ELECTRONIC SUPPLEMENTARY INFORMATION

Comparing Conventional and Microwave-Assisted Heating in PET Degradation Mediated by Imidazolium-Based Halometallate Complexes†

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1. X-ray crystal structure of $(dimim)_2[Fe_2Cl_6(\mu\text{-}O)]$

Table S1 Crystallographic data and structure refinement details of $(dimim)_2[Fe_2Cl_6(\mu\text{-}O)]$.

	$(dimim)_2[Fe_2Cl_6(\mu\text{-}O)]$
Empirical formula	$C_{10}H_{18}Cl_6Fe_2N_4O$
Formula weight	550.47
Crystal system	triclinic
Space group	$P\bar{1}$
a (Å)	7.322(1)
b (Å)	7.5071(8)
c (Å)	10.492(1)
α (º)	103.00(1)
β (º)	100.47(1)
γ (º)	92.43(1)
V (Å^3)	550.5(1)
Z	1
ρ (g·cm^{-3})	1.613
μ (mm^{-1})	17.321
Reflections collected	3365
Unique data/parameters	2130/109
R	0.0430
Goodness of fit (S)[a]	1.088
R_1[b]/wR^2[c] [$I>2\sigma(I)$]	0.0865/0.2671
R_1[b]/wR^2[c] [all data]	0.0970/0.2806

[a] $S = [\sum w(F_0^2 - F_c^2)^2 / (N_{obs} - N_{param})]^{1/2}$. [b] $R_1 = \sum||F_0|-|F_c|| / \sum|F_0|$; [c] $wR2 = [\sum w(F_0^2)^2 - F_c^2)^2 / \sum w(F_0^2)^2]^{1/2}$; $w = 1/[\sigma^2(F_0^2) + (aP)^2 + bP]$ where $P = (\max(F_0^2,0) + 2Fc^2)/3$, being a = 0.1687, b = 0.3119.

Table S2 Selected bond lengths and angles of $[Fe_2Cl_6(\mu\text{-}O)]^{2-}$ anion.

	Bond lengths (Å)
Fe1–O1	1.848(2)
Fe1–Cl1	2.217(2)
Fe1–Cl2	2.211(2)
Fe1–Cl3	2.206(4)
	Angles (º)
O1–Fe1–Cl1	103.1(6)
O1–Fe1–Cl2	104.3(7)
O1–Fe1–Cl3	124.5(5)
Cl1–Fe1–Cl2	106.1(1)
Cl1–Fe1–Cl3	110.3(1)
Cl2–Fe1–Cl3	107.2(2)

2. Recycling Experiments

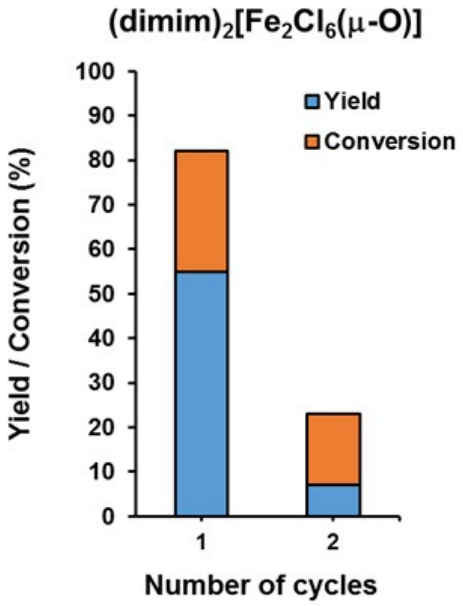

Fig. S1 Reuse of $(dimim)_2[Fe_2Cl_6(\mu\text{-}O)]$ in the glycolysis of PET. Reagents and conditions: **2** (0.0425 mmol), PET (125 mg), EG (0.8 mL), 170 ºC, 24 h.

