

Optically Active Transition-metal Compounds.^{†,*} Stereochemistry and Crystal Structure Determination of $[(\eta^5\text{-C}_5\text{H}_5)\text{CoI-NC}_5\text{H}_4\text{-C(R)=N-CH(CH}_3\text{)(C}_6\text{H}_5\text{)}]^+\text{I}^-$, $\text{R} = \text{CH}_3$

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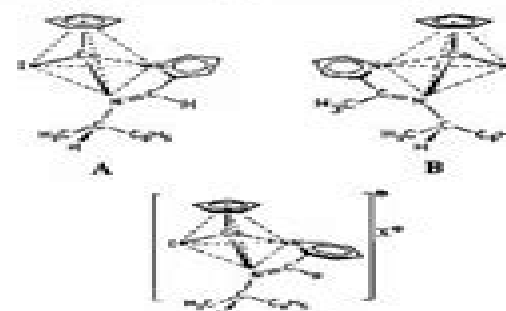
Abstract

The crystal structure and absolute configuration of the title compound has been determined by single-crystal X-ray diffraction. The crystals are orthorhombic with $a = 11.837(6)$, $b = 12.206(6)$ and $c = 14.523(7)$ Å, space group $P2_12_12_1$ and $d(\text{calc.}, Z = 4) = 1.91 \text{ gm cm}^{-3}$. The structure was refined to the final agreement factors of $R(F) = 0.061$ and $R_w(F) = 0.059$. The Co–I bond is 2.584(2) Å 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) Å) than the Co–N (pyridine) one (1.91(1) Å). The configuration around the chiral carbon and the Co atom has been determined using the Bijvoet method. The conformation of the $\text{CH(CH}_3\text{)(C}_6\text{H}_5\text{)}$ substituent with respect to the plane of the chelate ring is in accord with the concept of minimal steric hindrance simultaneously allowing for phenyl/ C_5H_5 attraction.

Introduction

From the reaction of $(\text{C}_5\text{H}_5)\text{Co(CO)}\text{I}_2$ with the Schiff bases NN^* , derived from 2-pyridine-carbaldehyde, 2-acetylpyridine, 2-benzoylpyridine, 2-pyrrole-carbaldehyde, 2-acetylpyrrole, (–)-1-phenylethylamine, and (–)-3-aminomethylpiperane, a number of new complexes has been prepared and characterized [1]. The compounds derived from pyrrole Schiff bases NN^* are neutral molecules $\text{C}_5\text{H}_5\text{Co(NN}^*)\text{I}$ because the chelate ligands NN^* are incorporated

as anions, whereas the complexes derived from pyridine Schiff bases NN^* are salts $[\text{C}_5\text{H}_5\text{Co(NN}^*)\text{I}]^+\text{X}^-$ with $\text{X} = \text{I}^-$ or PF_6^- 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 chelate ring (Scheme 1), and compared their conforma-



	I	II	III	IV	V	VI
R	H	H	CH ₃	CH ₃	C ₆ H ₅	C ₆ H ₅
X	I	PF ₆	I	PF ₆	I	PF ₆

Scheme 1.

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 $\text{C}_5\text{H}_5\text{Co(CO)}\text{I}_2$ 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

[†]Part 22 of Ivan Bernal's series. For part 22 see ref. 4.^{*}Simultaneously part 89 of Henri Brunner's series. For part 88 see ref. 4.^{††}Authors to whom correspondence should be addressed.

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