Supplementary Information

Figure S1. Picture of wired crystal of **11** for conductivity measurement.

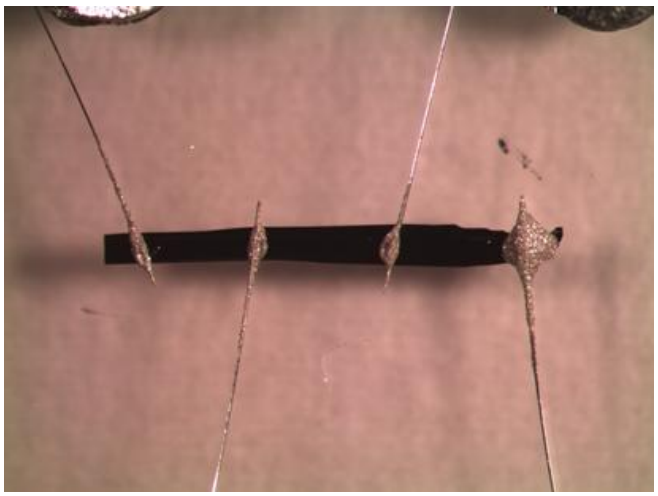

Figure S2. EPR spectra of radical **11** at room temperature.

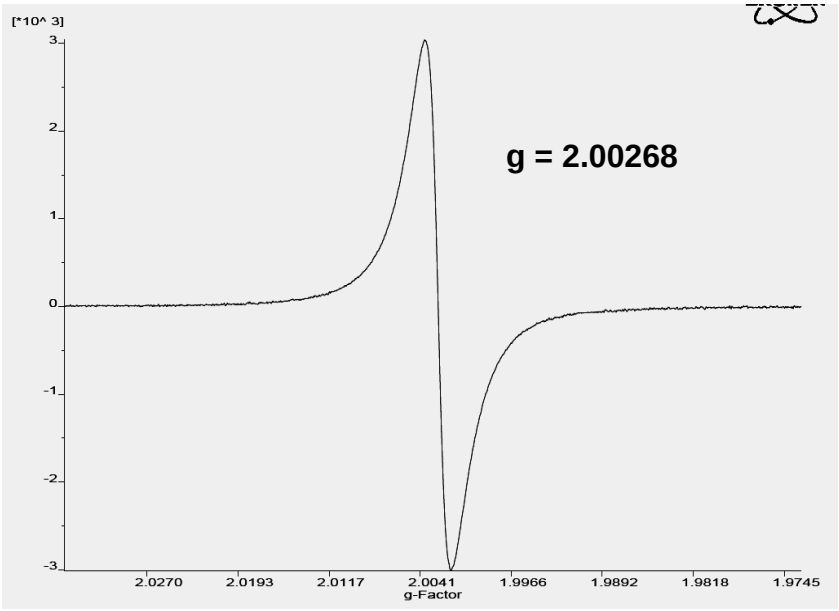

Table S1–S5. Details of crystallographic data for **11**; crystallographic cif file.

Table S1. Crystal data and structure refinement for 11.

