Article

The Influence of the Substrate Structure in the Tellurocyclofunctionalization Reaction of γ,δ -Unsaturated Carboxylic Acids and their Corresponding Benzyl Esters*

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Ácidos carboxílicos γ,δ -insaturados contendo ligações duplas monossubstituídas reagem com tricloreto de ariltelúrio, fornecendo as telurolactonas esperadas; reação dos ésteres benzílicos correspondentes fornece o produto de adição dos tricloreto de ariltelúrio à ligação dupla. Reação de ácidos carboxílicos γ,δ -insaturados contendo ligações duplas 1,1-disubstituídas, leva a uma mistura das telurolactonas esperadas e o produto de adição de ácido clorídrico à ligação dupla; os ésteres benzílicos correspondentes fornecem telurolactonas como único produto. A estereoseletividade da reação é baixa; formam-se misturas das duas possíveis lactonas diastereoméricas em relação aproximadamente 1:1.

γ,δ -Unsaturated carboxylic acids containing monosubstituted double bonds react with aryltellurium trichlorides to give the expected tellurolactone. Reaction of the corresponding benzyl esters gives the addition product of the aryltellurium trichlorides to the double bond. γ,δ -Unsaturated carboxylic acids containing 1,1-disubstituted double bonds lead to a mixture of the expected tellurolactone and the product of hydrochloric acid addition to the double bond; the corresponding benzyl ester gives the tellurolactone as the only product. The stereoselectivity of the reaction is low; mixtures of the two possible diastereomeric lactones are formed in approximately 1:1 ratios.

Keywords: *tellurocyclofunctionalization, tellurolactones*

Introduction

The tellurocyclofunctionalization was discovered at the same time as the selenocyclofunctionalization¹. Since then the selenocyclofunctionalization became a valuable synthetic tool²; however its tellurium counterpart has received relatively little attention. Some time ago we reported a systematic study on the lactonization of γ,δ -monosubstituted acyclic and cyclic carboxylic acids with *p*-methoxyphenyltellurium trichloride³. The detelluration of the tellurolactones was achieved by Bu_3SnH reduction⁴. These are the only reports on the lactonization of unsaturated acids with aryltellurium trichlorides. As several other aspects of this reaction were not yet investigated our group initiated a study to determine the scope and limitations of the tellurolactonization reaction.

In this work we studied the influence of the tellurium electrophile and the olefin structure in the course of the tel-

lurolactonization of γ,δ -unsaturated carboxylic acids extending the investigation to their benzyl esters. As the reaction leads to mixtures of diastereomeric lactones, the question of the stereoselectivity of this process was addressed.

The γ,δ -unsaturated carboxylic acids **1** and the corresponding benzyl ester **2**⁵ used are shown in Scheme 1.

Two tellurium electrophiles *p*-methoxyphenyltellurium trichloride **3** and *p*-phenoxyphenyltellurium trichloride **4**^{1d} were employed (see Fig. 1).

In all cases, the aryltellurium trichloride **4** reacted faster with **1** and **2** than the aryltellurium trichloride **3** (Table 1). Probably this difference in reactivity is associated to the higher solubility of **4** in chloroform and the lower electron density on the tellurium atom due to the conjugation of the oxygen lone electron pair with the second phenyl group.

*Dedicated to Prof. Helena M.C. Ferraz on the occasion of her 50th birthday

R =	CH ₃ ;	R ¹ =	H	1a	68%	R =	CH ₃ ;	R ¹ =	H	2a	85%
	Ph		H	1b	79%		Ph		H	2b	78%
	CH ₃		CH ₃	1c	72%		CH ₃		CH ₃	2c	82%
	Ph		CH ₃	1d	75%		Ph		CH ₃	2d	82%

Scheme 1.

Figure 1.

The structure of the substrate has a decisive influence in the course of the reaction and in the nature of the products formed. Carboxylic acid **1a** reacted with aryltellurium trichloride **3** and **4** leading to the tellurolactone **5a,b** in good yields. The corresponding benzyl ester **2a** did not give lactones **5a,b**. The products were the carbon-carbon double bond adducts with the aryltellurium trichlorides (**6**) (Scheme 2).

This result can be rationalized in terms of a lower nucleophilicity of the carboxylic oxygen of **2a**. Probably the first

Table 1. Reaction of aryltellurium trichlorides with γ,δ -unsaturated carboxylic acids and benzyl esters.

