0.790

TABLE 2

ATOMIC COORDINATES (×10^4, ×10^3 FOR H) AND DISPLACEMENT PARAMETERS (IN Å^2,×10^3) OF COMPLEX I

Atom	x	y	z	U_{eq}
Pd(1)	2235(1)	1607(1)	2855(1)	41(1)
Se(1a)	1988(1)	587(1)	3980(1)	57(1)
Se(1b)	2458(1)	537(1)	1782(1)	61(1)
C(2)	4173(7)	3372(4)	3434(4)	45(1)
N(1a)	2639(6)	2420(3)	4114(3)	38(1)
C(2a)	374(7)	3133(4)	4199(4)	41(1)
C(3a)	3434(8)	3685(4)	4980(5)	49(2)
C(4a)	2756(8)	3489(4)	5723(5)	49(2)
C(5a)	1441(8)	2405(5)	6428(5)	57(2)
C(6a)	949(9)	1633(6)	6409(5)	63(2)
C(7a)	1062(8)	1080(5)	5667(5)	55(2)
C(8a)	1636(8)	1348(4)	4920(5)	48(2)
C(9a)	2100(7)	2165(4)	4890(4)	43(1)
C(10a)	2092(7)	2706(4)	5693(4)	43(1)
C(4)	2818(10)	4071(6)	6540(6)	69(2)
N(1b)	1859(6)	2368(3)	1556(4)	41(1)
C(2b)	1154(7)	3089(4)	1429(4)	43(1)
C(3b)	1090(8)	3592(4)	609(4)	46(2)
C(4b)	1797(8)	3372(4)	-89(5)	48(2)
C(5b)	3151(8)	2246(5)	-731(4)	51(2)
C(6b)	3644(9)	1453(5)	-656(5)	57(2)
C(7b)	3470(8)	942(5)	88(5)	58(2)
C(8b)	2860(7)	1243(4)	821(4)	44(1)
C(9b)	2417(7)	2075(4)	799(4)	41(1)
C(10b)	2472(7)	2576(4)	-18(4)	45(2)
C(2')	341(7)	3379(4)	2165(4)	46(1)
C(4')	1778(9)	3923(5)	-939(6)	65(2)
H(2a)	4041(7)	2944(4)	2950(4)	68
H(2b)	5257(7)	3454(4)	3751(4)	68
H(2c)	3727(7)	3870(4)	3115(4)	68
H(3a)	3932(8)	4186(4)	4999(5)	58
H(5a)	1356(8)	2752(5)	6932(5)	69
H(6a)	520(9)	1456(6)	6899(5)	75
H(7a)	751(8)	538(5)	5683(5)	66
H(4a)	2297(10)	3838(6)	6981(6)	104
H(4b)	2318(10)	4574(6)	6272(6)	104
H(4c)	3880(10)	4179(6)	6896(6)	104
H(3b)	554(8)	4085(4)	541(4)	55
H(5b)	3258(8)	2572(5)	-1248(4)	61
H(6b)	4110(9)	1249(5)	-1116(5)	68
H(7b)	3762(8)	395(5)	99(5)	70
H(2'1)	475(7)	2981(4)	2683(4)	69
H(2'2)	-744(7)	3447(4)	1837(4)	69
H(2'3)	774(7)	3892(4)	2442(4)	69
H(4'1)	2330(9)	3667(5)	-1349(6)	97
H(4’2)	2267(9)	4433(5)	-692(6)	97
H(4'3)	726(9)	4022(5)	-1321(6)	97

RESULTS AND DISCUSSION

The crystal structure of complex I consists of the neutral asymmetric molecules $Pd[C_9H_4(2\text{-}CH_3,4\text{-}CH_3)NSe]_2$. The common view of the molecule with the assignment of atoms is shown in Fig. 1.

