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## Data article

## Structural and thermal properties of acidic and potassium high acyl gellan



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## ABSTRACT

Acidic and potassium high acyl gellans, AchAG and KHAG, respectively, were prepared from a commercial product (LT-100). The average content of potassium in KHAG (1.01%, dry weight, dw) was 2.24 times higher than in LT-100 and approximately 34 times more than in AchAG. X-ray powder diffraction and <sup>13</sup>C NMR analysis revealed structural differences between AchAG and KHAG, which have been explained on the basis of the effect of different organization of both forms in the solid-state. The FTIR-ATR spectra of AchAG showed well defined amide I and amide II bands attributed to amino acid residues. TG-DTG profiles were different for AchAG and KHAG, suggesting that cations have an important role in gellan structure organization, consequently in its thermal stability and the macroscopic physicochemical properties.

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## Specifications table.

Subject area	Biopolymer chemistry
Compounds	Acid and potassium forms of high acyl gellan
Data category	Chemical, element and physicochemical
Data acquisition format	NMR, IR, Elemental analysis and TG-DTG
Data type	Analyzed
Procedure	Polymer modification, thermal and structure characterization
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## 1. Rationale

Knowing the structure and properties discussed in this article for the modified forms of high-acyl gellan is important to study the fundamental aspects of applications of the polysaccharide in an aqueous environment. One such aspect is related to its functionality as a gelling agent which is characterized by its sol–gel–sol transition behavior. This behavior is strongly influenced by the content of cations and polysaccharide affinity to mono and divalent counterions. The commercial preparation from which the acid and potassium forms were obtained contains large amounts of intrinsic counterions, yet it is used in many food applications. However, elucidation of the behavior of the polysaccharide in an aqueous medium is easier to study with modified cation-specific forms because the amount and type of counterion can be controlled and the ionic strength better known. Thus, the presence of counterions different to those of the specific form that could influence the conformational transition through which the functionality of the polysaccharide is expressed is strongly limited. As a consequence, characterization of the structure and properties of the modified form provides fundamental information about the particular traits of such form. Therefore, the generated data have fundamental value as they are valid only for the particular salt.

## 2. Procedure

### 2.1. Materials

A food grade commercial form of high acyl gellan (LT-100) was obtained from CPKelco (San Diego, CA, USA). Other materials included hydrochloric acid and sodium hydroxide (NaOH) (J.T. Baker, Xalostoc, Edo. de Méx., México), potassium chloride (Mallinckrodt Chemical Works, St. Louis, MO, USA) and Amberlite® IR-120 (plus) resin (Sigma-Aldrich, St. Louis, MO, USA). All solutions were prepared with deionized water, and all reagents were analytical grade.

### 2.2. Preparation of modified gellan

KHAG and AchAG were prepared following the methodology reported previously [1]. Briefly, the resin was separately transformed into the  $H^+$  or  $K^+$  forms. The acid or potassium Amberlite form was suspended in a 0.7% LT-100 solution and kept under constant agitation at 80 °C for 1 h. After the ionic exchange, the resin was removed by filtration and the modified gellan solution was recovered. Dry KHAG or AchAG were obtained by lyophilization (Labconco Corporation, Kansas City, MO, USA).

### 2.3. Atomic absorption

Ion concentrations were determined in an atomic absorption spectrophotometer (Varian SpectraAA 200 A) equipped with a deuterium background corrector and a hollow-cathode lamp, using an air-acetylene flame. Wavelengths employed to identify  $Na^+$ ,  $K^+$ ,  $Ca^{2+}$ ,  $Mg^{2+}$  590, 770, 420, 280 nm, respectively.

### 2.4. Elemental analysis

The KHAG and AchAG were analyzed in an elemental analyzer (Perkin-Elmer 2400 Series II CHNS/O; Perkin Elmer Inc., Waltham, MA, USA).

### 2.5. Soluble protein

The Lowry method was used to evaluate hydrosoluble protein in the polysaccharides, with bovine serum albumin (Sigma-Aldrich, USA) as a protein standard [2]. Absorbance was measured at 750 nm using a UV/vis spectrophotometer (Thermo Spectronic Genesys 10 UV, Thermo Fischer Scientific Inc., Waltham, MA, USA).

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