The Journal of Organic Chemistry

JOC Article

Supramolecular Catalysis at Work. Diastereoselective Synthesis of a Molecular Bowl with Dynamic Inner Space

Zhiqing Yan, Troy McCracken, Shijing Xia, Veselin Maslak, Judith Gallucci, Christopher M. Hadad, and Jovica D. Badjić*

Department of Chemistry, The Ohio State University, 100 W. 18th Avenue, Columbus, OH 43210

badjic@chemistry.ohio-state.edu

Supporting Information

Table of Contents

General: All chemicals were purchased from commercial sources, and used as received unless stated otherwise. All solvents were dried prior to use according to standard literature protocols. Chromatography purifications were performed with silica gel 60 (40-75 μm, 200 x 400 mesh). Thin-layer chromatography (TLC) was performed with silica-gel plates w/UV254 (200 μm). Chromatograms were visualized by UV-light, and if needed by staining with 20% phosphomolybdic acid in ethanol. ^{1}H and ^{13}C NMR spectra were recorded on 500 MHz and 125 MHz NMR spectrometer, unless stated otherwise. The spectra were referenced using the solvent residual signal as internal standard. The chemical shift values are expressed as δ values and the coupling constants values (J) are in Hertz (Hz). The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; t, triplet; m, multiplet; and br, broad. MALDI-TOF mass spectra were measured with 2,5-Dihydroxybenzoic acid as matrix. The calorimetric experiments were performed using a commercial isothermal titration calorimeter. The heat of reaction was corrected for the heat of dilution of the guest solution, determined in separate experiments. Computer simulations (curve fitting) were performed with software adapted for ITC data analysis.

Figure S1. ^{1}H NMR spectrum of **1**$_{syn}$ in $CDCl_3$, at 298 K (400 MHz).

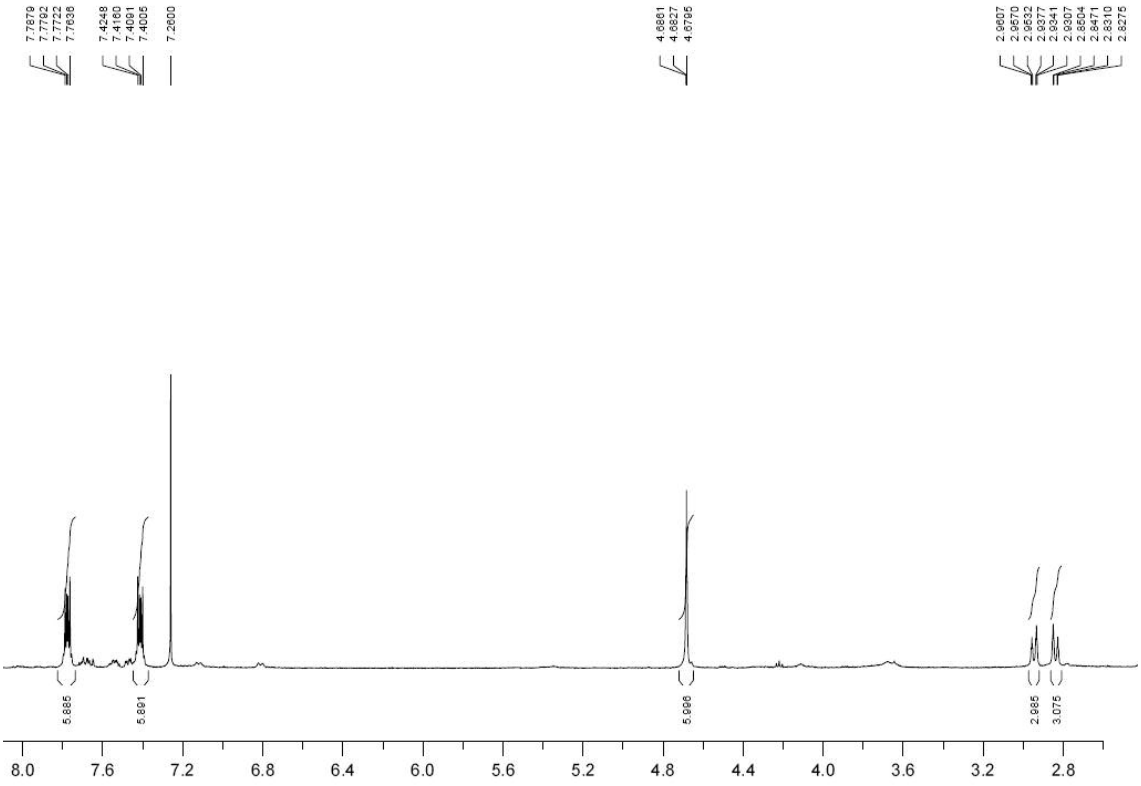


Figure S2. ^{13}C NMR spectrum of **1**$_{syn}$ in $CDCl_3$, at 298 K (100 MHz).

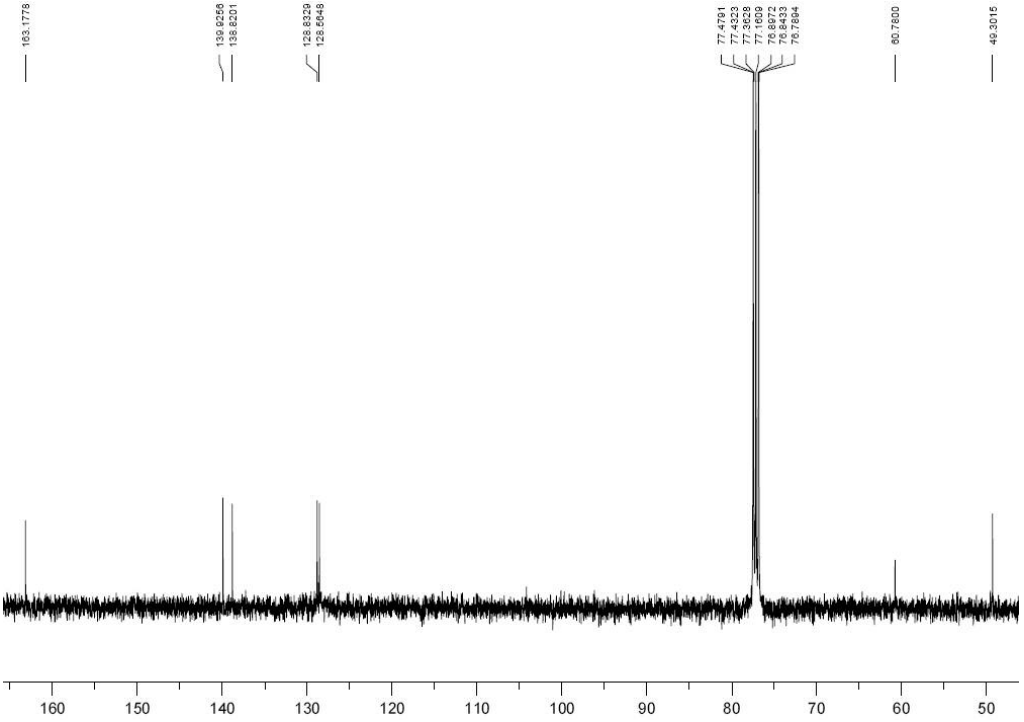


Figure S3. ^{1}H NMR spectrum of **1**$_{anti}$ in $CDCl_3$, at 298 K (400 MHz).

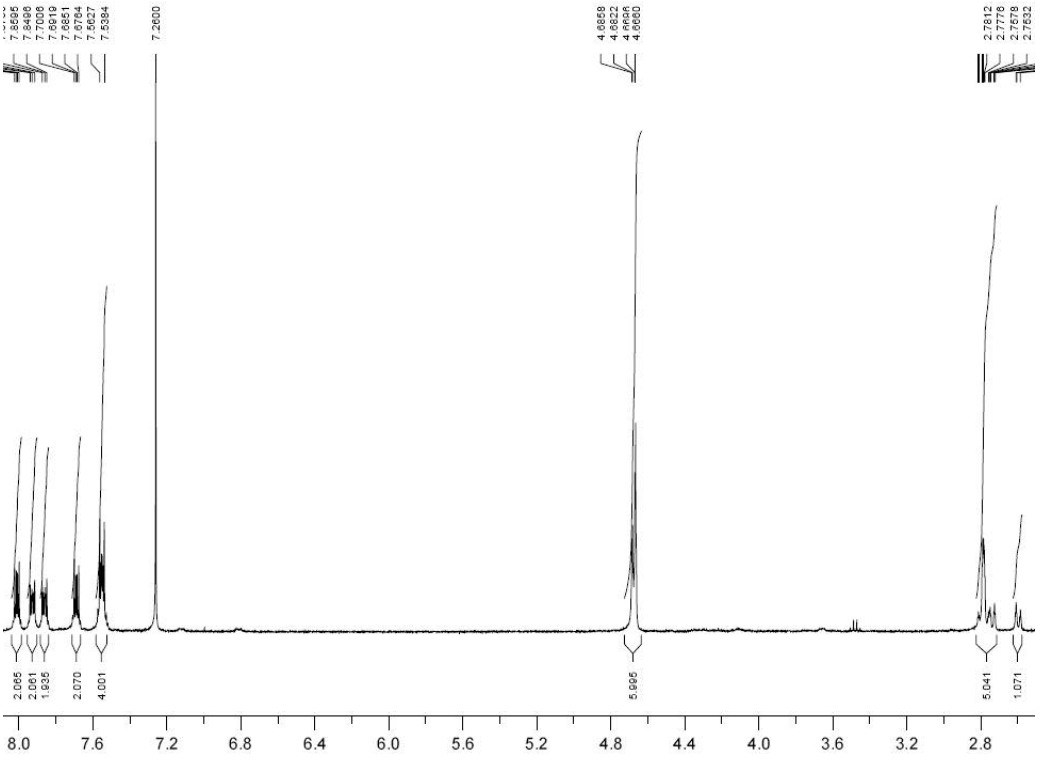


Figure S4. ^{13}C NMR spectrum of **1**$_{anti}$ in $CDCl_3$, at 298 K (100 MHz).

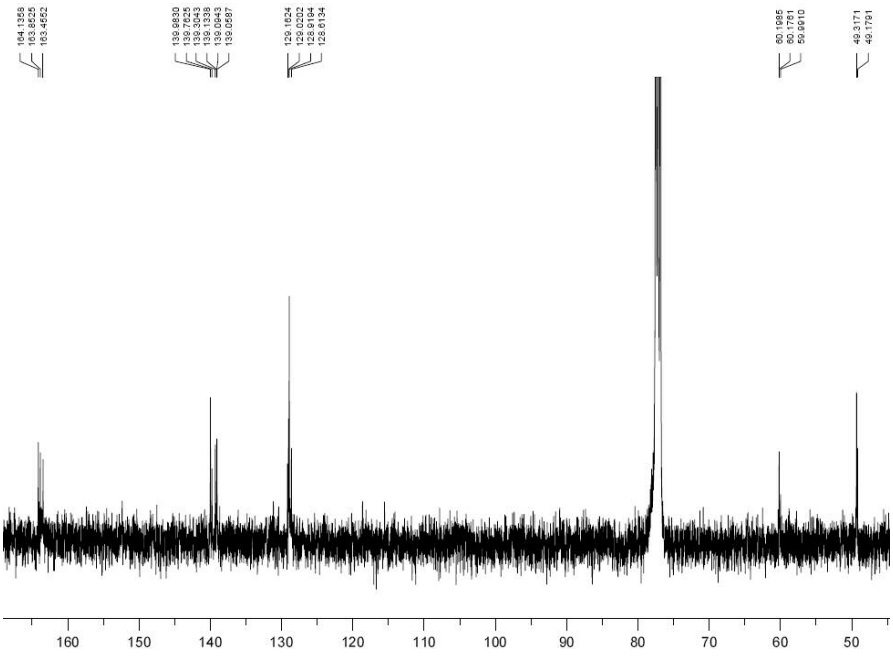


Figure S5. ^{1}H NMR spectrum of compound **2** in $CDCl_3$, at 298 K (250 MHz).[11]

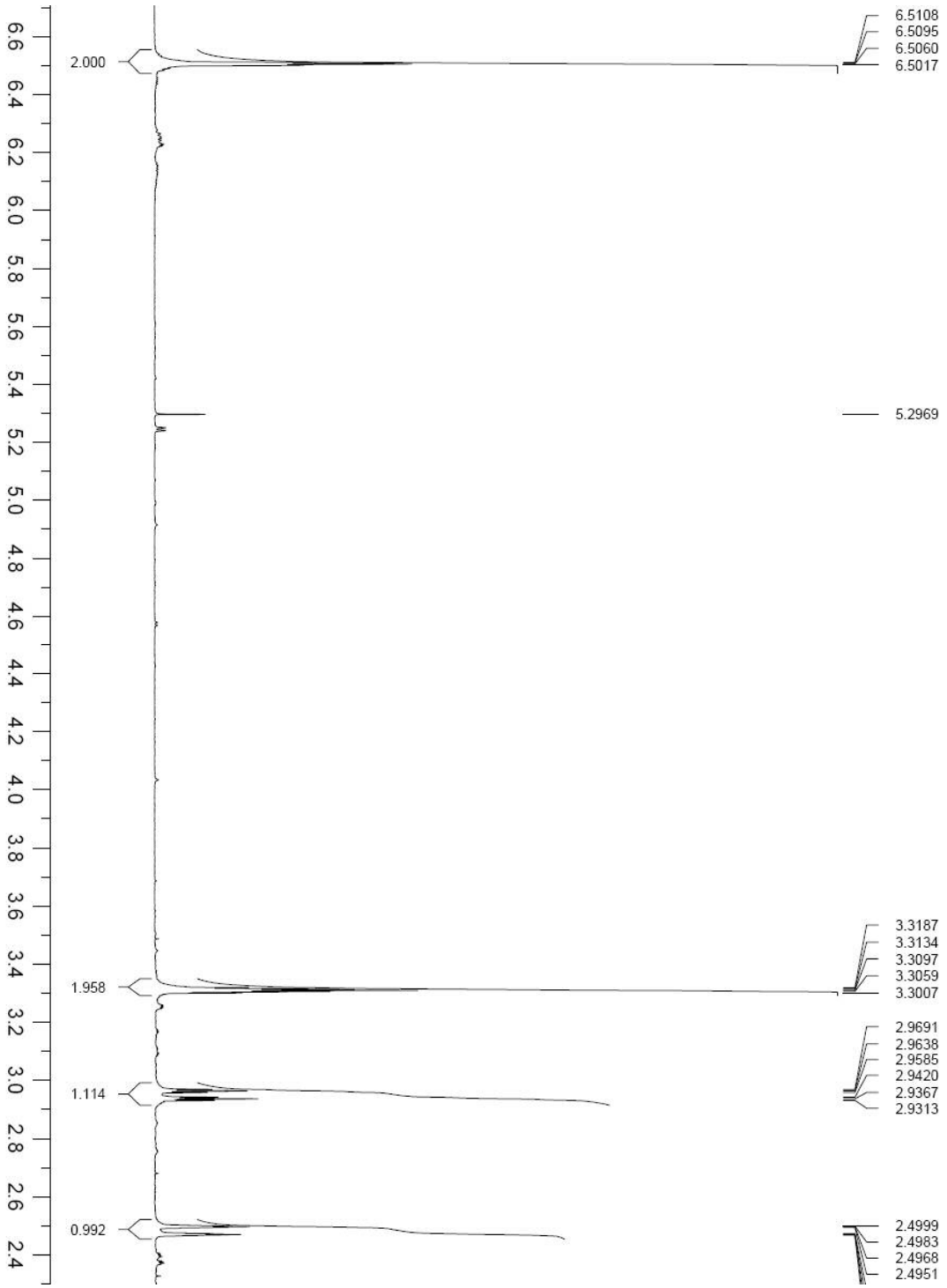


Figure S6. ^{1}H NMR spectrum of compound **4** in $CDCl_3$, at 298 K (400 MHz).

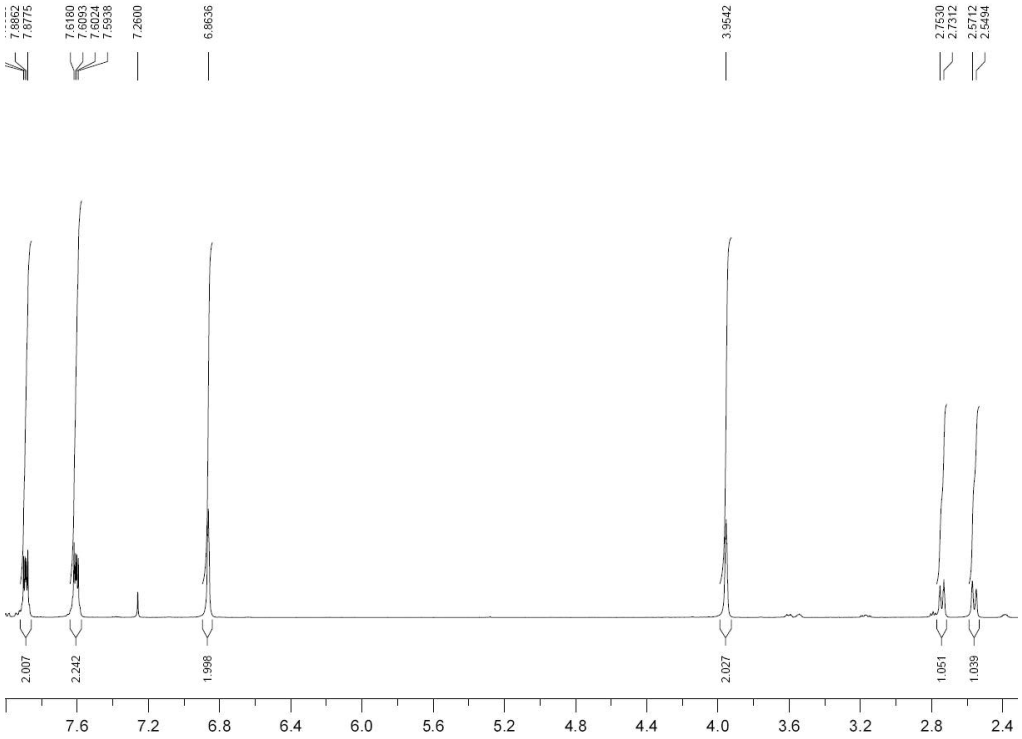


Figure S7. ^{13}C NMR spectrum of compound **4** in $CDCl_3$, at 298 K (100 MHz).

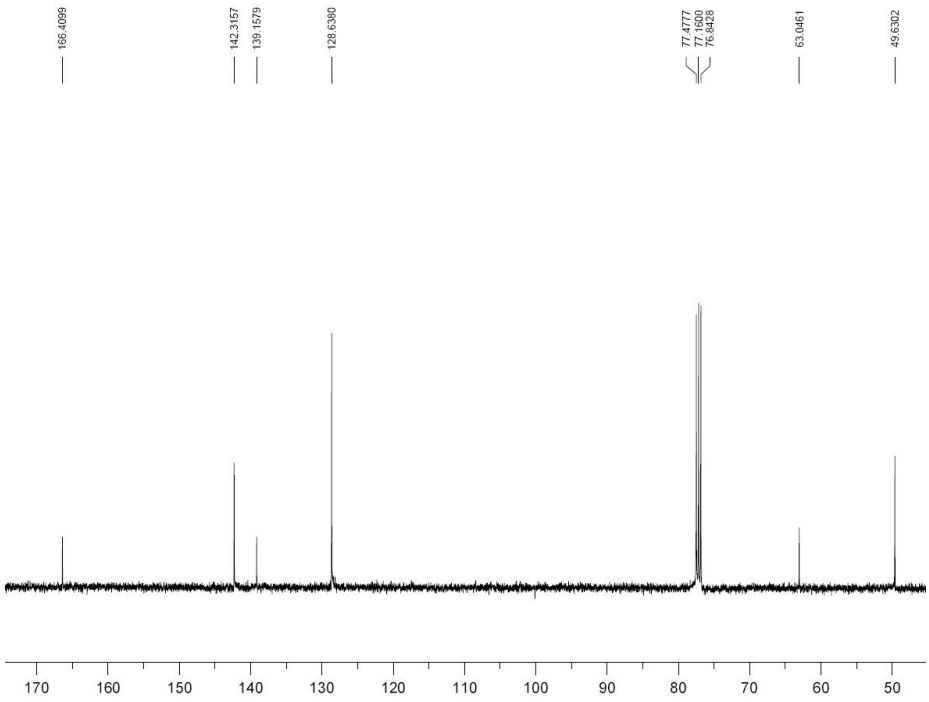


Figure S8. ^{1}H NMR spectrum of compound **5**$_{a}$ in $CDCl_3$, at 298 K (400 MHz).

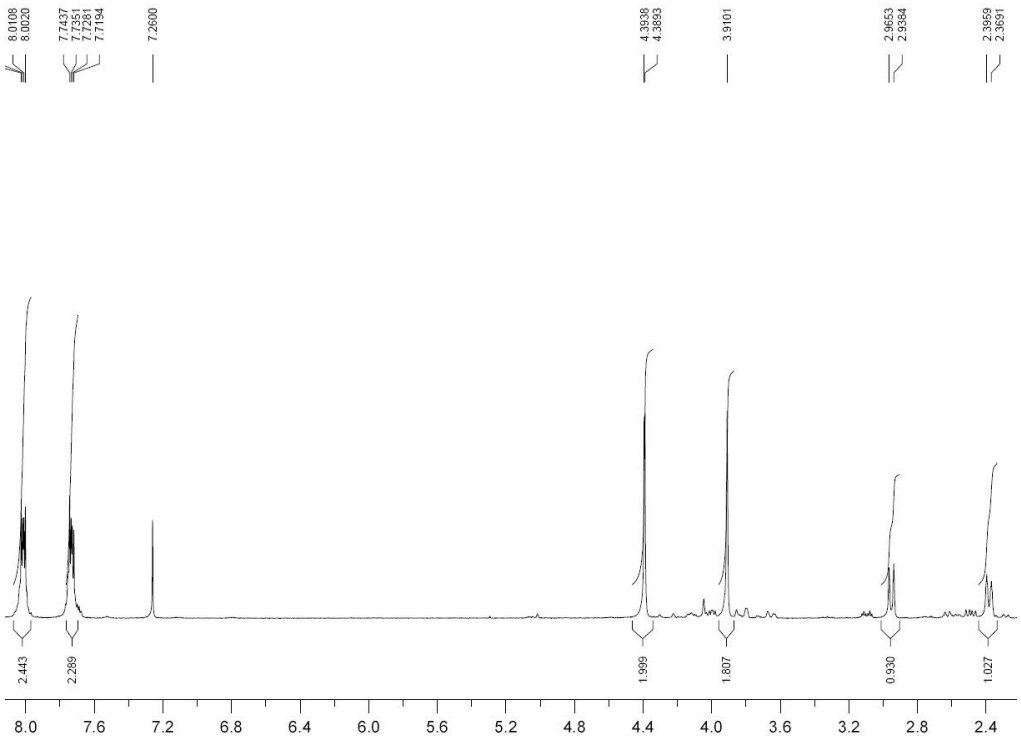


Figure S9. ^{13}C NMR spectrum of compound **5**$_{a}$ in $CDCl_3$, at 298 K (100 MHz).

