

- N. Bresciani-Pahor, J. D. Orbell, and L. Randaccio** **Steric Influences in Octahedral Cobaloximes. The Crystal and Molecular Structure of trans-methylbis(dimethylglyoximate) (phosphite)cobalt(III) Complexes with Phosphite= $P(OMe)_2Ph$  and  $P(OMe)Ph_2$**   
The crystal structures of  $(P(OMe)_2Ph)Co(DH)_2Me$  (I) and  $(P(OMe)Ph_2)(DH)_2Me$  (II) are reported. In both compounds the cobalt atom has a distorted octahedral geometry. Linear correlation between Co—P bond lengths and Tolman's cone angles in the series  $R_3PCo(DH)_2Me$  has been found  
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- M. J. Malinar, P. N. Radivojša, K. Marković, D. Belić, and M. B. Čelap** **Synthesis and Configuration of New Isomers of the Bis(aminocarboxylato)-carbonatocobaltate(III) Ion**  
The reaction of potassium tricarbonatocobaltate(III) with glycine as well as  $\beta$ -alanine, gave two new geometrical isomers. The configuration of the isomers was determined using its electronic spectrum and by means of PMR spectroscopy. . . .  
443—449
- P. Radivojević, N. Milinski, B. Ribár, and D. Lazar** **The Crystal Structure of the Complex  $[Y(H_2O)_5(NO_3)_2] [Y(H_2O)_2(NO_3)_4]$**   
The structure contains two crystallographically and chemically different complex ions, with yttrium atoms as the center of complexes. . . . .  
451—455
- E. C. Alyea, S. A. Dias, G. Ferguson, and P. Y. Siew** **Structural Studies of Steric Effects in Phosphine Complexes. Part XII<sup>1</sup>. Synthesis, Characterisation, and Crystal and Molecular Structure of Bis (trifluoroacetato) (trimesitylphosphine) mercury-(II) Dimer,  $[Hg(CF_3CO_2)_2P(mesityl)_3]_2$**   
The synthesis and crystal and molecular structure of the title compound with the bulkiest known phosphine, trimesitylphosphine are reported. The  $Pmes_3$  ligand has a regular propeller conformation, enlarged C—P—C angles, decreased Hg—P—C angles, and a maximum cone angle of  $208^\circ$ .  
457—465

W. H. Watson and  
W. W. Holley

**The Structures of Four Complexes of  
2,2,6,6-Tetramethyl-3,5-heptanedione  
Containing One, Four, Four and Nine  
Cu(II) Ions**

Bis-(2,2,6,6-tetramethyl-3,5-heptanediona-  
toCu(II) is a planar molecule with weak  
packing interactions. Di- $\mu_3$ -methoxy-tetra-  
kis[(2,2,6,6-tetramethyl-3,5-heptanediona-  
to)Cu(II)] is a step tetramer.  $\mu_4$ -oxa-bis-  
pyrazolatotetrakis [(2,2,6,6-tetramethyl-3,  
-6-heptanedionato)Cu(II)] has four Cu(II)  
ions tetrahedrally coordinated to a central  
oxygen atom. Hexa- $\mu_3$ -hydroxy- $\mu_6$ -(hydro-  
gendioxo-O, O')-nonakis[(2,2,6,6-tetramet-  
hyl-3,5-heptanedionato)Cu(II)] has six Cu-  
(II) ions occupying the corners of a tri-  
gonal prism and three lying above the rect-  
angular faces.

467—476

P. Bronzan-Planinić  
and H. Meider

**Synthesis and Characterization of Co-  
balt(II), Nickel(II) and Copper(II) Chlo-  
ride Complexes with Bis[(diphenylpho-  
sphinyl)methyl]phenylphosphine Oxide  
and Bis[(diphenylphosphiny)methyl]-  
phosphinic Acid**

Cobalt(II), nickel(II) and copper(II) chlori-  
de complexes with the tripod organopho-  
sphorus compounds: bis[diphenylphosphi-  
nyl)methyl]phenylphosphine oxide (RPPH)  
and bis[(diphenylphosphiny)methyl]pho-  
sphinic acid were studied. The compounds  
were characterized by infrared and elec-  
tronic spectral data and magnetic and  
conductivity measurements. The isolated  
complexes were of the general formulae  
[M(RPPH)<sub>3</sub>] [MCl<sub>4</sub>]·4H<sub>2</sub>O and [M(RPOH)Cl·  
nH<sub>2</sub>O]<sub>m</sub> (M=Co(II), Ni(II) or Cu(II); n =  
= 0—4; m = 1, 2 or more)

