

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

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Received December 14, 1984

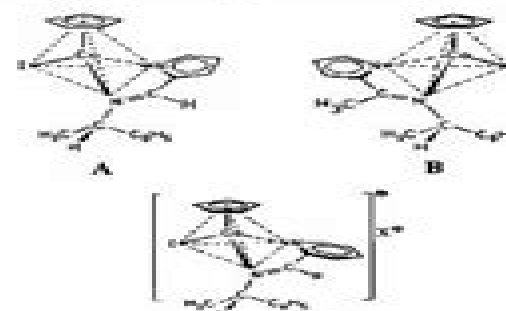
Abstract

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 $\text{X} = \Gamma^-$ 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 Γ^- 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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Bodie E. Douglas, Yoshihiko Saito



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Stereochemistry of Optically Active Transition Metal Compounds Bodie Eugene Douglas, Yoshihiko Saitō, American Chemical Society. Division of Inorganic Chemistry, 1980 *Stereochemistry of Optically Active Transition Metal Compounds* Bodie E. Douglas, Yoshihiko Saito, 1980-01-01 STEREOCHEMISTRY OF OPTICALLY ACTIVE TRANSITION METAL COMPOUNDS. B.E. DOUGLAS (ED.), *Topics in Stereochemistry* Ernest L. Eliel, Samuel H. Wilen, Norman L. Allinger, 2009-09-17 This seminal series first edited by Ernest Eliel responsible for some of the major advances in stereochemistry and the winner of the ACS Priestley Medal in 1996 provides coverage of the major developments of the field of stereochemistry The scope of this series is broadly defined to encompass all fields of chemical and biological sciences that are founded on molecular and supramolecular interactions Insofar as chemical physical and biological properties are determined by molecular shape and structure the importance of stereochemistry is fundamental to and consequential for all natural sciences Topics in Stereochemistry serves as a multidisciplinary series that enriches all of chemistry Aimed at advanced students university professors and teachers as well as researchers in pharmaceutical agricultural biotechnological polymer materials and fine chemical industries Topics in Stereochemistry publishes definitive and scholarly reviews in stereochemistry and has long been recognized as the gold standard reference work in this field Covering the effect of chirality on all aspects of molecular interaction from the fundamental physical chemical properties of molecules and their molecular physics to the application of chirality in new areas such as its applications in materials science Topics in Stereochemistry explores a wide variety of properties both physical and chemical of isomers with a view to their applications in a number of disciplines from biochemistry to materials science Molecular Optical Activity and the Chiral Discriminations Stephen F. Mason, 1982-10-14 Good No Highlights No Markup all pages are intact Slight Shelfwear may have the corners slightly dented may have slight color changes slightly damaged spine **Topics in Stereochemistry** Scott E. Denmark, 2003-04-10 Topics in Stereochemistry covers the fundamental principles of physical chemistry and molecular physics while dealing with certain stereochemical aspects of organic chemistry and biochemistry *Mössbauer Spectroscopy and Transition Metal Chemistry* P. Gülich, R. Link, A. Trautwein, 2013-11-11 Two decades have passed since the original discovery of recoilless nuclear gamma resonance by Rudolf Mossbauer the spectroscopic method based on this resonance effect referred to as Mossbauer spectroscopy has developed into a powerful tool in solid state research The users are chemists physicists biologists geologists and scientists from other disciplines and the spectrum of problems amenable to this method has become extraordinarily broad In the present volume we have confined ourselves to applications of Mossbauer spectroscopy to the area of transition elements We hope that the book will be useful not only to non Mossbauer specialists with problem Oriented activities in the chemistry and physics of transition elements but also to those actively working in the field of Mossbauer spectroscopy on systems compounds as well as alloys of transition elements The first five

chapters are directed to introducing the reader who is not familiar with the technique to the principles of the recoilless nuclear resonance effect the hyperfine interactions between nuclei and electronic properties such as electric and magnetic fields some essential aspects about measurements and the evaluation of Mossbauer spectra Chapter 6 deals with the interpretation of Mossbauer parameters of iron compounds Here we have placed emphasis on the information about the electronic structure in correlation with quantum chemical methods because of its importance for chemical bonding and magnetic properties

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Fundamental Research in Homogeneous Catalysis M. Tsutsui,2012-12-06

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