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

Table 1. Crystal data and structure refinement for compound 4.

Empirical formula	$C_{48}H_{34}N_4$
Formula weight	666.79
Crystallization solvent	CH_2Cl_2/Petroleum ether
Crystal shape	Fragment
Crystal size	0.26 x 0.15 x 0.11 mm
Crystal color	Yellow
Data Collection	
Preliminary photos	None
Type of diffractometer	CAD-4
Wavelength	0.71073Å MoKα
Data collection temperature	85 K
Lattice determination from	25 reflections
Theta range for reflections used in lattice determination	7.1 to 15.2°
Unit cell dimensions	a = 8.509(6)Å α= 90° b = 9.352(6)Å β = 99.69(5)° c = 22.57(2)Å γ = 90°
Volume	1770.6Å^3
Z	2
Crystal system and space group	Monoclinic $P2_1/n$
Density (calculated)	1.251 g/cm^3
Absorption coefficient	0.074 mm^{-1}
F(000)	700
Theta range for data collection	1.8 to 25.0°
Index ranges	$-10 \le h \le 9$, $-11 \le k \le 11$, $0 \le l \le 26$
Data collection scan type	ω scans
Reflections collected	6840
Independent reflections	3098 [R_{merge} = 0.058 GOF_{merge} = 1.01]
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	3098 / 0 / 303
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.302
Final R indices [$I>2\sigma(I)$]	R1 = 0.0557, *w*R2 = 0.0825
R indices (all data)	R1 = 0.1011, *w*R2 = 0.0962
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	0.366 and -0.263 e.Å^{-3}

Special Notes

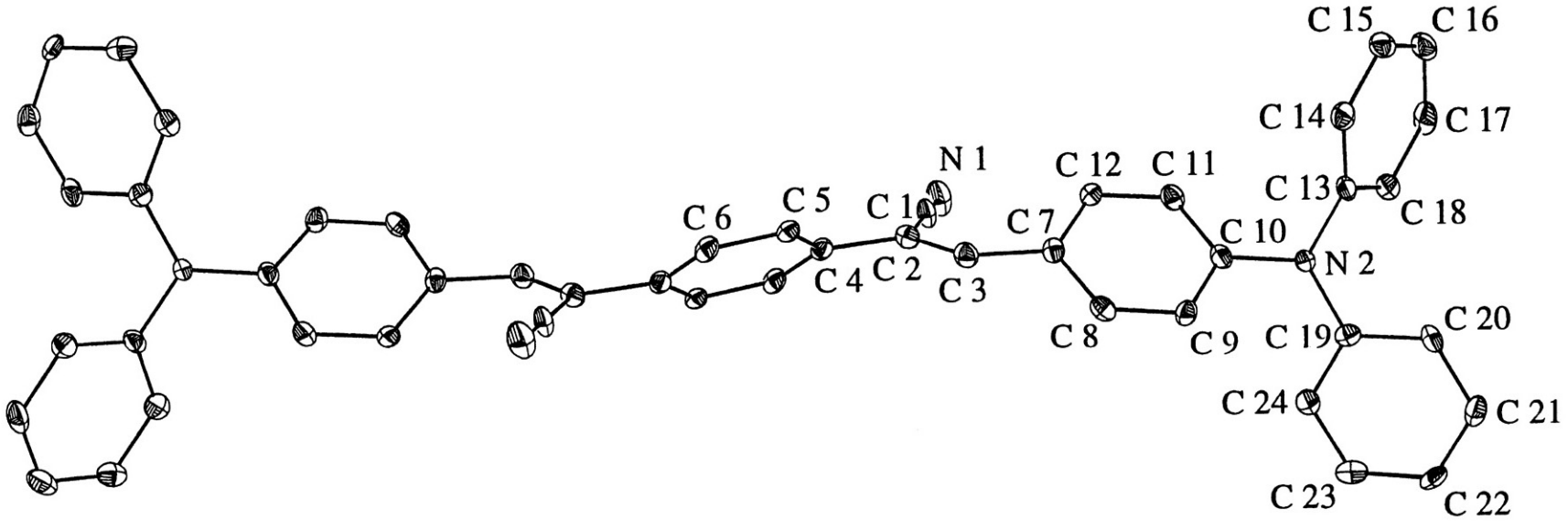

Figure 1: View of compound 4 (less hydrogen atoms). All unique atoms are labeled. All atoms are shown as 50% probability ellipsoids.

