The Journal of Physical Chemistry A

SUPPORTING INFORMATION

One- and Two-Photon Spectroscopy of Donor-Acceptor-Donor Bis(styryl)benzene Derivatives: Effect of Cyano Substitution and Distortion from Planarity

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X-ray report for 2,5-dicyano-1,4-bis[2-(4-diphenylamino-phenyl)vinyl]-benzene (compound 2)

Table 1. Crystal data and structure refinement for compound 2

Empirical formula	$C_{48}H_{34}N_4$
Formula weight	666.79
Crystallization solvent	$CHCl_3$\Petroleum ether
Crystal shape	Fragment
Crystal size	0.11 x 0.19 x 0.29 mm
Crystal color	Red--orange
Data Collection	
Preliminary photos	
Type of diffractometer	CAD-4
Wavelength	0.71073 Å MoKα
Data collection temperature	85 K
Lattice determination from	25 reflections
Theta range for reflections used in lattice determination	9.8 to 11.5°
Unit cell dimensions	a = 11.089(3)Å α = 90° b = 15.914(3)Å β = 90° c = 19.842(5)Å γ = 90°
Volume	3501.5Å^3
Z	4
Crystal system and space group	Orthorhombic Pbca
Density (calculated)	1.265 g/cm^3
Absorption coefficient	0.074 mm^{-1}
F(000)	1400
Theta range for data collection	2.0 to 25.0°
Index ranges	$0 \le h \le 13$, $-18 \le k \le 18$, $0 \le l \le 23$
Data collection scan type	ω scans
Reflections collected	6994
Independent reflections	3067 [R_{merge} = 0.057 GOF_{merge} = 0.955]
Absorption correction	None
Number of standards	3 reflections measured every 75 min.
Variation of standards	Within counting statistics, zero %.

Table 1 (cont).

Structure solution and Refinement

Structure solution program	SHELXS-86 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	3064 / 0 / 303
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.292
Final R indices [$I>2\sigma(I)$]	R1 = 0.0631, *w*R2 = 0.0853
R indices (all data)	R1 = 0.1164, *w*R2 = 0.1010
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	0.386 and -0.233 $e^{-}Å^{-3}$