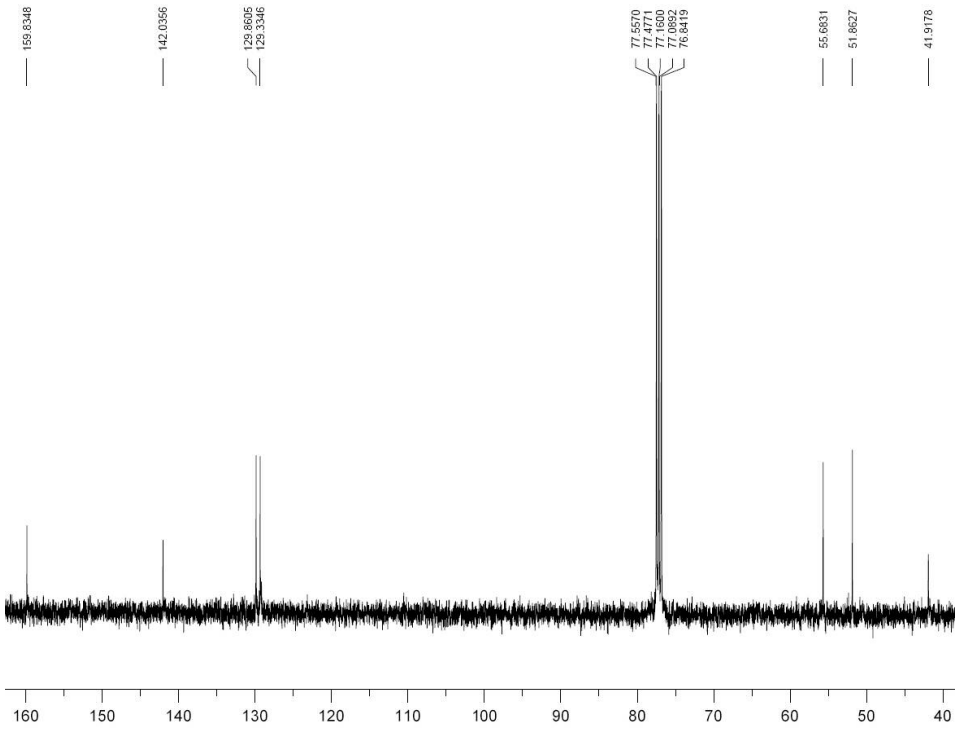


Figure S10. ^{1}H NMR spectrum of compound $\mathbf{5}_b$ in $CDCl_3$, at 298 K (400 MHz).

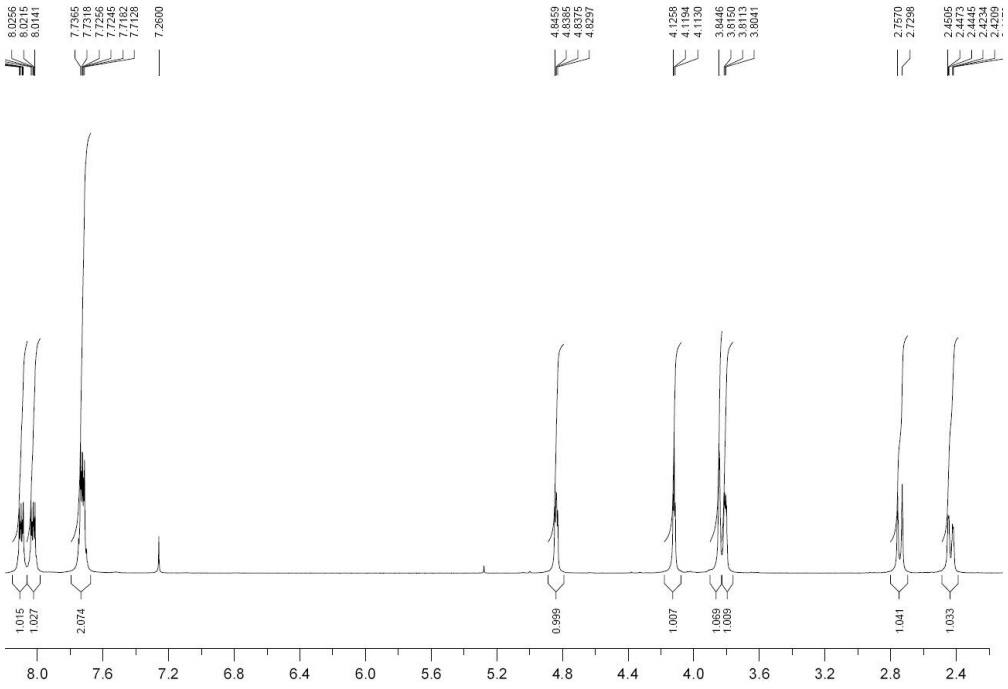


Figure S11. ^{13}C NMR spectrum of compound $\mathbf{5}_b$ in $CDCl_3$, at 298 K (100 MHz).

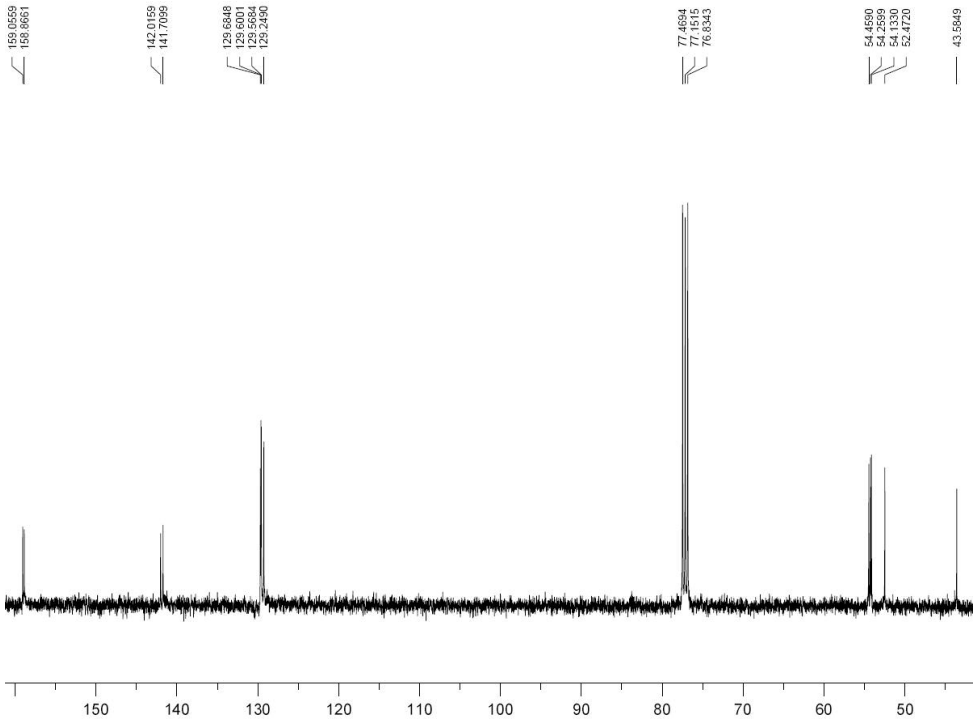


Figure S12. ^{1}H NMR spectrum of compound **6** in $CDCl_3$, at 298 K (400 MHz).

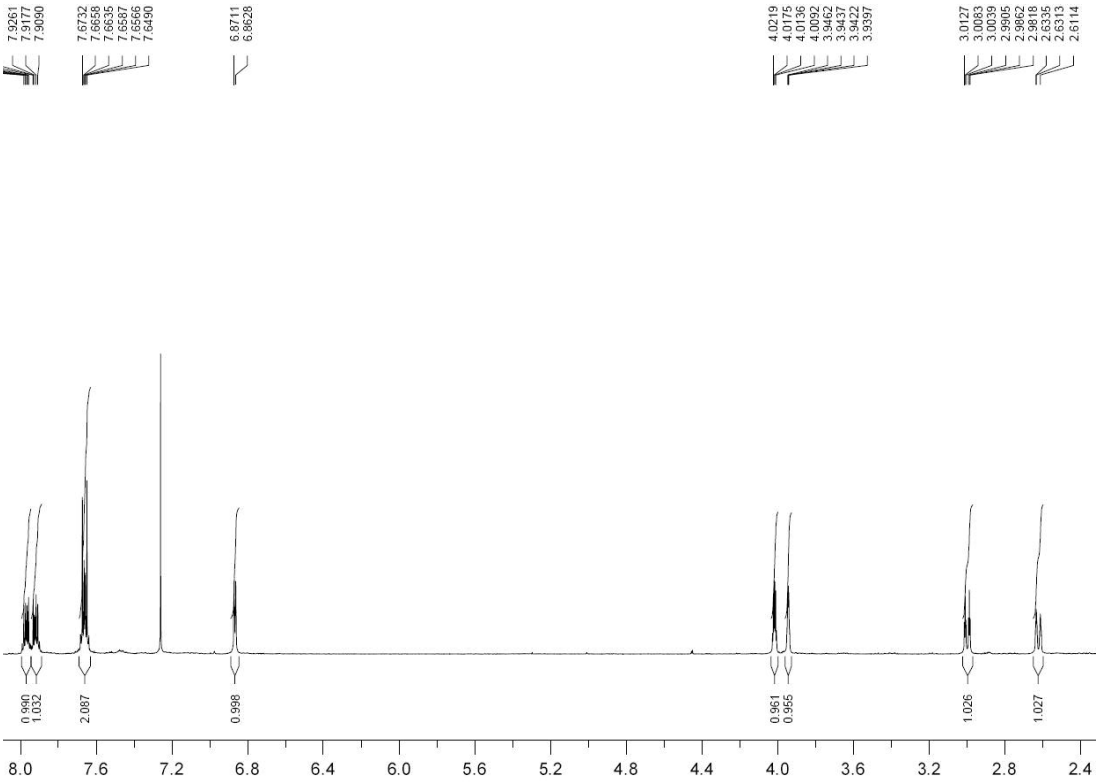


Figure S13. ^{13}C NMR spectrum of compound **6** in $CDCl_3$, at 298 K (100 MHz).

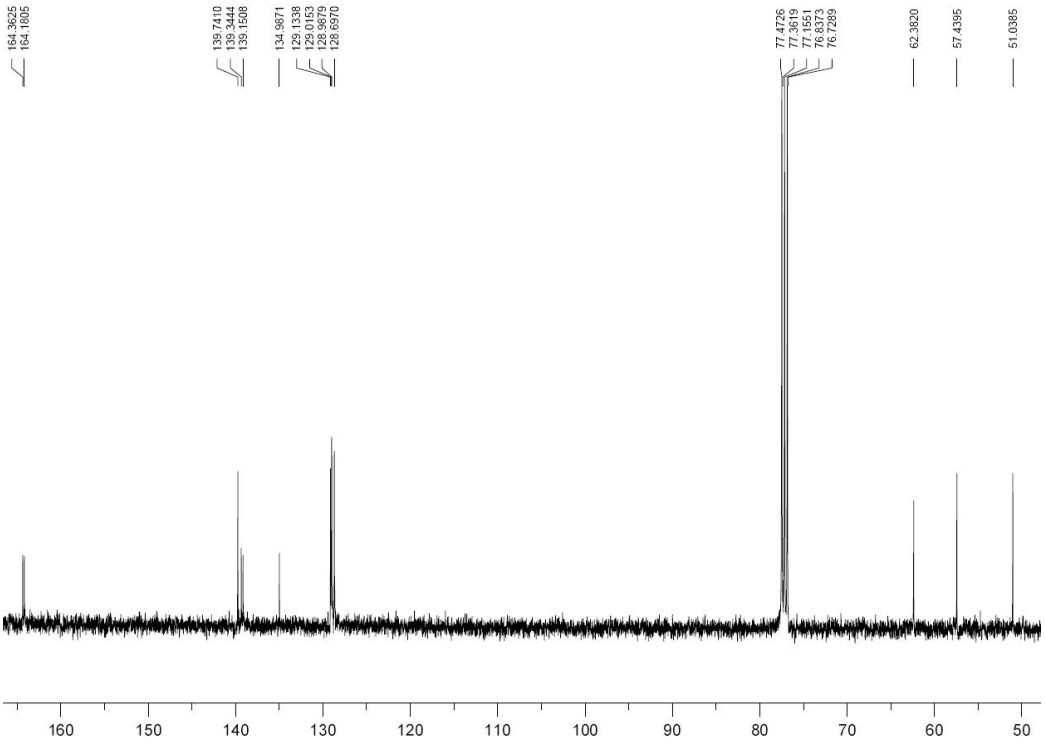


Figure S14. ^{1}H NMR spectrum of compound **7** in $CDCl_3$, at 298 K (400 MHz).

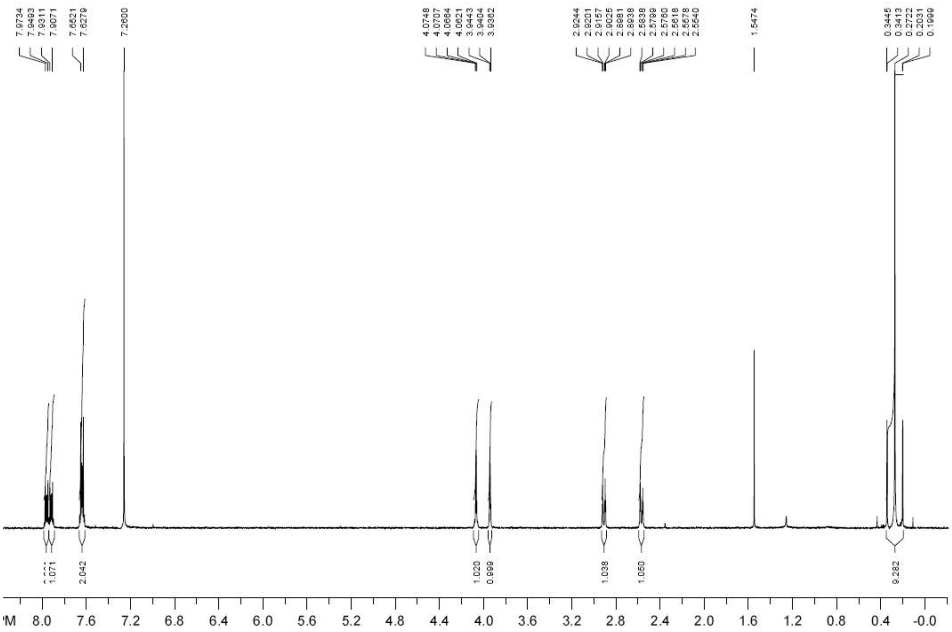


Figure S15. ^{13}C NMR spectrum of compound **7** in $CDCl_3$, at 298 K (100 MHz).

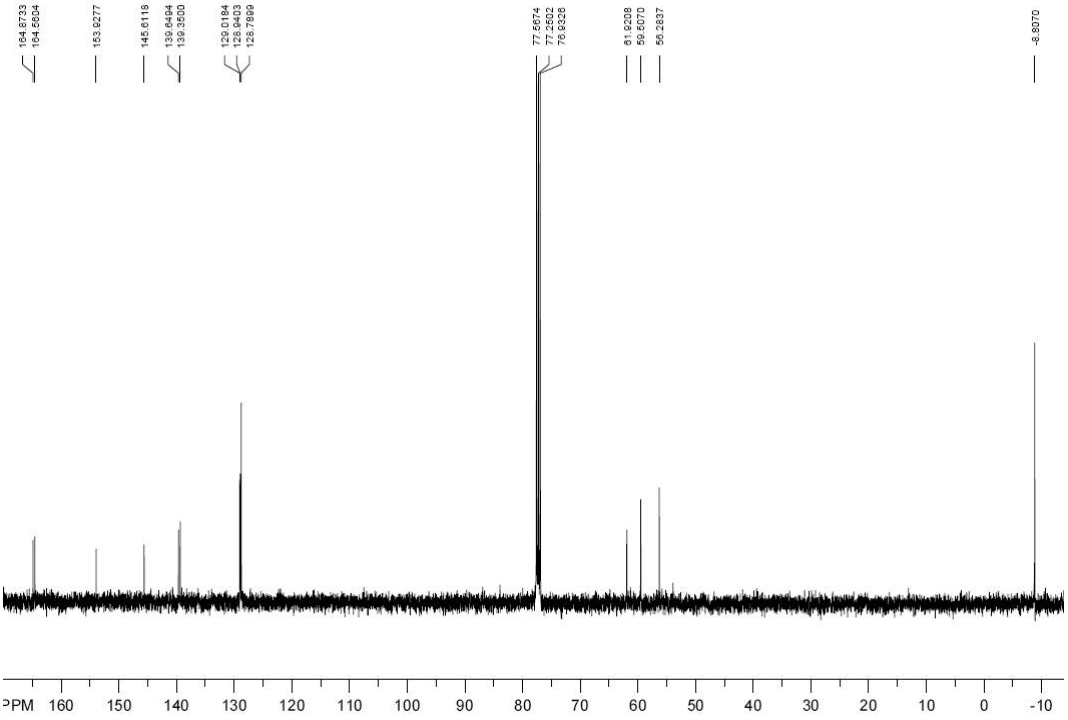


Figure S16. ^{1}H NMR spectrum of compound **8** in $CDCl_3$, at 298 K (400 MHz).

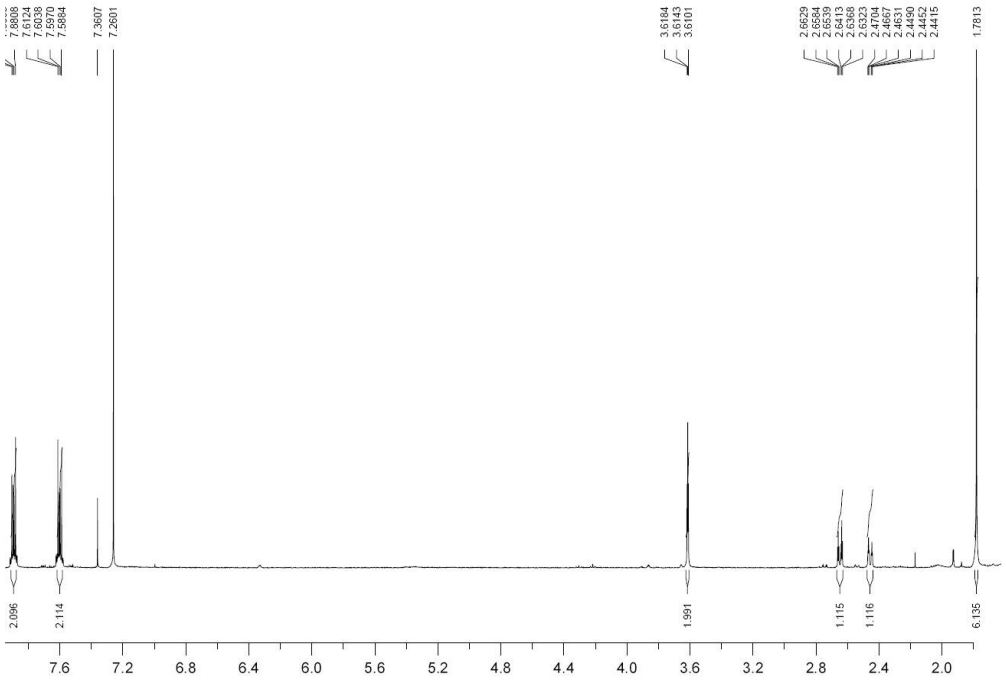


Figure S17. ^{13}C NMR spectrum of compound **8** in $CDCl_3$, at 298 K (100 MHz).

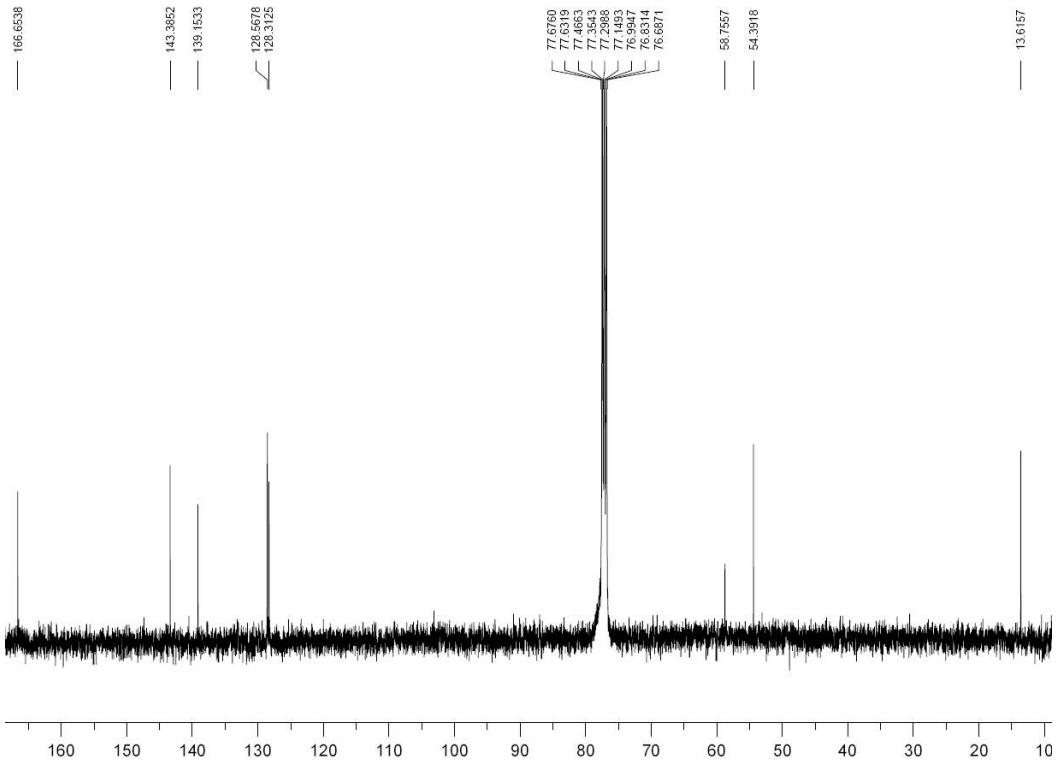


Figure S18. A series of ^{1}H NMR spectra (500 MHz, 298 K, CD_3SOCD_3), recorded on addition of a 1.32 M standard solution of $CsClO_4$ to a 3.50 mM solution of **1**$_{syn}$.

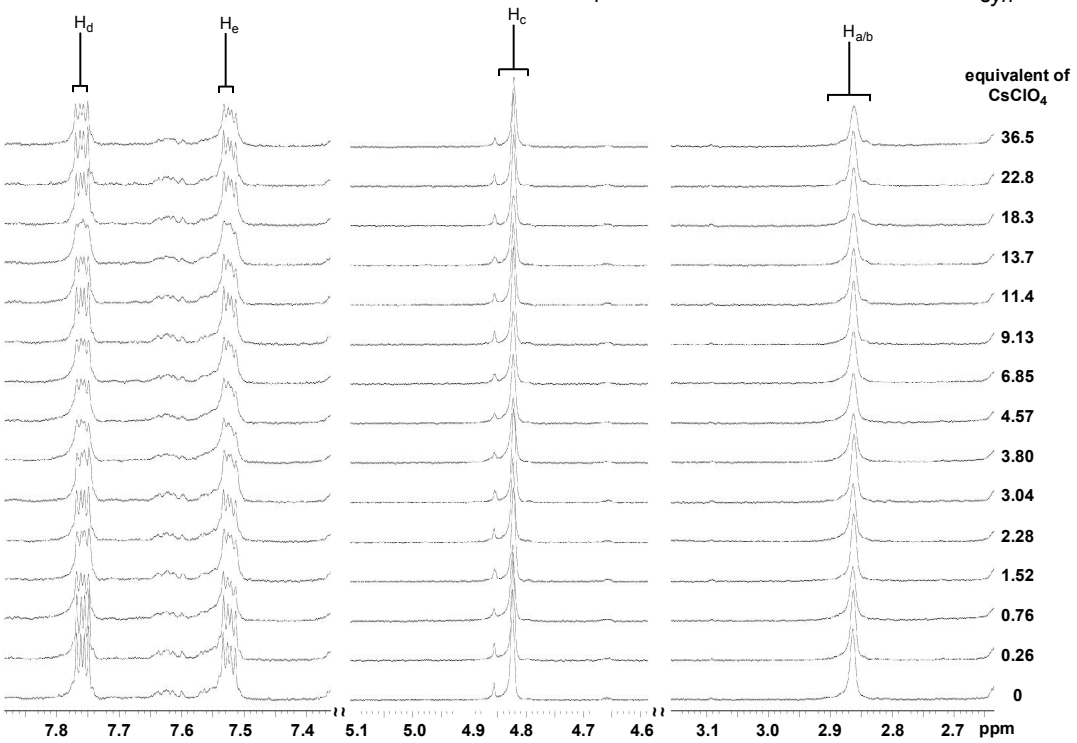


Figure S19. A series of ^{1}H NMR spectra (500 MHz, 298 K, CD_3CN:$CDCl_3$, 5:1), recorded on addition of a 1.91 M standard solution of $[Cu(CH_3CN)_4]PF_6$ to a 10.8 mM solution of **1**$_{syn}$.

