Electronic Supplementary Information

of the manuscript:

A rigid sublimable naphthalenediimide cyclophane as model compound for UHV STM experiments

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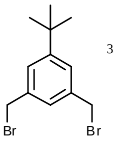
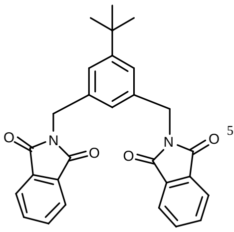
Synthetic protocols and analytical data

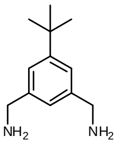
General: All chemicals were directly used for the synthesis without purification. The solvents for chromatography and extractions were once distilled before use. ^{1}H-NMR and ^{13}C-NMR were recorded at 298 K on a *Bruker DPX-NMR* (400 MHz) spectrometer. Chemical shifts (δ) are reported in ppm relative to residual solvent peaks and coupling constants (*J*) are in Hertz (Hz). NMR solvents were obtained from *Cambridge Isotope Laboratories, Inc.* (Andover, MA, USA). $CDCl_3$ was filtered through basic alumina before use. The multiplicity's are written as: s = singulett, d = doublet, t = triplet, m = multiplet and br = broad. The solvents for spectroscopic studies were of spectroscopic grade and used as received. UV/Vis absorption spectra were recorded on a *Agilent 8453* diode array spectrophotometer. The IR spectra were recorded on a FT-IR *RX1* from Perkin Elmer; wavenumbers measured in cm^{-1}. The elementary analysis were measured on a *Analysator 240* from Perkin-Elmer. The mass spectra were recorded on a esquire 3000 plus (Bruker) for Electron Spray Ionisation (ESI) and / or on a *finnigan MAT 95Q* for Electron Impact (EI) and on a *finnigan MAT 8400* for Fast Atom Bombardment (FAB). As matrix m-Nitro-Benzenealcohol (NBA) or glycine (GLY) was used; measured in m/z (%). Melting points were measured on a SMP3 from Stuart in °C. TLC was carried out on *Silica gel 60 F_{254}* glass plates with a thickness of 0.25 mm from Merck. The detection was observed through fluorescence at 254 nm with a UV-lamp from Camag. For column chromatography *silica gel 60* (40-63 μm) from Merck, was used with distilled solvents.



5-tert-Butyl-1,3-bis(bromomethyl)benzene **(3)***:* A suspension of 5-*tert*.-Butyl-1,3-xylene (**2**) (32.45 g, 200 mmol), NBS (80.45 g, 452 mmol) and AIBN (0.2 g, 1.2 mmol) in 400 ml methyl formate was irradiated with a 500-W bulb for 3h. The solvent was evaporated and the residue was dissolved in 300 ml CH_2Cl_2. The organic phase was washed twice with concentrated $NaHCO_3$ solution and water, then dried over Na_2SO_4 and concentrated under reduced pressure. Recrystallization of the solid residue from hexane gave the desired 5-*tert*-Butyl-1,3-bis(bromomethyl)benzene (**3**) as colorless crystals (30.77 g, 48 %). R_f=0.66 (Hex/EtOAc 3:1); ^{1}H-NMR (400MHz, $CDCl_3$): δ=7.33 (d, 2H, $^4J_{HH}$=1.5 Hz, 4-H, 6-H), 7.25 (t, 1H, $^4J_{HH}$=1.5 Hz, 2-H), 4.48 (s, 4H, $BrCH_2$ Ph), 1.32 ppm (s, 9H, $C(CH_3)_3$); ^{13}C-NMR (400MHz, $CDCl_3$): δ=152.5, 137.9, 126.8, 126.2, 34.7, 33.4, 31.2 ppm; M.p.: 113°C.



5-tert-Butyl-1,3-bis(phthalimido-methyl)benzene **(4)***:* A mixture of 5-*tert*-Butyl-1,3-bis(bromomethyl)benzene (**3**) (8.47 g, 27 mmol), potassium phthalimide (10.78 g, 58 mmol) and K_2CO_3 (21.95 g, 159 mmol) in 200 ml of anhydrous CH_3CN was heated under reflux for 5h. The reaction mixture was cooled to room temperature and quenched with 200 ml water. After extraction with EtOAc, the combined organic phases were washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (Hex/EtOAc 3:1 to 1:3) to provide 5-*tert*-Butyl-1,3-bis(phthalimidomethyl)benzene (**4**) as a white solid (10.31 g, 86 %). R_f=0.62 (Hex/EtOAc 2:3); ^{1}H-NMR (400MHz, $CDCl_3$): δ=7.84-7.82, 7.71-7.68 (m, 8H, Pht-H), 7.38 (d, 2H, $^4J_{HH}$=1.5 Hz, 4-H, 6-H), 7.32 (t, 1H, $^4J_{HH}$=1.5 Hz, 2-H), 4.80 (s, 4H, Pht-CH_2-Ph), 1.27 ppm (s, 9H, $C(CH_3)_3$); ^{13}C-NMR (400MHz, $CDCl_3$): δ=168.0, 152.2, 136.4, 133.9, 132.1, 126.1, 125.4, 123.3, 41.7, 34.6, 31.2 ppm; ESI-MS: m/z: 475 [M^++Na]; EI-MS: m/z: 452 [M^+], 437 [$C_{28}H_{25}N_2O_3^+$], 395 [$C_{24}H_{15}N_2O_4^+$], 305 [$C_{20}H_{19}NO_2^+$], 290 [$C_{20}H_{20}NO^+$], 160 [$C_{12}H_{16}^+$]; elemental analysis calcd. (%) for $C_{28}H_{24}N_2O_4$: C, 74.32; H, 5.35; N, 6.19; found: C, 74.17; H, 5.42; N, 6.05; M.p.: 183-184°C.



1,3-Bis(aminomethyl)-5-tert-butylbenzene **(5)***:*[1] Hydrazine monohydrate (31 ml, 638 mmol) was slowly added to a suspension of 5-*tert*-Butyl-1,3-bis(phthalimidomethyl) benzene (**4**) (11.1 g, 25 mmol) in 300 ml MeOH. The resulting solution was refluxed for 2h. After cooling to room temperature the reaction mixture was quenched with 200 ml 5 M NaOH solution and extracted with CH_2Cl_2 (4 x 100 ml). The solvent was evaporated and the remaining yellow oil was distilled under reduced pressure (1 mbar) to afford 1,3-Bis(aminomethyl)-5-*tert*-butylbenzene (**5**) as an air-sensitive colorless oil, which was stored under argon (3.88 g, 82 %). ^{1}H-NMR (400MHz, $CDCl_3$): δ=7.20 (d, 2H, $^4J_{HH}$=1.5 Hz, 4-H, 6-H), 7.10 (t, 1H,

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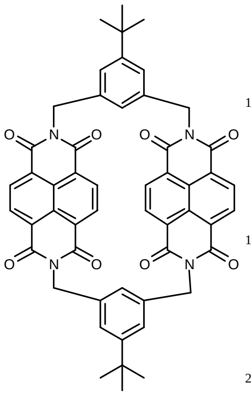
$^4J_{HH}$=1.5 Hz, 2-H), 3.85 (s, 4H, NH_2-CH_2-Ph), 1.32 ppm (s, 9H, $C(CH_3)_3$); ^{13}C-NMR (400MHz, $CDCl_3$): δ=151.7, 143.2, 122.9, 122.6, 46.7, 34.6, 31.3 ppm; ESI-MS: m/z: 385 [$2xM^+$+H]; 215 [M^++Na] 193 [M^++H]; EI-MS: m/z: 191 [M^+], 162 [$C_{11}H_{16}N^+$], 135 [$C_8H_{11}N_2^+$], 57 [$C_4H_9^+$].



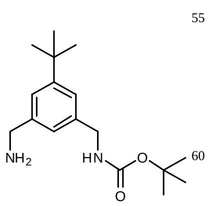
1,5(1,4,5,8)-Dinaphthalenetetracarboxylic acid diimide-3,7(3,5)-Di-1-tert-butyl-benzenacyclooctaphane-nodan **(1)***:*

a) The yellow suspension of Naphthalene-1,4,5,8-tetracarboxylic acid dianhydride (**6**) (0.87 g, 3.2 mmol) and 1,3-Bis(aminomethyl)-5-*tert*-butylbenzene (**5**) (0.62 g, 3.2 mmol) in 0.2 ml Et_3N and 170 ml *i*-PrOH was refluxed for 3 d. The reaction mixture was cooled to room temperature and filtered. The solvent was evaporated and the residue was purified by column chromatography on silica gel (CH_2Cl_2/EtOAc 10:1) to provide the symmetric NDI cyclophane **1** as a white solid (32.1 mg, 1.2 %).

b) Naphthalene-1,4,5,8-tetracarboxylic acid dianhydride (**6**) (1.93 g, 7.2 mmol) was solved at 120°C in 200 ml DMF with 20 ml CH_3COOH. Then 50 ml of a solution of 1,3-Bis(aminomethyl)-5-*tert*-butylbenzene (**5**) (0.55 g, 2.8 mmol) in 50 ml DMF was dropped in through a dropping funnel over 1h. This reaction mixture was refluxed for 4d. Then the reaction mixture was cooled to room temperature and filtered. The solvent was evaporated and the residue was purified by column chromatography on silica gel (CH_2Cl_2/EtOAc 10:1) to provide the symmetric NDI cyclophane as a white solid (44.5 mg, 3.4 %).

c) The yellow suspension of Naphthalene-1,4,5,8-tetracarboxylic acid dianhydride (**6**) (61 mg, 0.23 mmol) and **9** (149 mg, 0.18 mmol) in 1 ml Et_3N and 450 ml *i*-PrOH was refluxed for 3 d. The reaction mixture was cooled to room temperature and filtered. The solvent was evaporated and the residue was purified by column chromatography on silica gel (CH_2Cl_2/EtOAc 10:1) to provide the symmetric NDI cyclophane **1** as a white solid (59 mg, 40 %).

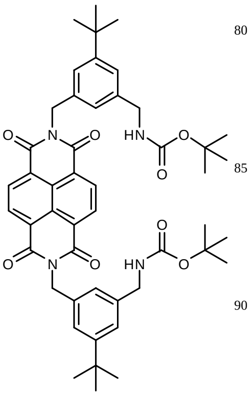
R_f=0.4 (CH_2Cl_2/EtOAc 10:1); UV/Vis (CH_3CN): λ_{max} (ε) = 232 (50 332), 343 (24 351), 358 (35 057), 379 nm (30 707 mol^{-1} dm^3 cm^{-1}); IR (ν/cm^{-1}): 3429, 3077, 2961, 1710 (νC=O), 1671 (νC=O), 1581, 1453, 1336, 1244, 1181, 1006, 772; ^{1}H-NMR (400MHz, $CDCl_3$): δ=8.60 (s, 8H, Napht.), 7.44 (d, 4H, $^4J_{HH}$=1.5 Hz, 2-H, 6-H), 7.31 (t, 1H, $^4J_{HH}$=1.5 Hz, 4-H), 5.34 (s, 8H, NDI-CH_2-Ph), 1.35 ppm (s, 18H, $C(CH_3)_3$); ^{13}C-NMR (400MHz, $CDCl_3$): δ=162.2, 151.3, 137.5, 130.7, 126.2, 126.1, 125.9, 124.4, 43.4, 34.7, 31.3 ppm; ESI-MS: m/z 2568 [$3xM^+$+Na], 1719 [$2xM^+$+Na], 871 [M^++Na]; FAB-MS: m/z 849 [M^+], 793 [$C_{48}H_{31}N_4O_8^+$]; elemental analysis calcd. (%) for $C_{53}H_{42}Cl_2N_4O_8$: C, 68.17; H, 4.53; N, 6.00; found: C, 68.59; H, 4.96; N, 5.59; M.p.: >349°C.



