Synthesis and styrene copolymerization of novel alkoxy ring-substituted octyl phenylcyanoacrylates

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Abstract

Novel alkoxy ring-substituted octyl phenylcyanoacrylates, RPhCH=\text{C(CN)CO}_2\text{CH}_2(\text{CH}_2)_n\text{CH}_3 (where R is 2-methoxy, 3-methoxy, 4-methoxy, 2-ethoxy, 3-ethoxy, 4-ethoxy, 4-propoxy, 4-butoxy, 4-hexyloxy) were prepared and copolymerized with styrene. The acrylates were synthesized by the piperidine catalyzed Knoevenagel condensation of ring-substituted benzaldehydes and octyl cyanoacetate, and characterized by CHN analysis, IR, $^1$H and $^{13}$C NMR. All the acrylates were copolymerized with styrene in solution with radical initiation (ABCN) at 70°C. The compositions of the copolymers were calculated from nitrogen analysis.
1. Introduction

4-Methoxy ring-substituted octyl phenylcyanoacrylate (PCA) is reported in synthesis and evaluation of octocrylene-inspired compounds for UV-filter activity [1]. 3-Methoxyphenyl ethyl PCA is mentioned in 2-pyridone synthesis under solvent-free conditions [2]; in synthesis of 3,3-dimethyl-5-methoxy-1-indanone and 9,9-dimethyl-2-methoxy-5-benzosuberone [3]; in synthesis of 2-substituted 4-arylpiperidines and benzomorphans as potential analgesics [4], and synthesis of 1,4-dialkyl-4-arylpiperidines [5]. 3-Butoxy ethyl PCA is involved in preparation, reactions, and studies of conjugated heteroenoid compounds [6, 7]; in studies of conformation and configuration of α,β-unsaturated carbonyl compounds from their NMR spectra [8], and in synthesis and reactions of conjugated compounds [9]. 1-Butoxy-3-ethenylbenzene is reported in Rhodium-catalyzed cross-coupling of organoboron compounds with vinyl acetate [10]; in preparation of negative-working resist compositions [11]; in manufacturing dry visual macrocapsules and cosmetic compositions [12, 13]. 4-(hexyloxy)-1-ethenylbenzene is reported in synthesis and optical properties of bipolar quinoxaline-triphenylamine based stilbene compounds [14]; in studies of impact of charge density on host-guest interactions within amphiphilic polymer assemblies in apolar media [15]; in synthesis of resveratrol derivatives as new analgesic drugs through desensitization of the TRPA1 receptor [16]; in synthesis of alkoxy-substituted hexastyrylbenzenes [17]; in Diels-Alder reaction on the fullerene core [18], and in synthesis of new liquid crystalline compounds based on 1,4-diarylbuta-1,3-dienes [19].
We have prepared octyl alkoxy ring-substituted phenylcyanoacrylates (OPCA), RPhCH=\(\text{C(CN)CO}_2\text{CH}_2\text{(CH}_2\text{oCH}_3\)), where R is 2-methoxy, 3-methoxy, 4-methoxy, 2-ethoxy, 3-ethoxy, 4-ethoxy, 4-propoxy, 4-butoxy, 4-hexyloxy, and explored the feasibility of their copolymerization with styrene. To the best of our knowledge, except synthesis of octyl 4-methoxyphenylcyanoacrylate [1], there have been no reports on either synthesis of these compounds, nor their copolymerization with styrene [20].

2. Experimental

2-Methoxy, 3-methoxy, 4-methoxy, 2-ethoxy, 3-ethoxy, 4-ethoxy, 4-propoxy, 4-butoxy, 4-hexyloxybenzaldehydes, octyl cyanoacetate (≥98.0%), piperidine (99%), styrene (≥99%), 1,1'-azobis(cyclohexanecarbonitrile) (98%), (ABCN), and toluene (98%) supplied from Sigma-Aldrich Co., were used as received. Instrumentation is reported in [21].

3. Results and discussion

3.1. Synthesis and characterization of octyl phenylcyanoacrylates

All octyl phenylcyanoacrylates (OPCA) compounds were synthesized by Knoevenagel condensation[22] of appropriate benzaldehydes with octyl cyanoacetate, catalyzed by base, piperidine (Scheme 1).
Scheme 1. Synthesis of octyl phenylcyanoacrylates where R is 2-methoxy, 3-methoxy, 4-methoxy, 2-ethoxy, 3-ethoxy, 4-ethoxy, 4-propoxy, 4-butoxy, 4-hexyloxy.