Substrate	Electrophile	Product ^a	Reaction time (h)	Yield ^b (%)
1a	3	5a	1.7	73
1a	4	5b	0.8	80
2a	3	6a	2.5	68
2a	4	6b	1.5	72
1b	3	5c	1.5	74
1b	4	5d	0.7	83
1c	3	5e	2.2	47

Table 1. (cont.)

Substrate	Electrophile	Product ^a	Reaction time (h)	Yield ^b (%)
1c	4	5f	1.2	53
2c	3	5e	4.2	62
2c	4	5f	3.5	85
1d	3	5g	2.5	52
1d	4	5h	1.5	43
2d	3	5g	4.3	76
2d	4	5h	3.7	79

^a Mixture of the two possible diastereomers; ^b Yield of the recrystallized products; ^c Obtained as oils. No satisfactory elemental analysis were obtained.

Scheme 2.

step consists on the formation of a π complex between the double bond and the electrophile. In the absence of a good internal nucleophile, the chloride ion originated from the aryltellurium trichloride attacks the complex leading to the adduct **6**.

Reaction of **3** and **4** with acid **1c** gave the expected lactone **5e,f** accompanied by the carbon-carbon double bond adduct with hydrochloric acid (**7**) (Eq. 1).

The hydrochloric acid liberated during the lactone formation attacks the carbon-carbon double bond leading to a tertiary carbenium ion which reacts with the chloride ion giving **7**. In the preceding case (Scheme 2) this side reaction was not observed in view of the lower stability of the carbenium ion, which is not formed. This problem could not be circumvented by adding an amine to the reaction me-

dium to trap the HCl formed since aryltellurium trichlorides react with amines⁶

On the contrary, reaction of **3** and **4** with the benzyl ester **2c** gave only the tellurolactones **5e,f** in good yields, since benzyl chloride instead of hydrogen chloride was formed as by-product. Similar results were obtained with acid **1d** and ester **2d** (Table 1).

Concerning the stereochemical course of the reaction it was observed a low stereoselectivity. Acids **1a** and **1b** gave the tellurolactone in a 3:1 *cis/trans* ratio. Acids **1c** and **1d** and esters **2c** and **2d** gave the tellurolactones in an approximately 1:1 *cis/trans* ratio (Scheme 3). The electrophile had no influence in the isomeric ratio.

The ratios were determined by NOE experiments with the mixture of isomers and by the relative integral of the methyl groups signals in the ¹H-NMR spectra of the crude mixture. In one case (lactone **5e**) one isomer was separated by successive recrystallizations and its structure was determined by X-ray analysis⁷. Comparison of the NMR spectrum of the pure isomer **5e** with the mixture confirmed the stereochemistry assigned by ¹H-NMR analysis.

In conclusion, the tellurolactonization of γ,δ -unsaturated acids containing monosubstituted olefins is successful, the tellurolactonization of γ,δ -unsaturated acids containing

disubstituted olefins is not satisfactory leading to a mixture of cyclization products and HCl addition products to the carbon-carbon double bond. However, tellurolactonization of benzyl esters derived from these last acids give good yields of the tellurolactones whereas the benzyl esters derived from the former acids give mixture of products, predominating the carbon-carbon double bond adduct with the aryltellurium trichlorides.

Experimental

General

Solvents were purified according to the literature⁸. Column chromatography (flash) was performed with 230-400 mesh, 60 Å (Merck) silica gel. TLC was performed on HF-254 (Merck) plates, visualizing with a 254 nm UV lamp and with I₂ vapor or with an acidic solution of vanilin. Proton Nuclear Magnetic Resonance spectra (¹H-NMR) were recorded on a Bruker AC 200 instrument. The chemical shifts are reported on the δ scale (ppm) downfield from tetramethylsilane. Carbon Nuclear Magnetic Resonance spectra (¹³C-NMR) were obtained at 50 MHz on a Bruker AC 200 spectrometer and are reported (ppm) relative to the centre line of a triplet at 77.00 ppm for CDCl₃. Infrared (IR) spectra were measured with a Perkin Elmer

Scheme 3.

1750-FT spectrometer. Elemental analysis were performed on a Perkin Elmer 2400 equipment. All analysis were performed by Central Analítica - Instituto de Química - USP.

