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IR SPECTROSCOPIC INVESTIGATION CARBONYL DERIVATIVES OF
FERROCENE

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Annotation: We obtained β -diketone-1-ferrocenylbutanedione-1,3 by Claisen condensation. Hydrazones of monocarboxylic acids 1-ferrocenylbutanedione-1,3 (H_2L) were synthesized by the interaction of carboxylic acid hydrazides with ferrocenoylacetone. The IR spectra of the synthesized compounds were studied. The research results showed that H_2L in solution exists in the form of a tautomeric mixture: hydrazone, α -hydroxyazine, and cyclic 5-hydroxypyrazoline forms.

Keywords: monoacetylferrocene, hydrazone, Claisen ester condensation, tautomerism, IR spectroscopy.

Ferrocene is a unique compound in terms of chemical and thermal stability, as well as the possibility of direct application in various organic reactions. This is due to its “sandwich” structure, which is a three-dimensional aromatic system. Thus, many ferrocene-containing compounds are widely studied as new materials and are used in coordination chemistry. Currently, a huge number of studies are being carried out to study the biological activity of ferrocene derivatives. A special degree of biological activity is inherent in hydrazone derivatives of ferrocene, which is due precisely to their chelating ability. Numerous experiments have established that the use of molecular and intracomplex compounds based on ferrocene-containing derivatives of trace elements, such as copper, nickel and zinc, leads to an improvement in the germination of plant seeds and is a potent pesticide and has a beneficial effect on the growth and development of plants. It has been established that the stimulating properties of complex compounds depend on the nature of the metal, methods of coordination of ligands, as well as the chemical composition and geometric structure of the complexes.

To expand the range of tridentate chelating ligand systems containing ferrocene fragments, we have synthesized a new ligand *m*-nitrobenzoylhydrazonerferrocenoylacetone (H_2L).

β -Dicarbonyl derivative of ferrocene, 1-ferrocenylbutanedione-1,3 (ferrocenoylacetone), was synthesized by Claisen condensation. H_2L was synthesized by the interaction of alcoholic solutions of equimolar amounts of 1-ferrocenylbutanedione-1,3 with an alcoholic solution of *meta*-nitrobenzoylhydrazide.

The IR spectra of all synthesized compounds showed characteristic absorption bands near 1040-1080, 1270-1300, 1535-1600, va 3190-3278 cm^{-1} , related to ν_s and ν_{as} vibrations of N–N, C–N, C=N and N–H bonds, respectively (Fig. 1). In the short-wavelength region of the spectrum, two absorption bands are noted, which are characteristic of ferrocene-containing compounds, attributed to torsional vibrations of the cyclopentadienyl fragments of the ligands about the fivefold axis of the metallocene.

In the IR spectrum of H_2L , absorption bands were recorded within 3230, 1540 and 1050 cm^{-1} , assigned to ν_s and ν_{as} vibrations of N–H, C=N, N–N bonds, respectively. The spectrum also contains high-intensity bands characteristic of ν_s and ν_{as} vibrations of NO_2 at 1535 cm^{-1} and 1346 cm^{-1} .

The IR spectra of all the compounds synthesized by us, in addition to the main characteristic bands, have absorption bands of average intensity of about 480-505 cm^{-1} , corresponding to the rotation of cyclopentadienyl rings.

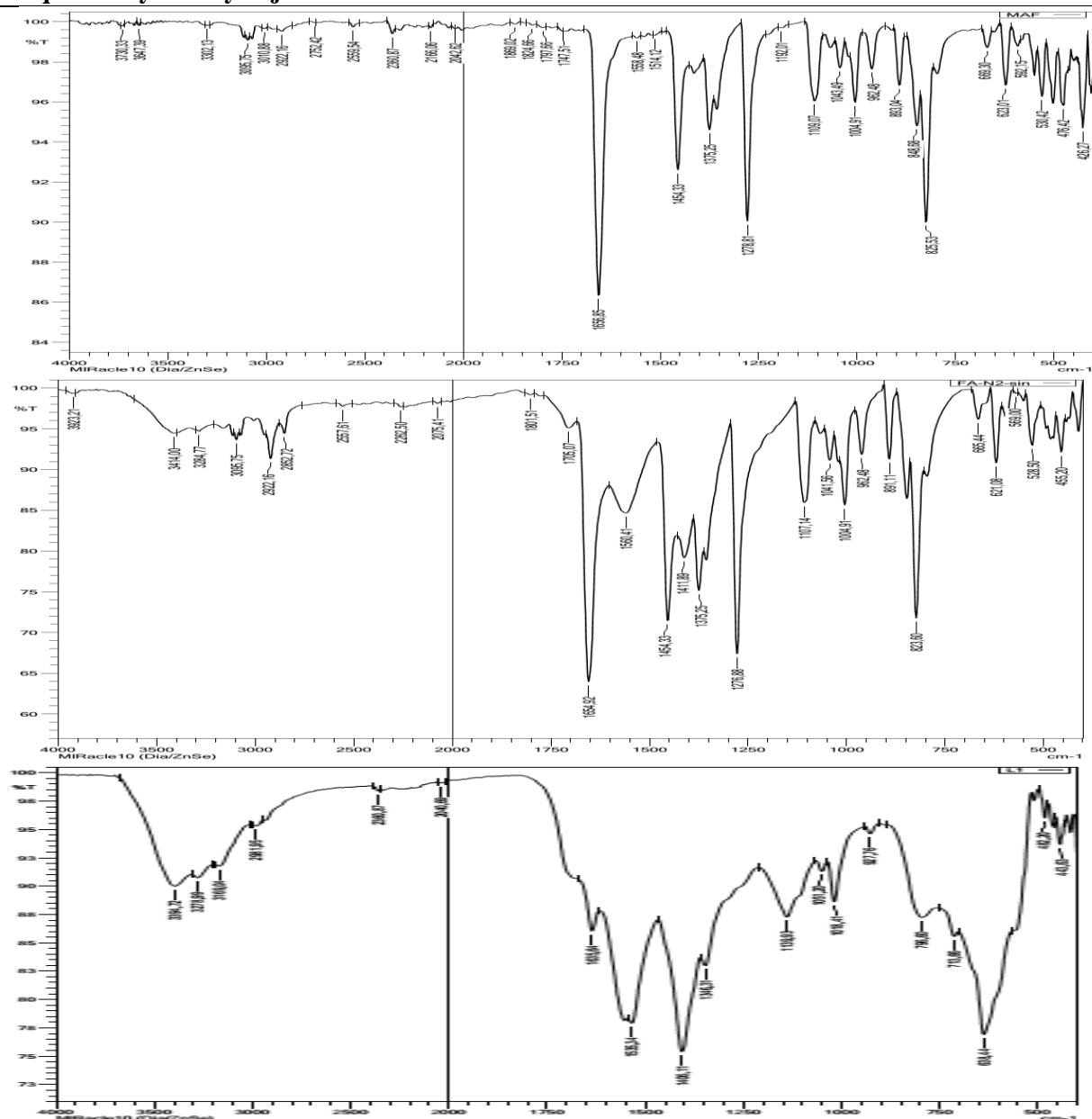


Fig.1. IR spectra of monoacetylferrocene (a), ferrocenoylacetone (b), H₂L ligand (c).

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