The preparation procedure was essentially the same for all the monomers. In a typical synthesis, equimolar amounts of octyl cyanoacetate and an appropriate benzaldehyde were mixed in equimolar ratio in a 20 mL vial. A few drops of piperidine were added with stirring. The product of the reaction was isolated by filtration and purified by crystallization from 2-propanol. The condensation reaction proceeded smoothly, yielding products, which were purified by conventional techniques. The compounds were characterized by IR, $^1$H and $^{13}$C NMR spectroscopies. No stereochemical analysis of the novel alkyl ring-substituted OPCA was performed since no stereoisomers (E or/and Z) of known configuration were available.

3.1.1. Octyl 2-methoxyphenylcyanoacrylate

Yield 78%; $^1$H NMR $\delta$ 8.8 (s, 1H, CH=), 8.4-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO$_2$CH$_2$), 3.9 (s, 3H, OCH$_3$), 1.7-1.8 (q, 2H, OCH$_2$CH$_2$), 1.6-1.5 (m, 6H, OCH$_2$CH$_2$(CH$_2$)$_3$), 1.4-1.2 (m, 4H, O(CH$_2$)$_3$(CH$_3$)$_2$), 0.9 (t, 3H, CH$_3$); $^{13}$C NMR $\delta$ 164 (C=O), 150 (HC=), 135, 129, 121, 111 (Ph), 116 (CN), 102 (C=), 67 (OCH$_2$), 56 (OCH$_3$), 32 (O(CH$_2$)$_5$ CH$_2$), 29 (O(CH$_2$)$_3$(CH$_2$)$_2$), 28 (OCH$_2$CH$_2$), 26 (O(CH$_2$)$_3$CH$_2$), 23 (CH$_2$CH$_3$), 14 (CH$_3$); IR (cm$^{-1}$): 2928 (m, C-H), 2222 (m, CN), 1728 (s, C=O), 1267 (s, C-O-CH$_3$), 756 (s, C-H out of plane). Anal. Calcd. for C$_{19}$H$_{25}$NO$_3$: C, 72.35; H, 7.99; N, 4.44; Found: C, 69.28; H, 7.78; N, 4.33.

3.1.2. Octyl 3-methoxyphenylcyanoacrylate.
Yield 87%; $^1$H NMR $\delta$ 8.2 (s, 1H, CH=), 7.7-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO$_2$CH$_2$), 3.9 (s, 3H, OCH$_3$), 1.8-1.7 (q, 2H, OCH$_2$CH$_2$), 1.6-1.5 (m, 6H, OCH$_2$CH$_2$(CH$_2$)$_3$), 1.4-1.2 (m, 4H, O(CH$_2$)$_3$(CH$_2$)$_2$), 0.9 (t, 3H, CH$_3$); $^{13}$C NMR $\delta$ 163 (C=O), 155 (HC=), 160, 135, 130, 125, 120, 115 (Ph), 116 (CN), 103 (C=), 67 (OCH$_2$), 56 (OCH$_3$), 32 (O(CH$_2$)$_3$CH$_2$), 29 (O(CH$_2$)$_3$(CH$_2$)$_2$), 28 (OCH$_2$CH$_2$), 26 (O(CH$_2$)$_2$CH$_2$), 23 (CH$_2$CH$_3$), 14 (CH$_3$); IR (cm$^{-1}$): 3100-2800 (m, C-H), 2224 (m, CN), 1730 (s, C=O), 1278 (s, C-O-CH$_3$), 762 (s, C-H out of plane). Anal. Calcd. for C$_{19}$H$_{25}$NO$_3$: C, 72.35; H, 7.99; N, 4.44; Found: C, 70.95; H, 8.00; N, 4.35.

