

## SUPPORTING INFORMATION

### Fullerene C<sub>60</sub> conjugated with phenols as new hybrid antioxidants increasing the oxidative stability of polymers at high temperatures.

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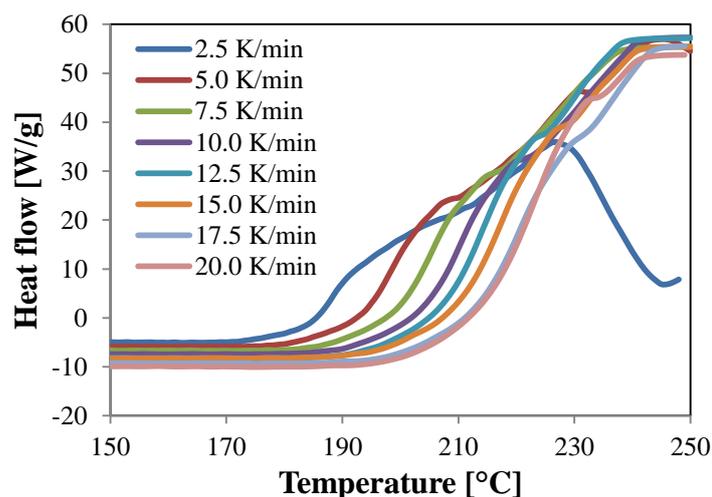
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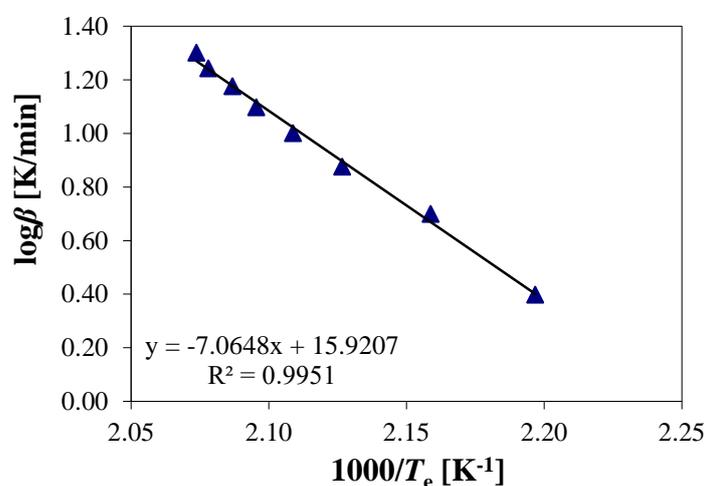
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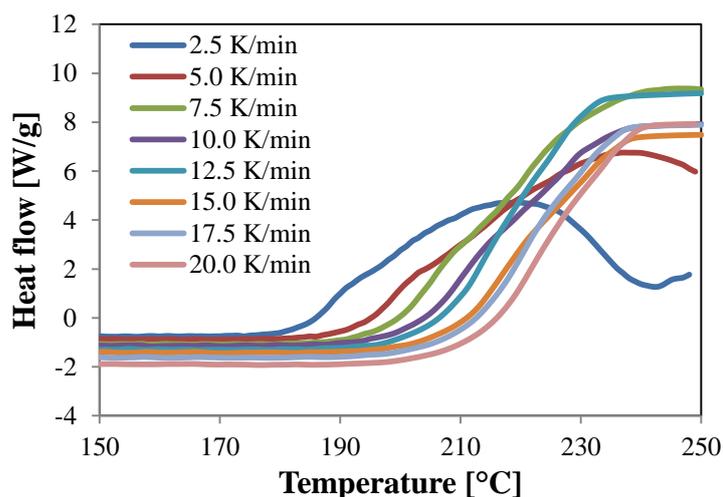
**Figure S1.** DSC curves of non-isothermal oxidative decomposition of pure HDPE.



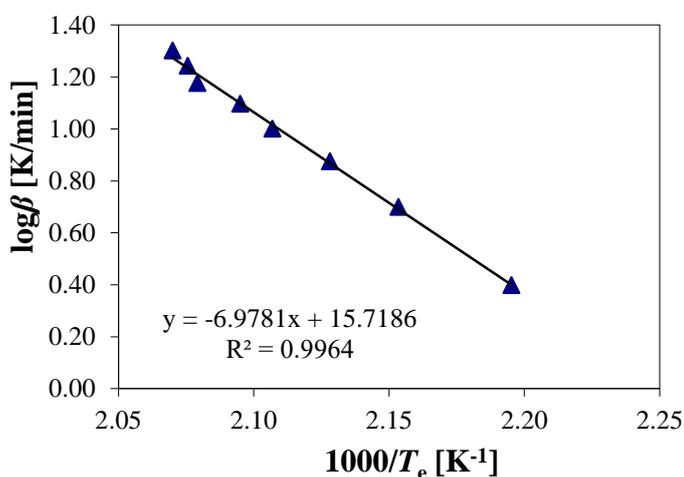
**Figure S2.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of pure HDPE.

**Table S1.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of pure HDPE. Symbols:  $\beta$  - heating rate  $T_e$  - temperature of extrapolated start of oxidation,  $a$ ,  $b$ ,  $R^2$  - statistical parameters of straight line equation  $\log\beta = a/T_e + b$  (eq. 1 in the main manuscript text),  $E_a$  - overall activation energy,  $Z$  - pre-exponential factor,  $k$  - overall rate constants of oxidation. The errors of  $E_a$  were calculated from the standard error  $\sigma$  of the slope  $a$  calculated with confidence level 90% ( $\sigma_{90\%}$ ).

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	455	$a = -7.0648$
5.0	463	$b = 15.9207$
7.5	470	$R^2 = 0.9951$
10.0	474	$E_a = 129 \pm 7 \text{ kJ/mol}$
12.5	477	$Z = 1.11 \times 10^{14} \text{ min}^{-1}$
15.0	479	$k(50^\circ\text{C}) = 1.80 \times 10^{-7} \text{ min}^{-1}$
17.5	481	$k(100^\circ\text{C}) = 1.10 \times 10^{-4} \text{ min}^{-1}$
20.0	482	$k(150^\circ\text{C}) = 1.47 \times 10^{-2} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 7.02 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.60 \times 10^1 \text{ min}^{-1}$



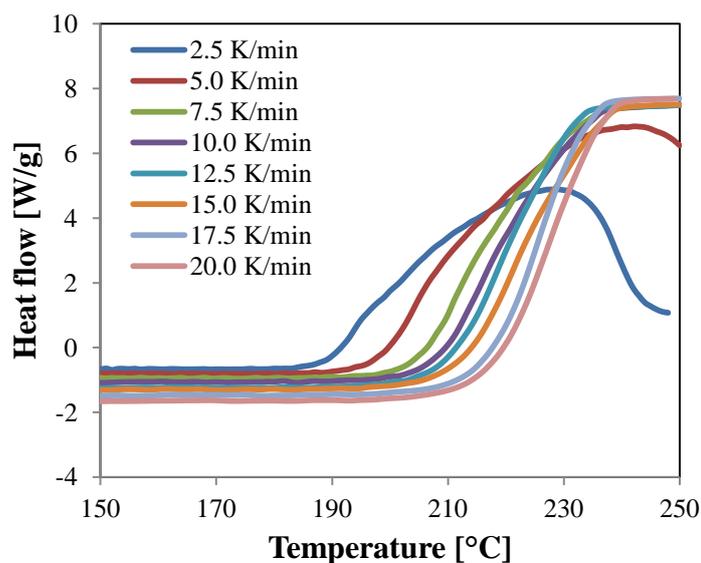
**Figure S3.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60** ( $C = 0.065\%$  w/w).



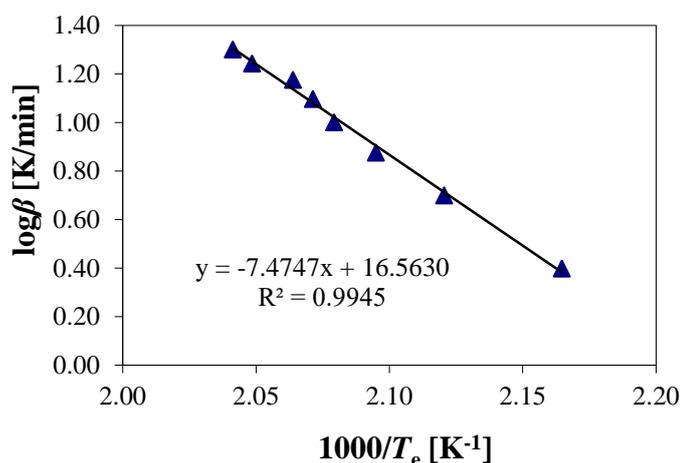
**Figure S4.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60** ( $C = 0.065\%$  w/w).

**Table S2.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60** ( $C = 0.065\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	455	$a = -6.9781$
5.0	464	$b = 15.7186$
7.5	470	$R^2 = 0.9964$
10.0	474	$E_a = 127 \pm 5 \text{ kJ/mol}$
12.5	477	$Z = 7.07 \times 10^{13} \text{ min}^{-1}$
15.0	480	$k(50^\circ\text{C}) = 2.06 \times 10^{-7} \text{ min}^{-1}$
17.5	481	$k(100^\circ\text{C}) = 1.16 \times 10^{-4} \text{ min}^{-1}$
20.0	482	$k(150^\circ\text{C}) = 1.47 \times 10^{-2} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 6.66 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.46 \times 10^1 \text{ min}^{-1}$



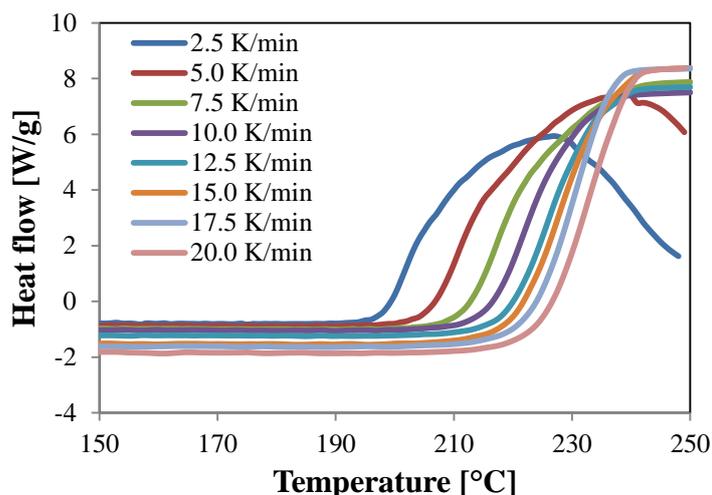
**Figure S5.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60** ( $C = 0.125\%$  w/w).



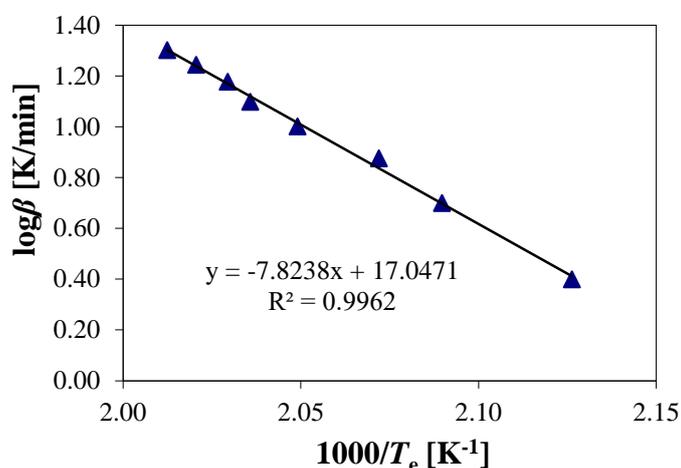
**Figure S6.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60** ( $C = 0.125\%$  w/w).

