Selective formation of dihydrofuran fused [60] fullerene derivatives by TEMPO mediated [3 + 2] cycloaddition of medium chain β-keto esters to C\textsubscript{60}†

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In this study, β-keto esters as readily available bio-based building blocks were used to decorate the C\textsubscript{60} sphere. Generally, cyclopropanated fullerene derivatives are obtained by the standard Bingel–Hirsch procedure. Herein, omitting the iodine from the reaction mixture and adding TEMPO afforded dihydrofuran fused C\textsubscript{60} fullerene derivatives. The mechanism of the reaction shifted from nucleophilic aliphatic substitution to oxidative [3 + 2] cycloaddition via fullerényl cations as an intermediate. This mechanism is proposed based on a series of control experiments with radical scavengers. Therefore, dihydrofuran-fused C\textsubscript{60} derivatives were selectively obtained in good yields and their structures were established based on UV-Vis, IR, NMR spectroscopy and mass spectrometry. The electrochemical properties of the synthesized compounds were investigated by cyclic voltammetry. DFT calculations were performed in order to investigate the difference in stability, electronic properties and π-electron delocalization between methano and furano fullerenes.

Results and discussion

Along this line, we explored nucleophilic cyclopropanation reaction, as one of the most efficient ways for obtaining methano fullerenes.\textsuperscript{12–14} Using the Bingel–Hirsch technique, C\textsubscript{60} 1 was treated with ethyl 3-oxoalkanoates 2a–d, iodine, and diazabicyclo[5.4.0]undec-7-ene (DBU) in toluene, at room temperature for 45 min, to afford derivatives 4a–d in 41–44% yield (Scheme 1).

We used medium chain β-keto esters 2a–d that differ in the length of the alkyl chain, starting with three methylene until nine methylene units. These materials were easily prepared...
mediated C-furan-fused fullerene derivatives were obtained. Enolate-piperidine.

These reactions were monitored by TLC, and when reactions were carried out simply by treating
C60 with anofullerenes base and iodine as oxidant.

Due to its ambiphilic nature, β-keto esters engage into [3 + 2]
cycloaddition reaction with alkenes affording substituted dihydrofurans, which are an important class of heterocyclic compounds. In reaction of β-keto esters with C60 different furan-fused fullerene derivatives were obtained. Enolate-mediated C-H activation occurs in the presence of a base usually with the aid of Cu(i)/Ag(I), Pd(II)/Cu(II) mixtures. Recently, Gao and Chen described the synthesis of furan-fused fullerenes by controlling the addition sequence of base and iodine as oxidant. In addition, Eguchi reported that furano fullerenes were obtained solely in the presence of piperidine. We were interested whether O-heteroannulation of C60 will occur if the iodine was removed from the previously described experimental protocol for the preparation of methanofullerenes 4a–d (Scheme 1).

Indeed, when reactions were carried out simply by treating C60 with β-keto esters 2a–d and DBU in toluene, at room temperature furan-fused fullerene derivatives 3a–d were obtained in 24–31% (Scheme 2).

