Two New Polymorphs of the Organic Semiconductor 9,10-Diphenylanthracene: Raman and X-ray Analysis

Tommaso Salzillo[1], Raffaele Guido Della Valle[1], Elisabetta Venuti[*,1], Aldo Brillante[1], Theo Siegrist[2], Matteo Masino[3], Francesco Mezzadri[3], and Alberto Girlando[*,3].

[1]Dip. di Chimica Industriale "Toso Montanari" and INSTM-UdR Bologna, Università di Bologna, Viale Risorgimento 4, I-40136 Bologna, Italy.

[2]Dept. of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Florida State University and Florida A&M University, Tallahassee, FL 32310-6046, U.S.A..

[3]Dip. di Chimica and INSTM-UdR Parma, Università degli Studi di Parma, Area delle Scienze 17/A I-43124 Parma, Italy.

E-mail: elisabetta.venuti@unibo.it; alberto.girlando@unipr.it

Supporting Information

SI content

1. Raman bands in the 0-150 cm^{-1} energy range

Table S 1. Wavenumber of the bands observed in the Raman spectra of the three DPA polymorphs in the energy range 0-150 cm^{-1}.

α-DPA (C2/c)		**β-DPA ($P2_1/a$)**		**γ-DPA ($P2_1/n$)**	
ω (cm^{-1})	*Pol.*	ω (cm^{-1})	*Pol.*	ω (cm^{-1})	*Pol.*
45	*(y,y) (x,y)*	33	*(y,y) (x,y)*	22	*(x,x) (y,y) (x,y)*
55	*(x,x) (y,y) (x,y)*	40	*(x,x) (y,y) (x,y)*	27	*(x,x) (y,y) (x,y)*
60	*(x,x) (y,y) (x,y)*	44	*(y,y) (x,y)*	41	*(x,x) (x,y)*
69	*(x,x) (x,y)*	50	*(x,x) (y,y) (x,y)*	45	*(x,x) (x,y)*
76	*(y,y) (x,y)*	59	*(y,y) (x,y)*	50	*(x,x) (x,y)*
95	*(y,y) (x,y)*	75	*(y,y) (x,y)*	61	*(x,x) (x,y)*
99	*(x,x) (y,y) (x,y)*	92	*(x,x) (x,y)*	78	*(x,x) (y,y) (x,y)*
110	*(x,x) (y,y) (x,y)*	99	*(y,y) (x,y)*	89	*(x,x) (y,y) (x,y)*
118	*(x,x) (x,y)*	115	*(y,y) (x,y)*	105	*(x,x) (y,y) (x,y)*
				116	*(x,x)*