**Table S3.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60** ( $C = 0.125\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	461	$a = -7.4747$
5.0	471	$b = 16.5630$
7.5	477	$R^2 = 0.9945$
10.0	480	$E_a = 136 \pm 8 \text{ kJ/mol}$
12.5	482	$Z = 4.61 \times 10^{14} \text{ min}^{-1}$
15.0	484	$k(50^\circ\text{C}) = 4.65 \times 10^{-8} \text{ min}^{-1}$
17.5	487	$k(100^\circ\text{C}) = 4.12 \times 10^{-5} \text{ min}^{-1}$
20.0	489	$k(150^\circ\text{C}) = 7.33 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 4.37 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.19 \times 10^1 \text{ min}^{-1}$



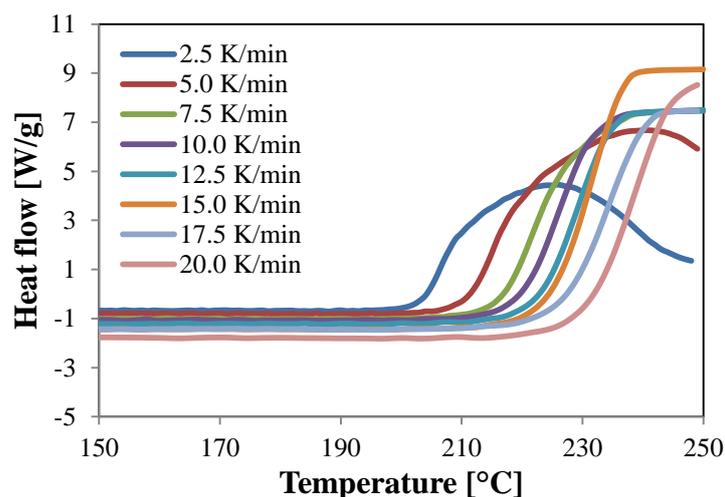
**Figure S7.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60** ( $C = 0.250\%$  w/w).



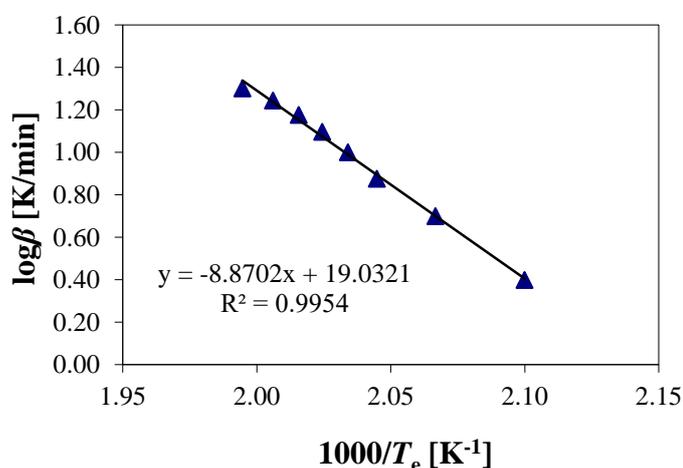
**Figure S8.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60** ( $C = 0.250\%$  w/w).

**Table S4.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60** ( $C = 0.250\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	470	$a = -7.8238$
5.0	478	$b = 17.0471$
7.5	482	$R^2 = 0.9962$
10.0	488	$E_a = 142 \pm 8 \text{ kJ/mol}$
12.5	491	$Z = 1.34 \times 10^{15} \text{ min}^{-1}$
15.0	493	$k(50^\circ\text{C}) = 1.27 \times 10^{-8} \text{ min}^{-1}$
17.5	495	$k(100^\circ\text{C}) = 1.55 \times 10^{-5} \text{ min}^{-1}$
20.0	497	$k(150^\circ\text{C}) = 3.51 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 2.53 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 8.05 \times 10^0 \text{ min}^{-1}$



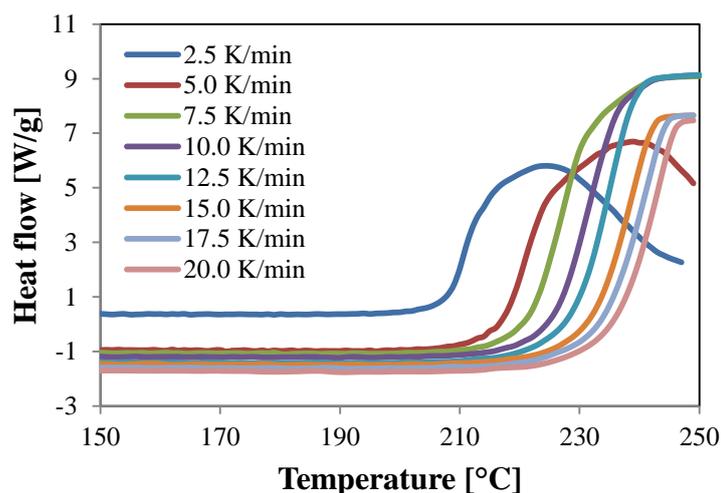
**Figure S9.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60** ( $C = 0.500\%$  w/w).



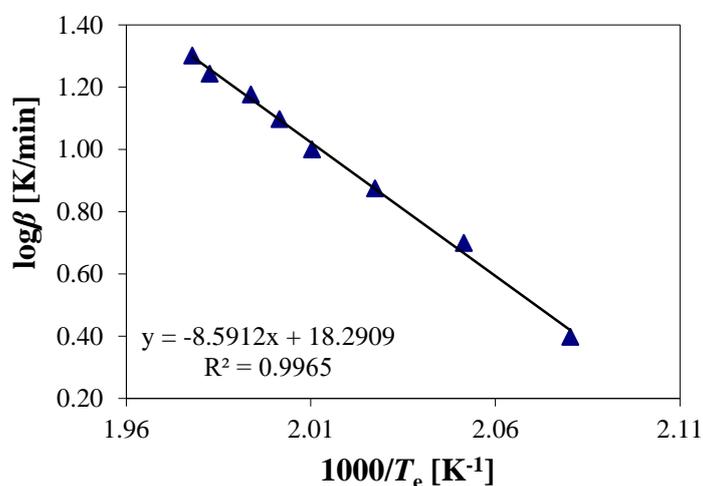
**Figure S10.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60** ( $C = 0.500\%$  w/w).

**Table S5.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60** ( $C = 0.500\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	476	$a = -8.8702$
5.0	483	$b = 19.0321$
7.5	488	$R^2 = 0.9954$
10.0	491	$E_a = 161 \pm 8 \text{ kJ/mol}$
12.5	493	$Z = 1.14 \times 10^{17} \text{ min}^{-1}$
15.0	496	$k(50^\circ\text{C}) = 9.03 \times 10^{-10} \text{ min}^{-1}$
17.5	499	$k(100^\circ\text{C}) = 2.84 \times 10^{-6} \text{ min}^{-1}$
20.0	501	$k(150^\circ\text{C}) = 1.33 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 1.70 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 8.59 \times 10^0 \text{ min}^{-1}$



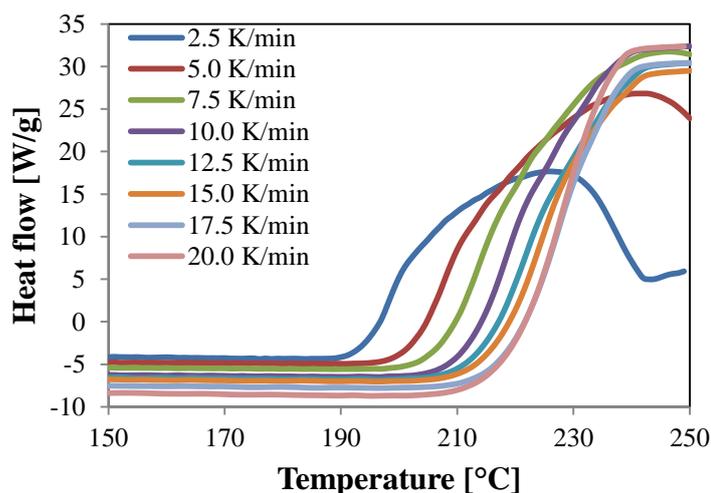
**Figure S11.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60** ( $C = 1.00\%$  w/w).



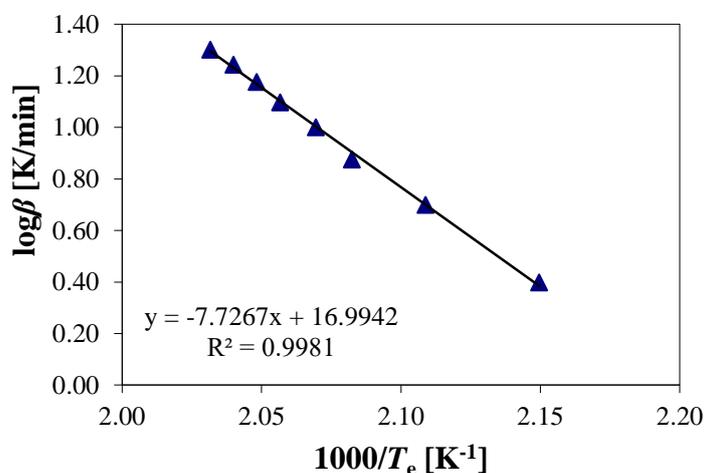
**Figure S12.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60** ( $C = 1.00\%$  w/w).

**Table S6.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60** ( $C = 1.00\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	480	$a = -8.5912$
5.0	487	$b = 18.2909$
7.5	493	$R^2 = 0.9965$
10.0	497	$E_a = 156 \pm 7 \text{ kJ/mol}$
12.5	499	$Z = 2.14 \times 10^{16} \text{ min}^{-1}$
15.0	501	$k(50^\circ\text{C}) = 1.12 \times 10^{-9} \text{ min}^{-1}$
17.5	504	$k(100^\circ\text{C}) = 2.73 \times 10^{-6} \text{ min}^{-1}$
20.0	505	$k(150^\circ\text{C}) = 1.06 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 1.16 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 5.17 \times 10^0 \text{ min}^{-1}$



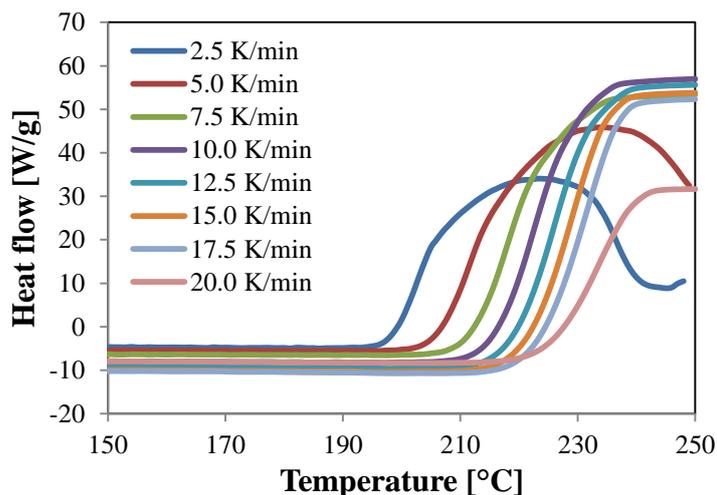
**Figure S13.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-I** ( $C = 0.065\%$  w/w).



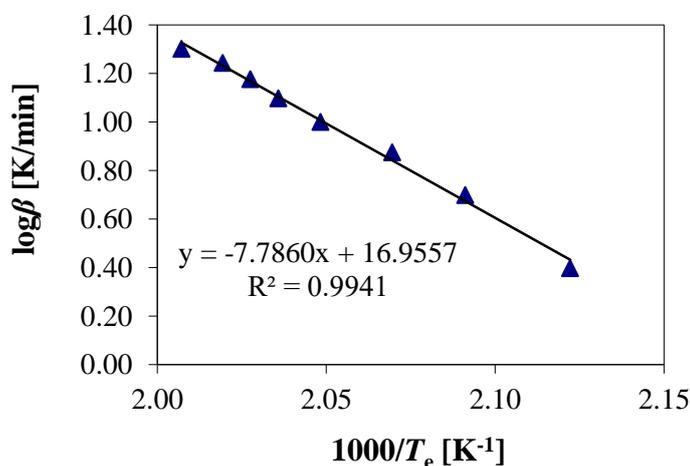
**Figure S14.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-I** ( $C = 0.065\%$  w/w).