3.1.3. Octyl 4-methoxyphenylcyanoacrylate.

Yield 81%; $^1$H NMR $\delta$ 8.2 (s, 1H, CH=), 8.1-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO$_2$CH$_2$), 3.9 (s, 3H, OCH$_3$), 1.8-1.7 (q, 2H, OCH$_2$CH$_2$), 1.5-1.3 (m, 6H, OCH$_2$CH$_2$(CH$_2$)$_3$), 1.4-1.2 (m, 4H, O(CH$_2$)$_3$(CH$_2$)$_2$), 0.9 (t, 3H, CH$_3$); $^{13}$C NMR $\delta$ 164 (C=O), 155 (HC=), 163, 134, 125, 115 (Ph), 116 (CN), 100 (C=), 67 (OCH$_2$), 56 (OCH$_3$), 32 (O(CH$_2$)$_3$CH$_2$), 29 (O(CH$_2$)$_3$(CH$_2$)$_2$), 28 (OCH$_2$CH$_2$), 26 (O(CH$_2$)$_2$CH$_2$), 23 (CH$_2$CH$_3$), 14 (CH$_3$); IR (cm$^{-1}$): 3100-2800 (m, C-H), 2222 (m, CN), 1724 (s, C=O), 1263 (s, C-O-CH$_3$), 835, 762, 714 (s, C-H out of plane). Anal. Calcd. for C$_{19}$H$_{25}$NO$_3$: C, 72.35; H, 7.99; N, 4.44; Found: C, 71.67; H, 8.60; N, 4.62.

3.1.4. Octyl 2-ethoxyphenylcyanoacrylate.

Yield 87%; $^1$H NMR $\delta$ 8.2 (s, 1H, CH=), 8.3-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO$_2$CH$_2$), 4.1 (q, 2H, OCH$_2$), 1.8-1.7 (q, 2H, OCH$_2$CH$_2$), 1.5-1.4 (m, 6H, OCH$_2$CH$_2$(CH$_2$)$_3$), 1.4-1.2 (m, 4H, O(CH$_2$)$_3$(CH$_2$)$_2$), 1.3 (t, 3H, PhOCH$_2$CH$_3$), 0.9 (t, 3H, CH$_3$); $^{13}$C NMR $\delta$ 163
(C=O), 150 (HC=), 159, 135, 130, 121, 112 (Ph), 116 (CN), 102 (C=), 67 (OCH₂), 64 (PhOCH₂), 56 (OCH₃), 32 (O(CH₂)₅CH₂), 29.3 (O(CH₂)₃(CH₂)₂), 28.6 (OCH₂CH₂), 26 (O(CH₂)₂CH₂), 23 (CH₂CH₃), 14.8 (PhOCH₂CH₃), 14.1 (CH₃); IR (cm⁻¹): 2955 (m, C-H), 2222 (m, CN), 1724 (s, C=O), 1240 (s, C-O-CH₃), 808 (s, C-H out of plane). Anal.

Calcd. for C₂₀H₂₇NO₃: C, 72.92; H, 8.26; N, 4.25; Found: C, 71.01; H, 8.41; N, 4.34.

3.1.5. Octyl 3-ethoxyphenylecyanacrylate.

Yield 86%; ¹H NMR δ 8.2 (s, 1H, CH=), 7.6-7.0 (m, 4H, Ph), 4.3 (t, 2H, CO₂CH₂), 4.1 (q, 2H, OCH₂), 1.8-1.7 (q, 2H, OCH₂CH₂), 1.5-1.4 (m, 6H, OCH₂CH₂(CH₂)₃), 1.4-1.2 (m, 4H, O(CH₂)₅(CH₂)₂), 1.3 (t, 3H, PhOCH₂CH₃), 0.9 (t, 3H, CH₃); ¹³C NMR δ 163 (C=O), 155 (HC=), 159, 133, 130, 125, 121, 112 (Ph), 115.3 (CN), 103 (C=), 67 (OCH₂), 64 (PhOCH₂), 56 (OCH₃), 32 (O(CH₂)₅CH₂), 29.3 (O(CH₂)₃(CH₂)₂), 28.5 (OCH₂CH₂), 26 (O(CH₂)₂CH₂), 23 (CH₂CH₃), 14.8 (PhOCH₂CH₃), 14.1 (CH₃); IR (cm⁻¹): 2926 (m, C-H), 2224 (m, CN), 1730 (s, C=O), 1240 (s, C-O-CH₃), 827, 787, 762 (s, C-H out of plane). Anal. Calcd. for C₂₀H₂₇NO₃: C, 72.92; H, 8.26; N, 4.25; Found: C, 73.65; H, 8.40; N, 4.28.