Special Notes

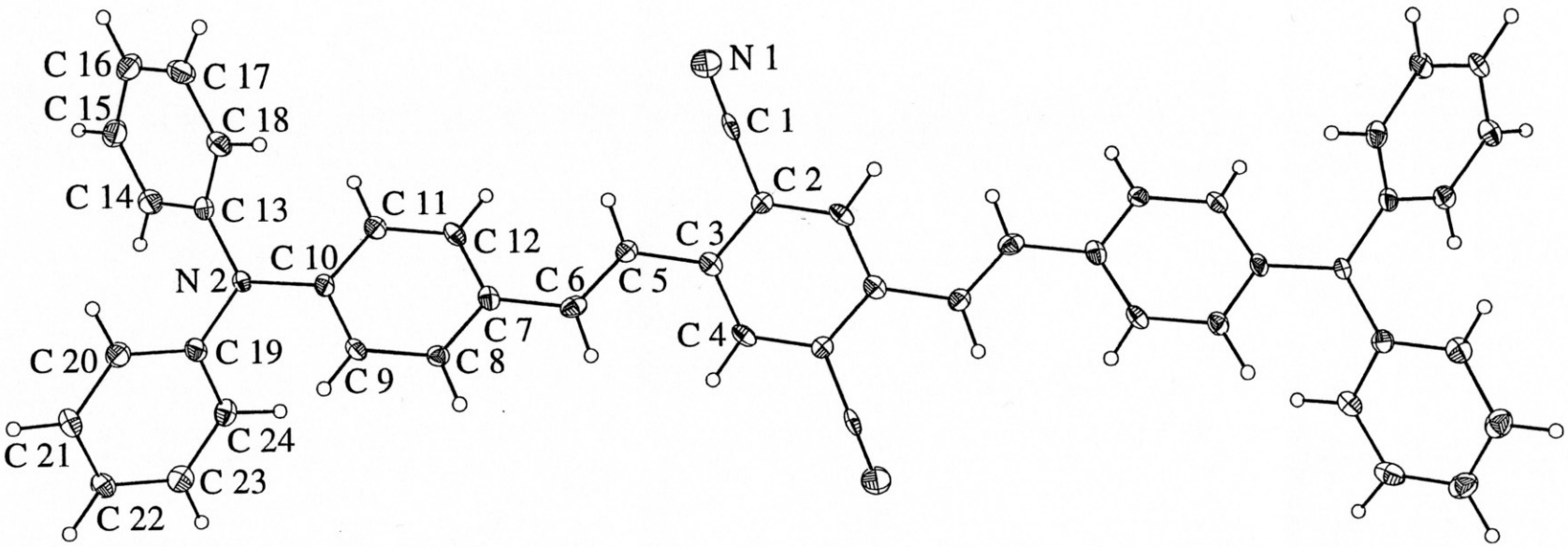

Figure 1: View of compound 2. All unique atoms are labeled.
Non-hydrogen atoms are shown as 50% probability ellipsoids.

