## Optically Active Transition-metal Compounds.<sup>1,\*</sup> Stereochemistry and Crystal Structure Determination of $[(\eta^5 - C_5H_5)CoI-NC_5H_4 - C(R) = N - CH(CH_3)(C_6H_5)]^*I$ , $R = CH_3$

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#### Abstract

The crystal structure and absolute configuration of the title compound has been determined by singlecrystal X-ray diffraction. The crystals are orthorhombic with a = 11.837(6), b = 12.206(6) and c= 14.523(7) A, space group P2,2,2, and d(calc., Z = 4) = 1.91 gm cm<sup>-3</sup>. The structure was refined to the final agreement factors of R(F) = 0.061 and Rw(F) = 0.059. The Co-1 bond is 2.584(2) A which is significantly shorter than that observed in related complexes where the metal is bonded to pyrrole instead of pyridine. The two Co-N bonds are quite different; the Co-N (imine) bond being longer (1.99(1) A) than the Co-N (pyridine) one (1.91(1) A). The configuration around the chiral carbon and the Co atom has been determined using the Bijvoet. method. The conformation of the CH(CH<sub>3</sub>)(C<sub>6</sub> H<sub>5</sub>) substituent with respect to the plane of the chelate ring is in accord with the concept of minimal steric hindrance simultaneously allowing for phenyl/Cattle adticaction.

#### Introduction

From the reaction of  $(C_sH_s)Co(CO)I_s$  with the Schiff bases NN\*, derived from 2-pyridine-carbaldehyde, 2-acetylpyridine, 2-benzoylpyridine, 2-pyrolecarbaidehyde, 2-acetylpyrrole, (-)-1-phenylethylamine, and (-)-3-aminomethylpisane, a number of new complexes has been prepared and characterized [1]. The compounds derived from pyrrole Schiff bases NN\* are neutral molecules  $C_sH_sCo(NN^*)$ 8 because the chelate ligands NN\* are incorporated.

tions with those found in solution [2]. We now report the crystal structure and absolute configuration of the ionic complex III obtained by the reaction between C<sub>2</sub>H<sub>2</sub>Co(CO)I<sub>2</sub> with the Schiff base, derived from 2-acetylpyridine and (S)-(-)-1-phenylethylamine, having I' as counterion. Compound III is one out of a set of six compounds differing

as anions, whereas the complexes derived from pyridine Schiff bases NN\* are salts  $[C_1\Pi_2Co(NN^*)\Pi]^TX$  with  $X = \Gamma$  or  $PF_a^-$  as counterions. Recently, we have determined the X-ray structures and absolute configurations of two neutral complexes A and B derived from the pyrrole Schiff bases differing only in the substituent at the imine carbon of the chelatering (Scheme 1), and compared their conforma-

<sup>\*</sup>Part 23 of Evan Bernal's scries. For part 22 see sef. 4.
\*Stoudtaneously part 89 of Henri Brunner's series. For part
88 see sef. 4.

<sup>\*\*</sup>Authors to whom correspondence should be addressed.

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