

Poly(butylene 2,5-thiophenedicarboxylate): an Added Value to the Class of High Gas Barrier Biopolyesters

Giulia Guidotti ¹, Matteo Gigli ^{2,*}, Michelina Soccio ¹, Nadia Lotti ^{1,*}, Massimo Gazzano ³,
Valentina Siracusa ⁴ and Andrea Munari ¹

¹ Department of Civil, Chemical, Environmental and Materials Engineering, University of Bologna, Via Terracini 28, 40131 Bologna, Italy; giulia.guidotti9@unibo.it (G.G.); m.soccio@unibo.it (M.S.); andrea.munari@unibo.it (A.M.)

² Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy;

³ Organic Synthesis and Photoreactivity Institute, CNR, Via Gobetti 101, 40129 Bologna, Italy; massimo.gazzano@cnr.it

⁴ Department of Chemical Science, University of Catania, Viale A. Doria 6, 95125 Catania, Italy; vsiracus@dmfci.unict.it

* Correspondence: matteo.gigli@uniroma2.it (M.G.); nadia.lotti@unibo.it (N.L.); Tel.: +39-067-259-4488 (M.G.); +39-051-209-0354 (N.L.)

Film Color Determination

In the Lab Color scale, the lightness coefficient (L^*) ranges from black (0) to white (100). For any L^* value, the coordinates a^* and b^* situate the color on a rectangular coordinate grid perpendicular to L^* axis. At the origin ($a^* = 0$ and $b^* = 0$) the color is achromatic (gray). Moving on the horizontal axis, a positive a^* value indicates a hue of red-purple, a negative a^* value indicates a hue of green. Moving on the vertical axis, a positive b^* value indicates a hue of yellow, a negative b^* value indicates a hue of blue (McGuire, R.G. Reporting of objective color measurements. HortScience 1992, 27, 1254-1255, 10.1016/S0190-9622(89)80314-7).

Table S1. L^* , a^* , b^* , total color difference (ΔE), C^* and h_{ab} of PBFT film.

Sample	L^*	a^*	b^*	ΔE	C^*	h_{ab}
white standard	66.4	-0.74	1.25	-	1.45	121
PBTF	62.5 ± 0.3	-0.47 ± 0.02	6.46 ± 0.37	6.53	6.48	94

$h_{ab} = 0^\circ$, red-purple; $h_{ab} = 90^\circ$, yellow; $h_{ab} = 180^\circ$, green; $h_{ab} = 270^\circ$, blue.

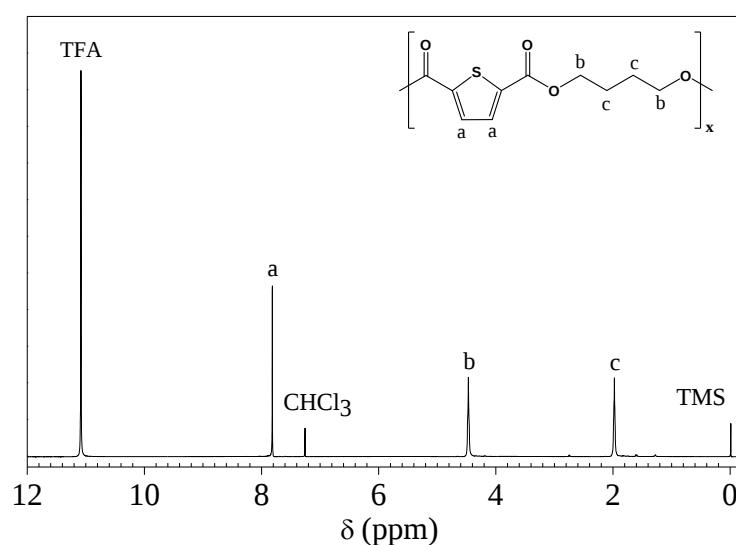
Table S2. Gas transmission rate (GTR) of N₂, O₂ and CO₂ in the range 5–45°C and perm-selectivity ratios for PBTF film (film thickness of 166 µm).

Temperature (°C)	GTR (cm ³ ·cm·m ⁻² ·d ⁻¹ ·bar ⁻¹)			Perm-selectivity		
	O ₂	N ₂	CO ₂	CO ₂ /O ₂	CO ₂ /N ₂	N ₂ /O ₂
5	0.016 ± 13E ⁻⁵	0.016 ± 8E ⁻⁵	0.023 ± 8E ⁻⁵	1.4	1.4	1.0
10	0.017 ± 8E ⁻⁵	0.017 ± 8E ⁻⁵	0.024 ± 13E ⁻⁵	1.4	1.4	1.0
15	0.018 ± 2E ⁻⁵	0.018 ± 2E ⁻⁵	0.024 ± 3E ⁻⁵	1.3	1.3	1.0
23	0.025 ± 10E ⁻⁵	0.023 ± 3E ⁻⁵	0.032 ± 10E ⁻⁵	1.3	1.4	1.0
35	0.035 ± 13E ⁻⁵	0.028 ± 7E ⁻⁵	0.036 ± 13E ⁻⁵	1.0	1.3	0.8
40	0.036 ± 55E ⁻⁵	0.029 ± 7E ⁻⁵	0.036 ± 18E ⁻⁵	1.0	1.2	0.8
45	0.036 ± 13E ⁻⁵	0.029 ± 7E ⁻⁵	0.037 ± 13E ⁻⁵	1.0	1.3	0.8

Table S3. Gas transmission rate (GTR) of PBTF with respect to other polyesters.

Polymer	O ₂ GTR, 35 °C (cm ³ ·cm·m ⁻² ·d ⁻¹ ·bar ⁻¹)	CO ₂ GTR, 35 °C (cm ³ ·cm·m ⁻² ·d ⁻¹ ·bar ⁻¹)
PBTF	0.035 ^a	0.036 ^a
PEF	0.0702 ^b	0.171 ^c
PPF	< 0.005 – 0.0472 ^d	/
PET	0.749 ^b	3.22 ^c
PLA	1.32 ^e	3.24 ^e

^athis work; ^b[³²]; ^c[³³]; ^d[³⁴], values dependent on the ageing time, RH50; ^e[³⁵], 23 °C.

**Figure S1.** ¹H-NMR spectrum of PBTF with resonance assignments.

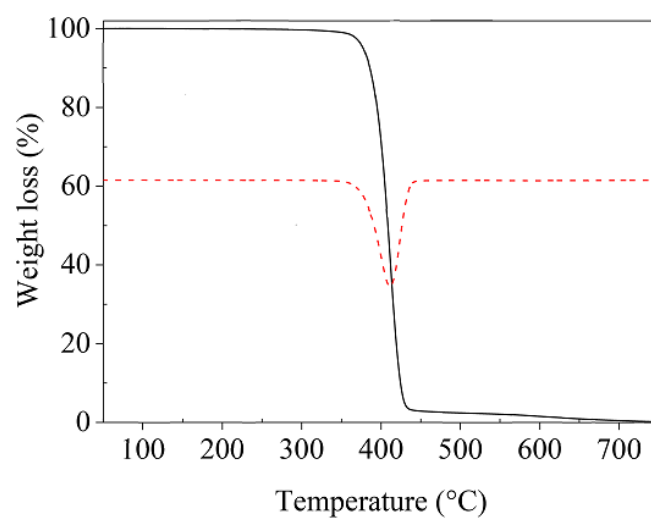


Figure S2. Thermogravimetric curve (solid line) under nitrogen flow of PBTF and its derivative (dashed line).