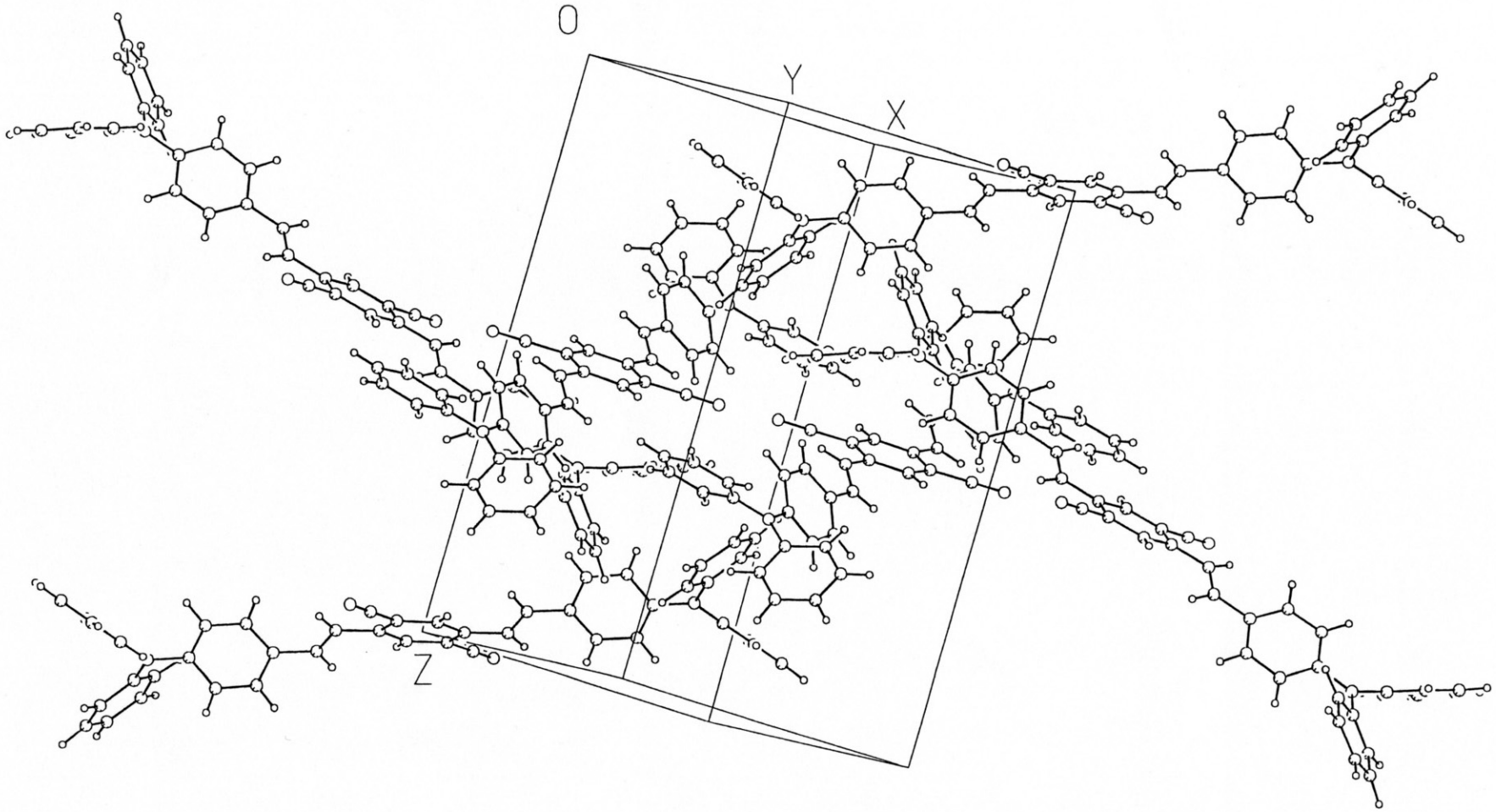

Figure 2: Crystal packing of compound 2. The unit cell boundaries are shown.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for comp. 2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	8256(2)	-1037(2)	4947(1)	30(1)
N(2)	10904(2)	3721(1)	6705(1)	17(1)
C(1)	7327(3)	-731(2)	4955(2)	18(1)
C(2)	6142(3)	-344(2)	4960(1)	13(1)
C(3)	6022(3)	502(2)	5183(1)	15(1)
C(4)	4851(3)	823(2)	5210(1)	15(1)
C(5)	7078(3)	1000(2)	5378(2)	15(1)
C(6)	7038(3)	1652(2)	5795(2)	17(1)
C(7)	8051(3)	2173(2)	6016(1)	15(1)
C(8)	7940(3)	2658(2)	6601(1)	14(1)
C(9)	8882(3)	3145(2)	6837(2)	15(1)
C(10)	9968(3)	3183(2)	6481(1)	14(1)
C(11)	10094(3)	2691(2)	5900(2)	16(1)
C(12)	9155(3)	2195(2)	5681(2)	16(1)
C(13)	12133(3)	3548(2)	6534(1)	16(1)
C(14)	12886(3)	4207(2)	6337(1)	19(1)
C(15)	14071(3)	4044(2)	6168(2)	23(1)
C(16)	14526(3)	3239(2)	6200(2)	24(1)
C(17)	13791(3)	2589(2)	6409(2)	23(1)
C(18)	12598(3)	2736(2)	6575(2)	19(1)
C(19)	10634(3)	4464(2)	7077(1)	17(1)
C(20)	11341(3)	4672(2)	7631(2)	19(1)
C(21)	11109(3)	5397(2)	7998(2)	22(1)
C(22)	10135(3)	5907(2)	7821(2)	21(1)
C(23)	9417(3)	5687(2)	7280(2)	20(1)
C(24)	9674(3)	4977(2)	6902(2)	17(1)