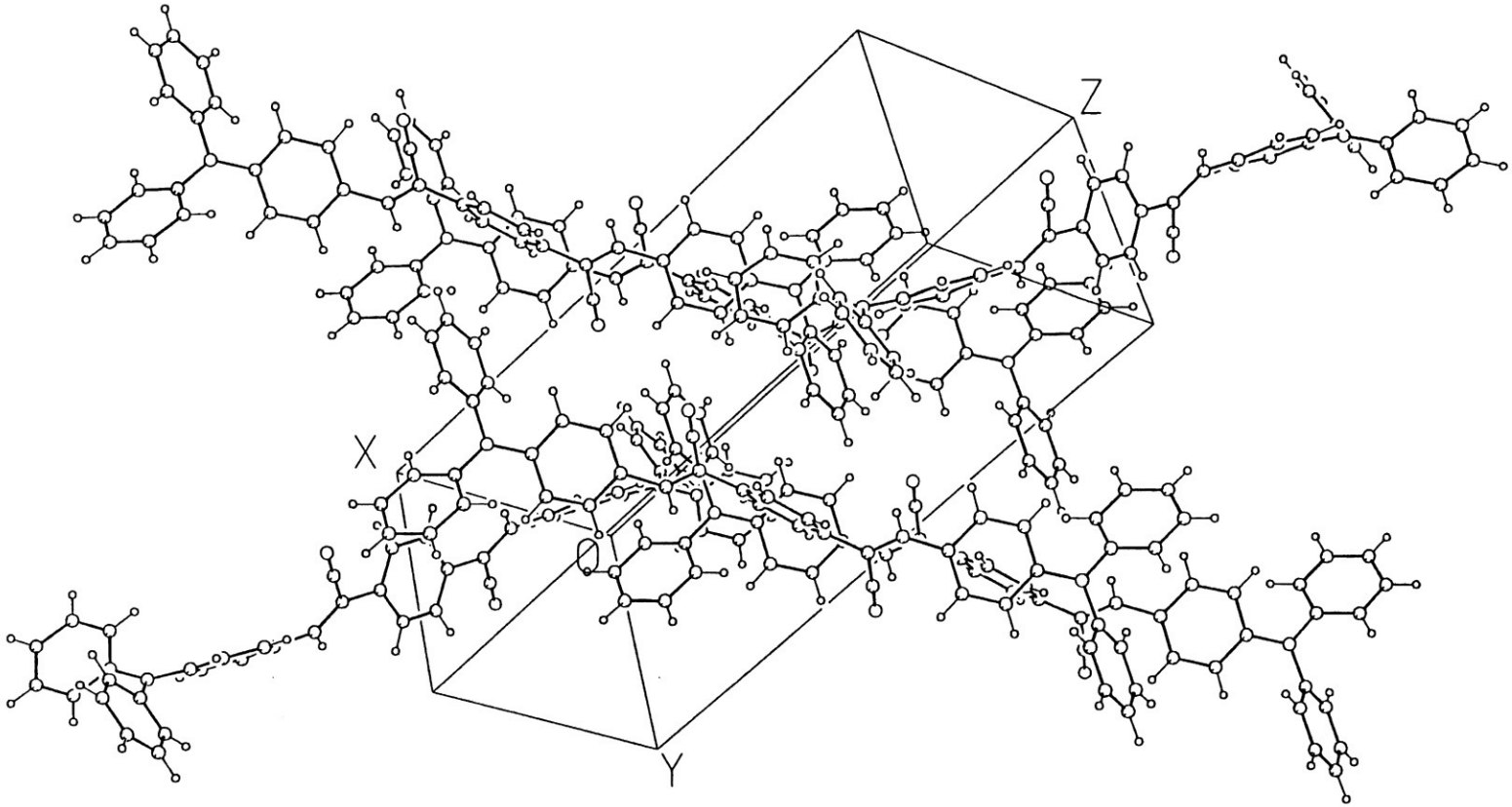

Figure 2: Crystal packing of compound 4. The unit cell boundaries are shown.