**Table S7.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-I** ( $C = 0.065\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	465	$a = -7.7267$
5.0	474	$b = 16.9942$
7.5	480	$R^2 = 0.9981$
10.0	483	$E_a = 141 \pm 5 \text{ kJ/mol}$
12.5	486	$Z = 1.2 \times 10^{15} \text{ min}^{-1}$
15.0	488	$k(50^\circ\text{C}) = 2.20 \times 10^{-8} \text{ min}^{-1}$
17.5	490	$k(100^\circ\text{C}) = 2.45 \times 10^{-5} \text{ min}^{-1}$
20.0	492	$k(150^\circ\text{C}) = 5.20 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 3.55 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.08 \times 10^1 \text{ min}^{-1}$



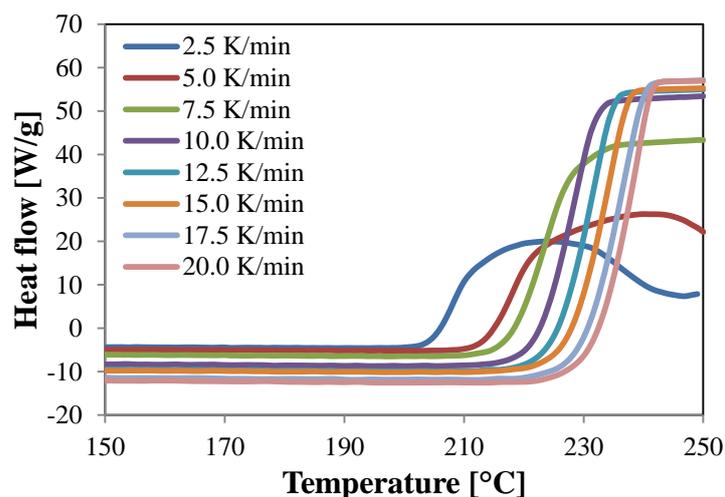
**Figure S15.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-I** ( $C = 0.125\%$  w/w).



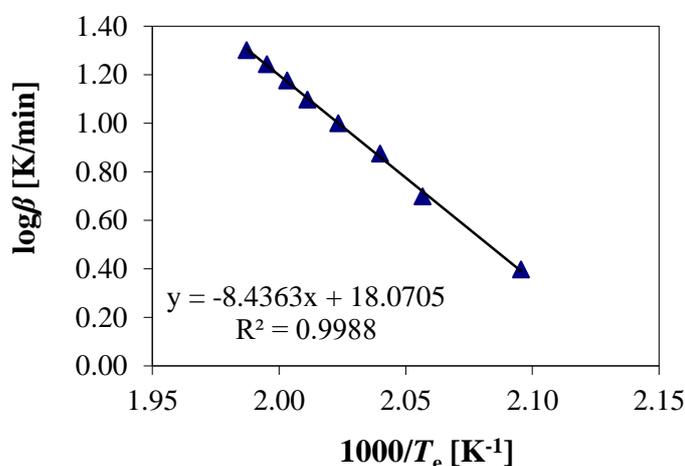
**Figure S16.** Plot of  $\log \beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-I** ( $C = 0.125\%$  w/w).

**Table S8.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-I** ( $C = 0.125\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	471	$a = -7.7860$
5.0	478	$b = 16.9557$
7.5	483	$R^2 = 0.9941$
10.0	488	$E_a = 142 \pm 8 \text{ kJ/mol}$
12.5	491	$Z = 1.1 \times 10^{15} \text{ min}^{-1}$
15.0	493	$k (50^\circ\text{C}) = 1.34 \times 10^{-8} \text{ min}^{-1}$
17.5	495	$k (100^\circ\text{C}) = 1.57 \times 10^{-5} \text{ min}^{-1}$
20.0	498	$k (150^\circ\text{C}) = 3.47 \times 10^{-3} \text{ min}^{-1}$
		$k (200^\circ\text{C}) = 2.45 \times 10^{-1} \text{ min}^{-1}$
		$k (250^\circ\text{C}) = 7.67 \times 10^0 \text{ min}^{-1}$



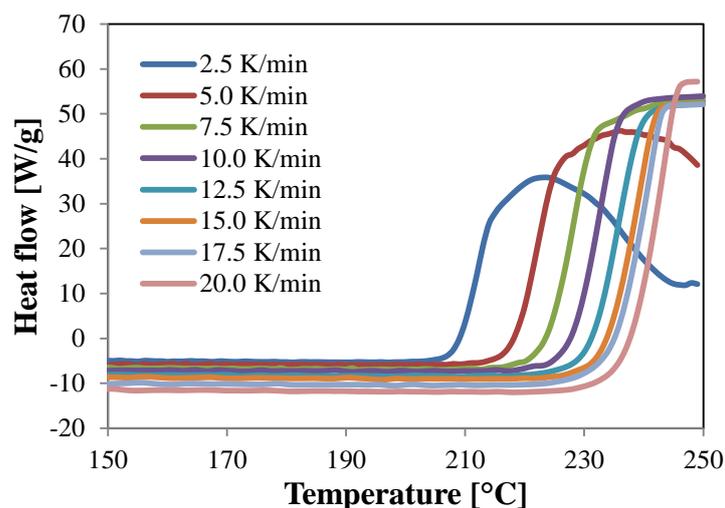
**Figure S17.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-I** ( $C = 0.250\%$  w/w).



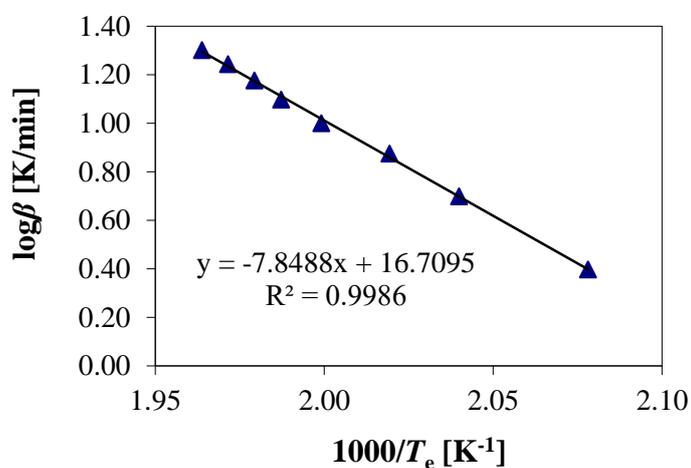
**Figure S18.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-I** ( $C = 0.250\%$  w/w).

**Table S9.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-I** ( $C = 0.250\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	477	$a = -8.4363$
5.0	486	$b = 18.0705$
7.5	490	$R^2 = 0.9988$
10.0	494	$E_a = 154 \pm 4$ kJ/mol
12.5	497	$Z = 1.31 \times 10^{16}$ min <sup>-1</sup>
15.0	499	$k(50^\circ\text{C}) = 1.96 \times 10^{-9}$ min <sup>-1</sup>
17.5	501	$k(100^\circ\text{C}) = 4.16 \times 10^{-6}$ min <sup>-1</sup>
20.0	503	$k(150^\circ\text{C}) = 1.44 \times 10^{-3}$ min <sup>-1</sup>
		$k(200^\circ\text{C}) = 1.45 \times 10^{-1}$ min <sup>-1</sup>
		$k(250^\circ\text{C}) = 6.07 \times 10^0$ min <sup>-1</sup>



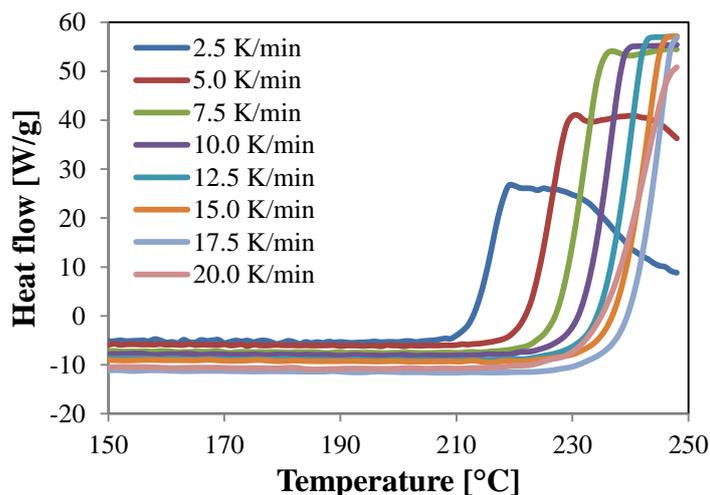
**Figure S19.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-I** ( $C = 0.500\%$  w/w).



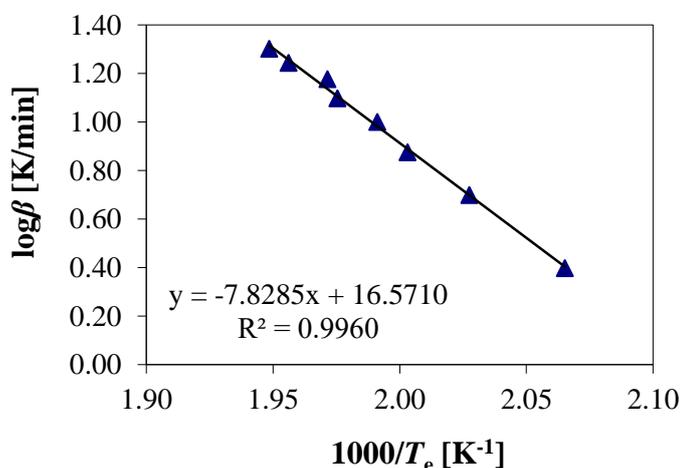
**Figure S20.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-I** ( $C = 0.500\%$  w/w).

**Table S10.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-I** ( $C = 0.500\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	481	$a = -7.8488$
5.0	490	$b = 16.7095$
7.5	495	$R^2 = 0.9986$
10.0	500	$E_a = 143 \pm 4$ kJ/mol
12.5	503	$Z = 6.15 \times 10^{14}$ min <sup>-1</sup>
15.0	504	$k(50^\circ\text{C}) = 4.52 \times 10^{-9}$ min <sup>-1</sup>
17.5	507	$k(100^\circ\text{C}) = 6.11 \times 10^{-6}$ min <sup>-1</sup>
20.0	509	$k(150^\circ\text{C}) = 1.41 \times 10^{-3}$ min <sup>-1</sup>
		$k(200^\circ\text{C}) = 1.03 \times 10^{-1}$ min <sup>-1</sup>
		$k(250^\circ\text{C}) = 3.32 \times 10^0$ min <sup>-1</sup>



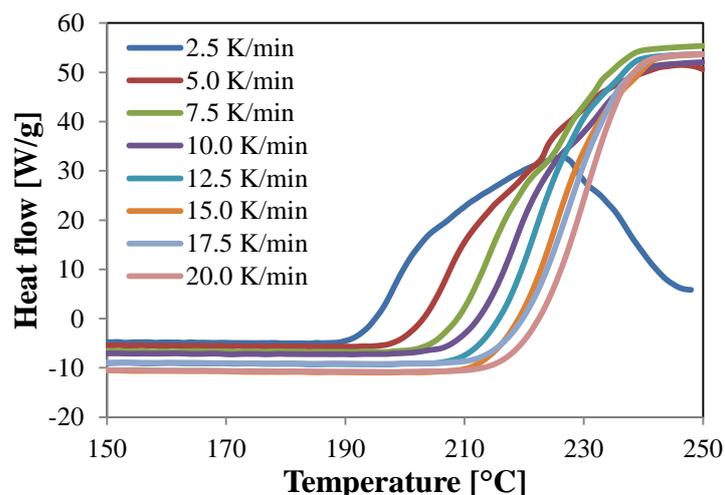
**Figure S21.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-I** ( $C = 1.00\%$  w/w).



