ISSN 1070-3284, Russian Journal of Coordination Chemistry, 2023, Vol. 49, No. 12, pp. 841–855. © Pleiades Publishing, Ltd., 2023.

3-(2-Methylphenyl)-2-selenoxo-2,3-dihydroquinazolin-4(1*H*)-one and Its Complex with Cd(II): Synthesis and Molecular and Crystal Structures

R. K. Askerov[a, *], E. V. Chipinskii[b], A. S. Peregudov[c], V. K. Osmanov[b], Zh. V. Matsulevich[b], G. N. Borisova[b], V. N. Khrustalev[d, e], O. N. Smirnova[f], A. M. Magerramov[a], and A. V. Borisov[b]

[a] *Baku State University, Baku, Azerbaijan*
[b] *Nizhni Novgorod State Technical University, Nizhni Novgorod, Russia*
[c] *Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russia*
[d] *Peoples' Friendship University of Russia, Moscow, Russia*
[e] *Zelinskii Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia*
[f] *National Research State University, Nizhni Novgorod, Russia*
**e-mail: rizvankam@bk.ru*

Received May 28, 2023; revised July 11, 2023; accepted July 21, 2023

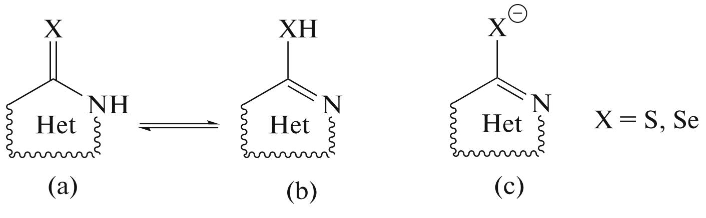
Abstract—The reaction of methyl anthranilate with 2-methylphenyl-*iso*-selenocyanate in boiling absolute ethanol affords a new compound: 3-(2-methylphenyl)-2-selenoxo-2,3-dihydroquinazolin-4(1*H*)-one (HL). Free ligand HL, which is selone, is preliminarily transformed into the corresponding sodium selenolate [$C_{15}H_{11}N_2OSeNa$] (**I**), which is then used without isolation in the reaction with cadmium chloride. This reaction leads to the formation of complex [$Cd_2(\mu\text{-}L)_2(L)_2(C_2H_5OH)_2$] (**II**). The structures of the compounds are determined by X-ray diffraction (XRD) (CIF files CCDC nos. 2142342 (HL) and 2246014 (**II**)) and NMR spectroscopy (^{1}H, ^{13}C, ^{15}N, and ^{77}Se). In the crystal, the molecules of HL form one-dimensional chains due to H...O and H...Se contacts and alternate in the syndiotactic order. Compound **II** is the centrosymmetric binuclear complex [$C_{64}H_{56}Cd_2N_8O_6Se_4$]. The cadmium atoms in complex **II** are hexacoordinated by two chelate anionic ligands L^-. According to the NMR data, in a DMSO-d_6 solution free ligand HL has the selone structure, whereas in cadmium complex **II** this ligand exists in the selenolate form, which is consistent with the XRD data on the crystal structures of the compounds.

Keywords: 3-(2-methylphenyl)-2-selenoxo-2,3-dihydroquinazolin-4(1*H*)-one, crystal structure, binuclear cadmium(II) complex, ^{1}H, ^{13}C, ^{15}N, and ^{77}Se NMR spectroscopy

DOI: 10.1134/S1070328423601061

INTRODUCTION

Heterocyclic thiones and selenols bearing the nitrogen atom near the C–SH or C–SeH group can exist due to tautomerism in both the thione or selone (a) and thiol or selenol form (b) [1–10] (Scheme 1). The thione or selone form (a) is considered to be more stable for heterocyclic compounds [1]. In addition, they can form thiolate or selenolate anions (c) in the presence of bases. Having several electron-donating centers, these forms of the reagents can be used as polydentate ligands in complex formation with diverse metals in order to synthesize various complexes and supramolecular structures.



Scheme 1. Tautomeric forms of thiones and selones (a, b, c).

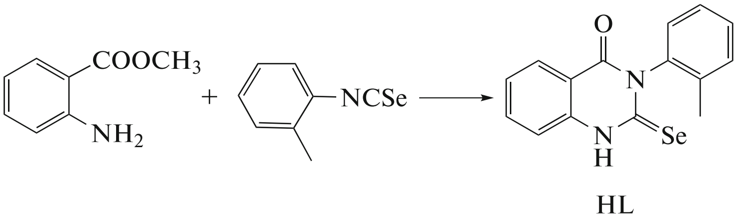
The reactions of heterocyclic thiones and thiolates with metal salts leading to the formation of various coordination compounds were described in many works [4–6, 9, 11–21]. For instance, we synthesized [4–6, 9, 20, 21] the cadmium complexes in which *N*-phenyl-1,4-dihydro-5*H*-tetrazole-5-thiones substituted in the benzene ring and related sodium thiolates acted as ligands. Unlike thiones and thiolates, heterocyclic selones, selenols, and metal selenolates are used, to a significantly lower extent, for the synthesis of coordination compounds. For example, a number of works is devoted to the synthesis of the metal (Hg, Pd, Ru, Au, Zn, Cu, and Cd) complexes with different imidazole- and benzimidazoleselones [22–25]. The synthesis of the 2-selenopyridin-1-oxide complexes with alkali metals, cadmium, and nickel was described [26–28].

The number of examples of using heterocyclic selones as ligands is lower because of a low stability of many Se-containing compounds [29] and the absence of available reagent-precursors.

Isoselenocyanates are known as universal building blocks for the preparation of diverse selenium-containing heterocyclic organoselenium compounds [8, 10, 30, 31].

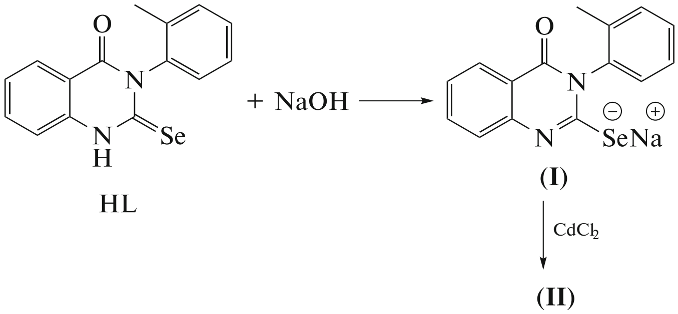
We have previously described a convenient synthesis of 2-selenoxo-1,2,3,4-tetrahydro-4-quinazolinones by the reactions of methyl anthranilate with aryl isoselenocyanates [10].

In this work continuing our previous studies [4–6, 9, 20, 21, 28], we studied the structure of the reaction product of cadmium chloride with sodium salt of ligand 3-(2-methylphenyl)-2-selenoxo-2,3-dihydroquinazolin-4(1*H*)-one (HL): [$C_{15}H_{11}N_2OSeNa$] (**I**). Ligand HL was synthesized by the reaction of methyl anthranilate with 2-methylphenylisoselenocyanate in boiling absolute ethanol [10] (Scheme 2).



Scheme 2.

Ligand HL was treated with sodium hydroxide to transform into the corresponding selenolate [$C_{15}H_{11}N_2OSeNa$] (**I**), which interacted with cadmium chloride without isolation affording complex [$Cd_2(\mu\text{-}L)_2(L)_2(C_2H_5OH)_2$] (**II**) (Scheme 3).



Scheme 3.

The structures of synthesized compounds HL and **II** were determined by XRD and NMR spectroscopy.

EXPERIMENTAL

Methyl anthranilate (Acros Organics, Belgium) was used as received. The starting reagents NaOH and $CdCl_2$ were no less than reagent grade. 2-Methylphenylisoselenocyanate was synthesized using a described procedure [32] and additionally purified by recrystallization in hexane at –20°C.