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

	x	y	z	U(eq)
N(1)	4829(3)	3441(3)	-657(1)	29(1)
N(2)	1493(3)	1333(2)	1694(1)	17(1)
C(1)	5849(3)	3481(3)	-260(1)	19(1)
C(2)	7148(3)	3614(3)	236(1)	16(1)
C(3)	6974(3)	3274(3)	804(1)	18(1)
C(4)	8612(3)	4298(3)	99(1)	16(1)
C(5)	10101(3)	3867(3)	400(1)	16(1)
C(6)	11477(3)	4579(3)	309(1)	16(1)
C(7)	5595(3)	2671(3)	1024(1)	15(1)
C(8)	5345(3)	3071(3)	1597(1)	16(1)
C(9)	4010(3)	2649(3)	1821(1)	16(1)
C(10)	2881(3)	1763(3)	1475(1)	16(1)
C(11)	3150(3)	1298(3)	914(1)	18(1)
C(12)	4500(3)	1751(3)	696(1)	17(1)
C(13)	757(3)	-2(3)	1499(1)	17(1)
C(14)	1677(3)	-1242(3)	1536(1)	19(1)
C(15)	970(3)	-2512(3)	1340(1)	20(1)
C(16)	-640(4)	-2591(3)	1113(1)	25(1)
C(17)	-1554(3)	-1356(3)	1073(1)	23(1)
C(18)	-862(3)	-71(3)	1266(1)	20(1)
C(19)	714(3)	2239(3)	2061(1)	16(1)
C(20)	-50(3)	1639(3)	2496(1)	19(1)
C(21)	-884(3)	2510(3)	2840(1)	21(1)
C(22)	-960(3)	3993(3)	2743(1)	18(1)
C(23)	-184(3)	4570(3)	2321(1)	20(1)
C(24)	655(3)	3715(3)	1973(1)	17(1)

Table 3. Bond lengths [Å] and angles [°] for compound 4.