2. Powder XRD

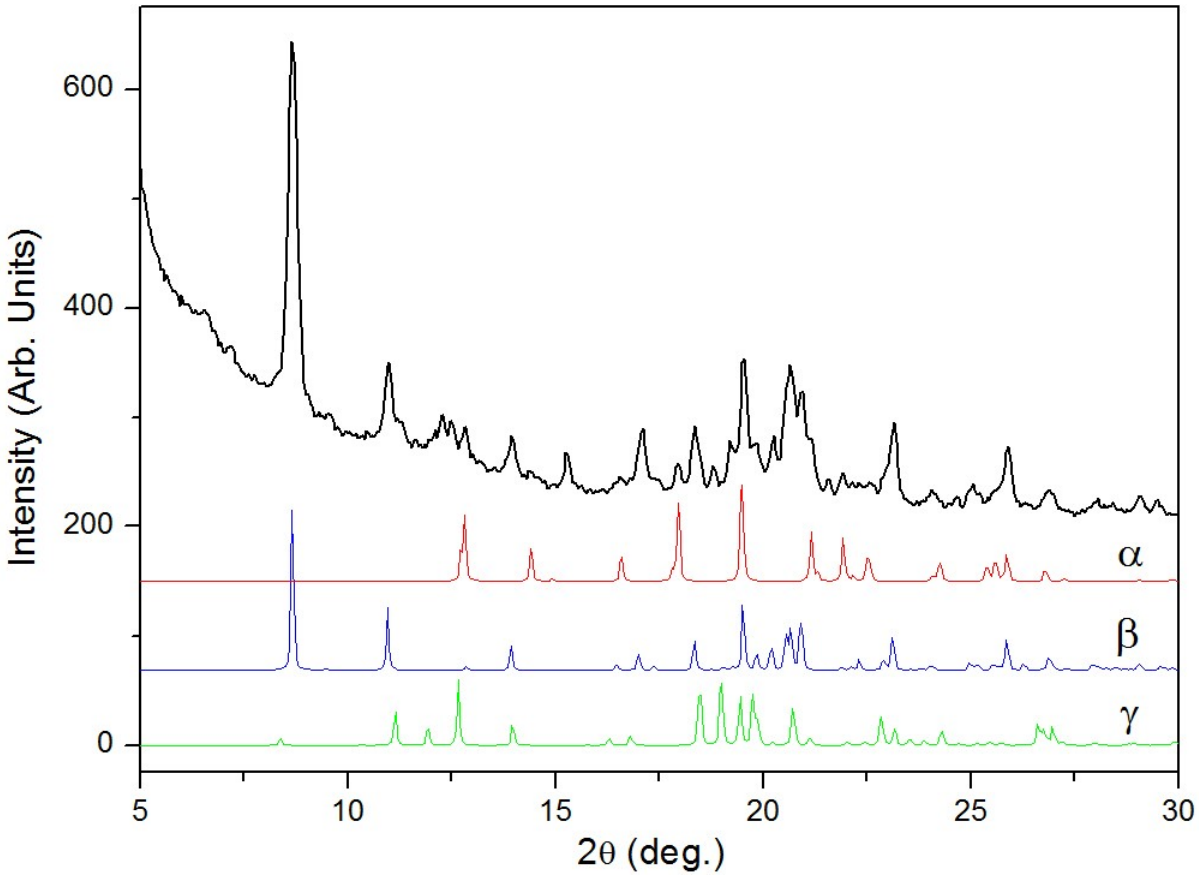

Figure S1. Powder X-ray diffraction of the micro-crystals compared with the simulated powder diffraction of the three polymorphs of DPA.

3. Computed free energy G(p,T) *vs* temperature T (at ambient p).

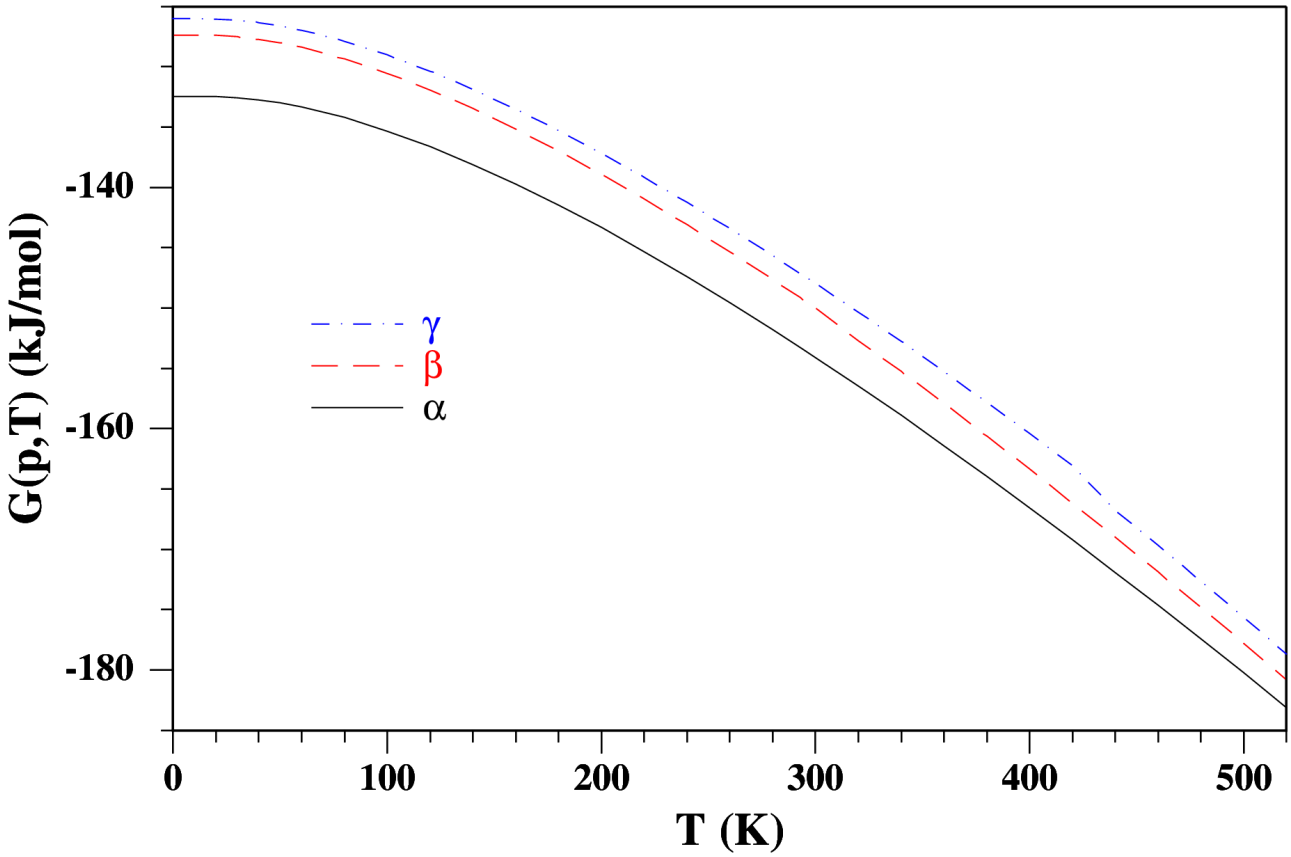

Figure S2. Free energy G(p,T) *vs* temperature T (at ambient pressure), computed for phases α, β and γ of DPA.

4. HOMO and LUMO hopping integrals for the DPA polymorphs

Table S2. Hopping integrals (meV) of the three DPA polymorphs, of Rubrene and of Anthracene

	DPA HOMO, LUMO	**DPA** HOMO, LUMO	**DPA** HOMO, LUMO	**Rubrene** HOMO, LUMO	**Anthracene** HOMO, LUMO
t_1	20, 5	33, 13	18, 14	84, 39	27, 38
t_2	4, 2	4, 0	1, 12	10, 4	
t_3	29, 5	0, 0			
t_4	0, 3				
t_5	5, 2				