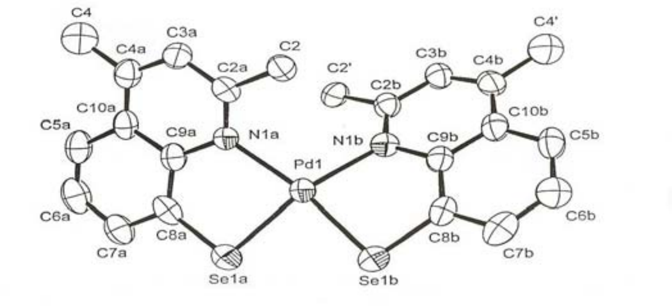

Fig. 1. Molecular structure of $Pd[C_9H_4(CH_3)_2NSe]_2$

The palladium atoms occupy the common places in the elementary cell, the atoms of selenium and nitrogen are bidentatically coordinated by the two non-identical ligands of 2,4-dimethyl-8-hydroselenoquinoline and are included in two metal-containing rings. The bonds Pd-Se ($l_{aver.}$=2.357Å) are nearly equal (Table 3).

TABLE 3

SELECTED BOND LENGTH OF COMPLEX I

Bond	l, Å	Bond	l, Å
Pd(1)-N(1b)	2.159(5)	C(7a)-C(8a)	1.372(9)
Pd(1)-N(1a)	2.162(5)	C(8a)-C(9a)	1.403(10)
Pd(1)-Se(1a)	2.3552(8)	C(9a)-C(10a)	1.438(9)
Pd(1)-Se(1b)	2.3587(9)	N(1b)-C(2b)	1.325(8)
Se(1a)-C(8a)	1.909(7)	N(1b)-C(9b)	1.390(8)
Se(1b)-C(8b)	1.893(7)	C(2b)-C(3b)	1.405(9)
C(2)-C(2a)	1.510(8)	C(2b)-C(2')	1.508(8)
N(1a)-C(2a)	1.328(8)	C(3b)-C(4b)	1.366(9)
N(1a)-C(9a)	1.383(7)	C(4b)-C(10b)	1.427(10)
C(2a)-C(3a)	1.412(9)	C(4b)-C(4')	1.495(10)
C(3a)-C(4a)	1.393(9)	C(5b)-C(6b)	1.364(10)
C(4a)-C(10a)	1.408(10)	C(5b)-C(10b)	1.424(9)
C(4a)-C(4)	1.482(10)	C(6b)-C(7b)	1.384(11)
C(5a)-C(6a)	1.333(11)	C(7b)-C(8b)	1.392(9)
C(5a)-C(10a)	1.418(9)	C(8b)-C(9b)	1.414(9)
C(6a)-C(7a)	1.409(11)	C(9b)-C(10b)	1.426(9)

They possess the expressed covalent nature, as their lengths are less than the sum of the covalent radii of the corresponding atoms (R_{Pd}+R_{Se}=2,534 Å [19]). The covalent nature of the Pd-Se bonds is expressed stronger than in the complex $Pd(C_9H_6NSe)_2$ (II), in which the bond lengths in the centrosymmetric *trans*-square coordination of palladium constitute 2.404(4) Å. The transfer from the planar *trans*-(complex II with non-substituted ligands) to *cis*-square coordination (complex I) is accompanied by the decrease in covalence and in elongation of the Pd-N bond from 2.065 Å (complex II) to $l_{aver.}$ = 2.161 Å (Table 4) in complex I (the sum of covalent radii R_{Pd} + R_N = 2.102Å [19]). This probably is due to the influence of the 4-CH_3 groups. It is necessary to emphasize that in platinum 2-methyl-8-hydroseleno-quinolinate, in which the coordination polyhedron of the platinum atom is a *trans*-square (2Se + 2N) with the Pt-N, bond length and the angle NPtN are not changed in contrast to $Pt(C_9H_6NSe)_2$ [2].