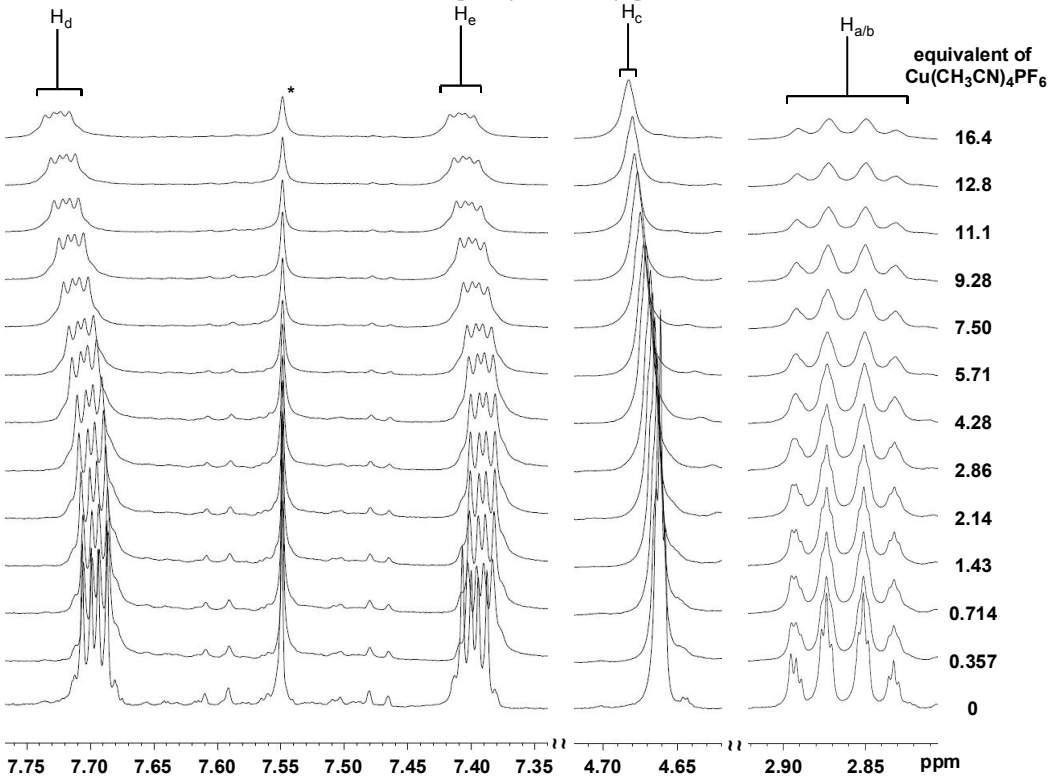


Figure S20. A series of ^{1}H NMR spectra (400 MHz, 298 K, $CDCl_3$:CD_3OD,1:1), recorded on addition of a 1.80 M standard solution of AgOTf to a 2.3 mM solution of **1**$_{syn}$.

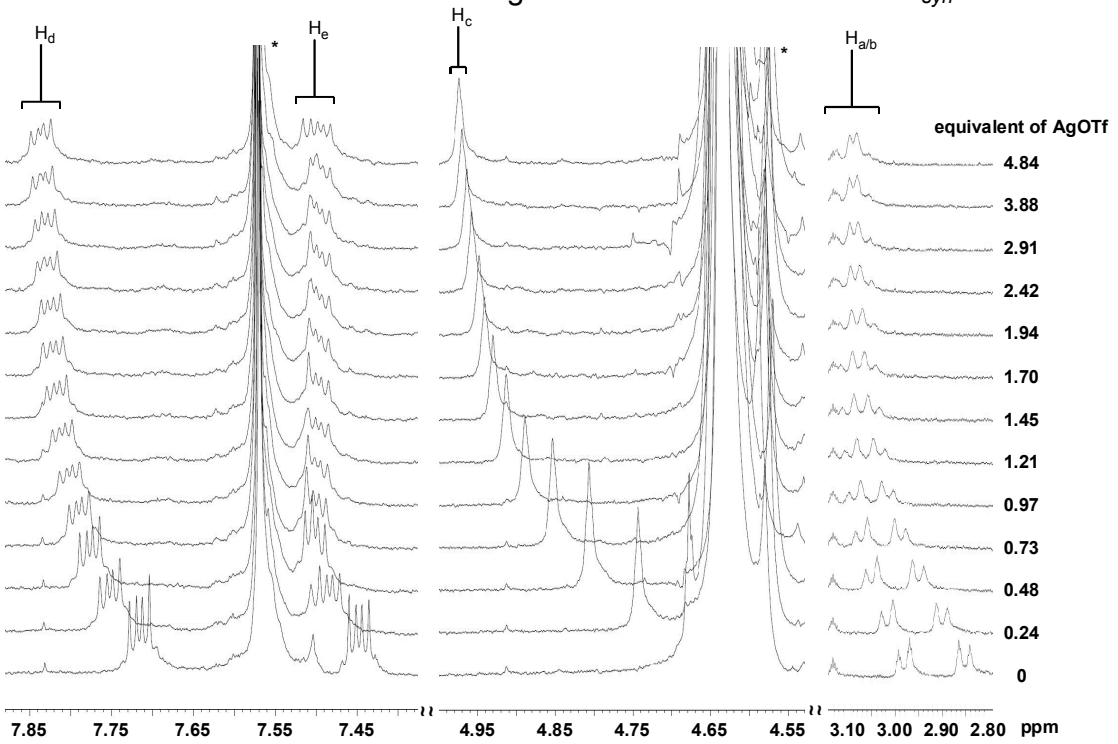


Figure S21. A series of ^{1}H NMR spectra (500 MHz, 298 K, CD_3CN), recorded on addition of a 0.68 M standard solution of [Au(PPh_3)]Cl to a 5.90 mM solution of **1**$_{syn}$.

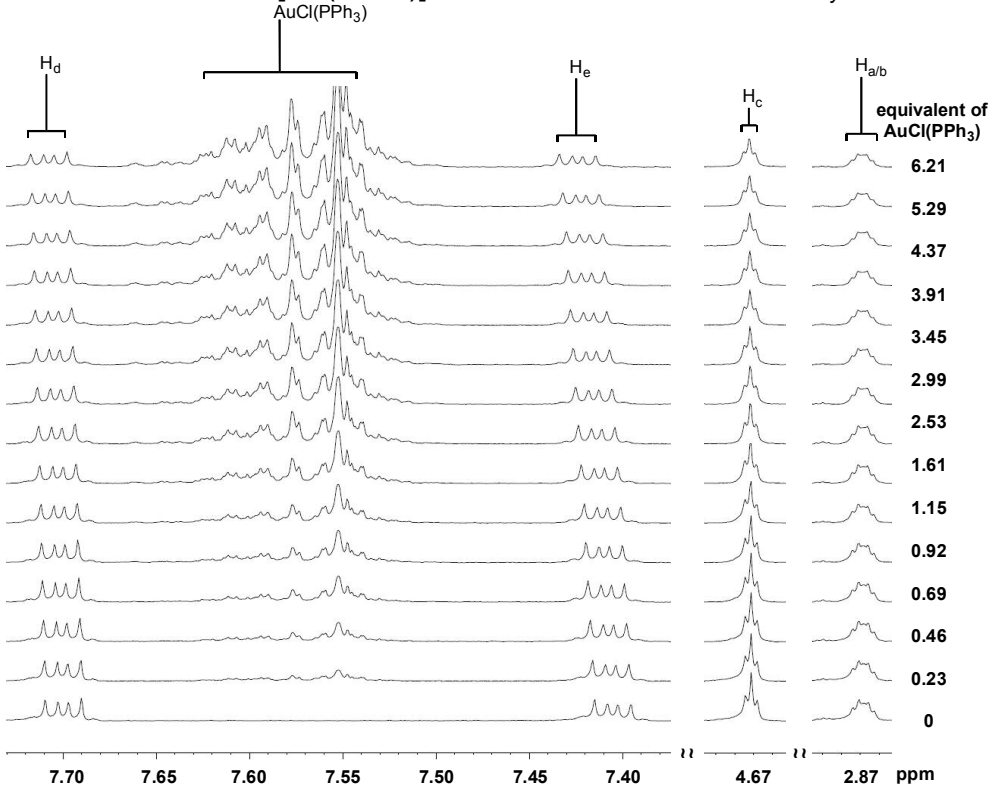


Figure S22. A series of ^{1}H NMR spectra (500 MHz, 298 K, CD_3CN:$CDCl_3$=5:1), recorded on addition of a 1.88 M standard solution of $[Cu(CH_3CN)_4]PF_6$ to a 9.36 mM mM solution of **1**$_{syn}$ containing 28.0 mM $CsPF_6$.

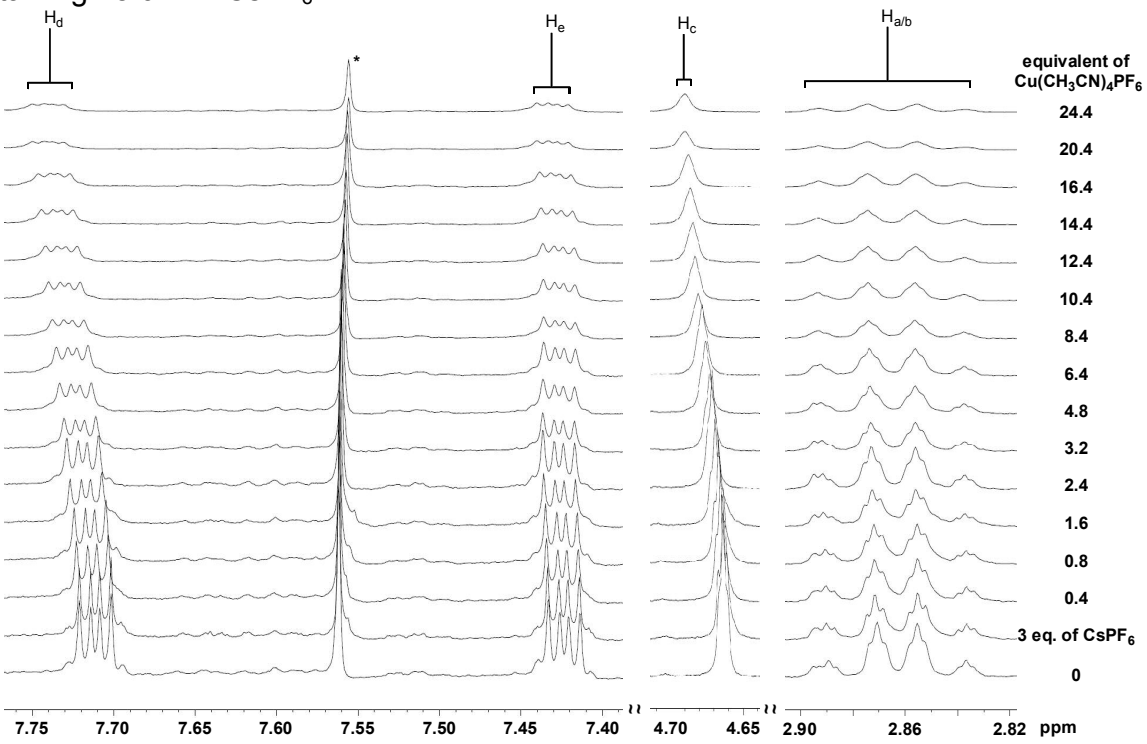


Figure S23. A series of ^{1}H NMR spectra (500 MHz, 298 K, CD_3OD:$CDCl_3$=1:1), recorded on addition of a 2.02 M standard solution of AgOTf to a 2.80 mM solution of **10**.

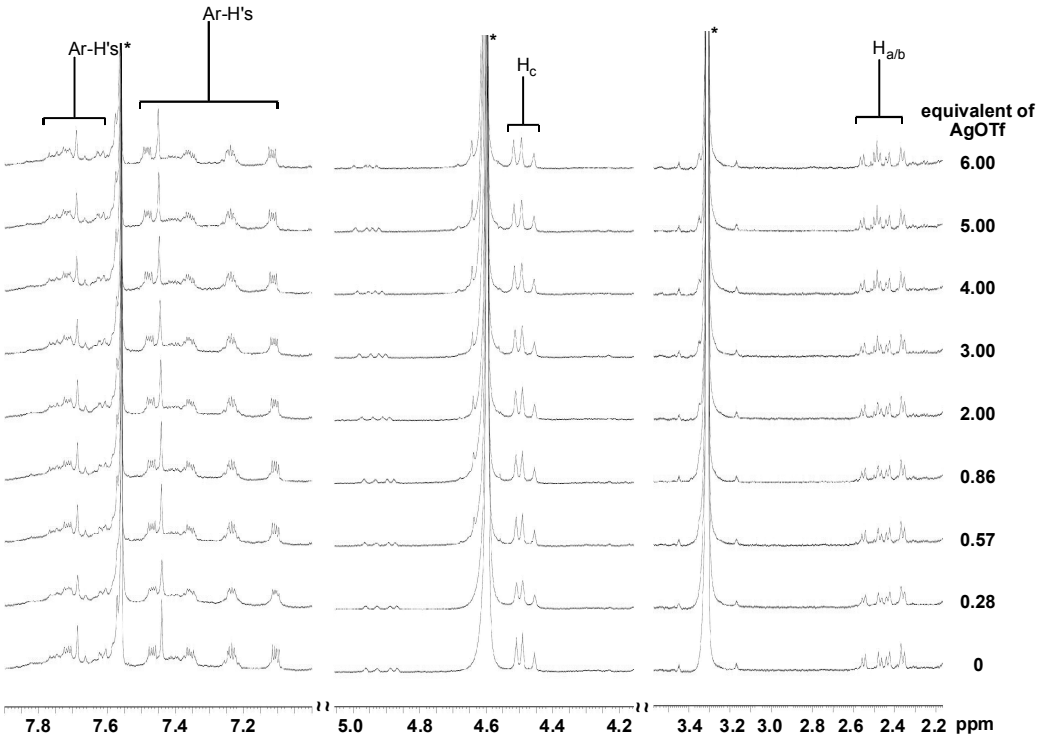
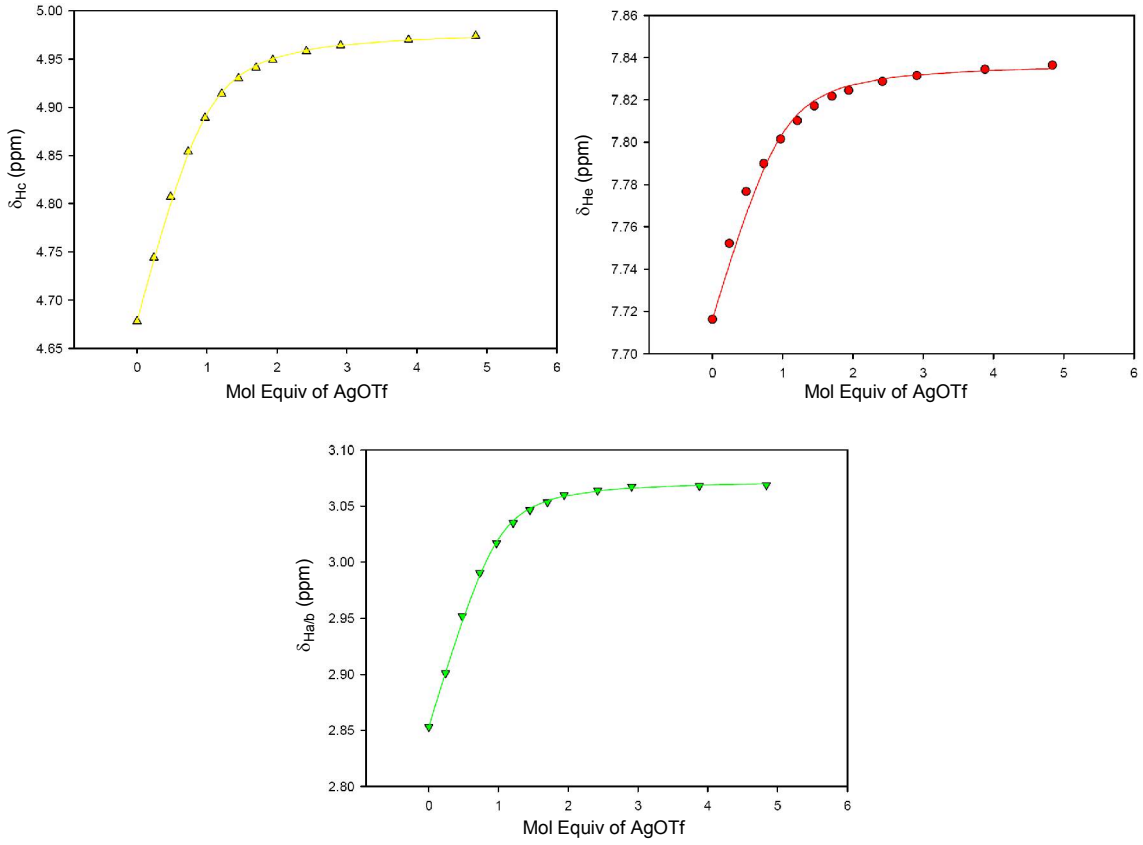


Figure S24. The non-linear curve fitting of the ^{1}H NMR chemical signals of the $\mathbf{H}_c$ $\mathbf{H}_e$ and $\mathbf{H}_{a/b}$ resonances in $\mathbf{1}_{syn}$ to a 1:1 equilibrium model. The NMR titration data was collected in an experiment whereby an incremental addition of 1.86 M standard solution of AgOTf ($CDCl_3/CD_3OD$ = 1:1) to 2.30 mM solution of **1** (500 MHz, $CDCl_3/CD_3OD$ = 1:1, 300K) was completed.



Proton	δ(ppm)	δ(saturated with Ag) (ppm)	$\Delta\delta$(ppm)	K_a(M^{-1})
$H_{a/b}$	2.85	3.07	0.22	9.1×10^3
H_c	4.68	4.97	0.29	3.7×10^3
H_e	7.72	7.84	0.12	4.1×10^3

The fitting equation:

$$\delta_{obs} = \delta_{\mathbf{1}} + \frac{\Delta\delta}{2\times[\mathbf{1}]}\times\left[[\mathbf{1}]+[Ag]+\frac{1}{K_a}-\sqrt{\left(\frac{1}{K_a}+[\mathbf{1}]+[Ag]\right)^2-(4\times[\mathbf{1}]\times[Ag])}\right]$$

$$K_{avg} = \frac{K_{H_{a/b}} + K_{H_c} + K_{H_e}}{3} = (5.6\pm1.6)\times10^3\,M^{-1}$$

Figure S25. The continuous variation plot (Job plot) for the interaction of **1**$_{syn}$ with AgOTf (6.1 mM). ^{1}H NMR spectroscopy was used to generate the data (500 MHz, $CDCl_3/CD_3OD$ = 1:1, 300K).

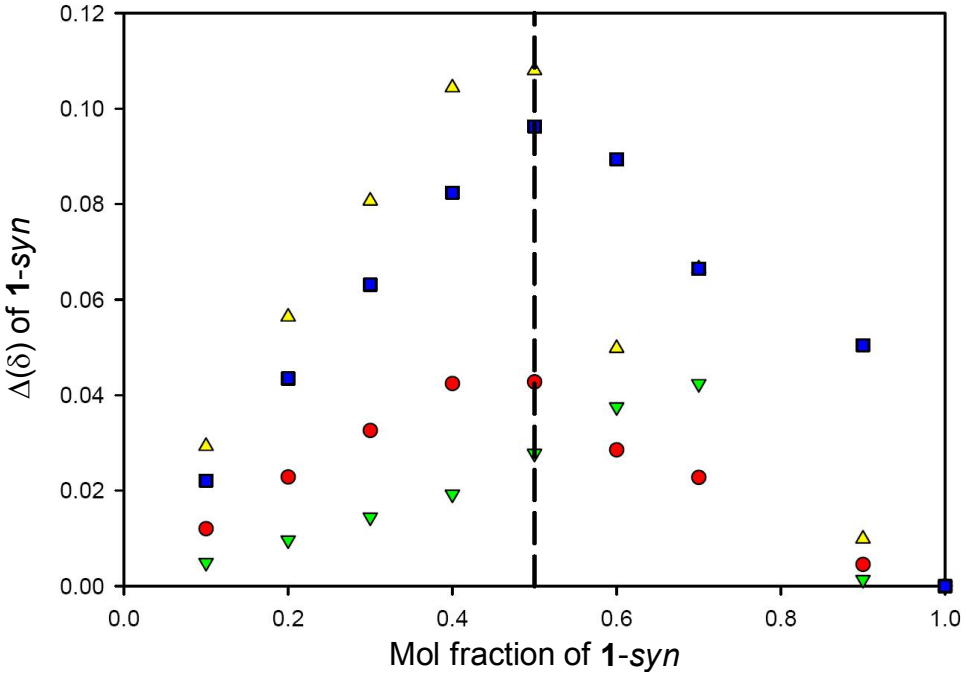


Figure S26. Low-resolution MALDI-TOF mass spectrum of **1**$_{syn}$ with a major peak at *m*/*z* 577.140 corresponding to the [**1** + H]$^{+}$ ion.

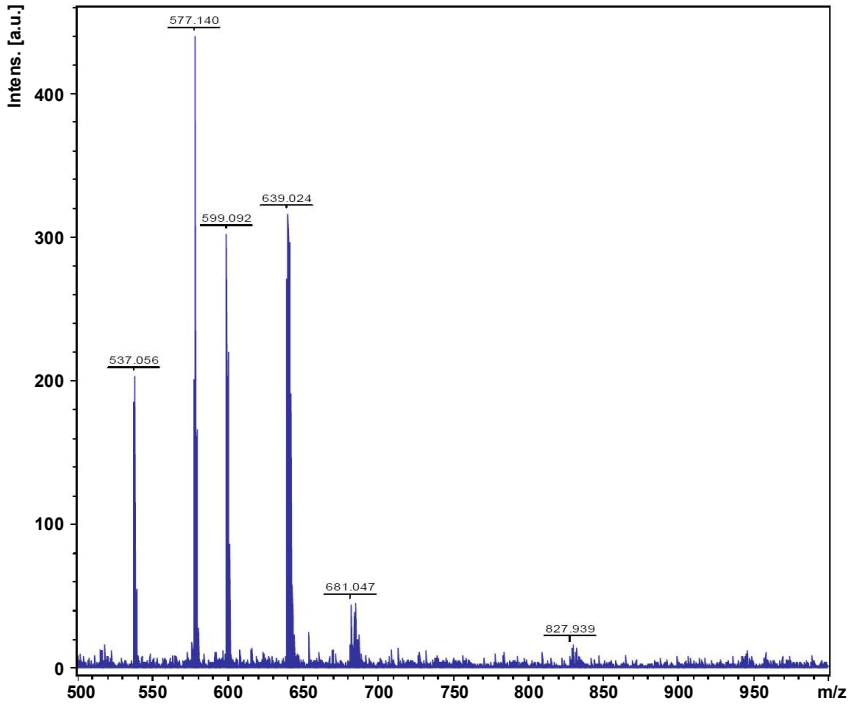


Figure S27. Low-Resolution MALDI-TOF mass spectrum of an equimolar **1**$_{syn}$/AgOTf mixture, with a major peak at *m*/*z* 683.075 corresponding to the [**1** : Ag]$^{+}$ ion.

