Selective Switching of Multiple Azobenzenes

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Supporting Information

General Information

Synthesis and Characterization

Chemicals were used as purchased from Sigma-Aldrich, Acros Organics, Alfa Aesar and TCI Europe. Anhydrous solvents were purchased from Acros Organics. Technical grade solvents used during workup and purification were distilled prior to use. Air and/or water-sensitive reactions were carried out under Schlenk-conditions. Solids were dried under high vacuum (oil pump, ca 10^{-3} mbar) at room temperature (rt), 50 °C or 60 °C when necessary. Flash column chromatography and column chromatography was carried out with Silica 60 M (0.04 – 0.063 mm) or Silica 60 (0.063 – 0.2 mm) from Macherey Nagel GmbH & Co. KG. Medium-pressure liquid chromatography (MPLC) was carried out on a Büchi Sepacore® flash chromatography system X-50 with Sepacore® Flash cartridges (particle size: 40–63 μm). Thin layer chromatography was performed on Polygram® SIL G/UV_{254} from Macherey Nagel GmbH & Co. KG. NMR spectra were measured on a Bruker Avance II 200 MHz, Avance II 400 MHz, Avance III 400 MHz HD or Avance III 600 MHz spectrometer at rt, if not stated otherwise. Chemical shifts are reported in parts per million (ppm) relative to the solvent peak, coupling constants (*J*) are reported in Hertz (Hz). Deuterated solvents were obtained from Deutero GmbH (Kastellaun, Germany) or Euriso-Top GmbH. For all azobenzenes, the thermodynamically more stable *E*-isomer is reported if not noted otherwise. ESI-MS spectra were recorded on a Bruker Daltonics Micro TOF. APCI mass spectra were obtained by using the same system with a Bruker APCI II ion source. Melting points were measured on a Krüss KSP1N capillary melting point apparatus with a heating rate of 1 °C min^{-1}.

Irradiation Experiments

Irradiation of the NMR or UV/Vis samples was conducted in an in house-built box using high power LEDs by Lumitronix or Nichia, purchased from leds.de. After the given irradiation times, the samples were immediately placed and measured in the corresponding spectrometer.

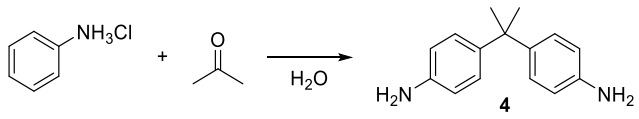
Table S1: LEDs used for all irradiation experiments with their specifications.

λmax / nm	ΔλFWHM / nm	Product name	Luminous flux / mW
365	9	NCSU276AT-U365	780
385	10	NCSU276AT-U385	900
405	12	NCSU276AT-U405	950
425-430	14	LHUV-0425-0650	675
448	20	LXML-PR01-0500	520
470	20	LXML-PB01-0030	44
500	30	NCSE119AT	143

Figure S1: In-house built LED irradiation box for UV/Vis cuvettes aswell as NMR tubes.

Synthesis

2,2-(4-Aminophenyl)propane (**4**)[1]



In a pressure tube, aniline hydrochloride (100 g, 764 mmol, 3.95 eq.) was suspended in water (80 mL) and acetone (14.2 mL, 193 mmol, 1.00 eq.). The tube was sealed and heated to 160 °C for 19.5 h. After cooling to rt, the solution was basified with aq. NaOH (25%) and EtOAc was added (130 mL). The organic phase was separated, washed with water (150 mL) and brine (150 mL) and was concentrated under reduced pressure. The resulting brown solution was distilled in vacuum to remove unreacted aniline and volatile byproducts to obtain a brown oil, which crystallized upon cooling to rt. The crude product was recrystallized from toluene to yield a beige solid (24.3 g, 56%).

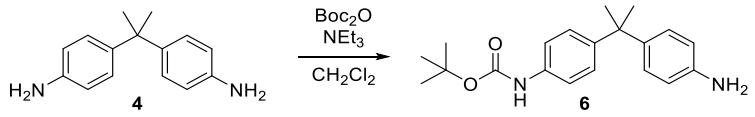
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.04 (d, *J*=8.6, 4H), 6.60 (d, *J*=8.6, 4H), 3.55 (s, 4H), 1.61 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.9, 141.6, 127.7, 114.9, 41.5, 31.1.

HRMS (ESI): *m*/*z* for $C_{15}H_{18}N_2Na^+$; calcd. 249.1362, found 249.1365

M.p. 132 °C.

2-(4-Aminophenyl)-2-(4'-*N*-Boc-aminophenyl)propane (**6**)



To an ice-cooled solution of 2,2-bis(4-aminophenyl)propane (5.01 g, 22.1 mmol, 1.00 eq.) and NEt_3 (3.2 mL, 23 mmol, 1.0 eq.) in CH_2Cl_2 (50 mL), di-*tert*-butyl dicarbonate (4.84 g, 22.2 mmol, 1.00 eq.) was added. The solution was stirred at 0 °C for 30 min and at rt overnight. After evaporation of the solvent under reduced pressure, the crude product was purified by column chromatography (SiO_2, cyclohexane/EtOAc; 3:2) to yield a colorless solid (3.31 g, 46%).

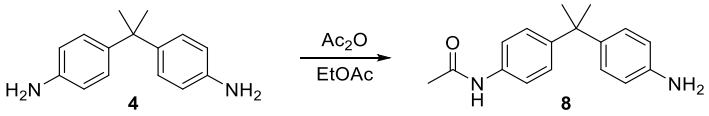
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.23 (d, *J*=8.4, 2H), 7.15 (d, *J*=8.6, 2H), 7.01 (d, *J*=8.6, 1H), 6.61 (d, *J*=8.6, 2H), 6.45 (s, 1H), 3.67 (s, 2H), 1.61 (s, 6H), 1.51 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 152.9, 146.0, 143.6, 141.2, 135.7, 127.6, 127.3, 118.3, 115.0, 80.3, 41.8, 30.9, 28.4.

HRMS (ESI): *m*/*z* for $C_{20}H_{26}N_2O_2Na^+$; calcd. 349.1886, found 349.1900.

M.p. 49.9 °C.

2-(4-Aminophenyl)-2-(4'-*N*-acetylamidophenyl)propane (**8**)



To an ice-cooled solution of 2,2-bis-(4-aminophenyl)propane (5.01 g, 22.1 mmol, 1.00 eq.) in EtOAc (125 mL), acetic ahnydride (2.28 g, 22.1 mmol, 1.00 eq.) in EtOAc (ca. 5 mL) was added. After stirring for 15 min, the ice-bath was removed and the solution was allowed to warm to rt within 2 h. After filtration of the precipitate, the filtrate was concentrated under reduced pressure to yield a slightly brown oil, which was purified by column chromatography (SiO_2, toluene/EtOAc; 1:5) to yield the product as a colorless solid (3.11 g, 52%).

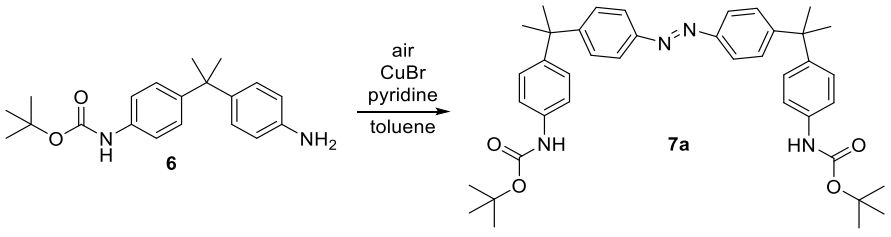
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.43 – 7.32 (m, 3H), 7.17 (d, *J*=8.5, 2H), 7.00 (d, *J*=8.6, 2H), 6.59 (d, *J*=8.5, 2H), 3.57 (s, 2H), 2.13 (s, 3H), 1.61 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 168.4, 147.5, 144.1, 140.9, 135.4, 127.7, 127.4, 119.8, 114.9, 42.0, 31.0, 24.6.

HRMS (ESI): *m*/*z* for $C_{17}H_{20}N_2ONa^+$; calcd. 291.1468, found 291.1477.

M.p. 160 °C.

