Ultrafast Dynamical Study of Pyrene-*N,N*-dimethylaniline (PyDMA) as an Organic Molecular Diode in Solid State

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Table S1. Crystal data and structure refinement for PyDMA.

Identification code	PyDMA	
Empirical formula	C24 H19 N	
Formula weight	321.40	
Temperature	100(2) K	
Wavelength	0.60000 Å	
Crystal system	Monoclinic	
Space group	*P*2(1)/*c*	
Unit cell dimensions	*a* = 6.1270(12) Å	α= 90°.
	b = 30.686(6) Å	β= 113.35(2)°.
	c = 9.478(3) Å	γ = 90°.
Volume	1636.0(7) Å^3	
Z	4	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	680	
Crystal size	0.30 x 0.15 x 0.10 mm^3	
Theta range for data collection	2.05 to 27.00°	
Index ranges	-8<=h<=9, -44<=k<=45, -14<=l<=14	
Reflections collected	47866	
Independent reflections	5872 [R(int) = 0.0630]	
Completeness to theta = 27.00°	98.7 %	
Max. and min. transmission	0.9925 and 0.9778	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5872 / 0 / 228	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0472, wR2 = 0.1295	
R indices (all data)	R1 = 0.0571, wR2 = 0.1352	
Largest diff. peak and hole	0.398 and -0.227 e.Å^{-3}	

Table S 2. Bond lengths [Å] and angles [°] for PyDMA.

N(1)-C(1)	1.3826(11)
N(1)-C(24)	1.4433(12)
N(1)-C(23)	1.4444(12)
C(24)-H(52D)	0.9800
C(24)-H(52E)	0.9800
C(24)-H(52F)	0.9800
C(23)-H(52A)	0.9800
C(23)-H(52B)	0.9800
C(23)-H(52C)	0.9800
C(21)-C(22)	1.3573(12)
C(21)-C(20)	1.4399(12)
C(21)-H(21)	0.9500
C(22)-C(17)	1.4317(12)
C(22)-H(22)	0.9500
C(20)-C(7)	1.4164(12)
C(20)-C(19)	1.4243(12)
C(19)-C(10)	1.4246(12)
C(19)-C(18)	1.4297(12)
C(18)-C(17)	1.4241(12)
C(18)-C(13)	1.4253(12)
C(17)-C(16)	1.4021(12)
C(16)-C(15)	1.3873(14)
C(16)-H(16)	0.9500
C(15)-C(14)	1.3896(14)
C(15)-H(15)	0.9500
C(14)-C(13)	1.4020(13)
C(14)-H(14)	0.9500
C(13)-C(12)	1.4376(13)
C(12)-C(11)	1.3564(13)
C(12)-H(12)	0.9500
C(11)-C(10)	1.4354(13)
C(11)-H(11)	0.9500
C(10)-C(9)	1.3993(12)
C(9)-C(8)	1.3846(13)

C(9)-H(9)	0.9500
C(8)-C(7)	1.3989(12)
C(8)-H(8)	0.9500
C(7)-C(4)	1.4851(12)
C(6)-C(5)	1.3861(12)
C(6)-C(1)	1.4099(12)
C(6)-H(6)	0.9500
C(5)-C(4)	1.3986(12)
C(5)-H(5)	0.9500
C(4)-C(3)	1.3967(12)
C(3)-C(2)	1.3880(12)
C(3)-H(3)	0.9500
C(2)-C(1)	1.4098(12)
C(2)-H(2)	0.9500