Synthesis of HL. 2-Methylphenylisoselenocyanate (1.961 g, 10 mmol) in absolute ethanol (20 mL) was added to a solution of methyl anthranilate (1.512 g, 10 mmol) in absolute ethanol (100 mL), and the mixture was refluxed for 6 h and then cooled to 0°C. The formed precipitate was filtered off, washed with ethanol (2 × 25 mL), and dried at 40°C. The yield of HL was 1.702 g (54%). Light brown crystals suitable for

XRD were recrystallized from ethanol. T_m = 210–211°C.

IR (ν, cm^{-1}): 3241, 1702, 1619, 1520, 1410, 1262, 1189, 753. HR-ESI MS: found, *m/z*: 317.0184; calculated for $[C_{15}H_{12}N_2OSe + H]^+$: 317.0188.

For $C_{15}H_{12}N_2OSe$

Anal. calcd., %	C, 57.15	H, 3.84	N, 8.89
Found, %	C, 57.35	H, 3.72	N, 8.78

Synthesis of complex II. A solution of sodium hydroxide (0.08 g, 2 mmol) in H_2O (2 mL) was added with stirring to a solution of selone HL (0.631 g, 2 mmol) in 95% ethanol (100 mL) at 50°C, and then a solution of $CdCl_2$ (0.183 g, 1 mmol) in H_2O (8 mL) was added. The reaction mixture was stored at 20°C for 24 h and then held at 0°C for 48 h. The formed precipitate was filtered off, washed with 95% ethanol cooled to 0°C (25 mL) and diethyl ether (2 × 25 mL), and dried at 60°C. The yield of white crystals was 0.293 g. The white crystals had T_m = 255–257°C (with decomp.). The crystals for XRD were used without additional recrystallization.

IR (ν, cm^{-1}): 3428, 1670, 1611, 1506, 1472, 1445, 1305, 1266, 1202, 959, 754.

The melting (decomposition) points were determined in evacuated sealed capillaries and are presented without corrections. Elemental analyses of the compounds were conducted on a Vario EL cube instrument. IR spectra were recorded on a Shimadzu IR Prestige-21 instrument in a range of 4000–400 cm^{-1} (KBr pellets, substance to KBr ratio 1 : 200). The NMR spectra for solutions of HL and **II** in DMSO-d$_6$ were recorded on a Bruker Avance^{TM}500 NMR spectrometer equipped with a cryosensor. The working frequency for ^{1}H, ^{13}C, ^{15}N, and ^{77}Se was 500.13, 125.77, 50.67, and 95.4 MHz, respectively. Signal assignment in the NMR spectra was performed using 2D correlation experiments: COSY(^{1}H,^{1}H), HSQC(^{1}H,^{13}C), HMBC(^{1}H,^{13}C), and HMBC(^{1}H,^{15}N). The standard pulse sequences from the Bruker library were used. The chemical shifts were determined as follows: in the ^{1}H NMR spectra, using the residual signal of DMSO-d$_6$ (2.50 ppm); in the ^{13}C NMR spectra, relative to the signal of DMSO-d$_6$ (40.00 ppm); in the ^{15}N NMR spectra, relative to liquid ammonia; and in the ^{77}Se NMR spectra, relative to Me_2Se. The HR-ESI mass spectrum of compound HL was detected on a Bruker micrOTOF II instrument. The measurements were carried out on positive ions (the voltage on the capillary was 4500 V). The scan range was *m/z* 50–3000, the internal calibration was used (Agilent Tuning Mix, Agilent), and *m/z* values for the most intense peak of the isotope cluster are presented. The substance as a solution in acetonitrile was injected with a syringe, and the flow rate was 5 μL/min. Nitrogen served as the spraying gas (4 L/min), and the temperature of the interface was 180°C.

XRD of compounds HL and **II** was carried out on a Rigaku Synergy S four-circle diffractometer equipped with a HyPix600HE two-dimensional detector (CuK_α radiation, λ = 1.54184 Å, *T* = 100 K, kappa geometry, ω scan mode). Experimental data were processed and an X-ray absorption correction was applied using the CrysAlisPro software [33]. The structures were solved by a direct method and refined by full-matrix least squares for F^2_{hkl} in the anisotropic approximation for non-hydrogen atoms. The hydrogen atom of the amino group in HL was revealed objectively in the difference Fourier syntheses and refined isotropically with the fixed shift parameters ($U_{iso}(H) = 1.2U_{eq}(N)$). The positions of other hydrogen atoms in HL and **II** were calculated geometrically and included into refinement with fixed positional parameters (riding model) and isotropic shift parameters ($1.5U_{iso}(C)$ for methyl groups and $U_{iso}(H) = 1.2U_{iso}(C)$ for all other groups). All calculations were performed using the SHELXTL software [34]. The crystallographic data and experimental XRD parameters are given in Table 1.

The structures were deposited with the Cambridge Crystallographic Data Centre (CIF files CCDC nos. 2142342 (HL**)** and 2246014 (**II**)).

RESULTS AND DISCUSSION

The thione or selone form is known to be more stable for heterocyclic thiols and selenols. The ^{1}H, ^{13}C, and ^{77}Se NMR spectra of compound HL detected in DMSO-d$_6$ contain only one set of indicatory signals, including somewhat broadened singlet at 14.38 ppm corresponding to the signal of the NH group of selone with an integral intensity of 1. The structure of the compound was confirmed by the XRD data.

Compound HL crystallizes in the monoclinic crystal system (space group $P2_1/c$) with two crystallographically independent molecules A and B. Molecules A and B are conformers relative to the mutual arrangement of two planar fragments (central bicycle and *o*-methylphenyl substituent) and are similar in structure (Fig. 1).

Compound HL consists of an almost planar dihydroquinazoline fragment (N(1)C(2)N(3)/C(4)–C(8)) (average deviation of the atoms from the plane is 0.0375 Å). A molecule of HL convolves around the N(3)–C(9) bond with a dihedral angle of 79.35°(7) for molecule A and 103.36(7)° for molecule B between the bicyclic dihydroquinazoline system (N(1)C(2)N(3)/ C(4)–C(8)) and substituted phenyl ring (C(9)–C(14)). The C(2)=Se(1) and C(4)=O(1) bond lengths are 1.824(2) and 1.225(3) Å in molecule A and 1.828(2) and 1.217(3) Å in molecule B and nearly coincide with the lengths of the corre-

Table 1. Selected crystallographic data and refinement parameters for the structures of compounds HL and **II**

Parameters	Value	
	HL	**II**
Empirical formula	$C_{15}H_{12}N_2OSe$	$C_{64}H_{56}N_8O_6Se_4Cd_2$
FW	315.23	1573.83
Temperature, K	100(2)	100(2)
Crystal sizes, mm	0.17 × 0.04 × 0.03	0.26 × 0.22 × 0.15
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	$P\bar{1}$
a, Å	18.80286(19)	10.7130(4)
b, Å	13.36157(11)	12.6510(6)
c, Å	10.51280(9)	13.0832(5)
α, deg	90	67.157(4)
β, deg	96.8825(9)	67.786(4)
γ, deg	90	80.560(3)
V, Å^3	2622.17(4)	1512.51(12)
Z	8	1
ρ_{calc}, g/cm^3	1.597	1.728
μ, mm^{-1}	3.816	8.859
F(000)	1264	776
Data collection range over θ, deg	79.641	78
Measured reflections	30554	27907
Independent reflections	5654	6195
Number of refined parameters	351	346
R_1 ($I > 2\sigma(I)$)	0.0336	0.0861
wR_2 (all data)	0.0887	0.2011
GOOF	1.039	1.063
T_{min}; T_{max}	0.555; 0.808	0.236; 1.000
Residual electron density ($\Delta\rho_{min}/\Delta\rho_{max}$), e Å^{-3}	–0.859/1.089	–2.842/2.922

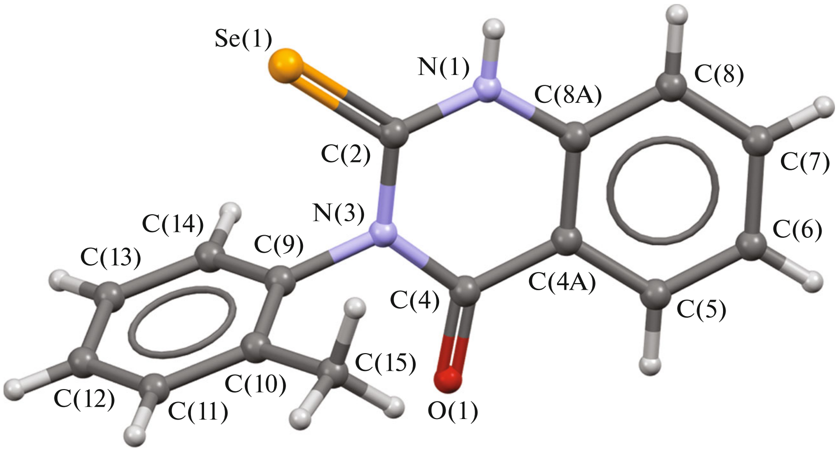


Fig. 1. Molecular structure of compound HL.

sponding double bonds in other 2-selenoxo-1,2,3,4-tetrahydro-4-quinazolines described earlier [10].

