

Chiral substituent containing perylene monoanhydride monoimide and its highly soluble symmetrical diimide: Synthesis, photophysics and electrochemistry from dilute solution to solid state

Sheida Amiralaei, Duygu Uzun and Huriye Icil

*Department of Chemistry, Faculty of Arts and Science, Eastern Mediterranean University,
Famagusta, N. Cyprus, Mersin 10, Turkey*

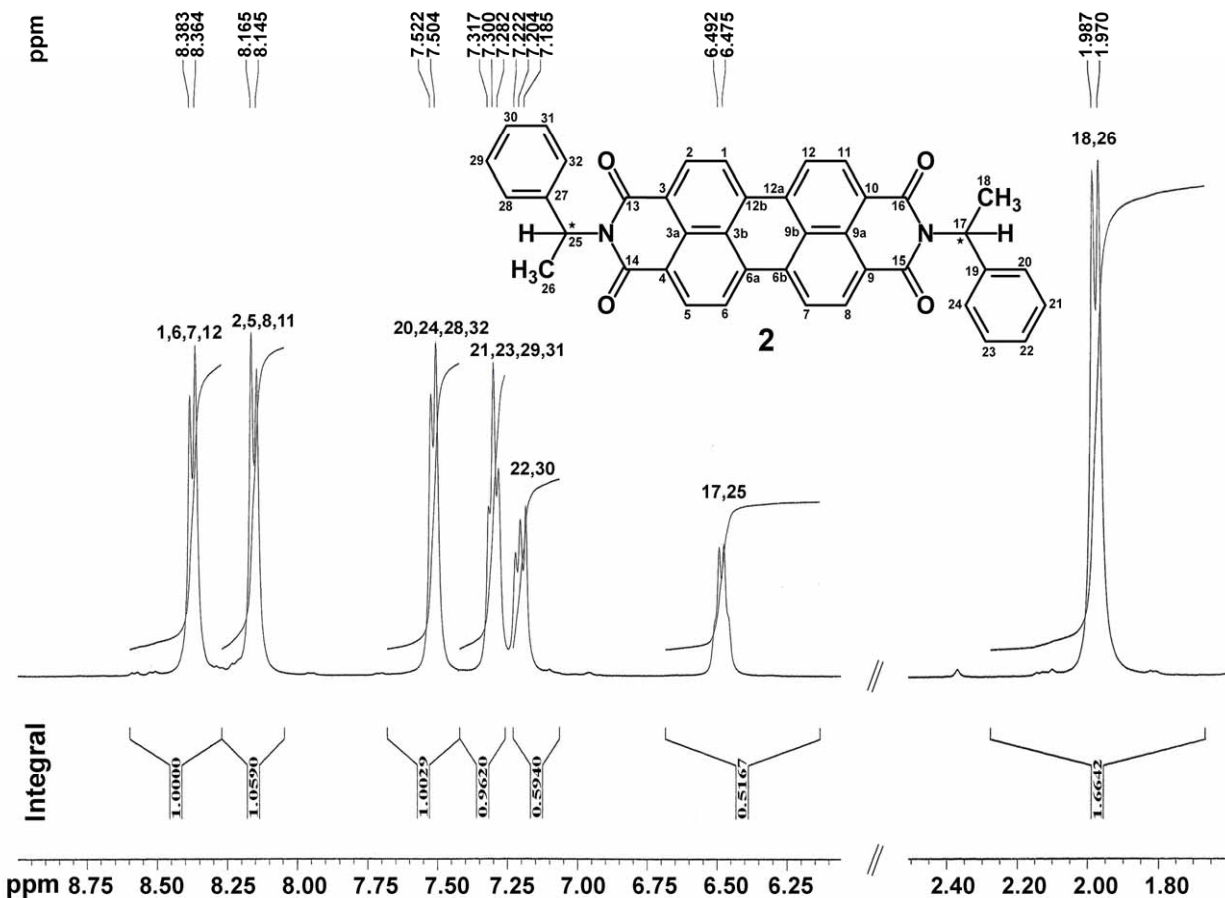


Fig. S1 ^1H NMR spectrum of **2** in CDCl_3