As evidence that reaction came to completion, the colour of the solution went from purple to dark brown in just 45 min, unlike similar procedures in the literature that lasted more than 30 h. These reactions were monitored by TLC, and when reactions completed the reaction mixtures were filtered through pad of silica-gel. On this way excess of DBU was efficiently removed. Solvents were evaporated and products were isolated after purification by column chromatography. However, insoluble polymeric mixture was formed when the reaction mixture concentrated before filtering. In these reactions excess of C60 were added and isolated yields were calculated in relation to the amount of added β-keto esters. To optimize the reaction conditions and discover possible steps in the mechanism, β-keto ester 2b was chosen as a model substrate. Firstly, we varied the amount of the base used in the reaction and no product was detected when 2.5 eq. of DBU was used. Increasing the amount of DBU gradually from 5 eq. to 20 eq. increased the yield of 3b from 3% to 30% (Table 1, entries 1–5). This suggested that the formation mechanism of furano fullerenes could involve oxidative cycloaddition as described in the literature (Scheme 3). With DBU β-keto ester 2 is deprotonated and enolate is formed which attacks C60 affording anion 5. This anion goes through oxidation steps to afford radical 6, which undergoes intramolecular cyclization with the abstraction of hydrogen to give the final product 3. Oxidation steps could be mediated by O2 or another molecule of C60. The neutral molecule of C60 probably contributes more to the oxidation since the reaction is not suppressed under an argon atmosphere. Indeed, when we used a smaller amount of C60 (1 eq. C60 : 1 eq. of 2b) the yield of 3b was reduced from 30% to 20%. Radical intermediate was also proposed in the synthesis of dihydrofuran-fused fullerenes via Cu(i)/Ag(i) mediated reactions and annulation reactions a slowed or completely suppressed in the presence of radical scavenger. In order to further clarify the mechanism of this transformation, we setup several control experiments with keto ester 2b in presence of different radical scavengers under the optimized conditions (Table 1). When we used 2,6-bis(1,1-dimethyl ethyl)-4-methylphenol (BHT) and galvinoxyl (2,6-di-tert-butyl-4-oxo-2,5 cyclohexadiene-1-ylidene)-p-tolyloxy as common radical scavengers, reactions proceeded and the product 3b was obtained in diminished yields of 8–21% (Table 1, entries 6–9). Surprisingly, the addition of 2 equivalents of 2,2,6,6-tetramethylpiperidine-1-oxo (TEMPO) to the reaction mixture resulted in a yield increase of 13%. When we used a larger amount of TEMPO (5 eq.) the yield of 3b was increased from 30% to 45% (Table 1, entries 10 and 11). TEMPO acts

using reaction sequence: Reformatsky reaction, than Collins oxidation (Scheme S1†). Monofunctionalized methanofullerenes were obtained directly, in good yields, under mild conditions and short reaction times. As predicted, derivatives containing longer alkyl chains 4c and 4d showed better solubility in organic solvents than the shorter ones 4a and 4b.

| Entry | DBU (eq.) | Additive (eq.) | Yield (%) |
|-------|-----------|---------------|-----------|
| 1     | 2.5       | —             | <1        |
| 2     | 5         | —             | 3         |
| 3     | 10        | —             | 7         |
| 4     | 15        | —             | 20        |
| 5     | 20        | —             | 30        |
| 6     | 20        | BHT (2)       | 21        |
| 7     | 20        | BHT (5)       | 20        |
| 8     | 20        | Galvinoxyl (2) | 20        |
| 9     | 20        | Galvinoxyl (5) | 8         |
| 10    | 20        | TEMPO (2)     | 43        |
| 11    | 20        | TEMPO (5)     | 45        |

* a (0.02 mmol), 2b (0.013 mmol), 15 mL toluene, Ar. Isolated yield was calculated in relation to the amount of added β-keto ester 2b.
either as a radical scavenger or as an oxidant.25,28 We proposed that in these reactions, TEMPO efficiently oxidized radical 6 into cation 7. Based on the above experimental results and literature data, reaction mechanism pathway involving fullerenylium cation is proposed (Scheme 3).21,27 Finally, enolization and intramolecular nucleophilic addition of 8 afford the furan-fused fullerenes 3 as the product of the reaction. Using the optimized reaction conditions the substrate scope was investigated with keto esters 2a–d and furano fused fullerenes 3a–d were obtained in moderate or good yields 34–54% (Scheme 2).

Furano fullerenes 3a–d and methano fullerenes 4a–d were synthesized for the first time and structure of these compounds are confirmed using HRMS,1H NMR,13C NMR and UV-Vis (see Synthetic procedures and ESL†). These products show good solubility in common organic solvents such as toluene, dichloromethane and chloroform (approx. 5–10 mg mL⁻¹). Given that the solubility of highly coloured compounds is difficult to estimate precisely, the solubility of 3b and 4b was determined by UV/vis spectroscopy in chloroform to be 8.15 and 31.74 mg mL⁻¹ respectively (detailed procedure is described in ESL†).