In the crystal of compound HL, two crystallographically independent molecules A and B form one-dimensional chains along the *b* axis via hydrogen bonds H(16)...O(2A) (2.45 Å), H(1E)...O(1F) (2.04 Å), and H(5F)...Se(1E) (3.015(3) Å), respectively (Fig. 2a). The molecules in the chains alternate in the syndiotactic order. Intermolecular contacts Se(2A)...H(11G) (2.84 Å) are observed between the chains, and they are substantially shorter than the sum of van der Waals radii of Se and H atoms (3.15 Å) [35].

The packing motif of the fir parquet (raking) type perpendicular to the direction of one-dimensional chains is observed in the crystal of HL (Fig. 2b). The chains of molecules A and B are packed as parallel rows along the *c* axis. The planes of the molecular chains between the adjacent rows are oriented at an angle of 80.6°. Note that the heterocyclic fragments of molecules A in the chains are arranged nearly in one plane, whereas analogous heterocycles of molecules B are shifted from one another at a distance of ~1 Å.

The molecular structure of complex $[Cd_2(\mu\text{-}L)_2(L)_2(C_2H_5OH)_2]$ (**II**) is shown in Fig. 3. Compound **II** is a centrosymmetric binuclear complex with a Cd...Cd intramolecular distance between the atoms of 4.0083(7) Å. In complex **II**, the cadmium atoms are coordinated by two anionic ligands L^- performing different functions. One of the ligands is (N, Se)-chelating terminal, whereas the second ligand is (N, Se)-chelating μ^2-bridging through the selenium atom. The coordination sphere of the metal builds up to an octahedron by the oxygen atom of the terminal ethanol molecule. Thus, the metal ion has the distorted $[Se_3N_2O]$ octahedral environment with small bond angles in the four-membered chelate rings responsible for the distortion of the ideal geometry. The Se(1,1A,2) and N(16) atoms lie in the octahedron base, the N(1) and O(3) atoms occupy the axial positions, and the N(1)Cd(1)O(3) angle is 148.6(3)°. The sum of the bond angles between the equatorial substituents is 359.89°. The dihedral angle between the chelating planar dihydroquinazoline fragments L^- at the Cd (II) atoms is 65.34°. The Cd–Se(2,1,1A) distances range from 2.708(1) to 2.892(1) Å at an average distance of 2.803(3) Å. The Cd–N(1,16) and Cd–O(3) bond lengths are 2.375(7), 2.441(6), and 2.335(6) Å, respectively. The turning angle of the phenyl fragments to the plane of the dihydroquinazoline cycles in complex **II** is 83.5(3)° and 101.0(2)°, respectively.

Unlike free ligand HL, which is selone, coordinated ligand L^- in complex **II** exists in the selenolate form. The C(2)–Se(1) and C(17)–Se(2) distances of chelating ligands L^- in complex **II** are 1.910(8) and 1.899(9) Å, which corresponds to the ordinary character of bond [35].

In the crystals, the molecules of complex **II** form unidimensional molecular chains along the crystallographic *a* axis via the H(3)...O(1B) hydrogen bonds (1.884(6) Å) (Fig. 4). The parallel packing of the dihydroquinazoline fragments of the chains propagating along the *b*0*c* diagonal is observed between the parallel chains along the *a* axis. The shortest C...C distances are observed between the carbon atoms C(19A)...C(21F) (3.36(1) Å) indicating π...π-stacking interactions. The distance between the centers of the planar fragments is 3.351(7) Å, which is within the geometric criteria for existence of the indicated π...π-stacking interactions [36].

The structures of synthesized compounds HL and **II** were studied by NMR spectroscopy. The NMR spectral data for ligand HL at 25°C and complex **II** at 70°C are given in Table 2.

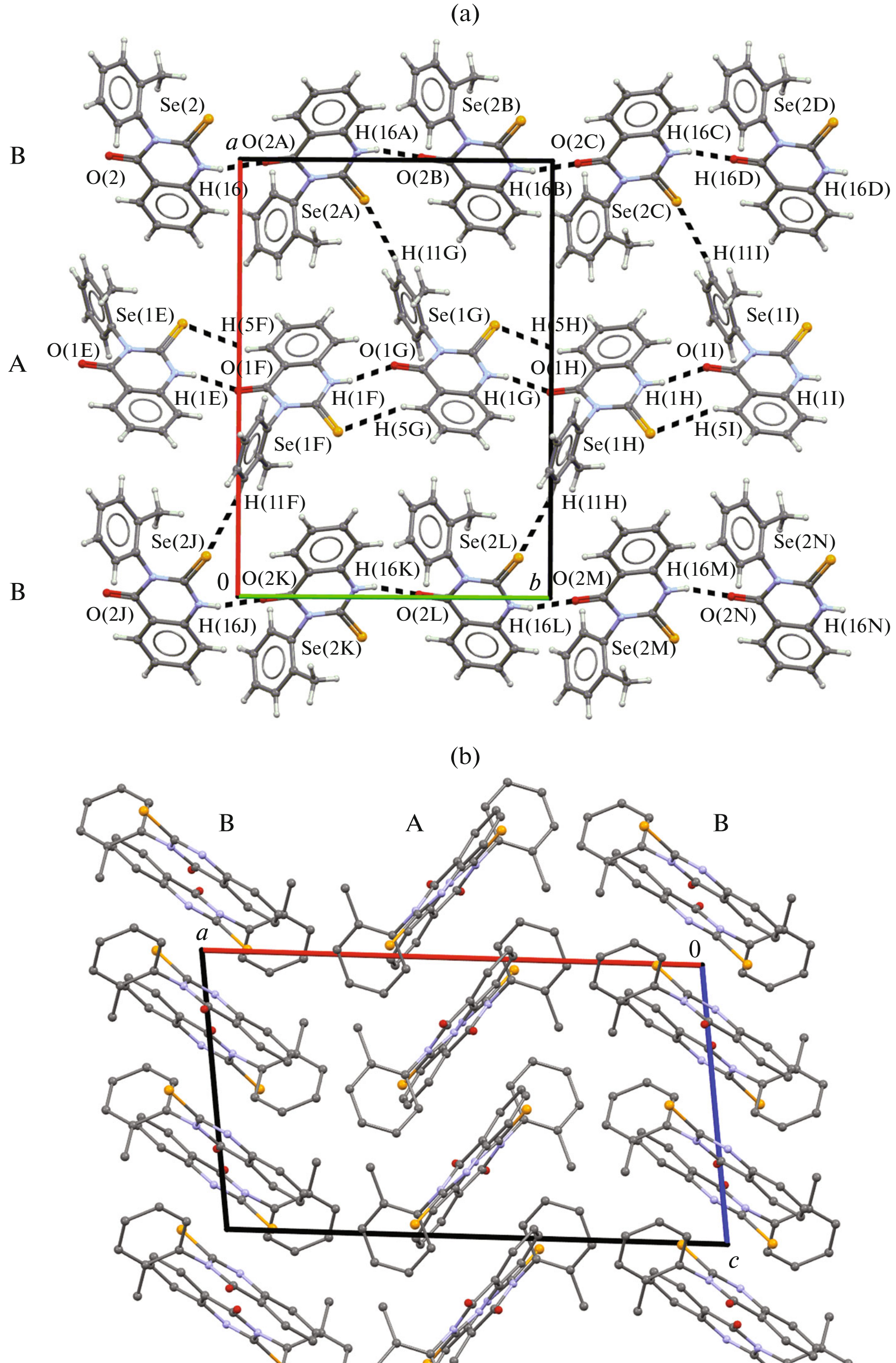


Fig. 2. Fragment of the crystal packing of compound HL in the (a) *x*0*y* and (b) *x*0*z* projections: (a) dashed lines show H...O and H...Se contacts, and conformer molecules are designated by letters A and B; and (b) hydrogen atoms are omitted for clarity.