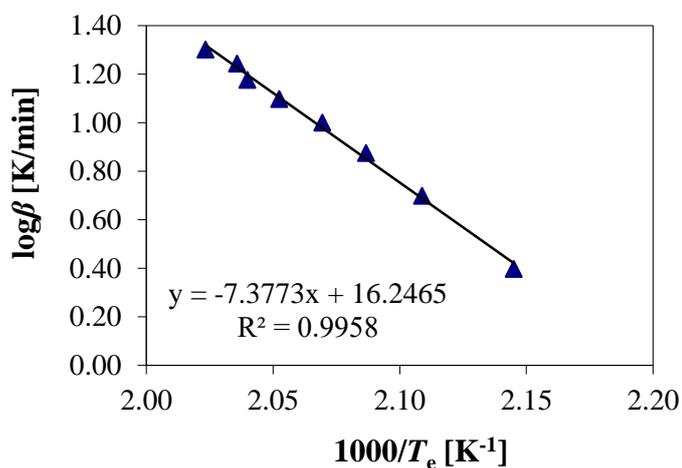
**Figure S22.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-I** ( $C = 1.00\%$  w/w).

**Table S11.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-I** ( $C = 1.00\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	481	$a = -7.8285$
5.0	490	$b = 16.5710$
7.5	495	$R^2 = 0.9960$
10.0	500	$E_a = 142 \pm 7 \text{ kJ/mol}$
12.5	503	$Z = 4.49 \times 10^{14} \text{ min}^{-1}$
15.0	504	$k(50^\circ\text{C}) = 4.12 \times 10^{-9} \text{ min}^{-1}$
17.5	507	$k(100^\circ\text{C}) = 5.02 \times 10^{-6} \text{ min}^{-1}$
20.0	509	$k(150^\circ\text{C}) = 1.14 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 8.26 \times 10^{-2} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 2.64 \times 10^0 \text{ min}^{-1}$



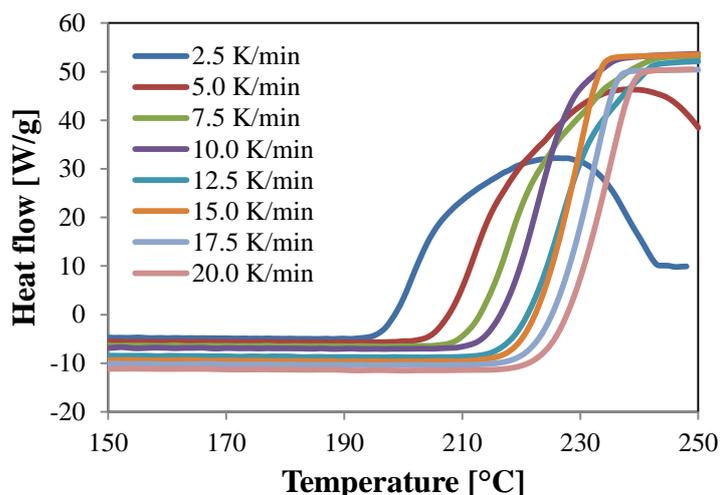
**Figure S23.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-II** ( $C = 0.065\%$  w/w).



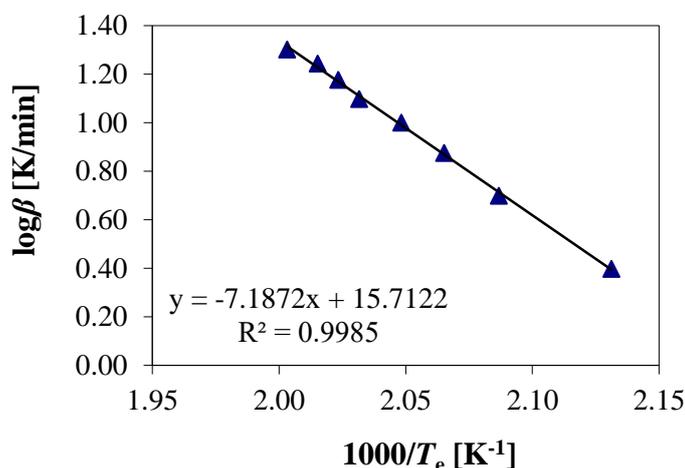
**Figure S24.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-II** ( $C = 0.065\%$  w/w).

**Table S12.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-II** ( $C = 0.065\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	466	$a = -7.3773$
5.0	474	$b = 16.2465$
7.5	479	$R^2 = 0.9958$
10.0	483	$E_a = 134 \pm 6 \text{ kJ/mol}$
12.5	487	$Z = 2.26 \times 10^{14} \text{ min}^{-1}$
15.0	490	$k(50^\circ\text{C}) = 4.40 \times 10^{-8} \text{ min}^{-1}$
17.5	491	$k(100^\circ\text{C}) = 3.56 \times 10^{-6} \text{ min}^{-1}$
20.0	494	$k(150^\circ\text{C}) = 5.93 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 3.35 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 8.75 \times 10^0 \text{ min}^{-1}$



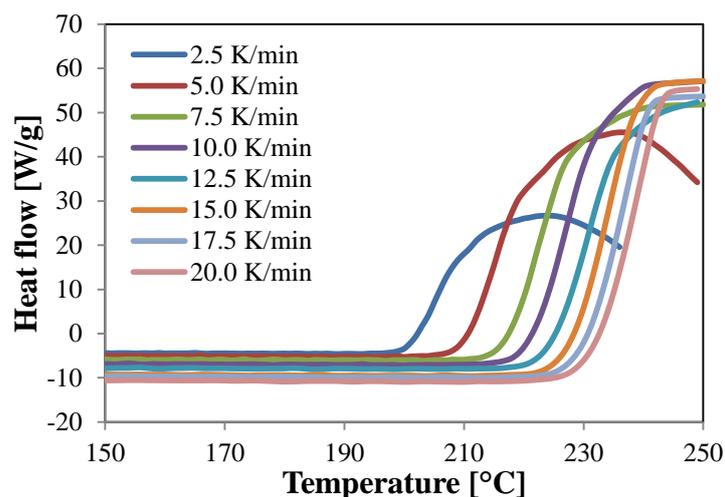
**Figure S25.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-II** ( $C = 0.125\%$  w/w).



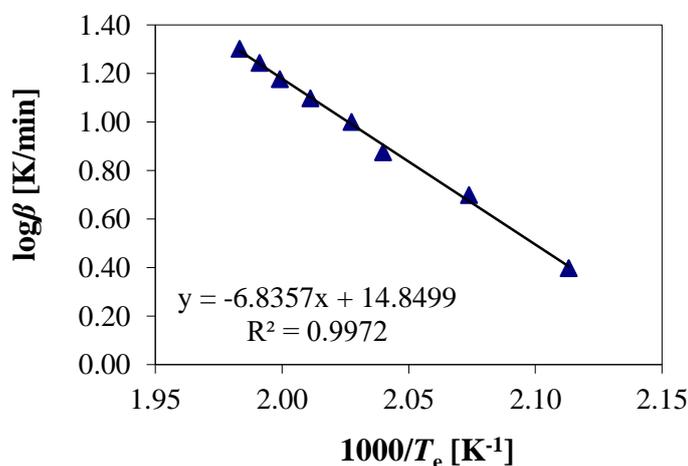
**Figure S26.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-II** ( $C = 0.125\%$  w/w).

**Table S13.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-II** ( $C = 0.125\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	469	$a = -7.1872$
5.0	479	$b = 15.7122$
7.5	474	$R^2 = 0.9985$
10.0	488	$E_a = 131 \pm 4 \text{ kJ/mol}$
12.5	492	$Z = 6.76 \times 10^{13} \text{ min}^{-1}$
15.0	494	$k(50^\circ\text{C}) = 4.79 \times 10^{-8} \text{ min}^{-1}$
17.5	496	$k(100^\circ\text{C}) = 3.26 \times 10^{-5} \text{ min}^{-1}$
20.0	499	$k(150^\circ\text{C}) = 4.76 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 2.42 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 5.82 \times 10^0 \text{ min}^{-1}$



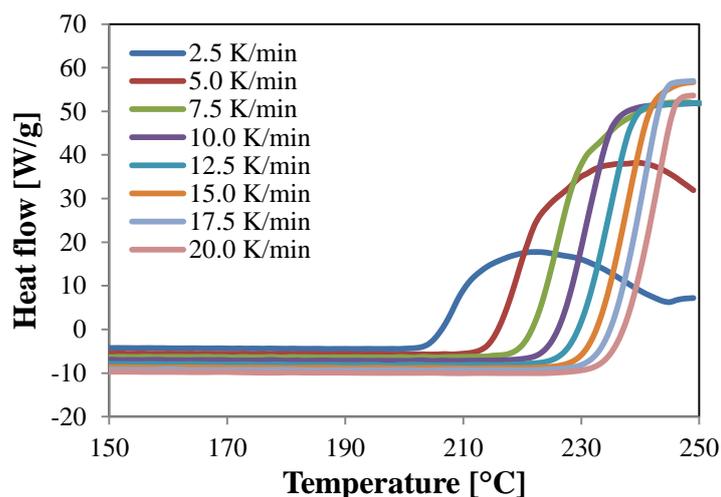
**Figure S27.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-II** ( $C = 0.250\%$  w/w).



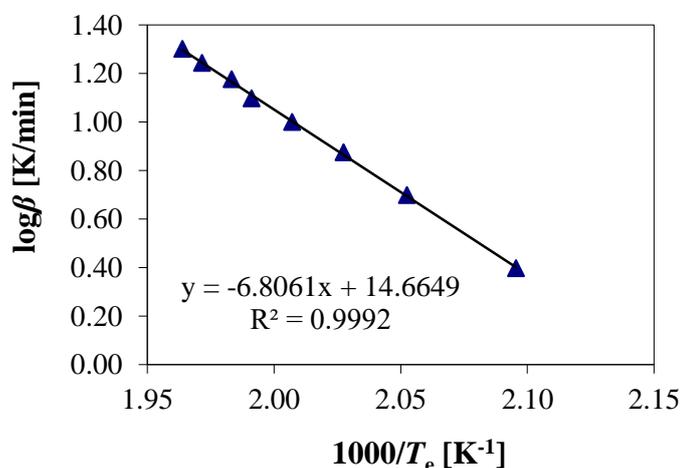
**Figure S28.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-II** ( $C = 0.250\%$  w/w).

**Table S14.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-II** ( $C = 0.250\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	473	$a = -6.8357$
5.0	482	$b = 14.8499$
7.5	490	$R^2 = 0.9972$
10.0	493	$E_a = 124 \pm 5 \text{ kJ/mol}$
12.5	497	$Z = 9.76 \times 10^{12} \text{ min}^{-1}$
15.0	500	$k(50^\circ\text{C}) = 7.48 \times 10^{-8} \text{ min}^{-1}$
17.5	502	$k(100^\circ\text{C}) = 3.70 \times 10^{-5} \text{ min}^{-1}$
20.0	504	$k(150^\circ\text{C}) = 4.24 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 1.78 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 3.66 \times 10^0 \text{ min}^{-1}$



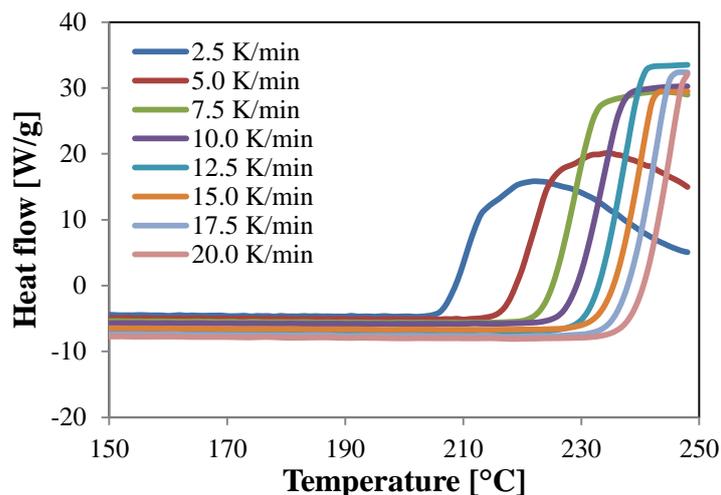
**Figure S29.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-II** ( $C = 0.500\%$  w/w).