This is very important property of furano fused fullerenes for their potential application and processability in material chemistry.

Electrochemical properties of the representative products 3b, 3d, and 4b, 4d along with C60 and 2b were investigated by cyclic voltammetry (CV) and their half-wave reduction potentials are summarized in Table 2. The obtained products exhibited essentially similar CV behaviors in the negative potential range of 0 to −2.5 V versus Fc/Fc⁺ (ESI†). β-Keto ester 2b showed one irreversible, 3b and 3d three, whilst 4b, 4d, and C60 showed four reversible, diffusion-controlled peaks. However, the first two reduction peaks obtained from the reaction products showed different peak heights for the reduction versus oxidation process. This is likely the consequence of a chemical reaction following the charge transfer step thus generating new electroactive species that are no longer available for oxidation. The first reduction potentials EI of the reaction products are similar to C₆₀, where in the case of 4b and 4d the values are even more positive than the pristine fullerene.

In general, when the C_{2v} symmetry of C₆₀ is broken it is harder for the derivative to accept the electron. In this case however, 4b and 4d with slightly more positive values for the first reduction showed to be the exception to the established rule. Both types of fullerene derivatives show essentially the same CV behaviour (Fig. 1). The observable reduction peaks differ less in the position in the potential range and more in heights of the corresponding oxidation peaks. This is especially pronounced for the first reduction process. As already mentioned, the 4a derivative could undergo a structural change under negative potential difference. The LUMO energies of furano fullerene 3b and 3d, and methano fullerene 4b and 4d were calculated using equation: E(LUMO) = −(E_{red1}^{1/2} + 4.80). LUMO/HOMO energy obtained by DFT calculation.

![Fig. 1 Cyclic voltammetry curves for 3a and 4a.](image-url)
their HOMO–LUMO energy gap, for compounds 3a–d and 4a–d are shown in Fig. 2. Also, 5-fold degenerated HOMO and 3-fold degenerated LUMO level of C\textsubscript{60}, calculated with the same method, are added for comparison. The frontier orbitals energies and distribution are practically not dependant on the size of alkyl chain attached to carbonyl group (Fig. 2), so we will limit our discussion only on compounds 3a and 4a as representatives for furano and methano fullerenes.

The 3-fold LUMO degeneracy found in C\textsubscript{60} is destroyed in furano fullerenes, but in HOMO level some degeneracy is preserved, since energy difference between HOMO and HOMO–1 orbitals are very small (0.005 eV for compound 3a) so they can be considered as a degenerate pair (Fig. 2). Relative to C\textsubscript{60}, energy of the HOMO level is raised by ~0.226 eV and, energy of the LUMO by ~0.078 eV, what makes HOMO–LUMO gap 0.148 eV smaller in furano fullerenes compared to C\textsubscript{60}. In methano fullerenes all frontier orbitals become non-degenerated, HOMO and LUMO are even higher in energy compared to furano fullerenes and, the HOMO–LUMO gap is further reduced to 1.491 eV (Fig. 2).

Frontier orbitals for 3a and 4a compounds are shown in Fig. 3. For both compounds LUMO orbital is localized almost exclusively on the fullerene part of the molecule. Results of the Becke orbital composition analysis have shown that 99.45% and 99.70% of LUMO is localized of fullerene cage for compounds 3a and 4a, respectively. On the other hand, nearly degenerate HOMO and HOMO–1 orbitals of compound 3a show significant amount of delocalization of electronic density between fullerene and β-keto ester part of the molecule; 17.0% and 11.8% of the HOMO and HOMO–1 are located at the β-keto ester part. That delocalization is much less pronounced in HOMO orbital of compound 4a; only 2.5% of HOMO electron density is located at β-keto ester part of the molecule (Fig. 3). Also, as the consequence of the C=C bond functionalization and overall symmetry lowering, the nodal plane, orthogonal to the plane of furane and cyclopropane ring is observed in fullerene part of HOMO orbitals of compounds 3a and 4a.