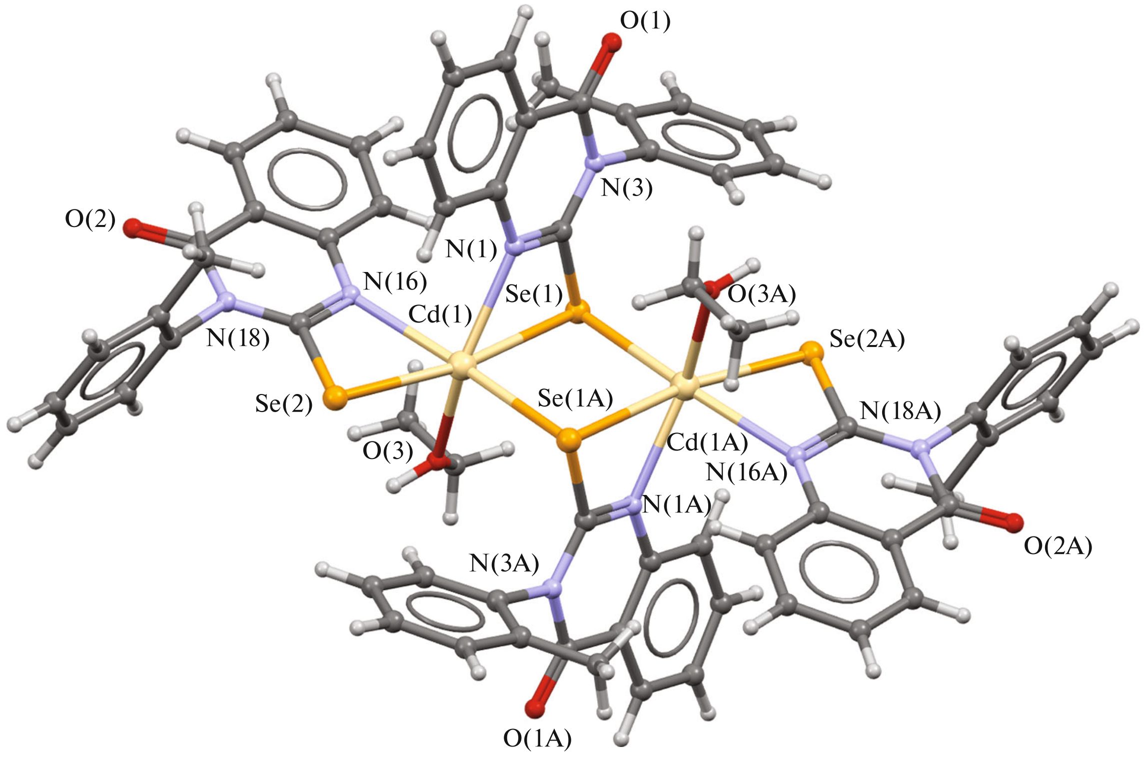
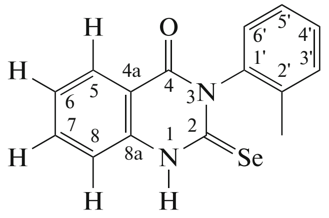


Fig. 3. Molecular structure of complex **II**.



(HL)

A comparison of the obtained spectral parameters for ligand HL and complex **II** provided the following conclusions.

• In the ^{1}H NMR spectrum of complex **II** at 25°C, the signals of the protons in positions 7 and 8 are strongly broadened and have no fine structure (Fig. 5a). With increasing temperature to 70°C, these signals become narrower and transform into the expected triplet and doublet (Fig. 5b) as observed in the initial ligand at room temperature (Fig. 6). With increasing temperature, the signals of the protons in positions 7 and 8 undergo a noticeable upfield shift (~0.2 ppm) compared to signals of other aromatic protons.

• The changes in chemical shifts (CS) of ^{13}C (~7–8 ppm) corresponding to an increase in their shielding on going from ligand HL (Fig. 7) to complex **II** (Fig. 8a) are most pronounced for positions 2, 8a, and 8. The signals of ^{13}C in these positions are strongly broadened (Fig. 8a), and increasing temperature to 70°C leads to narrowing of these signals (Fig. 8b).

• The signal from ^{77}Se in ligand HL is rather narrow (half-width at half-height 8 Hz) with CS = 442.5 ppm, which is characteristic of the selone form of quinozalinone [1]. At the same time, the signal from ^{77}Se in complex **II** is strongly broadened (the signal width at the half-height is 210 Hz) and undergoes an upfield shift by ~130 ppm (CS = 311.6 ppm). As the temperature increases to 70°C, this signal undergoes an appreciable narrowing to 102 Hz and an insignificant upfield shift (309.0 ppm) (Fig. 9).

• The CS of ^{15}N were determined by 2D HMBC (^{1}H–^{15}N) correlation spectra. The spectrum of ligand HL at room temperature (Fig. 10) exhibits correlation signals with the H(8) doublet, which corresponds to ^{15}N in position 1 with CS = 157 ppm and with the H(3') doublet corresponding to ^{15}N in position 3 with CS = 192 ppm. The correlation with H(6') occurs via four rather than three bonds due to their W-like geometry. In addition, this spectrum contains the doublet signal corresponding to the direct correlation with NH(1) and correlation via three bonds with N(3).