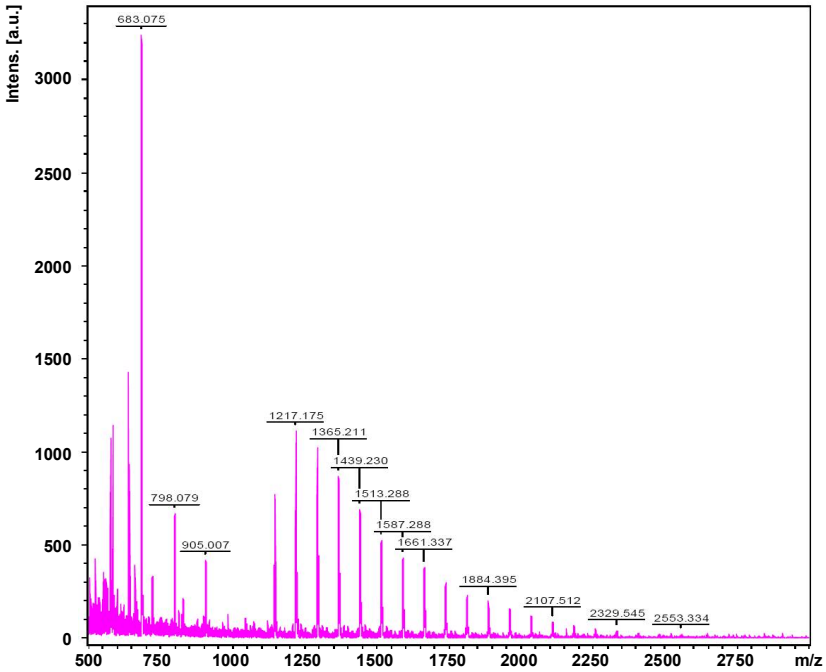
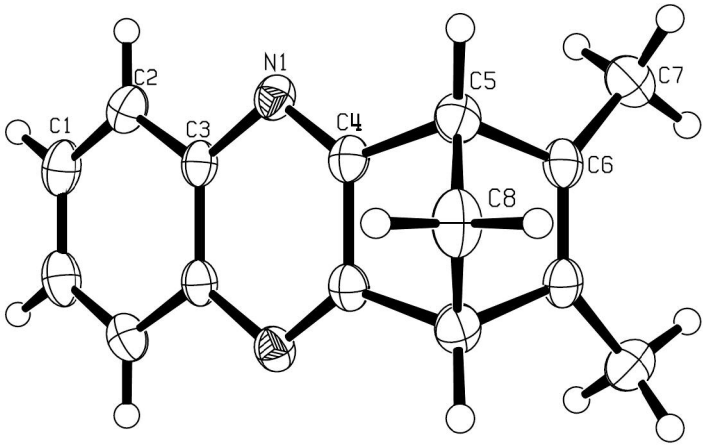


Figure S28. ORTEP representation of the solid-state structure of compound **8**.



Molecular formula: $C_{15}H_{14}N_2$, M_r = 222.28, Temperature: 150(2) K, 0.12 x 0.35 x 0.38 mm^3, orthorhombic, P$\bar{n}$ma, a=10.6543(2) Å, b=11.9382(2) Å, c=9.1044(2) Å, Vol=1158.02(4) Å^3, Z=4, ρ_{calcd}=1.275 Mg/m^3, μ=0.076 mm^{-1}, MoKα radiation (λ = 0.71073 Å), Theta range for data collection: 2.81 to 27.49°, 17881 measured reflections, 1381 independent reflections with R_{int}=0.049, R1(on I>2σ(I))=0.0415, wR2(on I>2σ(I))=0.0990, R1(on all data)=0.0689, wR2(on all data)=0.1110, Largest diff. peak and hole: 0.174 and -0.193 e/Å^3. Structure was solved by direct methods in SHELXS-97. Full matrix least-squares refinements were done on F^2 in SHELXL-97 as incorporated in the WinGX package. *

* The data collection crystal was a yellow plate. Examination of the diffraction pattern on a diffractometer indicated an orthorhombic crystal system. All work was done at 150 K using a cryostream Cooler. The data collection strategy was set up to measure an octant of reciprocal space with a redundancy factor of 5.0, which means that 90% of the reflections were measured at least 5.0 times. Phi and omega scans with a frame width of 1.0° were used. Integration, scaling and merging of the data was done computationally. Merging the data and averaging the symmetry equivalent reflections resulted in a Rint value of 0.049. The structure was solved by the direct methods procedure. Full-matrix least-squares refinements based on F2 were computed, as incorporated in a software package. The molecule contains a crystallographic mirror plane. For the methyl group, the hydrogen atoms were added at calculated positions using a riding model with U(H) = 1.5 * Ueq(bonded carbon atom). The torsion angle, which defines the orientation of the methyl group about the C-C bond, was refined. The remaining hydrogen atoms were included in the model at calculated positions using a riding model with U(H) = 1.2 * Ueq(attached atom). The final refinement cycle was based on 1381 intensities and 80 variables and resulted in agreement factors of R1(F) = 0.069 and wR2(F^2) = 0.111. For the subset of data with I > 2*sigma(I), the R1(F) value is 0.042 for 992 reflections. The final difference electron density map contains maximum and minimum peak heights of 0.17 and -0.19 e/$Å^3$. Neutral atom scattering factors were used and include terms for anomalous dispersion.

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	8721(1)	3711(1)	206(1)	26(1)
C(1)	11123(1)	3084(1)	-2555(1)	36(1)
C(2)	10325(1)	3668(1)	-1649(1)	31(1)
C(3)	9502(1)	3093(1)	-716(1)	24(1)
C(4)	8022(1)	3104(1)	1064(1)	24(1)
C(5)	7105(1)	3450(1)	2253(1)	29(1)
C(6)	7748(1)	3059(1)	3675(1)	26(1)
C(7)	8373(1)	3868(1)	4685(2)	37(1)
C(8)	6131(2)	2500	2068(2)	35(1)

Table S2. Bond lengths [Å] and angles [°] for compound **8**.

N(1)-C(4)	1.3003(15)	N(1)-C(3)-C(2)	118.67(11)
N(1)-C(3)	1.3934(15)	N(1)-C(3)-C(3)#1	121.99(6)
C(1)-C(2)	1.3741(19)	C(2)-C(3)-C(3)#1	119.33(8)
C(1)-C(1)#1	1.394(3)	N(1)-C(4)-C(4)#1	123.92(7)
C(1)-H(1)	0.9500	N(1)-C(4)-C(5)	130.22(11)
C(2)-C(3)	1.4009(17)	C(4)#1-C(4)-C(5)	105.83(7)
C(2)-H(2)	0.9500	C(4)-C(5)-C(6)	103.38(9)
C(3)-C(3)#1	1.416(2)	C(4)-C(5)-C(8)	98.92(11)
C(4)-C(4)#1	1.441(2)	C(6)-C(5)-C(8)	99.69(11)

C(4)-C(5)	1.5160(16)	C(4)-C(5)-H(5)	117.3
C(5)-C(6)	1.5370(17)	C(6)-C(5)-H(5)	117.3
C(5)-C(8)	1.5467(18)	C(8)-C(5)-H(5)	117.3
C(5)-H(5)	1.0000	C(6)#1-C(6)-C(7)	130.36(8)
C(6)-C(6)#1	1.336(2)	C(6)#1-C(6)-C(5)	107.66(7)
C(6)-C(7)	1.4905(18)	C(7)-C(6)-C(5)	121.51(11)
C(7)-H(7A)	0.9800	C(6)-C(7)-H(7A)	109.5
C(7)-H(7B)	0.9800	C(6)-C(7)-H(7B)	109.5
C(7)-H(7C)	0.9800	H(7A)-C(7)-H(7B)	109.5
C(8)-C(5)#1	1.5467(18)	C(6)-C(7)-H(7C)	109.5
C(8)-H(8A)	0.9900	H(7A)-C(7)-H(7C)	109.5
C(8)-H(8B)	0.9900	H(7B)-C(7)-H(7C)	109.5
C(4)-N(1)-C(3)	114.07(11)	C(5)-C(8)-C(5)#1	94.31(14)
C(2)-C(1)-C(1)#1	120.48(8)	C(5)-C(8)-H(8A)	112.9
C(2)-C(1)-H(1)	119.8	C(5)#1-C(8)-H(8A)	112.9
C(1)#1-C(1)-H(1)	119.8	C(5)-C(8)-H(8B)	112.9
C(1)-C(2)-C(3)	120.20(13)	C(5)#1-C(8)-H(8B)	112.9
C(1)-C(2)-H(2)	119.9	H(8A)-C(8)-H(8B)	110.3
C(3)-C(2)-H(2)	119.9		

Symmetry transformations used to generate equivalent atoms:

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

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **8**. 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}
N(1)	25(1)	29(1)	24(1)	3(1)	0(1)	3(1)
C(1)	29(1)	52(1)	26(1)	5(1)	5(1)	-6(1)
C(2)	30(1)	36(1)	27(1)	5(1)	0(1)	-4(1)
C(3)	21(1)	32(1)	19(1)	1(1)	-2(1)	1(1)
C(4)	20(1)	30(1)	21(1)	2(1)	-3(1)	3(1)
C(5)	26(1)	32(1)	28(1)	1(1)	3(1)	7(1)
C(6)	22(1)	33(1)	23(1)	-1(1)	5(1)	2(1)
C(7)	39(1)	37(1)	36(1)	-7(1)	2(1)	0(1)
C(8)	19(1)	55(1)	30(1)	0	2(1)	0

Table S4. Calculated hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for compound **8**.

	x	y	z	U(eq)
H(1)	11679	3479	-3185	43
H(2)	10332	4463	-1656	37
H(5)	6786	4237	2225	34
H(7A)	8715	3464	5533	56
H(7B)	7760	4423	5023	56
H(7C)	9056	4248	4164	56
H(8A)	5728	2500	1088	41
H(8B)	5485	2500	2850	41

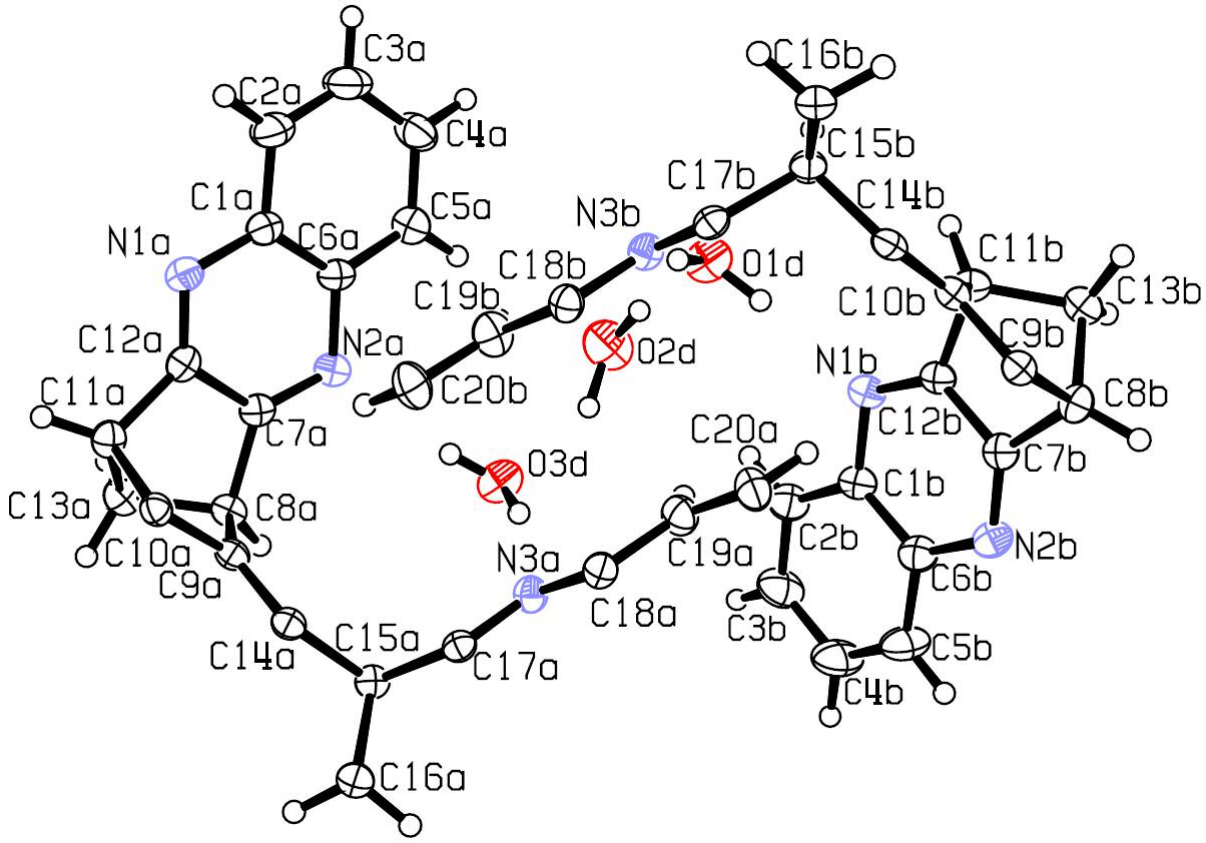
Table S5. Torsion angles [°] for compound **8**.

C(1)#1-C(1)-C(2)-C(3)	-0.04(14)
C(4)-N(1)-C(3)-C(2)	-177.84(11)
C(4)-N(1)-C(3)-C(3)#1	1.00(11)
C(1)-C(2)-C(3)-N(1)	178.90(11)
C(1)-C(2)-C(3)-C(3)#1	0.04(14)
C(3)-N(1)-C(4)-C(4)#1	-1.02(12)
C(3)-N(1)-C(4)-C(5)	176.99(11)
N(1)-C(4)-C(5)-C(6)	-111.33(14)
C(4)#1-C(4)-C(5)-C(6)	66.95(9)
N(1)-C(4)-C(5)-C(8)	146.40(13)
C(4)#1-C(4)-C(5)-C(8)	-35.32(9)
C(4)-C(5)-C(6)-C(6)#1	-68.29(9)
C(8)-C(5)-C(6)-C(6)#1	33.39(9)
C(4)-C(5)-C(6)-C(7)	104.55(13)
C(8)-C(5)-C(6)-C(7)	-153.77(12)
C(4)-C(5)-C(8)-C(5)#1	54.88(13)
C(6)-C(5)-C(8)-C(5)#1	-50.45(14)

Symmetry transformations used to generate equivalent atoms:

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

Figure S29. ORTEP representation of the solid-state structure of $\mathbf{1}_{syn}$ clearly indicating a repeating motif in the solid state comprising two fully entangled molecular bowls by π-π stacking with three water molecules.



Molecular formula: $C_{39}H_{24}N_6$ + $3H_2O$, M_r = 630.69, Temperature: 150(2) K, 0.12 x 0.19 x 0.35 mm^3, orthorhombic, $P\bar{b}cm$, a=17.6837(2) Å, b=20.8217(2) Å, c=19.9034(2) Å, Vol=7328.53(13) $Å^3$, Z=8, ρ_{calcd}=1.143 Mg/m^3, μ=0.074 mm^{-1}, MoKα radiation (λ = 0.71073 Å), Theta range for data collection: 2.05 to 27.48°, 73462 measured reflections, 8642 independent reflections with R_{int}=0.054, R1(on I>2σ(I))=0.0583, wR2(on I>2σ(I))=0.1599, R1(on all data)=0.0989, wR2(on all data)=0.1750, Largest diff. peak and hole: 0.290 and -0.274 e/$Å^3$. Structure was solved by direct methods in SHELXS-97. Full matrix least-squares refinements were done on F^2 in SHELXL-97 as incorporated in the WinGX package.

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **1**$_{syn}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1D)	3368(1)	5811(1)	4617(1)	39(1)
O(2D)	2543(1)	4963(1)	5489(1)	57(1)
O(3D)	1711(1)	4165(1)	4582(1)	37(1)
C(1A)	4138(1)	2849(1)	4121(1)	27(1)
C(2A)	4915(1)	2997(1)	4163(1)	41(1)
C(3A)	5161(1)	3493(1)	4561(1)	45(1)
C(4A)	4642(1)	3869(1)	4916(1)	38(1)
C(5A)	3880(1)	3750(1)	4873(1)	31(1)
C(6A)	3618(1)	3237(1)	4480(1)	24(1)
C(7A)	2659(1)	2618(1)	4088(1)	22(1)
C(8A)	1884(1)	2340(1)	3948(1)	23(1)
C(9A)	1739(1)	2468(1)	3201(1)	21(1)
C(10A)	2271(1)	2081(1)	2843(1)	22(1)
C(11A)	2735(1)	1717(1)	3368(1)	25(1)
C(12A)	3195(1)	2230(1)	3728(1)	23(1)
C(13A)	2103(1)	1617(1)	3910(1)	26(1)
C(14A)	1235(1)	2845(1)	2857(1)	21(1)
C(15A)	615(1)	3309(1)	3078(1)	23(1)
C(16A)	32(1)	3197(1)	2500	26(1)
C(17A)	909(1)	3961(1)	2864(1)	21(1)

C(18A)	1409(1)	4963(1)	2857(1)	24(1)
C(19A)	1680(1)	5504(1)	3201(1)	30(1)
C(20A)	1933(1)	6028(1)	2851(1)	34(1)
N(1A)	3915(1)	2332(1)	3728(1)	27(1)
N(2A)	2840(1)	3119(1)	4446(1)	24(1)
N(3A)	1155(1)	4437(1)	3226(1)	24(1)
C(1B)	1400(1)	6665(1)	4531(1)	26(1)
C(2B)	1169(1)	6152(1)	4945(1)	32(1)
C(3B)	410(1)	6019(1)	5009(1)	41(1)
C(4B)	-132(1)	6378(1)	4662(1)	47(1)
C(5B)	83(1)	6874(1)	4253(1)	41(1)
C(6B)	855(1)	7035(1)	4185(1)	29(1)
C(7B)	1765(1)	7668(1)	3751(1)	24(1)
C(8B)	2198(1)	8187(1)	3371(1)	25(1)
C(9B)	2668(1)	7829(1)	2844(1)	22(1)
C(10B)	3214(1)	7458(1)	3201(1)	21(1)
C(11B)	3086(1)	7590(1)	3946(1)	23(1)
C(12B)	2323(1)	7300(1)	4109(1)	22(1)
C(13B)	2837(1)	8313(1)	3895(1)	26(1)
C(14B)	3725(1)	7086(1)	2859(1)	21(1)
C(15B)	4345(1)	6619(1)	3077(1)	23(1)
C(16B)	4923(1)	6730(1)	2500	25(1)

C(17B)	4043(1)	5968(1)	2863(1)	22(1)
C(18B)	3544(1)	4969(1)	2857(1)	25(1)
C(19B)	3284(1)	4422(1)	3203(1)	33(1)
C(20B)	3036(1)	3895(1)	2851(1)	36(1)
N(1B)	2168(1)	6801(1)	4476(1)	24(1)
N(2B)	1047(1)	7549(1)	3770(1)	28(1)
N(3B)	3796(1)	5494(1)	3225(1)	24(1)

Table S7. Bond lengths [Å] and angles [°] for **1**$_{syn}$.

O(1D)-H(1D)	0.95(3)	C(2A)-C(1A)-C(6A)	118.65(15)
O(1D)-H(2D)	0.96(3)	C(3A)-C(2A)-C(1A)	120.39(17)
O(2D)-H(3D)	1.04(3)	C(3A)-C(2A)-H(2A)	119.8
O(2D)-H(4D)	1.08(3)	C(1A)-C(2A)-H(2A)	119.8
O(3D)-H(5D)	0.95(3)	C(2A)-C(3A)-C(4A)	120.35(18)
O(3D)-H(6D)	0.85(3)	C(2A)-C(3A)-H(3A)	119.8
C(1A)-N(1A)	1.389(2)	C(4A)-C(3A)-H(3A)	119.8
C(1A)-C(2A)	1.411(2)	C(5A)-C(4A)-C(3A)	120.82(17)
C(1A)-C(6A)	1.416(2)	C(5A)-C(4A)-H(4A)	119.6
C(2A)-C(3A)	1.373(3)	C(3A)-C(4A)-H(4A)	119.6
C(2A)-H(2A)	0.9500	C(4A)-C(5A)-C(6A)	119.74(17)
C(3A)-C(4A)	1.398(3)	C(4A)-C(5A)-H(5A)	120.1
C(3A)-H(3A)	0.9500	C(6A)-C(5A)-H(5A)	120.1

C(4A)-C(5A)	1.374(3)	N(2A)-C(6A)-C(5A)	119.02(15)
C(4A)-H(4A)	0.9500	N(2A)-C(6A)-C(1A)	120.95(14)
C(5A)-C(6A)	1.403(2)	C(5A)-C(6A)-C(1A)	120.02(16)
C(5A)-H(5A)	0.9500	N(2A)-C(7A)-C(12A)	124.09(15)
C(6A)-N(2A)	1.398(2)	N(2A)-C(7A)-C(8A)	129.00(15)
C(7A)-N(2A)	1.304(2)	C(12A)-C(7A)-C(8A)	106.88(13)
C(7A)-C(12A)	1.437(2)	C(7A)-C(8A)-C(9A)	105.34(12)
C(7A)-C(8A)	1.513(2)	C(7A)-C(8A)-C(13A)	98.77(13)
C(8A)-C(9A)	1.531(2)	C(9A)-C(8A)-C(13A)	99.34(12)
C(8A)-C(13A)	1.558(2)	C(7A)-C(8A)-H(8A)	116.8
C(8A)-H(8A)	1.0000	C(9A)-C(8A)-H(8A)	116.8
C(9A)-C(14A)	1.371(2)	C(13A)-C(8A)-H(8A)	116.8
C(9A)-C(10A)	1.429(2)	C(14A)-C(9A)-C(10A)	120.12(15)
C(10A)-C(10A)#1	1.363(3)	C(14A)-C(9A)-C(8A)	133.80(15)
C(10A)-C(11A)	1.530(2)	C(10A)-C(9A)-C(8A)	106.08(13)
C(11A)-C(12A)	1.521(2)	C(10A)#1-C(10A)-C(9A)	119.95(9)
C(11A)-C(13A)	1.566(2)	C(10A)#1-C(10A)-C(11A)	133.16(9)
C(11A)-H(11A)	1.0000	C(9A)-C(10A)-C(11A)	106.86(13)
C(12A)-N(1A)	1.292(2)	C(12A)-C(11A)-C(10A)	105.20(12)
C(13A)-H(13A)	0.9900	C(12A)-C(11A)-C(13A)	98.71(13)
C(13A)-H(13B)	0.9900	C(10A)-C(11A)-C(13A)	98.89(13)
C(14A)-C(14A)#1	1.422(3)	C(12A)-C(11A)-H(11A)	117.0