Bis-*N*-Boc-azobenzene **7a**[2]



2-(4-Aminophenyl)-2-(4'-*N*-Boc-aminophenyl)propane (**6**) (324 mg, 993 µmol, 1.00 eq.) was dissolved in toluene (5 mL). CuBr (11 mg, 80 µmol, 8 mol%) and pyridine (18.5 µL, 228 µmol, 23 mol%) were added and the reaction mixture was heated to 60 °C under air exposure for 18.5 h. After cooling to rt, the solvent was evaporated under reduced pressure to yield a black solid, which was purified by column chromatography (SiO_2, cyclohexane/EtOAc; 4:1) to yield the product as an orange solid (278 mg, 86%).

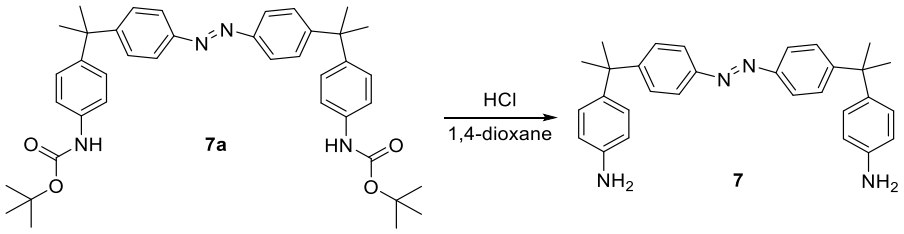
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J*=8.5, 4H), 7.35 (d, *J*=8.6, 4H), 7.29 – 7.23 (m, 4H), 7.17 (d, *J*=8.7, 4H), 6.43 (s, 2H), 1.69 (s, 12H), 1.51 (s, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 154.0, 153.0, 151.0, 145.1, 136.2, 127.6, 127.5, 122.5, 118.5, 80.6, 42.9, 30.9, 28.5.

HRMS (ESI): *m*/*z* for $C_{40}H_{48}N_4O_4Na^+$; calcd. 671.3568, found 671.3570.

M.p. 105 °C.

Azodianiline **7**



Bis-*N*-Boc-azobenzene **7a** (881 mg, 1.36 mmol, 1.00 eq.) was treated with HCl in dioxane (4 mol/L, 5.5 mL, 22 mmol, 16 eq.). The resulting suspension was stirred at rt for 60 min (TLC control showed full conversion after 45 min). The reaction was quenched by the consecutive addition of aq. NaOH (4 mol/L, 11 mL) and EtOAc (10 mL). After phase separation, the aqueous phase was extracted with EtOAc (5 mL) and the combined organic phases were dried over $MgSO_4$. Filtration and removal of the solvents under reduced pressure afforded an orange solid, which was dried in high vacuum at 50 °C overnight (588 mg, 97%).

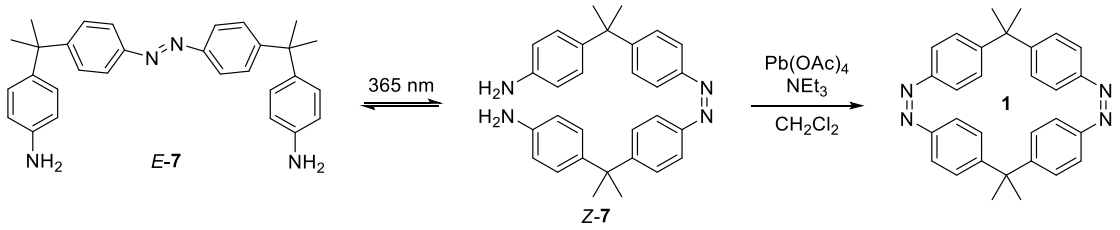
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J*=8.6, 4H), 7.37 (d, *J*=8.6, 4H), 7.04 (d, *J*=8.5, 4H), 6.62 (d, *J*=8.5, 4H), 3.56 (s, 4H), 1.68 (s, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 154.4, 150.8, 144.1, 140.4, 127.7, 127.5, 122.3, 114.9, 42.5, 30.8.

HRMS (ESI): *m*/*z* for $C_{30}H_{33}N_4^+$; calcd. 449.2700, found 449.2700.

M.p. 175 – 177 °C.

(*Z*,*Z*)-Bisazo macrocycle **1**[3]



Azodianiline **7** (180 mg, 401 µmol, 1.00 eq.) and NEt_3 (0.30 mL, 2.1 mmol, 5.3 eq.) were dissolved in CH_2Cl_2 (40 mL). The flask was placed in an empty Dewar bowl for best light reflection and was covered with tin foil for protection from ambient light. Under irradiation of the azo solution with a LED at 365 nm, a solution of $Pb(OAc)_4$ (565 mg, 95%, 1.21 mmol, 3.02 eq.) in CH_2Cl_2 (20 mL) was added dropwise within 55 min. After stirring for further 30 min, the solution was concentrated, and the residue was filtered through a silica plug (EtOAc wash). The obtained crude product was purified by flash column chromatography (SiO_2, toluene/EtOAc; 25:1) to yield the product as a red, crystalline solid (34 mg, 19%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.97 (d, *J*=8.6, 8H), 6.68 (d, *J*=8.5, 8H), 1.61 (s, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 151.2, 150.8, 126.9, 120.8, 42.7, 30.0.

HRMS (ESI): m/z for $C_{30}H_{28}N_4Na^+$; calcd. 467.2206, found 467.2203.

M.p. 267 °C (decomposition).

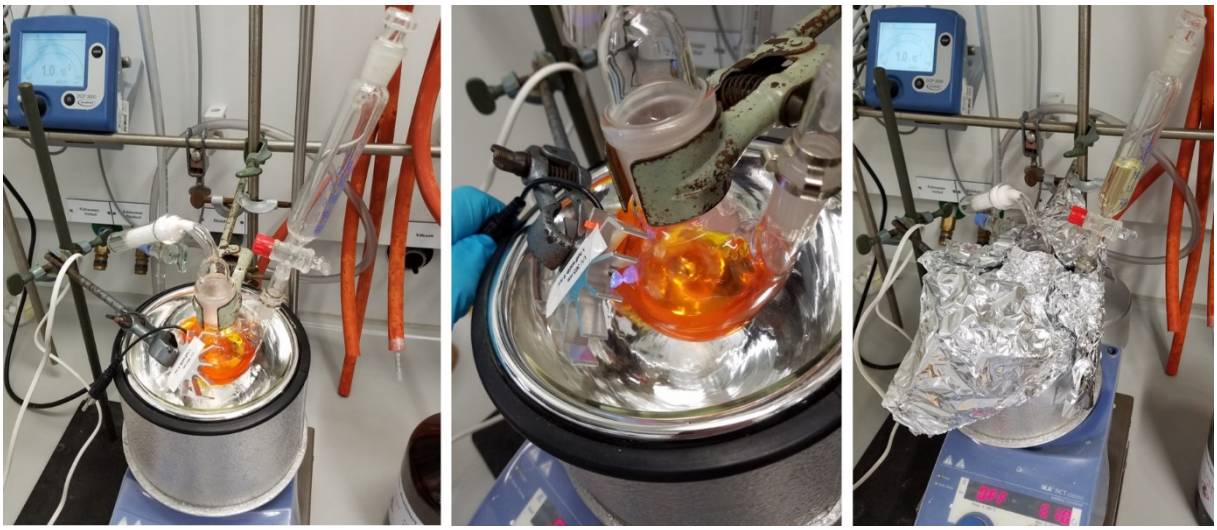
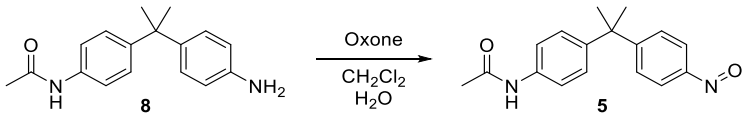


Figure S2: Macrocyclization setup for the synthesis of bisazo macrocycle **1**.