Tellurium tetrachloride^{1d}, p-methoxyphenyltellurium trichloride^{1d}, p-phenoxyphenyltellurium trichloride^{1d}, were obtained by literature procedures.

Reaction of γ,δ -unsaturated carboxylic acids (1) with aryltellurium trichlorides (3 or 4)

A mixture of the aryltellurium trichloride (3 or 4) (1.1 mmol) and the γ,δ -unsaturated carboxylic acid (1) (1.0 mmol) in dry chloroform (15 mL) was refluxed until the consumption of the starting carboxylic acid. The reaction was monitored by TLC. Then the solvent was evaporated and the residue was filtered through a silica gel column eluting with chloroform. The solution was dried over magnesium sulfate, the solvent was evaporated and the product was recrystallized from chloroform / petroleum ether to give the crude oil with the yields given in Table 1. When the hydrochloric acid adduct was formed it was separated by column chromatography eluting with a mixture of hexane / ethyl acetate (4:1) and then with chloroform to remove the tellurolactone.

Reaction of γ,δ -unsaturated benzyl esters (2) with aryltellurium trichlorides (3 or 4)

The same procedure described above for the reaction was used. The residue obtained after evaporation of the chloroform was chromatographed on silica gel eluting first with hexane / ethyl acetate (8:1) to remove the benzyl chloride and the non reacted benzyl ester and then with chloroform to remove the tellurated products (5 or 6).

5-[[Dichloro(4-phenoxyphenyl)-[λ]⁴-tellanyl]methyl]-3-methyl dihydro-2(3H)-furanone (5a)

¹H-NMR, 200 MHz (CDCl₃) δ 8.13-8.05 (m, 2 H), 7.10-7.04 (m, 2 H), 5.42-5.31 (m, 1 H), 5.30-5.15 (m, 1 H), 3.92-3.75 (m, 5 H), 2.93-2.80 (m, 1 H), 2.78-2.63 (m, 1 H), 2.33-2.16 (m, 1 H), 1.77 (ddd, J = 11.5, 10.95, 10.39 Hz, 1 H), 1.34 (d, J = 6.54 Hz, 3 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 177.82, 177.38, 162.12, 120.44, 115.56, 115.52, 73.05, 72.60, 55.45, 54.34, 37.68, 36.44, 35.64, 33.41, 15.27, 14.88; IR (cm⁻¹) 3350, 3478, 3415, 1783, 1594, 1571, 1493, 1300, 1261, 1183, 1139, 1029, 1007; Anal. calc. for C₁₃H₁₆Te: C, 37.26, H, 3.82; found: C, 37.48, H, 3.68.

5-[[Dichloro(4-methoxyphenyl)-[λ]⁴-tellanyl]methyl]-3-methyl dihydro-2(3H)-furanone (5b)

¹H-NMR, 200 MHz (CDCl₃) δ 8.14-8.07 (m, 2 H), 7.45-7.05 (m, 7 H), 5.44-5.33 (m, 1 H), 5.30-5.15 (m, 1 H), 3.95-3.75 (m, 2 H), 2.94-2.78 (m, 1 H), 2.68 (ddd, J = 11.95, 8.30, 5.20, 1 H), 2.33-2.24 (m, 1 H), 1.77 (ddd, J = 11.63, 11.50, 10.40 Hz, 1 H), 1.34 (d, J = 6.78 Hz, 3 H); ¹³C-NMR,

50 MHz (CDCl₃) δ 177.71, 177.27, 160.88, 154.93, 135.39, 135.13, 135.08, 134.77, 130.04, 124.82, 122.75, 121.97, 120.16, 118.77, 118.73, 72.97, 72.55, 56.10, 54.77, 37.75, 36.53, 35.70, 33.48, 15.35, 14.95; IR (cm⁻¹) 3417, 2933, 1770, 1574, 1487, 1286, 1250, 1174, 1145, 1006, 697; Anal. calc. for C₁₈H₁₈Cl₂O₃Te: C, 44.94, H, 3.74; found: C, 44.83, H, 3.51.