TABLE 4

SELECTED BOND ANGLES OF COMPLEX I

Angle	ω, deg	Angle	ω, deg
N(1b)Pd(1)N(1a)	107.0(2)	C(8a)C(9a)C(10a)	119.4(6)
N(1b)Pd(1)Se(1a)	163.1(1)	C(4a)C(10a)C(5a)	123.6(6)
N(1a)Pd(1)Se(1a)	84.65(13)	C(4a)C(10a)C(9a)	119.0(6)
N(1b)Pd(1)Se(1b)	84.45(14)	C(5a)C(10a)C(9a)	117.4(7)
N(1a)Pd(1)Se(1b)	163.1(1)	C(2b)N(1b)C(9b)	117.9(5)
Se(1a)Pd(1)Se(1b)	87.14(3)	C(2b)N(1b)Pd(1)	125.3(4)
C(8a)Se(1a)Pd(1)	94.3(2)	C(9b)N(1b)Pd(1)	116.8(4)
C(8b)Se(1b)Pd(1)	94.4(2)	N(1b)C(2b)C(3b)	122.3(6)
C(2a)N(1a)C(9a)	118.2(5)	N(1b)C(2b)C(2')	119.6(5)
C(2a)N(1a)Pd(1)	125.1(4)	C(3b)C(2b)C(2')	118.0(6)
C(9a)N(1a)Pd(1)	116.8(4)	C(4b)C(3b)C(2b)	121.5(6)
N(1a)C(2a)C(3a)	122.4(6)	C(3b)C(4b)C(10b)	117.8(6)
N(1a)C(2a)C(2)	119.3(6)	C(3b)C(4b)C(4')	121.4(7)
C(3a)C(2a)C(2)	118.3(6)	C(10b)C(4b)C(4')	120.7(6)
C(4A)C(3A)C(2a)	120.9(6)	C(6b)C(5b)C(10b)	120.0(7)
C(3a)C(4a)C(10a)	117.3(6)	C(5b)C(6b)C(7b)	121.7(7)
C(3a)C(4a)C(4)	120.7(7)	C(6b)C(7b)C(8b)	120.4(7)
C(10a)C(4a)C(4)	121.8(6)	C(7b)C(8b)C(9b)	119.5(6)
C(6a)C(5a)C(10a)	121.2(7)	C(7b)C(8b)Se(1b)	121.0(6)
C(5a)C(6a)C(7a)	121.7(7)	C(9b)C(8b)Se(1b)	119.4(4)
C(8a)C(7a)C(6a)	119.4(7)	N(1b)C(9b)C(8b)	118.5(5)
C(7a)C(8a)C(9a)	120.5(7)	N(1b)C(9b)C(10b)	121.9(6)
C(7a)C(8a)Se(1a)	120.1(6)	C(8b)C(9b)C(10b)	119.6(6)
C(9a)C(8a)Se(1a)	119.1(5)	C(5b)C(10b)C(9b)	118.4(7)
N(1a)C(9a)C(8a)	119.1(6)	C(5b)C(10b)C(4b)	123.8(6)
N(1a)C(9a)C(10a)	121.4(6)	C(9b)C(10b)C(4b)	117.8(6)

The chelate angles SePdN in complex I (Table 4) are equal within the limits of the error ($\omega_{aver.}$ = 84.55^o). The coordination polyhedron of the palladium atom in complex I is a slightly tetrahedrally distorted *cis*-square (2Se+2N). The degree of distortion of the planar environment of the palladium atom is characterized by the values of the diagonal angles SePdN ($\omega_{aver.}$=163.1^o) (Table 4) and by the dihedral angle between the coordination planes SePdN amounting to 20.15(1)^o.

The values of deviations of the palladium, selenium and nitrogen atoms from the mean square show that the mentioned atoms of palladium, selenium are located approximately in the same plane. The nitrogen and carbon atoms of the CH_3 groups are remote from this plane and are located in the opposite sides. The interligand repulsion of the selenium atom and CH_3 group in the *cis*-square coordination of the palladium atom is decreased due to the essential deviations of the palladium, selenium, carbon (methyl) atoms from the planes of the corresponding quinoline nuclei. The distance Pd…C(2) equals 3.344(5) and 3.357(5) Å.

The Se-C bond (Table 4) ($l_{aver.}$=1.901 Å) also possesses the covalent nature (the sum of the corresponding covalent radii $R_{Se} + R_C$ = 1.933 Å) and is near to the value 1.893 Å given in [20] for the Se(II)-Csp^2 fragment. The valence angles PdSeC ($\omega_{aver.}$=94.35°) (Table 4) give the evidence on the octahedral disposition of the electrons of the external electron layer of the selenium atom and on the additional strengthening of the Pd-Se bond due to the direct donor–acceptor π-bond [21].

The steric hindrance due to the presence of the 2-CH_3 group in the ligands and the tendency to preserve the approximate planarity of the coordination knot (Pd+2Se+2N) at the formation of the complex is accompanied by the bend of the five-membered metal-containing rings –Pd-Se-C(8)-C(9)-N- along the line Se…N. The dihedral angles of the bending of the metal-containing rings equal 22.56 and 23.44°, i.e., one of the greatest bending occurrences in the metal-containing rings, consequently, the five-membered metal-containing rings –Pd-Se-C(8)-C(9)-N- in complex I possess the "sloped" configuration.