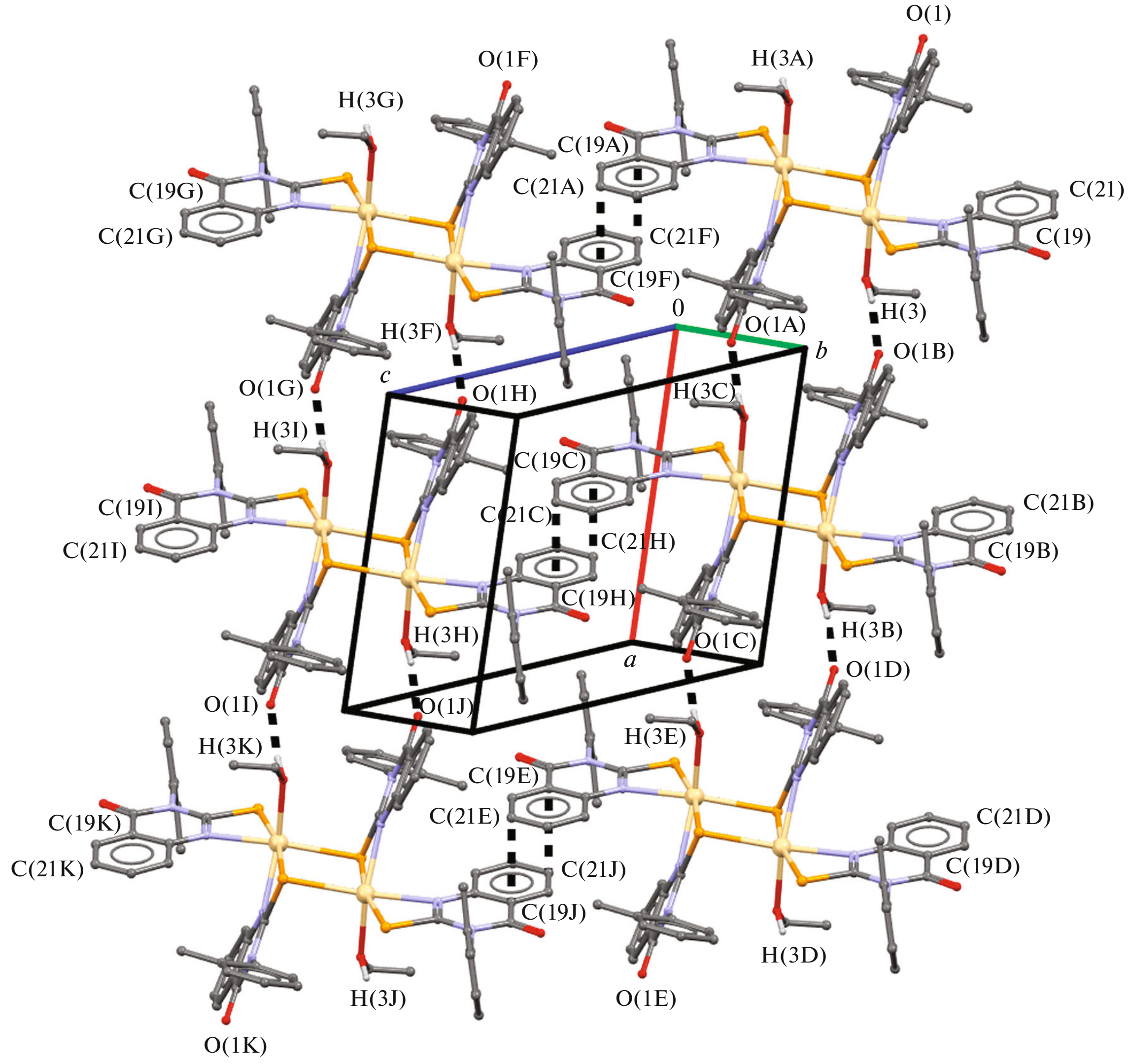


Fig. 4. Fragment of the crystal packing of complex **II** (dashed lines show H...O and C...C contacts, and the hydrogen atoms that are not involved in hydrogen bonds are omitted for clarity).

The spectrum of complex **II** at 70°C (Fig. 11), as well as that of the starting ligand HL, exhibits two correlation peaks between two doublets of H(8) at 7.43 ppm and H(3') at 7.16 ppm. The ^{15}N(1) and ^{15}N(3) chemical shifts determined from these spectra are 235 and 189 ppm, respectively.

A comparison of the ^{15}N chemical shift in ligand HL and complex **II** shows that in complex **II** the ^{15}N(3) shielding increases weakly (~3 ppm), whereas the ^{15}N(1) nuclei are strongly deshielded (~80 ppm). This is due to the fact that ligand HL exists in the selone tautomeric form (a), whereas in complex **II** ligand L^- has the selenolate structure (c) (Scheme 1).

The temperature dependence of the NMR spectra of different types observed for complex **II** and manifested most distinctly in the ^{1}H NMR spectra (Figs. 5a and 5b) can be caused by several factors. According to the XRD data, complex **II** has the structure of a tetragonal bipyramid in which the central metal atom coordinates to three quinazalinone ligands. Two ligands (along with the Se–Cd bond) have coordination bonds with the N(1) atom, whereas the third ligand has only the Se–Cd bond. In principle, one of possible reasons for the dynamic behavior in solution can be related to the transcoordination of these ligands due to their exchange along the Se–Cd bonds. Another possible explanation of this behavior is tautomerism of the selone–selenol type. The temperature dependence of the spectra can also be associated with hindered conformational transitions in the complex, which are

Table 2. NMR spectral data for ligand HL and complex **II**[a]

No of atom in ligand	Ligand HL				Complex **II**			
	^{1}H	^{13}C	^{77}Se	^{15}N	^{1}H	^{13}C	^{77}Se	^{15}N
1	13.43 br.s			156				235
2		175.70[b]	442.5			168.06	311.6	
3				192				189
4		160.84				160.64		
4a		116.88				119.43		
5	7.99 dd (7.8; 1.3 Hz)	129.05			7.96 dd	127.09		
6	7.43 td (7.5; 1.2 Hz)	126.60			[e]	124.60		
7	7.81 td (7.7; 1.2 Hz)	136.41			7.56 t	134.73		
8	7.60 d (8.2 Hz)	116.61			7.43 d	124.08		
8a		140.51				148.15		
1'		135.55				135.55		
2'		140.08				141.48		
CH_3	2.08	17.57			2.07	17.63		
3'	7.20 d (7.7 Hz)	130.96			7.18 d	129.14		
4'	[c]	[d]			[e]	[f]		
5'	[c]	[d]			[e]	[f]		
6'	[c]	[d]			[e]	[f]		

[a] According to the XRD data, the coordination sphere of cadmium contains one ethanol molecule along with three ligand molecules. Correspondingly, the ^{13}C and ^{1}H NMR spectra of the complex exhibit signals of ethanol, whose integral intensity corresponds to the ratio of the ligand to ethanol molecule (3 : 1) (marked with asterisks on the spectra in Figs. 5 and 8).

[b] $^1J(^{13}C,^{77}Se) = 224.2$ Hz.

[c] Multiplet from 7.28 to 7.34 ppm.

[d] Signals at 127.28, 128.03, and 129.44 ppm.

[e] Multiplet from 7.27 to 7.35 ppm.

[f] Signals at 127.09, 128.97, and 130.95 ppm.

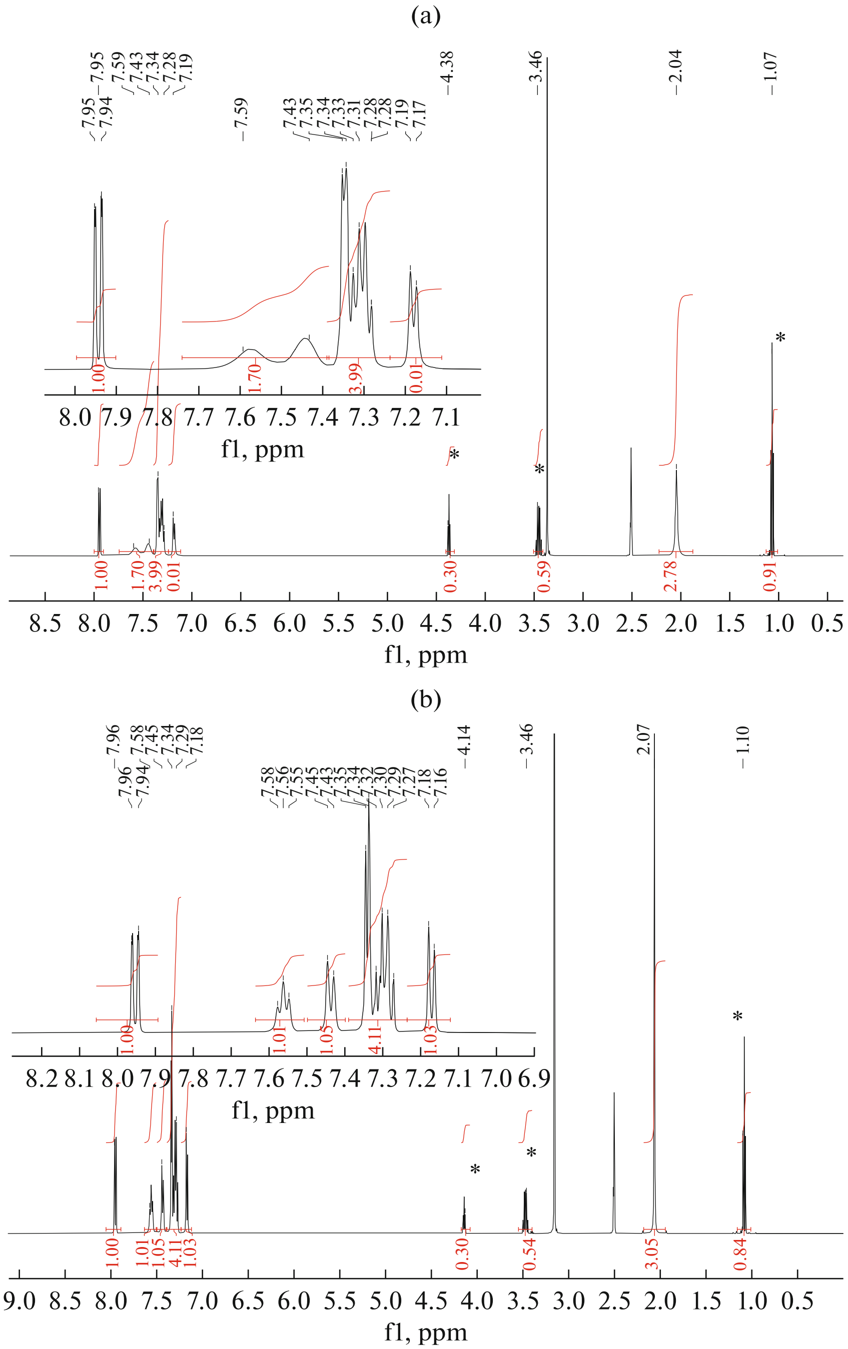


Fig. 5. ^{1}H NMR of complex **II** at (a) 25 and (b) 70°C.