C(14A)-C(15A)	1.527(2)	C(10A)-C(11A)-H(11A)	117.0
C(15A)-C(17A)	1.515(2)	C(13A)-C(11A)-H(11A)	117.0
C(15A)-C(16A)	1.561(2)	N(1A)-C(12A)-C(7A)	123.91(15)
C(15A)-H(15A)	1.0000	N(1A)-C(12A)-C(11A)	130.04(15)
C(16A)-C(15A)#1	1.561(2)	C(7A)-C(12A)-C(11A)	106.05(14)
C(16A)-H(16A)	0.9900	C(8A)-C(13A)-C(11A)	94.67(12)
C(16A)-H(16B)	0.9900	C(8A)-C(13A)-H(13A)	112.8
C(17A)-N(3A)	1.3014(19)	C(11A)-C(13A)-H(13A)	112.8
C(17A)-C(17A)#1	1.447(3)	C(8A)-C(13A)-H(13B)	112.8
C(18A)-N(3A)	1.3916(19)	C(11A)-C(13A)-H(13B)	112.8
C(18A)-C(19A)	1.403(2)	H(13A)-C(13A)-H(13B)	110.3
C(18A)-C(18A)#1	1.423(3)	C(9A)-C(14A)-C(14A)#1	119.93(9)
C(19A)-C(20A)	1.369(2)	C(9A)-C(14A)-C(15A)	133.37(14)
C(19A)-H(19A)	0.9500	C(14A)#1-C(14A)-C(15A)	106.70(8)
C(20A)-C(20A)#1	1.396(4)	C(17A)-C(15A)-C(14A)	103.87(12)
C(20A)-H(20A)	0.9500	C(17A)-C(15A)-C(16A)	98.80(13)
C(1B)-N(1B)	1.392(2)	C(14A)-C(15A)-C(16A)	99.68(13)
C(1B)-C(2B)	1.410(2)	C(17A)-C(15A)-H(15A)	117.2
C(1B)-C(6B)	1.413(2)	C(14A)-C(15A)-H(15A)	117.2
C(2B)-C(3B)	1.376(3)	C(16A)-C(15A)-H(15A)	117.2
C(2B)-H(2B)	0.9500	C(15A)#1-C(16A)-C(15A)	94.85(18)
C(3B)-C(4B)	1.399(3)	C(15A)#1-C(16A)-H(16A)	112.8

C(3B)-H(3B)	0.9500	C(15A)-C(16A)-H(16A)	112.8
C(4B)-C(5B)	1.369(3)	C(15A)#1-C(16A)-H(16B)	112.8
C(4B)-H(4B)	0.9500	C(15A)-C(16A)-H(16B)	112.8
C(5B)-C(6B)	1.411(2)	H(16A)-C(16A)-H(16B)	110.2
C(5B)-H(5B)	0.9500	N(3A)-C(17A)-C(17A)#1	123.64(9)
C(6B)-N(2B)	1.395(2)	N(3A)-C(17A)-C(15A)	129.94(14)
C(7B)-N(2B)	1.294(2)	C(17A)#1-C(17A)-C(15A)	106.35(8)
C(7B)-C(12B)	1.438(2)	N(3A)-C(18A)-C(19A)	119.07(15)
C(7B)-C(8B)	1.525(2)	N(3A)-C(18A)-C(18A)#1	121.79(8)
C(8B)-C(9B)	1.531(2)	C(19A)-C(18A)-C(18A)#1	119.13(10)
C(8B)-C(13B)	1.560(2)	C(20A)-C(19A)-C(18A)	120.28(17)
C(8B)-H(8B)	1.0000	C(20A)-C(19A)-H(19A)	119.9
C(9B)-C(9B)#1	1.371(3)	C(18A)-C(19A)-H(19A)	119.9
C(9B)-C(10B)	1.427(2)	C(19A)-C(20A)-C(20A)#1	120.58(11)
C(10B)-C(14B)	1.370(2)	C(19A)-C(20A)-H(20A)	119.7
C(10B)-C(11B)	1.524(2)	C(20A)#1-C(20A)-H(20A)	119.7
C(11B)-C(12B)	1.513(2)	C(12A)-N(1A)-C(1A)	114.03(14)
C(11B)-C(13B)	1.573(2)	C(7A)-N(2A)-C(6A)	114.12(14)
C(11B)-H(11B)	1.0000	C(17A)-N(3A)-C(18A)	114.55(14)
C(12B)-N(1B)	1.2996(19)	N(1B)-C(1B)-C(2B)	118.88(15)
C(13B)-H(13C)	0.9900	N(1B)-C(1B)-C(6B)	121.17(15)
C(13B)-H(13D)	0.9900	C(2B)-C(1B)-C(6B)	119.95(16)

C(14B)-C(14B)#1	1.430(3)	C(3B)-C(2B)-C(1B)	119.34(17)
C(14B)-C(15B)	1.529(2)	C(3B)-C(2B)-H(2B)	120.3
C(15B)-C(17B)	1.519(2)	C(1B)-C(2B)-H(2B)	120.3
C(15B)-C(16B)	1.556(2)	C(2B)-C(3B)-C(4B)	120.95(17)
C(15B)-H(15B)	1.0000	C(2B)-C(3B)-H(3B)	119.5
C(16B)-C(15B)#1	1.556(2)	C(4B)-C(3B)-H(3B)	119.5
C(16B)-H(16C)	0.9900	C(5B)-C(4B)-C(3B)	120.49(18)
C(16B)-H(16D)	0.9900	C(5B)-C(4B)-H(4B)	119.8
C(17B)-N(3B)	1.2966(19)	C(3B)-C(4B)-H(4B)	119.8
C(17B)-C(17B)#1	1.443(3)	C(4B)-C(5B)-C(6B)	120.26(18)
C(18B)-N(3B)	1.3902(19)	C(4B)-C(5B)-H(5B)	119.9
C(18B)-C(19B)	1.407(2)	C(6B)-C(5B)-H(5B)	119.9
C(18B)-C(18B)#1	1.420(3)	N(2B)-C(6B)-C(1B)	122.75(16)
C(19B)-C(20B)	1.375(2)	N(2B)-C(6B)-C(5B)	118.25(16)
C(19B)-H(19B)	0.9500	C(1B)-C(6B)-C(5B)	118.99(16)
C(20B)-C(20B)#1	1.397(4)	N(2B)-C(7B)-C(12B)	123.88(15)
C(20B)-H(20B)	0.9500	N(2B)-C(7B)-C(8B)	129.94(15)
H(1D)-O(1D)-H(2D)	106(2)	C(12B)-C(7B)-C(8B)	106.18(14)
H(3D)-O(2D)-H(4D)	102(3)	C(7B)-C(8B)-C(9B)	105.54(12)
H(5D)-O(3D)-H(6D)	108(2)	C(7B)-C(8B)-C(13B)	98.72(13)
N(1A)-C(1A)-C(2A)	118.52(15)	C(9B)-C(8B)-C(13B)	98.40(13)
N(1A)-C(1A)-C(6A)	122.82(15)	C(7B)-C(8B)-H(8B)	117.0

		C(9B)-C(8B)-H(8B)	117.0

Symmetry transformations used to generate equivalent atoms:

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

Table S8. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1**$_{syn}$. 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(1D)	42(1)	49(1)	27(1)	-4(1)	-2(1)	6(1)
O(2D)	61(1)	56(1)	54(1)	2(1)	-4(1)	-8(1)
O(3D)	39(1)	47(1)	25(1)	2(1)	0(1)	7(1)
C(1A)	24(1)	29(1)	29(1)	0(1)	-1(1)	2(1)
C(2A)	24(1)	47(1)	52(1)	-11(1)	1(1)	3(1)
C(3A)	22(1)	54(1)	57(1)	-9(1)	-1(1)	-4(1)
C(4A)	35(1)	39(1)	41(1)	-7(1)	-4(1)	-9(1)
C(5A)	31(1)	33(1)	28(1)	-1(1)	1(1)	-1(1)
C(6A)	21(1)	30(1)	23(1)	5(1)	-1(1)	-1(1)
C(7A)	23(1)	26(1)	18(1)	5(1)	-1(1)	0(1)
C(8A)	23(1)	26(1)	19(1)	1(1)	1(1)	-3(1)
C(9A)	22(1)	23(1)	19(1)	0(1)	0(1)	-4(1)
C(10A)	23(1)	19(1)	22(1)	1(1)	-2(1)	-2(1)
C(11A)	30(1)	24(1)	21(1)	2(1)	-2(1)	2(1)
C(12A)	26(1)	24(1)	18(1)	4(1)	1(1)	3(1)
C(13A)	32(1)	26(1)	21(1)	4(1)	-2(1)	-4(1)

C(14A)	20(1)	23(1)	21(1)	2(1)	2(1)	-4(1)
C(15A)	23(1)	24(1)	21(1)	2(1)	1(1)	-1(1)
C(16A)	24(1)	27(1)	25(1)	0	0	-2(1)
C(17A)	19(1)	23(1)	19(1)	0(1)	1(1)	2(1)
C(18A)	26(1)	24(1)	22(1)	0(1)	-1(1)	2(1)
C(19A)	35(1)	28(1)	28(1)	-5(1)	-2(1)	1(1)
C(20A)	38(1)	24(1)	39(1)	-3(1)	-2(1)	-3(1)
N(1A)	24(1)	31(1)	27(1)	0(1)	-1(1)	3(1)
N(2A)	24(1)	28(1)	19(1)	2(1)	0(1)	-2(1)
N(3A)	27(1)	24(1)	23(1)	-1(1)	1(1)	1(1)
C(1B)	24(1)	32(1)	21(1)	-3(1)	1(1)	-2(1)
C(2B)	30(1)	37(1)	29(1)	2(1)	2(1)	-3(1)
C(3B)	37(1)	47(1)	39(1)	10(1)	3(1)	-13(1)
C(4B)	27(1)	60(1)	52(1)	8(1)	4(1)	-10(1)
C(5B)	22(1)	57(1)	44(1)	6(1)	2(1)	0(1)
C(6B)	26(1)	33(1)	27(1)	-2(1)	3(1)	0(1)
C(7B)	27(1)	26(1)	19(1)	-5(1)	2(1)	1(1)
C(8B)	28(1)	25(1)	21(1)	-1(1)	2(1)	4(1)
C(9B)	23(1)	22(1)	21(1)	0(1)	0(1)	-2(1)
C(10B)	23(1)	23(1)	17(1)	0(1)	0(1)	-5(1)
C(11B)	23(1)	31(1)	15(1)	-2(1)	-2(1)	-1(1)
C(12B)	23(1)	26(1)	15(1)	-5(1)	-1(1)	-1(1)

C(13B)	30(1)	29(1)	20(1)	-4(1)	2(1)	-4(1)
C(14B)	20(1)	23(1)	21(1)	1(1)	-3(1)	-6(1)
C(15B)	22(1)	25(1)	22(1)	0(1)	-4(1)	0(1)
C(16B)	21(1)	29(1)	25(1)	0	0	-1(1)
C(17B)	21(1)	25(1)	21(1)	1(1)	-3(1)	3(1)
C(18B)	28(1)	24(1)	23(1)	-1(1)	0(1)	1(1)
C(19B)	41(1)	31(1)	26(1)	4(1)	0(1)	-2(1)
C(20B)	45(1)	27(1)	37(1)	4(1)	1(1)	-7(1)
N(1B)	25(1)	29(1)	17(1)	-2(1)	0(1)	-3(1)
N(2B)	25(1)	34(1)	25(1)	-1(1)	3(1)	4(1)
N(3B)	26(1)	24(1)	21(1)	1(1)	-1(1)	1(1)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $\mathbf{1}_{syn}$.

	x	y	z	U(eq)
H(1D)	3011(15)	6139(12)	4530(12)	74(8)*
H(2D)	3496(13)	5633(10)	4186(13)	64(7)*
H(3D)	2883(18)	5244(14)	5178(17)	118(11)*
H(4D)	2114(16)	4801(12)	5143(15)	91(9)*
H(5D)	1550(13)	4319(10)	4157(13)	62(7)*
H(6D)	2006(16)	3848(12)	4521(13)	77(9)*
H(2A)	5271	2750	3915	49
H(3A)	5687	3582	4595	53

H(4A)	4819	4212	5189	46
H(5A)	3531	4014	5110	37
H(8A)	1470	2459	4267	27
H(11A)	3012	1326	3213	30
H(13A)	1684	1342	3748	31
H(13B)	2304	1449	4340	31
H(15A)	425	3268	3549	27
H(16A)	-179	2757	2500	31
H(16B)	-382	3518	2500	31
H(19A)	1688	5508	3678	36
H(20A)	2110	6395	3087	40
H(2B)	1533	5900	5177	38
H(3B)	252	5678	5294	49
H(4B)	-653	6277	4710	56
H(5B)	-289	7111	4014	49
H(8B)	1902	8567	3213	30
H(11B)	3512	7488	4258	28
H(13C)	2642	8485	4325	32
H(13D)	3242	8594	3718	32
H(15B)	4537	6658	3548	28
H(16C)	5337	6410	2500	30
H(16D)	5134	7171	2500	30

H(19B)	3281	4418	3680	39
H(20B)	2862	3527	3088	43

*Refined isotropically

Table S10. Torsion angles [°] for **1**$_{syn}$.

N(1A)-C(1A)-C(2A)-C(3A)	-178.23(18)	N(1B)-C(1B)-C(2B)-C(3B)	179.18(15)
C(6A)-C(1A)-C(2A)-C(3A)	2.0(3)	C(6B)-C(1B)-C(2B)-C(3B)	-0.3(3)
C(1A)-C(2A)-C(3A)-C(4A)	-1.6(3)	C(1B)-C(2B)-C(3B)-C(4B)	1.1(3)
C(2A)-C(3A)-C(4A)-C(5A)	0.0(3)	C(2B)-C(3B)-C(4B)-C(5B)	-0.4(3)
C(3A)-C(4A)-C(5A)-C(6A)	1.2(3)	C(3B)-C(4B)-C(5B)-C(6B)	-1.0(3)
C(4A)-C(5A)-C(6A)-N(2A)	179.58(15)	N(1B)-C(1B)-C(6B)-N(2B)	0.3(2)
C(4A)-C(5A)-C(6A)-C(1A)	-0.8(3)	C(2B)-C(1B)-C(6B)-N(2B)	179.82(15)
N(1A)-C(1A)-C(6A)-N(2A)	-1.0(2)	N(1B)-C(1B)-C(6B)-C(5B)	179.46(15)
C(2A)-C(1A)-C(6A)-N(2A)	178.83(15)	C(2B)-C(1B)-C(6B)-C(5B)	-1.1(2)
N(1A)-C(1A)-C(6A)-C(5A)	179.47(15)	C(4B)-C(5B)-C(6B)-N(2B)	-179.13(18)
C(2A)-C(1A)-C(6A)-C(5A)	-0.7(3)	C(4B)-C(5B)-C(6B)-C(1B)	1.7(3)
N(2A)-C(7A)-C(8A)-C(9A)	110.83(18)	N(2B)-C(7B)-C(8B)-C(9B)	-112.98(19)
C(12A)-C(7A)-C(8A)-C(9A)	-67.48(15)	C(12B)-C(7B)-C(8B)-C(9B)	66.56(16)
N(2A)-C(7A)-C(8A)-C(13A)	-146.90(16)	N(2B)-C(7B)-C(8B)-C(13B)	145.72(17)
C(12A)-C(7A)-C(8A)-C(13A)	34.80(15)	C(12B)-C(7B)-C(8B)-C(13B)	-34.74(15)
C(7A)-C(8A)-C(9A)-C(14A)	-113.73(19)	C(7B)-C(8B)-C(9B)-C(9B)#1	116.45(11)
C(13A)-C(8A)-C(9A)-C(14A)	144.41(18)	C(13B)-C(8B)-C(9B)-C(9B)#1	-142.01(9)
C(7A)-C(8A)-C(9A)-C(10A)	67.07(15)	C(7B)-C(8B)-C(9B)-C(10B)	-66.41(16)

C(13A)-C(8A)-C(9A)-C(10A)	-34.78(15)	C(13B)-C(8B)-C(9B)-C(10B)	35.13(15)
C(14A)-C(9A)-C(10A)-C(10A)#1	-0.68(17)	C(9B)#1-C(9B)-C(10B)-C(14B)	-1.96(18)
C(8A)-C(9A)-C(10A)-C(10A)#1	178.64(7)	C(8B)-C(9B)-C(10B)-C(14B)	-179.56(13)
C(14A)-C(9A)-C(10A)-C(11A)	-179.15(13)	C(9B)#1-C(9B)-C(10B)-C(11B)	177.18(7)
C(8A)-C(9A)-C(10A)-C(11A)	0.18(16)	C(8B)-C(9B)-C(10B)-C(11B)	-0.42(16)
C(10A)#1-C(10A)-C(11A)-C(12A)	114.45(11)	C(14B)-C(10B)-C(11B)-C(12B)	-113.80(19)
C(9A)-C(10A)-C(11A)-C(12A)	-67.38(15)	C(9B)-C(10B)-C(11B)-C(12B)	67.22(15)
C(10A)#1-C(10A)-C(11A)-C(13A)	-143.94(9)	C(14B)-C(10B)-C(11B)-C(13B)	144.82(17)
C(9A)-C(10A)-C(11A)-C(13A)	34.24(15)	C(9B)-C(10B)-C(11B)-C(13B)	-34.16(15)
N(2A)-C(7A)-C(12A)-N(1A)	0.9(3)	N(2B)-C(7B)-C(12B)-N(1B)	1.6(3)
C(8A)-C(7A)-C(12A)-N(1A)	179.35(15)	C(8B)-C(7B)-C(12B)-N(1B)	-177.95(14)
N(2A)-C(7A)-C(12A)-C(11A)	-178.30(14)	N(2B)-C(7B)-C(12B)-C(11B)	179.40(15)
C(8A)-C(7A)-C(12A)-C(11A)	0.11(16)	C(8B)-C(7B)-C(12B)-C(11B)	-0.17(16)
C(10A)-C(11A)-C(12A)-N(1A)	-112.21(18)	C(10B)-C(11B)-C(12B)-N(1B)	110.74(18)
C(13A)-C(11A)-C(12A)-N(1A)	146.05(17)	C(13B)-C(11B)-C(12B)-N(1B)	-147.70(16)
C(10A)-C(11A)-C(12A)-C(7A)	66.97(16)	C(10B)-C(11B)-C(12B)-C(7B)	-66.90(15)
C(13A)-C(11A)-C(12A)-C(7A)	-34.78(15)	C(13B)-C(11B)-C(12B)-C(7B)	34.67(15)
C(7A)-C(8A)-C(13A)-C(11A)	-53.78(13)	C(7B)-C(8B)-C(13B)-C(11B)	53.71(13)
C(9A)-C(8A)-C(13A)-C(11A)	53.48(14)	C(9B)-C(8B)-C(13B)-C(11B)	-53.55(13)
C(12A)-C(11A)-C(13A)-C(8A)	53.90(13)	C(12B)-C(11B)-C(13B)-C(8B)	-53.77(13)
C(10A)-C(11A)-C(13A)-C(8A)	-53.10(13)	C(10B)-C(11B)-C(13B)-C(8B)	53.59(14)
C(10A)-C(9A)-C(14A)-C(14A)#1	0.68(17)	C(9B)-C(10B)-C(14B)-C(14B)#1	1.96(17)

C(8A)-C(9A)-C(14A)-C(14A)#1	-178.42(13)	C(11B)-C(10B)-C(14B)-C(14B)#1	-176.91(13)
C(10A)-C(9A)-C(14A)-C(15A)	-179.22(15)	C(9B)-C(10B)-C(14B)-C(15B)	-176.81(15)
C(8A)-C(9A)-C(14A)-C(15A)	1.7(3)	C(11B)-C(10B)-C(14B)-C(15B)	4.3(3)
C(9A)-C(14A)-C(15A)-C(17A)	112.05(18)	C(10B)-C(14B)-C(15B)-C(17B)	110.82(19)
C(14A)#1-C(14A)-C(15A)-C(17A)	-67.86(11)	C(14B)#1-C(14B)-C(15B)-C(17B)	-68.07(11)
C(9A)-C(14A)-C(15A)-C(16A)	-146.30(18)	C(10B)-C(14B)-C(15B)-C(16B)	-147.36(18)
C(14A)#1-C(14A)-C(15A)-C(16A)	33.79(11)	C(14B)#1-C(14B)-C(15B)-C(16B)	33.76(11)
C(17A)-C(15A)-C(16A)-C(15A)#1	53.88(16)	C(17B)-C(15B)-C(16B)-C(15B)#1	53.37(17)
C(14A)-C(15A)-C(16A)-C(15A)#1	-51.93(16)	C(14B)-C(15B)-C(16B)-C(15B)#1	-52.22(16)
C(14A)-C(15A)-C(17A)-N(3A)	-109.50(18)	C(14B)-C(15B)-C(17B)-N(3B)	-109.47(18)
C(16A)-C(15A)-C(17A)-N(3A)	148.17(17)	C(16B)-C(15B)-C(17B)-N(3B)	148.25(17)
C(14A)-C(15A)-C(17A)-C(17A)#1	67.61(11)	C(14B)-C(15B)-C(17B)-C(17B)#1	67.96(11)
C(16A)-C(15A)-C(17A)-C(17A)#1	-34.72(12)	C(16B)-C(15B)-C(17B)-C(17B)#1	-34.32(11)
N(3A)-C(18A)-C(19A)-C(20A)	-179.91(16)	N(3B)-C(18B)-C(19B)-C(20B)	-179.65(16)
C(18A)#1-C(18A)-C(19A)-C(20A)	0.7(2)	C(18B)#1-C(18B)-C(19B)-C(20B)	0.1(2)
C(18A)-C(19A)-C(20A)-C(20A)#1	-0.7(2)	C(18B)-C(19B)-C(20B)-C(20B)#1	-0.1(2)
C(7A)-C(12A)-N(1A)-C(1A)	1.1(2)	C(7B)-C(12B)-N(1B)-C(1B)	-3.5(2)
C(11A)-C(12A)-N(1A)-C(1A)	-179.81(15)	C(11B)-C(12B)-N(1B)-C(1B)	179.28(14)
C(2A)-C(1A)-N(1A)-C(12A)	179.14(16)	C(2B)-C(1B)-N(1B)-C(12B)	-177.00(15)
C(6A)-C(1A)-N(1A)-C(12A)	-1.1(2)	C(6B)-C(1B)-N(1B)-C(12B)	2.5(2)
C(12A)-C(7A)-N(2A)-C(6A)	-2.9(2)	C(12B)-C(7B)-N(2B)-C(6B)	1.4(2)
C(8A)-C(7A)-N(2A)-C(6A)	179.08(14)	C(8B)-C(7B)-N(2B)-C(6B)	-179.17(15)

C(5A)-C(6A)-N(2A)-C(7A)	-177.59(15)	C(1B)-C(6B)-N(2B)-C(7B)	-2.2(2)
C(1A)-C(6A)-N(2A)-C(7A)	2.8(2)	C(5B)-C(6B)-N(2B)-C(7B)	178.65(16)
C(17A)#1-C(17A)-N(3A)-C(18A)	1.18(16)	C(17B)#1-C(17B)-N(3B)-C(18B)	1.62(16)
C(15A)-C(17A)-N(3A)-C(18A)	177.85(15)	C(15B)-C(17B)-N(3B)-C(18B)	178.65(15)
C(19A)-C(18A)-N(3A)-C(17A)	179.50(15)	C(19B)-C(18B)-N(3B)-C(17B)	178.20(15)
C(18A)#1-C(18A)-N(3A)-C(17A)	-1.16(16)	C(18B)#1-C(18B)-N(3B)-C(17B)	-1.59(16)

Symmetry transformations used to generate equivalent atoms:

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

Table S11. Hydrogen bonds for **1**$_{syn}$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1D)-H(1D)...N(1B)	0.95(3)	2.03(3)	2.971(2)	171(2)
O(1D)-H(2D)...N(3B)	0.96(3)	2.01(3)	2.9463(19)	165.5(18)
O(2D)-H(3D)...O(1D)	1.04(3)	1.84(3)	2.874(2)	172(3)
O(2D)-H(4D)...O(3D)	1.08(3)	1.87(3)	2.860(2)	150(2)
O(3D)-H(5D)...N(3A)	0.95(3)	2.00(3)	2.929(2)	167.3(18)
O(3D)-H(6D)...N(2A)	0.85(3)	2.12(3)	2.967(2)	173(2)

Symmetry transformations used to generate equivalent atoms:

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

Figure S30. Energy minimized structure of compound **1**$_{syn}$

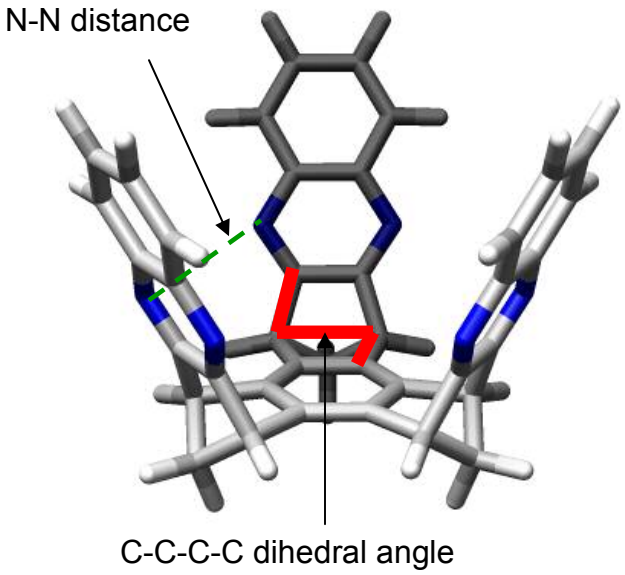


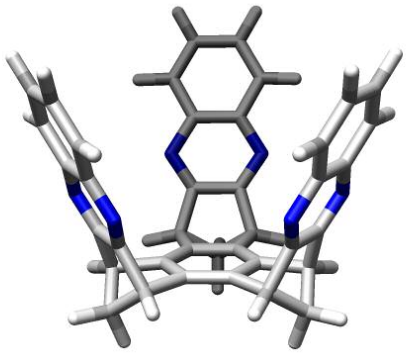
Table S12. Calculated energies, for relaxed potential energy scan, along the N-N distance in **1**$_{syn}$.