1-tert-Butoxycarbonyl-1,3-bis(aminomethyl)-5-tert-butylbenzene **(7)***:*

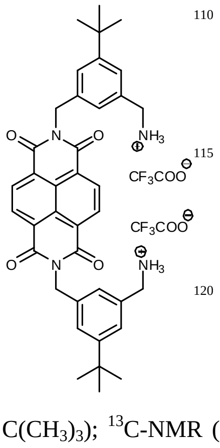
A solution of Di-*tert*-butyl-dicarbonate (1.1 g, 5 mmol) in 80 ml dry dioxane was added dropwise to a stirred solution of 1,3-Bis(aminomethyl)-5-*tert*-butylbenzene (**5**) (2.4 g, 12.5 mmol) in 500 ml dry dioxane at 0°C over 1 h. This reaction mixture was then warmed up to room temperature and quenched with water. After extraction with CH_2Cl_2, evaporation of the solvent and drying one isolated 1-*tert*-Butoxycarbonyl-1,3-bis(aminomethyl)-5-*tert*-butylbenzene (**7**) as a yellow oil (0.7 g, 47%). Further purification by extraction gave a colorless oil (22%). IR (ν/cm^{-1}): 3344, 2956, 2867, 1694 (νC=O), 1517, 1372, 1261, 1167, 906, 728; ^{1}H-NMR (400MHz, $CDCl_3$): δ=7.23 (m, 1H, 6-H), 7.18 (m, 1H, 4-H), 7.06 (m, 1H, 2-H), 4.30 (d, 2H, $^3J_{HH}$=5.6 Hz, NHBoc-CH_2-Ph), 3.85 (s, 2H, NH_2-CH_2-Ph), 1.47 (s, 9H, Boc $C(CH_3)_3$), 1.31 ppm (s, 9H, $C(CH_3)_3$); ^{13}C-NMR (400MHz, $CDCl_3$): δ=155.9, 152.0, 138.8, 123.5, 123.3, 123.2, 110.0, 46.5, 44.9, 34.7, 31.4, 28.4 ppm; ESI-MS: m/z 585 [$2xM^+$+H], 293 [M^++H]; FAB-MS: m/z 293 [M^+], 220 [$C_{13}H_{20}N_2O^+$], 176 [$C_{12}H_{19}N^+$], 57 [$C_4H_9^+$].

N,N'-Di-(1'-tert-Butoxycarbonyl-1',3'-bis(aminomethyl)-5'-tert-butylbenzene)-naphthalene-1,4,5,8-tetracarboxylic acid bisimide **(8)***:*



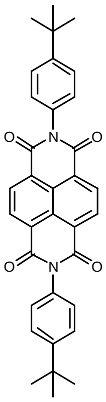
A suspension of 1-*tert*-Butoxycarbonyl-1,3-bis(aminomethyl)-5-*tert*-butylbenzene (**7**) (353 mg, 1.2 mmol), Naphthalene-1,4,5,8-tetracarboxylic acid dianhydride (**6**) (162 mg, 0.6 mmol) and 1 ml Et_3N in 70 ml *i*-PrOH was refluxed under an argon atmosphere for 3 days. After cooling to room temperature the solvent was evaporated and the residue was purified by column chromatography on silica gel (Hex/EtOAc 2:1) to provide the protected NDI semicircle **8** as a yellow solid (217 mg, 44%). R_f=0.3 (EtOAc/Hex 1:2); IR (ν/cm^{-1}): 3397, 2966, 1705 (νC=O), 1667 (νC=O), 1505, 1453, 1367, 1326, 1245, 1172, 910, 734; UV/Vis (CH_3CN): λ_{max} (ε) =235 (65 453), 342 (26 023), 359 (43 156), 379 nm (52 026 mol^{-1} dm^3 cm^{-1}); ^{1}H-NMR (400MHz, CDCl3): δ=8.66 (s, 4H, Napht.), 7.53, 7.26, 7.24 (s, 6H, 2-H, 4-H, 6-H), 5.35 (s, 4H, NDI-CH_2-Ph), 4.27 (d, 4H, $^3J_{HH}$=5.6 Hz, NHBoc-CH_2-Ph), 1.43 (s, 18H, Boc $C(CH_3)_3$), 1.31 ppm (s, 18H, $C(CH_3)_3$); ^{13}C-NMR (400MHz, $CDCl_3$): δ=162.4, 155.9, 151.9, 138.9, 136.4, 130.9, 126.3, 126.2, 125.8, 125.6, 124.4, 79.3, 44.8, 44.0, 34.7, 31.3, 28.3 ppm; ESI-MS: m/z 855 [M^++K], 839 [M^++Na]; FAB-MS: m/z 817 [M^+], 601 [$C_{35}H_{29}N_4O_6^+$], 57 [$C_4H_9^+$]; elemental analysis calcd. (%) for $C_{48}H_{56}N_4O_8$: C, 70.57; H, 6.91; N, 6.86; found: C, 70.03; H, 7.01; N, 6.50.

N,N'-Di-(1',3'-Bis(aminomethyl)-5'-tert-butylbenzene)-naphthalene-1,4,5,8-tetracarboxylic acid bisimide **(9)***:*



The protected NDI semicircle **8** (217 mg, 0.26 mmol) was solved in CH_2Cl_2 and 5 ml trifluoroacetic acid was dropped to the stirred solution at room temperature. This reaction mixture was stirred for 3 h under an argon atmosphere. After evaporation of the solvent one isolated the deprotected NDI semicircle **9** as a yellow salt in quantitative yield. ^{1}H-NMR (400MHz, DMSO): δ=8.73 (s, 4H, Napht.), 8.19 (br s, 6H, NH_3^+), 7.51, 7.43, 7.21 (s, 6H, 2-H, 4-H, 6-H), 5.30 (s, 4H, NDI-CH_2-Ph), 3.96 (br s, 4H, NH_2-CH_2-Ph), 1.29 ppm (s, 18H, $C(CH_3)_3$); ^{13}C-NMR (400MHz, DMSO): δ=162.7, 151.3, 137.1, 134.0, 130.8, 126.3, 124.8, 124.8, 124.3, 43.5, 42.3, 34.5, 31.0 ppm; ; ESI-MS: m/z 617 [M^++H]; FAB-MS: m/z 617 [M^++H], 600 [$C_{35}H_{29}N_4O_6^+$]; elemental analysis calcd. (%) for

$C_{48}H_{45}F_{15}N_4O_{14}$: C, 48.57; H, 3.82; N, 4.72; found: C, 48.71; H, 4.09; N, 4.71.



2,7-Bis(4-tert-butylphenyl)benzo[lmn][3,8]phenanthroline-1,3,6,8-tetrone **(11)**:[2] Naphthalene-1,4,5,8-tetracarboxylic acid dianhydride (**6**) (118 mg, 0.44 mmol), 4-*tert*-butylaniline (0.18 ml, 1.12 mmol) and 5 ml acetic acid were refluxed for 24 h. After cooling to room temperature the reaction mixture was quenched with water, extracted with CH_2Cl_2 and dried over Na_2SO_4. The solvent was evaporated and the residue was purified by column chromatography on silica gel (CH_2Cl_2) to provide the linear NDI model compound **11** as a yellow solid (86 mg, 37%). R_f=0.4 (CH_2Cl_2); UV/Vis (CH_3CN): λ_{max} (ε) = 235 (45 732), 341 (17 066), 357 (27 428), 377 nm (31 016 mol^{-1} dm^3 cm^{-1}); IR (ν/cm^{-1}): 3400, 3069, 2956, 2856, 1706 (νC=O), 1672 (νC=O), 1578, 1511, 1444, 1350, 1250, 1194, 1111, 978, 839, 761, 711, 556; ^{1}H-NMR (400MHz, $CDCl_3$): δ=8.84 (s, 4H, Napht.), 7.60 (d, 4H, $^3J_{HH}$=8.6 Hz, Phe), 7.27 (d, 4H, $^3J_{HH}$=8.6 Hz, Phe), 1.40 ppm (s, 18H, $6CH_3$); ^{13}C-NMR (400MHz, $CDCl_3$): δ=163.0, 152.0, 131.7, 131.4, 127.7, 127.1, 127.0, 126.6, 34.8, 31.3 ppm; ESI-MS: m/z 531 [M^++H], 553 [M^++Na]; EI-MS: m/z 530 [M^+], 515 [$C_{33}H_{27}N_2O_4^+$]; elemental analysis calcd. (%) for $C_{34}H_{30}N_2O_4$: C, 76.96; H, 5.70; N, 5.28; found: C, 76.93; H, 5.74; N, 5.10; M.p.: >349°C.

Solid state structures of the cyclophane 1

As mentioned in the main text, single crystals suitable for x-ray analysis of the cyclophane 1 were obtained by slow evaporation of solutions either from CH_2Cl_2 or from technical grade xylene. In both cases, the arrangement of the cyclophane framework was very comparable. As displayed in the figures SI-1 and SI-2, the planes of both NDI chromophores are tilted with respect to each other opening a cavity to one side. The interlinking *tert*.butyl phenyl spacers are both pointing towards the side of the open cavity resulting in the crescent type structure of the cyclophane 1. The entry of the cavity of 1 is partially filled by a solvent molecule. As displayed in figure SI-1, crystals obtained from CH_2Cl_2 comprise a CH_2Cl_2 molecule at the cavities entry.

Single crystals obtained from technical xylene (figure SI-2) comprise a *para*-xylene molecule partially penetrating the cavity. Furthermore, an additional solvent molecule is present at a general position in the asymmetric unit cell of the molecule. This position is occupied either with meta-xylene (0.4-occupancy) or with 3-ethyltoluene (0.6-occupancy). This additional solvent molecule is not displayed in figure SI-2.

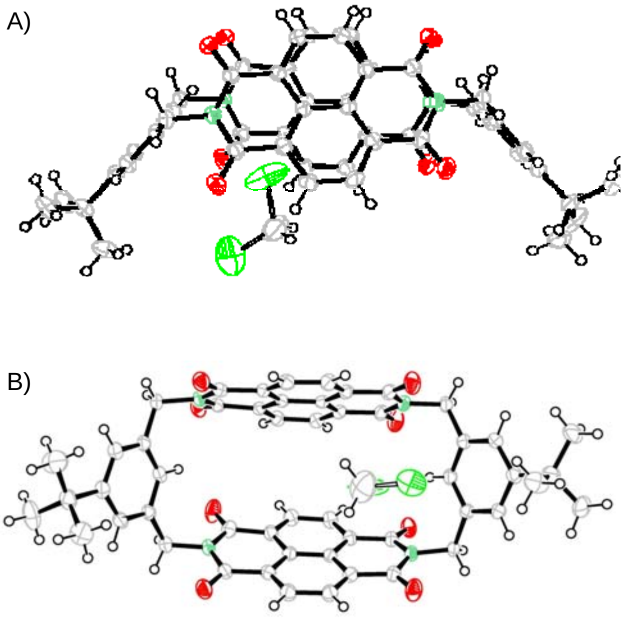


Fig. SI-1 Solid state structure of the cyclophane **1** obtained by evaporation of a CH_2Cl_2 solution comprising the partially penetrating CH_2Cl_2 molecule. A) top view, B) front viev.

