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Determination of the Absolute Configuration of Complex K[Co((S)-Pro)$_2$CO$_3$] by ^{1}H-NMR Spectroscopy

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^{1}H-NMR spectroscopy can be used for the determination of the absolute configuration of individual isomers of complex K[Co((S)-Pro)$_2$CO$_3$], because reciprocal positions of rigid rings of coordinated amino acids are specifically determined in them. As a result of various dipole–dipole interactions between protons of these rings, there occurs a characteristic rise in the multiplicity of ^{1}H-NMR signals for the given isomer.

Preparation and study of isomers of the complex K[Co((S)-Pro)$_2$CO$_3$] is described in our paper [1]. ^{1}H-NMR spectra of isolated isomers *cis*(N)*cis*(O) and *cis*(N)*trans*(O) have been measured on a Varian XL 100 instrument in D_2O. Chemical shift of the proton signals of amino acids was related to DSS as an internal standard.

With separate Λ- and Δ-*cis*(N)*cis*(O) and *cis*(N)-*trans*(O) isomers K[Co((S)-Pro)$_2$CO$_3$] a consequent rise of multiplicity of ^{1}H-NMR signals was noted relative to the multiplicity of signals of non-coordinated (S)-proline (Fig. 1).

Λ-cis*(N)*cis*(O) isomer*

- rise of multiplicity of signals ‘b’ caused by an expensive dipole–dipole interaction of protons CH_3 ‘b’ and CH'_2 ‘b’
- multiplicity of signals ‘a’ and ‘c’ remains preserved

Δ-cis*(N)*cis*(O) isomer*

- rise of multiplicity of signals ‘b’ and ‘c’ caused by a weaker dipole–dipole interaction of protons CH_2 ‘b’ and CH' ‘c’

Λ-cis*(N)*trans*(O) isomer*

- no rise of multiplicity of signals occurs, because of pyrrolidin rings of bound aminoacids being oriented in such a way that dipole–dipole interaction of protons is quite negligible

Δ-cis*(N)*trans*(O) isomer*

- an expressive rise of multiplicity of all signals occurs, while this effect is most expressive with signal ‘b’. This rise can be moved by an expressive dipole–dipole interaction of protons of groups CH_2 ‘a_2’ with CH'_2 ‘a_2’, and further by interaction CH_2 ‘a_1’ with CH'_2 ‘b’ and weaker interaction CH_2 ‘b’ with CH' ‘c’.

From our results it follows that the determination of an absolute configuration of isomers of complex K[Co((S)-Pro)$_2$CO$_3$] must be an ^{1}H-NMR experiment, because the change of multiplicity ^{1}H-NMR signals of protons of amino acids is specific for their absolute configuration.

Reference

1 B. Hájek, D. Sýkorová and J. Chyba, *Collection Czechoslov. Chem. Commun.* (in press).

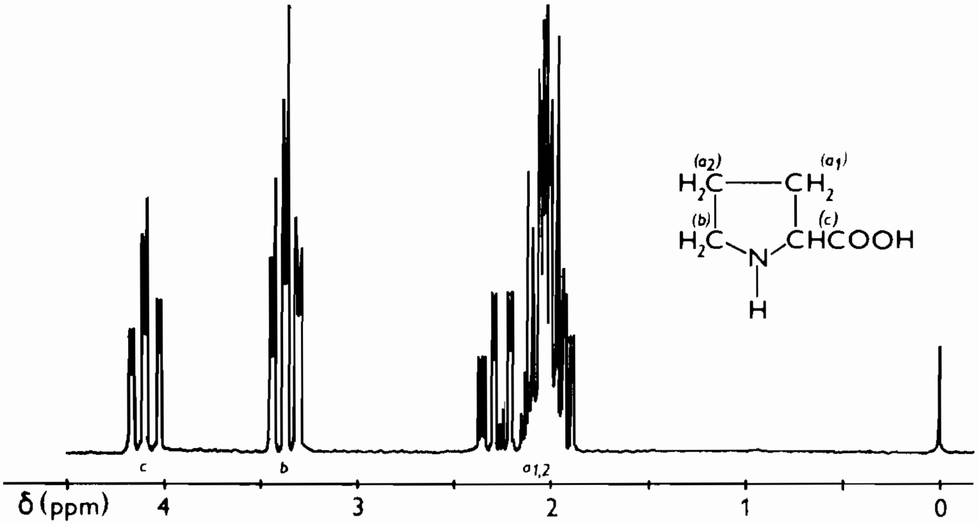

Fig. 1. 100 MHz ^{1}H-NMR spectrum of (S)-proline in D_2O.

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