Finally, the different HOMO orbital delocalization between fullerene and β-keto ester part in the methano and furano fullerenes prompted us to investigate possible π-electron resonance (delocalization) between two parts of the molecule. First, Mayer bond order analysis\textsuperscript{29} using all-electron PBEPBE/6-

![Fig. 2](image2.png) Energy levels and HOMO–LUMO gaps of C\textsubscript{60} and furano (3a–3d) and methano (4a–4d) fullerenes calculated with PBEPBE/6-311G(d,p) method. All energies are given in eV.

![Fig. 3](image3.png) Frontier orbitals of compounds 3a and 4a.

Synthetic procedures

**Preparation of dihydrofuranofullerenes (3a–d)**

Procedure A. DBU (40 mg, 0.26 mmol, 20 equiv.) was added to the solution of C\textsubscript{60} 1 (15 mg, 0.02 mmol, 1.5 equiv.), β-keto ester 2a–d (0.013 mmol, 1 equiv.) in toluene (15 mL). The reaction mixture was stirred for 45 min at room temperature, under argon atmosphere. After the reaction was completed, the
reaction mixture was filtrated through a silica gel pad and washed with toluene. The solvent was removed under reduced pressure, and the residue was chromatographed on a silica gel column with petrol ether as eluent, to recover unreacted C₆₀. Further elution with petrol ether/toluene (7:3 v/v) gave pure products 3a–d.

Procedure B. DBU (40 mg, 0.26 mmol, 20 equiv.) was added to the solution of C₆₀ 1 (15 mg, 0.02 mmol, 1.5 equiv.), β-keto ester 2a–d (0.013 mmol, 1 equiv.) and TEMPO (4.1 mg, 0.026 mmol, 2 equiv.) in toluene (15 mL). The reaction mixture was stirred for 45 min at room temperature, under argon atmosphere. After the reaction was completed, the reaction mixture was filtrated through a silica gel pad and washed with toluene. The solvent was removed under reduced pressure, and the residue was chromatographed on a silica gel column with petrol ether as eluent, to recover unreacted C₆₀. Further elution with petrol ether/toluene (7:3 v/v) gave pure products 3a–d.

Compound 3a. 5.7 mg (50%) (procedure B); 3.5 mg (31%) (procedure A); brown solid; 1H NMR (500 MHz, CDCl₃): δ 4.35 (q, J = 7.1 Hz, 2H), 3.31–3.28 (t, 2H, J = 7.3 Hz), 2.16–2.08 (sex, J = 7.4 Hz, 2H), 1.33 (t, J = 7.0 Hz, 3H), 1.32 (t, J = 7.3 Hz, 3H ppm); 13C NMR (100 MHz, CDCl₃, all 1C unless indicated): δ 172.6, 164.2, 148.7, 147.4, 146.5, 146.2 (2C), 146.0 (2C), 145.7, 145.4, 145.2, 140.5, 144.8, 144.5 (2C), 142.2, 141.3, 142.8 (2C), 142.7, 142.6, 142.5, 142.3, 141.6, 141.5, 139.9, 133.4, 137.4, 135.2, 104.8, 103.0 (sp³-C of C₆₀), 71.6 (sp³-C of C₆₀), 60.5, 30.8, 21.0, 14.4, 14.2 ppm; IR (ATR): ν 2951, 2926, 2866, 2730, 1700, 1630, 1539, 1458, 1309, 1223, 1084, 795, 525 cm⁻¹; UV-Vis (CHCl₃): λ 429, 457, 483, 687 nm (ε = 3444, 2745, 2264, 227 dm³ mol⁻¹ cm⁻¹). Positive HRMS: calcd for [M + Na]⁺ [C₆₀H₁₂O₂Na⁺]: 983.1618; found, 983.1618.