3. Characterization of BHET product

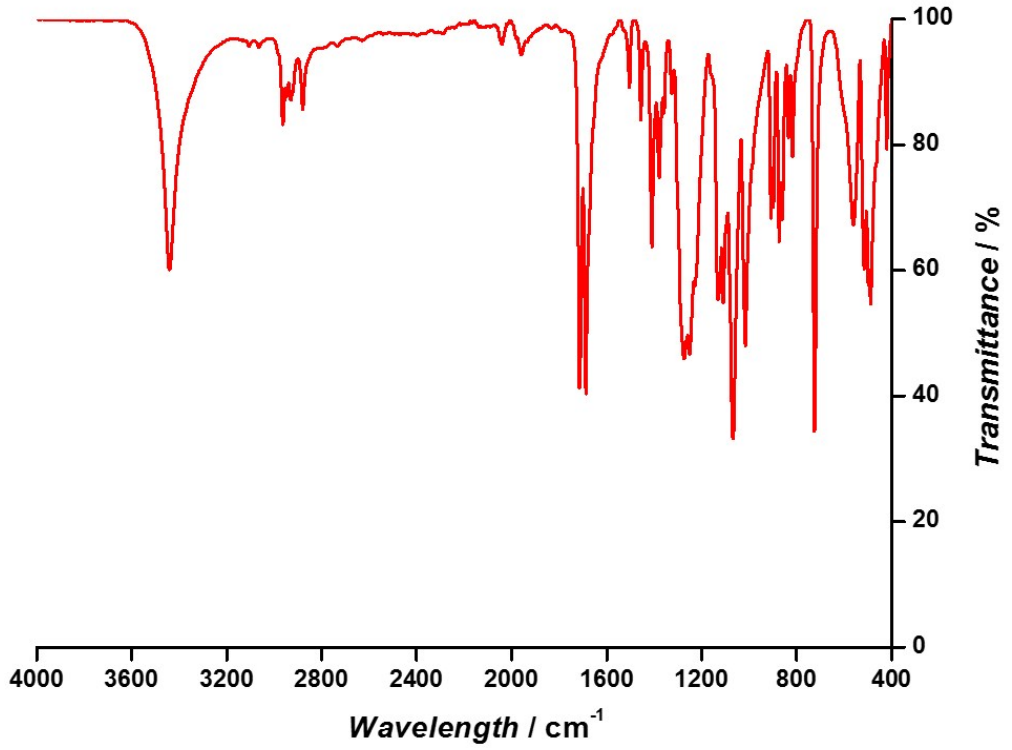

Fig. S2 IR spectrum of BHET product.

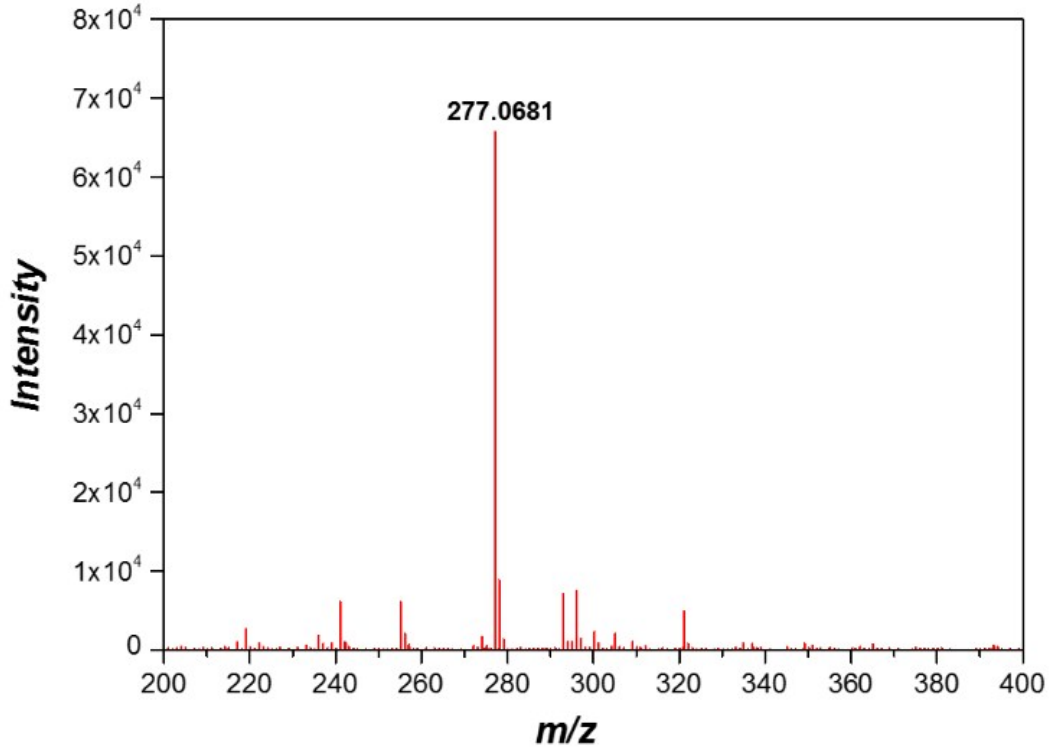

Fig. S3 ESI-MS spectrum of BHET product.