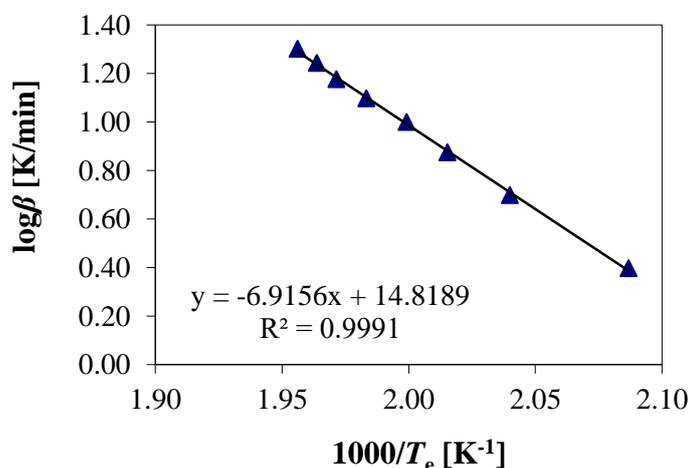
**Figure S30.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-II** ( $C = 0.500\%$  w/w).

**Table S15.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-II** ( $C = 0.500\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	477	$a = -6.8061$
5.0	487	$b = 14.6649$
7.5	493	$R^2 = 0.9992$
10.0	498	$E_a = 124 \pm 3 \text{ kJ/mol}$
12.5	502	$Z = 6.41 \times 10^{12} \text{ min}^{-1}$
15.0	504	$k(50^\circ\text{C}) = 5.99 \times 10^{-8} \text{ min}^{-1}$
17.5	507	$k(100^\circ\text{C}) = 2.89 \times 10^{-5} \text{ min}^{-1}$
20.0	509	$k(150^\circ\text{C}) = 3.24 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 1.34 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 2.72 \times 10^0 \text{ min}^{-1}$



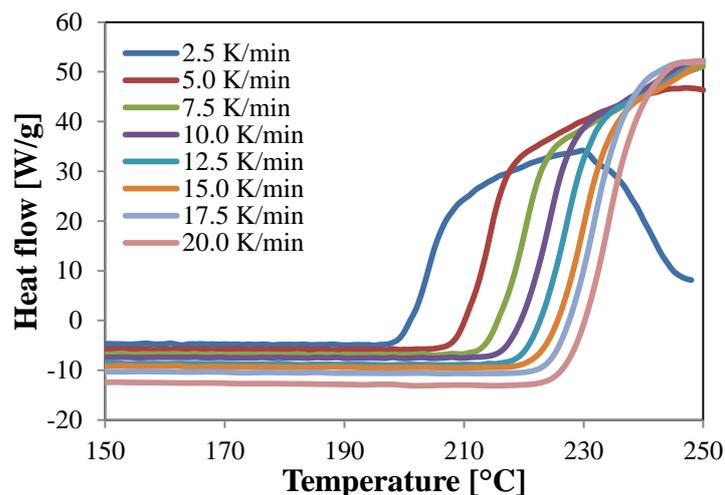
**Figure S31.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-II** ( $C = 1.00\%$  w/w).



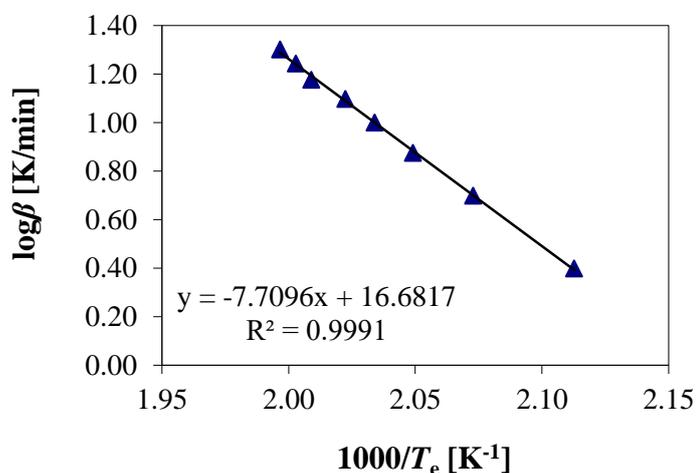
**Figure S32.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-II** ( $C = 1.00\%$  w/w).

**Table S16.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-II** ( $C = 1.00\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	479	$a = -6.9156$
5.0	490	$b = 14.8189$
7.5	496	$R^2 = 0.9991$
10.0	500	$E_a = 126 \pm 3 \text{ kJ/mol}$
12.5	504	$Z = 8.99 \times 10^{12} \text{ min}^{-1}$
15.0	507	$k(50^\circ\text{C}) = 4.01 \times 10^{-8} \text{ min}^{-1}$
17.5	509	$k(100^\circ\text{C}) = 2.13 \times 10^{-5} \text{ min}^{-1}$
20.0	511	$k(150^\circ\text{C}) = 2.58 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 1.13 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 2.41 \times 10^0 \text{ min}^{-1}$



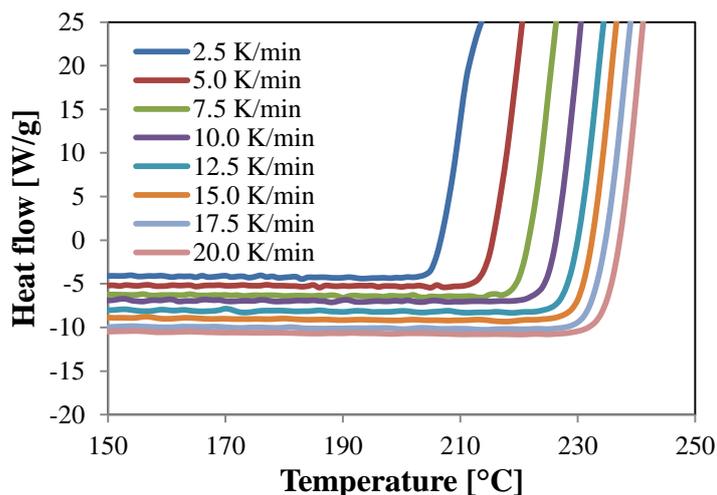
**Figure S33.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-III** ( $C = 0.065\%$  w/w).



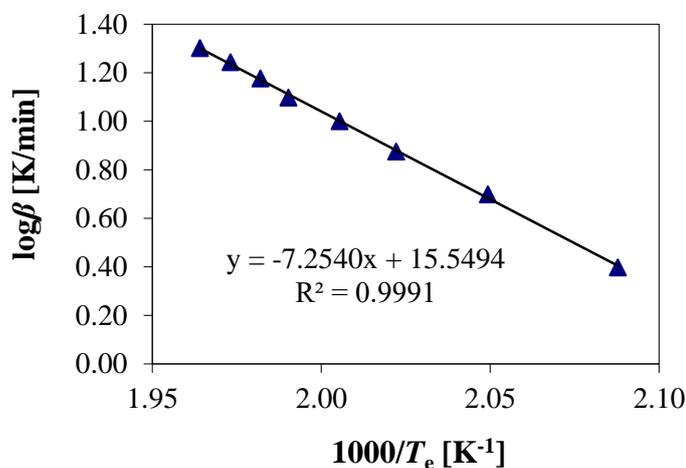
**Figure S34.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-III** ( $C = 0.065\%$  w/w).

**Table S17.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-III** ( $C = 0.065\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	473	$a = -7.7096$
5.0	482	$b = 16.6817$
7.5	488	$R^2 = 0.9991$
10.0	491	$E_a = 140 \pm 3 \text{ kJ/mol}$
12.5	494	$Z = 5.88 \times 10^{14} \text{ min}^{-1}$
15.0	498	$k(50^\circ\text{C}) = 1.21 \times 10^{-8} \text{ min}^{-1}$
17.5	499	$k(100^\circ\text{C}) = 1.32 \times 10^{-5} \text{ min}^{-1}$
20.0	501	$k(150^\circ\text{C}) = 2.77 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 1.88 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 5.68 \times 10^0 \text{ min}^{-1}$



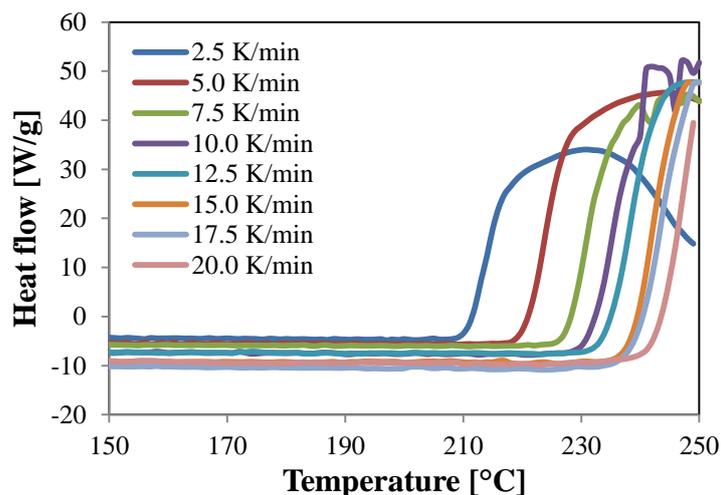
**Figure S35.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-III** ( $C = 0.125\%$  w/w).



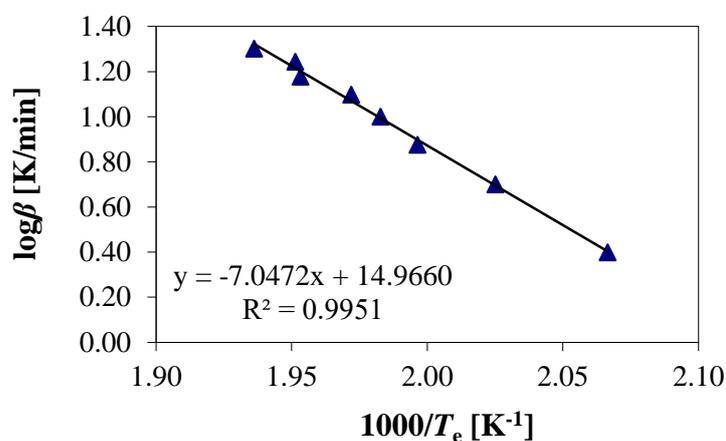
**Figure S36.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-III** ( $C = 0.125\%$  w/w).

**Table S18.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-III** ( $C = 0.125\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	479	$a = -7.2540$
5.0	488	$b = 15.5494$
7.5	494	$R^2 = 0.9991$
10.0	498	$E_a = 132 \pm 3$ kJ/mol
12.5	502	$Z = 4.61 \times 10^{13}$ min <sup>-1</sup>
15.0	504	$k(50^\circ\text{C}) = 2.07 \times 10^{-8}$ min <sup>-1</sup>
17.5	507	$k(100^\circ\text{C}) = 1.50 \times 10^{-5}$ min <sup>-1</sup>
20.0	509	$k(150^\circ\text{C}) = 2.29 \times 10^{-3}$ min <sup>-1</sup>
		$k(200^\circ\text{C}) = 1.21 \times 10^{-1}$ min <sup>-1</sup>
		$k(250^\circ\text{C}) = 3.00 \times 10^0$ min <sup>-1</sup>



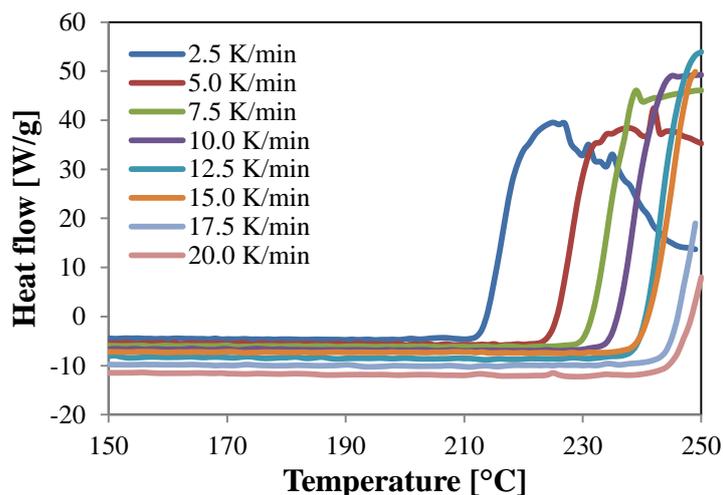
**Figure S37.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-III** ( $C = 0.250\%$  w/w).