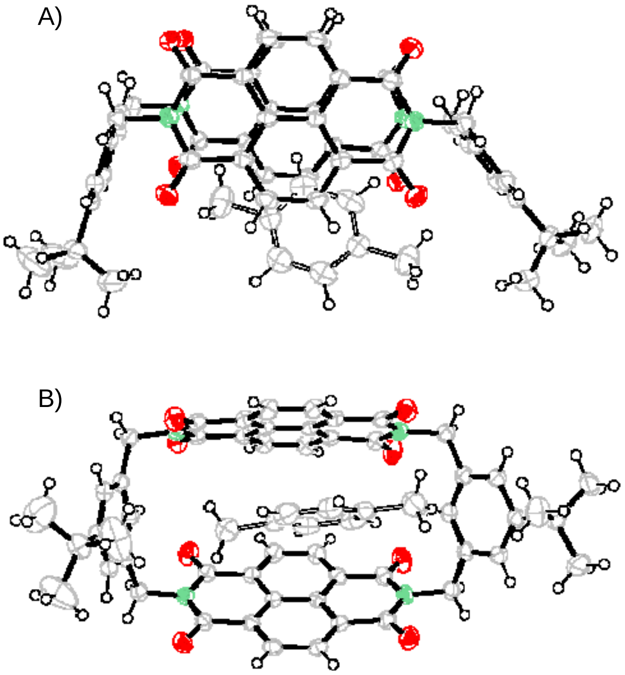


Fig. SI-2 Solid state structure of the cyclophane **1** obtained by evaporation of a solution of **1** in technical grade xylene, comprising the partially penetratin *para*-xylene molecule. A) top view, B) front viev.

UHV STM investigations

The experiments were performed with a low-temperature STM operated at 5.7 K in ultrahigh vacuum (below 10^{-10} mbar). The Au (111) samples as well as etched W tips were prepared by argon-ion bombardment and annealing. Cyclophane 1 was deposited from a tantalum crucible maintained at 300°C and at a rate of approximately 0,2 ML/min as monitored by a quartz microbalance. During deposition a residual gas pressure in the 10^{-8} mbar range was maintained and the sample was kept at room temperature. The data shown correspond to coverages of approximately 0.05 monolayer. All images were recorded in a constant-current mode.

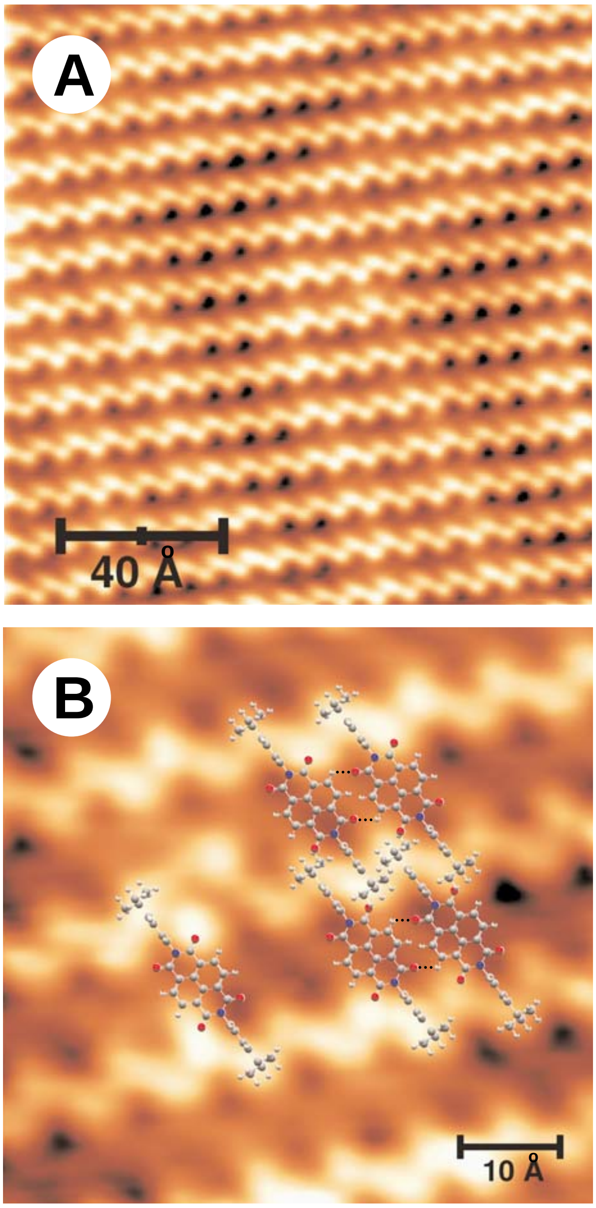


Fig. SI-3 Self-assembled monolayers obtained by sublimation of the NDI-model compound **11**; A) large area self assembly in parallel stripes; B) High resolution image comprising overlaid molecules **11**. Intermolecular hydrogen bonds are indicated by dotted lines.

To demonstrate the deposition of the cyclophane **1** without disruption, the resulting monolayers are compared with the monolayers obtained for the model compound **11** consisting of a single NDI chromophore.

As displayed in figure SI-3, the NDI molecule **11** self assembles in densely packed, regular parallel rows with a distance of about 1.5 nm. In figure SI-3 B) the molecular structure of **11** is overlaid suggesting a pair of hydrogen bonds between neighbouring molecules stabilizing the arrangement in stripes. The spatial proximity of the carbonyl oxygen and the naphthalene hydrogen of the neighbouring NDI chromophore indicate the formation of two hydrogen bonds between two neighbours in a row.

Also the cyclophane **1** self assembles in parallel stripes on the Au(111) surface with a pair of hydrogen bonds stabilizing the arrangement in rows (figure 2b of the main text and figure SI-4). However, comparing the surface structure emerging from the self assembly of the cyclophane **1** and the one obtained by the model compound **11** displays numerous phenomenological differences.

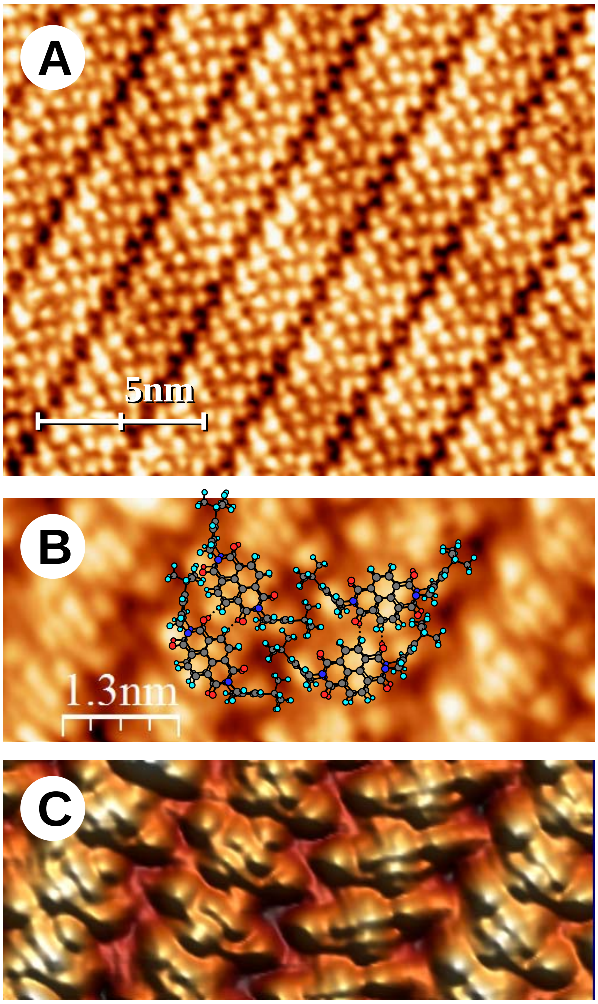


Fig. SI-4 Self-assembled monolayers obtained by sublimation of the cyclophane **1**; A) large area self assembly in parallel stripes; B) High resolution image comprising overlaid molecules **1**. Intermolecular hydrogen bonds are indicated by dotted lines; C) Topographical high resolution image of the same area as displayed in B).

While the molecular structure forming the self assembled pattern is linear in the case of **11** (figure SI-3B), it is crescent-shaped in the case of **1** (figure SI-4 B and C) resembling the solid state structure of **1** (figures SI-1 and SI-2). The perfectly regular parallel rows with a periodicity of 1.5 nm in the case of **11** arise from the intercalation of hydrogen-bond stabilized ribbons of the molecule rod **11**. In contrast to that, the parallel rows of **1** display a periodicity of 2.7 nm. As already reported in the main text and displayed in further details in figures SI-4 B) and SI-4 C), the stripes consists of two rows of intercalated cyclophane molecules which are rotated by about 120° with respect to each other. Each row is stabilized by a pair of intermolecular hydrogen bonds, formed between the carbonyl oxygens and the naphthalene hydrogens of the surface immobilized NDI chromophores (dotted lines in Figure SI-4 B). The intercalation of both rows as well as the densely packed arrangement of the parallel stripes seems to be driven by maximisation of the surface coverage.

The reconstruction of the underlying Au surface can still be observed in figure SI-5 indicating that the interaction between the molecule and the substrate is weak, similar to the case of supramolecular polymers on Au(111).[3] A stronger interaction and charge transfer between the molecule and the Au(111) would lead to lifting of the reconstruction as observed, e.g., in the case of C60 on Au(111).[4]