477—490

G. B. Carpenter

**The Conventional Bravais Unit Cell  
from Diffractometer Data**

This paper (a) describes how possible unit  
cell axes are found from 15—25 accurately  
centered reflections; (b) provides a proce-  
dure for deriving the reduced cell; and (c)  
indicates how International Tables for X-  
Ray Crystallography can be used to de-  
duce the conventional Bravais cell from  
reduced cell.

491—497

**P. Engel and  
W. Nowacki**

**Refinement of the Crystal Structure of  
Synthetic  $Tl_3AsS_4$**

The crystal structure of a synthetic sulfosalt  $Tl_3AsS_4$  has been determined and refined by X-ray diffraction method. Two types of the Tl coordination polyhedra, deformed octahedron with one vertex split and distorted trigonal bipyramid form a three-dimensional framework. The  $AsS_4$  tetrahedra are isolated. . . . .

499—505

**P. Doppelt,  
J. Fischer, and  
R. Weiss**

**Synthesis and Structure of a Dimer-  
capto-Iron(III) Porphyrin Derivative:  
 $[Fe(SC_6HF_4)_2]TPP \cdot Na \subset 18C_6 \cdot C_6H_6$**

A low-spin di-mercapto-iron(III)-meso-tetraphenylporphyrin complex with a d type hyperspectrum in the solid state has been synthesized. Structural parameters include relatively long equatorial Fe—Np bond distances of 1.998(3) Å and relatively short axial Fe—S bond distances of 2.312(1) Å. . . . .

507—518

**A. Kálmán, G.  
Argay, B. Ribár,  
S. Vladimirov, and  
D. Živanov-Stakić**

**Crystal and Molecular Structure of 3 $\beta$ -  
-Hydroxy-14,15 $\beta$ -epoxy-5 $\beta$ ,14 $\beta$ -card-  
-20,22-enolide (Digirezigenin)**

Digirezigenin and its methyl-suberate ester are quasiisostructural with those of the related compound digitoxigenin ( $C_{23}H_{34}O_4$ ). The conformation of the title compound is also compared with that of a bufa-20,-22-dienolide (cinofubagin). . . . .

519—528

**N. Brničević,  
Š. Mesarić, and  
H. Schäfer**

**Cluster Hydroxides of the Composition  
 $M_2[Ta_6Cl_{12}](OH)_6 \cdot nH_2O$ , With  $M=Na, K,$   
 $Rb, (CH_3)_4N^+$ ; Air Oxidation of the Clu-  
ster Unit  $[Ta_6Cl_{12}]^{2+}$  in Alkaline Medium**

Air oxidized methanol or methanol-water alkaline solutions of  $[Ta_6Cl_{12}]Cl_2 \cdot 8H_2O$  were used for the preparation of cluster hydroxides. Aspects of air oxidation of the cluster unit in the alkaline medium are discussed . . . . .

529—535

**B. Nowitzki und  
R. Hoppe**

**Eine Bemerkung über  $K_2[NiO_2]$**

Single crystals of  $K_2[NiO_2]$  have been obtained anew by reaction of surplus  $KO_{0,74}$  with the sidewall of Ni-cylinders. The structure of  $K_2[NiO_2]$  has been refined. The