^1H NMR (CDCl_3 , 400 MHz, ppm): δ_{H} 8.38–8.36 (d, $J = 7.7$ Hz, 4 Ar–H, H–C(1), H–C(6), H–C(7), H–C(12)); 8.17–8.15 (d, $J = 7.8$ Hz, 4 Ar–H, H–C(2), H–C(5), H–C(8), H–C(11)); 7.52–7.50 (d, $J = 7.2$ Hz, 4 Ar–H, H–C(20), H–C(24), H–C(28), H–C(32)); 7.32–7.28 (t, $J = 7.1$ Hz, 4 Ar–H, H–C(21), H–C(23), H–C(29), H–C(31)); 7.22–7.19 (t, $J = 7.3$ Hz, 2 Ar–H, H–C(22), H–C(30)); 6.49–6.48 (q, $J = 6.9$ Hz, 2 CH, H–C(17), H–C(25)); 1.99–1.97 ppm (d, $J = 6.8$ Hz, 2 CH_3 , H_3C (18), H_3C (26)).

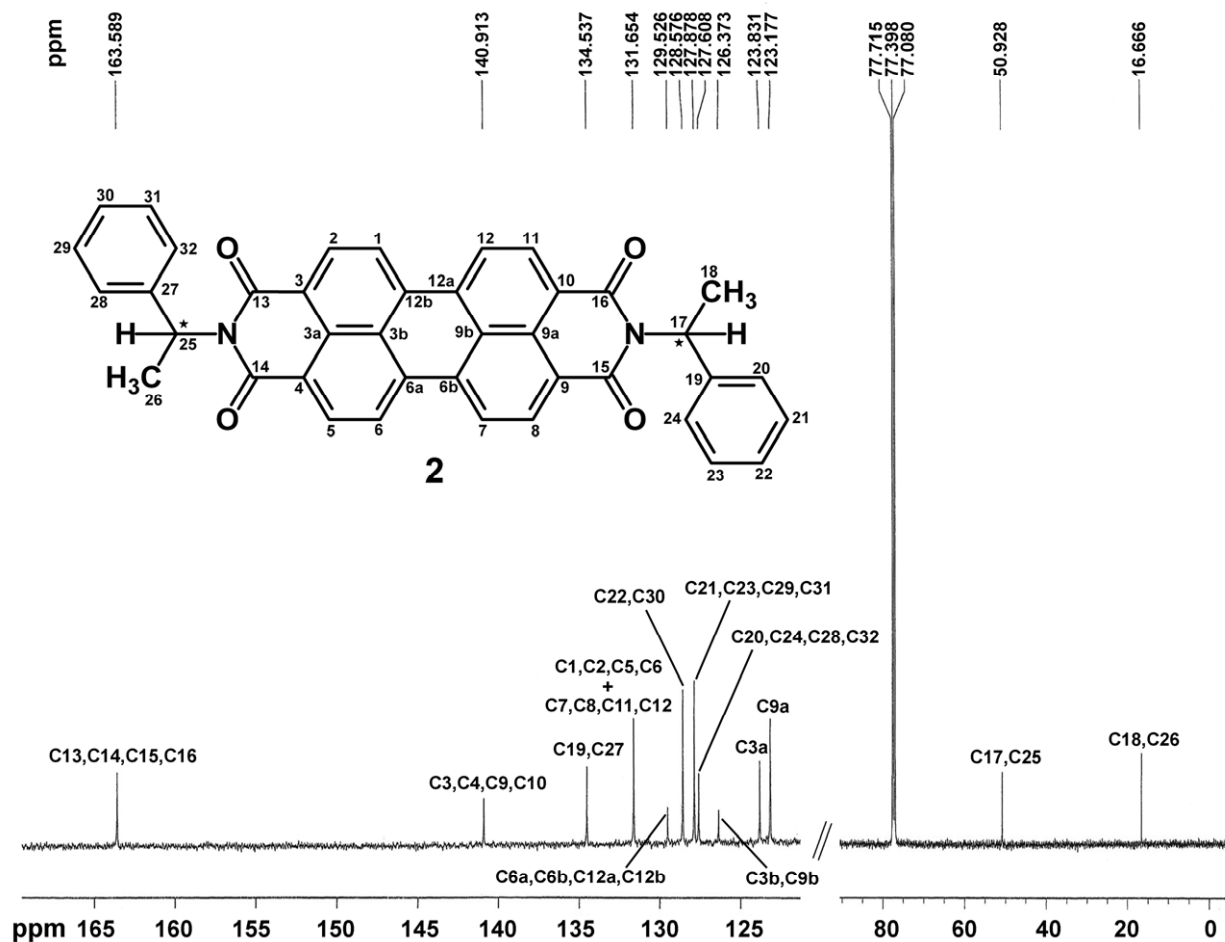


Fig. S2 ^{13}C NMR spectrum of **2** in CDCl_3 .