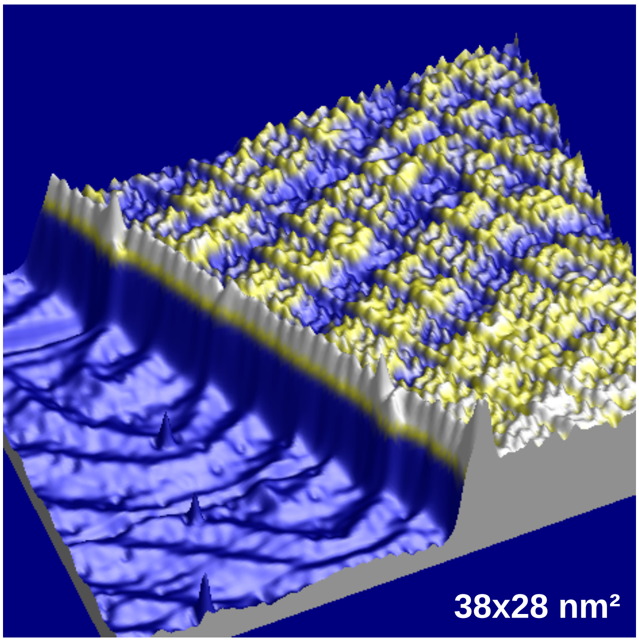
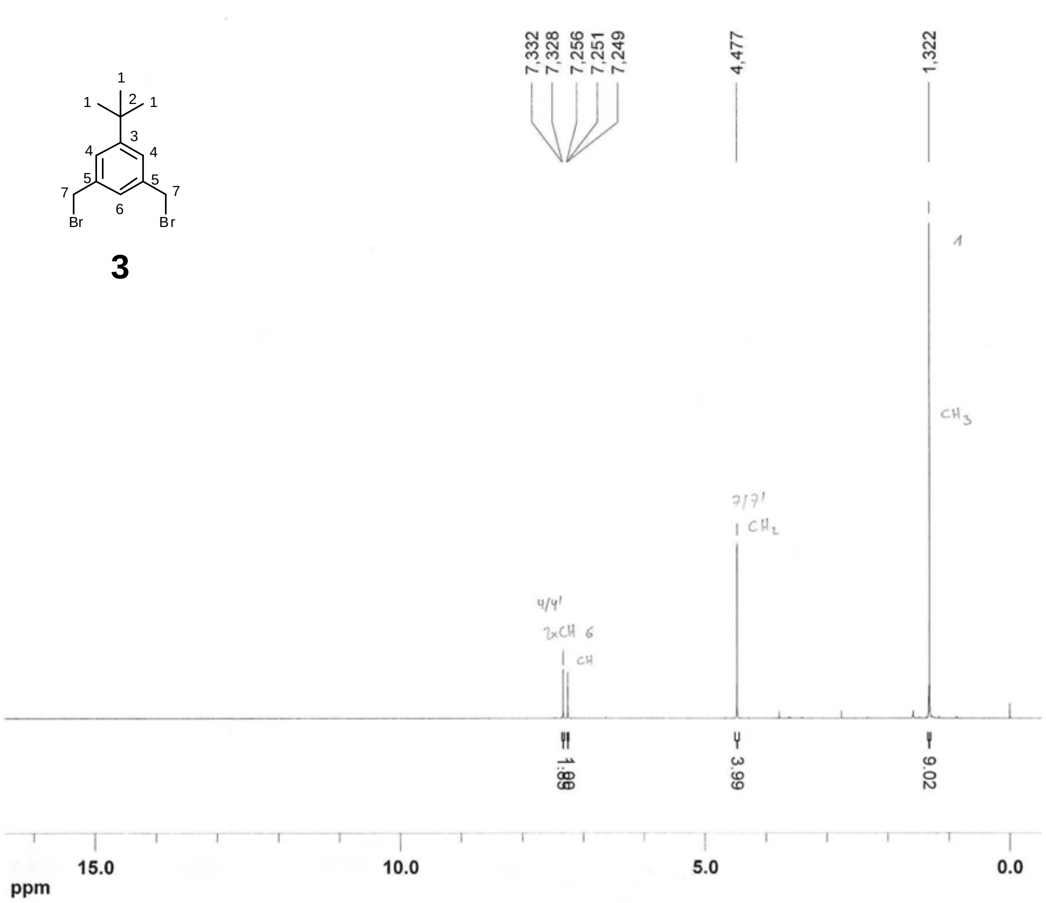


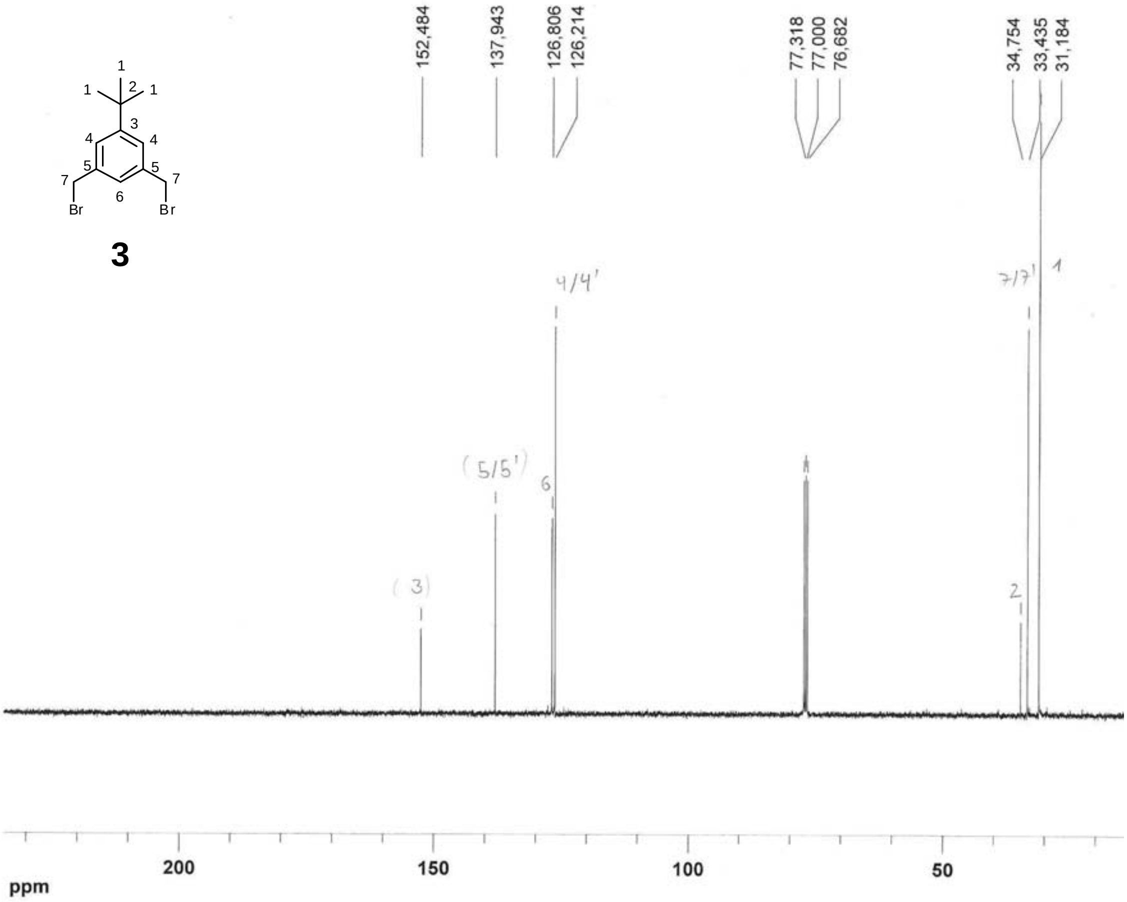
Fig. SI-5 Topographical picture of the self-assembled monolayers obtained by sublimation of the cyclophane **1** displaying the reconstruction of the underlying Au(111) surface.

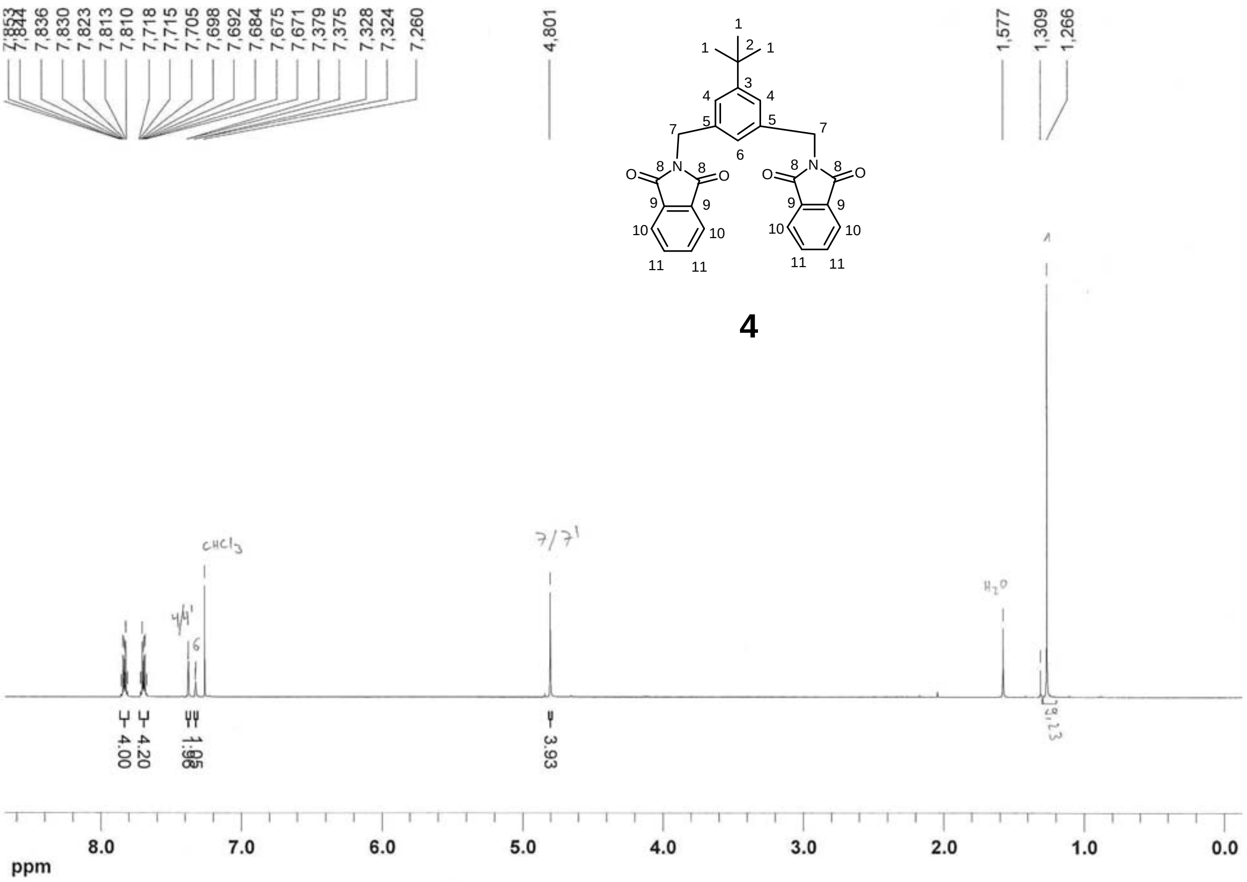
References

1 G. L. Succaw, T. J. R. Weakley, F. Han, K. M. Doxsee, *Crystal Growth & Design*, 2005, **5**, 2288.
2 H. Langhals, H. Jaschke, *Chem. Eur. J.*, 2006, **12**, 2815.
3 F. Vonau, D. Aubel, L. Bouteiller, G. Reiter, L. Simon, *Phys. Rev. Lett.*, 2007, **99**, 086103.
4 E. I. Altman, R. J. Colton, *Surf. Sci.*, 1992, **279**, 49.