- interatomic distances and the Madelung Part of Lattice Energy, MAPLE, were calculated. . . . . 537—543
- L. P. Battaglia, A. Bonamartini Corradi, and M. Nardelli** **Structural Aspects of 2-Thioimidazolidine Coordination in Silver(I) Halide Complexes**  
The crystal structure of  $\text{AgCl} \cdot 2\text{etu}$  and  $\text{AgBr} \cdot 2\text{etu}$  have been determined as well as the uncomplexed etu ( $\text{etu} = \text{SC}(\text{NHCH}_2)_2$ ). In both complexes Ag has a distorted tetrahedral coordination. . . . . 545—563
- Lj. Golič, I. Leban, and P. Šegedin** **Behaviour of Dimolybdenum Tetraacetate in Aqueous Solutions of Hydrogen Halides. Synthesis and Crystal Structures of  $(\text{pyH})_2[\text{Mo}_2(\text{O}_2\text{CCH}_3)_4\text{Br}_2]$  and two Modifications of  $(\text{pyH})_2[\text{Mo}_2(\text{O}_2\text{CCH}_3)_4\text{I}_2]$  (py = pyridine)**  
Two modifications of axial diadducts  $(\text{pyH})_2[\text{Mo}_2(\text{O}_2\text{CCH}_3)_4\text{I}_2]$ , and bromine analog were prepared. The crystal structures have been determined by X-ray diffraction method. . . . . 565—576
- B. V. Prelesnik and R. M. Herak** **The Crystal Structure of *trans*( $\text{NO}_2$ ,  $\text{N}=\text{C}-\text{CH}_3$ )-(N-ethylidene-ethylenediamine) glycyglycinatonitrocobalt(III) Monohydrate,  $[\text{Co}(\text{glygly})\text{NO}_2(\text{CH}_3\text{CH}=\text{en})] \cdot \text{H}_2\text{O}$**   
Crystal structure of title compound has been determined by X-ray diffraction method. The crystal structure consists of enantiomeric pairs of complex molecules and water molecules. The coordination around the cobalt atoms is distorted octahedral. . . . . 577—585
- Lj. Manojlović-Muir and K. W. Muir** **A Novel Pt(II)-Pt(IV) Mixed Valence Complex: The Crystal and Molecular Structure of  $[\text{LPt}(\mu\text{-I})(\mu\text{-Me-2PCH}_2\text{PeM}_2)_2\text{PtMe}_3] [\text{I}_3]$ ,  $\text{L} = 0.45\text{I} + 0.55\text{Me}$**   
The crystal structure is built up of symmetrical, linear  $[\text{I}_3]^-$  anions and partially disordered cations. In the cations the Pt(II) and Pt(IV) centres are characterized by square planar and octahedral coordination geometries. . . . . 587—595

N. Galešić,  
B. Matković,  
M. Topić,  
E. Coffou, and  
M. Šljukić

**The Crystal Structure of Disodium Thorium Bisphosphate,  $\text{Na}_2\text{Th}(\text{PO}_4)_2$**

Crystals of the title compound crystallize in two different space groups,  $C2/c$  and  $P2_1/c$ , retaining the same unit cell and practically the same structural arrangement. The metal polyhedra, formed by O atoms, are connected by common corners, edges, and planes. . . . .

597—608

M. Herceg  
B. Matković,  
D. Sevdic, D.  
Matković-Čalogović,  
and A. Nagl

**A Folded Conformation of 1,4,8,11-Tetrathiacyclotetradecane in its Mercury Compound: 1,4,8,11-Tetrathiacyclotetradecanedipycratomercury(II) Heminitromethane,**



The structure was solved from diffractometer data and refined to  $R = 0.030$ . Coordination polyhedron of the mercury atom is a distorted octahedron. The macrocycle is folded so that three sulfur atoms are in an equatorial and the fourth in an apical position. The conformation of coordinated macrocycle is compared to the conformation of free crystalline macrocycle and to the conformation of cyclotetradecane at 116 K. . . . .

609—619

I. Matijašić,  
G. D. Andreetti,  
P. Sgarabotto,  
A. Bezjak, and  
D. Fleš

**Crystal and Molecular Structure of (S)- $\alpha$ -(*p*-Bromobenzenesulphonamido)- $\beta$ -propiothiolactone**

Crystal structure of title compound has been determined by X-ray diffraction method. Heterocyclic four-membered ring has a puckering angle of  $8.9(4)^\circ$ . Discrete molecules are connected by intermolecular N—H...O hydrogen bonds. . . . .

621—628

L. Colombo,  
G. Baranović,  
J. R. During,  
and A. E. Stanley

**Polarized Infrared Spectra of Tolane Single Crystal**

Polarized infrared spectra of the oriented and very thin tolane crystal have been measured in the  $3500\text{--}50\text{ cm}^{-1}$  region. The application of the vibrational spectroscopy in studying the conformation of the free tolane molecule is discussed. . . . .