N(1)-C(1)	1.137(3)	C(19)-N(2)-C(13)	118.3(2)
N(2)-C(10)	1.412(3)	N(1)-C(1)-C(2)	176.8(3)
N(2)-C(19)	1.425(3)	C(3)-C(2)-C(1)	121.6(2)
N(2)-C(13)	1.432(3)	C(3)-C(2)-C(4)	122.0(2)
C(1)-C(2)	1.440(4)	C(1)-C(2)-C(4)	116.0(2)
C(2)-C(3)	1.354(4)	C(2)-C(3)-C(7)	129.3(3)
C(2)-C(4)	1.478(3)	C(2)-C(3)-H(3)	116(2)
C(3)-C(7)	1.462(4)	C(7)-C(3)-H(3)	115(2)
C(3)-H(3)	0.96(2)	C(6)#1-C(4)-C(5)	119.1(2)
C(4)-C(6)#1	1.390(3)	C(6)#1-C(4)-C(2)	120.7(2)
C(4)-C(5)	1.393(4)	C(5)-C(4)-C(2)	120.1(2)
C(5)-C(6)	1.392(4)	C(6)-C(5)-C(4)	120.5(2)
C(5)-H(5)	0.99(3)	C(6)-C(5)-H(5)	122(2)
C(6)-C(4)#1	1.390(3)	C(4)-C(5)-H(5)	117(2)
C(6)-H(6)	0.98(2)	C(5)-C(6)-C(4)#1	120.4(3)
C(7)-C(12)	1.387(4)	C(5)-C(6)-H(6)	120.4(14)
C(7)-C(8)	1.398(3)	C(4)#1-C(6)-H(6)	119.0(14)
C(8)-C(9)	1.376(4)	C(12)-C(7)-C(8)	117.9(2)
C(8)-H(8)	1.00(3)	C(12)-C(7)-C(3)	124.3(2)
C(9)-C(10)	1.402(4)	C(8)-C(7)-C(3)	117.8(2)
C(9)-H(9)	0.92(2)	C(9)-C(8)-C(7)	121.8(3)
C(10)-C(11)	1.395(4)	C(9)-C(8)-H(8)	117(2)
C(11)-C(12)	1.390(4)	C(7)-C(8)-H(8)	121(2)
C(11)-H(11)	1.05(2)	C(8)-C(9)-C(10)	119.7(3)
C(12)-H(12)	0.97(3)	C(8)-C(9)-H(9)	121(2)
C(13)-C(18)	1.391(4)	C(10)-C(9)-H(9)	119(2)
C(13)-C(14)	1.394(4)	C(11)-C(10)-C(9)	119.2(2)
C(14)-C(15)	1.370(4)	C(11)-C(10)-N(2)	120.2(2)
C(14)-H(14)	1.06(3)	C(9)-C(10)-N(2)	120.6(2)
C(15)-C(16)	1.382(4)	C(12)-C(11)-C(10)	119.9(2)
C(15)-H(15)	0.99(3)	C(12)-C(11)-H(11)	116.6(13)
C(16)-C(17)	1.387(4)	C(10)-C(11)-H(11)	123.5(13)
C(16)-H(16)	0.96(3)	C(11)-C(12)-C(7)	121.4(3)
C(17)-C(18)	1.376(4)	C(11)-C(12)-H(12)	119(2)
C(17)-H(17)	0.99(3)	C(7)-C(12)-H(12)	120(2)
C(18)-H(18)	0.94(2)	C(18)-C(13)-C(14)	119.6(3)
C(19)-C(20)	1.383(4)	C(18)-C(13)-N(2)	120.7(2)
C(19)-C(24)	1.395(4)	C(14)-C(13)-N(2)	119.7(2)
C(20)-C(21)	1.398(4)	C(15)-C(14)-C(13)	119.4(3)
C(20)-H(19)	0.89(2)	C(15)-C(14)-H(14)	120(2)
C(21)-C(22)	1.404(4)	C(13)-C(14)-H(14)	120.2(14)
C(21)-H(21)	0.92(3)	C(14)-C(15)-C(16)	121.4(3)
C(22)-C(23)	1.359(4)	C(14)-C(15)-H(15)	118(2)
C(22)-H(22)	0.91(3)	C(16)-C(15)-H(15)	120(2)
C(23)-C(24)	1.399(4)	C(17)-C(16)-C(15)	119.3(3)
C(23)-H(23)	0.99(3)	C(17)-C(16)-H(16)	120(2)
C(24)-H(24)	0.99(2)	C(15)-C(16)-H(16)	121(2)
		C(16)-C(17)-C(18)	120.0(3)
C(10)-N(2)-C(19)	122.2(2)	C(16)-C(17)-H(17)	122(2)
C(10)-N(2)-C(13)	119.3(2)	C(18)-C(17)-H(17)	118(2)