Table 3. Bond lengths [Å] and angles [°] for compound 2

N(1)-C(1)	1.139(4)	N(1)-C(1)-C(2)	179.5(3)
N(2)-C(10)	1.417(3)	C(4)#1-C(2)-C(3)	121.5(3)
N(2)-C(19)	1.426(3)	C(4)#1-C(2)-C(1)	119.1(2)
N(2)-C(13)	1.431(3)	C(3)-C(2)-C(1)	119.2(3)
C(1)-C(2)	1.451(4)	C(4)-C(3)-C(2)	116.4(3)
C(2)-C(4)#1	1.381(4)	C(4)-C(3)-C(5)	122.4(3)
C(2)-C(3)	1.424(4)	C(2)-C(3)-C(5)	121.2(3)
C(3)-C(4)	1.396(4)	C(2)#1-C(4)-C(3)	122.0(3)
C(3)-C(5)	1.467(4)	C(2)#1-C(4)-H(4)	116(2)
C(4)-C(2)#1	1.381(4)	C(3)-C(4)-H(4)	122(2)
C(4)-H(4)	1.00(3)	C(6)-C(5)-C(3)	124.1(3)
C(5)-C(6)	1.328(4)	C(6)-C(5)-H(5)	117(2)
C(5)-H(5)	0.95(3)	C(3)-C(5)-H(5)	118(2)
C(6)-C(7)	1.463(4)	C(5)-C(6)-C(7)	127.2(3)
C(6)-H(6)	0.92(2)	C(5)-C(6)-H(6)	117(2)
C(7)-C(8)	1.398(4)	C(7)-C(6)-H(6)	116(2)
C(7)-C(12)	1.394(4)	C(8)-C(7)-C(12)	117.4(3)
C(8)-C(9)	1.384(4)	C(8)-C(7)-C(6)	119.6(3)
C(8)-H(8)	0.99(3)	C(12)-C(7)-C(6)	123.0(3)
C(9)-C(10)	1.398(4)	C(7)-C(8)-C(9)	121.7(3)
C(9)-H(9)	0.93(3)	C(7)-C(8)-H(8)	120(2)
C(10)-C(11)	1.401(4)	C(9)-C(8)-H(8)	118(2)
C(11)-C(12)	1.377(4)	C(10)-C(9)-C(8)	120.2(3)
C(11)-H(11)	1.02(2)	C(10)-C(9)-H(9)	122(2)
C(12)-H(12)	0.95(2)	C(8)-C(9)-H(9)	117(2)
C(13)-C(18)	1.392(4)	C(9)-C(10)-C(11)	118.6(3)
C(13)-C(14)	1.397(4)	C(9)-C(10)-N(2)	119.9(3)
C(14)-C(15)	1.381(4)	C(11)-C(10)-N(2)	121.5(3)
C(14)-H(14)	0.96(2)	C(12)-C(11)-C(10)	120.3(3)
C(15)-C(16)	1.378(4)	C(12)-C(11)-H(11)	119.2(14)
C(15)-H(15)	1.02(3)	C(10)-C(11)-H(11)	120.5(14)
C(16)-C(17)	1.380(4)	C(11)-C(12)-C(7)	121.9(3)
C(16)-H(16)	0.96(3)	C(11)-C(12)-H(12)	117(2)
C(17)-C(18)	1.384(4)	C(7)-C(12)-H(12)	121(2)
C(17)-H(17)	1.00(3)	C(18)-C(13)-C(14)	119.4(3)
C(18)-H(18)	1.01(3)	C(18)-C(13)-N(2)	121.2(3)
C(19)-C(24)	1.387(4)	C(14)-C(13)-N(2)	119.4(3)
C(19)-C(20)	1.390(4)	C(15)-C(14)-C(13)	119.7(3)
C(20)-C(21)	1.387(4)	C(15)-C(14)-H(14)	120(2)
C(20)-H(20)	1.00(3)	C(13)-C(14)-H(14)	120(2)
C(21)-C(22)	1.395(4)	C(16)-C(15)-C(14)	120.8(3)
C(21)-H(21)	1.00(3)	C(16)-C(15)-H(15)	121(2)
C(22)-C(23)	1.381(4)	C(14)-C(15)-H(15)	119(2)
C(22)-H(22)	1.00(3)	C(15)-C(16)-C(17)	119.6(3)
C(23)-C(24)	1.386(4)	C(15)-C(16)-H(16)	119(2)
C(23)-H(23)	0.97(3)	C(17)-C(16)-H(16)	122(2)
C(24)-H(24)	1.00(3)	C(16)-C(17)-C(18)	120.6(3)
		C(16)-C(17)-H(17)	129(2)
C(10)-N(2)-C(19)	120.7(2)	C(18)-C(17)-H(17)	110(2)
C(10)-N(2)-C(13)	120.5(2)	C(13)-C(18)-C(17)	119.8(3)
C(19)-N(2)-C(13)	118.8(2)	C(13)-C(18)-H(18)	123(2)

C(17)-C(18)-H(18)	117(2)	C(21)-C(22)-C(23)	119.6(3)
C(24)-C(19)-C(20)	119.4(3)	C(21)-C(22)-H(22)	119(2)
C(24)-C(19)-N(2)	121.3(3)	C(23)-C(22)-H(22)	121(2)
C(20)-C(19)-N(2)	119.3(3)	C(24)-C(23)-C(22)	120.6(3)
C(21)-C(20)-C(19)	120.5(3)	C(24)-C(23)-H(23)	121(2)
C(21)-C(20)-H(20)	119(2)	C(22)-C(23)-H(23)	119(2)
C(19)-C(20)-H(20)	121(2)	C(23)-C(24)-C(19)	120.1(3)
C(20)-C(21)-C(22)	119.7(3)	C(23)-C(24)-H(24)	119(2)
C(20)-C(21)-H(21)	121(2)	C(19)-C(24)-H(24)	121(2)
C(22)-C(21)-H(21)	119(2)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1