Crystal Parameters	**Values**
Empirical formula	$C_{40}H_{40}BN_2O_2$
Formula weight	591.56
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 21.4373(15) Å α= 90 °. b = 6.1623(4) Å β= 97.597 °. c = 23.2775(16) Å γ = 90 °.
Volume	3048.0(4) $Å^3$
Crystal Parameters	Values
Z	4
Density (calculated)	1.289 Mg/m^3
Absorption coefficient	0.078 mm^{-1}
F(000)	1260
Crystal size	0.40 × 0.39 × 0.15 mm^3
Theta range for data collection	1.77 to 27.52 °
Index ranges	$-25 \le h \le 27$, $-8 \le k \le 7$, $-30 \le l \le 30$
Reflections collected	19619
Independent reflections	3460 [R(int) = 0.0323]
Completeness to theta = 27.52 °	98.7 º
Absorption correction	Sadabs
Max. and min. transmission	0.9884 and 0.9694
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3460/0/265
Goodness-of-fit on F^2	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0401, wR2 = 0.1005
R indices (all data)	R1 = 0.0607, wR2 = 0.1157
Largest diff. Peak and hole	0.303 and −0.197 $e.A^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **11**. *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	*U*(eq)
B(1)	0	7343(4)	2500	20(1)
O(1)	−200(1)	8778(2)	2941(1)	22(1)
N(1)	−544(1)	5835(2)	2243(1)	21(1)
C(1)	−738(1)	8511(2)	3167(1)	20(1)
C(2)	−879(1)	9986(2)	3591(1)	23(1)
C(3)	−1408(1)	9728(2)	3856(1)	24(1)
C(4)	−2349(1)	7557(3)	4014(1)	28(1)
C(5)	−2722(1)	5749(3)	3886(1)	30(1)
C(6)	−2589(1)	4273(3)	3467(1)	28(1)
C(7)	−1932(1)	3187(2)	2714(1)	24(1)
C(8)	−1446(1)	3567(2)	2405(1)	24(1)
C(9)	−1036(1)	5381(2)	2530(1)	20(1)
C(20)	−410(1)	4411(2)	1769(1)	22(1)
C(21)	−842(1)	4697(2)	1199(1)	22(1)
C(22)	−633(1)	3125(2)	756(1)	27(1)
C(23)	−1031(1)	3323(3)	163(1)	30(1)
C(24)	−1052(1)	5644(3)	-58(1)	30(1)
C(25)	−1274(1)	7186(3)	386(1)	30(1)
C(26)	−855(1)	7012(2)	970(1)	25(1)
C(3A)	−1818(1)	7936(2)	3726(1)	22(1)
C(6A)	−2077(1)	4608(2)	3161(1)	23(1)
C(9A)	−1152(1)	6789(2)	2997(1)	19(1)
C(9B)	−1683(1)	6448(2)	3294(1)	20(1)

Table S3. Bond lengths [Å] and angles [°] for **11.**

Bond	Bond Length (Å)	Bond	Bond Length (Å)
B(1)-O(1)#1	1.4622(16)	B(1)-O(1)	1.4622(16)
B(1)-N(1)	1.5477(17)	B(1)-N(1)#1	1.5477(17)
O(1)-C(1)	1.3387(16)	N(1)-C(9)	1.3511(18)
N(1)-C(20)	1.4682(17)	C(1)-C(2)	1.4045(19)
C(1)-C(9A)	1.4066(19)	C(2)-C(3)	1.368(2)
C(2)-H(2)	0.962(19)	C(3)-C(3A)	1.419(2)
C(3)-H(3)	0.986(18)	C(4)-C(5)	1.380(2)
C(4)-C(3A)	1.414(2)	C(4)-H(4)	1.001(18)
C(5)-C(6)	1.390(2)	C(5)-H(5)	0.953(18)
C(6)-C(6A)	1.400(2)	C(6)-H(6)	1.002(18)
C(7)-C(8)	1.362(2)	C(7)-C(6A)	1.426(2)
C(7)-H(7)	0.986(18)	C(8)-C(9)	1.428(2)
C(8)-H(8)	0.979(18)	C(9)-C(9A)	1.4373(19)
C(20)-C(21)	1.5238(18)	C(20)-H(20A)	0.993(18)
C(20)-H(20B)	1.014(18)	C(21)-C(26)	1.5224(19)
C(21)-C(22)	1.526(2)	C(21)-H(21)	1.047(18)
C(22)-C(23)	1.528(2)	C(22)-H(22A)	1.005(18)
C(22)-H(22B)	0.977(18)	C(23)-C(24)	1.519(2)