5-[[Dichloro(4-phenoxyphenyl)-[λ]⁴-tellanyl]methyl]-3-phenyl dihydro-2(3H)-furanone (5c)

¹H-NMR, 200 MHz (CDCl₃) δ 8.12-8.06 (m, 2 H), 7.41-7.24 (m, 5 H), 7.08-7.03 (m, 2 H), 5.55-5.29 (m, 1 H), 4.11-3.81 (m, 5 H), 2.95 (ddd, J = 12.6, 8.6, 5.6 Hz, 1 H), 2.72 (ddd, J = 13.33, 8.35, 7.45 Hz, 1 H), 2.58 (ddd, J = 13.39, 9.36, 4.7 Hz), 2.27 (ddd, J = 12.44, 12.38, 10.13 Hz); ¹³C-NMR, 50 MHz (CDCl₃) δ 175.05, 174.69, 135.85, 135.55, 135.30, 134.98, 129.09, 128.97, 128.05, 127.92, 127.68, 122.54, 120.17, 119.47, 115.73, 73.19, 73.14, 55.77, 55.57, 54.56, 47.65, 45.09, 38.55, 36.72; IR (cm⁻¹) 3086, 3061, 3032, 2942, 1776, 1583, 1570, 1494, 1456, 1298, 1258, 1183, 1158, 1137; Anal. calc. for C₁₈H₁₈Cl₂O₃Te: C, 44.94, H, 3.74; found: C, 44.66, H, 3.62.

5-[[Dichloro(4-methoxyphenyl)-[λ]⁴-tellanyl]methyl]-3-phenyl dihydro-2(3H)-furanone (5d)

¹H-NMR, 200 MHz (CDCl₃) δ 8.08 (d, J = 9.56 Hz, 2 H), 7.43-7.04 (m, 12 H), 5.58-5.49 (m, 1 H), 5.49-5.29 (m, 1 H), 4.10-3.81 (m, 3 H), 2.93 (ddd, J = 12.57, 8.52, 5.61 Hz, 1 H), 2.71 (ddd, J = 13.28, 8.31, 7.33 Hz, 1 H), 2.27 (ddd, J = 12.40, 12.39, 9.99 Hz, 1 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 175.17, 174.80, 160.98, 154.94, 135.82, 135.49, 135.20, 135.15, 134.84, 130.11, 129.08, 128.83, 127.88, 127.69, 124.90, 122.64, 121.94, 120.24, 118.85, 118.79, 73.17, 73.11, 55.72, 54.45, 47.63, 45.04, 38.46, 36.61; IR (cm⁻¹) 3061, 1775, 1575, 1486, 1243, 1197, 1175, 1143, 1006, 697; Anal. calc. for C₂₃H₂₀Cl₂O₃Te: C, 50.86, H, 3.68; found: C, 50.65, H, 3.57.

5-[[Dichloro(4-phenoxyphenyl)-[λ]⁴-tellanyl]methyl]-3,5-dimethyl dihydro-2(3H)-furanone (5e)

¹H-NMR, 200 MHz (CDCl₃) δ 8.11-8.03 (d, 2H), 7.07-7.02 (m, 2 H), 4.09 (d, J = 11.05 Hz, 1 H), 3.92 (d, J = 11.21 Hz, 1 H), 3.86 (s, 3 H), 3.07-2.85 (m, 1 H), 2.64 (dd, J = 13.14, 8.71 Hz, 1 H), 2.52 (dd, J = 12.80, 8.86 Hz, 1 H), 2.34 (dd, J = 12.09, 11.62 Hz, 1 H), 1.90 (dd, J = 12.52, 12.15 Hz, 1 H), 1.87 (s, 3 H), 1.73 (s, 3 H), 1.35 (d, J = 7.03 Hz, 3 H), 1.31 (d, J = 6.96 Hz, 3 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 177.22, 177.12, 162.24, 135.03, 134.97, 134.72, 120.16, 120.01, 115.63, 80.90, 62.52, 61.17, 55.55, 43.92, 43.67, 35.36, 34.88, 29.19, 28.31, 15.22, 14.86; IR (cm⁻¹) 2972, 2939, 1781, 1765, 1585, 1572, 1493, 1455, 1300,

1261, 1183, 1159, 1022; Anal. calc. for $C_{14}H_{18}Cl_2O_3Te$: C, 38.83, H, 4.16; found: C, 38.71, H, 4.12.