accelerated with increasing temperature and result in shielding averaging in the case of H(7) and H(8). This can also appear as narrowing of the signals of ^{13}C in positions 7, 8, 8a, and 2 (Fig. 8b) and additionally of the ^{77}Se signal (Fig. 9). The further studies of the temperature dependence of the NMR spectra of the Cd(II) complexes with 2-selenoxo-1,2,3,4-tetrahydro-4-quinazolinone ligands bearing different substituents in the phenyl ring [10] in various solvents would help to establish the nature of the indicated dynamic process.

Thus, two new organoselenium compounds, 3-(2-methylphenyl)-2-selenoxo-2,3-dihydroquinazolin-4(1*H*)-one (HL) and its complex with cadmium (**II**), were synthesized and characterized by XRD and NMR spectroscopy. The structure of ligand HL was determined by

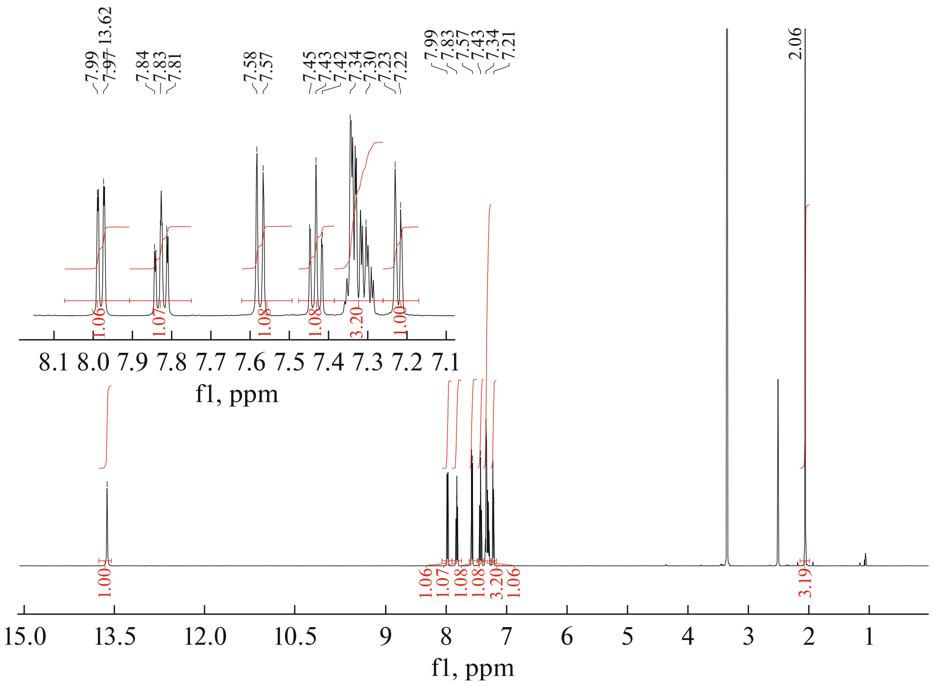


Fig. 6. ^{1}H NMR spectrum of ligand HL at 25°C.

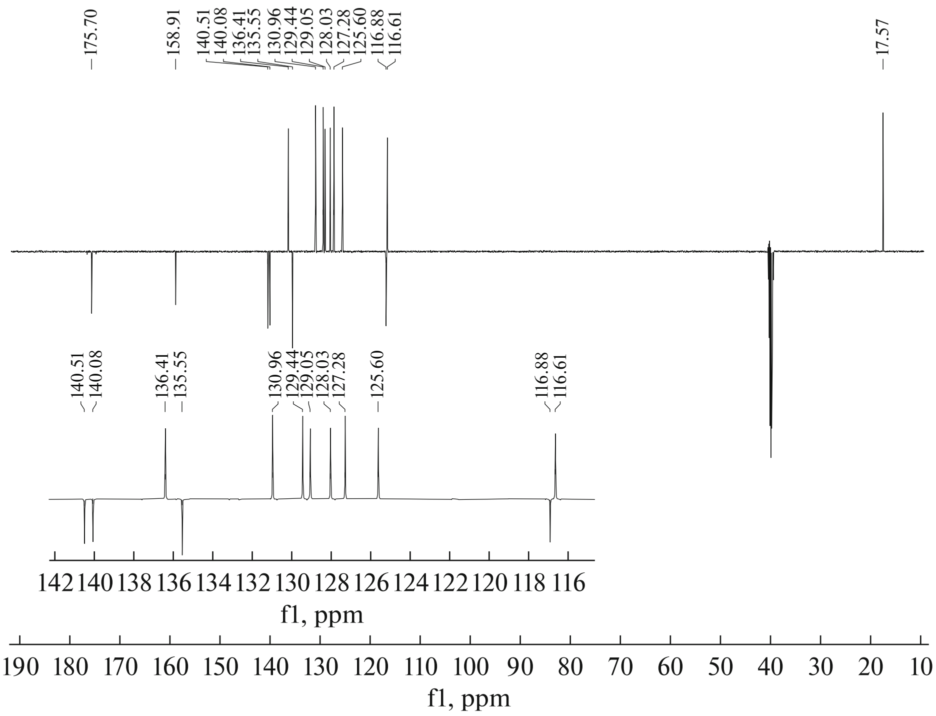


Fig. 7. ^{13}C NMR spectrum of ligand HL at 25°C recorded in the JMODECHO mode.