Nitrosoacetamide **5**[4]



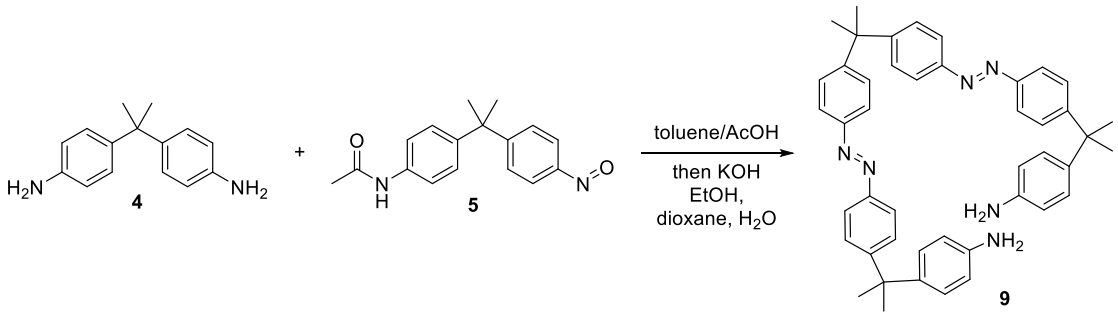
To a solution of 2-(4-Aminophenyl)-2-(4'-*N*-acetylamidophenyl)propane (**8**) (3.02 g, 11.3 mmol, 1.00 eq.) in CH_2Cl_2 (240 mL) under a nitrogen atmosphere a solution of Oxone® (13.8 g, 22.5 mmol, 2.00 eq.) in water (970 mL) was added. The biphasic mixture was vigorously stirred for 20 h at rt and the phases were separated afterwards. The organic phase was washed with 1 M HCl (200 mL), sat. aq. $NaHCO_3$ (200 mL) and brine (200 mL) and was dried over $MgSO_4$. After filtration and evaporation of the solvent under reduced pressure, a green oil was obtained, which was purified by medium pressure liquid chromatography (SiO_2, cyclohexane/EtOAc; 0 to 35% EtOAc) to yield the product as a green, crystalline solid (2.51 g, ca. 79%). The product was immediately used without further purification.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.80 (d, *J*=8.5, 2H), 7.51 – 7.38 (m, 4H), 7.24 – 7.09 (m, 3H), 2.16 (s, 3H), 1.71 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 168.4, 165.1, 159.2, 145.2, 136.1, 127.7, 127.4, 121.1, 120.0, 43.6, 30.5, 24.7.

HRMS (ESI): *m*/*z* for $C_{17}H_{18}N_2O_2Na^+$; calcd. 305.1260, found 305.1266.

Bisazodianiline **9**[5]



A solution of nitroso compound **5** (2.50 g, 8.85 mmol, 2.20 eq.) and AcOH (461 µL, 8.06 mmol, 2.00 eq.) in toluene (80 mL) was degassed in a nitrogen stream for 20 min. Then, 2,2-bis(4-aminophenyl)propane (911 mg, 4.03 mmol, 1.00 eq.) was added and the solution was stirred at 60 °C under a nitrogen atmosphere for 18 h. Then, AcOH (240 mL) was added and stirring at 60 °C was continued for further 5 d. Evaporation of the solvents under reduced

pressure led to a brown solid, which was suspended in a solution of KOH (85%, 72 g, 1.1 mol) in a mixture of EtOH/1,4-dioxane/H_2O (7:3:1, 250 mL, ca 4 mol/L KOH). The mixture was heated to reflux for 23 h, cooled to rt and was poured on ice (ca 200 g). After the addition of CH_2Cl_2 (400 mL), the organic phase was separated, dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography (SiO_2, toluene/EtOAc; 2:1) to yield a red solid (2.81 g, ca. 97% over two steps). An analytically pure sample was obtained by a second flash column chromatography (SiO_2, toluene/EtOAc; 2:1).

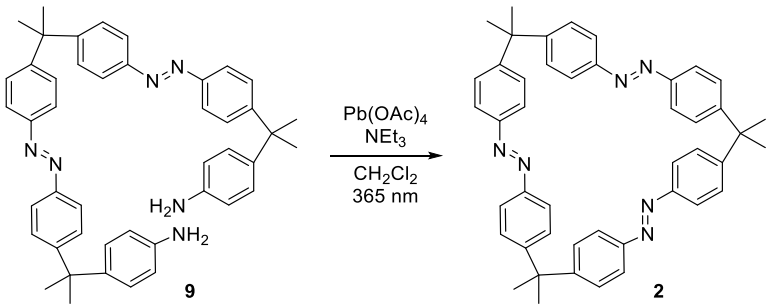
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.88 – 7.75 (m, 8H), 7.44 – 7.35 (m, 8H), 7.04 (d, *J*=8.4, 4H), 6.62 (d, *J*=8.3, 4H), 3.59 (s, 4H), 1.78 (s, 6H), 1.69 (s, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 154.6, 153.3, 151.1, 150.8, 144.3, 140.5, 127.8, 127.7, 127.6, 122.6, 122.5, 115.0, 43.6, 42.6, 30.9, 30.8.

HRMS (ESI): *m*/*z* for $C_{45}H_{47}N_6^+$; calcd. 671.3857, found 671.3858.

M.p. 197 °C.

Trisazo macrocycle **2**[6]



A three-necked flask was equipped with two 250 mL dropping funnels. One funnel was loaded with a solution of bisazodianiline precursor **9** (337 mg, 0.502 mmol, 1.00 eq.) and NEt_3 (1.04 mL, 7.48 mmol, 14.9 eq,) in CH_2Cl_2 (165 mL, 3 mmol/L) and the other dropping funnel was loaded with a solution of $Pb(OAc)_4$ (699 mg, 95%, 1.50 mmol, 2.98 eq.) in CH_2Cl_2 (165 mL). Both solutions were added dropwise into CH_2Cl_2 (150 mL) within 1 h 20 min, while the bisazo-precursor solution was irradiated at 365 nm with a LED continuously. After complete addition, the solution was stirred at rt for 30 min and was concentrated under reduced pressure. The residue was filtered over a silica plug (CH_2Cl_2 wash) and the solvent was evaporated. The oily dark red residue was purified by flash column

chromatography (SiO_2, toluene) to yield a red solid, which was dried in high vacuum (9 mg, 3%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.53 (d, *J*=8.7, 12H), 7.30 – 7.11 (m, 12H), 1.92 (s, 18H).

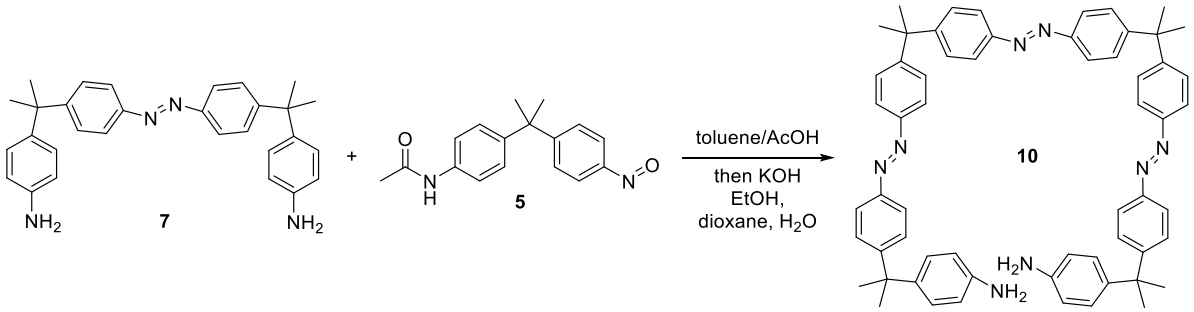
^{13}C NMR (101 MHz, $CDCl_3$) δ = 152.3, 150.9, 126.7, 123.0, 43.0, 27.0.

HRMS (ESI): *m*/*z* for $C_{45}H_{42}N_6Na^+$; calcd. 689.3363, found 689.3363.

M.p. >360 °C.

Figure S3: Macrocyclization setup for the synthesis of trisazo macrocycle **2**.

