



FOOD CONTACT COATNIGS: IDENTIFICATION BY FTIR AND ANALYSIS BY GC-MS

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INTRODUCTION

Metal cans are internally coated with a polymeric coating to protect the food. The coating may contain different components including resins, cross-linking agents, additives and solvents. Fourier Transform Infrared (FTIR) analysis has shown to be a simple, fast and useful analytical tool for the identification of polymers. In this work, a FTIR spectrometer equipped with an ATR (attenuated total reflectance) accessory was used to identify two polymeric can coatings. The identification was achieved based on the spectral comparison with KnowItAll® 17.4.135.B IR Spectral Libraries of Polymers & Related Compounds (Bio-Rad Laboratories, Inc.). In the second part of the work, the semi-volatile compounds present in the samples, were investigated. For that purpose, methanolic extracts were obtained and analysed by GC-MS (EI).

INSTRUMENTATION

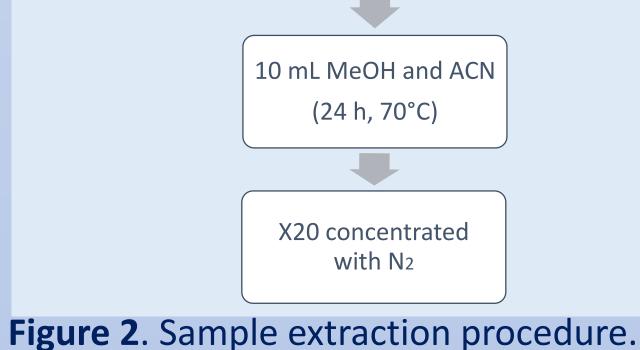
Column	Rxi-5SilMS (30 m x 0.25 mm, 0.25 µm)	100 cm ²
Injection Volume	$1 \mu L$	

Carrier gas flow (He)	1 mL/ min				
Full scan range	35-500 m/z				
Injector Temperature	300 °C				
Transfer line Temperature	300 °C				
Ramp Temperature	40-300 °C				
Mode of injection	Splitless				
Table 1. Chromatographic conditions.					





Figure 1. GC-MS.



Characterization of the coating	ng Extraction of the coating		Tr (min)	Fragment ions (m/z)	Identification	CAS	SI			DIO1 ACN	DI04 MeOH	DI04 ACN	DI06 MeOH	DI06 ACN
			17.1	74, 87	Dodecanoic acid, methyl ester	111-82-0	939	949	Х	-	-	-	х	-
0.3 0.275			19.7	74, 87	Tetradecanoic acid, methyl ester	124-10-7	920	943	х	-	-	-	х	-
	The polymeric coatings were	polymeric coatings were	20.2	73, 60, 129	Tetradecanoic acid	544-63-8	911	911	Х	Х	Х	х	Х	x
			21.4	43, 73, 129	Pentadecanoic acid Hexadecanoic acid,	1002-84-2	814	883	Х	Х	Х	Х	Х	Х
	identified as organosols and			74, 87	methyl ester	112-39-0	929	939	х	-	х	-	Х	-
	epoxy resin by ATR-FTIR.		22.3	55, 69	Carboxylic acid	57 40 0	007		X	X	X	X	X	X
	epoxy resin by Arn-Frin.		22.5 22.9	43 <i>,</i> 60, 73 148, 178	Hexadecanoic acid acid structure	57-10-3	907	952	X	X	X X	X	X	X
0.025 4000 3800 3600 3400 3200 2800 2600 2400 2200 1800 1600 1400 1200 1000 800 6d0 4d0 cm ⁻¹				55, 69	9-octadecanoic	112-62-9	902	914	X	_	X	-	-	-
Figure 3. Spectra of one of the			24.2	74, 87	octadecanoic acid, methyl ester	112-61-8	833	834	х	-	-	-	х	x
sample analysed by ATR-FTIR.			24.4	55, 69	9-octadecanoic acid (Z)	112-80-1	858	931	х	х	х	x	х	X
		• •	24.6	43, 60, 73	octadecanoic acid	57-11-4		951		Х	Х	х	Х	Х
	Esters and carboxylic acids were the most abundant compound	24.8	213, 119, 228, 91	2,4´-Bisphenol A	837-08-1	828	850	х	x	x	x	Х	x	
		compound	25.9	220, 91	octadecanoic acid, 9, 10-epoxy, methyl		020							
	identified by G	C-MS. Some		55, 74	ester, cis-	2566-91-8	851	851		-	-	-	Х	-
			26.9	69	ester				Х	-	-	-	-	-



Figure 4. FTIR Spectrometer.

unknown	compound	were	n				
possible its identification.							

Triphenylphosphine 277, 278 28.1 791-28-6 856 902 X X - - X X oxide 1,3-Bis(4methoxyphenyl)-1,3-propanedione 18362-51-1 652 659 X 136, 284 28.8 55*,* 264 29.5 Ester structure 69, 81 30.4 alkene

Table 2. Majority compounds identificated by GC-MS analysis.

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