Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and Properties of a Trapezoid Shaped Macrocycle with Different [*n*]yne Units

Maude Desroches and Jean-François Morin*

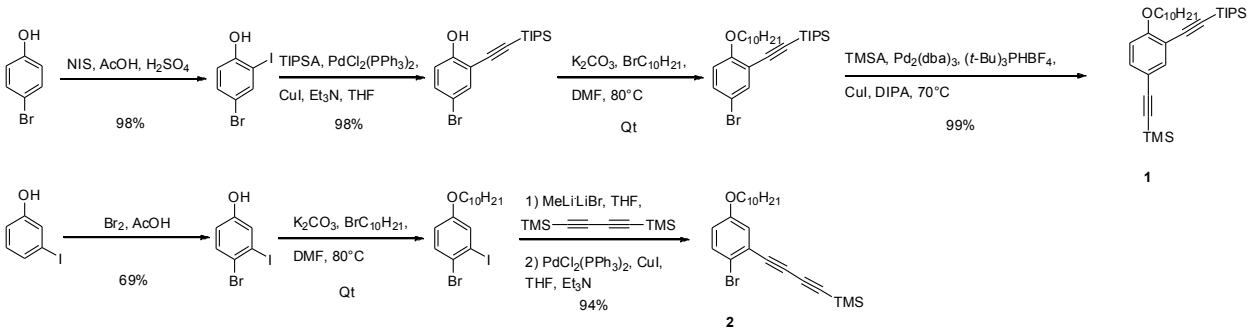
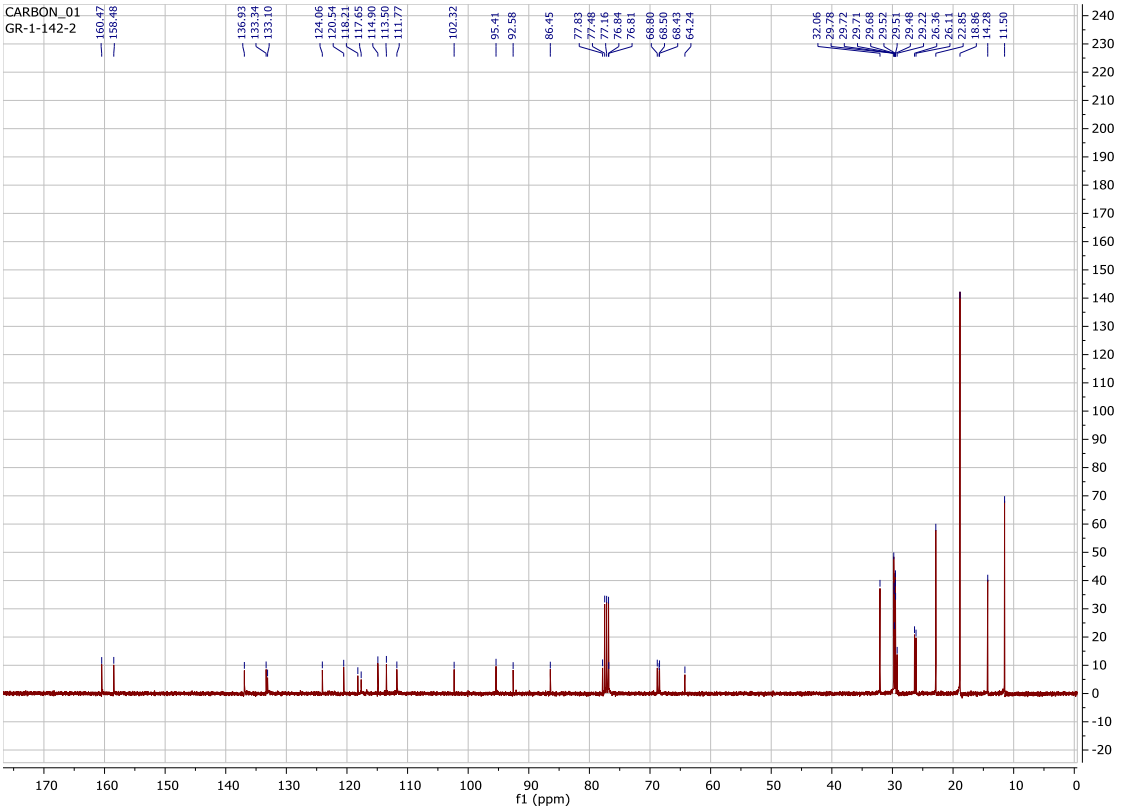
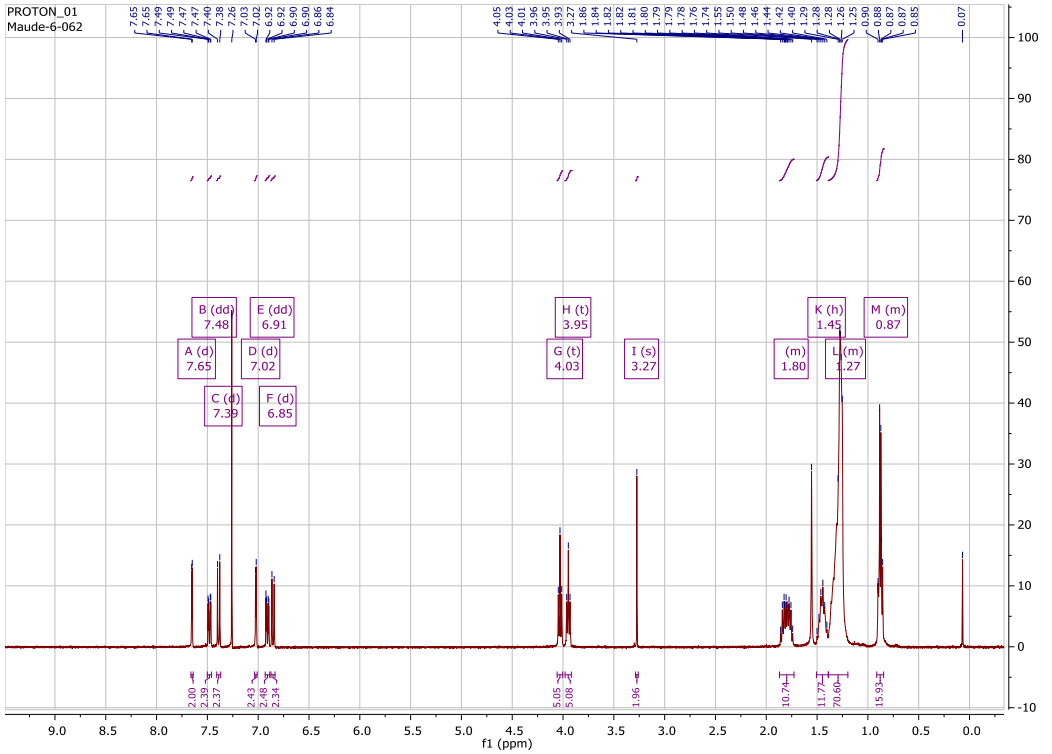


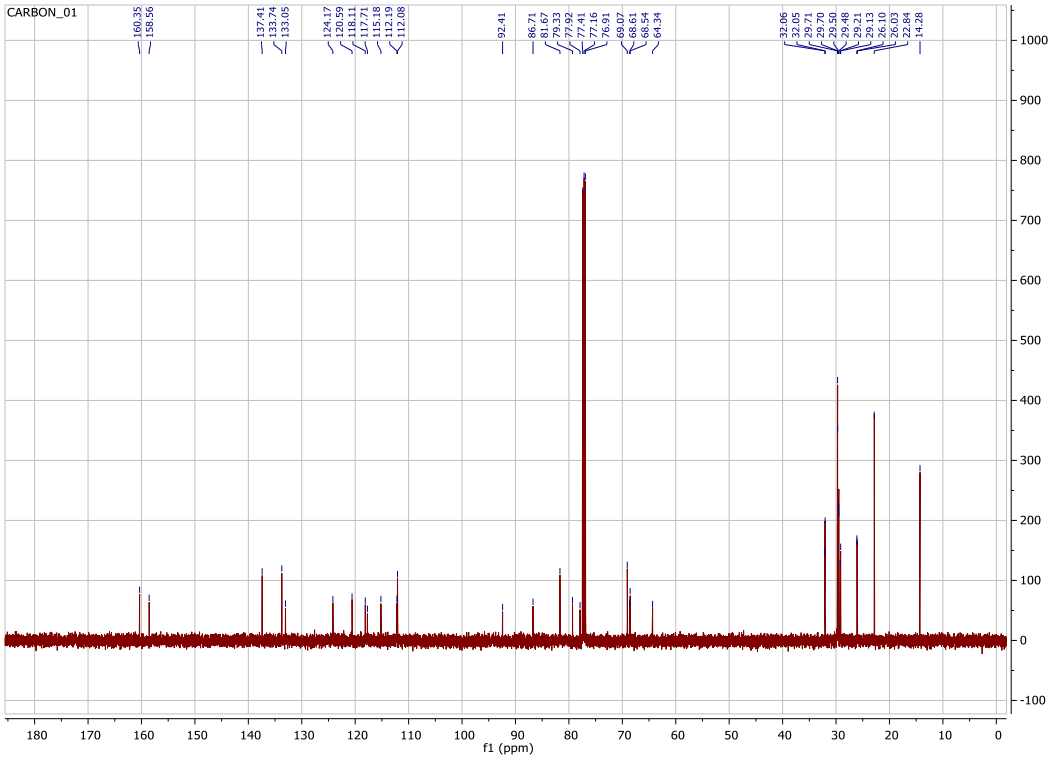
Figure S1. Synthetic scheme for compound **1** and **2** according to the literature procedure[1]

1,8-bis(5-(decyloxy)-2-((4-(decyloxy)-3-((triisopropylsilyl)ethynyl)phenyl)ethynyl)phenyl)octa-1,3,5,7-tetrayne (4)

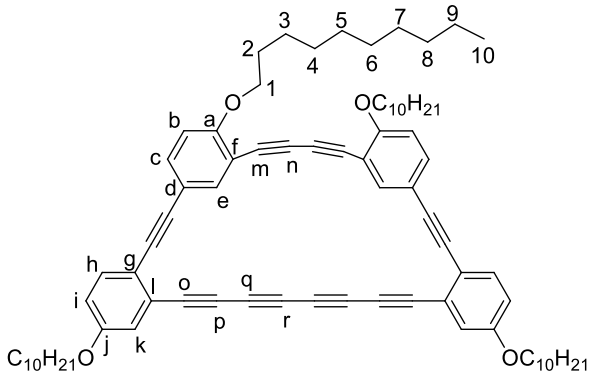


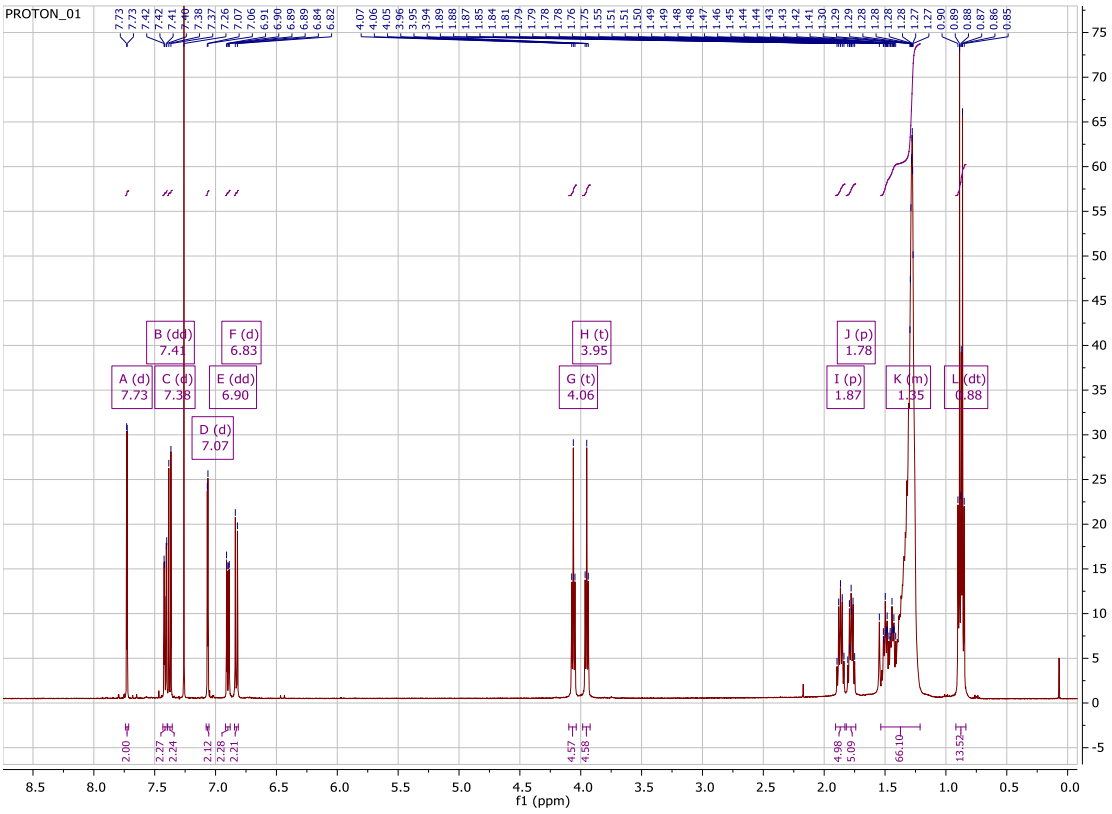
1,8-bis(5-(decyloxy)-2-((4-(decyloxy)-3-ethynylphenyl)ethynyl)phenyl)octa-1,3,5,7-tetrayne (5)

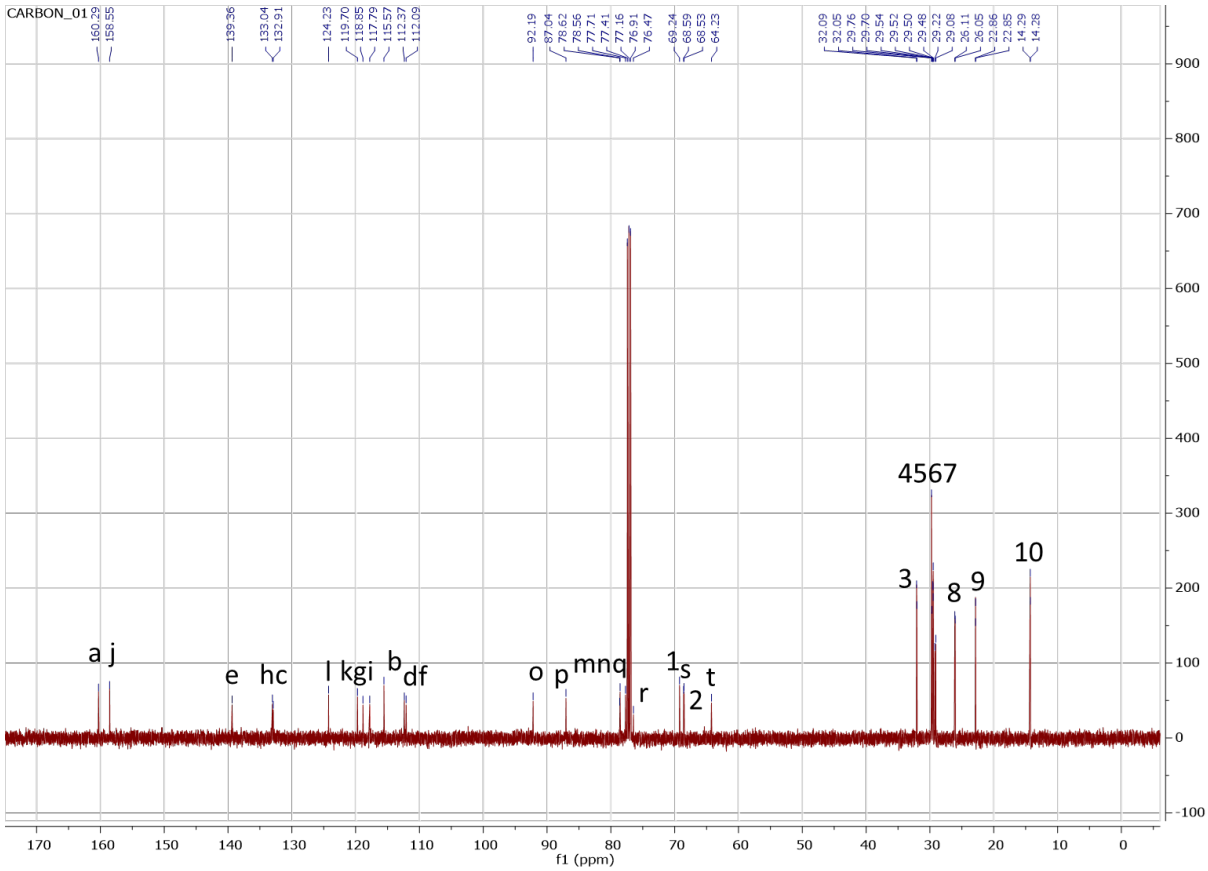




Macrocycle-tetrayne (6)



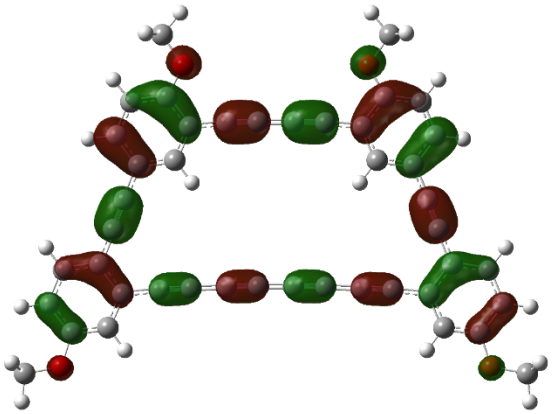




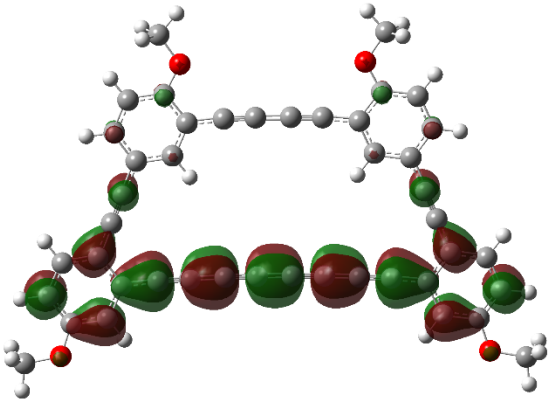
Computational method:

For computation time considerations, the decyl alkyl chains were replaced by a simple methyl group. Unless otherwise specified, the rest of the models used for calculations are identical to the reported compounds. Calculations were performed with the GAUSSIAN 09 suite of programs.[2] Geometries were optimized using the B3LYP functional in combination with the 6-31+G** basis set for all atoms, including hydrogen.[3] The stationary points were characterized as minima on the potential energy surface by full vibration frequencies calculations (no imaginary frequency). All geometry optimizations were carried out without any symmetry constraints. The crystal structure of compound **6** was used as a starting model for the dimerization energy in the gas phase. Absorption bands were calculated on the previously optimized models by TD-DFT using the long-range corrected functional ωB97xD[4] along with the 6-31+G* basis set using the PCM solvation model[5] with the experimental solvent (chloroform).

Structures, optimized geometries and cartesian coordinates for compound 6:



HOMO



LUMO

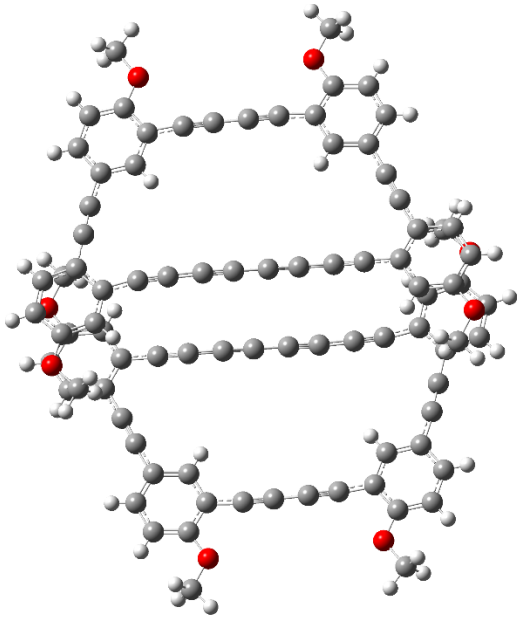
Sum of electronic and thermal Enthalpies= -1988.784739
Sum of electronic and thermal Free Energies= -1988.863240

C	7.81706900	-4.28166300	-0.00008200
C	6.43295800	-4.08778000	-0.00005700
C	5.88492100	-2.79719900	-0.00003400
C	6.75065100	-1.65954400	-0.00003400
C	8.13594300	-1.88708200	-0.00005900
C	8.67351100	-3.17091800	-0.00008400
H	5.78273600	-4.95481000	-0.00005400
H	8.80101900	-1.03002300	-0.00006100
H	9.74945200	-3.29468700	-0.00010400
C	4.47493900	-2.64673300	-0.00000300
C	3.25188700	-2.58399700	0.00002700
C	1.90345000	-2.52627500	0.00006400
C	0.67203600	-2.50219100	0.00006500
C	6.23594300	-0.33715300	-0.00001100
C	5.80812000	0.80184800	0.00000400
C	5.26712900	2.11766700	0.00001300
C	3.87465400	2.30986200	-0.00000100
C	6.09768300	3.25346900	0.00003500
C	3.31061900	3.59281200	0.00000600
H	3.21579200	1.44931700	-0.00001800
C	5.55861400	4.53723100	0.00004300
H	7.17483600	3.12416600	0.00004500
C	4.17213600	4.72303500	0.00002900
H	6.22633100	5.38990800	0.00006000
C	-0.67223900	-2.50232000	0.00004300
C	-1.90365000	-2.52658100	0.00001000
C	-3.25208600	-2.58432300	-0.00001300
C	-4.47513900	-2.64704900	-0.00001600
C	-5.88515300	-2.79722600	0.00001600
C	-6.43345700	-4.08769300	0.00004300
C	-6.75064600	-1.65939300	0.00001700
C	-7.81760900	-4.28128700	0.00007000
H	-5.78341400	-4.95485800	0.00004100
C	-8.13598600	-1.88664100	0.00004500
C	-8.67382100	-3.17036500	0.00007100
H	-8.80088300	-1.02944300	0.00004700
H	-9.74978700	-3.29391100	0.00009300
C	-6.23565400	-0.33711200	-0.00000600
C	-5.80761900	0.80180900	-0.00002300
C	-5.26671200	2.11766300	-0.00004400
C	-6.09732900	3.25341800	-0.00007200
C	-3.87424800	2.30993500	-0.00003600
C	-5.55833400	4.53721100	-0.00009100
H	-7.17447600	3.12405400	-0.00007800
C	-3.31028600	3.59291700	-0.00005500
H	-3.21533900	1.44942800	-0.00001500
C	-4.17186500	4.72309200	-0.00008300
H	-6.22609800	5.38985000	-0.00011200
C	1.89996300	3.74365200	-0.00001100
C	0.67925100	3.77479800	-0.00002700
C	-0.67892600	3.77496100	-0.00003100
C	-1.89963800	3.74383700	-0.00004300
O	-3.55715900	5.93157200	-0.00010000
O	3.55736000	5.93147900	0.00003400
O	-8.23104100	-5.57896000	0.00009600
O	8.23023200	-5.57942200	-0.00010500
C	9.62585700	-5.84392000	-0.00010600
H	9.72424600	-6.93002100	-0.00010500
H	10.11438700	-5.43723400	-0.89444900
H	10.11438800	-5.43723200	0.89423600
C	4.35915500	7.10440900	0.00005700

H	4.99155700	7.15988400	0.89469700
H	4.99157800	7.15990500	-0.89456700
H	3.66031200	7.94135300	0.00005800
C	-4.35902400	7.10445400	-0.00012800
H	-4.99143200	7.15988600	-0.89476600
H	-4.99144600	7.15991800	0.89449900
H	-3.66023000	7.94143900	-0.00013700
C	-9.62672100	-5.84316800	0.00009700
H	-9.72533500	-6.92924900	0.00009800
H	-10.11516600	-5.43637900	0.89444000
H	-10.11516800	-5.43638000	-0.89424500

Dimer of compound **6**:

Sum of electronic and thermal Enthalpies= -3977.614372
Sum of electronic and thermal Free Energies= -3977.745482



O	12.21802700	5.05850200	15.66299400
O	16.38306400	3.54220900	10.37844200
O	12.04078500	8.06315000	-0.25442000
O	1.86683700	11.07027600	12.59744800
C	10.85079200	6.08536000	14.07515800
C	5.22892900	9.60021600	12.19720900
C	4.01945300	10.22650500	11.85310200
H	3.85590000	10.48374700	10.95317500
C	16.09809900	4.02223200	9.13654300
C	13.70685300	6.56683700	3.24126100
C	8.79101200	7.18761900	14.68863300
C	5.46157300	9.20831200	13.51872800
C	14.86937100	4.68988900	9.02260300
C	10.15018300	6.12167600	16.37256400
H	10.29310400	5.89166300	17.28316700
C	9.71032800	6.80395400	13.72922000
H	9.56145400	7.03427400	12.82014100
C	14.30891300	6.02755400	4.43099500
C	6.20247000	9.34555400	11.18197000
C	12.45375100	7.19040100	3.29281600
C	6.66633500	8.52767900	13.91622100

C	14.04534600	4.90431600	10.16917100
C	12.50228000	4.67101900	17.01303700
H	11.79845100	4.06232900	17.34875500
H	12.52883800	5.47007600	17.59737900
C	7.62332500	7.92824700	14.29266500
C	12.52432500	7.60430900	0.92738200
C	14.47005900	5.18363400	7.78665300
H	13.63095000	5.62167100	7.70886300
C	11.07391000	5.74607500	15.41772600
C	3.07495100	10.46424300	12.81861600
C	14.80064800	5.56888600	5.41938900
C	11.77749900	5.70865800	13.06418900
C	12.51281200	5.44788000	12.14748400
C	17.67606100	2.93489700	10.58710300
H	18.39465400	3.56811900	10.33695400
H	17.76486400	2.12157800	10.02884300
C	16.49839500	4.39899600	6.80283500
H	17.06429100	4.30728500	6.04476100
C	10.74193500	8.67943400	-0.25167400
H	10.73639800	9.46049600	0.35692000
H	10.05811800	8.03579700	0.05796100
C	15.27051500	5.04993600	6.66845600
C	11.86851800	7.69959500	2.12931800
H	11.01312600	8.11282300	2.17202600
C	13.33040100	5.14276300	11.10112900
C	14.36412500	6.50256000	2.00881900
H	15.22750600	6.10826500	1.96001000
C	16.90906500	3.88344800	8.02612500
H	17.74422900	3.43750600	8.09934000
C	9.01627900	6.83268500	16.00801700
H	8.38581300	7.08013600	16.67304800
C	11.74917700	7.37510900	4.52403800
C	13.78187000	7.00309900	0.86637000
H	14.23732800	6.93824900	0.03508200
C	4.48798400	9.47154400	14.47051500
H	4.63821200	9.22015400	15.37349200
C	7.89158500	8.85727200	9.31195300
C	1.57825700	11.49823300	11.25518400
H	1.58203700	10.72212400	10.64201400
H	2.26252000	12.14438800	10.94859900
C	6.99837900	9.13432400	10.30797300
C	3.30459600	10.09046100	14.13189900
H	2.64879700	10.26171500	14.79692900
C	11.06369300	7.63493400	5.46362200
C	10.25010100	7.93966900	6.51913000
C	8.67030500	8.59179400	8.43185500
C	9.51640200	8.25704400	7.42363200
O	5.73812200	15.47181300	-0.41000000
O	1.57308400	16.98810600	4.87455200
O	5.91536300	12.46716500	15.50741400
O	16.08931200	9.46003900	2.65554600
C	7.10535700	14.44495500	1.17783600
C	12.72722000	10.93009900	3.05578500
C	13.93669500	10.30381000	3.39989200
H	14.10024900	10.04656800	4.29981900
C	1.85804900	16.50808300	6.11645100
C	4.24929600	13.96347800	12.01173300
C	9.16513600	13.34269600	0.56436100
C	12.49457600	11.32200300	1.73426500
C	3.08677700	15.84042600	6.23039000
C	7.80596600	14.40863900	-1.11957000

H	7.66304500	14.63865200	-2.03017300
C	8.24582000	13.72636100	1.52377400
H	8.39469400	13.49604100	2.43285300
C	3.64723500	14.50276100	10.82199900
C	11.75367900	11.18476100	4.07102400
C	5.50239700	13.33991400	11.96017800
C	11.28981400	12.00263600	1.33677200
C	3.91080200	15.62599900	5.08382300
C	5.45386900	15.85929600	-1.76004300
H	6.15769800	16.46798600	-2.09576100
H	5.42731100	15.06023900	-2.34438500
C	10.33282400	12.60206800	0.96032800
C	5.43182400	12.92600600	14.32561200
C	3.48609000	15.34668100	7.46634000
H	4.32519800	14.90864400	7.54413100
C	6.88223800	14.78424000	-0.16473200
C	14.88119800	10.06607200	2.43437800
C	3.15550100	14.96143000	9.83360500
C	6.17864900	14.82165700	2.18880500
C	5.44333700	15.08243500	3.10551000
C	0.28008700	17.59541800	4.66589100
H	-0.43850600	16.96219600	4.91604000
H	0.19128500	18.40873700	5.22415000
C	1.45775400	16.13131900	8.45015900
H	0.89185700	16.22303000	9.20823200
C	7.21421400	11.85088100	15.50466800
H	7.21975000	11.06981900	14.89607400
H	7.89803000	12.49451800	15.19503200
C	2.68563300	15.48037900	8.58453700
C	6.08763000	12.83072000	13.12367600
H	6.94302200	12.41749200	13.08096800
C	4.62574700	15.38755200	4.15186500
C	3.59202300	14.02775500	13.24417500
H	2.72864200	14.42205000	13.29298400
C	1.04708400	16.64686700	7.22686800
H	0.21191900	17.09280900	7.15365400
C	8.93986900	13.69763000	-0.75502300
H	9.57033600	13.45017900	-1.42005400
C	6.20697200	13.15520600	10.72895600
C	4.17427900	13.52721600	14.38662400
H	3.71882000	13.59206600	15.21791200
C	13.46816500	11.05877100	0.78247900
H	13.31793600	11.31016100	-0.12049900
C	10.06456300	11.67304300	5.94104100
C	16.37789200	9.03208200	3.99781000
H	16.37411200	9.80819100	4.61098000
H	15.69362900	8.38592700	4.30439500
C	10.95776900	11.39599100	4.94502100
C	14.65155300	10.43985400	1.12109500
H	15.30735100	10.26860000	0.45606500
C	6.89245600	12.89538100	9.78937100
C	7.70604700	12.59064600	8.73386400
C	9.28584300	11.93852100	6.82113900
C	8.43974600	12.27327100	7.82936200
H	4.50465800	16.35309900	-1.76762700
H	0.20350200	17.84940400	3.62929800
H	0.61250500	11.95884700	11.26275800
H	7.42576300	11.53980500	16.50635600
H	13.45149100	4.17721600	17.02062100
H	17.75264600	2.68091100	11.62369600
H	10.53038600	8.99051000	-1.25336200

H 17.34364400 8.57146700 3.99023600

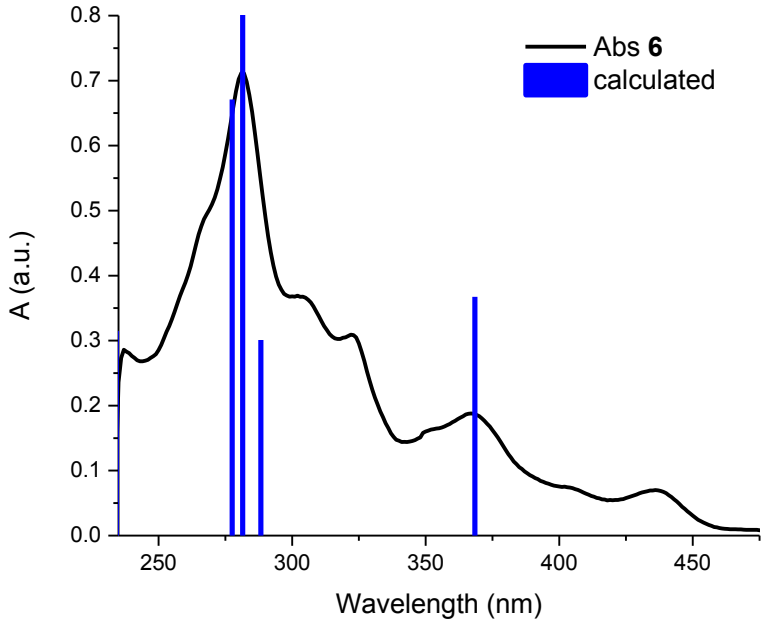


Figure S2. Absorption spectra of macrocycle **6** and calculated band by TD-DFT.

X-ray Diffraction

An orange stick-shaped crystal with a size of 0.32 x 0.28 x 0.06 mm^3 was mounted on CryoLoops with Paratone-N and optically aligned on a Bruker SMART APEX-II X-ray diffractometer with 1K CCD detector using a digital camera. Initial intensity measurements were performed using a fine-focused sealed tube, graphite-monochromated, X-ray source (Mo $K\alpha$, λ = 0.71073 Å) at 50 kV and 30 mA. Standard APEX-II[6] software package was used for determining the unit cells, generating the data collection strategy, and controlling data collection. SAINT[7] was used for data integration including Lorentz and polarization corrections. The structures of all compounds were solved by direct methods and refined by full-matrix least-squares methods with SHELX-97 in the SHELXTL6.14 package.[8] All the H atoms (on C atoms) were generated geometrically and refined in riding mode. Crystallographic information for all obtained phases is summarized in Table 1. Atomic coordinates and additional structural information are provided in the .cif files of the Supporting Information. Crystallographic data have been deposited with CCDC (CCDC 1531790). These data can be obtained upon request from the Cambridge

Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, E-mail: deposit@ccdc.cam.ac.uk, or via the Internet at www.ccdc.cam.ac.uk.

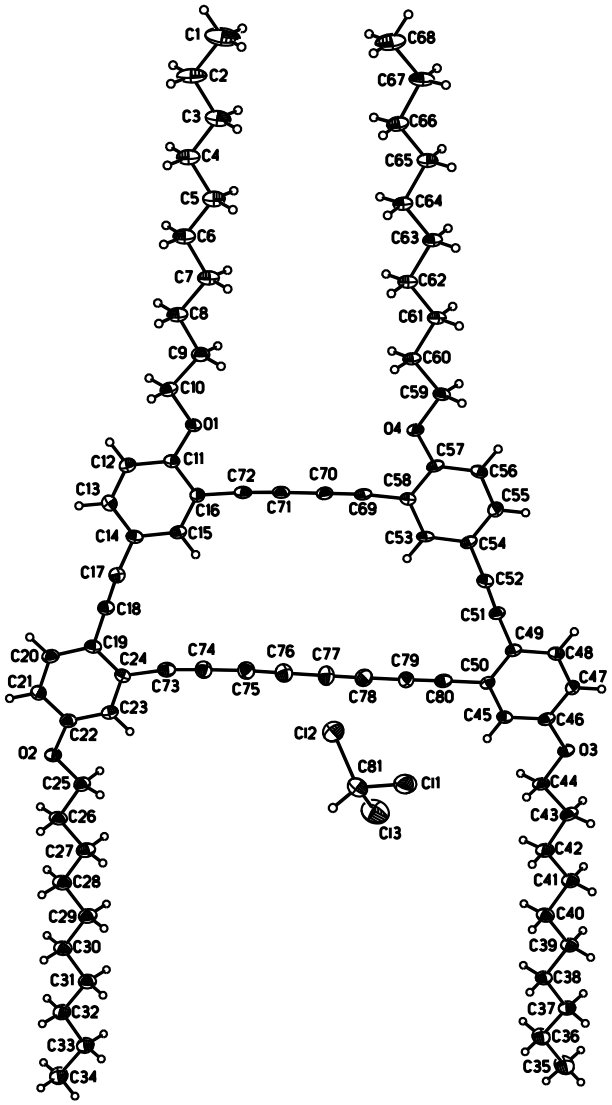


Figure S3. ORTEP of macrocycle **6** with thermal ellipsoids set at the 50% probability level. H atoms are shown as spheres with arbitrary radii.

Table 1. Crystal data and structure refinement for MUD0316.

Identification code	MUD0316
Empirical formula	C81 H97 Cl3 O4
Formula weight	1240.93

Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 15.3201(15) Å	α= 72.8140(10)°.
	b = 15.8949(15) Å	β= 83.465(2)°.
	c = 16.0521(15) Å	γ = 87.082(2)°.
Volume	3709.5(6) $Å^3$	
Z	2	
Density (calculated)	1.111 Mg/m^3	
Absorption coefficient	0.170 mm^{-1}	
F(000)	1332	
Crystal size	0.32 x 0.28 x 0.06 mm^3	
Theta range for data collection	1.335 to 24.558°.	
Index ranges	-17<=h<=17, -18<=k<=18, -18<=l<=18	
Reflections collected	29228	
Independent reflections	12345 [R(int) = 0.0467]	
Completeness to theta = 25.242°	91.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.990 and 0.947	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12345 / 0 / 797	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0610, wR2 = 0.1526	
R indices (all data)	R1 = 0.1106, wR2 = 0.1763	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.473 and -0.356 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MUD0316. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	8154(1)	9033(1)	8903(1)	57(1)
Cl(2)	8804(1)	7802(1)	7950(1)	53(1)
Cl(3)	7230(1)	8837(1)	7520(1)	67(1)
O(4)	6741(1)	175(1)	10269(1)	29(1)
O(1)	9870(1)	236(1)	6804(1)	31(1)
O(2)	7608(1)	5128(1)	-167(1)	35(1)
O(3)	-7(1)	4551(1)	8259(1)	36(1)
C(58)	5923(2)	1127(2)	9228(2)	24(1)
C(50)	2264(2)	3702(2)	7997(2)	23(1)
C(45)	1477(2)	4163(2)	7771(2)	26(1)
C(11)	9753(2)	777(2)	5990(2)	26(1)
C(19)	8508(2)	3514(2)	2125(2)	28(1)
C(54)	4500(2)	1703(2)	9630(2)	27(1)
C(49)	2339(2)	3201(2)	8863(2)	26(1)
C(16)	8936(2)	1219(2)	5915(2)	25(1)
C(56)	5308(2)	708(2)	10734(2)	29(1)
C(53)	5178(2)	1646(2)	9001(2)	27(1)
C(18)	8838(2)	2945(2)	2905(2)	28(1)
C(80)	2977(2)	3737(2)	7331(2)	29(1)
C(24)	7666(2)	3896(2)	2159(2)	26(1)
C(51)	3121(2)	2696(2)	9124(2)	27(1)
C(72)	8313(2)	1134(2)	6667(2)	29(1)
C(59)	6848(2)	-329(2)	11154(2)	28(1)
C(52)	3740(2)	2246(2)	9370(2)	28(1)
C(60)	7743(2)	-769(2)	11161(2)	28(1)

C(22)	7859(2)	4612(2)	608(2)	30(1)
C(15)	8743(2)	1768(2)	5105(2)	26(1)
C(57)	5988(2)	655(2)	10108(2)	26(1)
C(46)	787(2)	4127(2)	8404(2)	31(1)
C(17)	9107(2)	2466(2)	3553(2)	30(1)
C(69)	6609(2)	1084(2)	8565(2)	28(1)
C(70)	7160(2)	1096(2)	7964(2)	28(1)
C(63)	9020(2)	-2301(2)	13018(2)	31(1)
C(10)	10720(2)	-187(2)	6941(2)	31(1)
C(13)	10160(2)	1463(2)	4460(2)	31(1)
C(61)	7917(2)	-1335(2)	12071(2)	30(1)
C(25)	6740(2)	5516(2)	-165(2)	32(1)
C(14)	9346(2)	1899(2)	4372(2)	28(1)
C(23)	7346(2)	4441(2)	1396(2)	29(1)
C(71)	7775(2)	1105(2)	7278(2)	30(1)
C(20)	9023(2)	3710(2)	1317(2)	33(1)
C(62)	8835(2)	-1739(2)	12107(2)	31(1)
C(12)	10362(2)	903(2)	5262(2)	32(1)
C(55)	4569(2)	1226(2)	10495(2)	29(1)
C(73)	7116(2)	3776(2)	2966(2)	32(1)
C(21)	8704(2)	4245(2)	568(2)	34(1)
C(9)	10703(2)	-693(2)	7898(2)	34(1)
C(48)	1630(2)	3184(2)	9487(2)	34(1)
C(64)	9952(2)	-2681(2)	13055(2)	31(1)
C(78)	4223(2)	3789(2)	6105(2)	38(1)
C(44)	-118(2)	5079(2)	7379(2)	31(1)
C(38)	-3295(2)	7991(2)	4471(2)	34(1)
C(39)	-3164(2)	7451(2)	5408(2)	35(1)
C(79)	3563(2)	3772(2)	6758(2)	33(1)
C(26)	6628(2)	6058(2)	-1081(2)	36(1)

C(4)	13411(2)	-3127(2)	10373(2)	40(1)
C(65)	10141(2)	-3262(2)	13957(2)	33(1)
C(47)	860(2)	3639(2)	9265(2)	35(1)
C(8)	11571(2)	-1160(2)	8104(2)	34(1)
C(27)	5719(2)	6491(2)	-1159(2)	38(1)
C(74)	6596(2)	3759(2)	3582(2)	37(1)
C(31)	3751(2)	8522(2)	-3274(2)	39(1)
C(41)	-2106(2)	6481(2)	6418(2)	36(1)
C(75)	5983(2)	3748(2)	4274(2)	38(1)
C(6)	12465(2)	-2161(2)	9259(2)	39(1)
C(42)	-1185(2)	6077(2)	6478(2)	36(1)
C(40)	-2245(2)	7047(2)	5493(2)	36(1)
C(43)	-1029(2)	5486(2)	7386(2)	36(1)
C(7)	11601(2)	-1662(2)	9073(2)	38(1)
C(32)	3669(2)	9024(2)	-4224(2)	39(1)
C(30)	4617(2)	8016(2)	-3140(2)	38(1)
C(66)	11073(2)	-3619(2)	13996(2)	37(1)
C(37)	-4208(2)	8415(2)	4366(2)	36(1)
C(28)	5582(2)	6993(2)	-2096(2)	40(1)
C(29)	4712(2)	7487(2)	-2202(2)	39(1)
C(77)	4800(2)	3791(2)	5528(2)	40(1)
C(5)	12536(2)	-2642(2)	10211(2)	40(1)
C(67)	11271(2)	-4206(2)	14893(2)	45(1)
C(76)	5432(2)	3774(2)	4867(2)	40(1)
C(33)	2816(2)	9545(2)	-4372(2)	41(1)
C(36)	-4370(2)	8850(3)	3424(2)	45(1)
C(3)	13500(2)	-3605(2)	11330(2)	48(1)
C(2)	14387(3)	-4078(2)	11492(3)	55(1)
C(34)	2777(2)	10068(3)	-5329(2)	48(1)
C(81)	8265(2)	8826(2)	7885(2)	40(1)

C(35)	-5288(2)	9250(3)	3327(2)	62(1)
C(68)	12202(3)	-4570(3)	14903(3)	64(1)
C(1)	14460(3)	-4542(3)	12453(3)	77(2)

Table 3. Bond lengths [Å] and angles [°] for MUD0316.

Cl(1)-C(81)	1.748(3)
Cl(2)-C(81)	1.768(4)
Cl(3)-C(81)	1.749(4)
O(4)-C(57)	1.357(3)
O(4)-C(59)	1.433(3)
O(1)-C(11)	1.362(3)
O(1)-C(10)	1.443(3)
O(2)-C(22)	1.356(3)
O(2)-C(25)	1.438(4)
O(3)-C(46)	1.369(3)
O(3)-C(44)	1.438(3)
C(58)-C(53)	1.392(4)
C(58)-C(57)	1.403(4)
C(58)-C(69)	1.422(4)
C(50)-C(49)	1.398(4)
C(50)-C(45)	1.405(4)
C(50)-C(80)	1.429(4)
C(45)-C(46)	1.372(4)
C(45)-H(45)	0.9500
C(11)-C(12)	1.381(4)
C(11)-C(16)	1.403(4)
C(19)-C(20)	1.398(4)
C(19)-C(24)	1.401(4)
C(19)-C(18)	1.438(4)
C(54)-C(53)	1.382(4)
C(54)-C(55)	1.385(4)
C(54)-C(52)	1.437(4)
C(49)-C(48)	1.387(4)

C(49)-C(51)	1.440(4)
C(16)-C(15)	1.390(4)
C(16)-C(72)	1.428(4)
C(56)-C(57)	1.380(4)
C(56)-C(55)	1.387(4)
C(56)-H(56)	0.9500
C(53)-H(53)	0.9500
C(18)-C(17)	1.195(4)
C(80)-C(79)	1.201(4)
C(24)-C(23)	1.398(4)
C(24)-C(73)	1.430(4)
C(51)-C(52)	1.191(4)
C(72)-C(71)	1.198(4)
C(59)-C(60)	1.506(4)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-C(61)	1.517(4)
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(22)-C(23)	1.373(4)
C(22)-C(21)	1.396(4)
C(15)-C(14)	1.381(4)
C(15)-H(15)	0.9500
C(46)-C(47)	1.384(4)
C(17)-C(14)	1.432(4)
C(69)-C(70)	1.204(4)
C(70)-C(71)	1.362(5)
C(63)-C(62)	1.520(4)
C(63)-C(64)	1.521(4)
C(63)-H(63A)	0.9900

C(63)-H(63B)	0.9900
C(10)-C(9)	1.506(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(13)-C(12)	1.390(4)
C(13)-C(14)	1.397(4)
C(13)-H(13)	0.9500
C(61)-C(62)	1.517(4)
C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900
C(25)-C(26)	1.492(4)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(23)-H(23)	0.9500
C(20)-C(21)	1.376(4)
C(20)-H(20)	0.9500
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(12)-H(12)	0.9500
C(55)-H(55)	0.9500
C(73)-C(74)	1.192(4)
C(21)-H(21)	0.9500
C(9)-C(8)	1.512(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(48)-C(47)	1.377(4)
C(48)-H(48)	0.9500
C(64)-C(65)	1.520(4)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900

C(78)-C(77)	1.205(5)
C(78)-C(79)	1.365(5)
C(44)-C(43)	1.509(4)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(38)-C(37)	1.526(4)
C(38)-C(39)	1.526(4)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(40)	1.520(4)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(26)-C(27)	1.523(4)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(4)-C(3)	1.517(5)
C(4)-C(5)	1.521(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(65)-C(66)	1.511(4)
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(47)-H(47)	0.9500
C(8)-C(7)	1.530(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(27)-C(28)	1.514(4)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(74)-C(75)	1.368(5)

C(31)-C(32)	1.514(4)
C(31)-C(30)	1.518(4)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(41)-C(42)	1.521(4)
C(41)-C(40)	1.524(4)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(75)-C(76)	1.207(5)
C(6)-C(5)	1.506(4)
C(6)-C(7)	1.520(4)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(42)-C(43)	1.521(4)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(32)-C(33)	1.514(4)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(30)-C(29)	1.511(4)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(66)-C(67)	1.520(4)
C(66)-H(66A)	0.9900

C(66)-H(66B)	0.9900
C(37)-C(36)	1.510(4)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(28)-C(29)	1.512(4)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(77)-C(76)	1.358(5)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(67)-C(68)	1.512(5)
C(67)-H(67A)	0.9900
C(67)-H(67B)	0.9900
C(33)-C(34)	1.521(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(36)-C(35)	1.518(5)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(3)-C(2)	1.531(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(2)-C(1)	1.515(5)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800

C(81)-H(81)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800

C(57)-O(4)-C(59)	118.3(2)
C(11)-O(1)-C(10)	117.9(2)
C(22)-O(2)-C(25)	117.7(2)
C(46)-O(3)-C(44)	117.4(2)
C(53)-C(58)-C(57)	119.5(3)
C(53)-C(58)-C(69)	119.6(3)
C(57)-C(58)-C(69)	120.8(3)
C(49)-C(50)-C(45)	120.0(3)
C(49)-C(50)-C(80)	120.5(3)
C(45)-C(50)-C(80)	119.5(3)
C(46)-C(45)-C(50)	119.9(3)
C(46)-C(45)-H(45)	120.1
C(50)-C(45)-H(45)	120.1
O(1)-C(11)-C(12)	125.1(3)
O(1)-C(11)-C(16)	115.2(3)
C(12)-C(11)-C(16)	119.8(3)
C(20)-C(19)-C(24)	118.3(3)
C(20)-C(19)-C(18)	121.0(3)
C(24)-C(19)-C(18)	120.7(3)

C(53)-C(54)-C(55)	118.8(3)
C(53)-C(54)-C(52)	119.5(3)
C(55)-C(54)-C(52)	121.7(3)
C(48)-C(49)-C(50)	118.6(3)
C(48)-C(49)-C(51)	119.3(3)
C(50)-C(49)-C(51)	122.2(3)
C(15)-C(16)-C(11)	119.5(3)
C(15)-C(16)-C(72)	119.7(3)
C(11)-C(16)-C(72)	120.7(3)
C(57)-C(56)-C(55)	120.3(3)
C(57)-C(56)-H(56)	119.9
C(55)-C(56)-H(56)	119.9
C(54)-C(53)-C(58)	121.1(3)
C(54)-C(53)-H(53)	119.5
C(58)-C(53)-H(53)	119.5
C(17)-C(18)-C(19)	179.4(4)
C(79)-C(80)-C(50)	178.4(3)
C(23)-C(24)-C(19)	120.4(3)
C(23)-C(24)-C(73)	117.5(3)
C(19)-C(24)-C(73)	122.0(3)
C(52)-C(51)-C(49)	176.5(3)
C(71)-C(72)-C(16)	176.7(3)
O(4)-C(59)-C(60)	107.9(2)
O(4)-C(59)-H(59A)	110.1
C(60)-C(59)-H(59A)	110.1
O(4)-C(59)-H(59B)	110.1
C(60)-C(59)-H(59B)	110.1
H(59A)-C(59)-H(59B)	108.4
C(51)-C(52)-C(54)	177.5(3)
C(59)-C(60)-C(61)	112.2(3)

C(59)-C(60)-H(60A)	109.2
C(61)-C(60)-H(60A)	109.2
C(59)-C(60)-H(60B)	109.2
C(61)-C(60)-H(60B)	109.2
H(60A)-C(60)-H(60B)	107.9
O(2)-C(22)-C(23)	124.7(3)
O(2)-C(22)-C(21)	115.4(3)
C(23)-C(22)-C(21)	119.9(3)
C(14)-C(15)-C(16)	121.3(3)
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-H(15)	119.4
O(4)-C(57)-C(56)	125.2(3)
O(4)-C(57)-C(58)	115.4(3)
C(56)-C(57)-C(58)	119.3(3)
O(3)-C(46)-C(45)	124.8(3)
O(3)-C(46)-C(47)	114.8(3)
C(45)-C(46)-C(47)	120.4(3)
C(18)-C(17)-C(14)	174.4(3)
C(70)-C(69)-C(58)	175.3(3)
C(69)-C(70)-C(71)	179.2(4)
C(62)-C(63)-C(64)	113.4(3)
C(62)-C(63)-H(63A)	108.9
C(64)-C(63)-H(63A)	108.9
C(62)-C(63)-H(63B)	108.9
C(64)-C(63)-H(63B)	108.9
H(63A)-C(63)-H(63B)	107.7
O(1)-C(10)-C(9)	107.7(2)
O(1)-C(10)-H(10A)	110.2
C(9)-C(10)-H(10A)	110.2
O(1)-C(10)-H(10B)	110.2

C(9)-C(10)-H(10B)	110.2
H(10A)-C(10)-H(10B)	108.5
C(12)-C(13)-C(14)	121.1(3)
C(12)-C(13)-H(13)	119.4
C(14)-C(13)-H(13)	119.4
C(62)-C(61)-C(60)	113.3(3)
C(62)-C(61)-H(61A)	108.9
C(60)-C(61)-H(61A)	108.9
C(62)-C(61)-H(61B)	108.9
C(60)-C(61)-H(61B)	108.9
H(61A)-C(61)-H(61B)	107.7
O(2)-C(25)-C(26)	107.6(3)
O(2)-C(25)-H(25A)	110.2
C(26)-C(25)-H(25A)	110.2
O(2)-C(25)-H(25B)	110.2
C(26)-C(25)-H(25B)	110.2
H(25A)-C(25)-H(25B)	108.5
C(15)-C(14)-C(13)	118.5(3)
C(15)-C(14)-C(17)	118.8(3)
C(13)-C(14)-C(17)	122.7(3)
C(22)-C(23)-C(24)	120.2(3)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(72)-C(71)-C(70)	178.4(3)
C(21)-C(20)-C(19)	121.1(3)
C(21)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(61)-C(62)-C(63)	113.7(3)
C(61)-C(62)-H(62A)	108.8
C(63)-C(62)-H(62A)	108.8

C(61)-C(62)-H(62B)	108.8
C(63)-C(62)-H(62B)	108.8
H(62A)-C(62)-H(62B)	107.7
C(11)-C(12)-C(13)	119.8(3)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(54)-C(55)-C(56)	121.0(3)
C(54)-C(55)-H(55)	119.5
C(56)-C(55)-H(55)	119.5
C(74)-C(73)-C(24)	171.9(3)
C(20)-C(21)-C(22)	120.1(3)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(10)-C(9)-C(8)	111.4(3)
C(10)-C(9)-H(9A)	109.3
C(8)-C(9)-H(9A)	109.3
C(10)-C(9)-H(9B)	109.3
C(8)-C(9)-H(9B)	109.3
H(9A)-C(9)-H(9B)	108.0
C(47)-C(48)-C(49)	121.3(3)
C(47)-C(48)-H(48)	119.3
C(49)-C(48)-H(48)	119.3
C(65)-C(64)-C(63)	114.1(3)
C(65)-C(64)-H(64A)	108.7
C(63)-C(64)-H(64A)	108.7
C(65)-C(64)-H(64B)	108.7
C(63)-C(64)-H(64B)	108.7
H(64A)-C(64)-H(64B)	107.6
C(77)-C(78)-C(79)	179.0(4)
O(3)-C(44)-C(43)	107.7(3)

O(3)-C(44)-H(44A)	110.2
C(43)-C(44)-H(44A)	110.2
O(3)-C(44)-H(44B)	110.2
C(43)-C(44)-H(44B)	110.2
H(44A)-C(44)-H(44B)	108.5
C(37)-C(38)-C(39)	114.0(3)
C(37)-C(38)-H(38A)	108.8
C(39)-C(38)-H(38A)	108.8
C(37)-C(38)-H(38B)	108.8
C(39)-C(38)-H(38B)	108.8
H(38A)-C(38)-H(38B)	107.7
C(40)-C(39)-C(38)	112.7(3)
C(40)-C(39)-H(39A)	109.1
C(38)-C(39)-H(39A)	109.1
C(40)-C(39)-H(39B)	109.1
C(38)-C(39)-H(39B)	109.1
H(39A)-C(39)-H(39B)	107.8
C(80)-C(79)-C(78)	178.4(4)
C(25)-C(26)-C(27)	112.0(3)
C(25)-C(26)-H(26A)	109.2
C(27)-C(26)-H(26A)	109.2
C(25)-C(26)-H(26B)	109.2
C(27)-C(26)-H(26B)	109.2
H(26A)-C(26)-H(26B)	107.9
C(3)-C(4)-C(5)	114.0(3)
C(3)-C(4)-H(4A)	108.7
C(5)-C(4)-H(4A)	108.7
C(3)-C(4)-H(4B)	108.7
C(5)-C(4)-H(4B)	108.7
H(4A)-C(4)-H(4B)	107.6

C(66)-C(65)-C(64)	113.9(3)
C(66)-C(65)-H(65A)	108.8
C(64)-C(65)-H(65A)	108.8
C(66)-C(65)-H(65B)	108.8
C(64)-C(65)-H(65B)	108.8
H(65A)-C(65)-H(65B)	107.7
C(48)-C(47)-C(46)	119.9(3)
C(48)-C(47)-H(47)	120.1
C(46)-C(47)-H(47)	120.1
C(9)-C(8)-C(7)	113.7(3)
C(9)-C(8)-H(8A)	108.8
C(7)-C(8)-H(8A)	108.8
C(9)-C(8)-H(8B)	108.8
C(7)-C(8)-H(8B)	108.8
H(8A)-C(8)-H(8B)	107.7
C(28)-C(27)-C(26)	112.2(3)
C(28)-C(27)-H(27A)	109.2
C(26)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27B)	109.2
C(26)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(73)-C(74)-C(75)	178.5(4)
C(32)-C(31)-C(30)	113.0(3)
C(32)-C(31)-H(31A)	109.0
C(30)-C(31)-H(31A)	109.0
C(32)-C(31)-H(31B)	109.0
C(30)-C(31)-H(31B)	109.0
H(31A)-C(31)-H(31B)	107.8
C(42)-C(41)-C(40)	112.4(3)
C(42)-C(41)-H(41A)	109.1

C(40)-C(41)-H(41A)	109.1
C(42)-C(41)-H(41B)	109.1
C(40)-C(41)-H(41B)	109.1
H(41A)-C(41)-H(41B)	107.9
C(76)-C(75)-C(74)	177.3(4)
C(5)-C(6)-C(7)	114.8(3)
C(5)-C(6)-H(6A)	108.6
C(7)-C(6)-H(6A)	108.6
C(5)-C(6)-H(6B)	108.6
C(7)-C(6)-H(6B)	108.6
H(6A)-C(6)-H(6B)	107.5
C(41)-C(42)-C(43)	113.9(3)
C(41)-C(42)-H(42A)	108.8
C(43)-C(42)-H(42A)	108.8
C(41)-C(42)-H(42B)	108.8
C(43)-C(42)-H(42B)	108.8
H(42A)-C(42)-H(42B)	107.7
C(39)-C(40)-C(41)	113.7(3)
C(39)-C(40)-H(40A)	108.8
C(41)-C(40)-H(40A)	108.8
C(39)-C(40)-H(40B)	108.8
C(41)-C(40)-H(40B)	108.8
H(40A)-C(40)-H(40B)	107.7
C(44)-C(43)-C(42)	110.6(3)
C(44)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43A)	109.5
C(44)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	108.1
C(6)-C(7)-C(8)	112.9(3)

C(6)-C(7)-H(7A)	109.0
C(8)-C(7)-H(7A)	109.0
C(6)-C(7)-H(7B)	109.0
C(8)-C(7)-H(7B)	109.0
H(7A)-C(7)-H(7B)	107.8
C(33)-C(32)-C(31)	114.0(3)
C(33)-C(32)-H(32A)	108.8
C(31)-C(32)-H(32A)	108.8
C(33)-C(32)-H(32B)	108.8
C(31)-C(32)-H(32B)	108.8
H(32A)-C(32)-H(32B)	107.7
C(29)-C(30)-C(31)	114.4(3)
C(29)-C(30)-H(30A)	108.7
C(31)-C(30)-H(30A)	108.7
C(29)-C(30)-H(30B)	108.7
C(31)-C(30)-H(30B)	108.7
H(30A)-C(30)-H(30B)	107.6
C(65)-C(66)-C(67)	114.5(3)
C(65)-C(66)-H(66A)	108.6
C(67)-C(66)-H(66A)	108.6
C(65)-C(66)-H(66B)	108.6
C(67)-C(66)-H(66B)	108.6
H(66A)-C(66)-H(66B)	107.6
C(36)-C(37)-C(38)	113.6(3)
C(36)-C(37)-H(37A)	108.9
C(38)-C(37)-H(37A)	108.9
C(36)-C(37)-H(37B)	108.9
C(38)-C(37)-H(37B)	108.9
H(37A)-C(37)-H(37B)	107.7
C(29)-C(28)-C(27)	114.3(3)

C(29)-C(28)-H(28A)	108.7
C(27)-C(28)-H(28A)	108.7
C(29)-C(28)-H(28B)	108.7
C(27)-C(28)-H(28B)	108.7
H(28A)-C(28)-H(28B)	107.6
C(30)-C(29)-C(28)	112.8(3)
C(30)-C(29)-H(29A)	109.0
C(28)-C(29)-H(29A)	109.0
C(30)-C(29)-H(29B)	109.0
C(28)-C(29)-H(29B)	109.0
H(29A)-C(29)-H(29B)	107.8
C(78)-C(77)-C(76)	177.8(4)
C(6)-C(5)-C(4)	113.3(3)
C(6)-C(5)-H(5A)	108.9
C(4)-C(5)-H(5A)	108.9
C(6)-C(5)-H(5B)	108.9
C(4)-C(5)-H(5B)	108.9
H(5A)-C(5)-H(5B)	107.7
C(68)-C(67)-C(66)	113.1(3)
C(68)-C(67)-H(67A)	109.0
C(66)-C(67)-H(67A)	109.0
C(68)-C(67)-H(67B)	109.0
C(66)-C(67)-H(67B)	109.0
H(67A)-C(67)-H(67B)	107.8
C(75)-C(76)-C(77)	178.7(4)
C(32)-C(33)-C(34)	112.2(3)
C(32)-C(33)-H(33A)	109.2
C(34)-C(33)-H(33A)	109.2
C(32)-C(33)-H(33B)	109.2
C(34)-C(33)-H(33B)	109.2

H(33A)-C(33)-H(33B)	107.9
C(37)-C(36)-C(35)	113.1(3)
C(37)-C(36)-H(36A)	109.0
C(35)-C(36)-H(36A)	109.0
C(37)-C(36)-H(36B)	109.0
C(35)-C(36)-H(36B)	109.0
H(36A)-C(36)-H(36B)	107.8
C(4)-C(3)-C(2)	113.8(3)
C(4)-C(3)-H(3A)	108.8
C(2)-C(3)-H(3A)	108.8
C(4)-C(3)-H(3B)	108.8
C(2)-C(3)-H(3B)	108.8
H(3A)-C(3)-H(3B)	107.7
C(1)-C(2)-C(3)	112.7(4)
C(1)-C(2)-H(2A)	109.0
C(3)-C(2)-H(2A)	109.0
C(1)-C(2)-H(2B)	109.0
C(3)-C(2)-H(2B)	109.0
H(2A)-C(2)-H(2B)	107.8
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
Cl(1)-C(81)-Cl(3)	109.88(19)
Cl(1)-C(81)-Cl(2)	110.89(18)
Cl(3)-C(81)-Cl(2)	110.06(19)
Cl(1)-C(81)-H(81)	108.7
Cl(3)-C(81)-H(81)	108.7

Cl(2)-C(81)-H(81)	108.7
C(36)-C(35)-H(35A)	109.5
C(36)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(36)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for MUD0316. 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}
Cl(1)	85(1)	46(1)	38(1)	-12(1)	-10(1)	18(1)
Cl(2)	64(1)	43(1)	51(1)	-16(1)	1(1)	6(1)
Cl(3)	61(1)	72(1)	66(1)	-9(1)	-24(1)	-5(1)
O(4)	28(1)	30(1)	28(1)	-4(1)	-11(1)	11(1)
O(1)	27(1)	34(1)	26(1)	2(1)	-6(1)	8(1)
O(2)	33(1)	38(1)	28(1)	0(1)	-10(1)	12(1)
O(3)	27(1)	39(1)	35(1)	0(1)	-9(1)	17(1)
C(58)	26(2)	20(2)	25(2)	-4(1)	-7(1)	2(1)
C(50)	23(2)	18(2)	29(2)	-9(1)	-4(1)	2(1)
C(45)	27(2)	25(2)	24(2)	-4(1)	-10(1)	3(1)
C(11)	27(2)	24(2)	24(2)	-4(1)	-7(1)	2(1)
C(19)	35(2)	23(2)	26(2)	-6(1)	-10(1)	2(1)
C(54)	21(2)	26(2)	34(2)	-9(1)	-10(1)	7(1)
C(49)	24(2)	23(2)	30(2)	-7(1)	-10(1)	5(1)
C(16)	24(2)	27(2)	24(2)	-6(1)	-5(1)	2(1)
C(56)	31(2)	30(2)	23(2)	-1(1)	-11(1)	5(1)
C(53)	30(2)	20(2)	28(2)	-2(1)	-13(1)	7(1)
C(18)	31(2)	26(2)	29(2)	-8(2)	-8(1)	2(1)
C(80)	28(2)	27(2)	33(2)	-8(2)	-13(2)	4(1)
C(24)	31(2)	23(2)	23(2)	-4(1)	-6(1)	-1(1)
C(51)	28(2)	26(2)	28(2)	-7(1)	-9(1)	8(2)
C(72)	28(2)	28(2)	29(2)	-2(1)	-12(2)	7(1)
C(59)	33(2)	25(2)	24(2)	-4(1)	-12(1)	6(1)
C(52)	31(2)	25(2)	27(2)	-5(1)	-9(1)	1(2)
C(60)	28(2)	25(2)	31(2)	-5(1)	-14(1)	7(1)

C(22)	33(2)	29(2)	26(2)	-6(1)	-10(1)	6(1)
C(15)	26(2)	25(2)	28(2)	-8(1)	-10(1)	5(1)
C(57)	22(2)	24(2)	33(2)	-8(1)	-13(1)	9(1)
C(46)	27(2)	29(2)	37(2)	-7(2)	-11(2)	11(1)
C(17)	32(2)	29(2)	31(2)	-9(2)	-5(2)	1(1)
C(69)	25(2)	26(2)	30(2)	-3(1)	-13(2)	9(1)
C(70)	28(2)	26(2)	29(2)	-5(1)	-9(2)	7(1)
C(63)	33(2)	26(2)	34(2)	-7(1)	-16(2)	6(1)
C(10)	29(2)	31(2)	35(2)	-9(2)	-10(1)	7(1)
C(13)	32(2)	31(2)	27(2)	-7(1)	-2(1)	-1(2)
C(61)	36(2)	21(2)	32(2)	-6(1)	-14(1)	6(1)
C(25)	32(2)	32(2)	32(2)	-9(2)	-9(1)	6(2)
C(14)	31(2)	25(2)	26(2)	-4(1)	-10(1)	2(1)
C(23)	28(2)	25(2)	34(2)	-8(1)	-9(1)	3(1)
C(71)	29(2)	28(2)	29(2)	-1(1)	-12(2)	8(1)
C(20)	32(2)	32(2)	32(2)	-6(2)	-11(2)	10(2)
C(62)	36(2)	22(2)	35(2)	-4(1)	-15(2)	5(1)
C(12)	30(2)	32(2)	33(2)	-6(2)	-6(2)	7(1)
C(55)	25(2)	32(2)	31(2)	-8(2)	-4(1)	3(1)
C(73)	36(2)	31(2)	31(2)	-8(2)	-12(2)	3(2)
C(21)	36(2)	38(2)	24(2)	-4(2)	-4(1)	8(2)
C(9)	36(2)	31(2)	33(2)	-5(2)	-10(2)	7(2)
C(48)	34(2)	36(2)	27(2)	-2(2)	-9(2)	12(2)
C(64)	33(2)	24(2)	37(2)	-6(1)	-15(2)	5(1)
C(78)	34(2)	40(2)	41(2)	-13(2)	-6(2)	1(2)
C(44)	27(2)	28(2)	35(2)	-3(2)	-12(1)	9(1)
C(38)	32(2)	35(2)	32(2)	-3(2)	-12(2)	7(2)
C(39)	31(2)	35(2)	36(2)	-4(2)	-14(2)	8(2)
C(79)	30(2)	36(2)	31(2)	-7(2)	-2(2)	2(2)
C(26)	36(2)	33(2)	34(2)	0(2)	-13(2)	6(2)

C(4)	45(2)	29(2)	48(2)	-9(2)	-22(2)	5(2)
C(65)	35(2)	28(2)	37(2)	-5(2)	-17(2)	4(1)
C(47)	29(2)	39(2)	30(2)	-2(2)	1(1)	13(2)
C(8)	39(2)	27(2)	38(2)	-10(2)	-18(2)	4(2)
C(27)	44(2)	34(2)	37(2)	-11(2)	-16(2)	8(2)
C(74)	37(2)	42(2)	32(2)	-11(2)	-6(2)	0(2)
C(31)	45(2)	35(2)	35(2)	-7(2)	-11(2)	8(2)
C(41)	35(2)	37(2)	35(2)	-6(2)	-13(2)	11(2)
C(75)	40(2)	42(2)	35(2)	-12(2)	-4(2)	1(2)
C(6)	43(2)	31(2)	44(2)	-8(2)	-20(2)	4(2)
C(42)	31(2)	33(2)	42(2)	-4(2)	-14(2)	7(2)
C(40)	30(2)	35(2)	38(2)	-2(2)	-12(2)	4(2)
C(43)	31(2)	33(2)	43(2)	-10(2)	-12(2)	14(2)
C(7)	45(2)	29(2)	41(2)	-7(2)	-19(2)	7(2)
C(32)	37(2)	42(2)	36(2)	-7(2)	-12(2)	10(2)
C(30)	35(2)	36(2)	39(2)	-3(2)	-14(2)	5(2)
C(66)	37(2)	33(2)	44(2)	-11(2)	-22(2)	8(2)
C(37)	32(2)	37(2)	36(2)	-6(2)	-13(2)	9(2)
C(28)	38(2)	36(2)	42(2)	-3(2)	-14(2)	4(2)
C(29)	42(2)	38(2)	37(2)	-8(2)	-14(2)	10(2)
C(77)	34(2)	48(2)	39(2)	-14(2)	1(2)	-4(2)
C(5)	44(2)	31(2)	46(2)	-8(2)	-19(2)	3(2)
C(67)	53(2)	34(2)	49(2)	-5(2)	-31(2)	10(2)
C(76)	39(2)	44(2)	38(2)	-12(2)	-5(2)	-2(2)
C(33)	34(2)	46(2)	40(2)	-6(2)	-11(2)	10(2)
C(36)	39(2)	56(2)	35(2)	-2(2)	-15(2)	11(2)
C(3)	55(2)	35(2)	51(2)	-3(2)	-26(2)	2(2)
C(2)	59(3)	32(2)	74(3)	-4(2)	-43(2)	7(2)
C(34)	36(2)	59(3)	43(2)	-6(2)	-13(2)	12(2)
C(81)	45(2)	40(2)	33(2)	-5(2)	-6(2)	-2(2)

C(35)	45(2)	83(3)	43(2)	4(2)	-19(2)	21(2)
C(68)	62(3)	56(3)	78(3)	-15(2)	-45(2)	20(2)
C(1)	91(4)	58(3)	81(3)	-2(2)	-62(3)	4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for MUD0316.

	x	y	z	U(eq)
H(45)	1423	4498	7181	31
H(56)	5347	388	11331	35
H(53)	5135	1966	8405	32
H(59A)	6386	-777	11374	33
H(59B)	6799	62	11537	33
H(60A)	8197	-312	10941	34
H(60B)	7789	-1141	10760	34
H(15)	8186	2059	5054	32
H(63A)	8601	-2791	13220	37
H(63B)	8918	-1938	13427	37
H(10A)	11185	260	6777	38
H(10B)	10843	-592	6575	38
H(13)	10584	1551	3963	37
H(61A)	7830	-970	12479	35
H(61B)	7484	-1813	12274	35
H(25A)	6669	5891	234	38
H(25B)	6294	5051	38	38
H(23)	6771	4693	1424	34
H(20)	9603	3471	1285	39
H(62A)	9268	-1261	11897	37
H(62B)	8920	-2108	11702	37
H(12)	10917	608	5310	39
H(55)	4104	1254	10931	35
H(21)	9060	4364	23	41

H(9A)	10230	-1132	8055	41
H(9B)	10570	-283	8256	41
H(48)	1675	2852	10079	41
H(64A)	10057	-3031	12634	37
H(64B)	10370	-2189	12865	37
H(44A)	-48	4708	6977	37
H(44B)	328	5545	7178	37
H(38A)	-2852	8460	4272	41
H(38B)	-3189	7604	4086	41
H(39A)	-3274	7834	5797	42
H(39B)	-3599	6974	5607	42
H(26A)	6721	5678	-1474	43
H(26B)	7078	6520	-1275	43
H(4A)	13487	-3560	10035	48
H(4B)	13891	-2697	10149	48
H(65A)	10020	-2917	14381	40
H(65B)	9734	-3763	14141	40
H(47)	381	3619	9701	42
H(8A)	12043	-720	7923	41
H(8B)	11692	-1579	7753	41
H(27A)	5268	6032	-929	45
H(27B)	5641	6900	-794	45
H(31A)	3262	8104	-3056	47
H(31B)	3696	8942	-2921	47
H(41A)	-2210	6847	6824	44
H(41B)	-2540	6004	6606	44
H(6A)	12544	-2593	8920	46
H(6B)	12951	-1738	9046	46
H(42A)	-754	6558	6302	44
H(42B)	-1077	5729	6055	44

H(40A)	-1813	7527	5309	43
H(40B)	-2130	6681	5087	43
H(43A)	-1101	5836	7808	43
H(43B)	-1471	5015	7578	43
H(7A)	11510	-1240	9423	46
H(7B)	11113	-2085	9263	46
H(32A)	4165	9434	-4442	47
H(32B)	3718	8601	-4573	47
H(30A)	4678	7611	-3509	45
H(30B)	5103	8439	-3346	45
H(66A)	11479	-3116	13815	44
H(66B)	11195	-3958	13567	44
H(37A)	-4654	7958	4636	43
H(37B)	-4284	8861	4689	43
H(28A)	6062	7419	-2336	48
H(28B)	5624	6573	-2449	48
H(29A)	4229	7060	-1994	47
H(29B)	4654	7889	-1830	47
H(5A)	12056	-3072	10425	48
H(5B)	12456	-2214	10554	48
H(67A)	11169	-3863	15320	54
H(67B)	10858	-4702	15082	54
H(33A)	2752	9954	-4008	49
H(33B)	2318	9135	-4182	49
H(36A)	-4280	8408	3097	54
H(36B)	-3934	9319	3158	54
H(3A)	13027	-4042	11552	57
H(3B)	13413	-3174	11670	57
H(2A)	14473	-4515	11159	66
H(2B)	14862	-3643	11269	66

H(34A)	3259	10488	-5515	72
H(34B)	2214	10389	-5395	72
H(34C)	2834	9665	-5691	72
H(81)	8624	9302	7454	49
H(35A)	-5723	8796	3613	92
H(35B)	-5370	9485	2703	92
H(35C)	-5362	9727	3602	92
H(68A)	12289	-4962	14529	96
H(68B)	12306	-4901	15504	96
H(68C)	12615	-4084	14682	96
H(1A)	14385	-4112	12785	115
H(1B)	15040	-4829	12521	115
H(1C)	14004	-4987	12673	115

Table 6. Torsion angles [°] for MUD0316.

C(49)-C(50)-C(45)-C(46)	0.7(4)
C(80)-C(50)-C(45)-C(46)	179.5(3)
C(10)-O(1)-C(11)-C(12)	5.3(4)
C(10)-O(1)-C(11)-C(16)	-175.4(3)
C(45)-C(50)-C(49)-C(48)	-1.0(4)
C(80)-C(50)-C(49)-C(48)	-179.9(3)
C(45)-C(50)-C(49)-C(51)	178.1(3)
C(80)-C(50)-C(49)-C(51)	-0.7(4)
O(1)-C(11)-C(16)-C(15)	-178.2(3)
C(12)-C(11)-C(16)-C(15)	1.2(4)
O(1)-C(11)-C(16)-C(72)	3.8(4)
C(12)-C(11)-C(16)-C(72)	-176.8(3)
C(55)-C(54)-C(53)-C(58)	-0.6(4)
C(52)-C(54)-C(53)-C(58)	-179.9(3)
C(57)-C(58)-C(53)-C(54)	-0.1(4)
C(69)-C(58)-C(53)-C(54)	-179.9(3)
C(20)-C(19)-C(24)-C(23)	1.7(4)
C(18)-C(19)-C(24)-C(23)	-179.3(3)
C(20)-C(19)-C(24)-C(73)	-176.0(3)
C(18)-C(19)-C(24)-C(73)	3.0(5)
C(57)-O(4)-C(59)-C(60)	-177.9(2)
O(4)-C(59)-C(60)-C(61)	-179.0(2)
C(25)-O(2)-C(22)-C(23)	-0.8(4)
C(25)-O(2)-C(22)-C(21)	179.4(3)
C(11)-C(16)-C(15)-C(14)	-1.1(5)
C(72)-C(16)-C(15)-C(14)	176.9(3)
C(59)-O(4)-C(57)-C(56)	0.6(4)
C(59)-O(4)-C(57)-C(58)	-179.5(3)

C(55)-C(56)-C(57)-O(4)	179.6(3)
C(55)-C(56)-C(57)-C(58)	-0.3(5)
C(53)-C(58)-C(57)-O(4)	-179.3(3)
C(69)-C(58)-C(57)-O(4)	0.4(4)
C(53)-C(58)-C(57)-C(56)	0.6(4)
C(69)-C(58)-C(57)-C(56)	-179.7(3)
C(44)-O(3)-C(46)-C(45)	-0.7(4)
C(44)-O(3)-C(46)-C(47)	179.2(3)
C(50)-C(45)-C(46)-O(3)	179.8(3)
C(50)-C(45)-C(46)-C(47)	-0.1(5)
C(11)-O(1)-C(10)-C(9)	176.1(3)
C(59)-C(60)-C(61)-C(62)	-176.3(3)
C(22)-O(2)-C(25)-C(26)	179.2(3)
C(16)-C(15)-C(14)-C(13)	0.2(5)
C(16)-C(15)-C(14)-C(17)	179.5(3)
C(12)-C(13)-C(14)-C(15)	0.6(5)
C(12)-C(13)-C(14)-C(17)	-178.7(3)
O(2)-C(22)-C(23)-C(24)	179.9(3)
C(21)-C(22)-C(23)-C(24)	-0.3(5)
C(19)-C(24)-C(23)-C(22)	-0.6(4)
C(73)-C(24)-C(23)-C(22)	177.2(3)
C(24)-C(19)-C(20)-C(21)	-1.9(5)
C(18)-C(19)-C(20)-C(21)	179.2(3)
C(60)-C(61)-C(62)-C(63)	179.4(3)
C(64)-C(63)-C(62)-C(61)	-178.2(3)
O(1)-C(11)-C(12)-C(13)	178.9(3)
C(16)-C(11)-C(12)-C(13)	-0.4(5)
C(14)-C(13)-C(12)-C(11)	-0.5(5)
C(53)-C(54)-C(55)-C(56)	0.9(5)
C(52)-C(54)-C(55)-C(56)	-179.8(3)

C(57)-C(56)-C(55)-C(54)	-0.5(5)
C(19)-C(20)-C(21)-C(22)	0.9(5)
O(2)-C(22)-C(21)-C(20)	-180.0(3)
C(23)-C(22)-C(21)-C(20)	0.2(5)
O(1)-C(10)-C(9)-C(8)	-180.0(3)
C(50)-C(49)-C(48)-C(47)	0.8(5)
C(51)-C(49)-C(48)-C(47)	-178.4(3)
C(62)-C(63)-C(64)-C(65)	-178.7(3)
C(46)-O(3)-C(44)-C(43)	-179.1(3)
C(37)-C(38)-C(39)-C(40)	-179.3(3)
O(2)-C(25)-C(26)-C(27)	179.1(3)
C(63)-C(64)-C(65)-C(66)	-178.5(3)
C(49)-C(48)-C(47)-C(46)	-0.2(5)
O(3)-C(46)-C(47)-C(48)	179.9(3)
C(45)-C(46)-C(47)-C(48)	-0.2(5)
C(10)-C(9)-C(8)-C(7)	178.2(3)
C(25)-C(26)-C(27)-C(28)	-176.4(3)
C(40)-C(41)-C(42)-C(43)	-178.3(3)
C(38)-C(39)-C(40)-C(41)	-178.2(3)
C(42)-C(41)-C(40)-C(39)	179.2(3)
O(3)-C(44)-C(43)-C(42)	178.3(3)
C(41)-C(42)-C(43)-C(44)	177.3(3)
C(5)-C(6)-C(7)-C(8)	178.1(3)
C(9)-C(8)-C(7)-C(6)	177.4(3)
C(30)-C(31)-C(32)-C(33)	-179.2(3)
C(32)-C(31)-C(30)-C(29)	-178.4(3)
C(64)-C(65)-C(66)-C(67)	-179.6(3)
C(39)-C(38)-C(37)-C(36)	-172.7(3)
C(26)-C(27)-C(28)-C(29)	-176.1(3)
C(31)-C(30)-C(29)-C(28)	-180.0(3)

C(27)-C(28)-C(29)-C(30)	177.2(3)
C(7)-C(6)-C(5)-C(4)	-179.5(3)
C(3)-C(4)-C(5)-C(6)	179.2(3)
C(65)-C(66)-C(67)-C(68)	178.5(3)
C(31)-C(32)-C(33)-C(34)	177.6(3)
C(38)-C(37)-C(36)-C(35)	178.6(3)
C(5)-C(4)-C(3)-C(2)	-179.0(3)
C(4)-C(3)-C(2)-C(1)	179.5(3)

Symmetry transformations used to generate equivalent atoms:

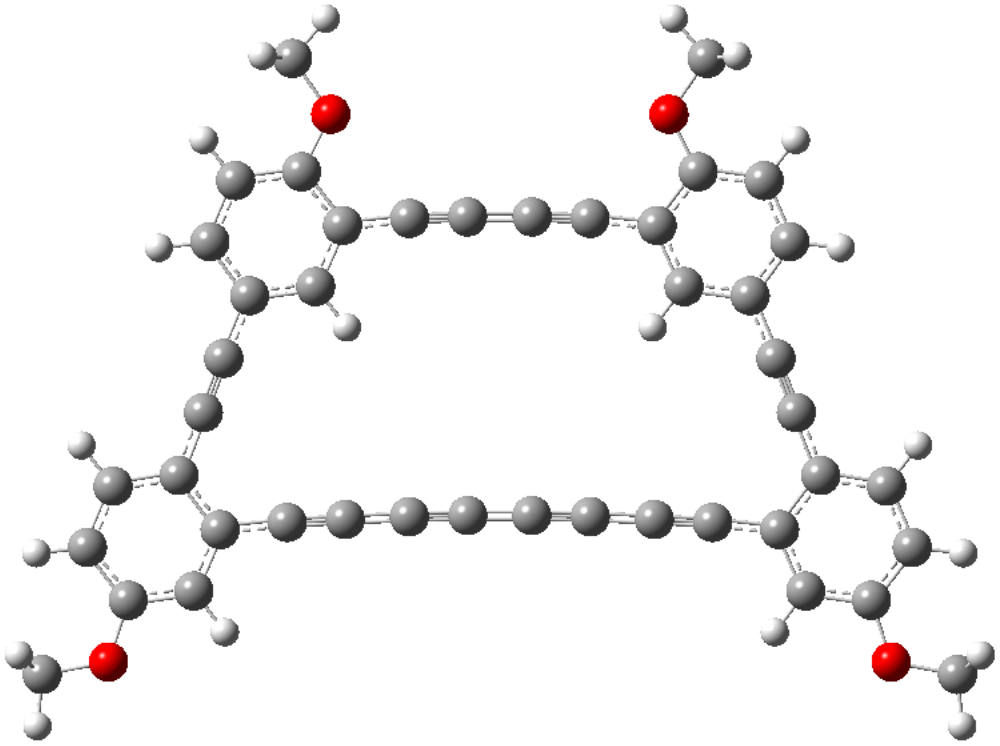


Figure S4. Model of macrocycle **6** optimized in the gas phase at the B3LYP/6-31G** level of theory.

References:

1) M. Desroches, M.-A. Courtemanche, G. Rioux and J.-F. Morin, *J. Org. Chem.*, 2015, **80**, 10634–10642.

2) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision C.01; Gaussian, Inc.: Wallingford CT, 2009.

3) (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652; (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789; (c) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* 1980, **58**, 1200-1211; (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* 1994, **98**, 11623-11627.

4) Chai, J.-D.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* 2008, **10**, 6615–6620.

5) Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* 2005, **105**, 2999-3093.

6) Bruker (2005). APEX 2 Version 2.0.2. Bruker AXS Inc., Madison, Wisconsin, USA.

7) Bruker (2003). SAINT Version 7.07a. Bruker AXS Inc., Madison, Wisconsin, USA.

8) Sheldrick, G.M. (1997). SHELXS-97 and SHELXL-97. Programs for the refinement of crystal structures. University of Gottingen, Germany.