^{1}H- and ^{13}C-NMR spectra



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7,813
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7,698
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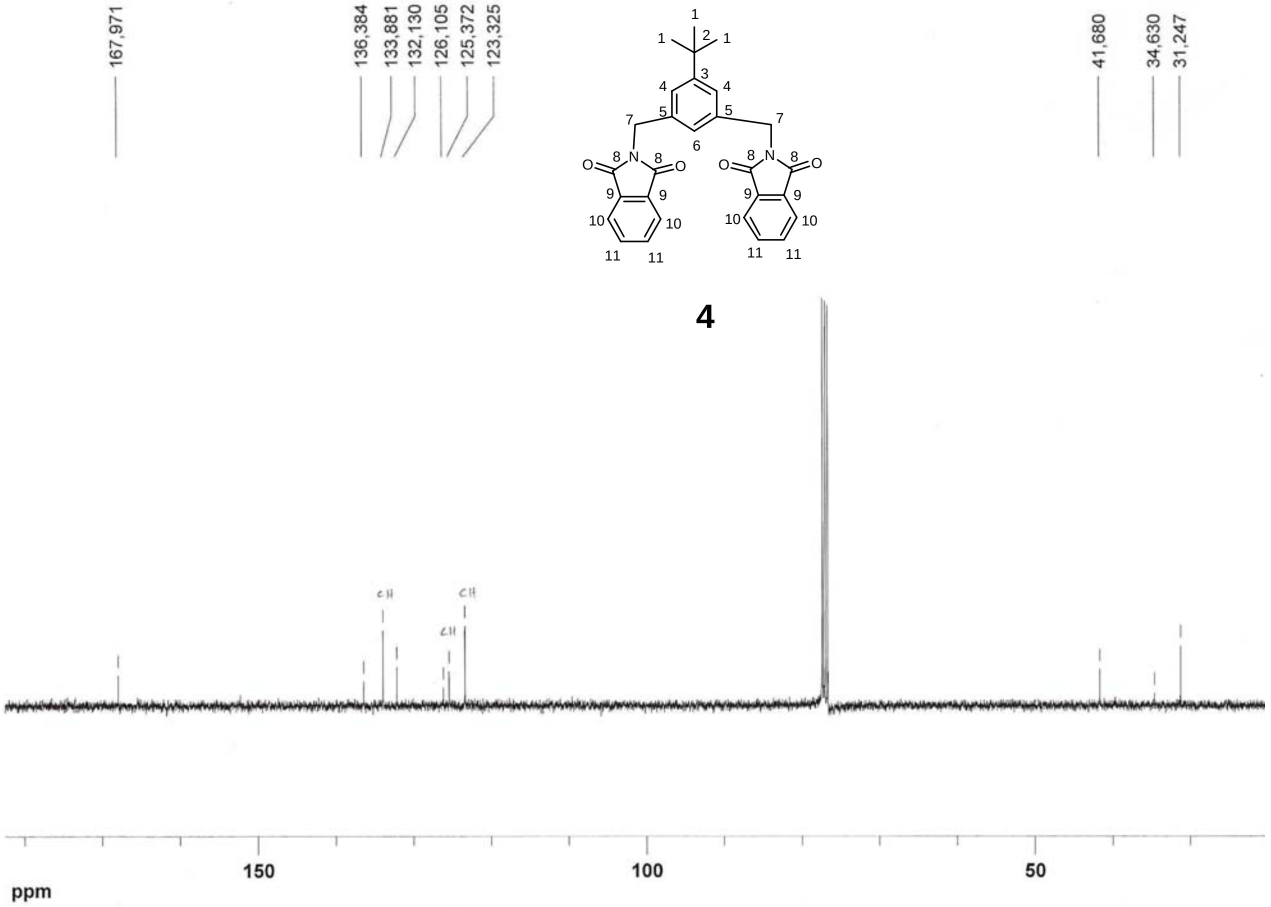
7,684
7,675
7,671
7,379
7,375
7,328
7,324
7,260
4,801
1,577
1,309
1,266
4
CHCl3
4/4'
6
7/7'
H2O
1
4.00
4.20
1.96
1.95
3.93
9.13
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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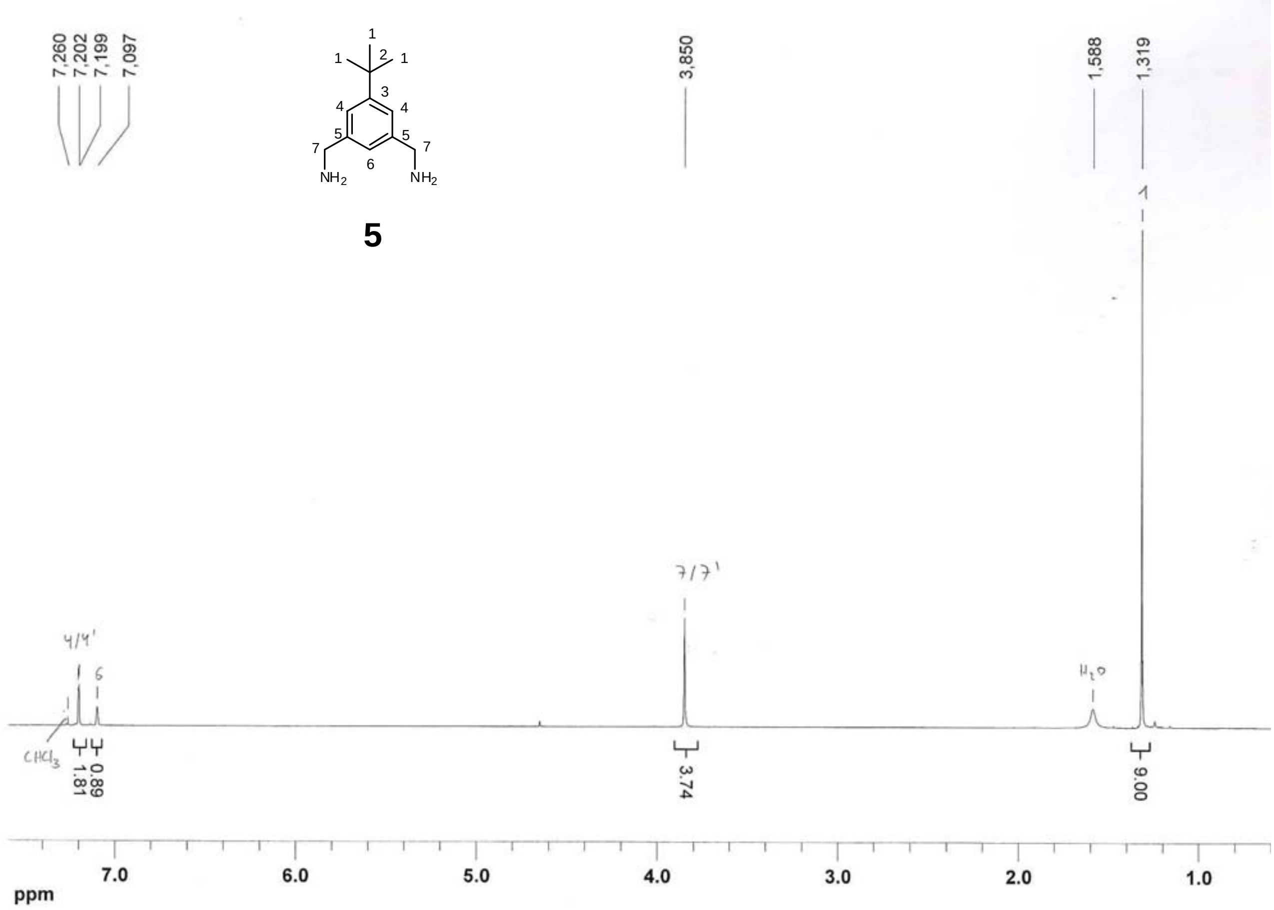
31,247
4
CH
CH
CH
150
100
50
ppm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7,202
7,199
7,097
1
1
2
1
3
4
4
5
5
7
7
6
NH2
NH2
5
3,850
1,588
1,319
1
7/7'
4/4'
6
CHCl3
H2O
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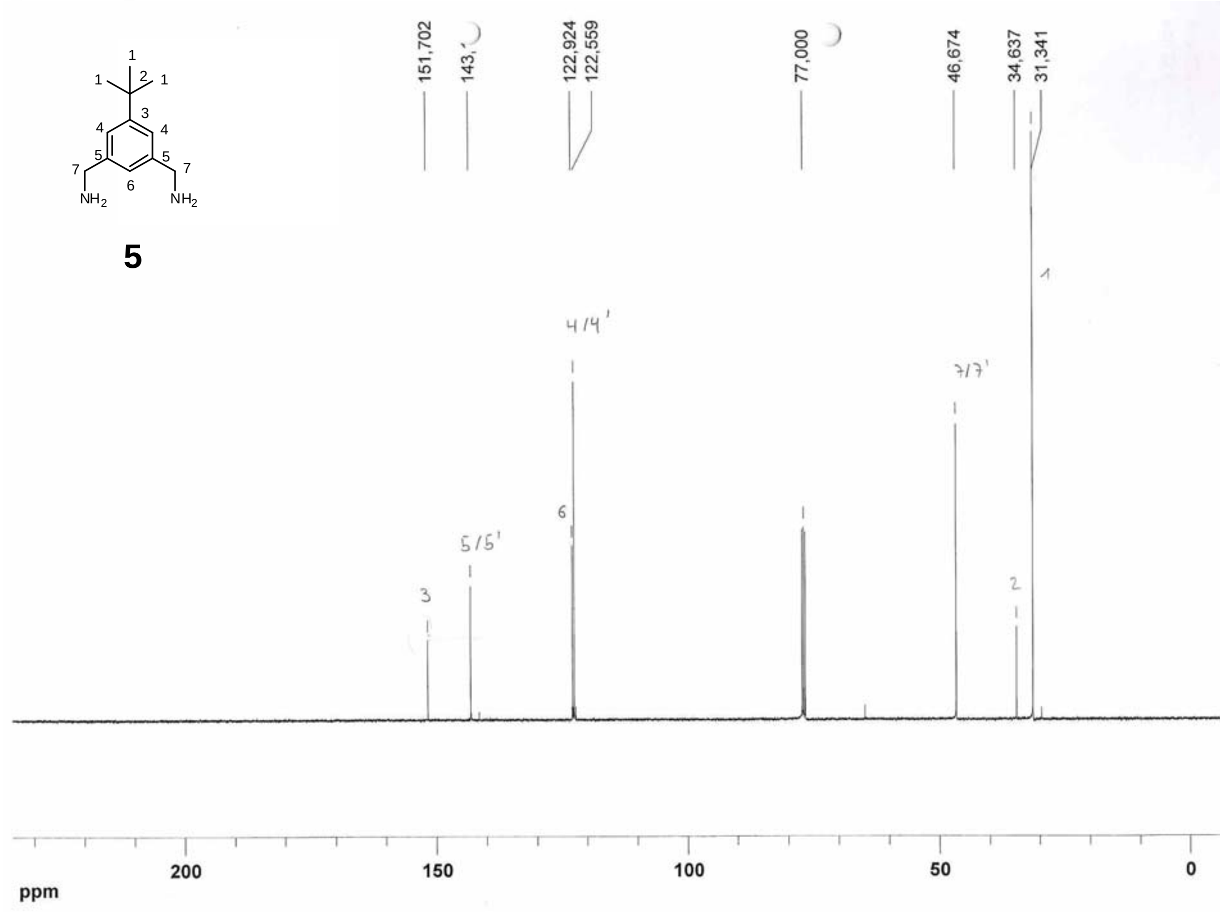
0.89
3.74
9.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm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1
2
1
3
4
4
5
5
7
7
6
NH2
NH2
5
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143,
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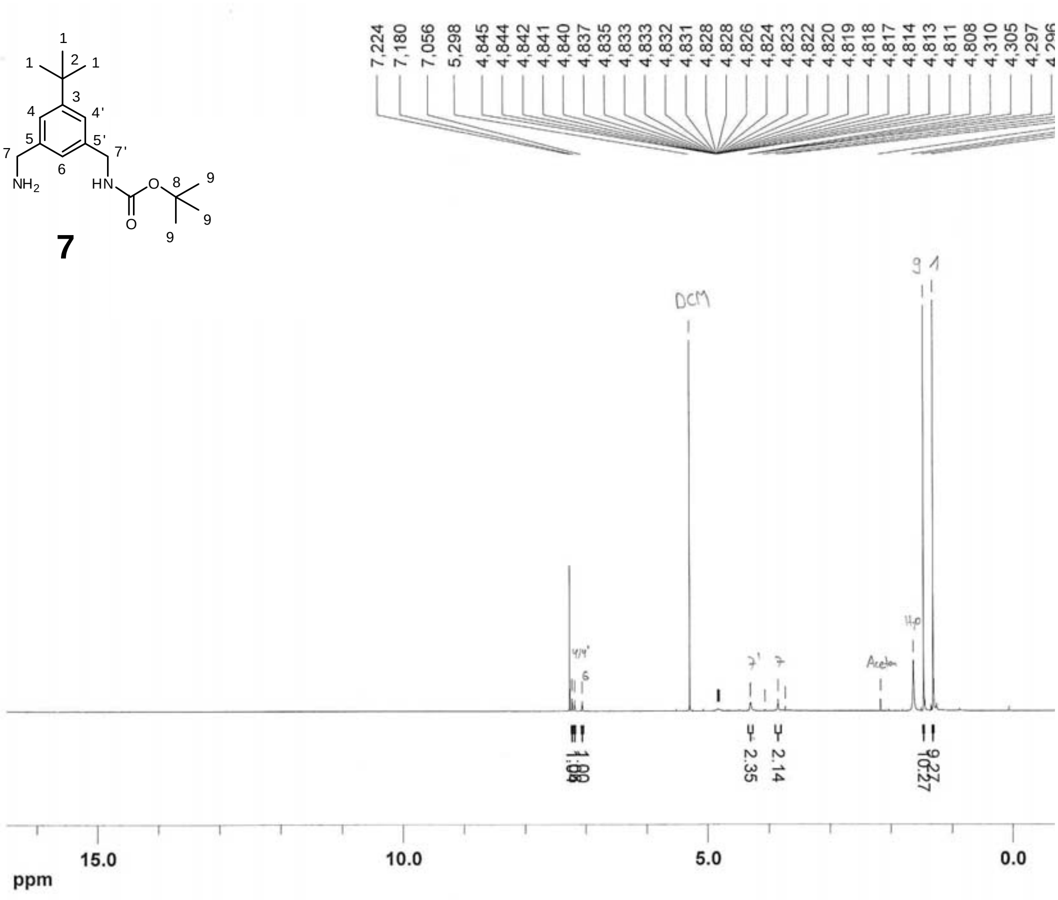
122,559
77,000
46,674
34,637
31,341
1
4/4'
7/7'
6
5/5'
3
2
200
150
100
50
0
ppm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4,840
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4,835
4,833
4,833
4,832
4,831
4,828
4,828
4,826
4,824
4,823
4,822
4,820
4,819
4,818
4,817
4,814
4,813
4,811
4,808
4,310
4,305
4,297
DCM
9
1
4/4'
6
7'
7
Aceton
H2O
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2.35
2.14
9.27
10.27
15.0
10.0
5.0
0.0
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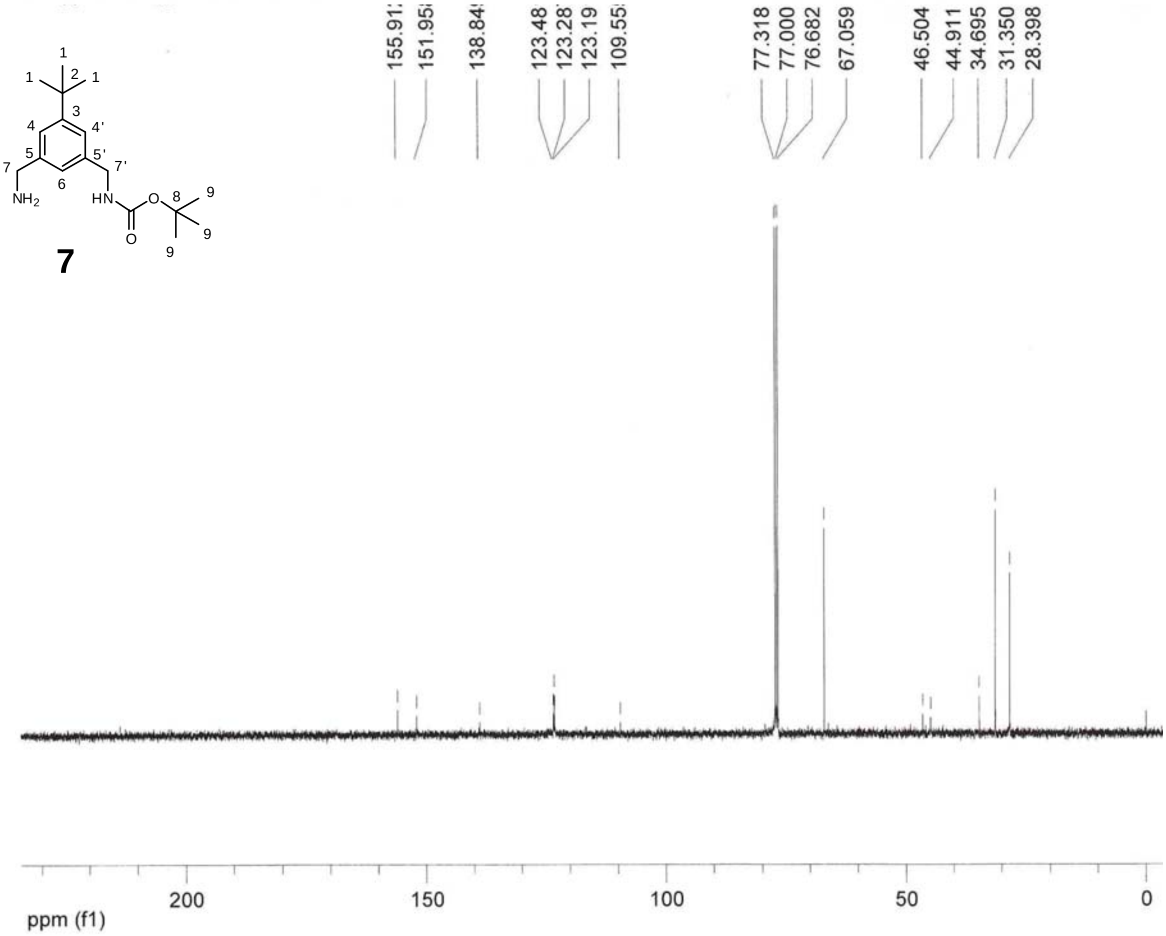
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34.695
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28.398
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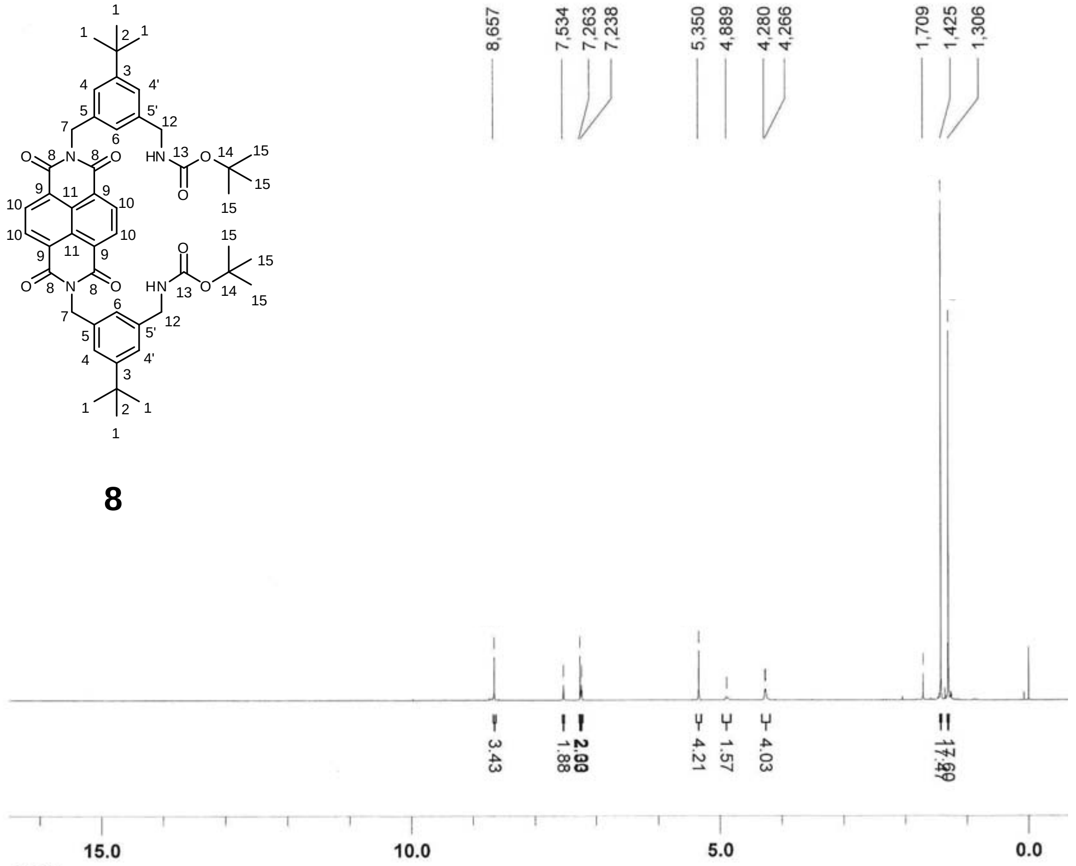
150
100
50
0
ppm (f1)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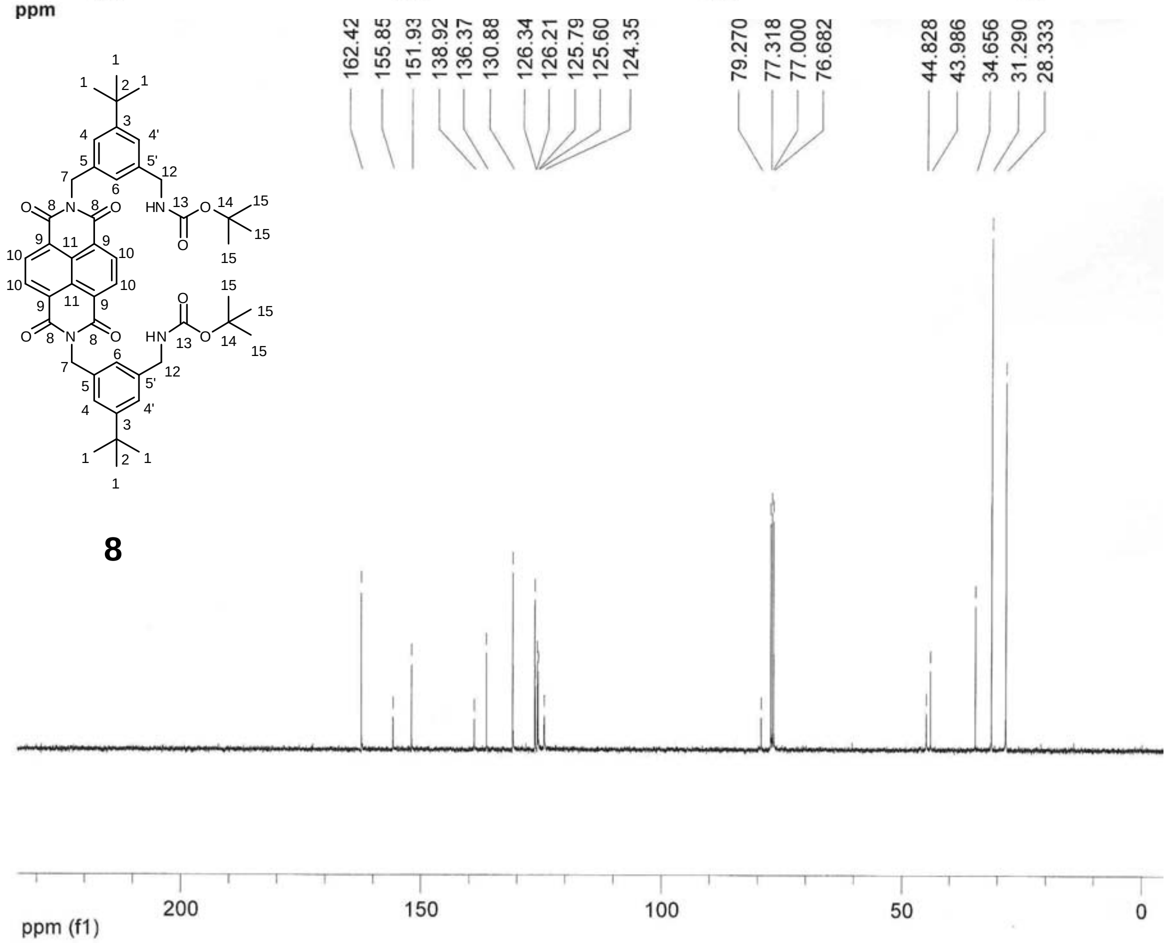
ppm