5-[[Dichloro(4-methoxyphenyl)-[λ]⁴-tellanyl]methyl]-3,5-dimethyl dihydro-2(3H)-furanone (5f)

¹H-NMR, 200 MHz (CDCl₃) δ 8.14-8.04 (m, 2 H), 7.45-7.05 (m, 7 H), 4.11 (d, J = 11.20 Hz, 1 H), 4.10 (s, 2 H), 3.95 (d, J = 11.22 Hz, 1 H), 3.11-2.85 (m, 1 H), 2.64 (dd, J = 13.16, 8.77 Hz, 1 H), 2.52 (dd, J = 12.81, 8.87 Hz, 1 H), 2.35 (dd, J = 12.14, 11.47 Hz, 1 H), 1.91 (dd, J = 12.48, 12.11, 1 H), 1.87 (s, 3 H), 1.74 (s, 3 H), 1.36 (d, J = 7.06 Hz, 3 H) 1.30 (d, J = 6.97 Hz, 3 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 177.15, 177.04, 161.02, 155.10, 135.28, 135.20, 130.15, 124.94, 122.41, 122.28, 120.27, 118.89, 80.86, 80.83, 62.90, 61.58, 44.01, 43.79, 35.41, 34.93, 29.27, 28.40, 15.27, 14.92; IR (cm⁻¹) 2976, 1767, 1596, 1572, 1479, 1236, 1223, 1176, 1170, 1124; Anal. calc.: C, 46.09, H, 4.04; found: C, 45.81, H, 3.96.

5-[[Dichloro(4-phenoxyphenyl)-[λ]⁴-tellanyl]methyl]-5-methyl-3-phenyldihydro-2(3H)-furanone (5g)

¹H-NMR, 200 MHz (CDCl₃) δ 8.14-8.07 (m, 2 H), 7.41-7.26 (m, 5 H), 7.10-7.04 (m, 2 H), 4.22 (dd, J = 12.35, 8.88 Hz, 1 H), 4.21 (d, J = 11.19 Hz, 1 H), 4.16 (d, J = 11.26 Hz, 1 H), 4.11 (d, J = 11.22 Hz, 1 H), 4.09 (dd, J = 11.25, 9.27 Hz, 1 H), 4.02 (d, J = 11.07 Hz, 1 H), 3.87 (s, 3 H), 2.92 (dd, J = 13.25, 8.88 Hz, 1 H), 2.82 (dd, J = 11.5, 10.9 Hz, 1 H), 2.76 (dd, J = 13.20, 9.50 Hz, 1 H), 2.39 (dd, J = 12.86, 12.77 Hz, 1 H), 1.93 (s, 3 H), 1.83 (s, 3 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 174.61, 162.30, 135.73, 135.55, 135.10, 135.03, 128.98, 128.92, 128.34, 128.13, 127.89, 127.82, 120.00, 115.70, 81.05, 62.54, 60.94, 55.58, 46.93, 46.16, 44.70, 44.57, 29.21, 28.25; IR (cm⁻¹) 1777, 1585, 1494, 1259, 1185, 1110; Anal. calc. for $C_{19}H_{20}Cl_2O_3Te$: C, 46.09, H, 4.04; found: C, 45.95, H, 4.03.

5-[[Dichloro(4-methoxyphenyl)-[λ]⁴-tellanyl]methyl]-5-methyl-3-phenyldihydro-2(3H)-furanone (5h)

¹H-NMR, 200 MHz (CDCl₃) δ 8.15-8.09 (m, 2 H), 7.45-7.05 (m, 12 H), 4.23 (d, J = 11.02 Hz, 1 H), 4.21 (dd, J = 13.13, 9.84 Hz, 1 H), 4.18 (d, J = 9.84 Hz, 1 H), 4.11 (d, J = 10.86 Hz, 1 H), 4.05 (dd, J = 11.37, 7.97 Hz, 1 H), 4.03 (d, J = 11.32 Hz, 1 H), 2.91 (dd, J = 13.55, 8.88 Hz, 1 H), 2.81 (dd, J = 11.5, 10.9 Hz, 1 H), 2.77 (dd, J = 13.20, 9.50 Hz, 1 H), 2.40 (dd, J = 12.86, 12.77 Hz, 1 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 174.50, 161.00, 155.05, 135.70, 135.59, 135.49, 135.29, 135.22, 134.98, 134.92, 130.12, 128.98, 128.92, 128.32, 127.89, 127.83, 124.92, 122.30, 122.03, 120.36, 120.24, 118.87, 118.66, 80.98, 80.92, 62.79, 61.24, 46.90, 46.13, 44.74, 44.57, 29.22, 28.26; IR (cm⁻¹) 1779, 1575, 1485, 1284, 1245, 1199, 1174, 1124; Anal. calc. for

$C_{24}H_{22}Cl_2O_3Te$: C, 51.74, H, 3.95; found: C, 51.54, H, 3.97.