C(17)-C(18)-C(13)	120.3(3)	C(22)-C(21)-H(21)	121(2)
C(17)-C(18)-H(18)	119(2)	C(23)-C(22)-C(21)	119.2(3)
C(13)-C(18)-H(18)	121(2)	C(23)-C(22)-H(22)	123(2)
C(20)-C(19)-C(24)	119.5(2)	C(21)-C(22)-H(22)	118(2)
C(20)-C(19)-N(2)	119.5(2)	C(22)-C(23)-C(24)	121.4(3)
C(24)-C(19)-N(2)	120.9(2)	C(22)-C(23)-H(23)	120(2)
C(19)-C(20)-C(21)	120.0(3)	C(24)-C(23)-H(23)	119(2)
C(19)-C(20)-H(19)	120(2)	C(19)-C(24)-C(23)	119.6(3)
C(21)-C(20)-H(19)	120(2)	C(19)-C(24)-H(24)	124(2)
C(20)-C(21)-C(22)	120.2(3)	C(23)-C(24)-H(24)	116(2)
C(20)-C(21)-H(21)	119(2)		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for comp. 4. 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)	27(2)	36(2)	23(1)	2(1)	3(1)	-11(1)
N(2)	16(1)	14(1)	23(1)	-4(1)	9(1)	-4(1)
C(1)	14(2)	22(2)	21(2)	2(1)	4(1)	-7(1)
C(2)	13(1)	15(1)	19(2)	0(1)	0(1)	0(1)
C(3)	14(2)	17(2)	20(2)	-1(1)	2(1)	-2(1)
C(4)	14(1)	19(1)	16(1)	-6(1)	4(1)	-3(1)
C(5)	19(2)	16(2)	13(1)	-3(1)	6(1)	0(1)
C(6)	10(1)	22(2)	17(2)	-2(1)	1(1)	2(1)
C(7)	11(1)	16(1)	18(1)	3(1)	2(1)	2(1)
C(8)	16(2)	16(1)	15(1)	0(1)	-2(1)	-3(1)
C(9)	19(2)	19(2)	13(1)	1(1)	6(1)	0(1)
C(10)	14(2)	13(1)	21(2)	2(1)	4(1)	-1(1)
C(11)	17(2)	17(1)	19(2)	-1(1)	1(1)	-4(1)
C(12)	20(2)	16(1)	17(2)	-2(1)	8(1)	-1(1)
C(13)	21(2)	15(1)	16(2)	-1(1)	6(1)	-6(1)
C(14)	22(2)	20(2)	15(1)	1(1)	4(1)	-1(1)
C(15)	29(2)	15(1)	16(1)	2(1)	5(1)	0(1)
C(16)	36(2)	20(2)	20(2)	-5(1)	8(1)	-11(2)
C(17)	17(2)	33(2)	20(2)	-4(1)	3(1)	-12(1)
C(18)	21(2)	17(2)	25(2)	1(1)	8(1)	0(1)
C(19)	13(1)	18(2)	15(1)	-4(1)	-1(1)	0(1)
C(20)	17(2)	16(2)	24(2)	6(1)	4(1)	-2(1)
C(21)	19(2)	30(2)	15(2)	0(1)	6(1)	-4(1)
C(22)	10(1)	27(2)	18(2)	-11(1)	3(1)	0(1)
C(23)	18(2)	18(2)	20(2)	-4(1)	-4(1)	5(1)
C(24)	18(2)	19(1)	13(1)	0(1)	0(1)	-3(1)

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

	x	y	z	U(eq)
H(3)	7859(30)	3518(25)	1111(11)	15(7)
H(5)	10135(32)	3006(27)	656(12)	25(8)
H(6)	12523(29)	4249(24)	506(10)	10(6)
H(8)	6133(32)	3685(27)	1863(12)	26(8)
H(9)	3821(30)	2965(25)	2189(12)	17(7)
H(11)	2388(29)	593(25)	639(10)	14(7)
H(12)	4649(31)	1450(26)	296(12)	26(8)
H(14)	2911(33)	-1203(27)	1716(11)	29(8)
H(15)	1647(32)	-3376(28)	1355(12)	28(8)
H(16)	-1133(35)	-3490(31)	983(13)	40(9)
H(17)	-2710(33)	-1360(28)	910(12)	29(8)
H(18)	-1492(29)	762(26)	1226(10)	13(7)
H(19)	15(32)	700(27)	2562(11)	21(8)
H(21)	-1336(31)	2104(26)	3143(12)	22(8)
H(22)	-1535(32)	4527(27)	2967(12)	25(8)
H(23)	-233(32)	5616(28)	2249(11)	27(8)
H(24)	1182(32)	4222(27)	1674(11)	23(7)