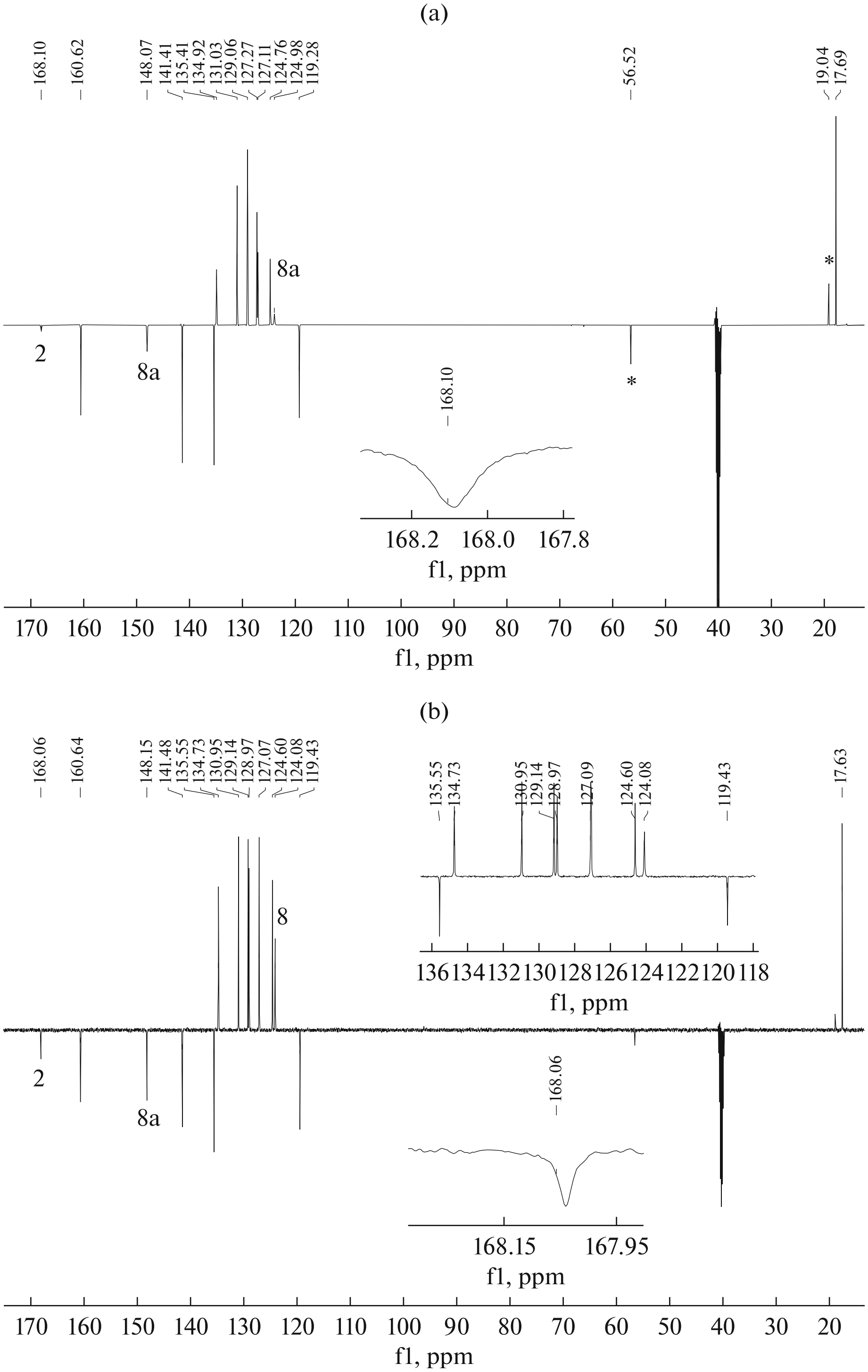


Fig. 8. ^{13}C NMR spectrum of complex **II** at (a) 25 and (b) 70°C recorded in the JMODECHO mode: (a) digits mark broadened signals and asterisks mark signals of ethanol, and (b) digits mark narrowed signals.

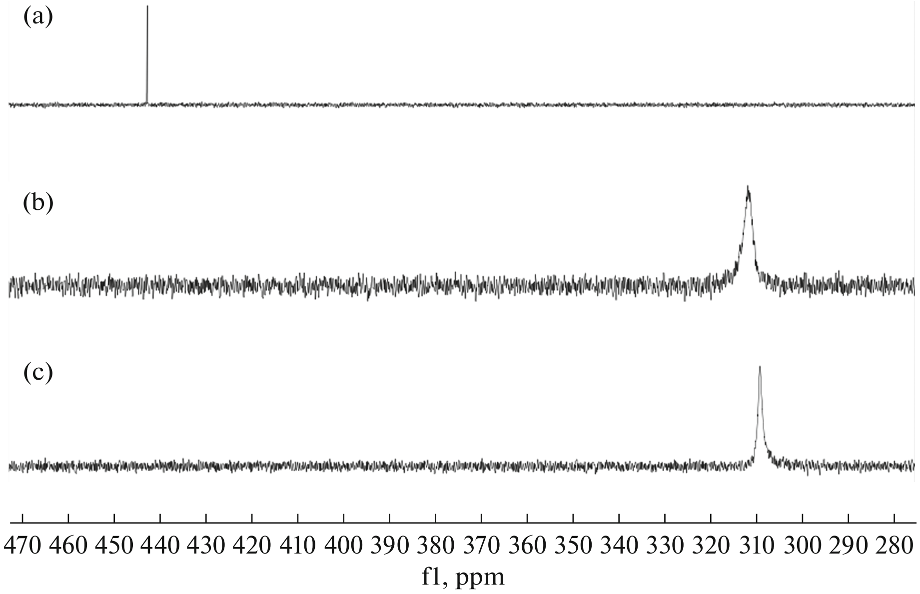


Fig. 9. ^{77}Se NMR spectra of (a) ligand HL and complex **II** at (b) 25 and (c) 70°C.

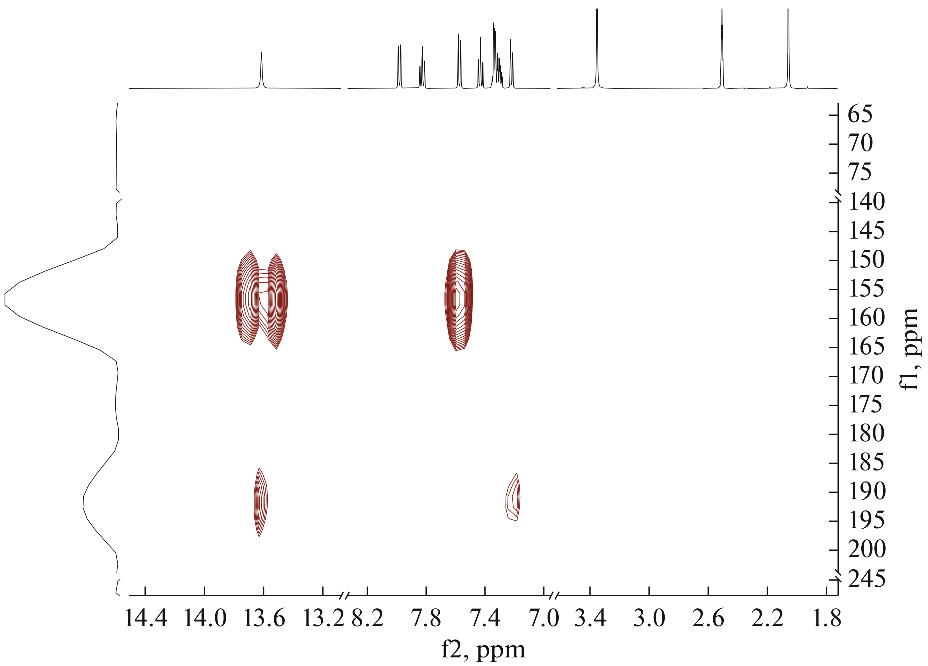


Fig. 10. HMBC (^{1}H,^{15}N) spectrum of ligand HL at 25°C.

XRD to be selone. A molecule of this compound contains several electron-donor centers and in complex **II** with cadmium behaves as the bi- and tridentate ligand performing the chelate-bridging function. In the crystals, the molecules of compounds HL and **II** form one-dimensional molecular chains due to the intermolecular Se...H and O...H bonds.

An analysis of the NMR spectra of ligand HL and cadmium complex **II** shows that in a DMSO-d$_6$ solution ligand HL exists in the selone form, and in complex **II** ligand L exists mainly in the selenolate form. This is consistent with the data on their crystal structures obtained by XRD. The study of the temperature dependence of the NMR spectra of complex **II** indi-

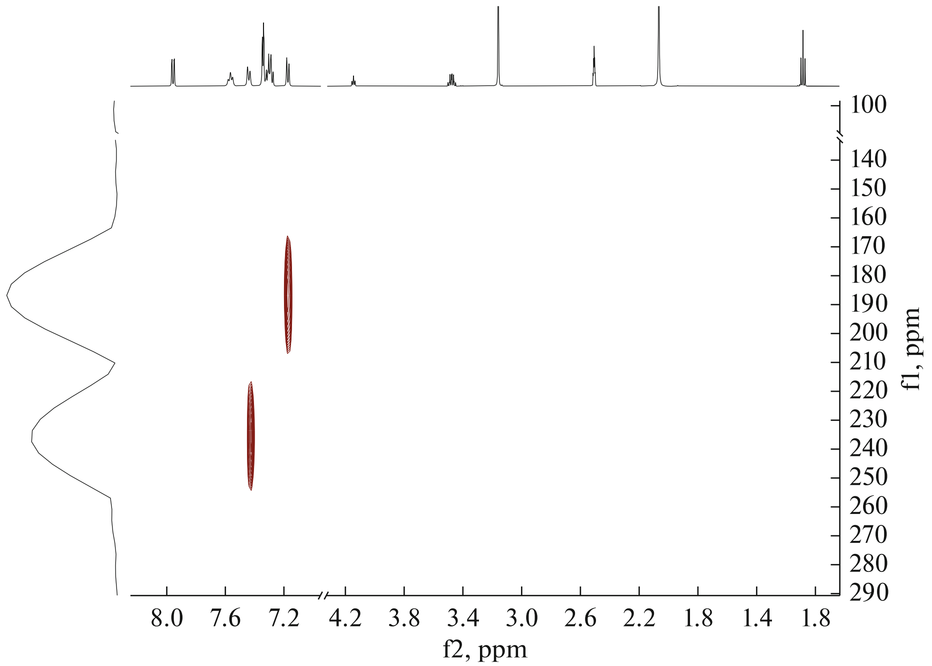


Fig. 11. HMBC ($^1H,^{15}N$) spectrum of complex **II** at 70°C.

cates that the dynamic process occurs in a DMSO-d_6 solution of complex **II**, the detailed mechanism of which is planned to be studied further.