Trisazodianiline **10**



Nitrosoacetamide **5** (873 mg, 3.09 mmol, 2.49 eq.) and AcOH (143 µL, 2.49 mmol, 2.00 eq.) were dissolved in toluene (28 mL) and the solution was degassed in a nitrogen-stream for 15 min. After the addition of azodianiline **7** (558 mg, 1.24 mmol, 1.00 eq.), the solution was stirred at 60 °C for 29 h. Following, AcOH (84 mL) was added and stirring was continued at 60 °C for further 38 h. After evaporation of the solvents under reduced pressure, the residue was recrystallized from toluene and washed with cold toluene and *n*-pentane. After drying in vacuum, the yellow to brown solid (708 mg, 0.724 mmol, 1.00 eq.) and KOH (85%, 11.5 g, 174 mmol, 240 eq.) were suspended in EtOH/1,4-dioxane/H_2O (7:3:1, 44 mL, ca 4 mol/L KOH) and heated to reflux for 21 h. Following, the mixture was poured on ice (ca 75 g) and CH_2Cl_2 (100 mL) was added. After phase separation, the aqueous phase was extracted with CH_2Cl_2 (2 x 50 mL) and the combined organic phases were washed with brine (100 mL), dried over $MgSO_4$, filtered and the solvents were evaporated under reduced pressure. The residue was suspended in hot toluene, the insoluble material was filtered off and was washed with hot toluene. The filtrate was evaporated under reduced pressure to yield a red to brown solid, which was recrystallized from few toluene. After cooling in an ice bath, a few drops of *n*-pentane were added to the cold solution to induce crystallization. The precipitate was filtered off, washed with *n*-pentane and was dried in high vacuum to yield a yellow to orange solid (542 mg, 49% over two steps).

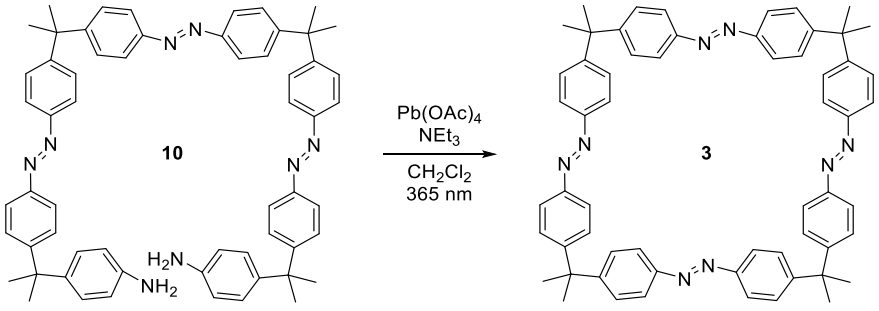
^{1}H NMR (400 MHz, $C_2D_2Cl_4$) δ = 7.86 – 7.75 (m, 12H), 7.44 – 7.35 (m, 12H), 7.05 (d, *J*=8.6, 4H), 6.62 (d, *J*=8.5, 4H), 3.63 (s, 4H), 1.79 (s, 12H), 1.69 (s, 12H).

^{13}C NMR (101 MHz, $C_2D_2Cl_4$) δ = 154.4, 153.2, 153.0, 150.7, 150.7, 150.4, 143.8, 140.1, 127.5, 127.4, 127.4, 122.5, 122.4, 122.2, 114.8, 43.3, 42.2, 30.6, 30.5.

HRMS (ESI): *m*/*z* for $C_{60}H_{61}N_8^+$; calcd. 893.5013, found 893.5013.

M.p. 125 − 127 °C.

Tetraazo macrocycle **3**



A solution of trisazodianiline **10** (149 mg, 0.167 mmol, 1.00 eq.) and NEt_3 (117 µL, 842 µmol, 5.05 eq.) in CH_2Cl_2 (170 mL) was continuously irradiated at 365 nm using a LED. To the stirred and irradiated solution, $Pb(OAc)_4$ (240 mg, 95%, 514 µmol, 3.08 eq.) in CH_2Cl_2 (85 mL) was added dropwise at rt within 1 h. After stirring for further 15 min, $Na_2EDTA \cdot 2\ H_2O$ (350 mg, 841 µmol, 5.04 eq.) in water (85 mL) was added and the biphasic mixture was stirred vigorously for 30 min. Then, the layers were separated, and the organic phase was washed with brine (150 mL), was dried over $MgSO_4$, filtered, and evaporated under reduced pressure to yield a dark red solid. The macrocycle was separated by column chromatography (SiO_2, toluene/EtOAc; 20:1) from the crude mixture. The obtained red solid was washed with CH_2Cl_2 and *n*-pentane to yield the product as an orange solid (17 mg 12%). It was found that the compound was insoluble in almost all common organic solvents except of 1,1,2,2-tetrachloroethane (solubility ca 1 mg/mL).

^{1}H NMR (400 MHz, $C_2D_2Cl_4$) δ = 7.75 (d, *J*=8.3, 16H), 7.30 (d, *J*=8.3, 16H), 1.83 (s, 24H).

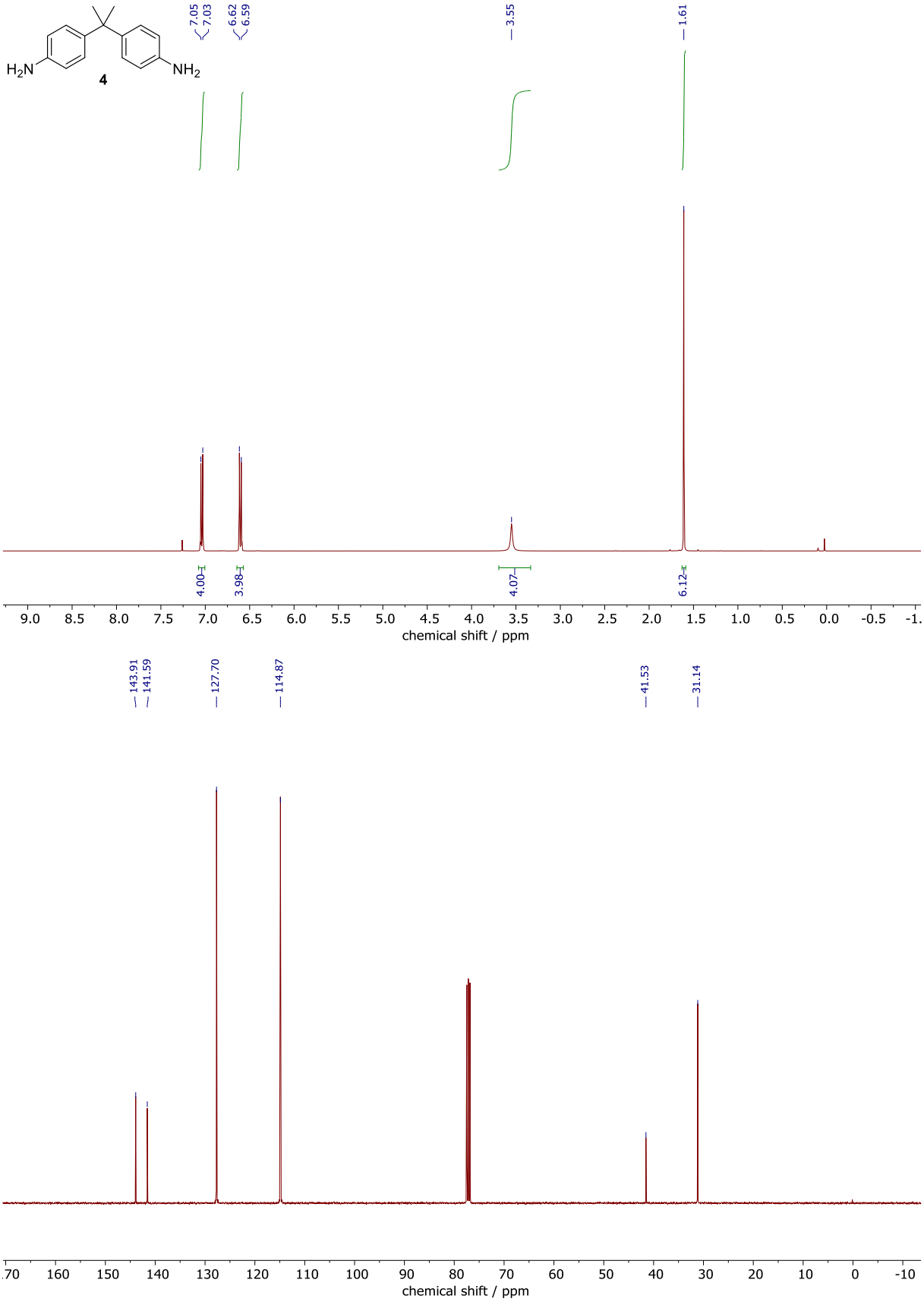
^{13}C NMR (101 MHz, $C_2D_2Cl_4$) δ = 153.3, 150.4, 127.2, 122.5, 42.9, 29.2.