C(1)-N(1)-C(24)	120.00(7)
C(1)-N(1)-C(23)	120.31(7)
C(24)-N(1)-C(23)	119.50(8)
N(1)-C(24)-H(52D)	109.5
N(1)-C(24)-H(52E)	109.5
H(52D)-C(24)-H(52E)	109.5
N(1)-C(24)-H(52F)	109.5
H(52D)-C(24)-H(52F)	109.5
H(52E)-C(24)-H(52F)	109.5
N(1)-C(23)-H(52A)	109.5
N(1)-C(23)-H(52B)	109.5
H(52A)-C(23)-H(52B)	109.5
N(1)-C(23)-H(52C)	109.5
H(52A)-C(23)-H(52C)	109.5
H(52B)-C(23)-H(52C)	109.5
C(22)-C(21)-C(20)	121.71(8)
C(22)-C(21)-H(21)	119.1
C(20)-C(21)-H(21)	119.1
C(21)-C(22)-C(17)	121.26(8)
C(21)-C(22)-H(22)	119.4
C(17)-C(22)-H(22)	119.4

C(7)-C(20)-C(19)	119.37(8)
C(7)-C(20)-C(21)	122.44(8)
C(19)-C(20)-C(21)	118.14(7)
C(20)-C(19)-C(10)	120.36(8)
C(20)-C(19)-C(18)	120.16(7)
C(10)-C(19)-C(18)	119.47(8)
C(17)-C(18)-C(13)	119.77(8)
C(17)-C(18)-C(19)	119.98(8)
C(13)-C(18)-C(19)	120.24(8)
C(16)-C(17)-C(18)	119.10(8)
C(16)-C(17)-C(22)	122.15(8)
C(18)-C(17)-C(22)	118.74(8)
C(15)-C(16)-C(17)	120.66(9)
C(15)-C(16)-H(16)	119.7
C(17)-C(16)-H(16)	119.7
C(16)-C(15)-C(14)	120.78(9)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(15)-C(14)-C(13)	120.63(9)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(14)-C(13)-C(18)	119.06(8)
C(14)-C(13)-C(12)	122.18(8)
C(18)-C(13)-C(12)	118.76(8)
C(11)-C(12)-C(13)	120.97(8)
C(11)-C(12)-H(12)	119.5
C(13)-C(12)-H(12)	119.5
C(12)-C(11)-C(10)	121.59(8)
C(12)-C(11)-H(11)	119.2
C(10)-C(11)-H(11)	119.2
C(9)-C(10)-C(19)	118.73(8)
C(9)-C(10)-C(11)	122.31(8)
C(19)-C(10)-C(11)	118.95(8)
C(8)-C(9)-C(10)	120.67(8)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7

C(9)-C(8)-C(7)	121.97(8)
C(9)-C(8)-H(8)	119.0
C(7)-C(8)-H(8)	119.0
C(8)-C(7)-C(20)	118.89(8)
C(8)-C(7)-C(4)	120.04(7)
C(20)-C(7)-C(4)	121.04(7)
C(5)-C(6)-C(1)	120.70(8)
C(5)-C(6)-H(6)	119.6
C(1)-C(6)-H(6)	119.6
C(6)-C(5)-C(4)	121.80(8)
C(6)-C(5)-H(5)	119.1
C(4)-C(5)-H(5)	119.1
C(3)-C(4)-C(5)	117.34(8)
C(3)-C(4)-C(7)	120.70(7)
C(5)-C(4)-C(7)	121.95(7)
C(2)-C(3)-C(4)	121.85(8)
C(2)-C(3)-H(3)	119.1
C(4)-C(3)-H(3)	119.1
C(3)-C(2)-C(1)	120.61(8)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
N(1)-C(1)-C(2)	121.37(7)
N(1)-C(1)-C(6)	120.99(7)
C(2)-C(1)-C(6)	117.64(8)

Symmetry transformations used to generate equivalent atoms:

Table S3. Torsion angles [°] for PyDMA.