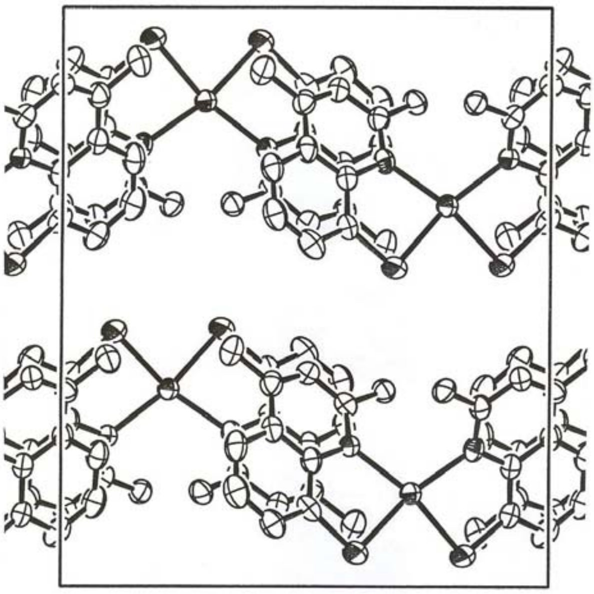

Fig. 2. The packing of complex I in the unit cell, projected onto the (001) plane

The dihedral angle between the planes of the quinoline nuclei is increased up to 38.71° due to the bending of the metal containing rings. The spatial disposition of the ligands in the molecule of palladium 2-methyl-8-mercaptoquinolinate is shown in Fig. 2. The quinoline rings are planar in the both ligands within the limits of error 3σ. The structure of the quinoline rings is usual: the bonds of the type N(1)-C(2) ($l_{aver.}$ =1.327 Å) are essentially shorter than the bonds of the type N(1)-C(9) ($l_{aver.}$ =1.387 Å) and exert the trend to double bonding (the length of the sesquibond Caryl-N equals 1.333-1.345 Å [20]. The alternating bonds C(3)-C(4), C(5)-C(6) C(7)-C(8) (Table 4) are shortened. The central bond of type C(9)-C(10) ($l_{aver.}$ =1.418 Å) occurs to be the most lengthened one. The angles CCC differ from 120° insignificantly (± 2.5). The value of the angle C(2)N(1)C(9) ($\omega_{aver.}$=118.1°) confirms the participation of the nitrogen atom in the donor–acceptor bond Pd-N.

Complex I is geometrically packed in the crystal structure in layers parallel to the xy plane. In this plane, there are the palladium atoms, and between them the layers of the parallel ligands occur (Fig. 2). The distance between the centrosymmetrically bonded planes of the quinoline rings is 3.733 Å.

Complex I has no isostructural analogue in the group of studied 8-mercaptoquinolinate.

CONCLUSIONS

Using the X-ray structural analysis method, the structure of complex I has been elucidated. Our studies have demonstrated that the introduction of the 2-CH_3 and 4-CH_3 groups in the 8-hydroselenoquinoline ligand causes the changes of both the molecular and crystal structure of the complex.

In complex I, if compared with complex II, the disproportion of the Pd-Se and Pd-N bond lengths occurs. The type of the coordination polyhedron of the central palladium atom and the spatial dislocation of the complex are also changed.

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Elga Siliņa, Jānis Ašaks, Sergejs Beļakovs, Andrejs Tokmakovs, Daina Zaruma. Pallādija 2,4-dimetil-8-selenolhinolināta sintēze un uzbūve

8-selenolhinolīna un tā atvasinājumu iekšēji komplekso savienojumu veidošanās aktivitātes un ķīmiskās saites M-Se dabas pētījumu jomā sintezēts un iegūts monokristālu veidā pallādija 2,4-dimetil-8-selenolhinolināts Pd$[C_9H_4(CH_3)_2]SeN]_2$ (I).

Ar rentgenstruktūranalīzes metodi (automātiskais difraktometrs Bruker-Nonius KappaCCD, λMoK_{α}, 4499 neatkarīgie refleksi ar $I > 2\sigma(I_{eksp.})$, R1 = 0.0477, wR2 = 0.1182) noteikta savienojuma I molekulārā un kristāliskā struktūra: monoklīnā singonija, telp.gr. $P2_1/n$, $a = 9.0092(4)$, $b = 16.3290(7)$, $c = 14.1073(6)$ Å, $\beta = 106.710(2)^{o}$, $V = 1987.7(2)$ Å^3, Z = 4, $\rho_{teorēt.} = 1.927$ g / cm^3.