Conformation #	**N-N distance** (Å)	**C-C-C-C** (º)	**Relative energy** (kcal/mol)
1	5.25	113.0	0.75
2	5.15	112.7	0.43
3	5.05	112.4	0.20
4	4.95	112.1	0.05
5 (opt)	4.85	111.8	0.00
6	4.65	111.3	0.30
7	4.45	110.8	0.00
8	4.25	110.3	1.61
9	4.05	109.8	2.82
10	3.85	109.3	4.50
11	3.65	108.9	6.76
12	3.45	108.5	9.94

RIDFT BP86 using TURBOMOLE

Compound **1**$_{syn}$

Structure



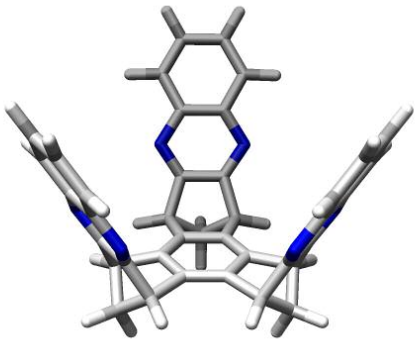
Coordinates

C	1.6375065	2.8362444	-3.1514093
C	0.3392670	2.8943491	-2.2759837
C	-0.0148130	1.4039582	-2.2682460
C	1.2232700	0.6891507	-2.2682460
C	2.3369464	1.7409884	-2.2759837
C	1.2232700	-0.6891507	-2.2682460
C	-0.0148130	-1.4039582	-2.2682460
C	-1.2084570	-0.7148076	-2.2682460
C	-1.2084570	0.7148076	-2.2682460
C	0.9895075	3.1554770	-0.9195418
C	2.2379695	2.4346771	-0.9195418
C	0.3392670	-2.8943491	-2.2759837
C	0.9895075	-3.1554770	-0.9195418
C	2.2379695	-2.4346771	-0.9195418
C	2.3369464	-1.7409884	-2.2759837
C	1.6375065	-2.8362444	-3.1514093
C	-2.6762133	1.1533607	-2.2759837
C	-3.2274769	0.7207999	-0.9195418
C	-3.2274769	-0.7207999	-0.9195418
C	-2.6762133	-1.1533607	-2.2759837
C	-3.2750129	0.0000000	-3.1514093
N	-3.6356903	1.4514158	0.0834363
C	-4.0751140	0.7194800	1.1735308
C	-4.0751140	-0.7194800	1.1735308
N	-3.6356903	-1.4514158	0.0834363
N	0.5608822	-3.8743080	0.0834363
C	1.4144691	-3.8888922	1.1735308
C	2.6606449	-3.1694123	1.1735308
N	3.0748081	-2.4228922	0.0834363
N	3.0748081	2.4228922	0.0834363
C	2.6606449	3.1694123	1.1735308
C	1.4144691	3.8888922	1.1735308
N	0.5608822	3.8743080	0.0834363
C	-4.5418445	1.4091705	2.3163269
C	-4.9893690	0.7069139	3.4219408
C	-4.9893690	-0.7069139	3.4219408
C	-4.5418445	-1.4091705	2.3163269
C	1.0505447	-4.6379380	2.3163269
C	1.8824791	-4.6743772	3.4219408
C	3.1068898	-3.9674634	3.4219408
C	3.4912997	-3.2287674	2.3163269
C	3.4912997	3.2287674	2.3163269
C	3.1068898	3.9674634	3.4219408
C	1.8824791	4.6743772	3.4219408
C	1.0505447	4.6379380	2.3163269
H	-2.8855700	-2.1885169	-2.5607553
H	-2.8855700	2.1885169	-2.5607553
H	3.3380962	-1.4047185	-2.5607553
H	-0.4525262	-3.5932354	-2.5607553

H	-0.4525262	3.5932354	-2.5607553
H	3.3380962	1.4047185	-2.5607553
H	-4.5308014	-2.4999149	2.2920049
H	-5.3446924	-1.2464030	4.3015640
H	-5.3446924	1.2464030	4.3015640
H	-4.5308014	2.4999149	2.2920049
H	4.4303905	-2.6738317	2.2920049
H	3.7517628	-4.0054379	4.3015640
H	1.5929296	-5.2518409	4.3015640
H	0.1004109	-5.1737465	2.2920049
H	0.1004109	5.1737465	2.2920049
H	1.5929296	5.2518409	4.3015640
H	3.7517628	4.0054379	4.3015640
H	4.4303905	2.6738317	2.2920049
H	-4.3745467	0.0000000	-3.1649626
H	-2.8805209	0.0000000	-4.1766611
H	2.1872733	-3.7884686	-3.1649626
H	1.4402604	-2.4946043	-4.1766611
H	2.1872733	3.7884686	-3.1649626
H	1.4402604	2.4946043	-4.1766611

Compound **1**$_{syn}$-1

Structure



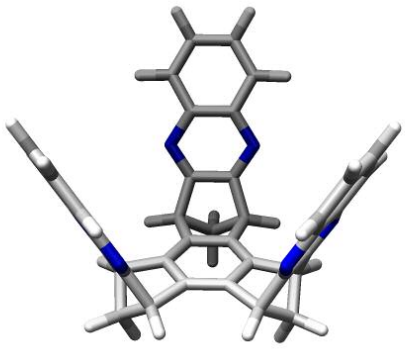
Coordinates

C	-1.6021595	2.7750217	3.0978120
C	-0.3380719	2.8929141	2.1758991
C	0.0148581	1.4046846	2.0706124
C	-1.2239216	0.6894748	2.0706124
C	-2.3363012	1.7392359	2.1758991
C	-1.2239216	-0.6894748	2.0706124
C	0.0148581	-1.4046846	2.0706124
C	1.2090635	-0.7152098	2.0706124
C	1.2090635	0.7152098	2.0706124
C	-1.0470755	3.2546291	0.8738343
C	-2.2950537	2.5341085	0.8738343
C	-0.3380719	-2.8929141	2.1758991
C	-1.0470755	-3.2546291	0.8738343
C	-2.2950537	-2.5341085	0.8738343
C	-2.3363012	-1.7392359	2.1758991
C	-1.6021595	-2.7750217	3.0978120
C	2.6743731	1.1536782	2.1758991
C	3.3421292	0.7205205	0.8738343
C	3.3421292	-0.7205205	0.8738343
C	2.6743731	-1.1536782	2.1758991
C	3.2043190	0.0000000	3.0978120
N	3.8669606	1.4500923	-0.0748794
C	4.4167996	0.7192479	-1.1138782
C	4.4167996	-0.7192479	-1.1138782
N	3.8669606	-1.4500923	-0.0748794
N	-0.6776636	-4.0739323	-0.0748794
C	-1.5855129	-4.1846846	-1.1138782
C	-2.8312867	-3.4654367	-1.1138782
N	-3.1892971	-2.6238400	-0.0748794
N	-3.1892971	2.6238400	-0.0748794

C	-2.8312867	3.4654367	-1.1138782
C	-1.5855129	4.1846846	-1.1138782
N	-0.6776636	4.0739323	-0.0748794
C	5.0016972	1.4092839	-2.2011923
C	5.5619184	0.7070410	-3.2542379
C	5.5619184	-0.7070410	-3.2542379
C	5.0016972	-1.4092839	-2.2011923
C	-1.2803730	-5.0362388	-2.2011923
C	-2.1686438	-5.1702831	-3.2542379
C	-3.3932747	-4.4632421	-3.2542379
C	-3.7213243	-3.6269549	-2.2011923
C	-3.7213243	3.6269549	-2.2011923
C	-3.3932747	4.4632421	-3.2542379
C	-2.1686438	5.1702831	-3.2542379
C	-1.2803730	5.0362388	-2.2011923
H	2.8615622	-2.1886904	2.4765555
H	2.8615622	2.1886904	2.4765555
H	-3.3262425	-1.3838404	2.4765555
H	0.4646804	-3.5725307	2.4765555
H	0.4646804	3.5725307	2.4765555
H	-3.3262425	1.3838404	2.4765555
H	4.9889055	-2.5000111	-2.1777118
H	6.0068234	-1.2464525	-4.0920529
H	6.0068234	1.2464525	-4.0920529
H	4.9889055	2.5000111	-2.1777118
H	-4.6595259	-3.0705133	-2.1777118
H	-4.0828712	-4.5788355	-4.0920529
H	-1.9239522	-5.8252879	-4.0920529
H	-0.3293796	-5.5705245	-2.1777118
H	-0.3293796	5.5705245	-2.1777118
H	-1.9239522	5.8252879	-4.0920529
H	-4.0828712	4.5788355	-4.0920529
H	-4.6595259	3.0705133	-2.1777118
H	4.2994887	0.0000000	3.1967151
H	2.7306505	0.0000000	4.0888588
H	-2.1497444	-3.7234664	3.1967151
H	-1.3653252	-2.3648127	4.0888588
H	-2.1497444	3.7234664	3.1967151
H	-1.3653252	2.3648127	4.0888588

Compound **1**$_{syn}$-2

Structure



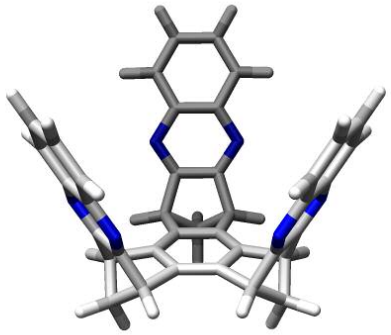
Coordinates

C	-1.6116941	2.7915360	3.1139975
C	-0.3386802	2.8938327	2.2036681
C	0.0148948	1.4045335	2.1230611
C	-1.2238090	0.6893675	2.1230611
C	-2.3367925	1.7402220	2.2036681
C	-1.2238090	-0.6893675	2.1230611
C	0.0148948	-1.4045335	2.1230611
C	1.2089143	-0.7151660	2.1230611
C	1.2089143	0.7151660	2.1230611
C	-1.0329578	3.2302308	0.8866649
C	-2.2809830	2.5096831	0.8866649

C	-0.3386802	-2.8938327	2.2036681
C	-1.0329578	-3.2302308	0.8866649
C	-2.2809830	-2.5096831	0.8866649
C	-2.3367925	-1.7402220	2.2036681
C	-1.6116941	-2.7915360	3.1139975
C	2.6754727	1.1536107	2.2036681
C	3.3139408	0.7205477	0.8866649
C	3.3139408	-0.7205477	0.8866649
C	2.6754727	-1.1536107	2.2036681
C	3.2233881	0.0000000	3.1139975
N	3.8095212	1.4506042	-0.0770607
C	4.3319346	0.7193233	-1.1300736
C	4.3319346	-0.7193233	-1.1300736
N	3.8095212	-1.4506042	-0.0770607
N	-0.6485005	-4.0244442	-0.0770607
C	-1.5430151	-4.1112270	-1.1300736
C	-2.7889195	-3.3919038	-1.1300736
N	-3.1610207	-2.5738400	-0.0770607
N	-3.1610207	2.5738400	-0.0770607
C	-2.7889195	3.3919038	-1.1300736
C	-1.5430151	4.1112270	-1.1300736
N	-0.6485005	4.0244442	-0.0770607
C	4.8866773	1.4091995	-2.2329228
C	5.4190108	0.7070099	-3.3002785
C	5.4190108	-0.7070099	-3.3002785
C	4.8866773	-1.4091995	-2.2329228
C	-1.2229361	-4.9365864	-2.2329228
C	-2.0972169	-5.0465060	-3.3002785
C	-3.3217939	-4.3394961	-3.3002785
C	-3.6637412	-3.5273869	-2.2329228
C	-3.6637412	3.5273869	-2.2329228
C	-3.3217939	4.3394961	-3.3002785
C	-2.0972169	5.0465060	-3.3002785
C	-1.2229361	4.9365864	-2.2329228
H	2.8684947	-2.1887276	2.5003243
H	2.8684947	2.1887276	2.5003243
H	-3.3297411	-1.3898255	2.5003243
H	0.4612463	-3.5785531	2.5003243
H	0.4612463	3.5785531	2.5003243
H	-3.3297411	1.3898255	2.5003243
H	4.8745985	-2.4999057	-2.2091428
H	5.8415170	-1.2464560	-4.1496330
H	5.8415170	1.2464560	-4.1496330
H	4.8745985	2.4999057	-2.2091428
H	-4.6022811	-2.9715733	-2.2091428
H	-4.0002211	-4.4356741	-4.1496330
H	-1.8412959	-5.6821302	-4.1496330
H	-0.2723174	-5.4714790	-2.2091428
H	-0.2723174	5.4714790	-2.2091428
H	-1.8412959	5.6821302	-4.1496330
H	-4.0002211	4.4356741	-4.1496330
H	-4.6022811	2.9715733	-2.2091428
H	4.3203909	0.0000000	3.1914490
H	2.7699172	0.0000000	4.1142427
H	-2.1601954	-3.7415682	3.1914490
H	-1.3849586	-2.3988187	4.1142427
H	-2.1601954	3.7415682	3.1914490
H	-1.3849586	2.3988187	4.1142427

Compound **1**$_{syn}$-3

Structure



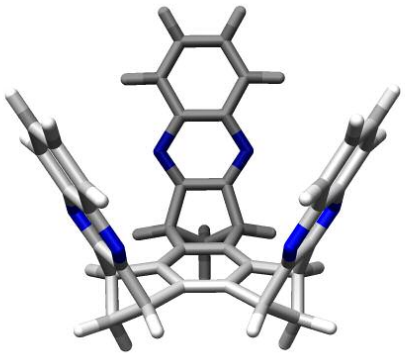
Coordinates

C	-1.6204916	2.8067738	3.1290356
C	-0.3390438	2.8942673	2.2299977
C	0.0148297	1.4042949	2.1734542
C	-1.2235699	0.6893046	2.1734542
C	-2.3369870	1.7407542	2.2299977
C	-1.2235699	-0.6893046	2.1734542
C	0.0148297	-1.4042949	2.1734542
C	1.2087402	-0.7149903	2.1734542
C	1.2087402	0.7149903	2.1734542
C	-1.0187960	3.2059120	0.8991782
C	-2.2670032	2.4852592	0.8991782
C	-0.3390438	-2.8942673	2.2299977
C	-1.0187960	-3.2059120	0.8991782
C	-2.2670032	-2.4852592	0.8991782
C	-2.3369870	-1.7407542	2.2299977
C	-1.6204916	-2.8067738	3.1290356
C	2.6760309	1.1535130	2.2299977
C	3.2857992	0.7206528	0.8991782
C	3.2857992	-0.7206528	0.8991782
C	2.6760309	-1.1535130	2.2299977
C	3.2409832	0.0000000	3.1290356
N	3.7519176	1.4508318	-0.0789191
C	4.2456891	0.7194158	-1.1455696
C	4.2456891	-0.7194158	-1.1455696
N	3.7519176	-1.4508318	-0.0789191
N	-0.6195015	-3.9746718	-0.0789191
C	-1.4998123	-4.0365825	-1.1455696
C	-2.7458769	-3.3171668	-1.1455696
N	-3.1324160	-2.5238400	-0.0789191
N	-3.1324160	2.5238400	-0.0789191
C	-2.7458769	3.3171668	-1.1455696
C	-1.4998123	4.0365825	-1.1455696
N	-0.6195015	3.9746718	-0.0789191
C	4.7705905	1.4091965	-2.2629370
C	5.2729081	0.7069614	-3.3447700
C	5.2729081	-0.7069614	-3.3447700
C	4.7705905	-1.4091965	-2.2629370
C	-1.1648953	-4.8360508	-2.2629370
C	-2.0242075	-4.9199530	-3.3447700
C	-3.2487005	-4.2129916	-3.3447700
C	-3.6056952	-3.4268543	-2.2629370
C	-3.6056952	3.4268543	-2.2629370
C	-3.2487005	4.2129916	-3.3447700
C	-2.0242075	4.9199530	-3.3447700
C	-1.1648953	4.8360508	-2.2629370
H	2.8745032	-2.1885995	2.5228457
H	2.8745032	2.1885995	2.5228457
H	-3.3326343	-1.3950930	2.5228457
H	0.4581311	-3.5836925	2.5228457
H	0.4581311	3.5836925	2.5228457
H	-3.3326343	1.3950930	2.5228457

H	4.7585776	-2.4999271	-2.2391770
H	5.6719403	-1.2463961	-4.2053739
H	5.6719403	1.2463961	-4.2053739
H	4.7585776	2.4999271	-2.2391770
H	-4.5442892	-2.8710855	-2.2391770
H	-3.9153809	-4.2888463	-4.2053739
H	-1.7565594	-5.5352425	-4.2053739
H	-0.2142884	-5.3710127	-2.2391770
H	-0.2142884	5.3710127	-2.2391770
H	-1.7565594	5.5352425	-4.2053739
H	-3.9153809	4.2888463	-4.2053739
H	-4.5442892	2.8710855	-2.2391770
H	4.3391204	0.0000000	3.1849314
H	2.8066952	0.0000000	4.1379709
H	-2.1695602	-3.7577885	3.1849314
H	-1.4033476	-2.4306694	4.1379709
H	-2.1695602	3.7577885	3.1849314
H	-1.4033476	2.4306694	4.1379709

Compound **1**$_{syn}$-4

Structure



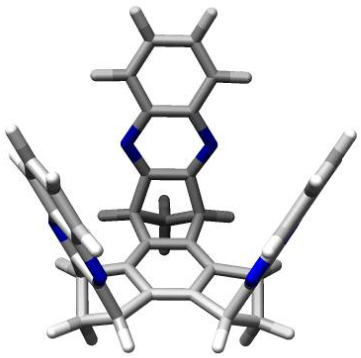
Coordinates

C	-1.6292015	2.8218599	3.1410872
C	-0.3392622	2.8944878	2.2537497
C	0.0148194	1.4041210	2.2215837
C	-1.2234141	0.6892265	2.2215837
C	-2.3370689	1.7410536	2.2537497
C	-1.2234141	-0.6892265	2.2215837
C	0.0148194	-1.4041210	2.2215837
C	1.2085948	-0.7148945	2.2215837
C	1.2085948	0.7148945	2.2215837
C	-1.0043746	3.1810698	0.9097962
C	-2.2527000	2.4603489	0.9097962
C	-0.3392622	-2.8944878	2.2537497
C	-1.0043746	-3.1810698	0.9097962
C	-2.2527000	-2.4603489	0.9097962
C	-2.3370689	-1.7410536	2.2537497
C	-1.6292015	-2.8218599	3.1410872
C	2.6763311	1.1534342	2.2537497
C	3.2570746	0.7207210	0.9097962
C	3.2570746	-0.7207210	0.9097962
C	2.6763311	-1.1534342	2.2537497
C	3.2584031	0.0000000	3.1410872
N	3.6943469	1.4511164	-0.0812057
C	4.1611605	0.7194573	-1.1599072
C	4.1611605	-0.7194573	-1.1599072
N	3.6943469	-1.4511164	-0.0812057
N	-0.5904697	-3.9249564	-0.0812057
C	-1.4575119	-3.9633993	-1.1599072
C	-2.7036486	-3.2439420	-1.1599072
N	-3.1038771	-2.4738400	-0.0812057
N	-3.1038771	2.4738400	-0.0812057
C	-2.7036486	3.2439420	-1.1599072
C	-1.4575119	3.9633993	-1.1599072

N	-0.5904697	3.9249564	-0.0812057
C	4.6570982	1.4092161	-2.2903806
C	5.1319836	0.7069603	-3.3845280
C	5.1319836	-0.7069603	-3.3845280
C	4.6570982	-1.4092161	-2.2903806
C	-1.1081321	-4.7377734	-2.2903806
C	-1.9537463	-4.7979083	-3.3845280
C	-3.1782374	-4.0909481	-3.3845280
C	-3.5489661	-3.3285573	-2.2903806
C	-3.5489661	3.3285573	-2.2903806
C	-3.1782374	4.0909481	-3.3845280
C	-1.9537463	4.7979083	-3.3845280
C	-1.1081321	4.7377734	-2.2903806
H	2.8802899	-2.1885571	2.5425820
H	2.8802899	2.1885571	2.5425820
H	-3.3354910	-1.4001257	2.5425820
H	0.4552011	-3.5886828	2.5425820
H	0.4552011	3.5886828	2.5425820
H	-3.3354910	1.4001257	2.5425820
H	4.6455957	-2.4999457	-2.2663509
H	5.5091667	-1.2463317	-4.2550003
H	5.5091667	1.2463317	-4.2550003
H	4.6455957	2.4999457	-2.2663509
H	-4.4878143	-2.7732310	-2.2663509
H	-3.8339382	-4.1479124	-4.2550003
H	-1.6752284	-5.3942441	-4.2550003
H	-0.1577814	-5.2731767	-2.2663509
H	-0.1577814	5.2731767	-2.2663509
H	-1.6752284	5.3942441	-4.2550003
H	-3.8339382	4.1479124	-4.2550003
H	-4.4878143	2.7732310	-2.2663509
H	4.3574509	0.0000000	3.1756740
H	2.8440038	0.0000000	4.1584096
H	-2.1787255	-3.7736632	3.1756740
H	-1.4220019	-2.4629796	4.1584096
H	-2.1787255	3.7736632	3.1756740
H	-1.4220019	2.4629796	4.1584096