HRMS (APCI): *m*/*z* for $C_{60}H_{57}N_8^+$; calcd. 889.4701, found 889.4697.

M.p. >360 °C.

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

4



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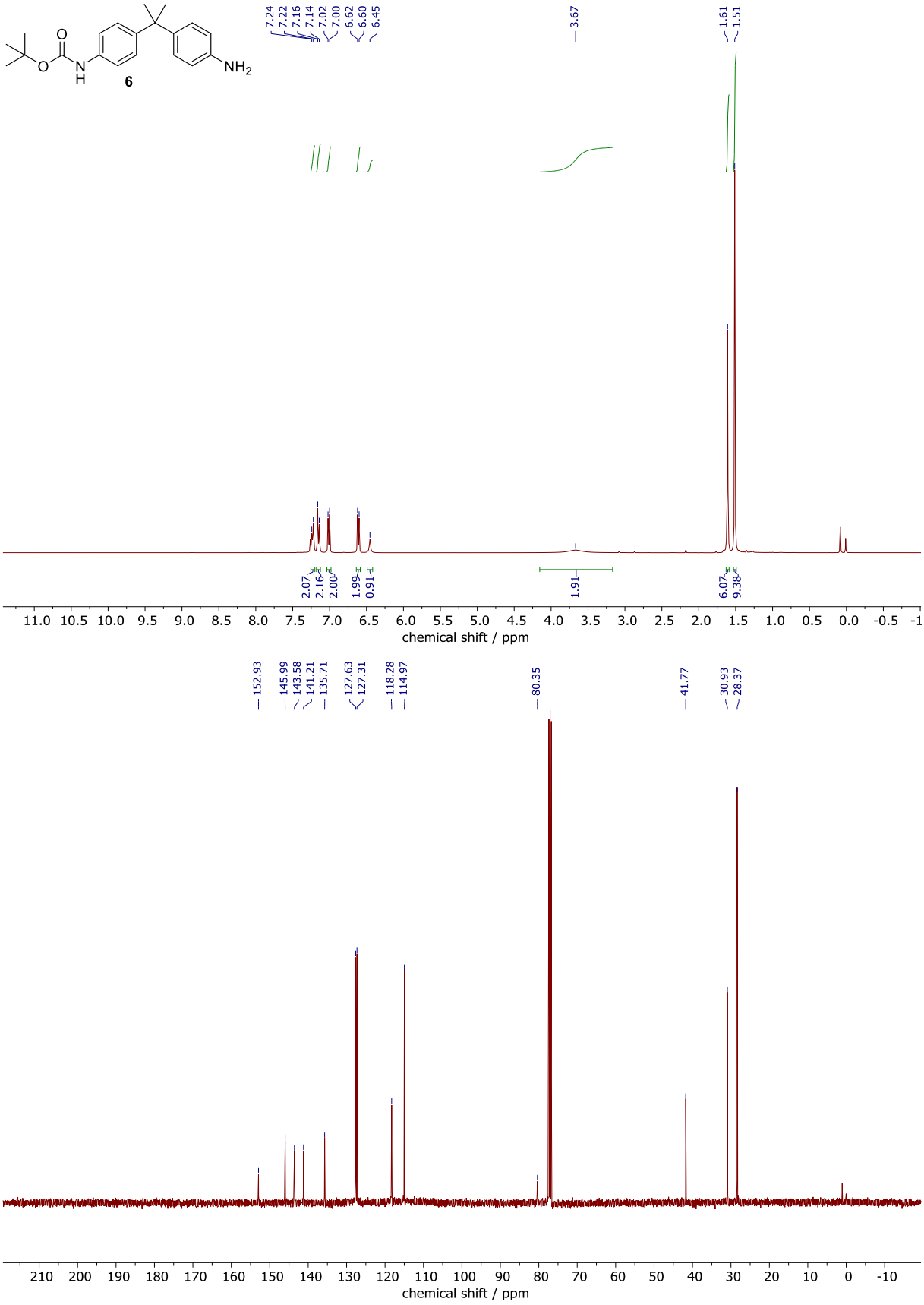
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7.22
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7.14
7.02
7.00
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6.45
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1.61
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2.07
2.16
2.00
1.99
0.91
1.91
6.07
9.38
chemical shift / ppm
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145.99
143.58
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127.31
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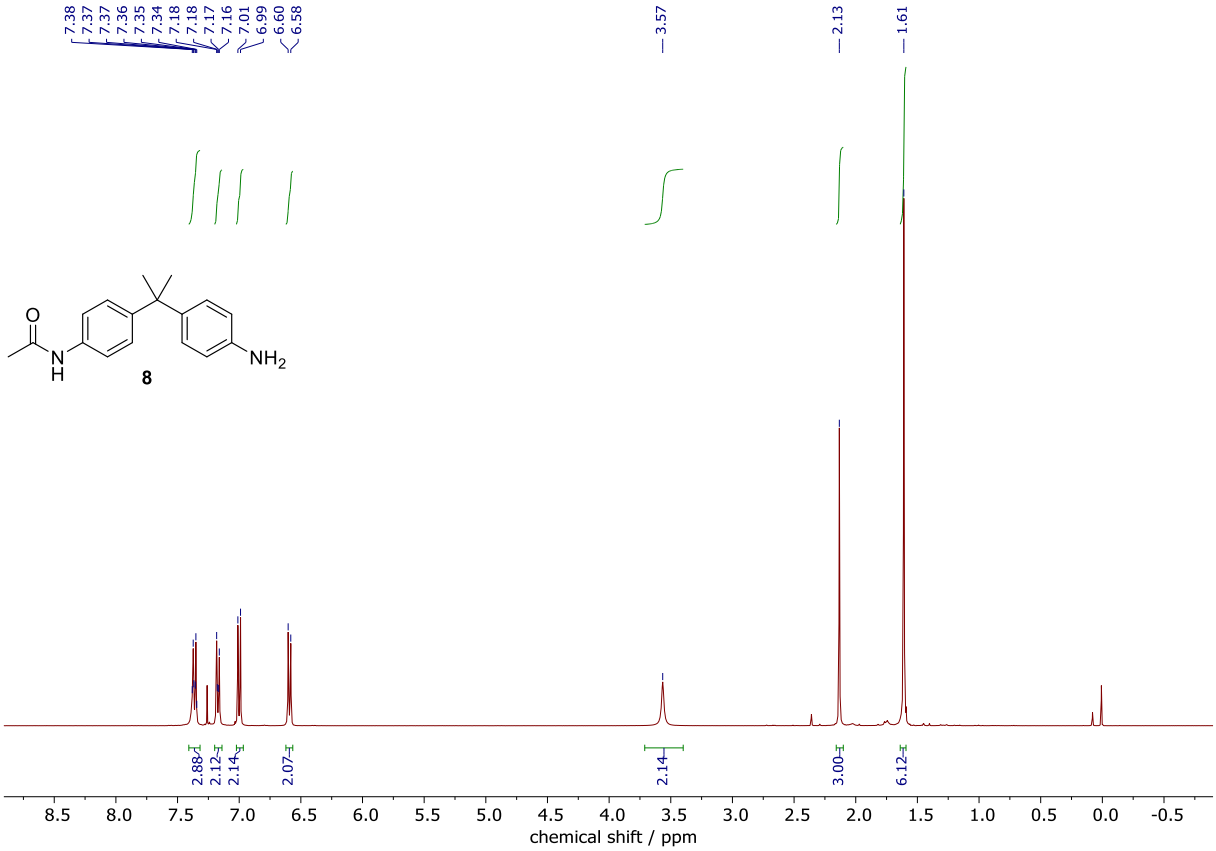
chemical shift / ppm