Savienojuma I kristālisko struktūru veido neitrāli asimetriski kompleksi Pd$[C_9H_4(CH_3)_2]SeN]_2$, kuros divi 2,4-dimetil-8-selenolhinolīna ligandi bidentāti (Se, N) koordinē pallādija atomu, veidojot kļūdas robežās vienādus SePdN koordinācijas leņķus (84.5^{o}). Pallādija atoma koordinācijas poliedrs – tetraedriski izkropļots *cis*-kvadrāts (2Se+2N), ko raksturo vienādi (163.1^{o}) diagonālie leņķi SePdN un divplakņu leņķis starp koordinācijas plaknēm SePdN / SePdN 20.15(1)^{o}. Saites Pd-Se (vid.2.357 Å) un Pd-N (vid.2.161 Å) kovalentas. Pieclocekļu metālciklu –Pd-Se-C(8)-C(9)-N- plāksnes ir stipri deformētas, to lauzuma divplakņu leņķi pa līniju Se...N ir attiecīgi 22.56 un 23.44^{o} .

Salīdzinot kompleksu Pd$[C_9H_5(CH_3)_2SeN]_2$ (I) un Pd$(C_9H_6SeN)_2$ (II) uzbūvi, kompleksa I veidošanās saistās ar pallādija atoma koordinācijas apkārtnes (2Se+2N) būtisku izmaiņu no plakanas centrsimetriskas *trans*- (II) uz asimetrisku tetraedriski izkropļotu *cis*- -kvadrātisku (I), kā arī ar saišu Pd-Se pastiprināšanos un saišu Pd-N pavājināšanos.

Элга Силинь, Янис Ашакс, Сергей Беляков, Андрей Токмаков, Дайна Зарума. Синтез и строение 2,4-диметил-8-селенолхинолината палладия

В рамках исследования комплексообразующей активности 8-селенолхинолина и его производных и природы связи Pd-Se синтезирован и получены монокристаллы 2,4-диметил-8-селенолхинолината палладия Pd$[C_9H_4(CH_3)_2]SeN]_2$ (I).

Методом рентгеноструктурного анализа (автоматический диффрактометр Bruker-Nonius KappaCCD, λMoK_{α}, R1=0.0477, wR2=0.1182 для 4499 независимых отражений с $I > 2\sigma(I_{eksp.})$) определена молекулярная и кристаллическая структура соединения I: моноклинная сингония, пр. гр. $P2_1/n$, $a = 9.0092(4)$, $b = 16.3290(7)$, $c = 14.1073(6)$ Å, $\beta = 106.710(2)^{o}$, $V = 1987.7(2)$ Å^3, Z = 4, $\rho_{теорет.} = 1.927$ g / cm^3.

Кристаллическая структура I состоит из нейтральных асимметричных комплексов Pd$[C_9H_4(CH_3)_2]SeN]_2$, где два лиганда 2,4-диметил-8-селенолхинолина бидентатно (Se,N) координируют атом палладия. Образуются одинаковые координационные углы SePdN, равные

84.5^o. Координационный полиэдр атома палладия- тетраэдрически искаженный *цис*-квадрат (2Se+2N), которого характеризуют одинаковые диагональные углы (163.1^o) и двугранный угол между координационными плоскостями SePdN / SePdN, равный 20.15(1)^o. Связи Pd-Se (средн. 2.357 Å) un Pd-N (средн. 2.161 Å) ковалентные. Плоскости пятичленных металлоциклов –Pd-Se-C(8)-C(9)-N- имеют большие перегибы по линии Se...N, равные 22.56 и 23.44^o соответственно.

Установлено, что образование комплекса I по сравнению с комплексом Pd(C_9H_6SeN)$_2$ (II) сопровождается существенными изменениями координационного окружения (2Se+2N) атома палладия от центросимметричного *транс*- квадрата в комплексе II до асимметричного тетраэдрически искаженного *цис*- квадрата в комплексе I, происходит также усиление связей Pd-Se и ослабление связей Pd-N.