Preparation of metanofullerenes (4a–d). DBU (0.032 mmol, 2.5 equiv.) was added to the solution of C₆₀ 1 (15 mg, 0.02 mmol, 1.5 equiv.), β-keto ester (0.013 mmol, 1 equiv.) 2a–d and iodine (0.02 mmol, 1.5 equiv.) in toluene (15 mL). The reaction mixture was stirred for 45 min at room temperature, under argon atmosphere. After the reaction was completed, the reaction mixture was filtrated through a silica gel pad and washed with toluene, the solvent was removed under reduced pressure. The obtained crude product was chromatographed on a silica gel column with petrol ether as eluent, to recover unreacted C₆₀. Further elution with petrol ether/toluene (7:3 v/v) gave pure products 4a–d.

Compound 4a. 5.0 mg (44%); brown solid; 1H NMR (500 MHz, CDCl₃): δ 4.58 (q, J = 7.1 Hz, 2H), 3.22 (t, J = 7.2 Hz, 2H), 1.94 (sex, J = 7.3 Hz, 2H), 1.50 (t, J = 7.1 Hz, 3H), 1.10 (t, J = 7.4 Hz, 3H ppm); 11C NMR (125 MHz, CDCl₃, all 1C unless indicated): δ 196.4, 162.4, 145.80, 145.48, 145.39, 145.36, 145.32 (2C), 145.27, 145.17, 144.97, 144.86 (3C), 144.71, 144.70, 144.00, 143.98, 143.30, 143.25, 143.17 (3C), 143.10, 143.26, 144.05, 141.16, 141.12, 139.40, 138.20, 72.52 (2C, sp³-C of C₆₀), 63.7, 59.4, 43.2, 17.6, 14.4, 13.9 ppm; IR (ATR): ν 2955, 2919, 1713, 1535, 1456, 1428, 1231, 1182, 579, 523 cm⁻¹; UV-Vis (CHCl₃): λ 409, 444, 483, 700 nm (ε = 2117, 1266, 152 cm⁻³ mol⁻¹ cm⁻¹). Positive HRMS: calcd for [M + Na]⁺ [C₆₀H₁₂O₂Na⁺]: 989.0679; found, 989.0681.

Compound 4b. 5.0 mg (43%); brown solid; 1H NMR (500 MHz, CDCl₃): δ 4.58 (q, J = 7.1 Hz, 2H), 3.23 (t, J = 7.3 Hz, 2H), 1.91 (quin, J = 7.3 Hz, 2H), 1.50 (t, J = 7.1 Hz, 3H), 1.10 (t, J = 7.4 Hz, 3H ppm); 11C NMR (125 MHz, CDCl₃, all 1C unless indicated): δ 196.6, 162.4, 145.81, 145.49, 145.40, 145.37, 145.33 (2C), 145.27, 145.17, 144.97, 144.86 (3C), 144.71, 144.70, 144.00, 143.98, 143.30, 143.25, 143.17 (3C), 143.10, 143.26, 144.05, 141.16, 141.12, 139.40, 138.20, 72.52 (2C, sp³-C of C₆₀), 63.7, 59.4, 43.2, 17.6, 14.4, 13.9 ppm; IR (ATR): ν 2955, 2919, 1713, 1535, 1456, 1428, 1231, 1182, 579, 523 cm⁻¹; UV-Vis (CHCl₃): λ 426, 492, 690 nm (ε = 2117, 1266, 152 cm⁻³ mol⁻¹ cm⁻¹). Positive HRMS: calcd for [M + Na]⁺ [C₆₀H₁₂O₂Na⁺]: 989.0679; found, 989.0681.
$\text{Compound 4c:}$ 5.1 mg (42%); brown solid; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 4.57 (q, $J$ = 7.4 Hz, 2H), 3.23 (t, $J$ = 7.3 Hz, 2H), 1.90 (quin, $J$ = 7.5 Hz, 2H), 1.50 (t, $J$ = 7.1 Hz, 3H), 1.48–1.43 (m, 2H), 1.42–1.37 (m, 2H), 1.35–1.30 (m, 4H), 0.90 (t, $J$ = 6.9 Hz, 3H) ppm; $^{13}$C NMR (125 MHz, CDCl$_3$, all 1C unless indicated): $\delta$ 196.6, 164.2, 145.81, 145.48, 145.39, 145.36, 145.32 (2C), 145.26, 145.17, 144.97, 144.86 (3C), 144.71, 144.69, 144.00, 143.98, 143.30, 143.25, 143.16 (3C), 143.10, 142.36, 142.05, 141.16, 141.11, 139.38, 138.20, 72.55 (2C, sp$^3$-C of C$_{60}$), 63.7, 59.4, 41.3, 31.8, 29.2, 24.1, 22.8, 14.4, 14.4 ppm; IR (ATR): v 2916, 2926, 2916, n, 2852, 1716, 1539, 1456, 1427, 1226, 1180, 579, 523 cm$^{-1}$.