^{13}C NMR (CDCl_3 , 100.6 MHz, ppm): δ_{C} 163.59 (4 C=O, C(13), C(14), C(15), C(16)); 140.91 (4 (C), C(3), C(4), C(9), C(10)); 134.54 (2 (C), C(19), C(27)); 131.65 (8 CH, C(1), C(2), C(5), C(6), C(7), C(8), C(11), C(12)); 129.53 (4 (C), C(6a), C(6b), C(12a), C(12b)); 128.58 (2 CH, C(22), C(30)); 127.88 (4 CH, C(21), C(23), C(29), C(31)); 127.61 (4 CH, C(20), C(24), C(28), C(32)); 126.37 (2 (C), C(3b), C(9b)); 123.83 ((C), C(3a)); 123.18 ((C), C(9a)); 50.93 (2 CH, C(17), C(25)); 16.67 ppm (2 CH_3 , C(18), C(26)).

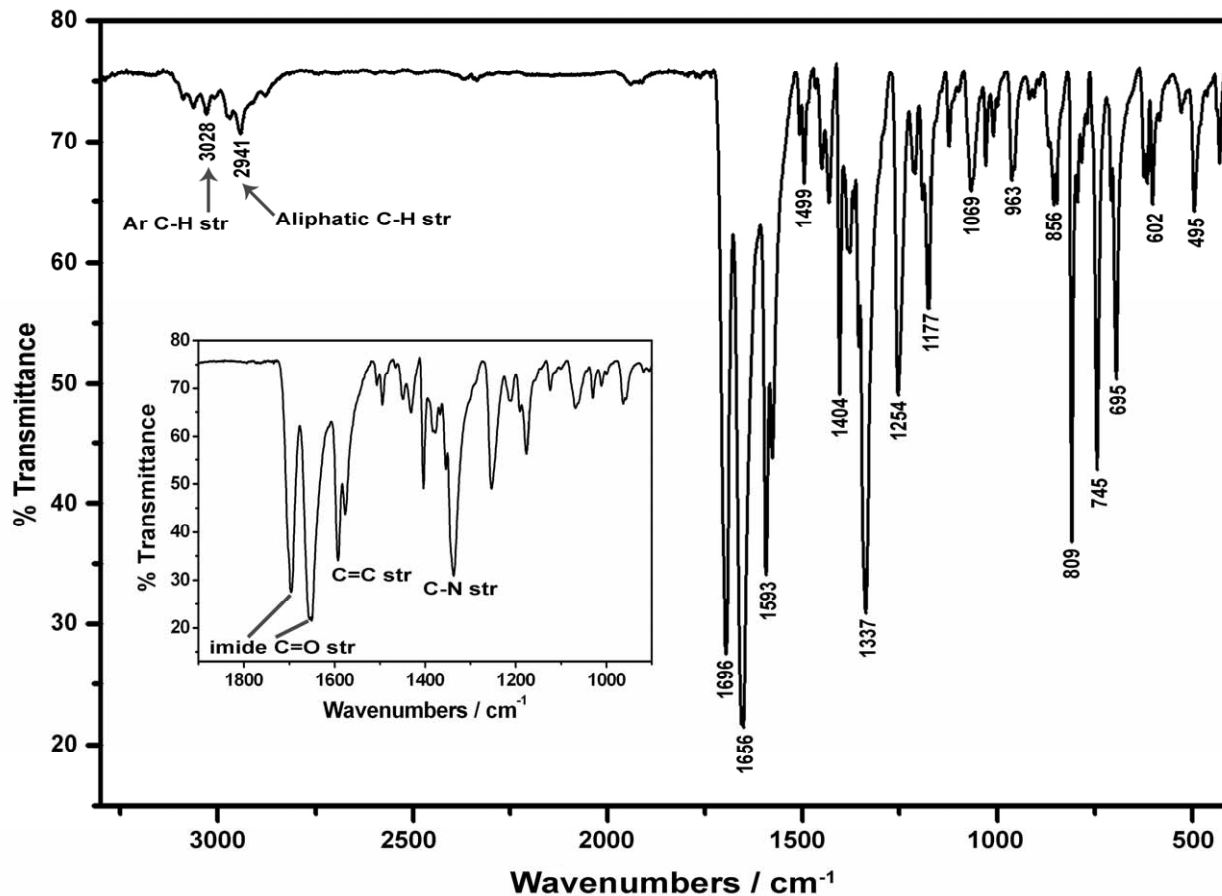


Fig. S3 Infrared spectra of **2**. Insets: The enlarged figures of the peaks.