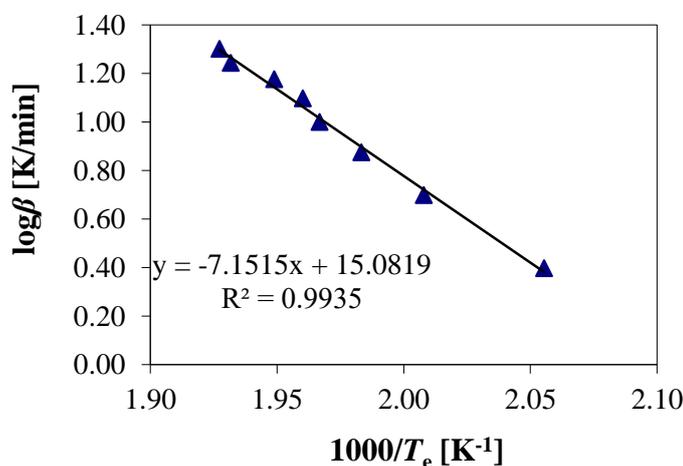
**Figure S38.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-III** ( $C = 0.250\%$  w/w).

**Table S19.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-III** ( $C = 0.250\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	483	$a = -7.0472$
5.0	494	$b = 14.9660$
7.5	501	$R^2 = 0.9951$
10.0	504	$E_a = 128 \pm 7 \text{ kJ/mol}$
12.5	507	$Z = 1.21 \times 10^{13} \text{ min}^{-1}$
15.0	512	$k(50^\circ\text{C}) = 2.26 \times 10^{-8} \text{ min}^{-1}$
17.5	512	$k(100^\circ\text{C}) = 1.36 \times 10^{-5} \text{ min}^{-1}$
20.0	516	$k(150^\circ\text{C}) = 1.80 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 8.47 \times 10^{-2} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.91 \times 10^0 \text{ min}^{-1}$



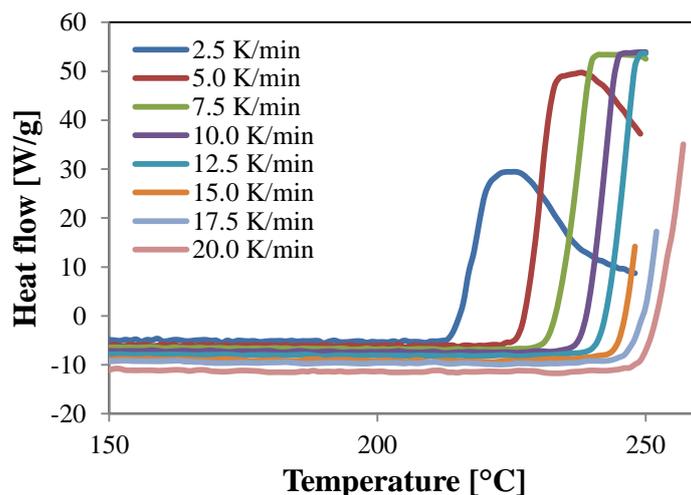
**Figure S39.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-III** ( $C = 0.500\%$  w/w).



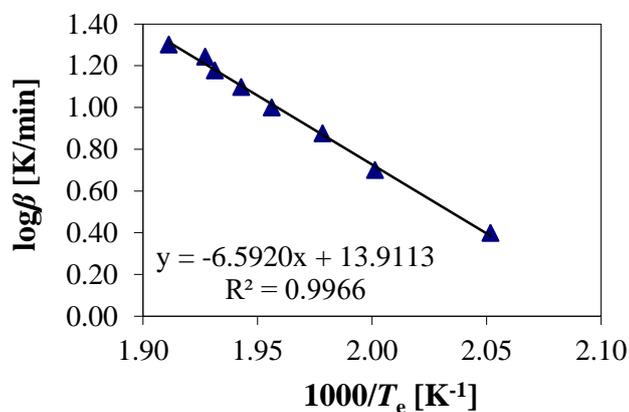
**Figure S40.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-III** ( $C = 0.500\%$  w/w).

**Table S20.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-III** ( $C = 0.500\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	486	$a = -7.1515$
5.0	498	$b = 15.0819$
7.5	504	$R^2 = 0.9935$
10.0	508	$E_a = 130 \pm 7 \text{ kJ/mol}$
12.5	510	$Z = 1.59 \times 10^{13} \text{ min}^{-1}$
15.0	513	$k(50^\circ\text{C}) = 1.43 \times 10^{-8} \text{ min}^{-1}$
17.5	517	$k(100^\circ\text{C}) = 9.47 \times 10^{-6} \text{ min}^{-1}$
20.0	519	$k(150^\circ\text{C}) = 1.35 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 6.73 \times 10^{-2} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.59 \times 10^0 \text{ min}^{-1}$



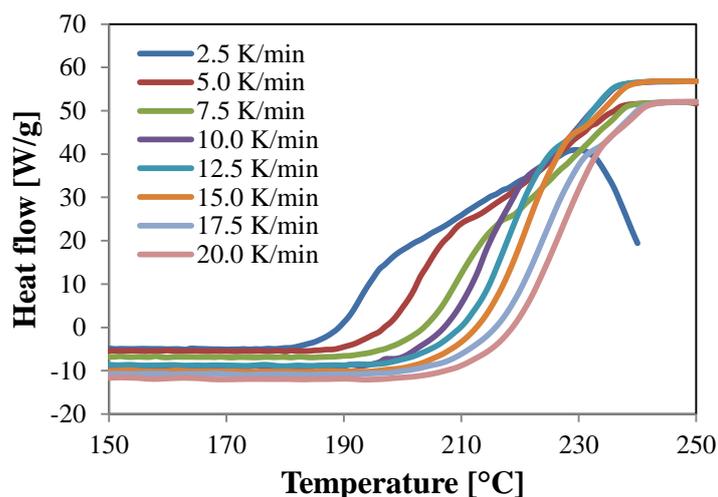
**Figure S41.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-III** ( $C = 1.00\%$  w/w).



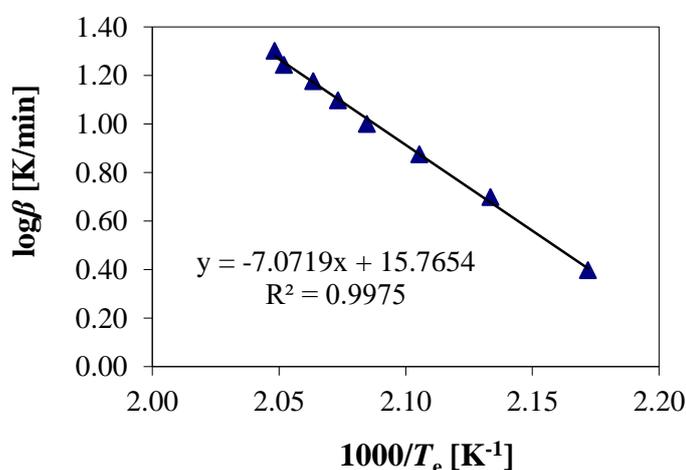
**Figure S42.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-III** ( $C = 1.00\%$  w/w).

**Table S21.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-III** ( $C = 1.00\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	487	$a = -6.5920$
5.0	499	$b = 13.9113$
7.5	505	$R^2 = 0.9966$
10.0	511	$E_a = 120 \pm 5$ kJ/mol
12.5	514	$Z = 1.17 \times 10^{12}$ min <sup>-1</sup>
15.0	518	$k(50^\circ\text{C}) = 4.66 \times 10^{-8}$ min <sup>-1</sup>
17.5	519	$k(100^\circ\text{C}) = 1.85 \times 10^{-5}$ min <sup>-1</sup>
20.0	523	$k(150^\circ\text{C}) = 1.79 \times 10^{-3}$ min <sup>-1</sup>
		$k(200^\circ\text{C}) = 6.57 \times 10^{-2}$ min <sup>-1</sup>
		$k(250^\circ\text{C}) = 1.21 \times 10^0$ min <sup>-1</sup>



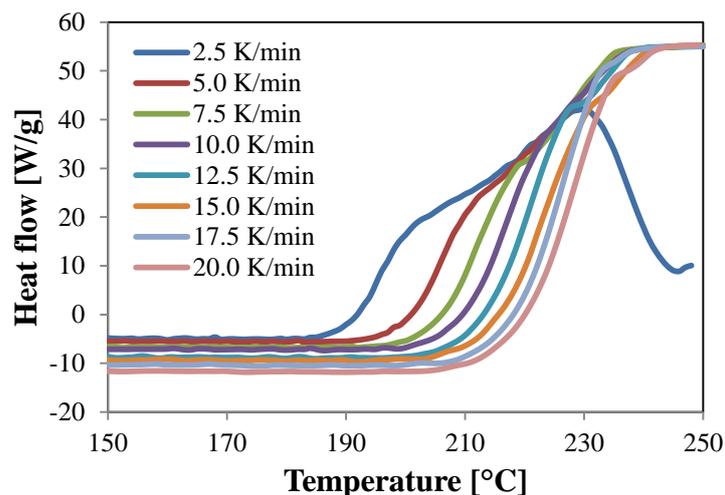
**Figure S43.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-IV** ( $C = 0.065\%$  w/w).



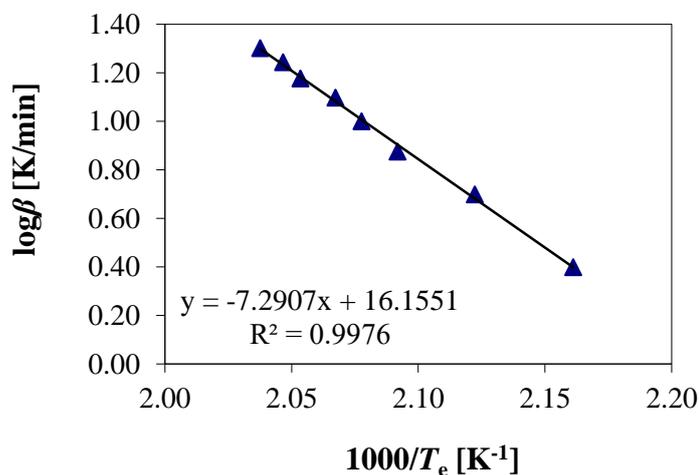
**Figure S44.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-IV** ( $C = 0.065\%$  w/w).