8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7.37
7.37
7.36
7.35
7.34
7.18
7.18
7.17
7.16
7.01
6.99
6.60
6.58
3.57
2.13
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N
H
NH2
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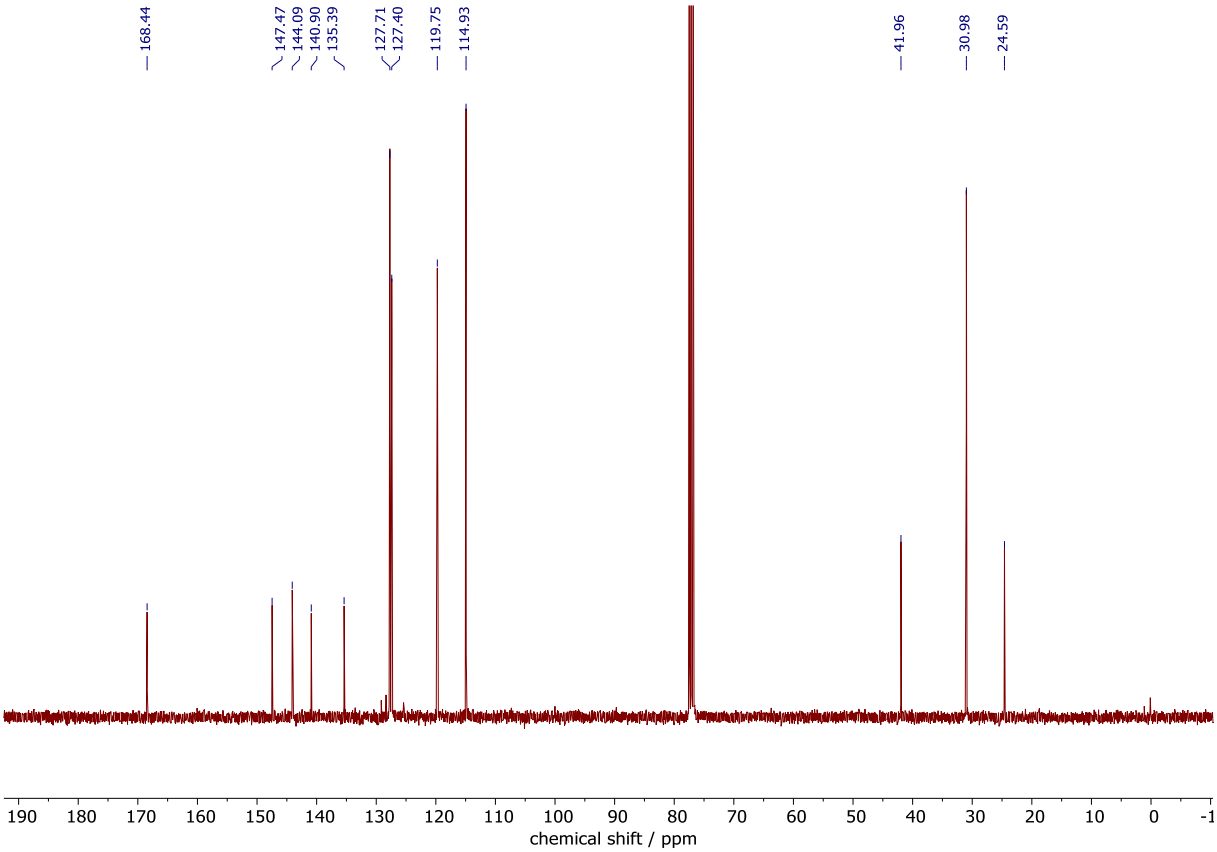
2.14
2.07
2.14
3.00
6.12
chemical shift / ppm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140.90
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127.40
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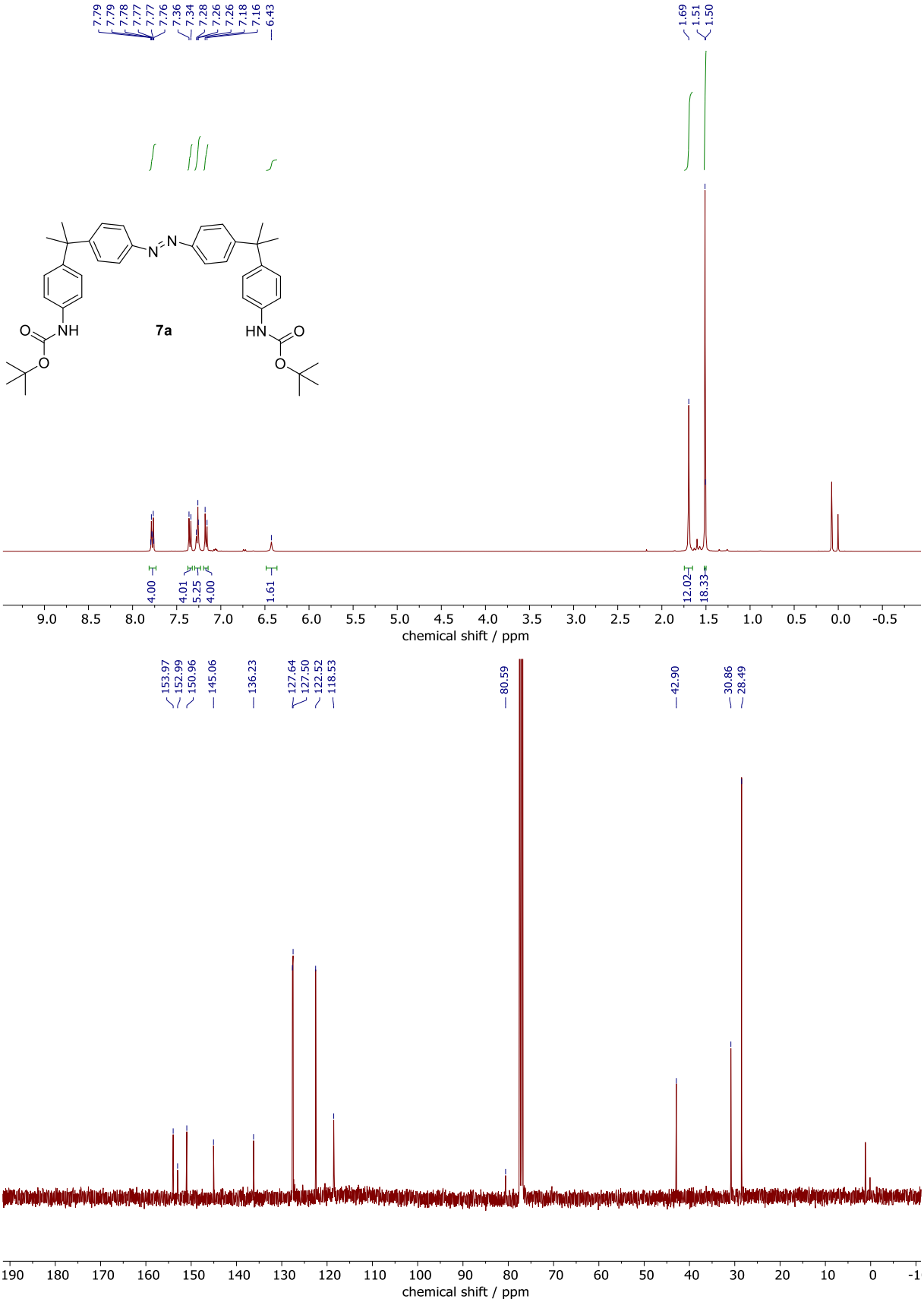
chemical shift / ppm