8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77.318
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150
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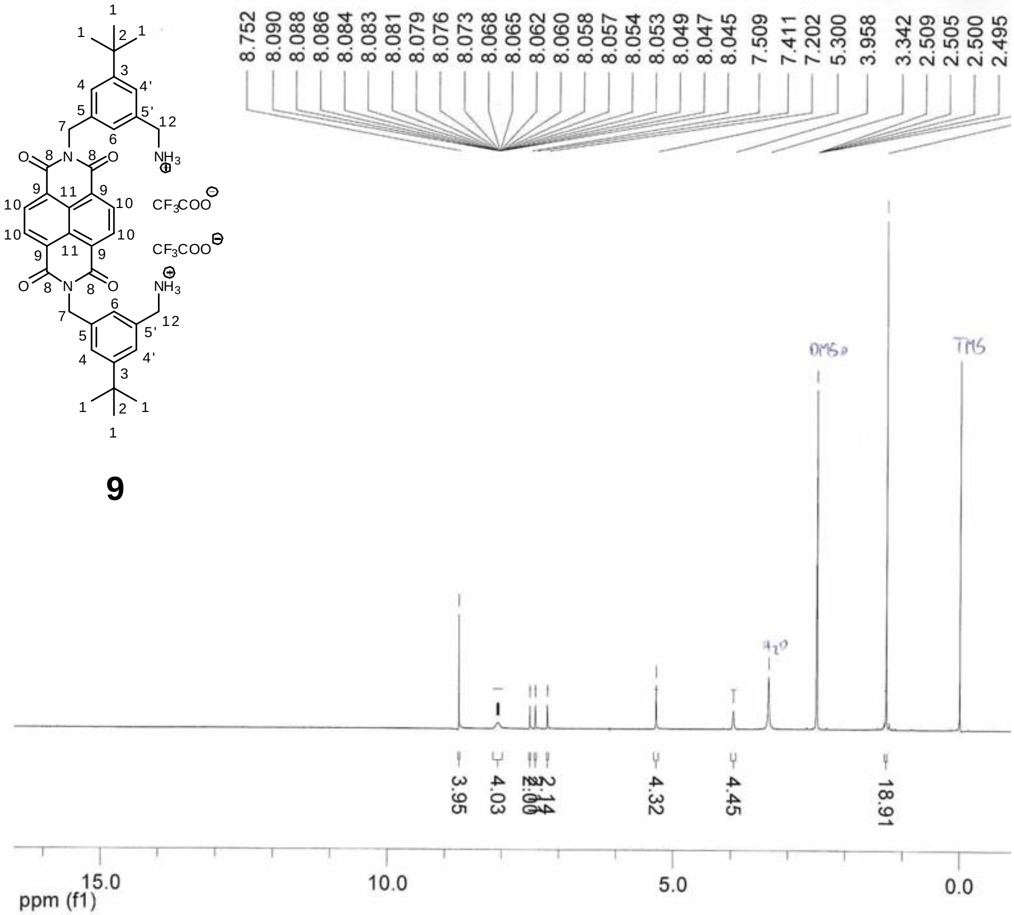
50
0
ppm (f1)