Table S3. *Cont.*

Bond	Bond Length (Å)	Bond	Bond Length (Å)
C(23)-H(23A)	1.012(18)	C(23)-H(23B)	1.040(18)
C(24)-C(25)	1.525(2)	C(24)-H(24A)	1.000(18)
C(24)-H(24B)	1.019(18)	C(25)-C(26)	1.530(2)
C(25)-H(25A)	1.036(18)	C(25)-H(25B)	1.011(18)
C(26)-H(26A)	1.017(18)	C(26)-H(26B)	1.021(18)
C(3A)-C(9B)	1.4194(19)	C(6A)-C(9B)	1.4238(19)
C(9A)-C(9B)	1.4223(19)		
O(1)#1-B(1)-O(1)	105.57(16)	O(1)#1-B(1)-N(1)	111.62(6)
O(1)-B(1)-N(1)	110.97(6)	O(1)#1-B(1)-N(1)#1	110.97(6)
O(1)-B(1)-N(1)#1	111.62(6)	N(1)-B(1)-N(1)#1	106.19(16)
C(1)-O(1)-B(1)	123.35(10)	C(9)-N(1)-C(20)	119.40(12)
C(9)-N(1)-B(1)	122.10(9)	C(20)-N(1)-B(1)	115.95(10)
O(1)-C(1)-C(2)	118.27(12)	O(1)-C(1)-C(9A)	121.76(12)
C(2)-C(1)-C(9A)	119.96(13)	C(3)-C(2)-C(1)	120.66(13)
C(3)-C(2)-H(2)	122.3(10)	C(1)-C(2)-H(2)	117.0(10)
C(2)-C(3)-C(3A)	121.39(13)	C(2)-C(3)-H(3)	121.1(10)
C(3A)-C(3)-H(3)	117.5(10)	C(5)-C(4)-C(3A)	120.73(14)
C(5)-C(4)-H(4)	121.5(10)	C(3A)-C(4)-H(4)	117.7(10)
C(4)-C(5)-C(6)	120.87(14)	C(4)-C(5)-H(5)	118.5(11)
C(6)-C(5)-H(5)	120.7(11)	C(5)-C(6)-C(6A)	120.45(14)
C(5)-C(6)-H(6)	121.3(10)	C(6A)-C(6)-H(6)	118.2(10)
C(8)-C(7)-C(6A)	122.42(13)	C(8)-C(7)-H(7)	120.5(10)
C(6A)-C(7)-H(7)	117.1(10)	C(7)-C(8)-C(9)	121.30(13)
C(7)-C(8)-H(8)	120.0(10)	C(9)-C(8)-H(8)	118.6(10)
N(1)-C(9)-C(8)	124.12(12)	N(1)-C(9)-C(9A)	118.25(12)
C(8)-C(9)-C(9A)	117.62(13)	N(1)-C(20)-C(21)	115.40(11)
N(1)-C(20)-H(20A)	109.6(10)	C(21)-C(20)-H(20A)	110.2(10)
N(1)-C(20)-H(20B)	106.9(10)	C(21)-C(20)-H(20B)	107.8(10)
H(20A)-C(20)-H(20B)	106.6(14)	C(26)-C(21)-C(20)	113.24(12)
C(26)-C(21)-C(22)	110.54(12)	C(20)-C(21)-C(22)	108.45(12)
C(26)-C(21)-H(21)	106.8(10)	C(20)-C(21)-H(21)	108.6(10)
C(22)-C(21)-H(21)	109.1(10)	C(21)-C(22)-C(23)	112.44(13)
C(21)-C(22)-H(22A)	109.7(10)	C(23)-C(22)-H(22A)	111.4(10)
C(21)-C(22)-H(22B)	107.8(10)	C(23)-C(22)-H(22B)	108.9(10)
H(22A)-C(22)-H(22B)	106.3(14)	C(24)-C(23)-C(22)	111.62(13)
C(24)-C(23)-H(23A)	110.5(10)	C(22)-C(23)-H(23A)	108.7(10)
C(24)-C(23)-H(23B)	108.2(10)	C(22)-C(23)-H(23B)	109.9(10)
H(23A)-C(23)-H(23B)	107.9(14)	C(23)-C(24)-C(25)	110.85(13)
C(23)-C(24)-H(24A)	108.4(10)	C(25)-C(24)-H(24A)	111.5(10)
C(23)-C(24)-H(24B)	109.6(10)	C(25)-C(24)-H(24B)	107.7(10)
H(24A)-C(24)-H(24B)	108.7(14)	C(24)-C(25)-C(26)	111.05(13)
C(24)-C(25)-H(25A)	109.1(10)	C(26)-C(25)-H(25A)	110.1(9)
C(24)-C(25)-H(25B)	109.5(10)	C(26)-C(25)-H(25B)	109.6(10)
H(25A)-C(25)-H(25B)	107.5(14)	C(21)-C(26)-C(25)	111.03(12)
C(21)-C(26)-H(26A)	107.2(10)	C(25)-C(26)-H(26A)	108.3(10)
C(21)-C(26)-H(26B)	109.0(10)	C(25)-C(26)-H(26B)	110.4(10)