Table 4. Anisotropic displacement parameters (Å x 10^3) for comp. 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
N(1)	24(2)	24(2)	41(2)	-4(1)	-5(2)	7(1)
N(2)	13(1)	12(1)	24(1)	-6(1)	0(1)	-3(1)
C(1)	24(2)	9(2)	22(2)	-5(1)	-3(2)	-5(1)
C(2)	14(2)	14(1)	12(2)	3(1)	-1(1)	0(1)
C(3)	20(2)	11(1)	13(2)	3(1)	2(1)	-1(1)
C(4)	24(2)	9(2)	13(2)	0(1)	1(1)	1(1)
C(5)	14(2)	15(2)	17(2)	1(1)	0(1)	0(1)
C(6)	14(2)	14(2)	22(2)	5(1)	2(2)	3(1)
C(7)	19(2)	8(1)	18(2)	3(1)	-5(1)	1(1)
C(8)	15(2)	12(2)	17(2)	0(1)	1(1)	1(1)
C(9)	19(2)	11(2)	14(2)	-3(1)	-2(1)	1(1)
C(10)	15(2)	7(1)	21(2)	1(1)	-3(1)	-1(1)
C(11)	18(2)	10(2)	19(2)	2(1)	0(1)	-1(1)
C(12)	22(2)	9(1)	15(2)	-1(1)	-1(2)	-1(1)
C(13)	15(2)	19(2)	15(2)	-4(1)	-3(1)	0(1)
C(14)	20(2)	18(2)	19(2)	0(1)	-2(1)	1(2)
C(15)	19(2)	30(2)	21(2)	-2(2)	-2(2)	-2(2)
C(16)	16(2)	34(2)	22(2)	-6(2)	-2(2)	2(2)
C(17)	26(2)	23(2)	20(2)	-7(2)	-3(2)	8(2)
C(18)	23(2)	15(2)	19(2)	-2(1)	-1(2)	1(1)
C(19)	17(2)	14(2)	20(2)	-2(1)	4(1)	-5(1)
C(20)	18(2)	15(2)	25(2)	0(1)	-1(2)	0(1)
C(21)	25(2)	20(2)	22(2)	-7(2)	-2(2)	-3(2)
C(22)	21(2)	10(2)	33(2)	-6(1)	1(2)	-1(1)
C(23)	21(2)	10(2)	30(2)	4(1)	-2(2)	1(1)
C(24)	18(2)	15(2)	20(2)	4(1)	-2(2)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for compound 2.

	x	y	z	U(eq)
H(4)	4686(24)	1420(17)	5336(13)	18(8)
H(5)	7853(26)	811(16)	5241(13)	22(8)
H(6)	6304(22)	1787(15)	5976(12)	1(7)
H(8)	7185(25)	2646(16)	6865(14)	23(8)
H(9)	8781(26)	3406(16)	7254(13)	19(8)
H(11)	10881(22)	2700(14)	5631(12)	4(7)
H(12)	9274(24)	1887(16)	5275(13)	13(8)
H(14)	12580(25)	4771(15)	6309(13)	15(8)
H(15)	14600(25)	4532(17)	6008(14)	26(9)
H(16)	15355(26)	3147(17)	6076(15)	25(9)
H(17)	13982(28)	1980(18)	6450(14)	36(10)
H(18)	12094(24)	2236(16)	6716(13)	17(8)
H(20)	12052(28)	4322(17)	7757(14)	36(10)
H(21)	11579(26)	5525(17)	8416(15)	31(9)
H(22)	9965(30)	6421(19)	8092(16)	51(11)
H(23)	8738(25)	6046(16)	7164(13)	21(8)
H(24)	9118(25)	4816(16)	6527(13)	21(8)