629—636

B. Kamenar,  
M. Penavić,  
and B. Marković

**The Crystal Structure of Pyridinium  $\mu$ -salicylato-tetrachloro- $\mu$ -oxo- $\mu$ -ethoxo-dioxodimolibdate(V)**

The crystal structure of the title complex is built up of  $\text{pyH}^+$  cations and  $[\text{Mo}_2\text{O}_3\text{Cl}_4(\text{C}_2\text{H}_5\text{O})(\text{HOC}_6\text{H}_4\text{CO}_2)]^{2-}$  anions. Each molybdenum atom of the binuclear anion is octahedrally coordinated. . . . . 637—643

**T. Balić-Žunić,  
S. Šćavničar,  
and Z. Grobrenski**

**The Structure of Thorium(IV) Ditungstate(IV) Oxide,  $\text{ThTi}_2\text{O}_6$**

The crystal structure of a modification of  $\text{ThTi}_2\text{O}_6$ , obtained from the melt at  $1100^\circ\text{C}$ , has been analysed by X-ray diffraction. The structure is based on a near-hexagonal close-packing of the oxygen atoms with the thorium and titanium atoms in »octahedral sites«. The Ti coordination polyhedra form layers parallel to the (100) which are connected by zig-zag chain of the Th coordination polyhedra running in the [001] direction. . . . . 645—651

**A. E. Elia,  
E. C. Lingafelter,  
and V. Schomaker**

**The Crystal Structure of (2,3,9,10-tetramethyl-1,4,8,11-tetraaza-1,3,8,10-cyclo-tetradecatetraone)copper(II) Tetraphenylborate**

The  $\text{CuTIM}$  cation, planar except for two methylene groups, is one of the rare cases of planar four-coordinate copper(II), although the apical regions of the coordination sphere are occupied by the centers of phenyl groups from two tetraphenylborate ions. . . . . 653—659

**B. Kojić-Prodić,  
Ž. Ružić-Toroš,  
G. Snatzke, and  
J.J. Herak**

**An Absolute Configuration of (1R,4R,5R)-4-Methoxy-8-acetyl-7,7-dimethyl-6-thia-3,8-diazabicyclo[3.2.1]octane-2-one,  $\text{C}_{10}\text{H}_{16}\text{N}_2\text{O}_3\text{S}$**

The crystal and molecular structure of the title compound was determined; its absolute configuration 1R,4R,5R was deduced from X-ray and CD spectral data. The conformation of the diazabicyclo[3.2.1]octane ring is boat-envelope-chair. Molecules are connected in an infinite chain by hydrogen bonds between amino and carbonyl groups. . . . . 661—668

**M. Pušelj, Z. Ban,  
and A. Szitula**

**The Crystal Structure and Magnetic Properties of the  $\text{Cu}_2\text{MnAl}_{1-x}\text{Hg}_x$  System**

- The system  $\text{Cu}_2\text{MnAl}_{1-x}\text{Hg}_x$  was studied by X-ray diffraction, neutron diffraction and magnetic susceptibility techniques. It is shown that the Curie temperature strongly depends upon the Hg concentration and all compounds with  $x > 0.4$  are ferromagnetic. . . . . 669—672
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- J.-P. Charland and A. L. Beauchamp** **Crystal Structure and Infrared Spectra of Anhydrous (Adeninato)methylmercury(II)**  
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Tris(chloromercuri)acetaldehyde, 2,2-bis(chloromercuri)propionaldehyde and 2,2-bis(chloromercuri)butyraldehyde were obtained by mercuration of the corresponding aldehyde in an aqueous mercury(II) chloride solution. The crystal structure of 2,2-bis(chloromercuri) butyraldehyde was determined using diffractometer X-ray diffraction data and refined by the least-squares procedure. The structure consists of discrete molecules. . . . . 689—694
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The crystal structure of  $\text{Te}[\text{CS}(\text{NH}_2)_2]_3\text{-(FHF)}_2$  was determined at 133 K. The trithiourea-tellurium(II) molecules crystallize as dimeric distorted square planar cations. . . . . 695—700

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