Table S3. *Cont.*

Bond	Bond Length (Å)	Bond	Bond Length (Å)
H(26A)-C(26)-H(26B)	110.8(14)	C(4)-C(3A)-C(3)	122.86(13)
C(4)-C(3A)-C(9B)	118.77(13)	C(3)-C(3A)-C(9B)	118.36(13)
C(6)-C(6A)-C(9B)	119.34(13)	C(6)-C(6A)-C(7)	122.84(13)
C(9B)-C(6A)-C(7)	117.82(13)	C(1)-C(9A)-C(9B)	119.35(12)
C(1)-C(9A)-C(9)	120.14(12)	C(9B)-C(9A)-C(9)	120.50(12)
C(3A)-C(9B)-C(9A)	120.03(12)	C(3A)-C(9B)-C(6A)	119.81(13)
C(9A)-C(9B)-C(6A)	120.16(12)		

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

Table S4. Anisotropic displacement parameters (Å^2 × 10^3) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a \times b \times U^{12}\ ]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	26(1)	19(1)	16(1)	0	2(1)	0
O(1)	26(1)	20(1)	21(1)	−3(1)	3(1)	−3(1)
N(1)	27(1)	19(1)	16(1)	−2(1)	1(1)	0(1)
C(1)	23(1)	19(1)	16(1)	2(1)	1(1)	1(1)
C(2)	30(1)	19(1)	19(1)	−2(1)	0(1)	−2(1)
C(3)	31(1)	22(1)	18(1)	−2(1)	2(1)	3(1)
C(4)	30(1)	29(1)	24(1)	0(1)	4(1)	4(1)
C(5)	27(1)	33(1)	31(1)	5(1)	7(1)	1(1)
C(6)	27(1)	26(1)	29(1)	5(1)	0(1)	−3(1)
C(7)	30(1)	21(1)	22(1)	1(1)	−3(1)	−5(1)
C(8)	32(1)	20(1)	17(1)	−1(1)	−2(1)	−2(1)
C(9)	26(1)	19(1)	15(1)	2(1)	−3(1)	1(1)
C(20)	28(1)	20(1)	18(1)	−2(1)	0(1)	2(1)
C(21)	30(1)	20(1)	17(1)	−1(1)	2(1)	1(1)
C(22)	39(1)	20(1)	20(1)	−2(1)	4(1)	3(1)
C(23)	49(1)	24(1)	18(1)	−3(1)	2(1)	3(1)
C(24)	46(1)	27(1)	18(1)	1(1)	3(1)	−1(1)
C(25)	42(1)	22(1)	23(1)	1(1)	−2(1)	3(1)
C(26)	35(1)	19(1)	20(1)	−1(1)	0(1)	3(1)
C(3A)	27(1)	23(1)	17(1)	3(1)	1(1)	3(1)
C(6A)	26(1)	22(1)	20(1)	4(1)	−2(1)	0(1)
C(9A)	24(1)	18(1)	15(1)	1(1)	−2(1)	1(1)
C(9B)	22(1)	20(1)	16(1)	3(1)	−3(1)	1(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **11.**

Atom	*x*	*y*	*z*	*U*(eq)
H(2)	−593(8)	11180(30)	3680(7)	32(1)
H(3)	−1514(8)	10770(30)	4149(8)	32(1)
H(4)	−2437(8)	8620(30)	4317(8)	32(1)
H(5)	−3074(8)	5540(30)	4090(7)	32(1)
H(6)	−2860(8)	2970(30)	3369(7)	32(1)
H(7)	−2202(8)	1900(30)	2632(7)	32(1)
H(8)	−1358(8)	2540(30)	2104(8)	32(1)
H(20A)	−413(8)	2870(30)	1897(7)	32(1)
H(20B)	35(9)	4740(30)	1694(8)	32(1)
H(21)	−1303(8)	4320(30)	1267(7)	32(1)
H(22A)	−637(8)	1600(30)	909(8)	32(1)
H(22B)	−196(9)	3450(30)	715(7)	32(1)
H(23A)	−851(8)	2320(30)	−119(8)	32(1)
H(23B)	−1490(9)	2830(30)	190(8)	32(1)
H(24A)	−1335(8)	5700(30)	−435(8)	32(1)
H(24B)	−612(8)	6120(30)	−125(7)	32(1)
H(25A)	−1736(8)	6820(30)	435(7)	32(1)
H(25B)	−1266(8)	8730(30)	238(7)	32(1)
H(26A)	−407(9)	7400(30)	910(8)	32(1)
H(26B)	−1014(8)	8020(30)	1266(8)	32(1)