3.1.6. Octyl 4-ethoxyphenylecyanacrylate.

Yield 71%; mp 45.4°C; ¹H NMR δ 8.2 (s, 1H, CH=), 8.1-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO₂CH₂), 4.1 (q, 2H, OCH₂), 1.8-1.7 (q, 2H, OCH₂CH₂), 1.5-1.4 (m, 6H, OCH₂CH₂(CH₂)₃), 1.4-1.2 (m, 4H, O(CH₂)₅(CH₂)₂), 1.3 (t, 3H, PhOCH₂CH₃), 0.9 (t, 3H, CH₃); ¹³C NMR δ 163 (C=O), 155 (HC=), 159, 134, 125, 115 (Ph), 116 (CN), 99 (C=), 67 (OCH₂), 64 (PhOCH₂), 32 (O(CH₂)₅CH₂), 29.3 (O(CH₂)₃(CH₂)₂), 28.5 (OCH₂CH₂),
26 (O(CH₂)₂CH₂), 23 (CH₂CH₃), 15 (PhOCH₂CH₃), 14 (CH₃); IR (cm⁻¹): 2928 (m, C-H), 2220 (m, CN), 1720 (s, C=O), 1263 (s, C-O-CH₃), 837, 762 (s, C-H out of plane). Anal. Calcd. for C₂₀H₂₇NO₃: C, 72.92; H, 8.26; N, 4.25; Found: C, 72.18; H, 8.45; N, 4.29.

3.1.7. Octyl 4-propanoxyphenylcyanoacrylate.

Yield 82%; mp 113.1°C; ¹H NMR δ 8.2 (s, 1H, CH=), 8.1-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO₂CH₂), 4.0 (q, 2H, PhOCH₂), 1.9-1.8 (m, 2H, OCH₂CH₂), 1.8-1.7 (m, 2H, Ph OCH₂CH₂), 1.5-1.4 (m, 6H, OCH₂CH₂(CH₂)₃), 1.4-1.2 (m, 4H, O(CH₂)₅(CH₂)₂), 1.1-1.0 (t, 3H, PhO(CH₂)₂CH₃), 0.9 (t, 3H, CH₃); ¹³C NMR δ 163 (C=O), 155 (HC=), 163, 134, 125, 115 (Ph), 116 (CN), 99 (C=), 70 (PhOCH₂), 67 (OCH₂), 32 (O(CH₂)₂CH₂), 29.3 (O(CH₂)₃(CH₂)₂), 28.7 (OCH₂CH₂), 26 (O(CH₂)₂CH₂), 22.8 (O(CH₂)₅CH₂), 22.5 (PhOCH₂CH₂), 14.3 (CH₂CH₃), 10.5 (PhOCH₂CH₂CH₂); IR (cm⁻¹): 2922 (m, C-H), 2220 (m, CN), 1717 (s, C=O), 1262 (s, C-O-CH₃), 841 (s, C-H out of plane). Anal. Calcd. for C₂₁H₂₉NO₃: C, 73.44; H, 8.51; N, 4.08; Found: C, 72.14; H, 8.87; N, 4.06.

3.1.8. Octyl 4-butoxyphenylcyanoacrylate.

Yield 79%; mp 84.6°C; ¹H NMR δ 8.2 (s, 1H, CH=), 8.1-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO₂CH₂), 4.0 (q, 2H, PhOCH₂), 1.9-1.8 (m, 2H, OCH₂CH₂), 1.8-1.7 (m, 2H, PhOCH₂CH₂), 1.6-1.4 (m, 6H, OCH₂CH₂(CH₂)₃), 1.4-1.2 (m, 4H, O(CH₂)₅(CH₂)₂), (m, 2H, PhO(CH₂)₂CH₂), 1.1-1.0 (t, 3H, PhO(CH₂)₃CH₂), 0.9 (t, 3H, CH₃); ¹³C NMR δ 163 (C=O), 155 (HC=), 163, 134, 124, 115 (Ph), 116 (CN), 99 (C=), 68 (PhOCH₂), 67 (OCH₂), 32 (O(CH₂)₅CH₂), 31 (PhOCH₂CH₂), 29.3 (O(CH₂)₃(CH₂)₂), 28.7 (OCH₂CH₂), 26 (O(CH₂)₂CH₂), 22.8 (O(CH₂)₅CH₂), 19 (PhO(CH₂)₂CH₂), 14.1 (CH₂CH₃), 13.8
(PhO(CH₂)₃CH₃); IR (cm⁻¹): 2916 (m, C-H), 2222 (m, CN), 1717 (s, C=O), 1273 (s, C-O-CH₃), 964, 836 (s, C-H out of plane). Anal. Calcd. for C₂₂H₃₁NO₃: C, 73.92; H, 8.74; N, 3.92; Found: C, 73.38; H, 8.57; N, 4.04.

