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mer-Tris(β-alaninato)cobalt(III): Crystal structure, solution properties and its DNA cleavage in the presence of ascorbic acid

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Abstract

In its crystal structure, *mer*-tris(β-alaninato)cobalt(III), *mer*-[Co(β-ala)$_3$], assumes a half-chair conformation. The complex has been additionally characterized by UV–Vis spectroscopy on its buffered solutions, electrospray ionization-mass spectroscopy (ESI-MS) and cyclic voltammetry. Its larger λ_{max} value (visible region) compared to cobalt(III) complexes of α-amino acids suggests that β-alaninate is a weaker field ligand. Compared to Co^{III} hexamine complexes with six nitrogen-ligating atoms, *mer*-[Co(β-ala)$_3$], with a N_3O_3 coordination sphere, is more easily reduced. The complex alone does not cleave DNA but can do so in the presence of ascorbic acid in TBE buffer pH 8.3. DNA cleavage can be attributed to ascorbate free radicals generated by one-electron transfer from ascorbate ions to *mer*-[Co(β-ala)$_3$]. This represents the first report of DNA cleavage by a cobalt chelated amino acid complex.

Keywords: Cobalt(III); β-alanine; Ascorbic acid; ESI-mass spectrometry; Cyclic voltammetry; Nuclease activity

1. Introduction

It is now well known that the anticancer property of *cis*-dichlorodiammineplatinum(II) (cisplatin) is due to its binding to DNA [1]. Certain cobalt(III) Schiff base complexes have been found to have anticancer properties and to be potent antiviral agents [2–4]. β-Alanine, a non-protein amino acid, can chelate to cobalt(III) to yield a *mer*- or *fac*-isomer of the tris(β-alaninato)cobalt(III) complex, [Co(β-ala)$_3$]. The importance of this amino acid is that it is a precursor of both vitamin pantothenate and the dipeptide L-carnosine, which has both neuroprotective and detoxificating effects on cytotoxic α,β-aldehydes [5,6]. Furthermore, β-amino acids and their derivatives (β-lactam) have recently been found to: (i) exhibit pharmacological properties (e.g., antibiotic), (ii) occur in other biologically active natural products, and (iii) form peptides which can resist enzymatic hydrolysis [7–9]. These properties have prompted us to examine the solution properties of [Co(β-ala)$_3$], and its interaction with DNA.

Our interest in exploring the possible nucleolytic ability of neutral [Co(β-ala)$_3$] has also been prompted by our recent findings that the redox active neutral copper(II) complexes of L-α-amino acids can oxidatively

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