FUNDING

This work was supported by the Russian Science Foundation (interdisciplinary projects nos. 20-62-47038 and 20-63-47107).

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

REFERENCES

1. Shtefan, E.D. and Vvedenskii, V.Y., *Russ. Chem. Rev.*, 1996, vol. 65, p. 307. https://doi.org/10.1070/ RC1996v065n04ABEH000212
2. Akkurt, M., Ozturk, S., Servi, S., et al., *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2004, vol. 60, p. 1507. https://doi.org/10.1107/S1600536804019099
3. Buzykin, B.I., Mironova, E.V., Gubaidullin, A.T., et al., *Russ. J. Gen. Chem.*, 2008, vol. 78, no. 4, p. 634. https://doi.org/10.1134/S107036320804021X
4. Askerov R.K., Mageramov A.M., Osmanov V.K., et al., *J. Struct. Chem.*, 2018, vol. 59, no. 7, p. 1658.
5. Askerov, R.K., Magerramov, A.M., Osmanov, V.K., et al., *Russ. J. Coord. Chem.*, 2019, vol. 45, no. 2, p. 112. https://doi.org/10.1134/S1070328419020039
6. Askerov, R.K., Magerramov, A.M., Osmanov, V.K., et al., *Russ. J. Coord. Chem.*, 2019, vol. 45, no. 8, p. 668. https://doi.org/10.1134/S1070328419070017
7. Rizvan, K.A., Maharramov, A.M., Khalilov, A.N., et al., *Acta Crystallogr., Sect. E: Crystallogr. Commun.,* 2020, p. 1007. https://doi.org/10.1107/S2056989020007033
8. Osmanov, V.K., Chipinski, E.V., Askerov, R.K., et al., *Russ. J. Coord. Chem.*, 2021, vol. 47, no. 1, p. 32. https://doi.org/10.1134/S1070328421010048
9. Askerov, R.K., Osmanov, V.K., and Kovaleva, O.N., *Russ. J. Coord. Chem.*, 2021, vol. 47, no. 11, p. 741. https://doi.org/10.1134/S1070328421110014
10. Osmanov, V.K., Chipinsky, E.V., and Khrustalev, V.N., *Molecules*, 2022, vol. 27, p. 5799. https://doi.org/10.3390/molecules27185799
11. Song, J.-F., Wang, J., Li, Si-Z., et al., *J. Mol. Struct.*, 2017, vol. 1129, p. 1.
12. Hernandez-Arganis, M., Moya-Cabrera, M., Jancik, V., et al., *Inorg. Chim. Acta*, 2018, vol. 475, p. 83. https://doi.org/10.1016/j.ica.2017.07.062
13. Hernandez-Arganis, M., Toscano, R.A., Moya-Cabrera, M., et al., *Z. Anorg. Allg. Chem.*, 2004, vol. 630, p. 1627. https://doi.org/10.1002/zaac.200400183
14. Muhammad, I., Andreas, M., Neumann, B., et al., *Dalton Trans.*, 2014, vol. 43, no. 39, p. 14737. https://doi.org/10.1039/C4DT01931H
15. Li, Y., Wang, C.Q., and Bian, H.D., *J. Coord. Chem.*, 2012, vol. 65, no. 20, p. 3665.
16. Ilie, A., Rat, C.I., Scheutzow, S., et al., *Inorg. Chem.*, 2011, vol. 50, p. 2675. https://doi.org/10.1021/ic102595d

17. Sanina, N.A., Kozub, G.I., Kondrat'eva, T.A., et al., *J. Mol. Struct.*, 2013, vol. 1041, p. 183. https://doi.org/10.1016/j.molstruc.2013.03.021
18. Bharty, M.K., Dani, R.K., Kushawaha, S.K., et al., *Polyhedron*, 2015, vol. 88, p. 208. https://doi.org/10.1016/j.poly.2015.05.045
19. Taheriha, M., Ghadermazi, M., and Amani, V., *J. Mol. Struct.*, 2016, vol. 1107, p. 57. https://doi.org/10.1016/j.molstruc.2015.11.012
20. Askerov, R.K., Youness, El. Bakri, and Osmanov, V.K., *J. Inorg. Biochem.*, 2022, vol. 231, p. 111791. https://doi.org/10.1016/j.jinorgbio.2022.111791
21. Askerov, R.K., Ashfaq, M., Chipinsky, E.V., et al., *Results Chem.*, 2022, vol. 4, p. 100600. https://doi.org/10.1016/j.rechem.2022.100600
22. Yadav, S., Deka, R., and Singh, H.B., *Chem. Lett.*, 2019, vol. 48, p. 65. https://doi.org/10.1246/cl.180748
23. Yadav, S., Singh, H.B., and Butcher, R.J., *Eur. J. Inorg. Chem.*, 2017, vol. 23, p. 2968. https://doi.org/10.1002/ejic.201700218
24. Karri, R., Chalana, A., Kumar, B., et al., *Chem.-Eur. J.*, 2019, vol. 25, no. 55, p. 12810. https://doi.org/10.1002/chem.201902578
25. Isab, A.A., Wazeer, M.I.M., Fettouhi, M., et al., *Polyhedron*, 2006, vol. 25, p. 2629. https://doi.org/10.1016/j.poly.2006.03.022
26. Henderson, R., Rothgery, E.F., and Schroeder, H.A., US Patent, no. 4496559, 1985.
27. CN Patent, no. 104447532A, 2015.
28. Askerov, R.K., Magerramov, A.M., Matsulevich, Z.V., et al., *Russ. J. Coord. Chem.*, 2019, vol. 45, p. 320. https://doi.org/10.1134/S1070328419030011
29. Ninomiya, M., Garud, D.R., and Koketsu, M., *Coord. Chem. Rev.*, 2011, vol. 255, p. 296. https://doi.org/10.1016/j.ccr.2011.07.009
30. Garud, D.R., Koketsu, M., Ishihara, H., et al., *Molecules*, 2007, vol. 2, p. 504. https://doi.org/10.3390/12030504
31. Heimgartner, H., Zhou, Y., Plamen, K., et al., *Phosphorus, Sulfur, Silicon Relat. Elem.*, 2008, vol. 183, p. 840. https://doi.org/10.1080/10426500801898135
32. Zakrzewski, J., Huras, B., and Kielczewska, A., *Synthesis*, 2016, vol. 48, no. p. 85. https://doi.org/10.1055/s-0035-1560481
33. *CrysAlisPro. Version 1.171.41.106a*, Rigaku Oxford Diffraction, 2021.
34. Sheldrick, G.M., *Acta Crystallogr., Sect. C: Struct. Chem.*, 2015, vol. 71, p. 3. https://doi.org/10.1107/S2053229614024218
35. Batsanov, S.S., *Zh. Neorg. Khim.*, 1991, vol. 36, no. 12, p. 3015.
36. Christoph, J., *Dalton Trans.*, 2000, p. 3885. https://doi.org/10.1039/B003010O

Translated by E. Yablonskaya