Compound **1**$_{syn}$-6

Structure



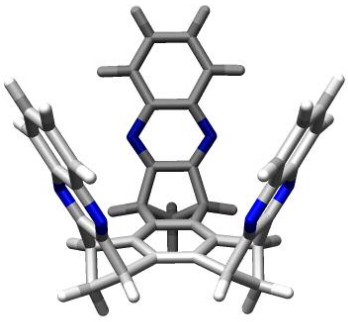
Coordinates

C	-1.6526435	2.8624625	-3.1661890
C	-0.3389560	2.8934910	-2.3144961
C	0.0147699	1.4037746	-2.3530372
C	-1.2230894	0.6890962	-2.3530372
C	-2.3363587	1.7402900	-2.3144961
C	-1.2230894	-0.6890962	-2.3530372
C	0.0147699	-1.4037746	-2.3530372
C	1.2083195	-0.7146784	-2.3530372
C	1.2083195	0.7146784	-2.3530372
C	-0.9607793	3.1058483	-0.9365550
C	-2.2093539	2.3849834	-0.9365550
C	-0.3389560	-2.8934910	-2.3144961
C	-0.9607793	-3.1058483	-0.9365550

C	-2.2093539	-2.3849834	-0.9365550
C	-2.3363587	-1.7402900	-2.3144961
C	-1.6526435	-2.8624625	-3.1661890
C	2.6753147	1.1532010	-2.3144961
C	3.1701332	0.7208649	-0.9365550
C	3.1701332	-0.7208649	-0.9365550
C	2.6753147	-1.1532010	-2.3144961
C	3.3052870	0.0000000	-3.1661890
N	3.5215700	1.4518981	0.0873396
C	3.9075431	0.7194097	1.1973696
C	3.9075431	-0.7194097	1.1973696
N	3.5215700	-1.4518981	0.0873396
N	-0.5034043	-3.7757181	0.0873396
C	-1.3307444	-3.7437364	1.1973696
C	-2.5767986	-3.0243267	1.1973696
N	-3.0181657	-2.3238200	0.0873396
N	-3.0181657	2.3238200	0.0873396
C	-2.5767986	3.0243267	1.1973696
C	-1.3307444	3.7437364	1.1973696
N	-0.5034043	3.7757181	0.0873396
C	4.3172381	1.4088664	2.3618420
C	4.7106262	0.7067801	3.4877821
C	4.7106262	-0.7067801	3.4877821
C	4.3172381	-1.4088664	2.3618420
C	-0.9385049	-4.4432711	2.3618420
C	-1.7432236	-4.4329120	3.4877821
C	-2.9674026	-3.7261319	3.4877821
C	-3.3787332	-3.0344046	2.3618420
C	-3.3787332	3.0344046	2.3618420
C	-2.9674026	3.7261319	3.4877821
C	-1.7432236	4.4329120	3.4877821
C	-0.9385049	4.4432711	2.3618420
H	2.8944135	-2.1883546	-2.5915671
H	2.8944135	2.1883546	-2.5915671
H	-3.3423774	-1.4124584	-2.5915671
H	0.4479639	-3.6008129	-2.5915671
H	0.4479639	3.6008129	-2.5915671
H	-3.3423774	1.4124584	-2.5915671
H	4.3068142	-2.4996689	2.3372862
H	5.0229416	-1.2462457	4.3836129
H	5.0229416	1.2462457	4.3836129
H	4.3068142	2.4996689	2.3372862
H	-4.3181839	-2.4799760	2.3372862
H	-3.5907513	-3.7268722	4.3836129
H	-1.4321904	-4.9731179	4.3836129
H	0.0113697	-4.9796450	2.3372862
H	0.0113697	4.9796450	2.3372862
H	-1.4321904	4.9731179	4.3836129
H	-3.5907513	3.7268722	4.3836129
H	-4.3181839	2.4799760	2.3372862
H	4.4045597	0.0000000	-3.1394698
H	2.9494153	0.0000000	-4.2054905
H	-2.2022799	-3.8144606	-3.1394698
H	-1.4747076	-2.5542685	-4.2054905
H	-2.2022799	3.8144606	-3.1394698
H	-1.4747076	2.5542685	-4.2054905

Compound **1**$_{syn}$-7

Structure



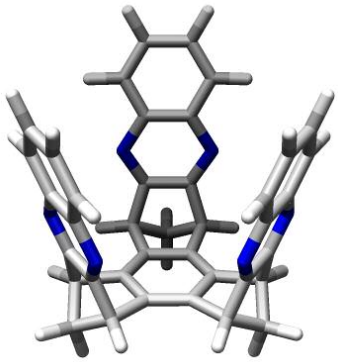
Coordinates

C	-1.6378866	2.8369028	3.1515115
C	-0.3392415	2.8943141	2.2766860
C	0.0148168	1.4039769	2.2699905
C	-1.2232881	0.6891568	2.2699905
C	-2.3369288	1.7409488	2.2766860
C	-1.2232881	-0.6891568	2.2699905
C	0.0148168	-1.4039769	2.2699905
C	1.2084713	-0.7148202	2.2699905
C	1.2084713	0.7148202	2.2699905
C	-0.9890896	3.1547158	0.9198038
C	-2.2375192	2.4339346	0.9198038
C	-0.3392415	-2.8943141	2.2766860
C	-0.9890896	-3.1547158	0.9198038
C	-2.2375192	-2.4339346	0.9198038
C	-2.3369288	-1.7409488	2.2766860
C	-1.6378866	-2.8369028	3.1515115
C	2.6761703	1.1533653	2.2766860
C	3.2266088	0.7207811	0.9198038
C	3.2266088	-0.7207811	0.9198038
C	2.6761703	-1.1533653	2.2766860
C	3.2757732	0.0000000	3.1515115
N	3.6318723	1.4513908	-0.0843778
C	4.0720691	0.7194949	-1.1741426
C	4.0720691	-0.7194949	-1.1741426
N	3.6318723	-1.4513908	-0.0843778
N	-0.5589948	-3.8709891	-0.0843778
C	-1.4129337	-3.8862628	-1.1741426
C	-2.6591354	-3.1667678	-1.1741426
N	-3.0728775	-2.4195982	-0.0843778
N	-3.0728775	2.4195982	-0.0843778
C	-2.6591354	3.1667678	-1.1741426
C	-1.4129337	3.8862628	-1.1741426
N	-0.5589948	3.8709891	-0.0843778
C	4.5387705	1.4091737	-2.3169529
C	4.9869103	0.7069444	-3.4223116
C	4.9869103	-0.7069444	-3.4223116
C	4.5387705	-1.4091737	-2.3169529
C	-1.0490051	-4.6352774	-2.3169529
C	-1.8812233	-4.6722632	-3.4223116
C	-3.1056870	-3.9653188	-3.4223116
C	-3.4897655	-3.2261037	-2.3169529
C	-3.4897655	3.2261037	-2.3169529
C	-3.1056870	3.9653188	-3.4223116
C	-1.8812233	4.6722632	-3.4223116
C	-1.0490051	4.6352774	-2.3169529
H	2.8858683	-2.1885136	2.5612421
H	2.8858683	2.1885136	2.5612421
H	-3.3382425	-1.4049785	2.5612421
H	0.4523742	-3.5934920	2.5612421
H	0.4523742	3.5934920	2.5612421
H	-3.3382425	1.4049785	2.5612421

H	4.5277110	-2.4999020	-2.2926399
H	5.3425165	-1.2463186	-4.3018306
H	5.3425165	1.2463186	-4.3018306
H	4.5277110	2.4999020	-2.2926399
H	-4.4288341	-2.6711618	-2.2926399
H	-3.7506018	-4.0035957	-4.3018306
H	-1.5919147	-5.2499143	-4.3018306
H	-0.0988769	-5.1710638	-2.2926399
H	-0.0988769	5.1710638	-2.2926399
H	-1.5919147	5.2499143	-4.3018306
H	-3.7506018	4.0035957	-4.3018306
H	-4.4288341	2.6711618	-2.2926399
H	4.3752874	0.0000000	3.1640751
H	2.8821933	0.0000000	4.1771042
H	-2.1876437	-3.7891101	3.1640751
H	-1.4410966	-2.4960526	4.1771042
H	-2.1876437	3.7891101	3.1640751
H	-1.4410966	2.4960526	4.1771042

Compound **1**$_{syn}$-8

Structure



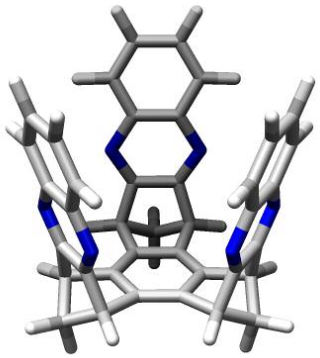
Coordinates

C	-1.6793698	2.9087539	-3.1753018
C	-0.3362114	2.8880186	-2.3737988
C	0.0145624	1.4034482	-2.5059862
C	-1.2227030	0.6891127	-2.5059862
C	-2.3329918	1.7351769	-2.3737988
C	-1.2227030	-0.6891127	-2.5059862
C	0.0145624	-1.4034482	-2.5059862
C	1.2081406	-0.7143355	-2.5059862
C	1.2081406	0.7143355	-2.5059862
C	-0.9008278	3.0023127	-0.9593254
C	-2.1496652	2.2812961	-0.9593254
C	-0.3362114	-2.8880186	-2.3737988
C	-0.9008278	-3.0023127	-0.9593254
C	-2.1496652	-2.2812961	-0.9593254
C	-2.3329918	-1.7351769	-2.3737988
C	-1.6793698	-2.9087539	-3.1753018
C	2.6692032	1.1528417	-2.3737988
C	3.0504930	0.7210166	-0.9593254
C	3.0504930	-0.7210166	-0.9593254
C	2.6692032	-1.1528417	-2.3737988
C	3.3587397	0.0000000	-3.1753018
N	3.2911270	1.4527592	0.0954509
C	3.5727119	0.7194988	1.2362617
C	3.5727119	-0.7194988	1.2362617
N	3.2911270	-1.4527592	0.0954509
N	-0.3874371	-3.5765792	0.0954509
C	-1.1632517	-3.4538086	1.2362617
C	-2.4094602	-2.7343099	1.2362617
N	-2.9036899	-2.1238200	0.0954509
N	-2.9036899	2.1238200	0.0954509
C	-2.4094602	2.7343099	1.2362617
C	-1.1632517	3.4538086	1.2362617

N	-0.3874371	3.5765792	0.0954509
C	3.8706849	1.4086188	2.4342756
C	4.1591676	0.7067213	3.5916934
C	4.1591676	-0.7067213	3.5916934
C	3.8706849	-1.4086188	2.4342756
C	-0.7154428	-4.0564209	2.4342756
C	-1.4675452	-3.9553054	3.5916934
C	-2.6916224	-3.2485841	3.5916934
C	-3.1552421	-2.6478020	2.4342756
C	-3.1552421	2.6478020	2.4342756
C	-2.6916224	3.2485841	3.5916934
C	-1.4675452	3.9553054	3.5916934
C	-0.7154428	4.0564209	2.4342756
H	2.9075885	-2.1881487	-2.6339564
H	2.9075885	2.1881487	-2.6339564
H	-3.3487866	-1.4239712	-2.6339564
H	0.4411981	-3.6121199	-2.6339564
H	0.4411981	3.6121199	-2.6339564
H	-3.3487866	1.4239712	-2.6339564
H	3.8625829	-2.4993601	2.4085540
H	4.3875381	-1.2462558	4.5125530
H	4.3875381	1.2462558	4.5125530
H	3.8625829	2.4993601	2.4085540
H	-4.0958009	-2.0954149	2.4085540
H	-3.2730582	-3.1765916	4.5125530
H	-1.1144799	-4.4228474	4.5125530
H	0.2332179	-4.5947750	2.4085540
H	0.2332179	4.5947750	2.4085540
H	-1.1144799	4.4228474	4.5125530
H	-3.2730582	3.1765916	4.5125530
H	-4.0958009	2.0954149	2.4085540
H	4.4528932	0.0000000	-3.0678324
H	3.0804328	0.0000000	-4.2380777
H	-2.2264466	-3.8563186	-3.0678324
H	-1.5402164	-2.6677330	-4.2380777
H	-2.2264466	3.8563186	-3.0678324
H	-1.5402164	2.6677330	-4.2380777

Compound **1**$_{syn}$-9

Structure



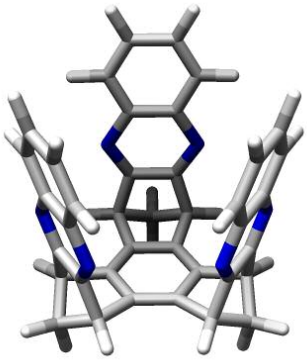
Coordinates

C	1.6902278	2.9275605	-3.1712906
C	0.3336148	2.8833284	-2.3950622
C	-0.0144231	1.4032665	-2.5719795
C	1.2224760	0.6891425	-2.5719795
C	2.3302282	1.7305831	-2.3950622
C	1.2224760	-0.6891425	-2.5719795
C	-0.0144231	-1.4032665	-2.5719795
C	-1.2080529	-0.7141240	-2.5719795
C	-1.2080529	0.7141240	-2.5719795
C	0.8701643	2.9495827	-0.9663536
C	2.1193314	2.2283757	-0.9663536
C	0.3336148	-2.8833284	-2.3950622
C	0.8701643	-2.9495827	-0.9663536

C	2.1193314	-2.2283757	-0.9663536
C	2.3302282	-1.7305831	-2.3950622
C	1.6902278	-2.9275605	-3.1712906
C	-2.6638430	1.1527453	-2.3950622
C	-2.9894957	0.7212070	-0.9663536
C	-2.9894957	-0.7212070	-0.9663536
C	-2.6638430	-1.1527453	-2.3950622
C	-3.3804556	0.0000000	-3.1712906
N	-3.1760147	1.4534489	0.0990832
C	-3.4065720	0.7196831	1.2512897
C	-3.4065720	-0.7196831	1.2512897
N	-3.1760147	-1.4534489	0.0990832
N	0.3292837	-3.4772339	0.0990832
C	1.0800222	-3.3100195	1.2512897
C	2.3265499	-2.5903364	1.2512897
N	2.8467311	-2.0237850	0.0990832
N	2.8467311	2.0237850	0.0990832
C	2.3265499	2.5903364	1.2512897
C	1.0800222	3.3100195	1.2512897
N	0.3292837	3.4772339	0.0990832
C	-3.6510812	1.4087135	2.4613998
C	-3.8874501	0.7067563	3.6308503
C	-3.8874501	-0.7067563	3.6308503
C	-3.6510812	-1.4087135	2.4613998
C	0.6055589	-3.8662858	2.4613998
C	1.3316561	-3.7200087	3.6308503
C	2.5557940	-3.0132524	3.6308503
C	3.0455223	-2.4575723	2.4613998
C	3.0455223	2.4575723	2.4613998
C	2.5557940	3.0132524	3.6308503
C	1.3316561	3.7200087	3.6308503
C	0.6055589	3.8662858	2.4613998
H	-2.9112325	-2.1880217	-2.6464465
H	-2.9112325	2.1880217	-2.6464465
H	3.3504987	-1.4271904	-2.6464465
H	-0.4392662	-3.6152122	-2.6464465
H	-0.4392662	3.6152122	-2.6464465
H	3.3504987	1.4271904	-2.6464465
H	-3.6447299	-2.4992699	2.4350050
H	-4.0747553	-1.2463304	4.5608014
H	-4.0747553	1.2463304	4.5608014
H	-3.6447299	2.4992699	2.4350050
H	3.9867962	-1.9067937	2.4350050
H	3.1167315	-2.9056764	4.5608014
H	0.9580238	-4.1520068	4.5608014
H	-0.3420663	-4.4060636	2.4350050
H	-0.3420663	4.4060636	2.4350050
H	0.9580238	4.1520068	4.5608014
H	3.1167315	2.9056764	4.5608014
H	3.9867962	1.9067937	2.4350050
H	-4.4703542	0.0000000	-3.0264601
H	-3.1392955	0.0000000	-4.2433753
H	2.2351771	-3.8714403	-3.0264601
H	1.5696478	-2.7187097	-4.2433753
H	2.2351771	3.8714403	-3.0264601
H	1.5696478	2.7187097	-4.2433753

Compound **1**$_{syn}$-10

Structure



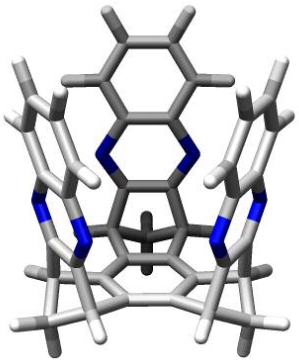
Coordinates

C	1.7004957	2.9453449	-3.1599731
C	0.3307236	2.8778252	-2.4109125
C	-0.0143531	1.4032261	-2.6334092
C	1.2224060	0.6891829	-2.6334092
C	2.3269079	1.7253277	-2.4109125
C	1.2224060	-0.6891829	-2.6334092
C	-0.0143531	-1.4032261	-2.6334092
C	-1.2080529	-0.7140432	-2.6334092
C	-1.2080529	0.7140432	-2.6334092
C	0.8386526	2.8954167	-0.9699082
C	2.0881781	2.1740028	-0.9699082
C	0.3307236	-2.8778252	-2.4109125
C	0.8386526	-2.8954167	-0.9699082
C	2.0881781	-2.1740028	-0.9699082
C	2.3269079	-1.7253277	-2.4109125
C	1.7004957	-2.9453449	-3.1599731
C	-2.6576316	1.1524975	-2.4109125
C	-2.9268307	0.7214139	-0.9699082
C	-2.9268307	-0.7214139	-0.9699082
C	-2.6576316	-1.1524975	-2.4109125
C	-3.4009914	0.0000000	-3.1599731
N	-3.0609209	1.4541004	0.1030587
C	-3.2432196	0.7197351	1.2637891
C	-3.2432196	-0.7197351	1.2637891
N	-3.0609209	-1.4541004	0.1030587
N	0.2711725	-3.3778854	0.1030587
C	0.9983009	-3.1685781	1.2637891
C	2.2449187	-2.4488430	1.2637891
N	2.7897483	-1.9237850	0.1030587
N	2.7897483	1.9237850	0.1030587
C	2.2449187	2.4488430	1.2637891
C	0.9983009	3.1685781	1.2637891
N	0.2711725	3.3778854	0.1030587
C	-3.4379391	1.4084477	2.4829088
C	-3.6284413	0.7067219	3.6608727
C	-3.6284413	-0.7067219	3.6608727
C	-3.4379391	-1.4084477	2.4829088
C	0.4992181	-3.6815664	2.4829088
C	1.2021815	-3.4956833	3.6608727
C	2.4262598	-2.7889614	3.6608727
C	2.9387210	-2.2731188	2.4829088
C	2.9387210	2.2731188	2.4829088
C	2.4262598	2.7889614	3.6608727
C	1.2021815	3.4956833	3.6608727
C	0.4992181	3.6815664	2.4829088
H	-2.9138397	-2.1877592	-2.6533647
H	-2.9138397	2.1877592	-2.6533647
H	3.3515749	-1.4295796	-2.6533647
H	-0.4377352	-3.6173388	-2.6533647
H	-0.4377352	3.6173388	-2.6533647
H	3.3515749	1.4295796	-2.6533647

H	-3.4333578	-2.4990070	2.4558357
H	-3.7786745	-1.2463462	4.5974991
H	-3.7786745	1.2463462	4.5974991
H	-3.4333578	2.4990070	2.4558357
H	3.8808824	-1.7238716	2.4558357
H	2.9687047	-2.6492551	4.5974991
H	0.8099698	-3.8956012	4.5974991
H	-0.4475246	-4.2228785	2.4558357
H	-0.4475246	4.2228785	2.4558357
H	0.8099698	3.8956012	4.5974991
H	2.9687047	2.6492551	4.5974991
H	3.8808824	1.7238716	2.4558357
H	-4.4848141	0.0000000	-2.9758790
H	-3.1988443	0.0000000	-4.2400505
H	2.2424071	-3.8839630	-2.9758790
H	1.5994221	-2.7702804	-4.2400505
H	2.2424071	3.8839630	-2.9758790
H	1.5994221	2.7702804	-4.2400505

Compound **1**$_{syn}$-11

Structure



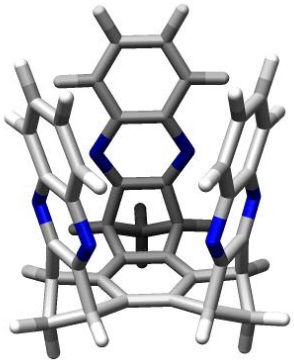
Coordinates

C	1.7095587	2.9610425	-3.1428603
C	0.3270788	2.8711173	-2.4215265
C	-0.0141124	1.4031828	-2.6896222
C	1.2222482	0.6893697	-2.6896222
C	2.3229211	1.7188172	-2.4215265
C	1.2222482	-0.6893697	-2.6896222
C	-0.0141124	-1.4031828	-2.6896222
C	-1.2081358	-0.7138131	-2.6896222
C	-1.2081358	0.7138131	-2.6896222
C	0.8066312	2.8402559	-0.9706955
C	2.0564181	2.1186911	-0.9706955
C	0.3270788	-2.8711173	-2.4215265
C	0.8066312	-2.8402559	-0.9706955
C	2.0564181	-2.1186911	-0.9706955
C	2.3229211	-1.7188172	-2.4215265
C	1.7095587	-2.9610425	-3.1428603
C	-2.6499999	1.1523001	-2.4215265
C	-2.8630494	0.7215648	-0.9706955
C	-2.8630494	-0.7215648	-0.9706955
C	-2.6499999	-1.1523001	-2.4215265
C	-3.4191174	0.0000000	-3.1428603
N	-2.9459222	1.4547669	0.1072210
C	-3.0846348	0.7197081	1.2737718
C	-3.0846348	-0.7197081	1.2737718
N	-2.9459222	-1.4547669	0.1072210
N	0.2130960	-3.2786269	0.1072210
C	0.9190319	-3.0312261	1.2737718
C	2.1656029	-2.3115181	1.2737718
N	2.7328261	-1.8238600	0.1072210
N	2.7328261	1.8238600	0.1072210
C	2.1656029	2.3115181	1.2737718
C	0.9190319	3.0312261	1.2737718

N	0.2130960	3.2786269	0.1072210
C	-3.2373360	1.4081749	2.4989693
C	-3.3872540	0.7066357	3.6828625
C	-3.3872540	-0.7066357	3.6828625
C	-3.2373360	-1.4081749	2.4989693
C	0.3991527	-3.5077027	2.4989693
C	1.0816625	-3.2867659	3.6828625
C	2.3055915	-2.5801302	3.6828625
C	2.8381833	-2.0995277	2.4989693
C	2.8381833	2.0995277	2.4989693
C	2.3055915	2.5801302	3.6828625
C	1.0816625	3.2867659	3.6828625
C	0.3991527	3.5077027	2.4989693
H	-2.9142815	-2.1875611	-2.6549317
H	-2.9142815	2.1875611	-2.6549317
H	3.3516242	-1.4300612	-2.6549317
H	-0.4373427	-3.6176223	-2.6549317
H	-0.4373427	3.6176223	-2.6549317
H	3.3516242	1.4300612	-2.6549317
H	-3.2363917	-2.4986963	2.4712752
H	-3.5067002	-1.2464052	4.6238385
H	-3.5067002	1.2464052	4.6238385
H	-3.2363917	2.4986963	2.4712752
H	3.7821304	-1.5534493	2.4712752
H	2.8327687	-2.4136889	4.6238385
H	0.6739315	-3.6600941	4.6238385
H	-0.5457386	-4.0521456	2.4712752
H	-0.5457386	4.0521456	2.4712752
H	0.6739315	3.6600941	4.6238385
H	2.8327687	2.4136889	4.6238385
H	3.7821304	1.5534493	2.4712752
H	-4.4955092	0.0000000	-2.9198530
H	-3.2557532	0.0000000	-4.2294250
H	2.2477546	-3.8932252	-2.9198530
H	1.6278766	-2.8195650	-4.2294250
H	2.2477546	3.8932252	-2.9198530
H	1.6278766	2.8195650	-4.2294250