C(20)-C(21)-C(22)-C(17)	-0.27(13)
C(22)-C(21)-C(20)-C(7)	177.85(8)
C(22)-C(21)-C(20)-C(19)	0.24(12)
C(7)-C(20)-C(19)-C(10)	0.69(11)
C(21)-C(20)-C(19)-C(10)	178.37(7)
C(7)-C(20)-C(19)-C(18)	-177.93(7)
C(21)-C(20)-C(19)-C(18)	-0.25(11)
C(20)-C(19)-C(18)-C(17)	0.30(12)
C(10)-C(19)-C(18)-C(17)	-178.34(7)
C(20)-C(19)-C(18)-C(13)	179.27(7)
C(10)-C(19)-C(18)-C(13)	0.63(12)
C(13)-C(18)-C(17)-C(16)	-0.39(12)
C(19)-C(18)-C(17)-C(16)	178.59(8)
C(13)-C(18)-C(17)-C(22)	-179.29(8)
C(19)-C(18)-C(17)-C(22)	-0.31(12)
C(21)-C(22)-C(17)-C(16)	-178.56(8)
C(21)-C(22)-C(17)-C(18)	0.30(12)
C(18)-C(17)-C(16)-C(15)	-0.45(13)
C(22)-C(17)-C(16)-C(15)	178.41(8)
C(17)-C(16)-C(15)-C(14)	0.95(15)
C(16)-C(15)-C(14)-C(13)	-0.61(15)
C(15)-C(14)-C(13)-C(18)	-0.23(13)
C(15)-C(14)-C(13)-C(12)	-179.17(9)
C(17)-C(18)-C(13)-C(14)	0.72(12)
C(19)-C(18)-C(13)-C(14)	-178.25(8)
C(17)-C(18)-C(13)-C(12)	179.69(7)
C(19)-C(18)-C(13)-C(12)	0.72(12)
C(14)-C(13)-C(12)-C(11)	177.63(8)
C(18)-C(13)-C(12)-C(11)	-1.31(13)
C(13)-C(12)-C(11)-C(10)	0.52(13)
C(20)-C(19)-C(10)-C(9)	-1.12(12)
C(18)-C(19)-C(10)-C(9)	177.51(8)
C(20)-C(19)-C(10)-C(11)	179.95(7)
C(18)-C(19)-C(10)-C(11)	-1.42(11)

C(12)-C(11)-C(10)-C(9)	-178.03(8)
C(12)-C(11)-C(10)-C(19)	0.86(13)
C(19)-C(10)-C(9)-C(8)	0.46(12)
C(11)-C(10)-C(9)-C(8)	179.35(8)
C(10)-C(9)-C(8)-C(7)	0.65(13)
C(9)-C(8)-C(7)-C(20)	-1.08(12)
C(9)-C(8)-C(7)-C(4)	-179.10(8)
C(19)-C(20)-C(7)-C(8)	0.39(12)
C(21)-C(20)-C(7)-C(8)	-177.18(7)
C(19)-C(20)-C(7)-C(4)	178.40(7)
C(21)-C(20)-C(7)-C(4)	0.82(12)
C(1)-C(6)-C(5)-C(4)	0.77(13)
C(6)-C(5)-C(4)-C(3)	1.44(13)
C(6)-C(5)-C(4)-C(7)	-177.38(8)
C(8)-C(7)-C(4)-C(3)	62.00(11)
C(20)-C(7)-C(4)-C(3)	-115.98(9)
C(8)-C(7)-C(4)-C(5)	-119.22(9)
C(20)-C(7)-C(4)-C(5)	62.80(11)
C(5)-C(4)-C(3)-C(2)	-2.21(13)
C(7)-C(4)-C(3)-C(2)	176.62(8)
C(4)-C(3)-C(2)-C(1)	0.79(13)
C(24)-N(1)-C(1)-C(2)	-179.67(8)
C(23)-N(1)-C(1)-C(2)	-4.74(13)
C(24)-N(1)-C(1)-C(6)	0.99(13)
C(23)-N(1)-C(1)-C(6)	175.91(8)
C(3)-C(2)-C(1)-N(1)	-177.93(8)
C(3)-C(2)-C(1)-C(6)	1.44(12)
C(5)-C(6)-C(1)-N(1)	177.17(8)
C(5)-C(6)-C(1)-C(2)	-2.20(12)

Symmetry transformations used to generate equivalent atoms: