

Supporting Information

for

Novel Macrocycles Embedding *p,p'*-Terphenyl Units: Synthesis, Characterization, Single Crystal X-ray Molecular Structures and Theoretical Investigations

by

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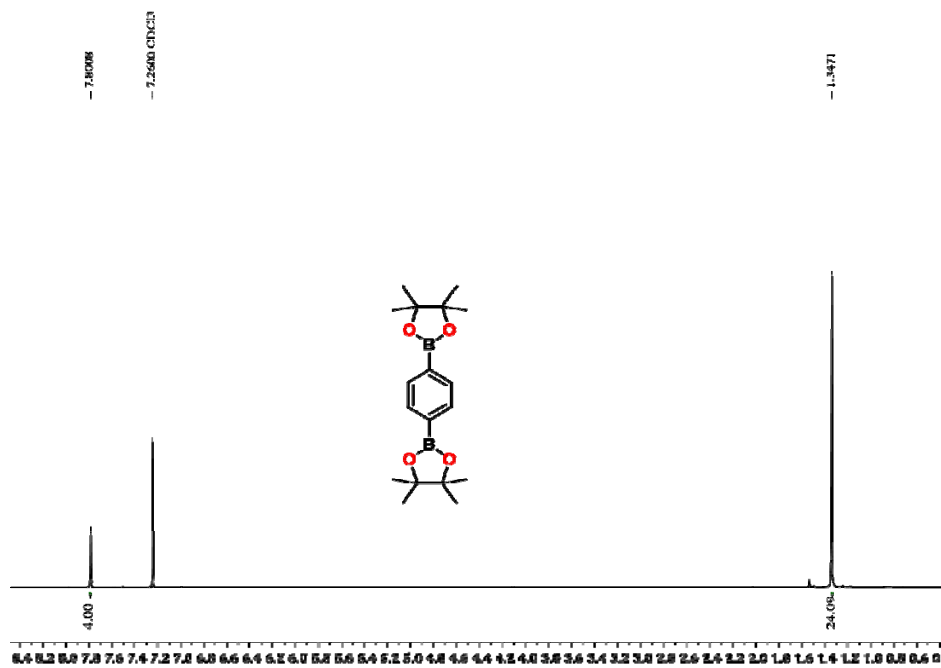
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General experimental data. ¹H and ¹³C NMR spectra were recorded at room temperature (rt) on a Bruker Avance 600 or a Bruker Avance 400 spectrometer. High resolution mass spectra were recorded in positive mode, on a ThermoScientific spectrometer equipped with Orbital Ion Trap mass analyzer using electrospray (ESI) or atmospheric pressure chemical ionization (APCI) techniques. Thin-layer chromatography was performed on Merck 60F 254 silica gel sheets, while Merck silica gel (40-60 µm) was used for preparative column chromatography. All chemicals of commercial grade were used without further purification. The crystals of 1 and 2 were mounted on MiTe GenmicroMountscryo loops and data were collected on a Bruker D8 VENTURE diffractometer using Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) from a I μ S 3.0 microfocus source with multilayer optics, at low temperature (100 K). The structures were refined with anisotropic thermal parameters for non-H atoms. Hydrogen atoms were placed in fixed, idealized positions and refined with a riding model and a mutual isotropic thermal parameter. For structure solving and refinement the Bruker APEX3 Software Packages were used.¹⁷ The drawings were created using the Diamond program¹⁸ Intermolecular contacts were found in Platon¹⁹. CCDC 2119430 and 2119431 contain the supplementary crystallographic data for compounds 1 and 2. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. Theoretical calculations were performed using the high-performance computational facility at Babeş-Bolyai University.....8

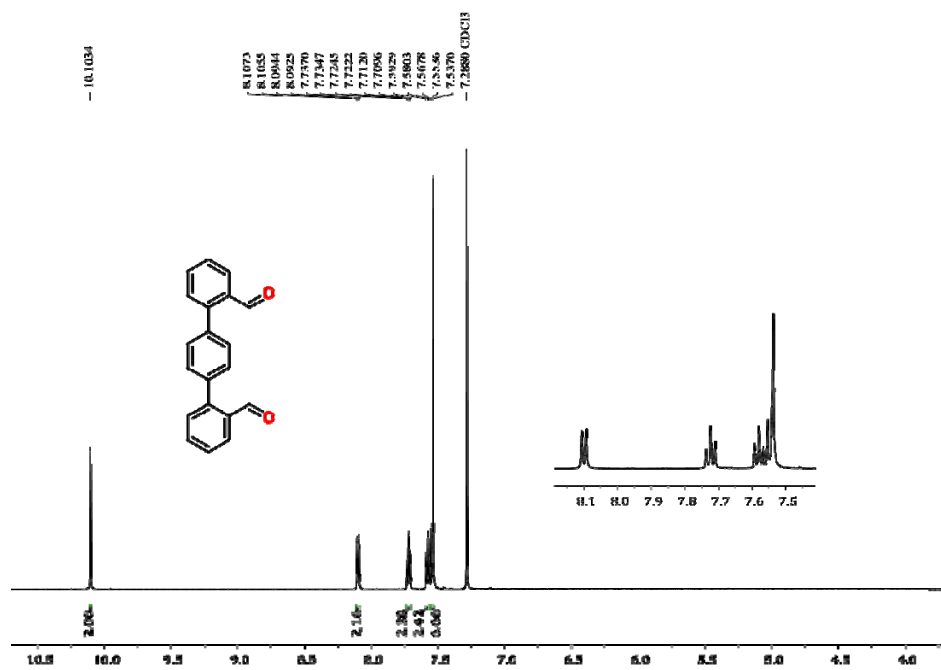
General procedure for the synthesis of macrocycles 1 and 2. A dry solution of dioxime3 (0.80 g, 0.252 mmol) and BuONa (53.3 mg, 0.556 mmol) in anhydrous DMF (6 mL) and anhydrous acetonitrile (50 mL) was stirred at 80°C under argon for one hour. To this mixture, ditosylated diethyleneglycol (135 mg, 0.328 mmol, for macrocycle 1) or 1,3-bis(bromomethyl)benzene (86.78 mg, 0.328 mmol, for macrocycle 2) solved in anhydrous acetonitrile (5 mL) were added dropwise under argon at 80°C during 10 h. The reaction mixture was stirred at reflux for 6 days. The reaction mixture was brought at rt, the solvents were removed in vacuum, the residue was dissolved in CH₂Cl₂ (30 mL) and washed with H₂O (3x25 mL). The organic phase was dried over anhydrous MgSO₄ and the solvent was removed in vacuum. Pure macrocycles 1 and 2 were isolated after column chromatography using silica gel as stationary phase and a mixture of pentane / acetone 8 / 2 as elution system. 9

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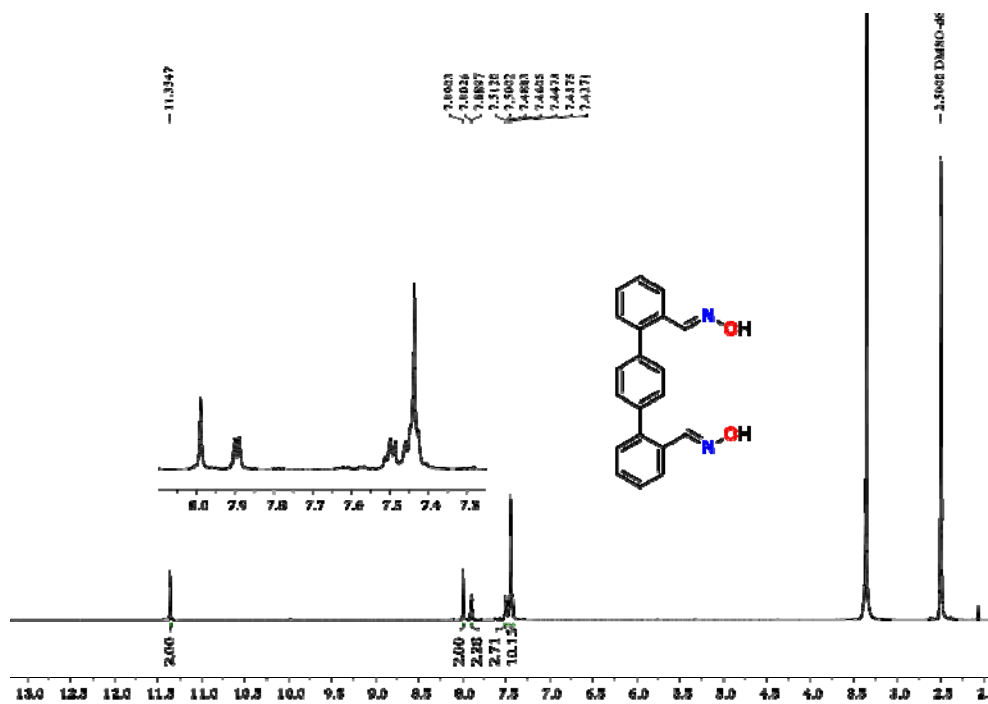
1 COPY OF ^1H AND ^{13}C NMR SPECTRA



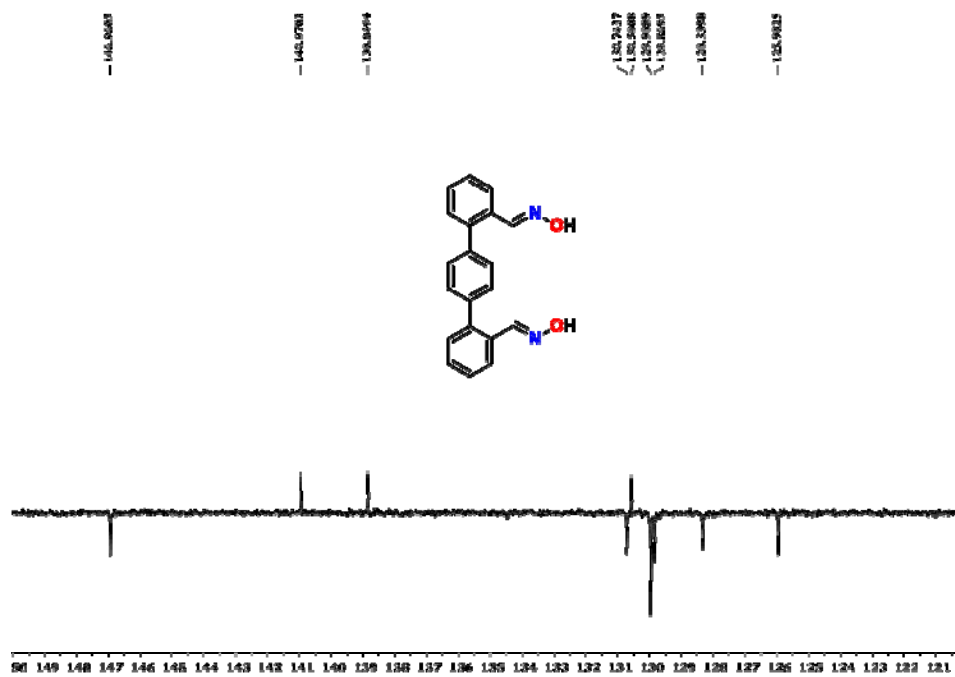
2 FIGURE S1. ^1H -NMR SPECTRUM (400 MHz, CDCl_3) OF 4



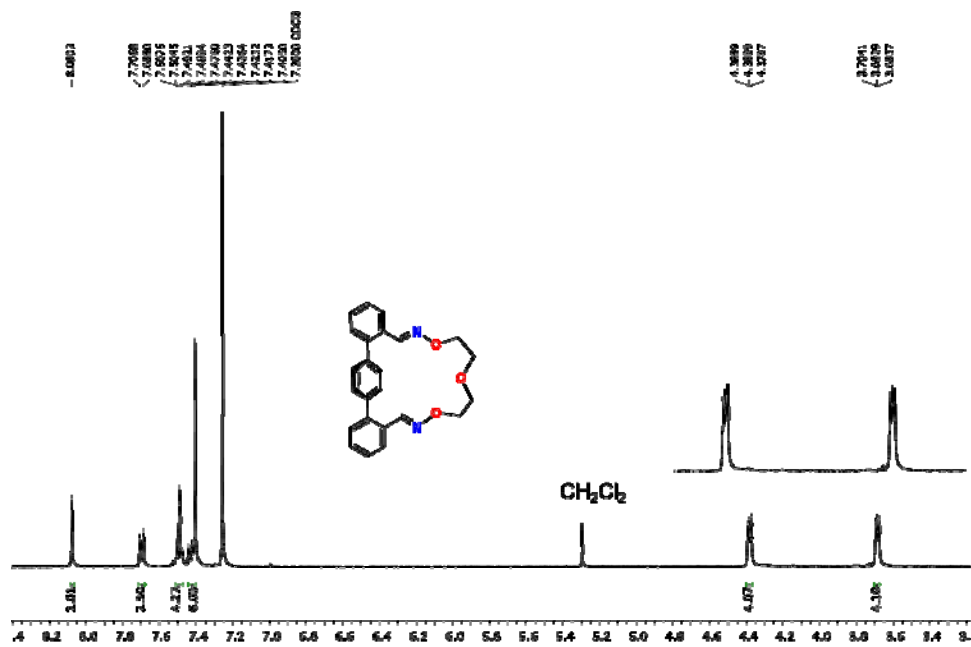
3 FIGURE S2. ^1H -NMR SPECTRUM (600 MHz, CDCl_3) OF 5.



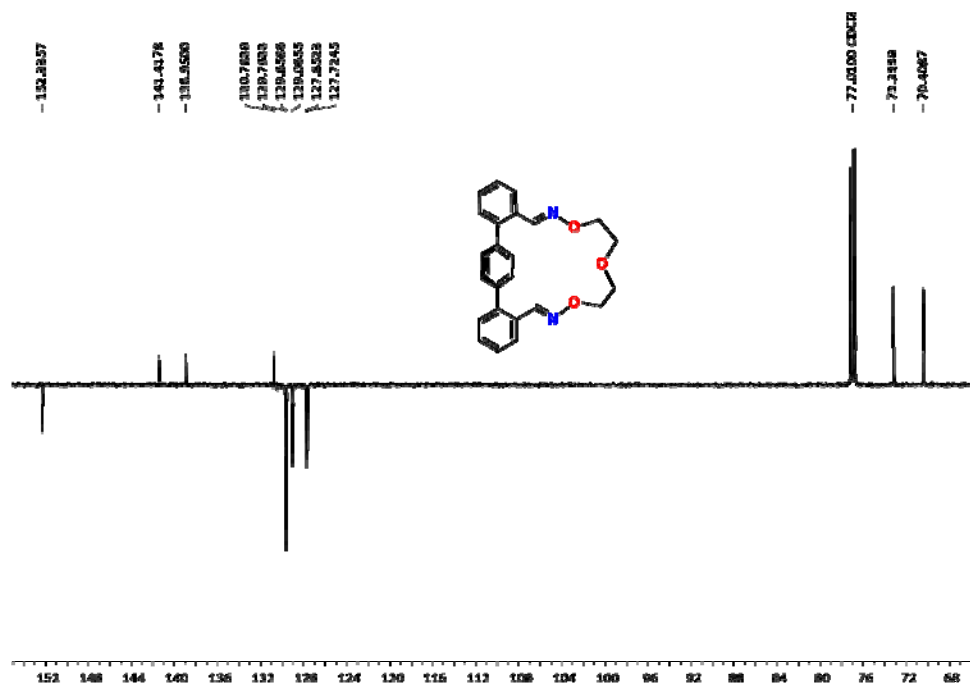
4 FIGURE S3. ^1H -NMR SPECTRUM (600 MHz, $\text{DMSO-}d_6$) OF 3.



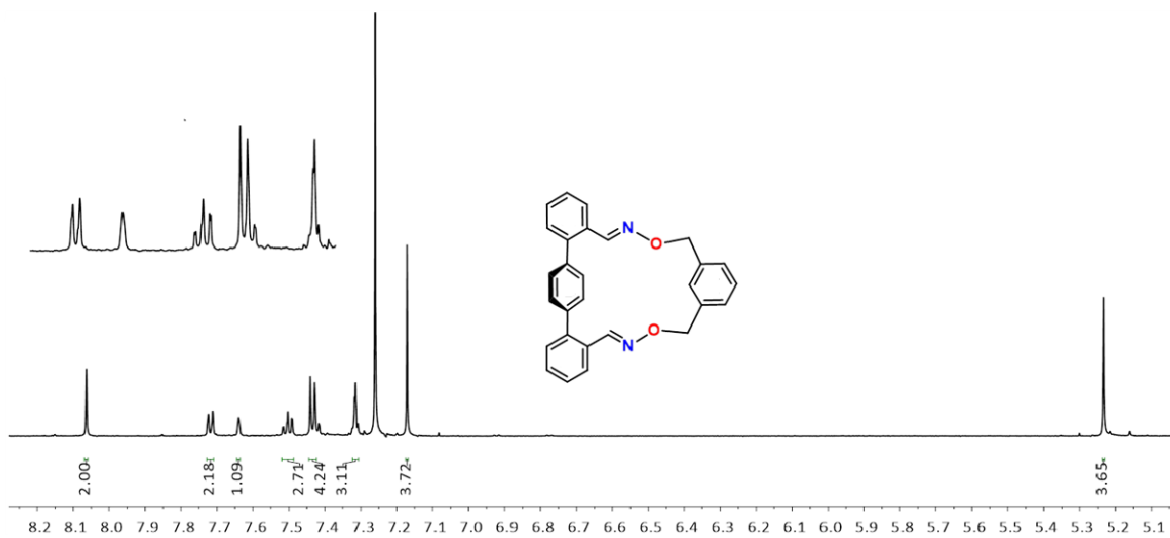
5 FIGURE S4. ^{13}C -APT-NMR SPECTRUM (150 MHz, CDCl_3) OF 3.



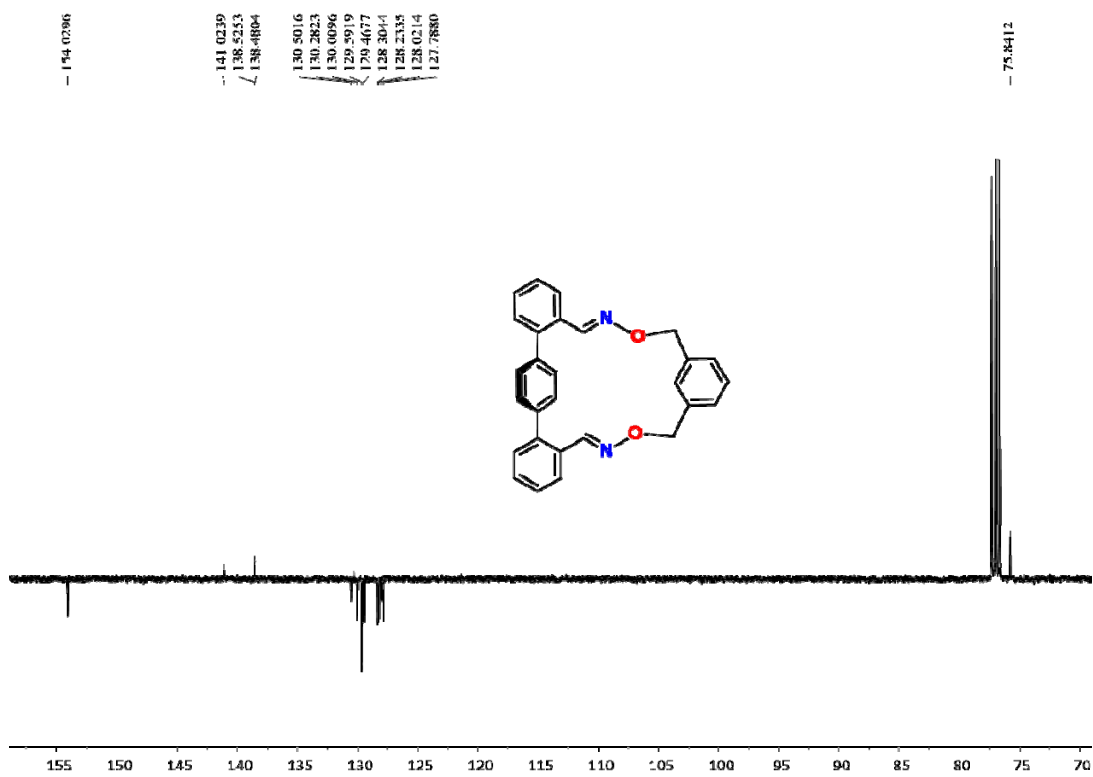
6 FIGURE S5. ¹H-NMR SPECTRUM (400 MHz, CDCl₃) OF **1**



7 FIGURE S6. ¹³C-APT-NMR SPECTRUM (150 MHz, CDCl₃) OF **1**.



8 FIGURE S7. $^1\text{H-NMR}$ SPECTRUM (600 MHz, CDCl_3) OF **2**



9 FIGURE S8. $^{13}\text{C-APT-NMR}$ SPECTRUM (100 MHz, CDCl_3) OF **2**.

10 TABLE 1. CRYSTAL DATA AND STRUCTURE REFINEMENT FOR **1** AND **2**

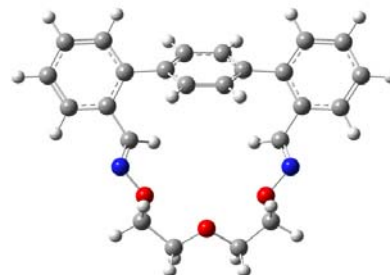
Empirical formula	$C_{24}H_{22}N_2O_3$	$C_{28}H_{22}N_2O_2$
Formula weight	386.43	418.47
Temperature	100(2) K	102(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	P 21/c	P 21/c
Unit cell dimensions	a = 15.6929(6) Å $\alpha = 90^\circ$ b = 9.1656(4) Å $\beta = 103.632(2)^\circ$ c = 14.3146(5) Å $\gamma = 90^\circ$	a = 12.3639(9) Å $\alpha = 90^\circ$ b = 22.7912(15) Å $\beta = 92.201(2)^\circ$ c = 7.5526(6) Å $\gamma = 90^\circ$
Volume	2000.94(14) Å ³	2126.7(3) Å ³
Z	4	4
Density (calculated)	1.283 Mg/m ³	1.307 Mg/m ³
Absorption coefficient	0.085 mm ⁻¹	0.083 mm ⁻¹
F(000)	816	880
Crystal size	0.133 x 0.113 x 0.068 mm ³	0.110 x 0.076 x 0.040 mm ³
Theta range for data collection	2.593 to 28.327°.	2.431 to 28.314°.
Index ranges	-20 ≤ h ≤ 20, -12 ≤ k ≤ 12, -19 ≤ l ≤ 18	-16 ≤ h ≤ 16, -30 ≤ k ≤ 29, -10 ≤ l ≤ 10
Reflections collected	32742	56491
Independent reflections	4978 [R(int) = 0.0707]	5275 [R(int) = 0.1690]
Completeness to theta = 25.242°	100.0 %	99.9 %
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	4978 / 0 / 262	5275 / 0 / 292
Goodness-of-fit on F ²	1.046	1.095
Final R indices [I > 2σ(I)]	R1 = 0.0510, wR2 = 0.0980	R1 = 0.0654, wR2 = 0.0964
R indices (all data)	R1 = 0.0891, wR2 = 0.1161	R1 = 0.1565, wR2 = 0.1230
Largest diff. peak and hole	0.319 and -0.238 e.Å ⁻³	0.252 and -0.293 e.Å ⁻³

12 DFT COORDINATES

1-C1

H (298 K, 1 atm) = -1262.360874 a.u.

O	-2.19616800	2.56118300	-0.45591700
O	2.19547300	2.56179900	-0.45598400
O	-0.00054800	4.08987500	0.42093100
N	-3.08367100	1.60107800	-0.01131500
N	3.08325700	1.60194800	-0.01139800
C	-2.73645000	0.45623300	-0.43220300
H	-1.82176200	0.35662500	-1.01416100
C	-3.53061300	-0.74910800	-0.14576400
C	-4.92164900	-0.68437200	-0.10039400
H	-5.39963300	0.27676400	-0.23735500
C	-5.67445400	-1.83085500	0.08999000
H	-6.75430000	-1.76901200	0.12114000
C	-5.04121600	-3.06007400	0.22207400
H	-5.62506800	-3.96051800	0.36198100
C	-3.65761600	-3.13326100	0.18655300
H	-3.15901500	-4.08537600	0.32171500
C	-2.88562900	-1.98646400	0.01786800
C	-1.40551100	-2.06369200	0.05823300
C	-0.69064200	-1.21778400	0.90718400
H	-1.22805600	-0.54723700	1.56616500
C	0.69107100	-1.21759000	0.90716800
H	1.22831200	-0.54689200	1.56613600
C	1.40615800	-2.06329800	0.05820100
C	0.69463400	-2.94985400	-0.74741300
H	1.23391500	-3.61347000	-1.41263900
C	-0.69375600	-2.95004700	-0.74739800
H	-1.23286600	-3.61381500	-1.41261200
C	2.88625300	-1.98564800	0.01780400
C	3.53087700	-0.74810800	-0.14585100
C	4.92189400	-0.68296900	-0.10050400
H	5.39959900	0.27830300	-0.23748200

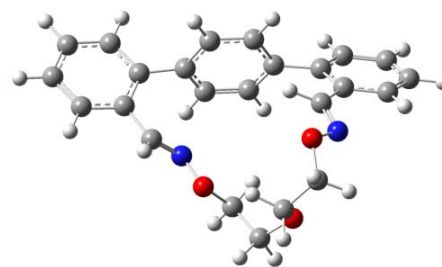


C	5.67503500	-1.82923200	0.08988000
H	6.75486300	-1.76707600	0.12101400
C	5.04215400	-3.05863300	0.22198600
H	5.62626800	-3.95890600	0.36189600
C	3.65857500	-3.13222100	0.18648800
H	3.16025000	-4.08447800	0.32166800
C	2.73636300	0.45700300	-0.43228400
H	1.82169700	0.35713200	-1.01423300
C	2.33781100	3.76036100	0.28177600
H	3.28848700	4.24463000	0.03908900
H	2.30727100	3.54461400	1.35204800
C	1.17879500	4.64584100	-0.10110400
H	1.34412100	5.65732800	0.29336300
H	1.11921700	4.71029200	-1.19484100
C	-1.18006900	4.64551100	-0.10105600
H	-1.12054900	4.70998700	-1.19479500
H	-1.34566700	5.65694800	0.29342500
C	-2.33881900	3.75969800	0.28185900
H	-2.30817700	3.54395100	1.35212800
H	-3.28964200	4.24369900	0.03921400

1-C2

H (298 K, 1 atm) = -1262.351092 a.u.

O	-1.53528900	2.22525500	0.30529400
O	1.99087500	2.25158400	-2.00793400
O	1.11174900	3.71397600	0.36030100
N	-2.07296000	0.96471500	0.42901700
N	2.84710300	1.63056100	-1.11605100
C	-2.96111800	0.72024100	-0.44012800
H	-3.25534700	1.48859900	-1.15588000
C	-3.66718600	-0.57583800	-0.47364000
C	-5.01723000	-0.54899200	-0.82443900
H	-5.47865400	0.40366900	-1.05681100
C	-5.77255100	-1.70872600	-0.86766700



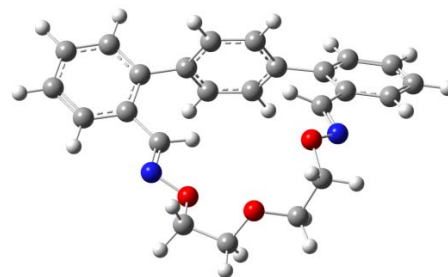
H	-6.82091900	-1.66277800	-1.13119800
C	-5.17348700	-2.92509100	-0.57722500
H	-5.75004300	-3.84024100	-0.61198200
C	-3.82422400	-2.96877300	-0.25756900
H	-3.34494300	-3.91853200	-0.05483100
C	-3.05443200	-1.81072000	-0.19978900
C	-1.59101300	-1.91641700	0.05611800
C	-1.04569100	-1.68833400	1.31369500
H	-1.70238600	-1.47465800	2.14688500
C	0.32875100	-1.64387400	1.48530900
H	0.74569700	-1.40621300	2.45666000
C	1.18741400	-1.82347600	0.40304100
C	0.63934300	-2.15172300	-0.83386600
H	1.29621900	-2.32994100	-1.67707100
C	-0.73557000	-2.19630200	-1.00536400
H	-1.15283500	-2.40736600	-1.98259400
C	2.64434000	-1.57454000	0.56626600
C	3.25560200	-0.47160300	-0.05409200
C	4.61190700	-0.22721900	0.16590700
H	5.06763500	0.62450600	-0.32144400
C	5.35545800	-1.05212400	0.99056500
H	6.40723800	-0.85194500	1.14783200
C	4.75057500	-2.13800900	1.61137600
H	5.32779000	-2.78925900	2.25487700
C	3.40434500	-2.39002700	1.40107000
H	2.92506900	-3.23344800	1.88292100
C	2.46743500	0.43929200	-0.89994500
H	1.53342500	0.09946800	-1.33613000
C	1.98279400	3.65676800	-1.83957200
H	1.86895600	4.08643800	-2.83650000
H	2.93182300	3.97702700	-1.40640300
C	0.82619100	4.08669700	-0.96787400
H	0.69700300	5.17592900	-1.03787900
H	-0.09049100	3.60234900	-1.31942000

C	0.02516300	3.78505400	1.25095800
H	-0.68870800	4.55841500	0.94323300
H	0.43161500	4.07116900	2.22335100
C	-0.68416300	2.46150500	1.42232800
H	0.04895000	1.65450900	1.49520400
H	-1.29042500	2.47926000	2.33337700

1-C3

H (298 K, 1 atm) = -1262.355595 a.u.

O	-1.87989900	2.29926500	0.86781500
O	1.99021100	2.50803400	-1.43432000
O	0.01599000	4.12748700	-0.14390400
N	-2.93956800	1.50775700	0.47879100
N	2.88276500	1.68926300	-0.77571600
C	-2.56252000	0.29692400	0.42014700
H	-1.52118800	0.07050100	0.63227000
C	-3.46897600	-0.80041500	0.05611400
C	-4.84815600	-0.60436500	-0.02177900
H	-5.24661500	0.37398600	0.21313700
C	-5.68549700	-1.64024800	-0.39431900
H	-6.75384800	-1.47702700	-0.44930300
C	-5.15510500	-2.88915600	-0.69614600
H	-5.80818100	-3.70160100	-0.98713500
C	-3.78627000	-3.09576500	-0.62152400
H	-3.36580900	-4.06580600	-0.85603400
C	-2.93297900	-2.06504000	-0.24154200
C	-1.45744500	-2.25817200	-0.18748100
C	-0.69778800	-2.17686200	-1.35112200
H	-1.19955200	-2.11098800	-2.30877100
C	0.68571400	-2.10593800	-1.28651000
H	1.26363000	-2.00227000	-2.19726000
C	1.34066300	-2.10611800	-0.05712700
C	0.58435400	-2.29277400	1.09803100
H	1.08386800	-2.31903400	2.05885300

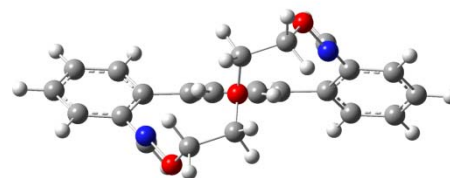


C	-0.79840800	-2.36937500	1.03358200
H	-1.37928200	-2.44844000	1.94472600
C	2.80071600	-1.84792900	0.05611500
C	3.35173900	-0.60365900	-0.29535600
C	4.71928500	-0.38760500	-0.11352200
H	5.13019100	0.57249300	-0.39587500
C	5.53125800	-1.37450000	0.41462700
H	6.58977100	-1.19066800	0.54388800
C	4.98593600	-2.60151100	0.77097300
H	5.61549200	-3.38087200	1.18022600
C	3.63099900	-2.82870600	0.59471600
H	3.19817700	-3.78264900	0.87018300
C	2.50644000	0.47732900	-0.82984100
H	1.54657600	0.24571900	-1.28143700
C	2.17557100	3.86182800	-1.06617700
H	3.23818700	4.05430600	-0.90590600
H	1.81737100	4.44669100	-1.91376200
C	1.38228900	4.22389600	0.16799000
H	1.64406400	5.24507200	0.47976800
H	1.63815200	3.53855000	0.98647400
C	-0.84835400	4.38992900	0.93336700
H	-0.41646400	4.02350400	1.87249000
H	-1.02451700	5.46810500	1.03503000
C	-2.15386500	3.67426100	0.68733000
H	-2.49902300	3.85762200	-0.33249700
H	-2.91929300	4.00578700	1.39544700

1-C4

H (298 K, 1 atm) = -1262.345259 a.u.

C	0.48034500	0.50964400	0.74386500
C	1.34750900	-0.41272800	3.24516500
C	0.42519400	-0.86238300	1.06071700
C	0.95608000	1.39343800	1.71062100
C	1.37997600	0.94242500	2.95111600
C	0.86989800	-1.30809200	2.30012100
H	1.02848300	2.44637500	1.46815400
H	1.75173100	1.64902400	3.68175600
H	0.82263900	-2.36705500	2.51871400
H	1.68843900	-0.77180300	4.20719500
C	0.11765900	0.99697900	-0.60871700
C	-0.53526200	1.83657600	-3.23237400
C	-0.50903600	2.22559600	-0.83763600
C	0.42249200	0.21500100	-1.71972500
C	0.05372400	0.59826100	-2.99037300
C	-0.80744000	2.64789900	-2.12657600
H	-0.76880300	2.86013000	0.00118900
H	0.96028400	-0.71250200	-1.61793300
H	0.23313200	-0.10108300	-3.78944700
H	-1.25759900	3.62227000	-2.27373100
C	-0.86168300	2.22732400	-4.62510300
C	-1.59663800	2.81481100	-7.26627700
C	-2.03495800	2.92463900	-4.90707100
C	-0.03875900	1.84023900	-5.70158000
C	-0.42094600	2.12684600	-7.00710400
C	-2.39907800	3.22279300	-6.21103200
H	-2.68900300	3.20260000	-4.09001100
H	0.22491000	1.81434600	-7.81741300
H	-3.31921900	3.75931400	-6.40287300
H	-1.88170000	3.03398200	-8.28674900
C	1.25415000	1.16775100	-5.44507600

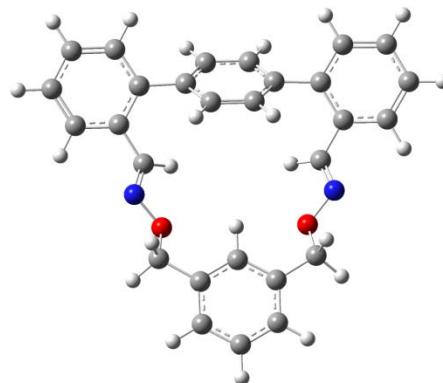


H	1.96821400	1.64082300	-4.77137000
C	-0.14827700	-1.82574200	0.09458200
H	-1.14935300	-1.64476500	-0.29622400
N	1.50276300	0.02184900	-5.92289800
N	0.53349700	-2.79730800	-0.34636000
O	-0.21040400	-3.54477700	-1.25471600
O	2.76575700	-0.40994800	-5.52782600
C	2.82481200	-1.82150700	-5.41152300
H	3.80935600	-2.11722100	-5.78169800
C	0.61334800	-4.14859300	-2.23787700
H	1.62813100	-4.25191400	-1.84723300
H	0.19451300	-5.14136200	-2.41928800
C	0.60000000	-3.36244900	-3.54195600
H	-0.42938300	-3.07375300	-3.76393600
H	0.95271400	-4.00595800	-4.35693600
C	2.68682800	-2.27208100	-3.96363900
H	3.30825200	-1.62835200	-3.33768600
H	3.05996600	-3.29868600	-3.86609600
O	1.36331200	-2.17567600	-3.47989100
H	2.05341000	-2.26999200	-6.04154700

2-C1

H (298 K, 1 atm) = -1339.550532 a.u.

O	2.20506500	17.61631700	1.22394500
O	5.52157200	20.74110900	2.10889100
N	2.09535700	16.31994400	1.68991200
N	6.64486700	20.60506800	2.90236400
C	8.47860000	19.11941300	3.31365300
C	9.43501100	20.07764000	3.64286200
H	9.22227200	21.11643100	3.42685500
C	10.64129500	19.70325300	4.20999100
H	11.37765600	20.45576400	4.45956300
C	10.90908300	18.35999100	4.44047100
H	11.85341200	18.06036300	4.87595900



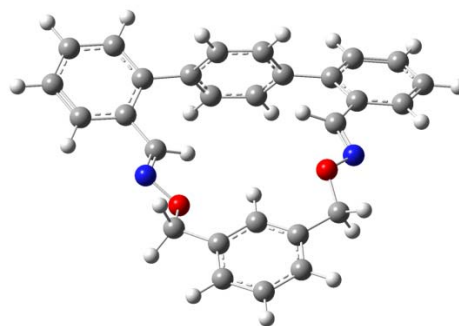
C	9.96028700	17.40075200	4.12388300
H	10.15277500	16.35567400	4.33380800
C	8.73329300	17.76231800	3.57215300
C	7.69897400	16.73097300	3.31506800
C	7.98357000	15.57186400	2.59561800
H	8.98357000	15.41956200	2.20771600
C	6.99144300	14.63774500	2.33189300
H	7.22145000	13.76057800	1.73917200
C	5.68696400	14.83643300	2.78022600
C	5.41416800	15.97621400	3.53832000
H	4.41520200	16.12836400	3.92828700
C	6.40232100	16.90662900	3.80095100
H	6.17187600	17.78220800	4.39540700
C	4.60259200	13.87221300	2.47356000
C	4.77399200	12.51647200	2.74421100
H	5.71811100	12.17932600	3.15440800
C	3.74476500	11.61261400	2.53364700
H	3.89431600	10.56434900	2.75717900
C	2.52100800	12.05538500	2.04822900
H	1.71350700	11.35366000	1.88605500
C	2.34104600	13.39636800	1.75444700
H	1.40514300	13.75386700	1.34546800
C	3.37289700	14.31082700	1.95506300
C	3.20511000	15.71878800	1.56385500
H	4.06344000	16.25781000	1.16569700
C	1.09585100	18.40880800	1.61227800
H	0.75830400	18.08303600	2.59940700
H	0.27046300	18.27763100	0.90656200
C	1.54509100	19.84675700	1.65232800
C	0.67516900	20.87581600	1.31152000
H	-0.32990400	20.64478800	0.97842200
C	1.09743500	22.19599800	1.38063600
H	0.41936900	22.99366800	1.10619900
C	2.39486000	22.49576100	1.77159600

H	2.72910500	23.52635200	1.79688800
C	3.27317000	21.47462900	2.11464200
C	2.83682800	20.15690600	2.05859700
H	3.52370300	19.35847700	2.30317200
C	4.67646700	21.78127800	2.57054200
H	5.01237100	22.74543900	2.17800100
H	4.72727000	21.81854400	3.66166300
C	7.23366100	19.51349800	2.63648900
H	6.80447200	18.84073100	1.89556700

2-C2

H (298 K, 1 atm) = -1339.545555 a.u.

C	-2.85912300	-2.44770500	-0.17697600
C	-3.50607400	-1.24387500	0.14826900
C	-4.89585700	-1.16237800	0.04954800
C	-5.64039300	-2.24875100	-0.37201700
C	-5.00215900	-3.43690700	-0.70582500
C	-3.62306400	-3.52887300	-0.61113200
H	-5.37719100	-0.22827500	0.30730100
H	-6.71763700	-2.17188300	-0.43888900
H	-5.57850600	-4.29180500	-1.03471400
H	-3.11961700	-4.45267000	-0.86856900
C	-1.37657900	-2.57191400	-0.12913800
C	-0.67668300	-2.49165400	1.07308200
C	-0.65357100	-2.73700700	-1.30814700
C	0.70951000	-2.50777800	1.08836700
H	-1.22559400	-2.39000000	2.00193100
C	0.73410500	-2.75836600	-1.29312000
H	-1.18552100	-2.81221700	-2.24876600
C	1.43187100	-2.61411400	-0.09781600
H	1.24233400	-2.40967900	2.02625800
H	1.28405300	-2.85073900	-2.22197800
C	2.91767200	-2.49618600	-0.07856900
C	3.52945600	-1.24814600	-0.27179300

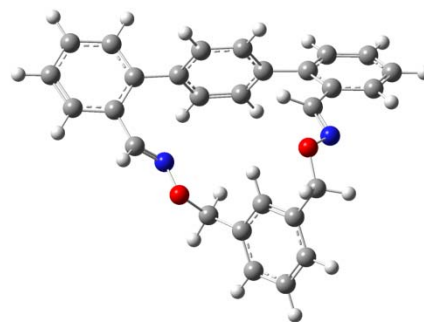


C	3.71121700	-3.60977200	0.17921900
C	4.91905300	-1.14477200	-0.20532700
C	5.09166100	-3.49707700	0.24252500
H	3.23354800	-4.56928600	0.33383700
C	5.69564000	-2.26040200	0.05173400
H	5.37461700	-0.17605000	-0.36315100
H	5.69568900	-4.37325300	0.43927500
H	6.77288800	-2.16896700	0.09768900
C	-2.72301200	-0.06419700	0.54275800
H	-1.71179600	-0.19175200	0.91878400
C	2.69656200	-0.06641700	-0.53436500
H	1.68629400	-0.20623800	-0.91336100
N	3.11706700	1.11003000	-0.30960000
N	-3.18725500	1.11143100	0.42110900
O	2.15102400	2.03110900	-0.65806500
O	-2.26287100	2.02975900	0.87771500
C	2.44695300	3.32144600	-0.15584300
H	3.13852700	3.83931600	-0.82737200
H	2.92902600	3.21976000	0.81978500
C	1.15370600	4.08531100	-0.02377500
C	-0.04775200	3.40573000	0.13289000
C	1.15487500	5.47526000	-0.01237800
C	-1.24154100	4.09368000	0.30977400
H	-0.05356000	2.32685800	0.11726600
C	-0.03235000	6.16944000	0.17376700
H	2.08430600	6.01694500	-0.14540600
C	-1.22722400	5.48328800	0.33954700
H	-0.02633700	7.25167400	0.18974200
H	-2.15054700	6.03115700	0.48893300
C	-2.54360600	3.34026700	0.42054700
H	-3.02921900	3.27797400	-0.55624500
H	-3.22657400	3.84347200	1.11175100

2-C3

H (298 K, 1 atm) = -1339.545291 a.u.

C	-0.33589100	-0.84745500	1.07073200
C	-0.40469800	-0.35446500	3.83308000
C	0.47102600	0.13531300	1.63425600
C	-1.21210000	-1.54667900	1.89636800
C	-1.24337000	-1.30755900	3.26251600
C	0.43330800	0.38143400	2.99731400
H	1.15522400	0.68604800	1.00299600
H	-1.86132800	-2.29869900	1.46440000
H	1.08269200	1.13295300	3.43002600
C	-0.37236300	-0.12149000	5.30208400
C	-0.23901300	0.41532600	8.04262400
C	0.12860100	-1.08770800	6.18792600
C	-0.78637300	1.10801300	5.80948100
C	-0.72665400	1.37735100	7.16748000
C	0.18654300	-0.80662100	7.55335000
H	-1.16360200	1.85459300	5.12147000
H	-1.06379200	2.33494400	7.54259800
H	0.57432300	-1.56514800	8.22020700
H	-0.19345000	0.61758900	9.10463200
C	-0.30605300	-1.15461500	-0.38677500
C	-0.46446800	-1.79960500	-3.11072500
C	-1.37742100	-0.72819500	-1.16971800
C	0.70668900	-1.91821200	-0.99051700
C	0.59782500	-2.24456900	-2.34361200
C	-1.45790700	-1.03336800	-2.51948600
H	-2.16071100	-0.14749600	-0.69827600
H	1.37001200	-2.85576400	-2.79581300
H	-2.29915500	-0.68302200	-3.10314400
H	-0.51991200	-2.05558500	-4.16048800
C	1.87417300	-2.46308000	-0.27383600
H	2.23896500	-3.44938400	-0.56134300
N	2.47461700	-1.80544400	0.62735500
O	3.50851300	-2.51863700	1.18638500

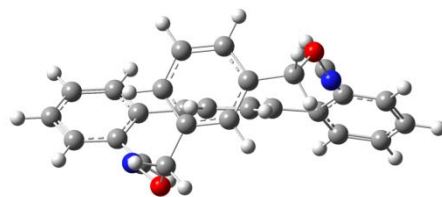


C	0.63536000	-2.37322000	5.68174900
H	0.24611200	-2.78385100	4.75368100
N	1.54324900	-2.99862300	6.30899300
O	1.81789200	-4.21338900	5.69875600
C	4.27290800	-1.68759600	2.05518500
H	3.63549100	-0.85930100	2.37173900
H	5.12856800	-1.28150400	1.50903000
C	3.14593900	-4.59923000	5.98359500
H	3.34624700	-4.46123000	7.04909700
H	3.18417600	-5.66604900	5.75501000
C	4.16357100	-3.85139200	5.15551800
C	6.06455400	-2.52372500	3.61295700
C	3.78480300	-3.15815400	4.01690800
C	5.50709700	-3.87083500	5.52383800
C	6.45335500	-3.21607300	4.75429500
C	4.72810300	-2.48531800	3.24459900
H	2.74256200	-3.13505500	3.72244300
H	5.81020700	-4.40055800	6.42009300
H	6.80381600	-2.00863000	3.01119800
H	7.49616300	-3.23976900	5.04308700
H	-1.91938100	-1.87089900	3.89503800

2-C4

H (298 K, 1 atm) = -1339.544435 a.u.

C	0.66267300	1.44724200	4.26852400
C	1.44561800	0.84213200	6.89812000
C	0.91061200	0.11891600	4.65550100
C	0.81239500	2.44819100	5.23045000
C	1.19026500	2.15472500	6.53019700
C	1.30799000	-0.16638400	5.95881500
H	0.66810300	3.48074200	4.94032000
H	1.30242700	2.95488600	7.25020900
H	1.49850300	-1.19761700	6.22550700
H	1.75216800	0.60462700	7.90811500



C	0.33594400	1.82649000	2.87161200
C	-0.10489900	2.69057600	0.21116400
C	-0.47650600	2.93006200	2.59278500
C	0.88445800	1.14310300	1.78627100
C	0.63888000	1.54340200	0.48598300
C	-0.67742500	3.36353100	1.29303700
H	-0.94645900	3.46774900	3.40656600
H	1.54791500	0.30552600	1.93886500
H	1.05262200	0.94965600	-0.31828600
H	-1.26788500	4.25410700	1.11525700
C	-0.26119600	3.18967000	-1.17677400
C	-0.61207200	4.06870900	-3.81503000
C	-1.48967200	3.68620400	-1.61140800
C	0.80641300	3.15200600	-2.09241300
C	0.61771000	3.58299700	-3.40201700
C	-1.66654700	4.12447200	-2.91384500
H	-2.32488100	3.69629100	-0.92217800
H	1.45490600	3.54140300	-4.08650000
H	-2.63187900	4.49899600	-3.22870100
H	-0.74658700	4.40540100	-4.83445600
C	2.12069100	2.64164700	-1.65985300
H	2.52591100	2.94881700	-0.69739500
C	0.74784400	-1.00764700	3.71230900
H	-0.19411300	-1.14902000	3.18255400
N	2.72363200	1.77016300	-2.35201500
N	1.72603600	-1.78438300	3.50666200
O	1.38277100	-2.83137600	2.65319200
O	3.89207200	1.35185900	-1.72320600
C	2.43430100	-3.04932800	1.72290700
H	3.38675400	-2.78613600	2.18582500
H	2.42402300	-4.12180200	1.51867700
C	2.21689400	-2.28753000	0.43514700
C	1.80298200	-1.06929900	-2.03730300
C	0.99216000	-2.41140100	-0.21692000

C	3.21578100	-1.51467300	-0.14848000
C	3.02180500	-0.90186300	-1.38691600
C	0.78608400	-1.80657800	-1.44592300
H	0.20623600	-2.99724800	0.24444900
H	4.16542400	-1.39422100	0.36350900
H	-0.16463300	-1.91703800	-1.95135300
H	1.64778700	-0.59822900	-2.99961300
C	4.08691700	-0.03092200	-2.01029700
H	4.10328900	-0.16703000	-3.09437800
H	5.06998200	-0.25950800	-1.60088100