09.4–31 BIS 2,2'BIPYRIDINE PLATINUM(II) DINITRATE MONOHYDRATE $Pt(bpy)_2(NO_3)_2H_2O$ AND RELATED STRUCTURES. By Alan Hazell, Chemistry Department, Aarhus University, DK-8000 Århus C, Denmark.

The dimensions of 2,2'bipyridine (bpy) and 1,10-phenanthroline (phen) are such that a planar arrangement of two of these about a metal atom, with normal M-N distances, will result in an impossibly close approach of H-atoms of opposing ligands. The strain can be relieved by a tetrahedral distortion which twists the ligands out of the plane, or by keeping the metal and nitrogen atoms in a plane and tilting the ligands whilst retaining their planarity, or by a bow-shaped distortion of the ligands. $Pt(phen)_2^{2+}$ (Hazell & Mukhopadhyay, Acta Cryst. (1980) B36, 1647) exhibits the twist deformation whereas $(Pt(bpy)_2^{2+}$ in its TCNQ salts has the bow deformation (Dong, Endres et al., Acta Cryst. (1977) B33, 2428. Endres, Keller et al., Acta Cryst. (1978) B34, 1823).

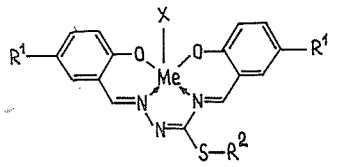
$Pt(bpy)_2(NO_3)_2.H_2O$ is monoclinic, C2/c, with a = 19.257(3), b = 15.482(2), c = 7.071(1) Å, β = 101.55(1), and Z = 4. The structure was determined from 3393 reflexions [$I>3\sigma(I)$] and found to have the twist conformation. The structure is not isomorphous with the corresponding Pd compound (Chieh, J. Chem. Soc. Dalton Trans. (1972) 1643), but is isomorphous with the nitrate of Pt bpy $phen^{2+}$ (Simonson (1984), private communication). The tetrahedral distortion is found to be smaller for the phenanthroline complexes than for those of 2-2'bipyridine.

09.4–32 THE COORDINATION ABILITY OF THIOSEMICARBAZIDDIACETIC ACID. ITS METAL COMPLEXES. By I.F. Burshtein, T.I. Malinovsky, L.I. Petuchov, N.V. Gerbeleu, O.A. Bologa, Institute of Applied Physics, Institute of Chemistry of Moldavian Academy of Sciences, Kishinev, USSR.

Thiosemicarbazidacetic acid, $H_2NC(S)NHN(CH_2COOH)_2 = H_2L$, is similar in structure to a well-known complexone - nitrilotriacetic acid. The residue L^{-2} has six atoms capable of coordinating a metal. The following complexes of Co(II), Cu(II) and Cd(II) with H_2L have been studied by X-ray methods: $CoL.H_2O$ (tricl., I, and rhomb., II); CoL.Thio (III); CuL (IV); $CdL.4H_2O$ (V); $CoLH_2.2H_2O$ (VI). Their crystallochemical features include: (1) The presence of monomeric (I, III, VI), dimeric (V) and polymeric (IV) structures. (2) The ability of the ligand to act as a O,O,N,S-tetradentate tripod ligand (I - III), a tetradentate and bridging ligand (IV, V), and a O,O,N,S-tetradentate tripod plus S-monodentate ligand (VI). The conformation of the monodentate ligand in VI is the same as that of the free acid, but is different from the conformation of the molecule when it acts as a tripod ligand. The results permit us to suppose that H_2L differs from its nearest analog in the series of complexones (nitrilotriacetic acid) by forming more variable metal complexes, due to a specific set of donor atoms of H_2L.

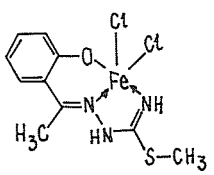
09.4–33 STRUCTURE AND PROPERTIES OF Fe(III), Cu(II) AND Zn(II) COMPLEXES WITH TRI- AND TETRADENTATE LIGANDS DERIVED FROM S-ALKYLISOTHIOSEMICARBAZIDES. By T.I.Malinowsky, Yu.A. Simonov, M.A.Yampol'skaya, S.G.Shova, M.D.Revenko, V.G.Rusu, Institute of Applied Physics and Institute of Chemistry, Academy of Sciences, Moldavian SSR, Kishinev, USSR

The Fe(III) and Zn(II) compounds with tetradentate ligands derived from S-alkylisothiosemicarbazides have been obtained by the method of the template reactions.

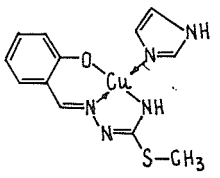


I	Me = Fe,	R^1 = H,	$R^2 = CH_3$,	$X = Cl^-$
II	Me = Fe,	R^1 = Cl,	$R^2 = C_3H_7$,	$X = Cl^-$
III	Me = Fe,	R^1 = H,	$R^2 = CH_3$,	$X = 1/2O^{-2}$
IV	Me = Fe,	$R^1 = CH_3$,	$R^2 = C_4H_9$,	$X = 1/2O^{-2}$
V	Me = Zn,	R^1 = H,	$R^2 = CH_3$,	X = Py

Complexes I and II are molecular monomers with the tetragonal-pyramidal coordination of the metal. The average bond distances are the following: Fe-O = 1.884, Fe-N = 2.094 Å. The displacement of Fe ion from the N_2O_2 plane is 0.534 (I) and 0.549 Å (II).
Complexes III and IV consist of dimeric molecules in which iron ions are bonded by the μ-oxo-bridge. The Fe-ligand bond lengths are in good agreement with those observed in I and II. The geometric characteristics of the μ-oxo-bridged system Fe-O-Fe are: $Fe-O_{(\mu)}$ = 1.769, 1.763 Å, ∠Fe-O-Fe = 156.4°, 157.89° for III and IV respectively.
The Mössbauer spectra data and the temperature variation of the average susceptibility of the powdered samples show that the ground state of Fe(III) in I-IV is $^6A_1$ (S_i = 5/2). Zn(II) in the complex V has a pyramidal coordination similar to that of I and II.
The crystal structure characteristics of I-V have been compared with those obtained early for Fe(III) and Cu(II) complexes (VI, VII) with related tridentate ligands.



VI



VII

The crystal data of the investigated complexes are shown in the table:

No	a	b	c	α	β	γ
I	7.933	16.943	12.181	90	90	91.76
II	9.331	9.445	12.807	80.48	68.93	89.79
III	16.449	17.785	14.275	90	90	120.49
IV	15.048	13.946	23.048	90	90	111.35
V	12.132	10.968	8.072	97.28	77.55	74.02
VI	7.719	7.990	12.072	88.62	76.11	69.42
VII	11.963	15.047	7.899	90	90	91.61