**Table S22.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-IV** ( $C = 0.065\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	460	$a = -7.0719$
5.0	469	$b = 15.7654$
7.5	475	$R^2 = 0.9975$
10.0	479	$E_a = 129 \pm 5 \text{ kJ/mol}$
12.5	482	$Z = 7.77 \times 10^{13} \text{ min}^{-1}$
15.0	484	$k(50^\circ\text{C}) = 1.20 \times 10^{-7} \text{ min}^{-1}$
17.5	487	$k(100^\circ\text{C}) = 7.37 \times 10^{-5} \text{ min}^{-1}$
20.0	488	$k(150^\circ\text{C}) = 9.93 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 4.75 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.08 \times 10^1 \text{ min}^{-1}$



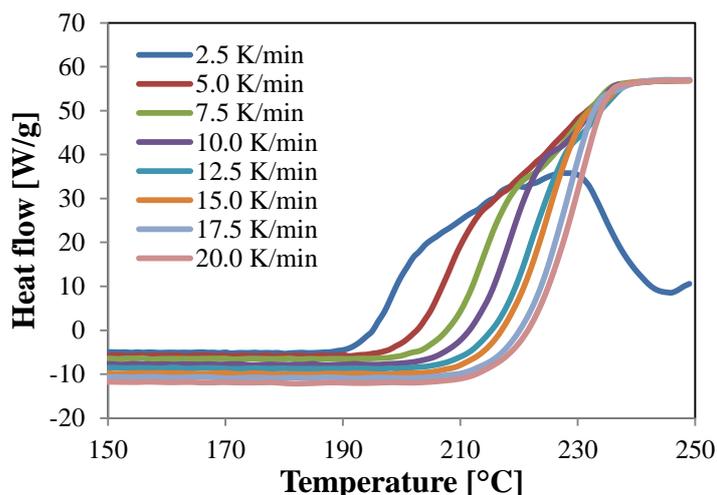
**Figure S45.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-IV** ( $C = 0.125\%$  w/w).



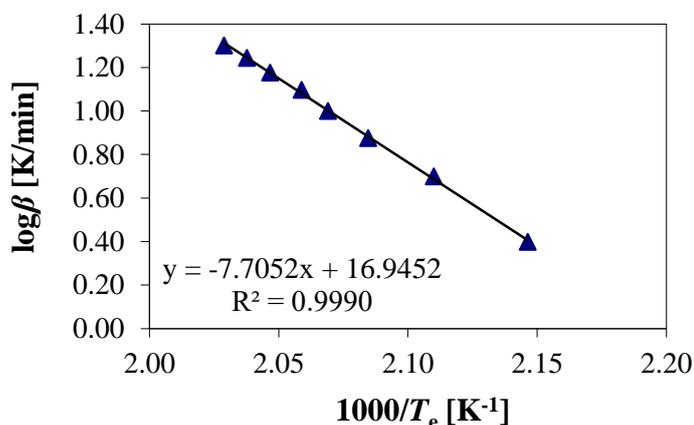
**Figure S46.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-IV** ( $C = 0.125\%$  w/w).

**Table S23.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-IV** ( $C = 0.125\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	463	$a = -7.2907$
5.0	471	$b = 16.1551$
7.5	478	$R^2 = 0.9976$
10.0	481	$E_a = 133 \pm 5 \text{ kJ/mol}$
12.5	484	$Z = 1.85 \times 10^{14} \text{ min}^{-1}$
15.0	487	$k(50^\circ\text{C}) = 6.48 \times 10^{-8} \text{ min}^{-1}$
17.5	488	$k(100^\circ\text{C}) = 4.86 \times 10^{-5} \text{ min}^{-1}$
20.0	491	$k(150^\circ\text{C}) = 7.61 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 4.10 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.03 \times 10^1 \text{ min}^{-1}$



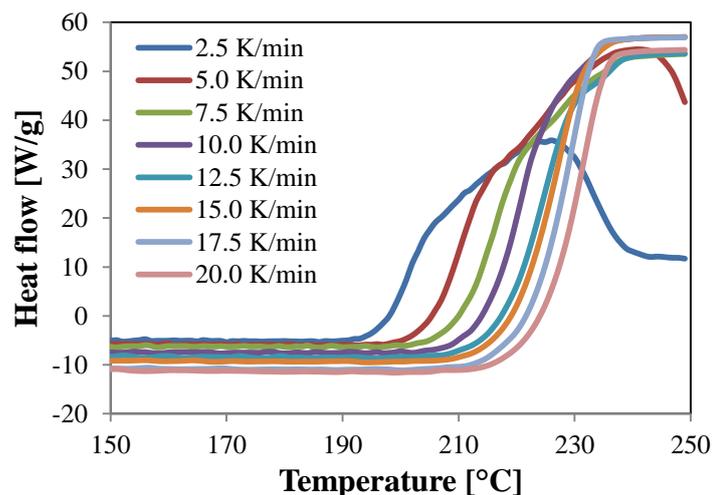
**Figure S47.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-IV** ( $C = 0.250\%$  w/w).



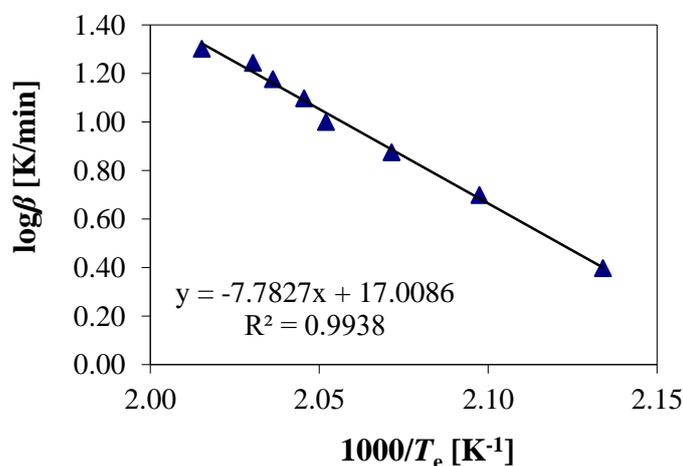
**Figure S48.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-IV** ( $C = 0.250\%$  w/w).

**Table S24.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-IV** ( $C = 0.250\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	466	$a = -7.7052$
5.0	474	$b = 16.9452$
7.5	480	$R^2 = 0.9990$
10.0	483	$E_a = 140 \pm 3 \text{ kJ/mol}$
12.5	486	$Z = 1.08 \times 10^{15} \text{ min}^{-1}$
15.0	488	$k(50^\circ\text{C}) = 2.28 \times 10^{-8} \text{ min}^{-1}$
17.5	491	$k(100^\circ\text{C}) = 2.49 \times 10^{-5} \text{ min}^{-1}$
20.0	493	$k(150^\circ\text{C}) = 5.20 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 3.52 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 1.06 \times 10^1 \text{ min}^{-1}$



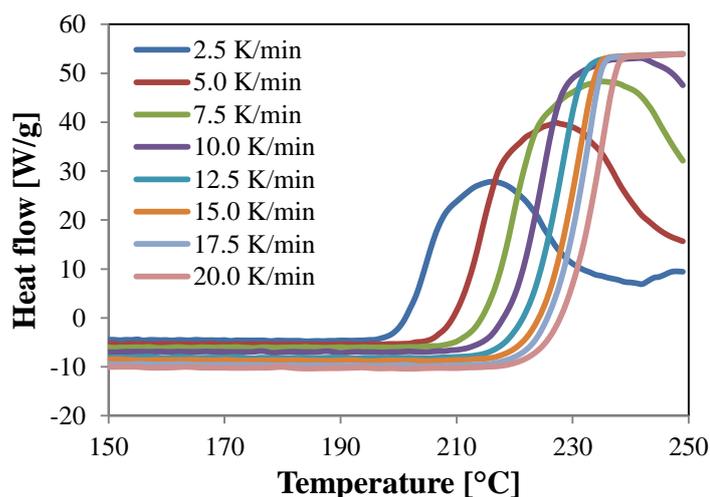
**Figure S49.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-IV** ( $C = 0.500\%$  w/w).



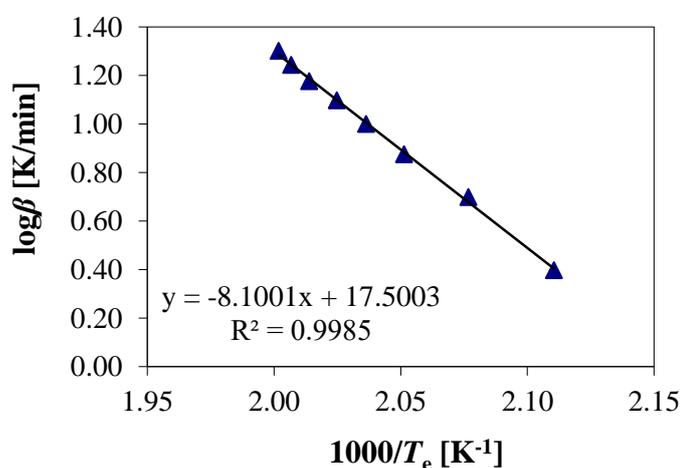
**Figure S50.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-IV** ( $C = 0.500\%$  w/w).

**Table S25.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-IV** ( $C = 0.500\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	486	$a = -7.7827$
5.0	498	$b = 17.0086$
7.5	504	$R^2 = 0.9938$
10.0	508	$E_a = 142 \pm 8 \text{ kJ/mol}$
12.5	510	$Z = 1.24 \times 10^{15} \text{ min}^{-1}$
15.0	513	$k(50^\circ\text{C}) = 1.55 \times 10^{-8} \text{ min}^{-1}$
17.5	517	$k(100^\circ\text{C}) = 1.81 \times 10^{-6} \text{ min}^{-1}$
20.0	519	$k(150^\circ\text{C}) = 3.99 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 2.81 \times 10^{-2} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 8.79 \times 10^0 \text{ min}^{-1}$



**Figure S51.** DSC curves of non-isothermal oxidative decomposition of HDPE with **C60-IV** ( $C = 1.00\%$  w/w).



**Figure S52.** Plot of  $\log\beta$  versus  $1000/T_e$  for oxidation of HDPE containing **C60-IV** ( $C = 1.00\%$  w/w).

**Table S26.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **C60-IV** ( $C = 1.00\%$  w/w). Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.5	474	$a = -8.1001$
5.0	481	$b = 17.5003$
7.5	487	$R^2 = 0.9985$
10.0	491	$E_a = 148 \pm 4 \text{ kJ/mol}$
12.5	494	$Z = 3.68 \times 10^{15} \text{ min}^{-1}$
15.0	496	$k(50^\circ\text{C}) = 5.37 \times 10^{-9} \text{ min}^{-1}$
17.5	498	$k(100^\circ\text{C}) = 8.38 \times 10^{-6} \text{ min}^{-1}$
20.0	499	$k(150^\circ\text{C}) = 2.30 \times 10^{-3} \text{ min}^{-1}$
		$k(200^\circ\text{C}) = 1.93 \times 10^{-1} \text{ min}^{-1}$
		$k(250^\circ\text{C}) = 6.94 \times 10^0 \text{ min}^{-1}$

**Table S27.** Results ( $T_e$ , statistical parameters of equation 1,  $E_a$ ,  $Z$ , and  $k$ ) obtained for oxidation of HDPE containing **BHT** ( $C = 0.5\%$  w/w).<sup>1</sup> Symbols are the same as explained in caption to Table S1.

$\beta$ [K/min]	$T_e$ [K]	Statistical and kinetic parameters
2.0	456	$a = -6.3126$
5.0	468	$b = 14.1667$
7.5	474	$R^2 = 0.9969$
10.0	480	$E_a = 115 \pm 5$ kJ/mol
12.5	483	$Z = 2.19 \times 10^{12}$ min <sup>-1</sup>
15.0	486	$k(50^\circ\text{C}) = 5.81 \times 10^{-7}$ min <sup>-1</sup>
17.5	489	$k(100^\circ\text{C}) = 1.79 \times 10^{-4}$ min <sup>-1</sup>
20.0	491	$k(150^\circ\text{C}) = 1.43 \times 10^{-2}$ min <sup>-1</sup>
		$k(200^\circ\text{C}) = 4.50 \times 10^{-1}$ min <sup>-1</sup>
		$k(250^\circ\text{C}) = 7.34 \times 10^0$ min <sup>-1</sup>

## Experimental Methods and Synthesis Section

**Materials.** High density polyethylene (HDPE for the use in spectroscopy, density 0.96 g/cm<sup>3</sup>, melting point 132-134°C, powder) was obtained from Merck and used as received. Fullerene C<sub>60</sub> was of 99+% purity (MER Corporation, Tucson). 4-hydroxy-3-methoxybenzaldehyde, 4-hydroxy-3-methoxycinnamaldehyde, N-methylglycine (sarcosine), potassium hydroxide, 2,6-xylenol, aluminum chloride (98,5%), isobutyraldehyde, carbon disulfide, dichloromethane, copper (I) bromide dimethyl sulfide complex, acetonitrile, methanol, ethanol, hexane were purchased from Sigma-Aldrich. 4-(2-tetrahydropyranyloxy)phenyl magnesium bromide (0.5 M in 2-methyltetrahydrofuran) was purchased from ABCR. Toluene (POCH 99.5%), THF (Sigma-Aldrich, 99.5%), 1,2-dichlorobenzene (Sigma-Aldrich, 99.5%) were dried and distilled before use, other solvents were analytical grade reagents and were used as received.

