

07-Crystallography of Organometallic and Coordination Compounds

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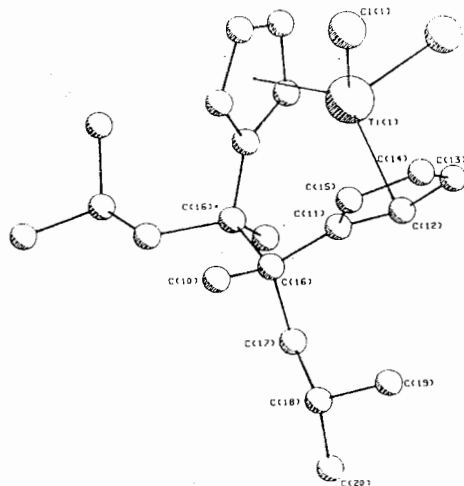
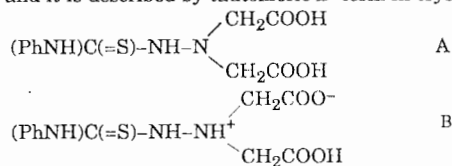


Fig. 1

PS-07.04.46 STRUCTURE OF 4-PHENYLTHIOSEMI CARBAZIDE DIACETIC ACID AND ITS COMPLEXES WITH Co, Ni AND VO by V.Ch.Kravtsov^a, Yu.A.Simonov^{a*}, J.Lipkowski^c, T.J.Malinowski^a, O.A.Bologa^b, N.V.Gerbeleu^b, V.I.Loza^b, ^aInstitute of Applied Physics and ^bInstitute of Chemistry; The Academy of Science of Moldova, Kishinev, 277028 Moldova; ^cInstitute of Physical Chemistry, The Academy of Sciences of Poland, Warsaw, 01224 Poland

Thio- and semicarbazide diacetic acids and their derivatives are perspective reagents as the complexones, e.g., the analogs of nitrilotriacetate. The structures of 4-phenylthiosemicarbazide diacetic acid (I-H₂L) and its complexes [Co.L(H₂O)₂]-II, [Ni.L(H₂O)₂]-III, [VO.L.H₂O]-IV were investigated. In I the molecule framework conformation differs from that one found for dimethyl ether of semicarbazide diacetic acid (Burstein I.F., Sotman S.S., Gerbelu N.V. et al. Kristallografiya. 1990, V.35, No1, P68) and it is described by tautomeric B-form in crystal:



In H₂L the arrangement of acetate branches is defined by two NH...O intramolecular hydrogen bonds and familiar to that one revealed for nitriloacetic acid. Such a mutual arrangement of the ligand branches ensures the most favourable conditions was found in II-IV. H₂L proves to be the metal through a set of donor atoms S,N,O,O. In II and III metal coordination is supplemented up to the octahedron by two water molecules, in IV - by water molecule and oxygen atom. The distances (A) in the coordination polyhedron are:

	M-S	M-N	M - O	M-H ₂ O (=O)
II	2.401	2.190	2.086	2.059
III	2.365	2.099	2.097	2.027
IV	2.423	2.351	1.999	1.962

The main changes in the ligand during complexation are connected with 4-phenylgroup rotation around C-N and N-C bonds:

	I	II	III	IV
φ1	0	1.1	3.0	14.0
φ2	90	97.5	78.1	45.2

Crystal data

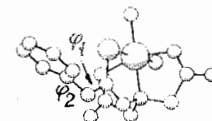
Sp.gr.	Pnam	P1	P1	P2 ₁ /n
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Sp.gr.	Pnam	P1	P1	P2 ₁ /n
a(A)	13.568	15.665	15.570	6.70
b(A)	10.601	7.411	7.333	12.47
c(A)	9.647	6.673	6.668	16.95
α(deg)	90	103.12	104.49	90
β(deg)	90	95.29	94.28	90
γ(deg)	90	98.18	97.90	95.1
Z	4	2	2	4
No refl.	968	1127	3049	2014
R(hkl)	0.067	0.053	0.043	0.067

PS-07.04.47 STRUCTURE OF THE BIS-2,5-DIMETHYL-1-PYRAZOLAMIDE SEMICARBAZIDE DIACETIC ACID AND OF THE PRODUCT OF ITS INTERACTION WITH COPPER ACETATE by T.J.Malinowski^{a*}, V.Ch.Kravtsov^a, Yu.A.Simonov^a, O.A.Bologa^b, N.V.Gerbeleu ^aInstitute of Applied Physics and ^bInstitute of Chemistry; The Academy of Sciences of Moldova, Kishinev, 277028 Moldova

Semicarbazide diacetic acid (I)-NH₂C(=O)NH-N(CH₂COOH)₂ is known as a perspective complexone. Its dentation is changed from one to six in the process of the metal coordination. Dihydrazide (II)-NH₂C(=O)NH-N(CH₂C(=O)-NH-NH₂)₂ was obtained from (I) in order to create the new coordination centers in the ligand. III was synthesized by interaction of II with acetyl acetone:

