Table 1. Crystal Data and Structure Refinement for **1**.

Identification code	spirobiradical **1**
Empirical formula	C35 H46 N4 O4
Formula weight	586.76
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions	a = 24.861(10) A
	b = 12.129(3) A deg.
	c = 12.258(6) A
	alpha = 90 deg.
	beta = 117.482(19)
	gamma = 90 deg.
Volume	3279(2) A^3
Z	4
Density (calculated)	1.189 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	1264
Crystal size	0.40 x 0.15 x 0.087 mm
Theta range for data collection	1.85 to 25.92 deg.
Index ranges	0<=h<=30, 0<=k<=14, -15<=l<=13
Reflections collected	3235
Independent reflections	3161 [R(int) = 0.0307]
Absorption correction	Semi-empirical \y scan
Max. and min. transmission	0.999522 and 0.949579
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3161 / 0 / 287
Goodness-of-fit on F^2	0.984
Final R indices [I>2sigma(I)]	R1 = 0.0612, wR2 = 0.1243
R indices (all data)	R1 = 0.2025, wR2 = 0.1645
Largest diff. peak and hole	0.215 and -0.217 e.A^-3

Table 2. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (A^2 x 10^3) for **1**. U(eq) is Defined as One Third of the Trace of the Orthogonalized U_{ij} Tensor.

	x	y	z	U(eq)
C(3)	4414(2)	2241(3)	843(3)	31(1)
C(4)	3851(1)	2685(3)	45(3)	30(1)
N(1)	3321(1)	4238(2)	-1408(3)	41(1)
C(1)	5000	743(4)	2500(3)	33(1)
O(1)	2891(1)	4403(2)	-1109(2)	53(1)
O(2)	4647(1)	3132(2)	-1123(2)	51(1)
N(2)	4156(1)	3657(2)	-1388(2)	37(1)
C(2)	4442(1)	1411(3)	1647(3)	29(1)
C(12)	3784(1)	3521(3)	-872(3)	32(1)
C(5)	3326(2)	2289(3)	72(3)	36(1)
C(7)	3925(2)	1024(3)	1661(3)	32(1)
C(8)	4051(2)	75(3)	2551(3)	44(1)
C(16)	3960(2)	4601(3)	-2291(3)	45(1)
C(9)	4745(2)	65(4)	3236(4)	45(1)
C(17)	4382(2)	5555(4)	-1621(5)	68(1)
C(18)	4036(3)	4258(5)	-3409(4)	68(2)
C(13)	3300(2)	4770(4)	-2522(4)	55(1)
C(14)	2836(2)	4081(7)	-3628(4)	88(2)
C(15)	3091(4)	5954(6)	-2591(9)	102(3)
C(6)	3362(2)	1454(3)	872(3)	38(1)
C(10)	3807(4)	-996(5)	1818(7)	103(3)
C(11)	3773(3)	253(7)	3401(7)	96(2)

Table 3. Bond Lengths [A] and Angles [deg] for **1**.

C(3)-C(2)	1.388(5)
C(3)-C(4)	1.394(4)
C(4)-C(5)	1.403(4)
C(4)-C(12)	1.465(4)
N(1)-O(1)	1.296(4)
N(1)-C(12)	1.348(4)
N(1)-C(13)	1.490(5)
C(1)-C(2)#1	1.527(4)
C(1)-C(2)	1.527(4)
C(1)-C(9)#1	1.555(4)
C(1)-C(9)	1.555(4)
O(2)-N(2)	1.279(3)
N(2)-C(12)	1.349(4)
N(2)-C(16)	1.508(4)
C(2)-C(7)	1.377(4)
C(5)-C(6)	1.384(5)
C(7)-C(6)	1.383(4)
C(7)-C(8)	1.516(5)
C(8)-C(11)	1.508(7)
C(8)-C(9)	1.533(5)
C(8)-C(10)	1.536(7)
C(16)-C(17)	1.523(6)
C(16)-C(18)	1.525(6)
C(16)-C(13)	1.544(5)
C(13)-C(15)	1.516(8)
C(13)-C(14)	1.557(7)

C(2)-C(3)-C(4)	118.9(3)
C(3)-C(4)-C(5)	119.6(3)
C(3)-C(4)-C(12)	121.8(3)
C(5)-C(4)-C(12)	118.5(3)
O(1)-N(1)-C(12)	126.3(3)
O(1)-N(1)-C(13)	120.6(3)
C(12)-N(1)-C(13)	112.8(3)
C(2)#1-C(1)-C(2)	116.0(4)
C(2)#1-C(1)-C(9)#1	101.1(2)
C(2)-C(1)-C(9)#1	111.55(19)
C(2)#1-C(1)-C(9)	111.55(19)
C(2)-C(1)-C(9)	101.1(2)
C(9)#1-C(1)-C(9)	116.2(5)
O(2)-N(2)-C(12)	126.8(3)
O(2)-N(2)-C(16)	120.7(3)
C(12)-N(2)-C(16)	112.3(3)
C(7)-C(2)-C(3)	121.0(3)
C(7)-C(2)-C(1)	111.7(3)
C(3)-C(2)-C(1)	127.1(3)
N(1)-C(12)-N(2)	107.9(3)
N(1)-C(12)-C(4)	126.1(3)
N(2)-C(12)-C(4)	125.8(3)
C(6)-C(5)-C(4)	120.7(3)

C(2)-C(7)-C(6)	120.7(3)
C(2)-C(7)-C(8)	112.6(3)
C(6)-C(7)-C(8)	126.6(3)
C(11)-C(8)-C(7)	112.3(4)
C(11)-C(8)-C(9)	112.4(4)
C(7)-C(8)-C(9)	101.9(3)
C(11)-C(8)-C(10)	110.0(6)
C(7)-C(8)-C(10)	109.1(4)
C(9)-C(8)-C(10)	110.8(5)
N(2)-C(16)-C(17)	105.8(3)
N(2)-C(16)-C(18)	108.8(4)
C(17)-C(16)-C(18)	110.6(4)
N(2)-C(16)-C(13)	101.0(3)
C(17)-C(16)-C(13)	114.0(4)
C(18)-C(16)-C(13)	115.6(3)
C(8)-C(9)-C(1)	109.6(3)
N(1)-C(13)-C(15)	109.1(4)
N(1)-C(13)-C(16)	100.9(3)
C(15)-C(13)-C(16)	116.3(4)
N(1)-C(13)-C(14)	105.3(4)
C(15)-C(13)-C(14)	111.3(5)
C(16)-C(13)-C(14)	112.7(4)
C(7)-C(6)-C(5)	119.1(3)

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

Table 4. Anisotropic Displacement Parameters ($A^2 \times 10^3$) for **1**. The Anisotropic Displacement Factor Exponent Takes the Form:

$-2\pi^2[h^2a^2U_{11} + \ldots + 2hkabU_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(3)	26(2)	35(2)	28(2)	-1(2)	11(2)	-4(2)
C(4)	34(2)	30(2)	23(2)	0(2)	10(2)	-1(2)
N(1)	37(2)	44(2)	40(2)	12(2)	17(2)	4(2)
C(1)	35(3)	33(3)	28(3)	0	13(2)	0
O(1)	50(2)	59(2)	60(2)	19(1)	33(1)	16(1)
O(2)	43(2)	67(2)	50(2)	19(2)	26(1)	12(1)
N(2)	32(2)	43(2)	36(2)	8(2)	15(1)	0(2)
C(2)	31(2)	31(2)	20(2)	-5(2)	7(1)	-2(2)
C(12)	31(2)	35(2)	28(2)	1(2)	12(2)	1(2)
C(5)	29(2)	42(2)	32(2)	4(2)	11(2)	-1(2)
C(7)	36(2)	33(2)	25(2)	3(2)	13(2)	-5(2)
C(8)	42(2)	51(2)	35(2)	12(2)	14(2)	-8(2)
C(16)	41(2)	53(3)	37(2)	17(2)	16(2)	1(2)
C(9)	37(2)	49(3)	39(2)	15(2)	8(2)	-6(2)
C(17)	62(3)	51(3)	77(4)	12(3)	20(3)	-11(3)
C(18)	67(3)	94(4)	47(3)	23(3)	31(3)	6(3)
C(13)	54(2)	67(3)	46(2)	29(2)	26(2)	9(2)
C(14)	53(3)	163(7)	33(2)	14(3)	7(2)	-20(4)
C(15)	105(5)	87(5)	145(7)	85(5)	84(6)	53(4)
C(6)	30(2)	44(2)	37(2)	4(2)	14(2)	-5(2)
C(10)	101(5)	50(3)	80(4)	28(3)	-24(4)	-35(3)
C(11)	83(4)	142(7)	85(5)	63(5)	56(4)	32(5)

Table 5. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(1)	4912(15)	-670(3)	3410(3)	46(11)
H(2)	2990(15)	1210(3)	900(3)	45(10)
H(3)	4770(12)	2480(2)	840(2)	16(8)
H(4)	2940(14)	2560(2)	-510(3)	36(9)
H(5)	3390(3)	6400(5)	-1620(5)	130(2)
H(6)	3750(2)	3540(4)	-3900(4)	84(15)
H(7)	4470(3)	4070(4)	-3170(5)	120(2)
H(8)	4255(19)	6240(4)	-2130(4)	79(14)
H(9)	3898(19)	4890(4)	-3910(4)	77(15)
H(10)	4800(2)	5300(4)	-1350(5)	109(19)
H(11)	3961(17)	1020(3)	3840(3)	52(14)
H(12)	3900(2)	-320(4)	3930(5)	97(18)
H(13)	4280(2)	5860(4)	-880(5)	103(18)
H(14)	3890(2)	-1530(4)	2420(5)	101(18)
H(15)	3830(4)	-1160(6)	1120(7)	180(4)
H(16)	2830(2)	4390(4)	-4310(5)	102(18)
H(17)	3380(3)	-940(4)	1430(6)	120(2)
H(18)	3130(2)	6180(4)	-3160(4)	72(17)
H(19)	2420(2)	4070(4)	-3590(4)	120(2)
H(20)	2950(3)	3190(5)	-3500(5)	140(3)
H(21)	3370(3)	420(4)	3080(5)	110(2)
H(22)	4876(18)	410(3)	4100(4)	75(13)
H(23)	2680(3)	5920(5)	-2710(6)	160(3)