Supplementary Material

Experimental

Tables S1 through S5 summarize the crystallographic data for crystals of compound **2c** grown by chlorobenzene/cyclohexane vapour diffusion.

Table S1. Crystal data and structure refinement for **2c**

Empirical formula	$C_{91}H_{62}B_2Cl_2N_{12}O_2$	
Formula weight	1448.05 g/mol	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 13.4143(4) Å	α= 90°.
	b = 18.7352(9) Å	β= 90.652(2)°.
	c = 27.6286(10) Å	γ = 90°.
Volume	6943.2(5) $Å^3$	
Z	4	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	0.159 mm^{-1}	
F(000)	3008	
Crystal size	0.30 x 0.24 x 0.03 mm^3	
Theta range for data collection	2.63 to 25.00°.	
Index ranges	-15<=h<=15, -22<=k<=22, -32<=l<=32	
Reflections collected	18179	
Independent reflections	6090 [R(int) = 0.0711]	
Completeness to theta = 25.00°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.992 and 0.753	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6090 / 0 / 501	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0593, wR2 = 0.1417	
R indices (all data)	R1 = 0.1122, wR2 = 0.1750	
Largest diff. peak and hole	0.901 and -0.497 e.$Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	1782(1)	3999(1)	3352(1)	33(1)
N(1)	929(2)	5764(1)	3971(1)	33(1)
N(2)	1138(2)	4523(1)	4136(1)	30(1)
N(3)	619(2)	3432(1)	4493(1)	35(1)
N(4)	188(2)	3707(1)	3679(1)	31(1)
N(5)	-881(2)	4145(1)	3058(1)	33(1)
N(6)	384(2)	4887(1)	3399(1)	30(1)
C(1)	1192(2)	5228(2)	4268(1)	31(1)
C(2)	1366(2)	5230(2)	4789(1)	34(1)
C(3)	1552(2)	5780(2)	5116(1)	39(1)
C(4)	1682(2)	5604(2)	5598(1)	44(1)
C(5)	1583(2)	4897(2)	5761(1)	43(1)
C(6)	1364(2)	4351(2)	5444(1)	38(1)
C(7)	1278(2)	4512(2)	4950(1)	34(1)
C(8)	1049(2)	4080(2)	4525(1)	33(1)
C(9)	142(2)	3276(2)	4077(1)	32(1)
C(10)	-661(2)	2771(2)	3972(1)	33(1)
C(11)	-1031(2)	2190(2)	4232(1)	39(1)
C(12)	-1848(2)	1834(2)	4041(1)	43(1)
C(13)	-2302(2)	2046(2)	3609(1)	41(1)
C(14)	-1956(2)	2625(2)	3350(1)	37(1)
C(15)	-1126(2)	2989(2)	3530(1)	32(1)
C(16)	-601(2)	3626(2)	3366(1)	31(1)
C(17)	-430(2)	4782(2)	3101(1)	31(1)
C(18)	-785(2)	5489(2)	2974(1)	31(1)
C(19)	-1564(2)	5717(2)	2677(1)	35(1)
C(20)	-1745(2)	6446(2)	2650(1)	39(1)
C(21)	-1188(2)	6937(2)	2918(1)	42(1)
C(22)	-431(2)	6714(2)	3227(1)	38(1)
C(23)	-224(2)	5989(2)	3251(1)	31(1)
C(24)	467(2)	5579(2)	3547(1)	32(1)

C(25)	2553(2)	4378(2)	3168(1)	31(1)
C(26)	3003(2)	4109(2)	2754(1)	33(1)
C(27)	3807(2)	4459(2)	2551(1)	35(1)
C(28)	4188(2)	5088(2)	2753(1)	32(1)
C(29)	3740(2)	5347(2)	3165(1)	32(1)
C(30)	2931(2)	4996(2)	3373(1)	32(1)
C(31)	5000	5530(2)	2500	33(1)
C(32)	5520(2)	6052(2)	2848(1)	34(1)
C(33)	5344(2)	6761(2)	2708(1)	37(1)
C(34)	5818(2)	7317(2)	2950(1)	44(1)
C(35)	6415(2)	7161(2)	3352(1)	49(1)
C(36)	6535(2)	6465(2)	3505(1)	46(1)
C(37)	6105(2)	5902(2)	3253(1)	40(1)
B(1)	944(2)	4282(2)	3623(1)	31(1)
C(38)	4078(3)	5052(3)	4724(2)	76(1)
C(39)	5039(3)	5290(2)	4509(1)	64(1)
C(40)	5763(3)	5522(3)	4894(2)	71(1)
Cl(1)	2860(1)	2543(1)	4574(1)	58(1)
Cl(1A)	6417(2)	3865(1)	3657(1)	71(1)
C(41)	3944(3)	2791(2)	4338(2)	60(1)
C(42)	4875(3)	2571(2)	4493(1)	52(1)
C(43)	5707(3)	2864(2)	4284(1)	52(1)
C(44)	5569(3)	3379(2)	3925(1)	58(1)
C(45)	4638(4)	3584(2)	3779(2)	68(1)
C(46)	3823(3)	3291(2)	3982(2)	67(1)

Table S3. Bond lengths [Å] and angles [°] for **2c**.

O(1)-C(25)	1.360(3)
O(1)-B(1)	1.457(4)
N(1)-C(1)	1.341(4)
N(1)-C(24)	1.363(4)
N(2)-C(8)	1.365(4)
N(2)-C(1)	1.371(4)
N(2)-B(1)	1.508(4)
N(3)-C(9)	1.342(4)
N(3)-C(8)	1.347(4)
N(4)-C(9)	1.366(4)
N(4)-C(16)	1.367(4)
N(4)-B(1)	1.490(4)
N(5)-C(17)	1.343(4)
N(5)-C(16)	1.343(4)
N(6)-C(24)	1.364(4)
N(6)-C(17)	1.376(4)
N(6)-B(1)	1.490(4)
C(1)-C(2)	1.455(4)
C(2)-C(3)	1.392(4)
C(2)-C(7)	1.422(4)
C(3)-C(4)	1.383(4)
C(4)-C(5)	1.405(5)
C(5)-C(6)	1.377(4)
C(6)-C(7)	1.400(4)
C(7)-C(8)	1.456(4)
C(9)-C(10)	1.462(4)
C(10)-C(11)	1.397(4)
C(10)-C(15)	1.425(4)
C(11)-C(12)	1.384(4)
C(12)-C(13)	1.392(5)
C(13)-C(14)	1.382(4)
C(14)-C(15)	1.393(4)
C(15)-C(16)	1.460(4)
C(17)-C(18)	1.448(4)

C(18)-C(19)	1.388(4)
C(18)-C(23)	1.420(4)
C(19)-C(20)	1.389(5)
C(20)-C(21)	1.392(5)
C(21)-C(22)	1.384(4)
C(22)-C(23)	1.389(4)
C(23)-C(24)	1.450(4)
C(25)-C(30)	1.383(4)
C(25)-C(26)	1.393(4)
C(26)-C(27)	1.385(4)
C(27)-C(28)	1.399(4)
C(28)-C(29)	1.382(4)
C(28)-C(31)	1.541(4)
C(29)-C(30)	1.398(4)
C(31)-C(32)#1	1.533(4)
C(31)-C(32)	1.533(4)
C(31)-C(28)#1	1.541(4)
C(32)-C(37)	1.387(4)
C(32)-C(33)	1.404(4)
C(33)-C(34)	1.388(4)
C(33)-C(33)#1	1.466(6)
C(34)-C(35)	1.393(5)
C(35)-C(36)	1.380(5)
C(36)-C(37)	1.387(5)
C(38)-C(39)	1.493(6)
C(38)-C(40)#2	1.521(6)
C(39)-C(40)	1.496(5)
C(40)-C(38)#2	1.521(6)
Cl(1)-C(41)	1.666(4)
C(41)-C(46)	1.368(6)
C(41)-C(42)	1.378(5)
C(42)-C(43)	1.377(5)
C(43)-C(44)	1.394(5)
C(44)-C(45)	1.363(6)
C(45)-C(46)	1.350(6)

C(25)-O(1)-B(1)	126.6(2)
C(1)-N(1)-C(24)	116.7(3)
C(8)-N(2)-C(1)	112.4(2)
C(8)-N(2)-B(1)	122.9(3)
C(1)-N(2)-B(1)	123.2(3)
C(9)-N(3)-C(8)	116.8(3)
C(9)-N(4)-C(16)	113.7(2)
C(9)-N(4)-B(1)	123.2(2)
C(16)-N(4)-B(1)	122.5(2)
C(17)-N(5)-C(16)	117.7(2)
C(24)-N(6)-C(17)	112.2(2)
C(24)-N(6)-B(1)	124.0(2)
C(17)-N(6)-B(1)	122.2(2)
N(1)-C(1)-N(2)	123.0(3)
N(1)-C(1)-C(2)	129.9(3)
N(2)-C(1)-C(2)	105.9(3)
C(3)-C(2)-C(7)	120.8(3)
C(3)-C(2)-C(1)	132.0(3)
C(7)-C(2)-C(1)	107.1(3)
C(4)-C(3)-C(2)	118.0(3)
C(3)-C(4)-C(5)	121.5(3)
C(6)-C(5)-C(4)	121.0(3)
C(5)-C(6)-C(7)	118.4(3)
C(6)-C(7)-C(2)	120.1(3)
C(6)-C(7)-C(8)	132.9(3)
C(2)-C(7)-C(8)	106.8(3)
N(3)-C(8)-N(2)	122.6(3)
N(3)-C(8)-C(7)	129.7(3)
N(2)-C(8)-C(7)	106.2(3)
N(3)-C(9)-N(4)	122.5(3)
N(3)-C(9)-C(10)	130.8(3)
N(4)-C(9)-C(10)	105.2(2)
C(11)-C(10)-C(15)	120.7(3)
C(11)-C(10)-C(9)	131.8(3)
C(15)-C(10)-C(9)	107.3(3)
C(12)-C(11)-C(10)	117.6(3)

C(11)-C(12)-C(13)	121.8(3)
C(14)-C(13)-C(12)	121.4(3)
C(13)-C(14)-C(15)	118.2(3)
C(14)-C(15)-C(10)	120.3(3)
C(14)-C(15)-C(16)	132.5(3)
C(10)-C(15)-C(16)	107.0(2)
N(5)-C(16)-N(4)	122.0(3)
N(5)-C(16)-C(15)	131.0(3)
N(4)-C(16)-C(15)	105.5(2)
N(5)-C(17)-N(6)	122.2(3)
N(5)-C(17)-C(18)	130.2(3)
N(6)-C(17)-C(18)	105.7(2)
C(19)-C(18)-C(23)	120.4(3)
C(19)-C(18)-C(17)	131.9(3)
C(23)-C(18)-C(17)	107.5(2)
C(18)-C(19)-C(20)	117.7(3)
C(19)-C(20)-C(21)	121.8(3)
C(22)-C(21)-C(20)	121.0(3)
C(21)-C(22)-C(23)	117.9(3)
C(22)-C(23)-C(18)	121.0(3)
C(22)-C(23)-C(24)	132.1(3)
C(18)-C(23)-C(24)	106.7(3)
N(1)-C(24)-N(6)	122.3(3)
N(1)-C(24)-C(23)	129.2(3)
N(6)-C(24)-C(23)	106.5(3)
O(1)-C(25)-C(30)	124.1(3)
O(1)-C(25)-C(26)	117.2(3)
C(30)-C(25)-C(26)	118.7(3)
C(27)-C(26)-C(25)	120.5(3)
C(26)-C(27)-C(28)	121.4(3)
C(29)-C(28)-C(27)	117.6(3)
C(29)-C(28)-C(31)	120.1(3)
C(27)-C(28)-C(31)	122.0(3)
C(28)-C(29)-C(30)	121.4(3)
C(25)-C(30)-C(29)	120.5(3)
C(32)#1-C(31)-C(32)	100.8(3)

C(32)#1-C(31)-C(28)	107.92(15)
C(32)-C(31)-C(28)	112.15(16)
C(32)#1-C(31)-C(28)#1	112.15(16)
C(32)-C(31)-C(28)#1	107.92(15)
C(28)-C(31)-C(28)#1	115.0(4)
C(37)-C(32)-C(33)	120.3(3)
C(37)-C(32)-C(31)	128.8(3)
C(33)-C(32)-C(31)	110.9(3)
C(34)-C(33)-C(32)	120.2(3)
C(34)-C(33)-C(33)#1	131.2(2)
C(32)-C(33)-C(33)#1	108.57(18)
C(33)-C(34)-C(35)	118.8(3)
C(36)-C(35)-C(34)	120.5(3)
C(35)-C(36)-C(37)	121.2(3)
C(36)-C(37)-C(32)	118.7(3)
O(1)-B(1)-N(4)	108.6(3)
O(1)-B(1)-N(6)	117.0(3)
N(4)-B(1)-N(6)	104.7(2)
O(1)-B(1)-N(2)	117.7(2)
N(4)-B(1)-N(2)	103.3(2)
N(6)-B(1)-N(2)	104.0(2)
C(39)-C(38)-C(40)#2	111.9(3)
C(38)-C(39)-C(40)	111.2(3)
C(39)-C(40)-C(38)#2	111.9(4)
C(46)-C(41)-C(42)	121.9(4)
C(46)-C(41)-Cl(1)	112.1(3)
C(42)-C(41)-Cl(1)	125.9(4)
C(43)-C(42)-C(41)	119.1(4)
C(42)-C(43)-C(44)	118.2(3)
C(45)-C(44)-C(43)	121.3(4)
C(46)-C(45)-C(44)	120.4(4)
C(45)-C(46)-C(41)	119.2(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 -x+1,-y+1,-z+1

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	31(1)	30(1)	38(1)	0(1)	7(1)	0(1)
N(1)	26(1)	39(2)	33(1)	-1(1)	5(1)	-2(1)
N(2)	26(1)	31(2)	33(1)	-2(1)	3(1)	-2(1)
N(3)	28(1)	40(2)	39(2)	2(1)	3(1)	3(1)
N(4)	31(1)	30(1)	31(1)	-1(1)	3(1)	-2(1)
N(5)	33(1)	34(2)	32(1)	-4(1)	3(1)	-2(1)
N(6)	29(1)	28(2)	33(1)	0(1)	4(1)	-2(1)
C(1)	25(2)	33(2)	35(2)	-1(2)	5(1)	-4(1)
C(2)	25(2)	41(2)	35(2)	-5(2)	4(1)	-1(1)
C(3)	35(2)	40(2)	41(2)	-6(2)	5(2)	3(2)
C(4)	40(2)	53(2)	39(2)	-14(2)	5(2)	1(2)
C(5)	38(2)	57(2)	36(2)	-4(2)	7(2)	5(2)
C(6)	33(2)	45(2)	37(2)	1(2)	6(1)	-3(2)
C(7)	25(2)	41(2)	37(2)	-2(2)	2(1)	1(1)
C(8)	28(2)	35(2)	35(2)	1(2)	5(1)	-1(1)
C(9)	29(2)	34(2)	32(2)	1(1)	5(1)	0(1)
C(10)	31(2)	29(2)	38(2)	-3(1)	6(1)	-1(1)
C(11)	41(2)	36(2)	41(2)	0(2)	5(2)	-3(2)
C(12)	43(2)	36(2)	49(2)	2(2)	7(2)	-10(2)
C(13)	39(2)	37(2)	46(2)	-2(2)	4(2)	-9(2)
C(14)	34(2)	40(2)	38(2)	-2(2)	0(1)	-4(2)
C(15)	29(2)	32(2)	36(2)	-3(1)	6(1)	1(1)
C(16)	30(2)	31(2)	32(2)	0(1)	4(1)	1(1)
C(17)	30(2)	35(2)	27(2)	-2(1)	3(1)	-2(1)
C(18)	29(2)	36(2)	27(2)	0(1)	8(1)	1(1)
C(19)	34(2)	42(2)	30(2)	0(2)	5(1)	0(2)
C(20)	38(2)	46(2)	34(2)	6(2)	1(1)	6(2)
C(21)	43(2)	36(2)	47(2)	5(2)	4(2)	4(2)
C(22)	37(2)	36(2)	40(2)	0(2)	6(2)	-3(2)
C(23)	30(2)	33(2)	29(2)	2(1)	6(1)	-1(1)
C(24)	29(2)	34(2)	34(2)	1(2)	9(1)	-4(1)

