Research paper

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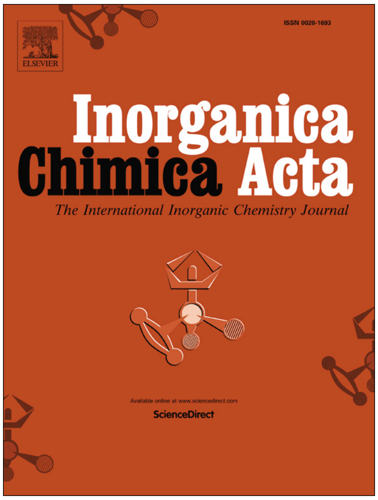

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Polarity of organometallic systems: Correlation analysis via substituent constants

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ABSTRACTS

The mechanism of the substituent influence on polarity of organometallics is poorly understood. In this work, literature data on the substituent influence on dipole moments μ as a measure of the bond polarity for 43 narrow series of organometallic complexes have been considered using correlation analysis. Generally, the μ values for series studied, including complexes of organometallics with benzene, were first established to depend on the joint influence of the inductive, resonance, polarizability, and steric effects of substituents. The presence or absence of certain effects are dictated by the type of series. The polarizability effect (an electrostatic ion-dipole interaction) is caused by an excess charge appearing on indicator centre as a result of the complexation. The contribution of the polarizability effect ranges up to about 50%.

Keywords:

Organometallics

Dipole moments

Classic electronic effects

Polarizability effect

1. Introduction

According to the traditional view, the basic characteristics of the chemical bond are its strength (which is more properly referred to as bond dissociation enthalpy BDE), length *l*, and polarity. As a rule, the dipole moment μ_b is taken to be a measure of the bond polarity. Recently we have considered in some detail the influence of the environment of the chemical bond on its properties BDE and *l* [1,2]. It has been found that in most cases this influence cannot be understood in the framework of the usual conventional concept of the inductive and resonance (conjugation) effects of substituents. By using the correlation analysis, the inductive, resonance, and polarizability effects of substituents were established to be in operation [1,2].

The dipole moments μ of organometallic systems have been studied over many years, see, for example, Refs. [3-22]. Nevertheless, to our knowledge no satisfactory explanation was provided for the mechanism of the influence of chemical environment on the dipole moments μ_b of individual

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