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INTERNATIONAL JOURNAL OF ARTIFICIAL INTELLIGENCE (ISSN: 2692-5206)
Volume 04, Issue 04, 2024
Published Date: - 03-07-2024

APPLICATION OF XRD IN COORDINATION CHEMISTRY

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Abstract: Currently, researchers are particularly attracted to ramified β- dicarbonyl compounds bearing aroyl-containing substituents, since such compounds are characterized by a number of important advantages in practice due to the presence of fluorine in the molecule: specific extracting ability, use in gas-liquid chromatography, spectrophotometric and luminescent analysis, use as chelating agents, complex compounds of fluorinated β-diketones are characterized by high volatility and good solubility. Of particular note is the use of a number of fluorinated lanthanides (especially europium and praseodymium) as shift reagents in NMR spectroscopy.

Keywords: Diketones, aromatic acid, molecules, diffractometer

Introduction

Among the wide variety of ligands capable of complex formation, polydentate multifunctional ligands occupy a special place.

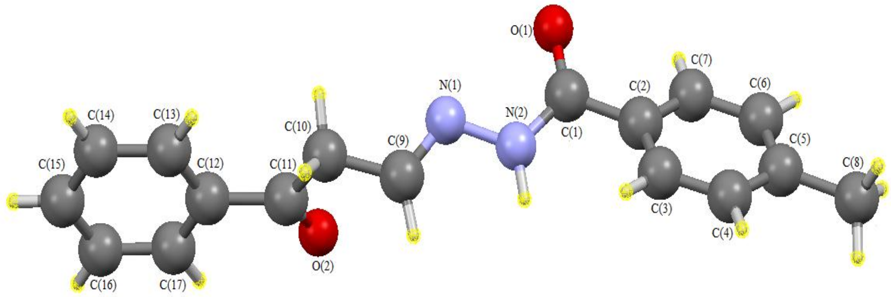
The condensation products of ketoaldehydes with aromatic acid hydrazides, according to previous studies, show a ring-chain equilibrium in which, along with the hydrazone or enhydrazine forms, the cyclic 5-hydroxypyrazoline form takes part. Unlike the condensation products of benzoylacetic aldehyde with acylhydrazines of aliphatic acids, the condensation products of benzoyl acetic aldehyde with substituted aroyl hydrazides in solutions are predominantly linear: E-hydrazone (AE) and E-enhydrazine (BE and BZ) forms.

The compounds are poorly soluble in
$CDCl_3$, therefore, DMSO was used as a solvent -d_6. When kept in solutions in DMSO -d_6 connections (H_2L^1-H_2L^4), Having electron-withdrawing substituents in the aromatic ring, a complex ring-chain equilibrium is established in which the hydrazone (A), enhydrazine (B) and cyclic 5-hydroxy-2-pyrazoline (C) forms take part.

Condensation products of benzoylacetic aldehyde with substituted aroylhydrazides (H_2L^1-H_2L^4) in solutions it is dominated by linear: E-hydrazone (AE) and enhydrazine (B_E and B_Z) forms.

This is evidenced by the parameters of the PMR spectra. To be fair, it should be noted that the signals of the protons of the phenyl substituent of aroylhydrazide compounds (H_2L^1-H_2L^4) In all four PMR spectra, parts of the molecules are partially present, thereby complicating the appearance of the spectra. The totality of spectral data shows that by varying the nature of the substituents in the hydrazide part of the molecules and the nature of the solvent used, various tautomeric equilibria can be realized in the series of acylhydrazones of β-ketoaldehydes. Some of them can be complex, including up to five and sometimes up to six configurational and conformational forms.

Regardless of the type of equilibrium for derivatives of substituted aroylhydrazones H_2L^1-H_2L^4 the presence of a cyclic (c) form is simply excluded and is not recorded in the time scale of PMR spectra from this tautomer; in the solid state and in solutions they exist mainly in the form of Z, E-enhydrazine tautomeric forms (BE and Bz). To unambiguously prove the conclusions of IR and NMR spectroscopy about the linear structure of the obtained organic ligands, we recrystallized the ligand H_2L^8 single crystals were grown $C_{17}H_{16}N_2O_4$ and the crystal structure was deciphered using the X-ray diffraction method. Ligand crystals belong to the triclinic system with unit cell parameters: a=15.6942(13), b=12.1515(13), c=8.0046(10), α=90, β=99.853(9), γ=90o, V=1504.0(3)Å^3, Z=4, pr.gr. $P2_1/c$. X-ray diffraction study was carried out on an automatic diffractometer "**Xcalibur, Oxford Diffraction**" (λ=1.5418 Å Cu$K\alpha$ - radiation, graphite monochromator ω- scanning, θ_{max}=75.8°, θ_{min}=4.6°). The structure was solved by the direct method using the SHELXS-97 program



Rice. Crystal structure of p-methylbenzoylhydrazone 3-phenyl-3-oxopropionaldehyde (H_2L^8).

Thus, as a result of studies using IR spectroscopy and X-ray diffraction, it was established that the ligands in the solid state are in a hydrazone (A_E) form.

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