Compound **1**$_{syn}$-12

Structure



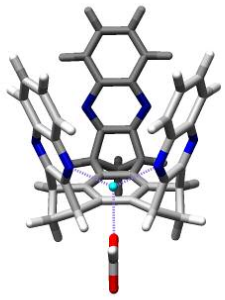
Coordinates

C	1.7175038	2.9748039	-3.1193431
C	0.3222247	2.8624971	-2.4272142
C	-0.0136200	1.4030664	-2.7417380
C	1.2219012	0.6897379	-2.7417380
C	2.3178828	1.7103034	-2.4272142
C	1.2219012	-0.6897379	-2.7417380
C	-0.0136200	-1.4030664	-2.7417380
C	-1.2082812	-0.7133285	-2.7417380
C	-1.2082812	0.7133285	-2.7417380
C	0.7734212	2.7831842	-0.9682980
C	2.0235976	2.0613945	-0.9682980
C	0.3222247	-2.8624971	-2.4272142
C	0.7734212	-2.7831842	-0.9682980

C	2.0235976	-2.0613945	-0.9682980
C	2.3178828	-1.7103034	-2.4272142
C	1.7175038	-2.9748039	-3.1193431
C	-2.6401076	1.1521937	-2.4272142
C	-2.7970188	0.7217897	-0.9682980
C	-2.7970188	-0.7217897	-0.9682980
C	-2.6401076	-1.1521937	-2.4272142
C	-3.4350077	0.0000000	-3.1193431
N	-2.8312799	1.4562006	0.1117158
C	-2.9368756	0.7199414	1.2815611
C	-2.9368756	-0.7199414	1.2815611
N	-2.8312799	-1.4562006	0.1117158
N	0.1545332	-3.1800606	0.1117158
C	0.8449503	-2.9033795	1.2815611
C	2.0919253	-2.1834382	1.2815611
N	2.6767467	-1.7238600	0.1117158
N	2.6767467	1.7238600	0.1117158
C	2.0919253	2.1834382	1.2815611
C	0.8449503	2.9033795	1.2815611
N	0.1545332	3.1800606	0.1117158
C	-3.0645065	1.4076711	2.5098854
C	-3.1912027	0.7064828	3.6966212
C	-3.1912027	-0.7064828	3.6966212
C	-3.0645065	-1.4076711	2.5098854
C	0.3131743	-3.3577760	2.5098854
C	0.9837693	-3.1169040	3.6966212
C	2.2074334	-2.4104212	3.6966212
C	2.7513322	-1.9501049	2.5098854
C	2.7513322	1.9501049	2.5098854
C	2.2074334	2.4104212	3.6966212
C	0.9837693	3.1169040	3.6966212
C	0.3131743	3.3577760	2.5098854
H	-2.9124732	-2.1875633	-2.6507012
H	-2.9124732	2.1875633	-2.6507012
H	3.3507220	-1.4284941	-2.6507012
H	-0.4382488	-3.6160575	-2.6507012
H	-0.4382488	3.6160575	-2.6507012
H	3.3507220	1.4284941	-2.6507012
H	-3.0689142	-2.4980235	2.4815702
H	-3.2939769	-1.2464008	4.6394514
H	-3.2939769	1.2464008	4.6394514
H	-3.0689142	2.4980235	2.4815702
H	3.6978089	-1.4087459	2.4815702
H	2.7264032	-2.2294673	4.6394514
H	0.5675737	-3.4758681	4.6394514
H	-0.6288947	-3.9067694	2.4815702
H	-0.6288947	3.9067694	2.4815702
H	0.5675737	3.4758681	4.6394514
H	2.7264032	2.2294673	4.6394514
H	3.6978089	1.4087459	2.4815702
H	-4.5023393	0.0000000	-2.8568074
H	-3.3117553	0.0000000	-4.2111464
H	2.2511696	-3.8991402	-2.8568074
H	1.6558776	-2.8680642	-4.2111464
H	2.2511696	3.8991402	-2.8568074
H	1.6558776	2.8680642	-4.2111464

Compound [$\mathbf{1}_{syn}$+Ag]

Structure



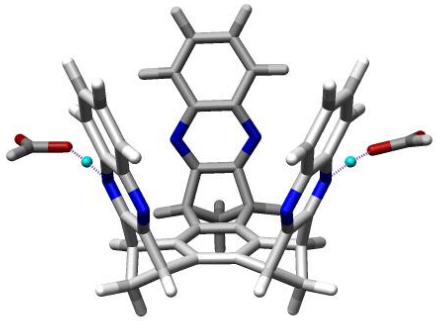
Coordinates

C	0.0348414	-3.6327368	3.7900376
C	-1.1267778	-3.1763818	2.8427654
C	-0.6900024	-1.7273060	2.6050940
C	0.7419463	-1.7296789	2.5903622
C	1.1787645	-3.1802210	2.8195111
C	1.4362984	-0.5581861	2.3583984
C	0.7133922	0.6584830	2.1822839
C	-0.6620852	0.6607844	2.1967186
C	-1.3850494	-0.5534295	2.3881844
C	-0.7083200	-3.9350482	1.5860572
C	0.7327045	-3.9376225	1.5716362
C	1.7314241	1.7552248	1.8677936
C	2.2131360	1.3452025	0.4863548
C	2.9882357	0.1393930	0.6453160
C	2.9180636	-0.2113555	2.1340440
C	2.9383895	1.2391205	2.7179507
C	-2.8701164	-0.2013230	2.1961970
C	-2.9719507	0.1504052	0.7095986
C	-2.1962955	1.3533632	0.5340366
C	-1.6827640	1.7611458	1.9046719
C	-2.8725724	1.2488749	2.7810321
N	-3.5490329	-0.4953560	-0.2678129
C	-3.3636857	0.0703133	-1.5171602
C	-2.5367867	1.2300434	-1.7192065
N	-1.9267757	1.8643206	-0.6460190
N	1.9189434	1.8563506	-0.6876474
C	2.5023954	1.2188541	-1.7741717
C	3.3291327	0.0565485	-1.5898778
N	3.5409132	-0.5089846	-0.3444789
N	1.4532794	-4.5005107	0.6386873
C	0.7103962	-5.1091694	-0.3587965
C	-0.7286971	-5.1064113	-0.3445424
N	-1.4493651	-4.4950763	0.6675200
C	-3.9806675	-0.5316990	-2.6377560
C	-3.7906904	-0.0122352	-3.9066482
C	-2.9738589	1.1242997	-4.1006885
C	-2.3543415	1.7348385	-3.0234751
C	2.2919765	1.7230729	-3.0744412
C	2.8847479	1.1094454	-4.1648614
C	3.7021208	-0.0295232	-3.9883202
C	3.9189093	-0.5483720	-2.7234544
C	1.3883932	-5.7575999	-1.4167861
C	0.6749731	-6.3791095	-2.4271160
C	-0.7388834	-6.3763807	-2.4131167
C	-1.4298721	-5.7522067	-1.3889501
H	0.0349395	-4.7164505	3.9752002
H	0.0453174	-3.0833194	4.7411880
H	-2.1587862	-3.3365656	3.1680239
H	2.2164817	-3.3437583	3.1241836
H	1.3919853	2.7940348	1.9748699
H	3.6631312	-0.9316161	2.4829242

H	3.8736567	1.7755938	2.5035544
H	2.7258889	1.2663643	3.7946922
H	-3.6097945	-0.9193152	2.5609942
H	-1.3374734	2.7986967	2.0044236
H	-3.8103609	1.7888284	2.5875061
H	-2.6363254	1.2749284	3.8528547
H	-4.5994626	-1.4123361	-2.4618931
H	-4.2715040	-0.4833514	-4.7651300
H	-2.8334041	1.5240872	-5.1059453
H	-1.7283116	2.6210734	-3.1505271
H	1.6665000	2.6114572	-3.1879678
H	2.7225647	1.5086880	-5.1670640
H	4.1622278	-0.5027783	-4.8569679
H	4.5384520	-1.4310216	-2.5607428
H	2.4792645	-5.7472208	-1.4040497
H	1.2052073	-6.8766501	-3.2408374
H	-1.2870000	-6.8718166	-3.2161940
H	-2.5202570	-5.7376264	-1.3547808
Ag	-0.0001068	3.1789296	-0.5915044
O	0.0131220	4.4642347	1.1919044
C	0.0110166	5.7677085	1.2935153
H	0.0008217	6.3136273	0.3100920
O	0.0189450	6.4034244	2.3445105

Compound [$\mathbf{1}_{syn}$+Ag_2]

Structure



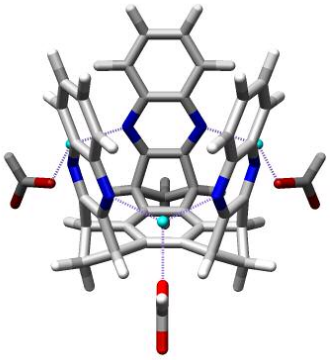
Coordinates

C	-2.9250587	-2.2725723	3.2309924
C	-2.9048868	-0.9605796	2.3762716
C	-1.4055227	-0.6443338	2.4322684
C	-0.7225909	-1.8998185	2.4613435
C	-1.8041590	-2.9857478	2.4047593
C	0.6564435	-1.9272874	2.4717345
C	1.3840371	-0.6976606	2.4659020
C	0.7252826	0.5117540	2.4157870
C	-0.7017633	0.5406004	2.3878076
C	-3.0932892	-1.5745112	1.0025625
C	-2.4196526	-2.8453552	1.0120710
C	2.8711503	-1.0638062	2.4133522
C	3.0354548	-1.6581372	1.0268173
C	2.3203781	-2.9069555	1.0167440
C	1.7004272	-3.0498016	2.4067529
C	2.8424377	-2.3891251	3.2462174
C	-1.1057004	2.0052910	2.1954625
C	-0.6269858	2.3239782	0.7764274
C	0.8111416	2.2924941	0.8140906
C	1.2009967	1.9564517	2.2522954

C	0.0436289	2.6977332	2.9990836
N	-1.3236726	2.5080301	-0.3126054
C	-0.5584493	2.7430949	-1.4419464
C	0.8817258	2.7073231	-1.4044917
N	1.5734375	2.4368984	-0.2365320
N	3.6349192	-1.1740583	-0.0391121
C	3.5772513	-1.9729627	-1.1799568
C	2.8785022	-3.2292776	-1.1524040
N	2.2253713	-3.6894581	-0.0243386
N	-2.3643622	-3.6541737	-0.0116013
C	-3.0118225	-3.1951108	-1.1436664
C	-3.6758178	-1.9204973	-1.1898179
N	-3.7002188	-1.1002084	-0.0636496
C	-1.2103944	3.0229420	-2.6650086
C	-0.4693959	3.2652626	-3.8087770
C	0.9442047	3.2334651	-3.7707196
C	1.6109553	2.9572258	-2.5896792
C	4.2132940	-1.5560667	-2.3668257
C	4.1648152	-2.3527771	-3.4978526
C	3.4810946	-3.5889341	-3.4768767
C	2.8493589	-4.0200394	-2.3241845
C	-3.0192033	-4.0094841	-2.2998222
C	-3.6513010	-3.5828465	-3.4542648
C	-4.2995660	-2.3281410	-3.4931608
C	-4.3128675	-1.5082562	-2.3775255
H	-3.8902902	-2.7969470	3.1908874
H	-2.6323844	-2.0909132	4.2735916
H	-3.5959845	-0.1520647	2.6368936
H	-1.5120567	-4.0008603	2.6868543
H	3.5889957	-0.2837595	2.6873800
H	1.3724595	-4.0584196	2.6720835
H	3.7882766	-2.9465419	3.2002591
H	2.5533000	-2.2143542	4.2907205
H	-2.1408347	2.2801362	2.4170619
H	2.2344959	2.1843101	2.5280541
H	0.0702161	3.7858655	2.8501568
H	0.0119888	2.4622311	4.0714329
H	-2.3007509	3.0582975	-2.6653791
H	-0.9781577	3.4923922	-4.7470627
H	1.5124187	3.4377806	-4.6795191
H	2.7003699	2.9461551	-2.5298729
H	4.7415746	-0.5987524	-2.3658796
H	4.6607914	-2.0231362	-4.4114769
H	3.4540238	-4.2051256	-4.3764244
H	2.3133195	-4.9685000	-2.2790385
H	-2.5115736	-4.9727295	-2.2413537
H	-3.6521801	-4.2175416	-4.3412757
H	-4.7946967	-2.0017645	-4.4084063
H	-4.8117768	-0.5355557	-2.3901715
Ag	-4.6379705	0.8106678	-0.0051085
Ag	4.5814406	0.7396015	-0.0045637
O	5.5319734	2.5571480	0.1025315
O	-5.5264913	2.6413377	0.2341920
C	6.8447046	2.6660989	0.1504237
H	7.4044306	1.6920307	0.1205628
C	-6.8026400	2.8590005	-0.0157813
H	-7.3706271	1.9697352	-0.4020004
O	7.4514953	3.7246922	0.2221071
O	-7.3666161	3.9311174	0.1438772

Compound [$\mathbf{1}_{syn}$+Ag_3]

Structure



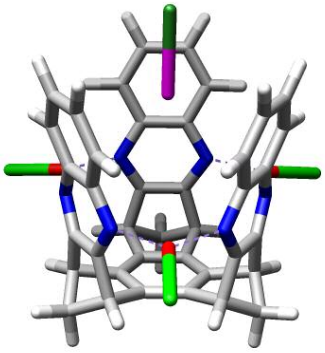
Coordinates

C	-1.6979295	2.9409002	2.7768868
C	-0.3288451	2.8873827	2.0243497
C	0.0134001	1.4033669	2.2160015
C	-1.2220515	0.6900787	2.2160015
C	-2.3361242	1.7284796	2.0243497
C	-1.2220515	-0.6900787	2.2160015
C	0.0134001	-1.4033669	2.2160015
C	1.2086514	-0.7132883	2.2160015
C	1.2086514	0.7132883	2.2160015
C	-0.8445125	2.9055979	0.5912186
C	-2.0940654	2.1841682	0.5912186
C	-0.3288451	-2.8873827	2.0243497
C	-0.8445125	-2.9055979	0.5912186
C	-2.0940654	-2.1841682	0.5912186
C	-2.3361242	-1.7284796	2.0243497
C	-1.6979295	-2.9409002	2.7768868
C	2.6649693	1.1589032	2.0243497
C	2.9385778	0.7214297	0.5912186
C	2.9385778	-0.7214297	0.5912186
C	2.6649693	-1.1589032	2.0243497
C	3.3958590	0.0000000	2.7768868
N	3.0050503	1.4365585	-0.5086122
C	3.1938461	0.7178964	-1.6815427
C	3.1938461	-0.7178964	-1.6815427
N	3.0050503	-1.4365585	-0.5086122
N	-0.2584290	-3.3207292	-0.5086122
C	-0.9752065	-3.1249001	-1.6815427
C	-2.2186396	-2.4070037	-1.6815427
N	-2.7466214	-1.8841706	-0.5086122
N	-2.7466214	1.8841706	-0.5086122
C	-2.2186396	2.4070037	-1.6815427
C	-0.9752065	3.1249001	-1.6815427
N	-0.2584290	3.3207292	-0.5086122
C	3.3735375	1.4064378	-2.8991660
C	3.5580551	0.7059004	-4.0791690
C	3.5580551	-0.7059004	-4.0791690
C	3.3735375	-1.4064378	-2.8991660
C	-0.4687579	-3.6247881	-2.8991660
C	-1.1676999	-3.4343163	-4.0791690
C	-2.3903553	-2.7284159	-4.0791690
C	-2.9047797	-2.2183503	-2.8991660
C	-2.9047797	2.2183503	-2.8991660
C	-2.3903553	2.7284159	-4.0791690
C	-1.1676999	3.4343163	-4.0791690
C	-0.4687579	3.6247881	-2.8991660
H	-2.2415190	3.8824248	2.6159861
H	-1.5884746	2.7513187	3.8520764
H	0.4592772	3.6135524	2.2632656
H	-3.3590668	1.4090305	2.2632656
H	0.4592772	-3.6135524	2.2632656
H	-3.3590668	-1.4090305	2.2632656

H	-2.2415190	-3.8824248	2.6159861
H	-1.5884746	-2.7513187	3.8520764
H	2.8997896	2.2045219	2.2632656
H	2.8997896	-2.2045219	2.2632656
H	4.4830380	0.0000000	2.6159861
H	3.1769492	0.0000000	3.8520764
H	3.3815775	2.4981279	-2.8753707
H	3.7097462	1.2467940	-5.0140033
H	3.7097462	-1.2467940	-5.0140033
H	3.3815775	-2.4981279	-2.8753707
H	0.4726535	-4.1775959	-2.8753707
H	-0.7751178	-3.8361314	-5.0140033
H	-2.9346284	-2.5893374	-5.0140033
H	-3.8542310	-1.6794680	-2.8753707
H	-3.8542310	1.6794680	-2.8753707
H	-2.9346284	2.5893374	-5.0140033
H	-0.7751178	3.8361314	-5.0140033
H	0.4726535	4.1775959	-2.8753707
Ag	2.0524874	3.5550124	-0.2188508
Ag	2.0524874	-3.5550124	-0.2188508
Ag	-4.1049747	0.0000000	-0.2188508
O	2.5601574	4.4343226	1.7063953
O	2.5601574	-4.4343226	1.7063953
O	-5.1203147	0.0000000	1.7063953
C	3.2030962	-5.5479254	1.9637707
H	3.5329640	-6.1192731	1.0536826
C	-6.4061924	0.0000000	1.9637707
H	-7.0659280	0.0000000	1.0536826
C	3.2030962	5.5479254	1.9637707
H	3.5329640	6.1192731	1.0536826
O	3.4518585	5.9787943	3.0837600
O	3.4518585	-5.9787943	3.0837600
O	-6.9037170	0.0000000	3.0837600

Compound [$\mathbf{1}_{syn}$+Cs+Cu_3]

Structure



Coordinates

C	-3.2459271	1.4060391	-1.9926781
C	-2.9988252	0.7181729	-0.7854938
C	-2.9988252	-0.7181729	-0.7854938
C	-3.2459271	-1.4060391	-1.9926781
C	-3.5108374	-0.7053432	-3.1612590
C	-3.5108374	0.7053432	-3.1612590
N	-2.7592408	1.4437563	0.3856176
C	-2.8250679	0.7125070	1.4904126
C	-2.8250679	-0.7125070	1.4904126
N	-2.7592408	-1.4437563	0.3856176
C	-2.6454493	-1.1506541	2.9389009
C	-3.4309919	0.0000000	3.6425896
C	-2.6454493	1.1506541	2.9389009
C	-1.2070498	-0.7138956	3.2419119
C	-1.2070498	0.7138956	3.2419119
C	-0.0147269	-1.4022836	3.2419119
C	1.2217767	-0.6883879	3.2419119

C	1.2217767	0.6883879	3.2419119
C	-0.0147269	1.4022836	3.2419119
C	2.3192203	-1.7156992	2.9389009
C	1.7154960	-2.9713262	3.6425896
C	0.3262290	-2.8663533	2.9389009
C	2.0295831	-2.0903271	1.4904126
C	0.7954848	-2.8028341	1.4904126
C	0.3262290	2.8663533	2.9389009
C	1.7154960	2.9713262	3.6425896
C	2.3192203	1.7156992	2.9389009
C	0.7954848	2.8028341	1.4904126
C	2.0295831	2.0903271	1.4904126
N	0.1292908	-3.1114507	0.3856176
C	0.8774566	-2.9561452	-0.7854938
C	2.1213685	-2.2379723	-0.7854938
N	2.6299500	-1.6676944	0.3856176
N	2.6299500	1.6676944	0.3856176
C	2.1213685	2.2379723	-0.7854938
C	0.8774566	2.9561452	-0.7854938
N	0.1292908	3.1114507	0.3856176
C	2.8406291	2.1080358	-1.9926781
C	2.3662638	2.6878028	-3.1612590
C	1.1445736	3.3931460	-3.1612590
C	0.4052980	3.5140749	-1.9926781
C	0.4052980	-3.5140749	-1.9926781
C	1.1445736	-3.3931460	-3.1612590
C	2.3662638	-2.6878028	-3.1612590
C	2.8406291	-2.1080358	-1.9926781
Cu	-1.8704766	3.2397604	0.4558232
Cl	-2.9351318	5.0837974	0.9511978
Cu	-1.8704766	-3.2397604	0.4558232
Cl	-2.9351318	-5.0837974	0.9511978
Cu	3.7409531	0.0000000	0.4558232
Cl	5.8702636	0.0000000	0.9511978
Cs	0.0000000	0.0000000	-2.8608072
F	0.0000000	0.0000000	-5.4419681
H	-4.5022160	0.0000000	3.4013523
H	-3.2850016	0.0000000	4.7305947
H	-2.9191453	2.1888724	3.1517186
H	-2.9191453	-2.1888724	3.1517186
H	3.3551917	-1.4336178	3.1517186
H	-0.4360464	-3.6224902	3.1517186
H	2.2511080	-3.8990335	3.4013523
H	1.6425008	-2.8448949	4.7305947
H	-0.4360464	3.6224902	3.1517186
H	3.3551917	1.4336178	3.1517186
H	2.2511080	3.8990335	3.4013523
H	1.6425008	2.8448949	4.7305947
H	-0.5247165	4.0866409	-1.9618001
H	0.7805768	3.8422481	-4.0853407
H	2.9371961	2.5971234	-4.0853407
H	3.8014931	1.5889026	-1.9618001
H	3.8014931	-1.5889026	-1.9618001
H	2.9371961	-2.5971234	-4.0853407
H	0.7805768	-3.8422481	-4.0853407
H	-0.5247165	-4.0866409	-1.9618001
H	-3.2767766	-2.4977383	-1.9618001
H	-3.7177729	-1.2451247	-4.0853407
H	-3.7177729	1.2451247	-4.0853407
H	-3.2767766	2.4977383	-1.9618001

Compound CH_3OH

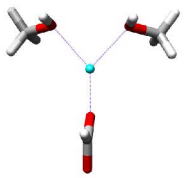
Structure

Coordinates

C	-0.0000037	0.7325841	0.0131724
H	0.8968593	1.1290840	0.5227053
H	0.0019480	1.1033718	-1.0193528
H	-0.8986878	1.1292170	0.5193969
O	-0.0000023	-0.6960859	-0.0644543
H	-0.0000396	-1.0423788	0.8433631

Compound [Ag+3CH_3OH]

Structure



Coordinates

Ag	-0.0343283	0.1417059	0.0000000
O	0.5448446	-1.8734790	0.0000000
C	-0.3328983	-2.8485663	0.0000000
H	-1.4109455	-2.5250728	0.0000000
O	-0.0506577	-4.0403390	0.0000000
O	-0.2929787	1.9272642	1.6397560
H	-1.2155497	2.1582447	1.8438513
O	-0.2929787	1.9272642	-1.6397560
H	-1.2155497	2.1582447	-1.8438513
C	0.3946228	1.6778612	-2.8909267
H	0.3691278	2.5731773	-3.5301612
H	1.4343810	1.4512834	-2.6332149
H	-0.0362582	0.8191176	-3.4271277
C	0.3946228	1.6778612	2.8909267
H	1.4343810	1.4512834	2.6332149
H	0.3691278	2.5731773	3.5301612
H	-0.0362582	0.8191176	3.4271277