**Proton nuclear magnetic resonance.** <sup>1</sup>H NMR spectra were recorded using Bruker AVANCE 300 MHz or Varian 200 MHz instruments.

**Differential Scanning Calorimetry.** Oxidation process of STA and LNA was monitored by Differential Scanning Calorimetry (Du Pont 910 apparatus with Du Pont 9900 thermal analyzer and normal pressure, recently refurbished cell was used). Temperature and cell constant were calibrated with ultrapure indium standard. TA Instruments software (General V4.01) was used for collecting the data and for determination of temperatures from DSC curves. The oxidations were performed under oxygen flow 6 dm<sup>3</sup>/h. Samples (3.0-3.5 mg) were heated from 50 to 250°C in open aluminium pan with linear heating rate  $\beta$  (2.5; 5.0; 7.5; 10.0; 12.5; 15.0; 17.5; 20.0 K/min). As a reference material an empty aluminium pan was used. Temperatures of extrapolated start of oxidation,  $T_e$ , were determined from the plots of heat flow versus temperature dependence for each  $\beta$ .

**Thermogravimetric analysis.** Thermogravimetric measurements of obtained C<sub>60</sub> derivatives were carried out with a Q50 TA Instruments apparatus under nitrogen flow 6 dm<sup>3</sup>/h in a platinum vessel. Samples of **C60-(I-IV)** were dried in vacuum in 40°C for 12h. In a typical TG

measurement a sample (6-7 mg) was heated at 5 K/min from 50 to 600°C. Universal V4.54 TA Instruments software was used for data collection and analysis.

**Synthesis** of derivatives **C60-(I-IV)** is described elsewhere (Ind. Eng. Chem. Res., **2016**, *55*, 9887-9894). In this ESI we are quoting the text at full length.

Four phenols were used as precursors for synthesis of conjugates with C<sub>60</sub> presented in Chart 1: 4-hydroxy-3-methoxybenzaldehyde, **I**, and 4-hydroxy-3-methoxycinnamaldehyde, **II**, 2,6-dimethylphenol, **III**, unsubstituted phenol, **IV**. Two C<sub>60</sub> adducts: N-methyl-2-[4-hydroxy-3-methoxyphenyl]-3,4-[60]fulleropyrrolidine, **C60-I**, and N-methyl-2-[2-(4-hydroxy-3-methoxyphenyl)vinyl]-3,4-[60]fulleropyrrolidine, **C60-II**, were prepared using the modified 1,3-dipolar cycloaddition of azomethine ylides to olefins (the Prato reaction, with the ylides formed by reaction of the corresponding aldehyde and N-methylglycine). Compound **C60-III** was synthesized by electrophilic addition of 2,6-dimethylphenol to C<sub>60</sub> in the presence of a strong Lewis acid, AlCl<sub>3</sub>. Derivative **C60-IV** was obtained using organo-magnesium compounds (Grignard compounds).

*Synthesis of N-methyl-2-[4-hydroxy-3-methoxyphenyl]-3,4-[60]fulleropyrrolidine, C60-I.*<sup>2</sup> A mixture of C<sub>60</sub> (100 mg, 0.14 mmol), sarcosine (61.4 mg, 0.69 mmol, 5 eq.), 4-hydroxy-3-methoxybenzaldehyde (21.1 mg, 0.14 mmol, 1 eq.) and 90 mL toluene was stirred in reflux for 24 h in 250 mL flask. The reaction mixture was cooled down and the solvent was removed under reduced pressure. The residue was purified by column chromatography to give 48 mg product **C60-I** as a brown solid (39% yield based on converted C<sub>60</sub>). Analysis: <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, TMS) δ: 2.81 (s, 3H), 3.90 (s, 3H), 4.21 – 4.26 (d, 1H), 4.85 (s, 1H), 4.96 – 4.99 (d, 1H), 6.91 – 6.95 (d, 1H), 7.18 – 7.22 (d, 1H), 7.38 (s, 1H) ppm; MS TOF ESI: m/z expected (C<sub>60</sub>(C<sub>10</sub>H<sub>13</sub>O<sub>2</sub>N)): 899.8577, found: 899.9668; FTIR (KBr) [cm<sup>-1</sup>]: 3300 (O-H); 2922 (C-H); 1512 (C-C); 1431 (C-C, C<sub>60</sub>); 1269 (C-O); 1180 (C-C, C<sub>60</sub>); 1032 (C-O); 768 (C-C, C<sub>60</sub>); 527 (C-C, C<sub>60</sub>). The weight loss was 27% at temperature range 250°C and 650°C, which corresponds to one group attached to the fullerene molecule.

*Synthesis of N-methyl-2-[2-(4-hydroxy-3-methoxyphenyl)vinyl]-3,4-[60]fulleropyrrolidine, C60-II.*<sup>2</sup> A mixture of C<sub>60</sub> (100 mg, 0.14 mmol), sarcosine (61.4 mg, 0.69 mmol, 5 eq.), 4-hydroxy-3-methoxycinnamaldehyde (21.1 mg, 0.14 mmol, 1 eq.) and 100 mL toluene was stirred in reflux for 24 h in 250 mL flask. The reaction mixture was cooled down and the solvent was removed under reduced pressure. The residue was purified by column chromatography to give 35 mg product **C60-II** as a brown solid (28% yield based on converted C<sub>60</sub>). Analysis: <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, TMS) δ: 2.91 (s, 3H), 3.90 (s, 3H), 4.12 – 4.17 (d, 1H), 4.42 – 4.46 (d, 1H), 4.88 – 4.93 (d, 1H), 5.02 (s, 1H), 6.47-6.60 (dd, 1H), 6.85 – 6.90 (d, 1H), 6.94-7.02 (d, 1H), 6.99 (s, 1H), 7.18 – 7.22 (d, 1H), ppm; MS TOF ESI: m/z expected (C<sub>60</sub>(C<sub>12</sub>H<sub>15</sub>O<sub>2</sub>N)): 899.8577, found: 763.42. FTIR (KBr) [cm<sup>-1</sup>]: 3300 (O-H), 2926 (C-H), 1510 (C-C), 1422 (C-C, C<sub>60</sub>), 1273 (C-O), 1175 (C-C, C<sub>60</sub>), 1026 (C-O), 521 (C-C, C<sub>60</sub>). Percentage weight loss at temperature range 150°C and 600°C was 21%, which corresponds to one group attached to the fullerene molecule.

*Synthesis of tetra-2,6-methyl-4-hydroxyphenyl[60]fullerene, C60-III.* C<sub>60</sub> derivative (**C60-III**) was obtained using the synthetic procedure reported by Shi *et al.*<sup>3</sup> Round-bottom flask (100 mL, two necks) was filled with C<sub>60</sub> (43 mg, 0.9 mmol), 2,6-xyleneol (100 mg, 0.9 mmol, 1 eq.), aluminum chloride (100 mg, 0.74 mmol, 0.8 eq.) and 20 mL carbon disulfide. This mixture was stirred at ambient temperature for 24 hours. Then 30 mL dichloromethane and 15 mL water was added. Water layer was extracted with dichloromethane (2 × 20 mL). The combined organic layers were dried (MgSO<sub>4</sub>) overnight, concentrated and purified on a silica gel column. The product was eluted with methanol: toluene (1:10 v/v) and dried overnight in 40°C in vacuum oven. The product **C60-III** was obtained as a brown solid (20.5 mg, 30%, based on converted C<sub>60</sub>). Analysis: <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, TMS) δ: 2.17 (s, 6H), 2.30 (s, 12H), 2.44 (s, 6H), 4.58 (s, 1H), 4.70 (s, 1H), 4.83 (s, 1H), 7.15 (s, 2H), 7.83 (s, 2H); MS TOF ESI: m/z expected: 1205.3 found: 708, 724, 781, 797, 855, 873, 929, 1004. FTIR (KBr) [cm<sup>-1</sup>]: 3440 (O-H), 2963 (C-H), 1489 (C-C), 1261 (C-O), 1198 (C-C, C<sub>60</sub>), 1026 (C-O), 527 (C-C, C<sub>60</sub>). Percentage weight loss at temperature range 150°C and 550°C was 40%, which corresponds to four group attached to the fullerene molecule.

*Synthesis of penta-(4-hydroxyphenyl)hydro[60]fullerene, C60-IV.* Derivative **C60-IV** was synthesized using a method reported by Matsuo and Nakamura.<sup>4</sup> A 50 mL two neck round-bottom flask was filled with CuBr•SMe<sub>2</sub> (576 mg, 2.8 mmol, 20 eq.), THF (20 mL) and a 0.5 M solution of 4-(THPO)C<sub>6</sub>H<sub>4</sub>MgBr (5.6 mL, 2.8 mmol, 20 eq.) in 2-MeTHF. The dark red suspension was stirred for 10 min and a solution of C<sub>60</sub> (100 mg, 0.139 mmol) in 1,2-dichlorobenzene (7.5 mL) was added. Stirring was continued for 2 hours. The reaction was stopped by addition of NH<sub>4</sub>Cl(aq) (0.5 mL) and the mixture was diluted by addition of toluene (20 mL). The mixture was filtered through a pad of silica gel. Then was condensed and after addition of EtOH precipitate was formed, collected and washed with EtOH. The orange solid was dissolved in CH<sub>2</sub>Cl<sub>2</sub>/MeOH (20 ml, 50% v/v) and p-toluene sulfonic acid (10 mg, 0.053 mmol) was added. The mixture was stirred for 24 h and neutralized with NaHCO<sub>3</sub>. Next was purified by filtration with a pad of celite. To obtain precipitates the solvent was evaporated. The powder was dissolved in few milliliters of EtOH. After addition of hexane, precipitates formed and were collected, washed with hexane, and dried to give 83 mg of product **C60-IV** (50%, based on converted C<sub>60</sub>). Analysis: <sup>1</sup>H NMR (200 MHz, acetone-d<sub>6</sub>) δ: 5.49 (s, 1H), 6.64 - 6.68 (d, 2H), 6.72 - 6.76 (d, 2H), 6.87 - 6.91 (d, 2H), 7.24 - 7.28 (d, 2H), 7.55 - 7.59 (d, 2H), 7.74 - 7.79 (d, 2H), FTIR (KBr) [cm<sup>-1</sup>]: 3300 (O-H), 2959 (C-H), 1508 (C-C), 1429 (C-C, C<sub>60</sub>), 1236 (C-O), 1174 (C-C, C<sub>60</sub>), 1015 (C-O), 538 (C-C, C<sub>60</sub>). Percentage weight at temperature range 150°C and 550°C was 35%, which corresponds to five group attached to the fullerene molecule.

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(3) Shi, Z.; Li, Y.; Wang, S.; Fang, H.; Zhu, D. Synthesis and antioxidative properties of polyphenol-fullerenes. *Chin. Sci. Bull.* **2001**, *46*, 1790-1792.

(4) Matsuo, Y.; Nakamura, E. Selective multiaddition of organocopper reagents to fullerenes. *Chem. Rev.* **2008**, *108*, 3016-3028.