4. X-ray crystal structure of BHET

Table S3 Crystallographic data and structure refinement details of BHET.

	BHET
Empirical formula	$C_{12}H_{14}O_6$
Formula weight	254.23
Crystal system	triclinic
Space group	$P\bar{1}$
a (Å)	8.2252(3)
b (Å)	9.3639(9)
c (Å)	16.501(1)
α (°)	87.306(7)
β (°)	84.160(5)
γ (°)	80.338(6)
V (Å^3)	1245.8(2)
Z	4
ρ (g·cm^{-3})	1.355
μ (mm^{-1})	1.844
Reflections collected	14759
Unique data/parameters	8599/330
R	0.0435
Goodness of fit (S)[a]	0.948
R_1[b]/wR^2[c] [$I>2\sigma(I)$]	0.0764/ 0.1975
R_1[b]/wR^2[c] [all data]	0.0968/ 0.2097

[a] $S = [\sum w(F_0^2 - F_c^2)^2 / (N_{obs} - N_{param})]^{1/2}$. [b] $R_1 = \sum||F_0|-|F_c|| / \sum|F_0|$; [c] $wR2 = [\sum w(F_0^2)^2 - F_c^2)^2 / \sum w(F_0^2)^2]^{1/2}$; $w = 1/[\sigma^2(F_0^2) + (aP)^2 + bP]$ where $P = (\max(F_0^2,0) + 2Fc^2)/3$, being a = 0.1502, b = 0.

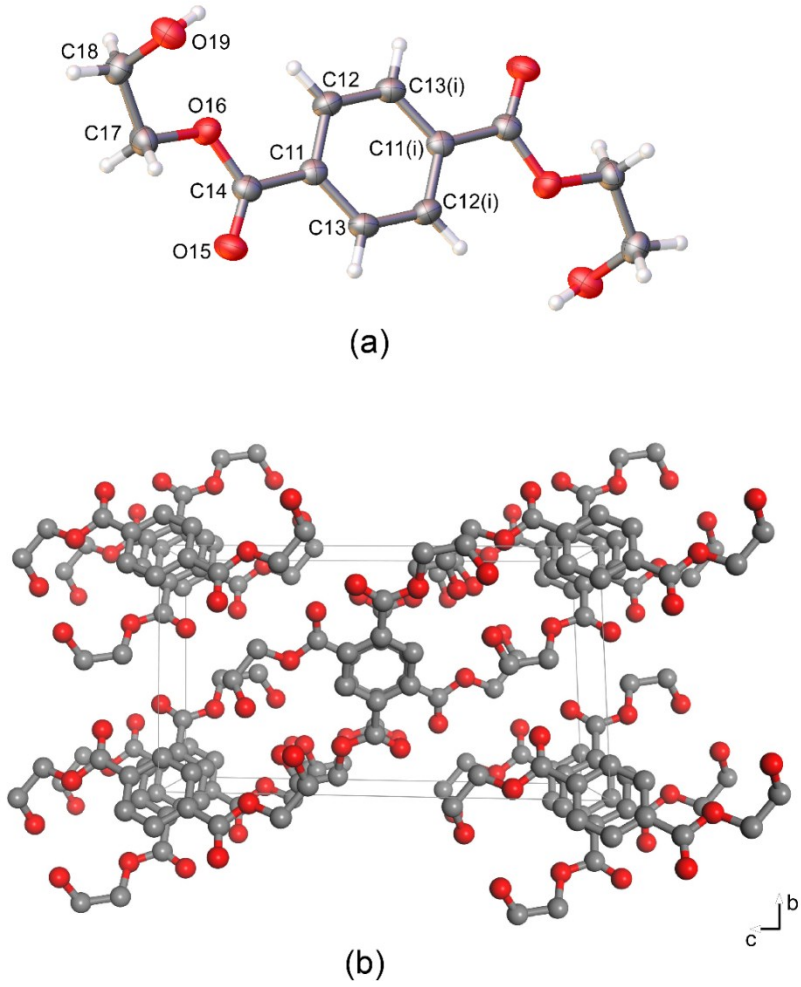

Fig. S4 Crystal structure of the new BHET ($P\bar{1}$) polymorph. (a) One of the four crystallographically independent BHET molecules showing the numbering scheme (i: -x, 1-y, 1-z). Thermal ellipsoids are drawn at 50% probability. (b) Perspective view of the crystal structure along the [100] direction. Hydrogen atoms were omitted for the sake of clarity.