C(25)	28(2)	32(2)	33(2)	4(1)	3(1)	-1(1)
C(26)	33(2)	30(2)	37(2)	-4(1)	4(1)	-2(1)
C(27)	37(2)	35(2)	34(2)	-1(1)	7(1)	1(2)
C(28)	32(2)	32(2)	31(2)	0(1)	6(1)	2(1)
C(29)	30(2)	33(2)	34(2)	-4(1)	2(1)	0(1)
C(30)	30(2)	36(2)	30(2)	-2(1)	5(1)	1(1)
C(31)	33(2)	32(3)	35(2)	0	5(2)	0
C(32)	29(2)	34(2)	40(2)	-3(2)	12(1)	-1(1)
C(33)	34(2)	33(2)	45(2)	-4(2)	16(1)	-1(1)
C(34)	37(2)	32(2)	63(2)	-8(2)	17(2)	-3(2)
C(35)	39(2)	46(2)	62(2)	-23(2)	11(2)	-7(2)
C(36)	37(2)	55(3)	47(2)	-12(2)	5(2)	-3(2)
C(37)	35(2)	38(2)	45(2)	-4(2)	8(2)	-1(2)
B(1)	31(2)	31(2)	32(2)	-3(2)	2(2)	-2(2)
C(38)	51(2)	109(4)	69(3)	-2(3)	-15(2)	10(3)
C(39)	73(3)	68(3)	52(2)	-3(2)	3(2)	10(2)
C(40)	63(3)	81(3)	67(3)	-16(3)	12(2)	-9(2)
Cl(1)	46(1)	66(1)	63(1)	9(1)	7(1)	2(1)
Cl(1A)	62(1)	76(2)	74(1)	5(1)	3(1)	-2(1)
C(41)	53(2)	69(3)	57(2)	-19(2)	7(2)	-1(2)
C(41A)	53(2)	69(3)	57(2)	-19(2)	7(2)	-1(2)
C(42)	61(2)	54(2)	40(2)	5(2)	-1(2)	0(2)
C(43)	52(2)	57(2)	46(2)	0(2)	-6(2)	10(2)
C(44)	80(3)	50(2)	45(2)	1(2)	-1(2)	-13(2)
C(44A)	80(3)	50(2)	45(2)	1(2)	-1(2)	-13(2)
C(45)	103(4)	44(2)	56(3)	3(2)	-30(3)	2(3)
C(46)	69(3)	59(3)	71(3)	-8(2)	-20(2)	20(2)

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

	x	y	z	U(eq)
H(3A)	1589	6262	5011	46
H(4A)	1843	5969	5825	53
H(5A)	1667	4794	6096	52
H(6A)	1275	3877	5557	46
H(11A)	-731	2046	4530	47
H(12A)	-2107	1433	4209	51
H(13A)	-2862	1787	3489	49
H(14A)	-2276	2771	3058	45
H(19A)	-1961	5386	2499	42
H(20A)	-2264	6615	2442	47
H(21A)	-1330	7432	2888	50
H(22A)	-63	7048	3417	45
H(26A)	2756	3683	2610	40
H(27A)	4106	4266	2270	42
H(29A)	3987	5773	3310	39
H(30A)	2638	5184	3658	39
H(34A)	5737	7796	2843	52
H(35A)	6741	7536	3523	59
H(36A)	6920	6370	3789	56
H(37A)	6210	5423	3355	47
H(38A)	3637	4864	4464	92
H(38B)	3741	5467	4872	92
H(39A)	4910	5692	4284	77
H(39B)	5331	4894	4321	77
H(40A)	5513	5961	5050	85
H(40B)	6410	5636	4743	85
H(41A)	3370	2591	4484	72
H(42A)	4941	2221	4740	62
H(43A)	6358	2720	4382	62
H(44)	6134	3591	3779	70

H(45A)	4562	3934	3532	82
H(46A)	3174	3431	3878	80