7a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6.43
1.69
1.51
1.50
N
N
O
NH
O
7a
HN
O
O
4.00
4.01
5.25
4.00
1.61
12.02
18.33
chemical shift / ppm
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152.99
150.96
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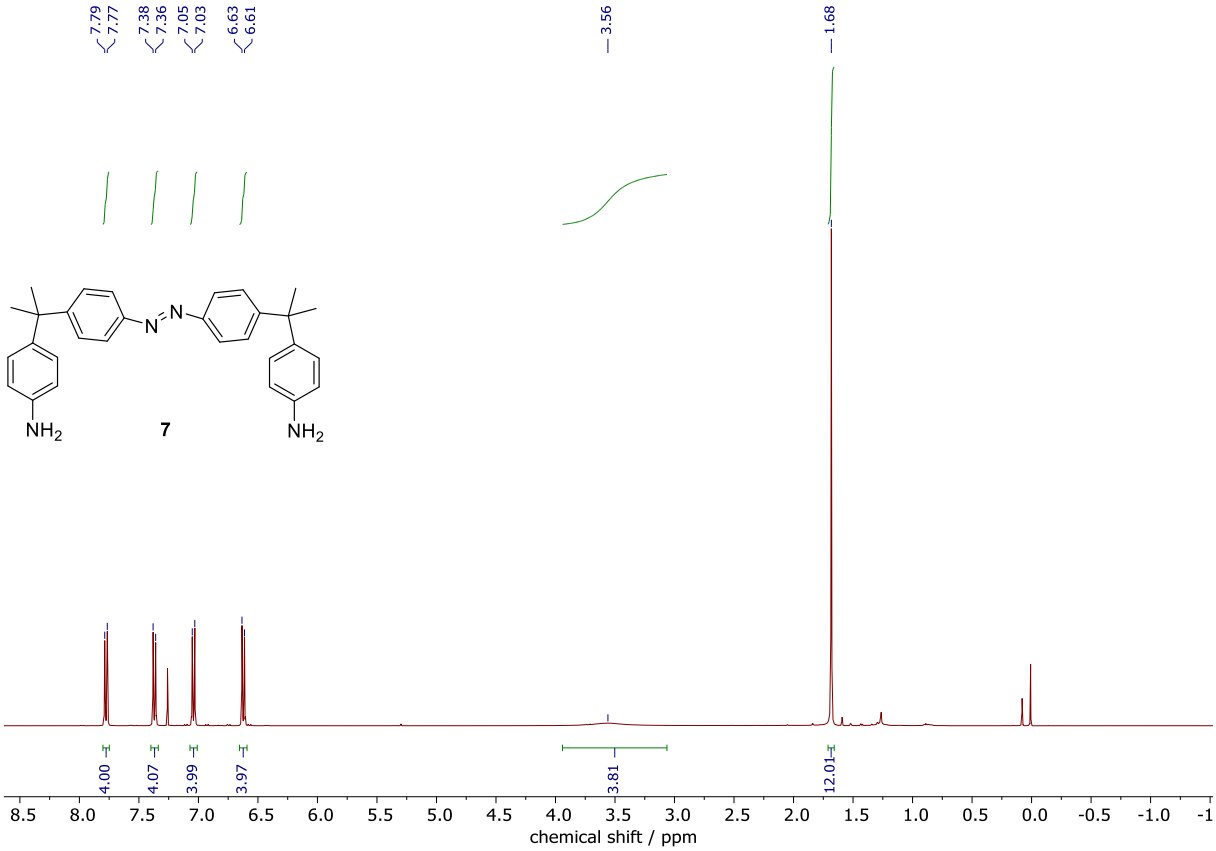
chemical shift / ppm

7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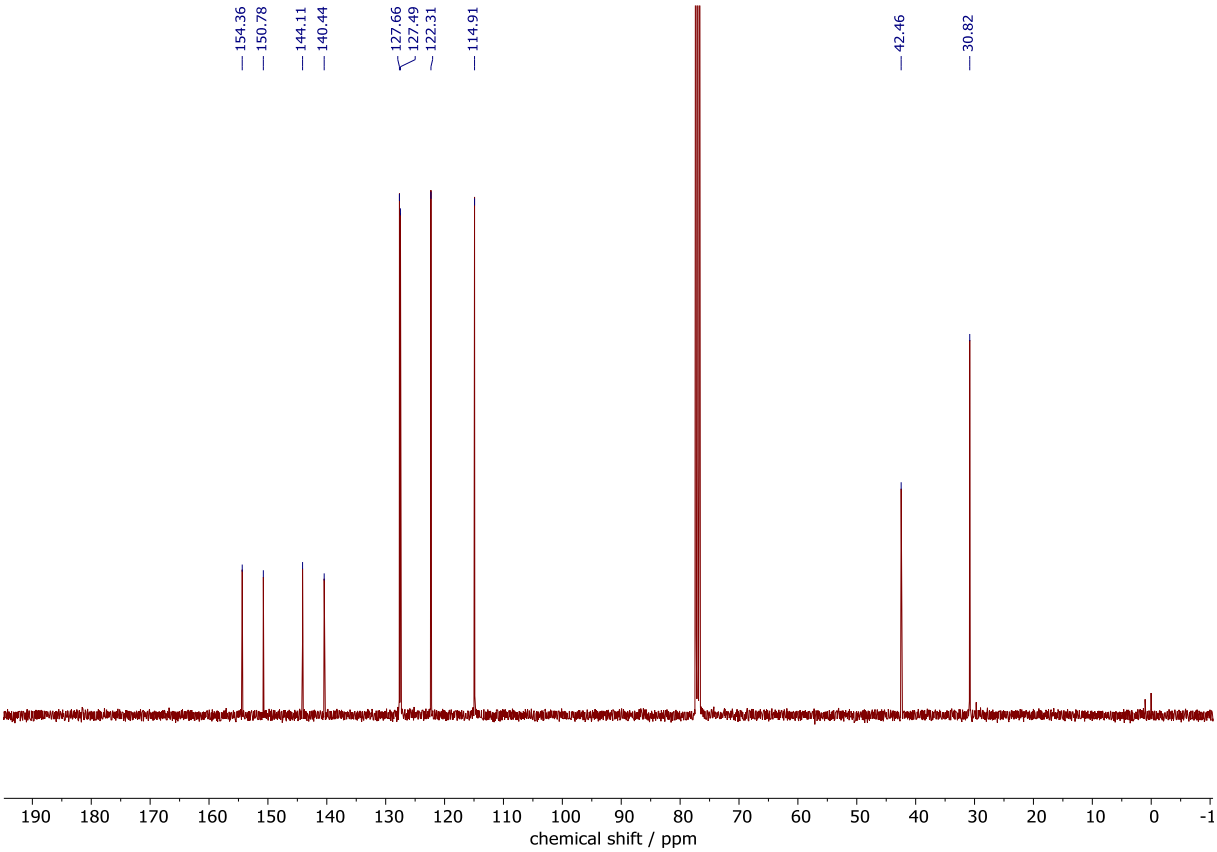
3.99
3.97
3.81
12.01
chemical shift / ppm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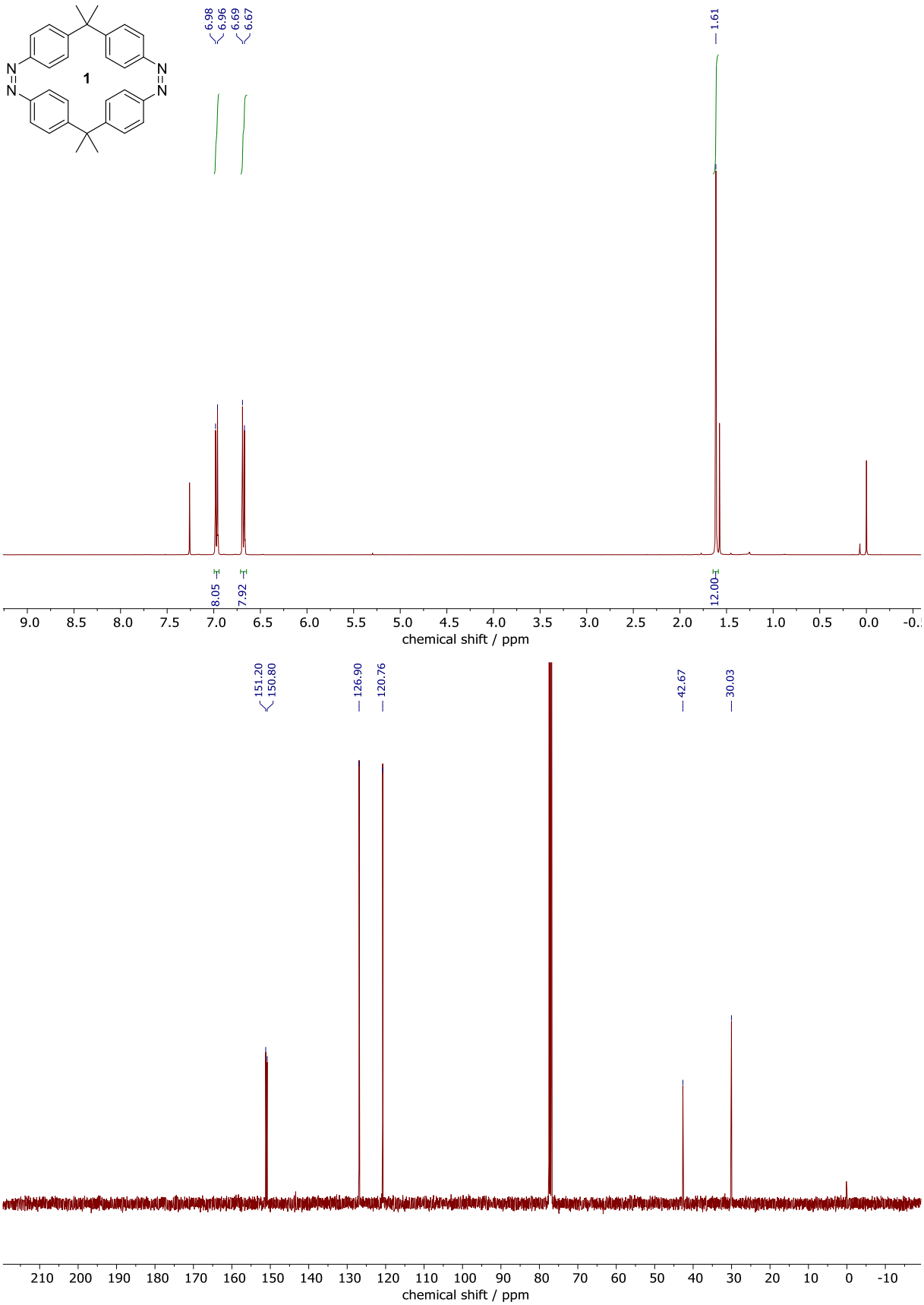
chemical shift / ppm

