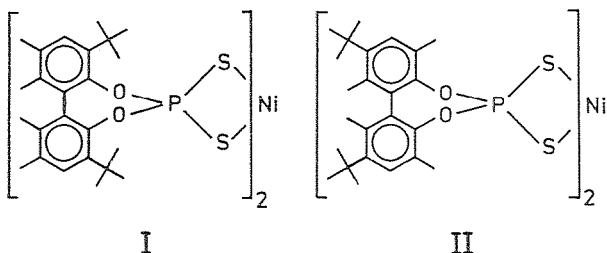


## 09. STRUCTURES OF ORGANIC, ORGANOMETALLIC AND COORDINATION COMPOUNDS

09.4-28 RELATION BETWEEN COLOUR AND CRYSTAL STRUCTURE IN TWO ISOMERIC NICKEL COMPLEXES. By W. Kuchen, D. Mootz, W. Poll, and R. Stephan, Institut für Anorganische Chemie und Strukturchemie, Universität Düsseldorf, D-4000 Düsseldorf, Germany.

Dithiophosphatonickel(II) complexes crystallize as violet solids with absorption maxima at about 530 and 710 nm. In our investigations on complexes with ligands possessing axial chirality (E. Hoffmann, W. Kuchen, W. Poll, and H. Wunderlich (1979). *Angew. Chem.* 91, 448; *Angew. Chem. Int. Ed. Engl.* 18, 415.) above values were observed for the pure enantiomorphs as well as for the racemic mixture. In contrast to that, the pure enantiomorphs of complex I were obtained as blue crystals (absorption maxima in remission at 558 and 756 nm), while the racemic mixture shows the normal violet colour. To clear up the reason for this effect, the crystal structure of the (+)-enantiomorph of complex I was determined by single crystal X-ray diffraction. Since the crystallization of the racemic mixture failed, the crystal structure of the isomeric complex (+)-II (violet in optical pure and racemic form) was also analysed for comparison. Complex II possesses a square planar  $NiS_4$  chromophore of the same kind previously reported (W. Poll and H. Wunderlich, *Acta Cryst.* (1980). B36, 1191). In complex I the  $NiS_4$  chromophore is no longer planar, but distorted towards a tetrahedral coordination of the Ni atom. The angle between the two planes  $NiS_2$  of the left and right halves of the molecule has a value of about 22 degrees. Also a slight bending of the whole molecule is observed due to the close neighbourhood of two tertiary butyl groups to the same side of the  $NiS_4$  plane.



09.4-29 SYSTEMATIC STUDIES OF BENZOTRIAZOLE COMPLEXES. By I. Sjøtofte and K. Nielsen, Structural Chemistry Group, Chemistry Dept. B, Technical University of Denmark, DK-2800 Lyngby, Denmark.

A summary and a comparison of crystal structures of metal complexes with benzotriazole concerning the geometry and the packing of the molecules will be presented.

The crystal structures involved in the analysis are complexes of the following transition metals:  $Mn^{2+}$ ,  $Ni^{2+}$ ,  $Cu^{1,2,3,8}$ ,  $Zn^{2+}$ ,  $Ag^{+}$ ,  $Cd^{2+}$ ,  $Ir^{3+}$  and  $Tl^{3+}$ .

Also, a comparison between the benzotriazole complexes and complexes with unsubstituted imidazole, pyrazole and 1,2,4-triazole will be discussed.

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09.4-30 THE STRUCTURE OF DICHLORO(TETRAPYRIDINE)-PLATINUM(II) TRIHYDRATE,  $[Pt(C_5H_5N)_4]^{2+} \cdot 2Cl^- \cdot 3H_2O$ .\* By Chin Hsuan Wei, Biology Division, and B. E. Hingerty, Health and Safety Research Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, U.S.A.

A compound of presumed formula  $Pt(Ado.Cl)_2$  was obtained by the reaction of  $K_2PtCl_4$  with adenosine. The brownish reaction product was crystallized from a mixed solution of pyridine and DMSO, which yielded yellow crystals that could be obtained in an untwinned form (I) from a solution of 1,2-dichloroethane. When I was treated further with pyridine and DMSO (volume ratio 9:1) in the presence of a small amount of water over a steam bath, large colorless crystals were obtained (II). Subsequent structural analyses by X-ray diffraction have shown I to be *trans*-dichloro(dipyridine)platinum(II) and II to be dichloro-(tetrapyridine)platinum(II) trihydrate.

The crystals of I are triclinic, space group  $P\bar{1}$ , with  $a = 5.5289(9)$ ,  $b = 7.090(1)$ ,  $c = 7.645(1)$  Å,  $\alpha = 79.12(1)^\circ$ ,  $\beta = 83.92(1)^\circ$ ,  $\gamma = 87.78(1)^\circ$  ( $Z = 1$ ). The resulting structural features were found to be essentially identical with those found earlier (P. Colamarino and P. L. Orioli, *J. Chem. Soc. Dalton Trans.* (1975) pp. 1656-1659) for *trans*-dichlorobispyridineplatinum(II).

The title compound crystallizes with four formula species in a unit cell of symmetry Cc and of dimensions  $a = 12.711(1)$ ,  $b = 12.856(1)$ ,  $c = 16.600(2)$  Å and  $\beta = 118.544(8)^\circ$ . All pyridine H atoms were included in the refinement. The final R(F) value was 2.1% for 3429 observed counter data collected with Mo K $\alpha$  radiation to 0.71 Å, and corrected for absorption and isotropic extinction. The four N atoms of pyridine rings display the usual square-planar coordination around the metal with an average Pt-N distance of 2.023(2) Å. The  $Cl^-$  ions and water molecules occupy space in crystal lattices. (\*Research supported by the Office of Health and Environmental Research, U.S. Department of Energy, under contract W-7405-eng-26 with the Union Carbide Corporation.)