FT-IR (KBr): ν/cm^{-1} 3028, 2941, 1696, 1656, 1593, 1499, 1404, 1337, 1254, 1177, 1069, 963, 856, 809, 745, 695, 602, 495.

As shown in the IR spectrum of **2**, the characteristic bands of the anhydride carbonyl stretching bands (1771 and 1730) had disappeared and were replaced by *N*-imides carbonyl stretching bands (1696 and 1656). Similarly, the characteristic band of the C–O–C stretching (1016 cm⁻¹) had disappeared and was replaced by C–N stretching band (1337 cm⁻¹). Other absorption bands of **2** were very similar to those of **1**. However, the absorption bands of **2** have become more intense; at 3028 (aromatic C–H stretch); 2941 (aliphatic C–H stretch); 1696, 1656 (imides C=O stretch); 1593 (conjugated C=C stretch); 1337 (C–N stretch); 809 and 745 (C–H bend) cm⁻¹. Moreover, the intrinsic chemical structure of perylene backbone was same in monoanhydride monoimide and diimide perylene structures.

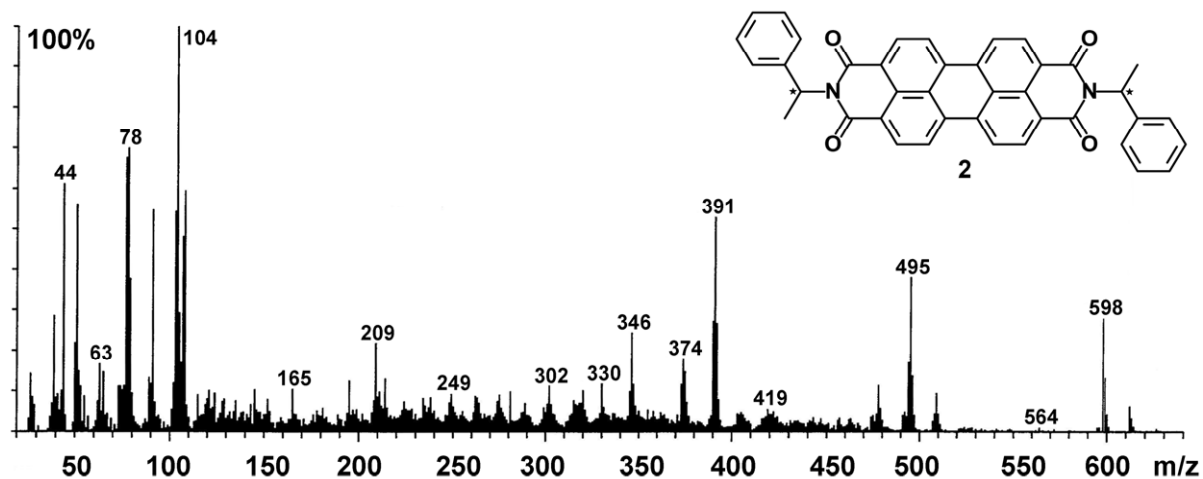


Fig. S4 Mass spectrum of **2** in DMF.

MS (m/z , (%)): 598 (M+1, 31), 564 (2), 495 (39), 419 (7), 391 (54), 374 (19), 346 (26), 330 (13), 302 (12), 249 (10), 209 (22), 165 (11), 104 (100), 78 (70), 63 (17), 44 (61).

The mass spectrum of the compound **2** showed the corresponding molecular ion peak at 598 m/z (M+1). The fragments of 495 and 391 m/z were produced by the breakage of Ph-CCH₂ and Ph-CCH₃ groups, respectively. Additionally, a fragment Ph-CCH₃ at 104 m/z was observed as a base peak.