3.1.9. Octyl 4-hexyloxyphenylcyanoacrylate.

Yield 88%; mp 80.1°C; ¹H NMR δ 8.2 (s, 1H, CH=), 8.1-6.9 (m, 4H, Ph), 4.3 (t, 2H, CO₂CH₂), 4.0 (q, 2H, PhOCH₂), 1.9-1.8 (m, 2H, OCH₂CH₂), 1.8-1.7 (m, 2H, PhOCH₂CH₂), 1.6-1.4 (m, 6H, OCH₂CH₂(CH₂)₃), 1.4-1.2 (m, 4H, O(CH₂)₅(CH₂)₂), (m, 2H, PhO(CH₂)₂(CH₂)₂, 1.0-0.8 (t, 3H, PhO(CH₂)₅CH₃), (t, 3H, CH₃); ¹³C NMR δ 163 (C=O), 155 (HC=), 163, 134, 125, 115 (Ph), 116 (CN), 99 (C=), 69 (PhOCH₂), 67 (OCH₂), 32 (O(CH₂)₅CH₂), 31.8 (PhOCH₂CH₂), 29.3 (O(CH₂)₅(CH₂)₂), 28.7 (OCH₂CH₂), 26 (O(CH₂)₂CH₂), 22.8 (O(CH₂)₆CH₂), 22.7 (PhO(CH₂)₆CH₂), 14.2 (CH₂CH₃), 14.1 (PhO(CH₂)₅CH₃); IR (cm⁻¹): 2922 (m, C-H), 2220 (m, CN), 1722 (s, C=O), 1265 (s, C-O-CH₃), 835 (s, C-H out of plane). Anal. Calcd. for C₂₄H₃₅NO₃: C, 74.77; H, 9.15; N, 3.63; Found: C, 73.31; H, 9.04; N, 3.72.

3.2. Synthesis and characterization of styrene – OPCA copolymers

Copolymers of the ST and the OPCA compounds, P(ST-co-OPCA) were prepared in 25-mL glass screw cap vials at ST/OPCA = 3 (mol) the monomer feed using 0.12 mol/L of ABCN at an overall monomer concentration 2.44 mol/L in 10 mL of toluene. The copolymerization was conducted at 70°C. After a predetermined time, the mixture was cooled to room temperature, and precipitated dropwise in methanol. The composition of the copolymers was determined based on the nitrogen content (cyano group in OPCA).
The novel synthesized OPCA compounds copolymerized readily with ST under free-radical conditions (Scheme 2) forming white flaky precipitates when their solutions were poured into methanol. The conversion of the copolymers was kept between 10 and 20% to minimize compositional drift (Table 1).

**Scheme 2.** Copolymerization of ST and the ring-substituted octyl phenylcyanoacrylates, where R is 2-methoxy, 3-methoxy, 4-methoxy, 2-ethoxy, 3-ethoxy, 4-ethoxy, 4-propany, 4-butoxy, 4-hexyloxy.

**Table 1.** Copolymerization of styrene and octyl phenylcyanoacrylates.

<table>
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<tr>
<th>R</th>
<th>Yield( ^a ) (wt%)</th>
<th>N (wt%)</th>
<th>ST in copol. (mol%)</th>
<th>OPCA in copol. (mol%)</th>
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<tr>
<td>2-Methoxy</td>
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<td>24.5</td>
</tr>
</tbody>
</table>
Nitrogen elemental analysis showed that between 19.8 and 26.2 mol% of OPCA is present in the copolymers prepared at ST/OPCA = 3 (mol), which is indicative of relatively high reactivity of the OPCA monomers towards ST radical which is typical of alkoxy ring-substituted PCA. Since OPCA monomers do not homopolymerize, the most likely structure of the copolymers would be isolated OPCA monomer units alternating with short ST sequences (Scheme 2).

The copolymers prepared in the present work are all soluble in ethyl acetate, THF, DMF and CHCl₃ and insoluble in methanol, ethyl ether, and petroleum ether.

4 Conclusions

Novel trisubstituted ethylenes, octyl alkoxyphenylcyanoacrylates, RPhCH=C(CN)CO₂CH₂(CH₂)₆CH₃ (where R is 2-methoxy, 3-methoxy, 4-methoxy, 2-ethoxy, 3-ethoxy, 4-ethoxy, 4-propoxy, 4-butoxy, 4-hexyloxy) were prepared and copolymerized with styrene.

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