Benzyl-4-chloro-5-[[Dichloro(4-methoxyphenyl)-[λ]⁴-tellanyl]-2-phenyl pentanoate (6a)

¹H-NMR, 200 MHz (CDCl₃) δ 8.01 (d, J = 8.80 Hz, 2 H), 7.94 (d, J = 8.81, 2 H), 7.32-7.18 (m, 10 H), 6.98 (d, J = 8.77, 2 H), 6.95 (d, J = 8.77 Hz, 2 H), 5.15 (d, J = 12.28 Hz, 1 H), 5.12 (d, J = 12.48 Hz, 1 H), 5.07 (d, J = 12.42 Hz, 1 H), 5.04 (d, J = 12.42 Hz, 1 H), 4.89-4.94 (m, 1 H), 4.56-4.52 (m, 1 H), 4.03 (dd, J = 10.35, 4.12 Hz, 1 H), 3.99-3.94 (m, 2 H), 3.84 (dd, J = 11.22 e 4.24 Hz, 1 H), 3.80 (s, 3 H), 3.78 (s, 3 H), 2.75 (ddd, J = 14.40, 10.58, 3.43 Hz, 1 H), 2.58 (ddd, J = 14.51, 9.75, 5.29 Hz, 1 H), 2.40 (ddd, J = 3.65, 9.82, 14.49 Hz, 1 H), 2.17 (ddd, J = 14.42, 9.86, 4.21 Hz, 1 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 172.37, 172.19, 162.07, 162.03, 137.58, 136.32, 135.54, 135.29, 134.98, 134.92, 128.90, 128.83, 128.33, 128.04, 127.89, 127.86, 127.79, 127.77, 127.65, 127.58, 120.26, 115.50, 115.45, 66.81, 66.74, 60.56, 60.31, 56.29, 55.69, 55.38, 48.79, 42.34, 41.42; IR (cm⁻¹) 3434, 3063, 1773, 1593, 1575, 1487, 1453, 1402, 1345, 1287, 1250, 1198, 1174, 1144, 1021.

Benzyl-4-chloro-5-[[Dichloro(4-phenoxyphenyl)-[λ]⁴-tellanyl]-2-phenyl pentanoate (6b)

¹H-NMR, 200 MHz (CDCl₃) δ 8.06 (d, J = 9.04, 2 H), 7.99 (d, J = 9.04, 2 H), 7.32-7.04 (m, 17 H), 5.16 (d, J = 12.51 Hz, 1 H), 5.12 (d, J = 12.40 Hz, 1 H), 5.06 (d, J = 12.41 Hz, 1 H), 5.05 (d, J = 12.56 Hz, 1 H), 4.98-4.90 (m, 1 H), 4.55 (m, 1 H), 4.04-3.96 (m, 3 H), 3.87 (dd, J = 11.15, 4.32 Hz, 1 H), 2.77 (ddd, J = 14.40, 10.47, 3.49 Hz, 1 H), 2.63 (ddd, J = 14.51, 9.58, 5.38 Hz, 1 H), 2.41 (ddd, J = 14.50, 9.72, 3.76 Hz, 1 H), 2.21 (ddd, J = 14.42, 9.76, 4.24 Hz, 1 H); ¹³C-NMR, 50 MHz (CDCl₃) δ 172.55, 172.38, 161.00, 160.98, 155.13, 155.10, 135.31, 135.26, 130.15, 129.09, 129.00, 128.59, 128.50, 128.43, 128.23, 128.22, 128.09, 128.06, 128.00, 127.97, 127.90, 127.83, 127.72, 127.30, 124.92, 122.63, 120.26, 118.93, 118.87, 67.12, 67.05, 61.77, 61.53, 56.44, 55.70, 48.98, 48.95, 42.54, 41.62; IR (cm⁻¹) 2971, 2934, 1773, 1575, 1487, 1454, 1402, 1287, 1250, 1174, 1145, 1005.

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