8


1
2
3
4
4'
5
5'
6
7
8
9
10
11
12
NH_3
CF_3COO

9

8.752
8.090
8.088
8.086
8.084
8.083
8.081
8.079
8.076
8.073
8.068
8.065
8.062
8.060
8.058
8.057
8.054
8.053
8.049
8.047
8.045
7.509
7.411
7.202
5.300
3.958
3.342
2.509
2.505
2.500
2.495
DMSO
TMS
H2O
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2.14
4.32
4.45
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10.0
5.0
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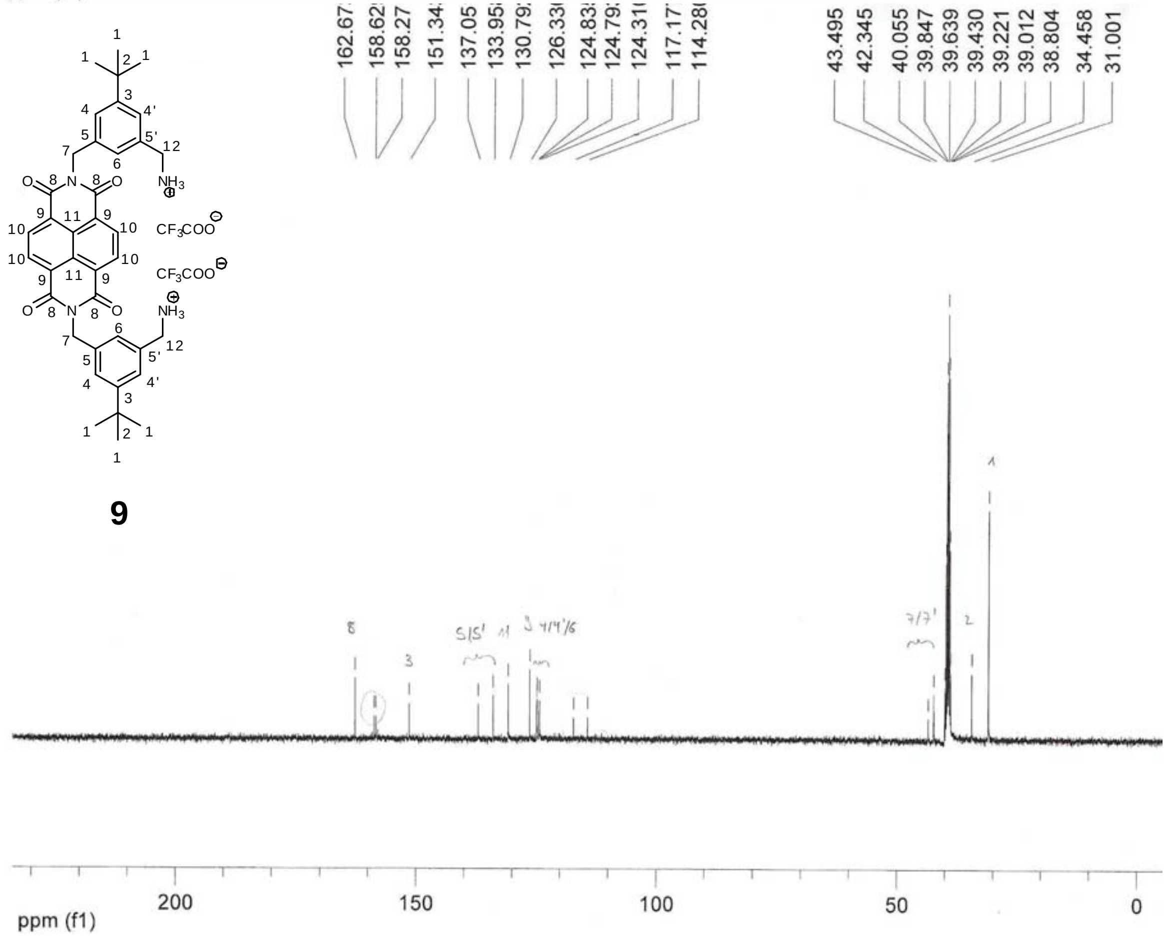
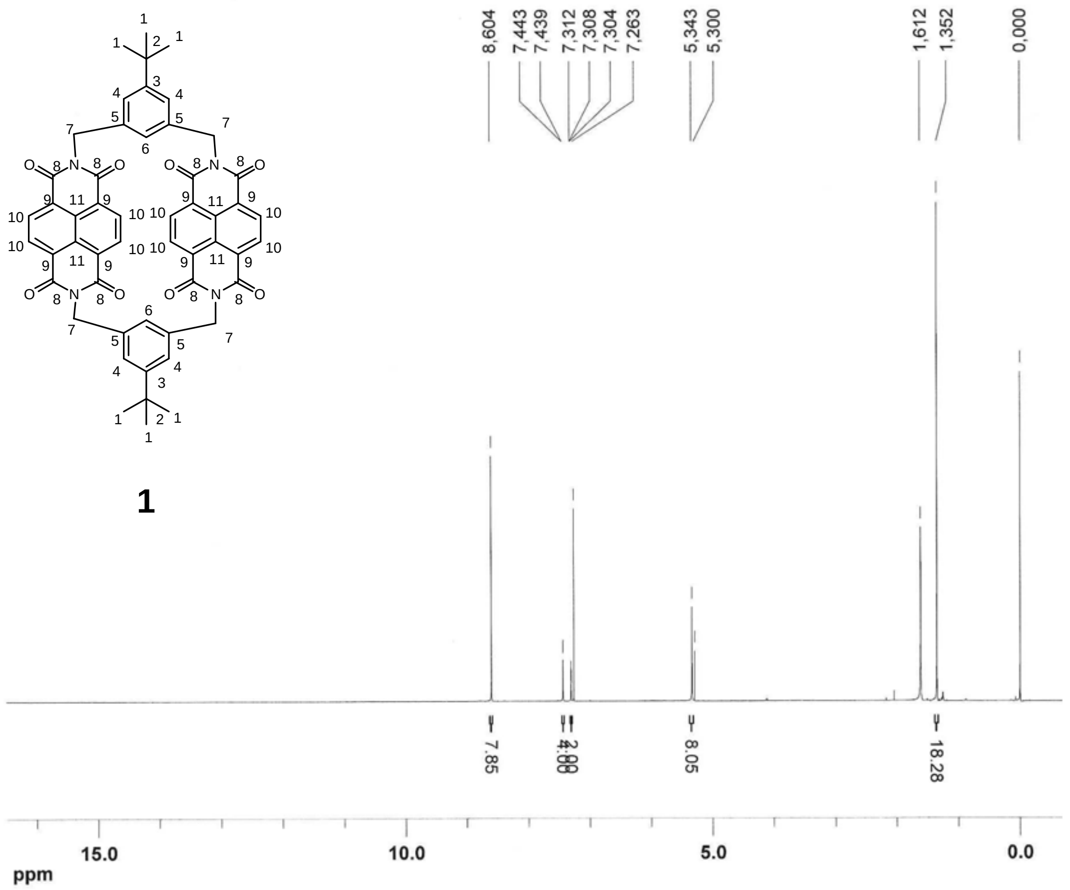
ppm (f1)