$\text{Compound 4d:}$ 5.1 mg (41%); brown solid; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 4.57 (q, $J$ = 7.4 Hz, 2H), 3.23 (t, $J$ = 7.3 Hz, 2H), 1.90 (quin, $J$ = 7.5 Hz, 2H), 1.50 (t, $J$ = 7.1 Hz, 3H), 1.48–1.42 (m, 2H), 1.41–1.35 (m, 2H), 1.34–1.25 (m, 8H), 0.89 (t, $J$ = 6.8 Hz, 3H) ppm; $^{13}$C NMR (125 MHz, CDCl$_3$, all 1C unless indicated): $\delta$ 196.6, 164.2, 145.81, 145.48, 145.39, 145.36, 145.32 (2C), 145.26, 145.17, 144.97, 144.86 (3C), 144.71, 144.69, 144.00, 143.98, 143.30, 143.25, 143.16 (3C), 143.10, 142.36, 142.05, 141.16, 141.11, 139.38, 138.20, 72.55 (2C, sp$^3$-C of C$_{60}$), 63.7, 59.4, 41.3, 32.0, 29.61, 29.57, 29.4, 29.3, 24.1, 22.8, 14.4, 14.4 ppm; IR (ATR): v 2920, 2849, 2733, 2679, 1722, 1539, 1459, 1428, 1229, 1182, 582, 525 cm$^{-1}$; UV-Vis (CHCl$_3$): $\lambda$ 426, 492, 690 nm ($\epsilon$ = 2186, 1303, 170 dm$^3$ mol$^{-1}$ cm$^{-1}$). Positive HRMS: calcd for [M + Na]$^+$ (C$_{72}$H$_{20}$O$_3$Na)$^+$: 955.1305; found, 955.1316.

$\text{Conclusions}$

In summary, we have developed a tuneable procedure for the preparation of methano and furano fused fullerenes in the reaction of C$_{60}$ with bioavailable medium chain $\beta$-keto esters in the presence of DBU and with or without iodine. Preparation of furano-fused fullerenes proceeds $via$ oxidative cycloaddition and the pathway involving fullerenyl cation intermediate is proposed. With the assistance of TEMPO reaction is more efficient and furano fused fullerenes were obtained in moderate or good yields. This reaction exhibits a useful route for preparation of different fullerene derivatives under mild reaction conditions with short reaction times. Furano-fused fullerenes 3b and 3d could make good candidates for acceptor component in organic photovoltaic devices based on values for the first reduction peak as well owing to their improved solubility and stability as rationalized by DFT calculations.

$\text{Author contributions}$

J. J., Z. T. V., and A. M. performed the experiments and analysed data. J. J. and V. M. designed the experiments. A. M. performed CV experiments and analysed data. M. M. performed electronic structure calculation and analysed data. V. M. supervised the project and prepared the original manuscript. All authors proofread, commented on, and approved the final manuscript for submission.

$\text{Conflicts of interest}$

There are no conflicts to declare.

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