1
2
3
4
4'
5
5'
6
7
8
9
10
11
12
NH_3
CF_3COO

9

162.67
158.62
158.27
151.34
137.05
133.95
130.79
126.33
124.83
124.79
124.31
117.17
114.28
43.495
42.345
40.055
39.847
39.639
39.430
39.221
39.012
38.804
34.458
31.001
8
3
5/5' 11
3 4/4'/6
7/7'
2
1
200
150
100
50
0
ppm (f1)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2.00
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10.0
5.0
0.0
ppm

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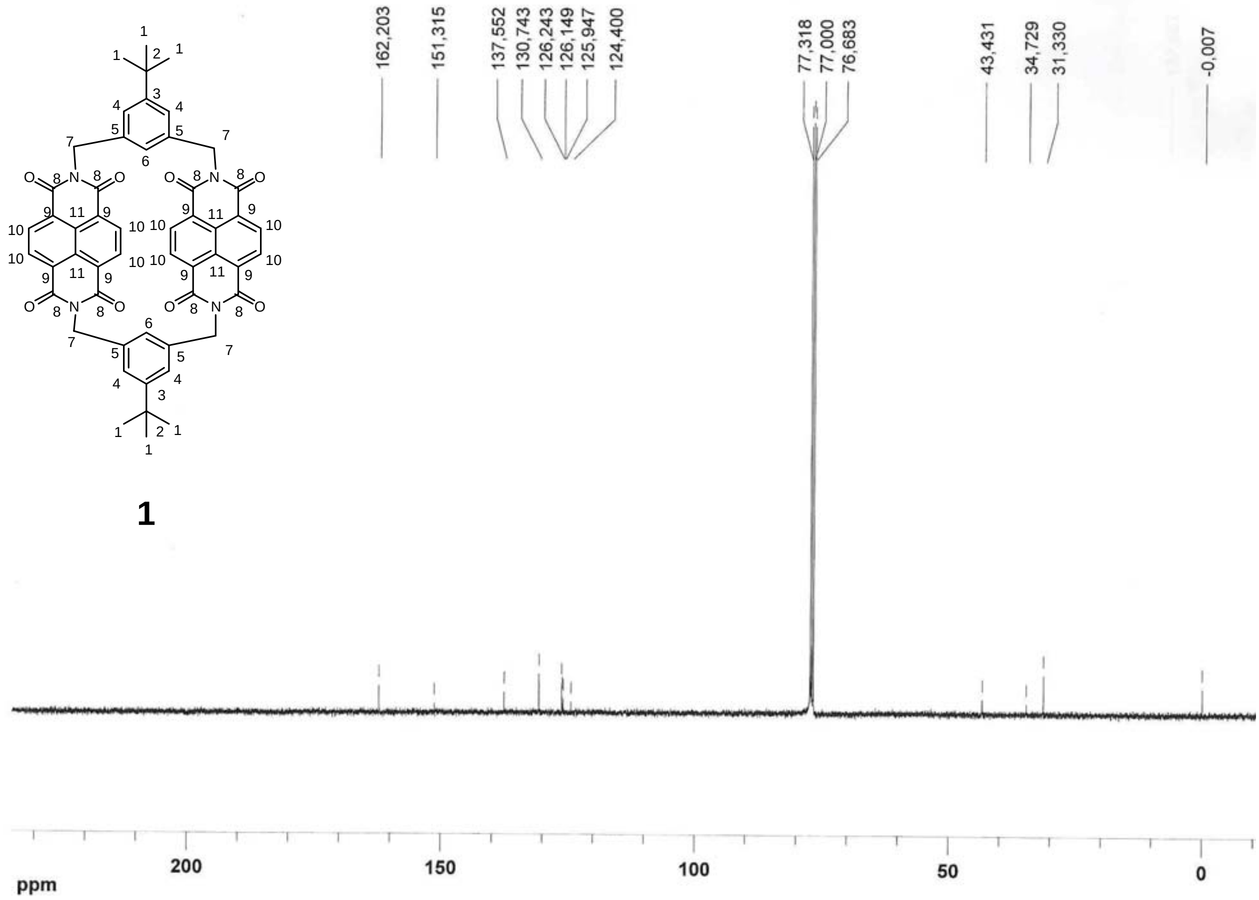
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100
50
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ppm

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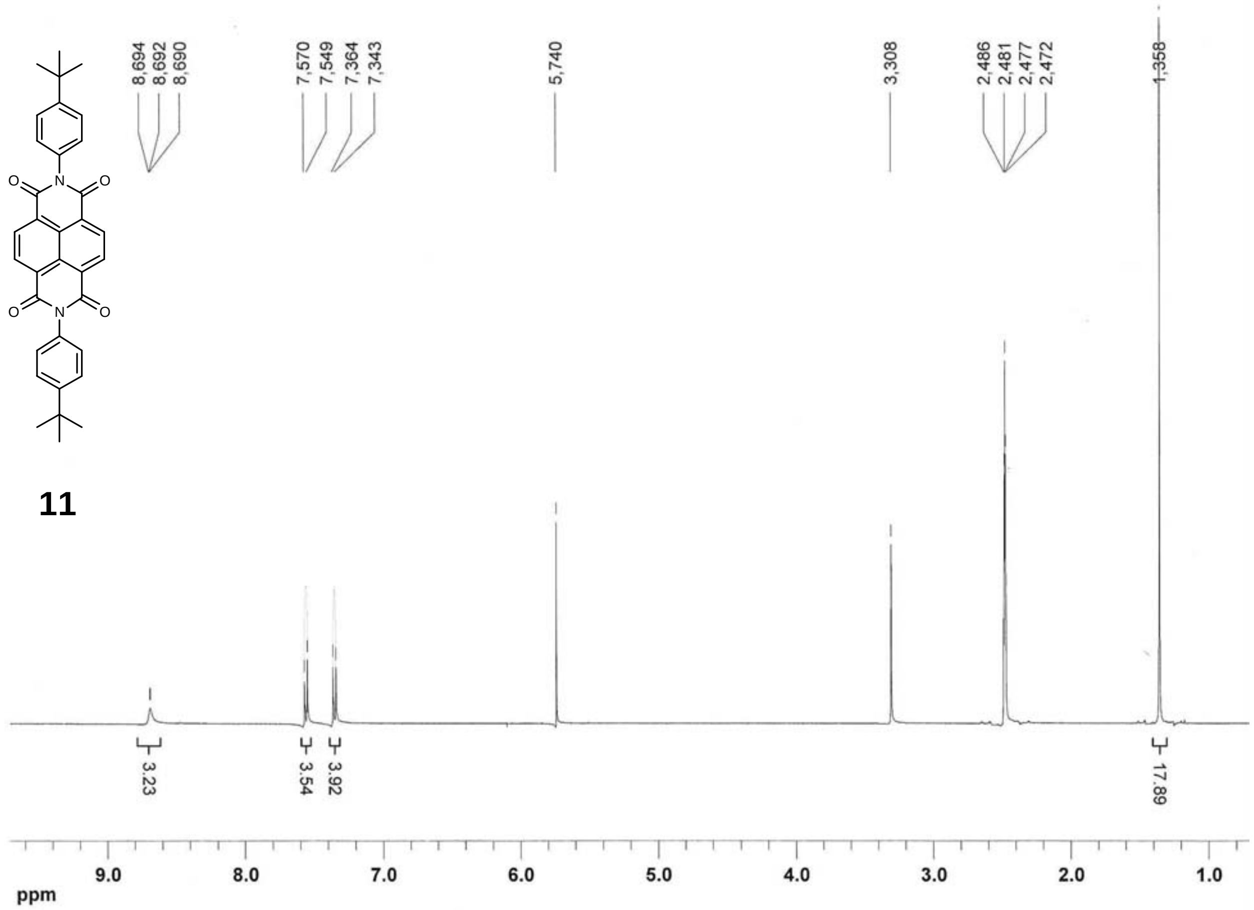
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2,481
2,477
2,472
1,358
3.23
3.54
3.92
17.89
9.0
8.0
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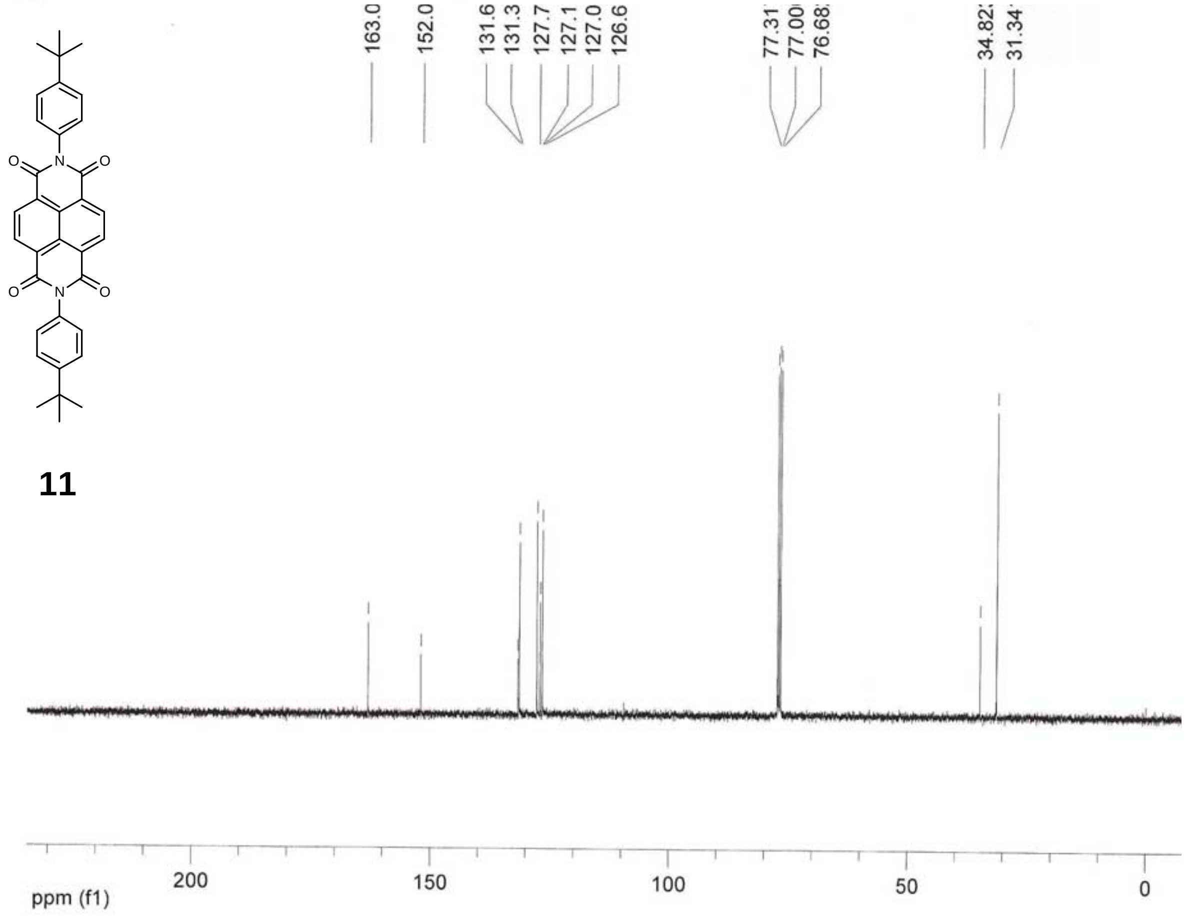
5.0
4.0
3.0
2.0
1.0
ppm
O
N
O
O
N
O

11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76.68
34.82
31.34
200
150
100
50
0
ppm (f1)
O
N
O
O
N
O

11