1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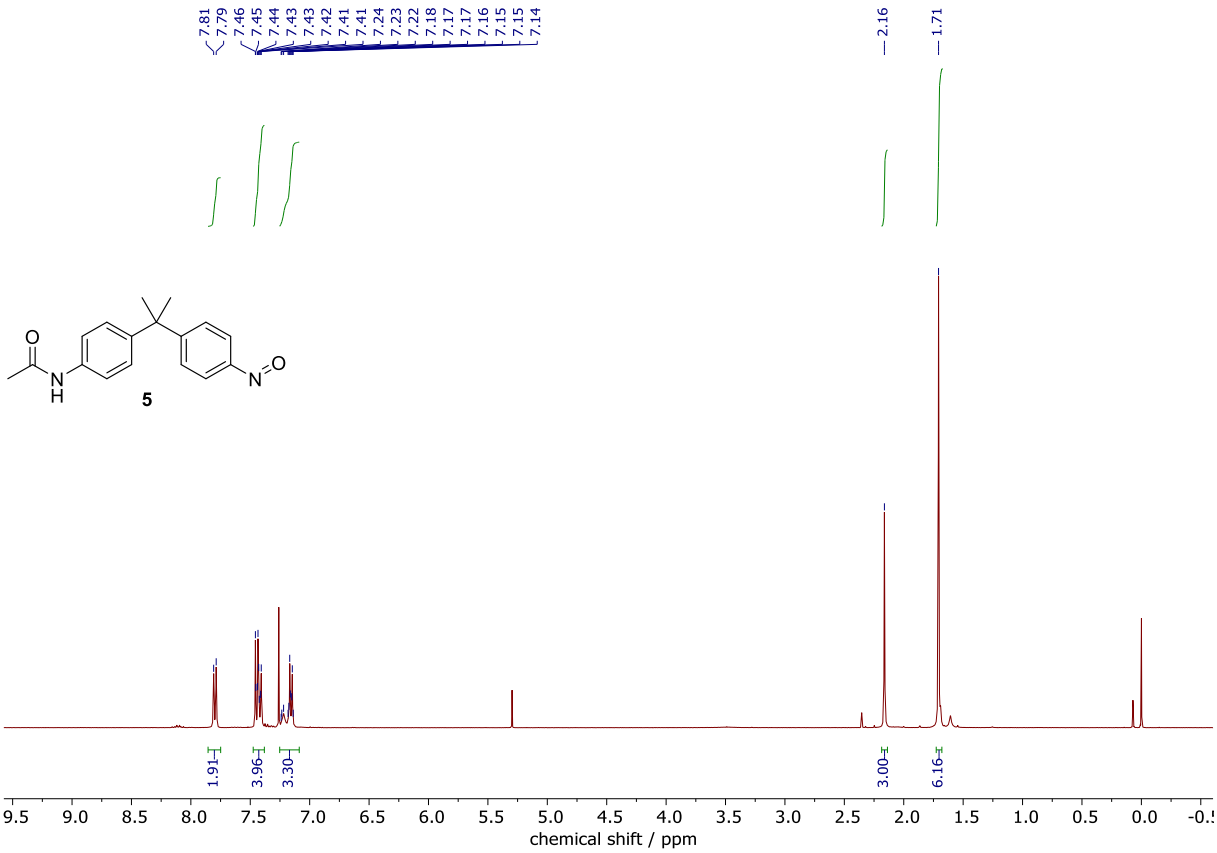
chemical shift / ppm

5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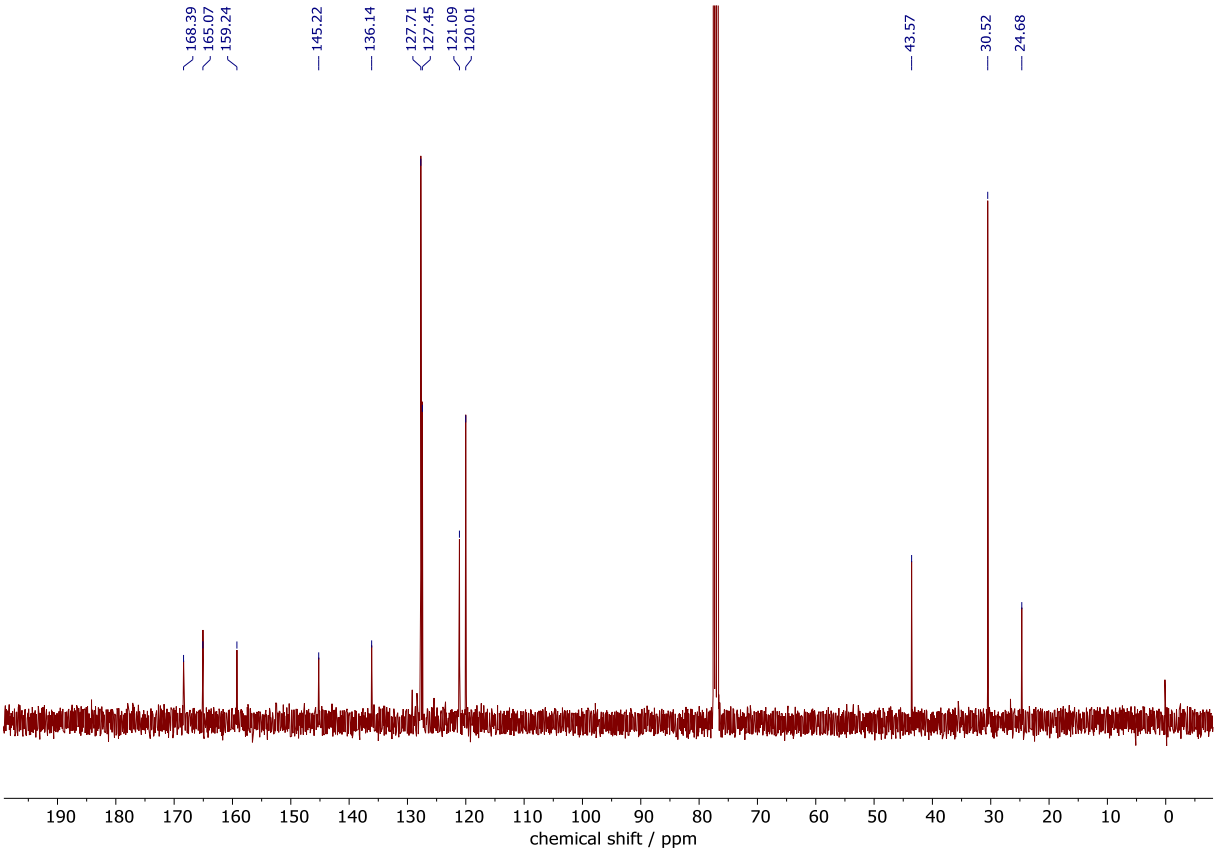
7.18
7.17
7.17
7.16
7.15
7.15
7.14
2.16
1.71
O
N
H
N
O
5
1.91
3.96
3.30
3.00
6.16
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
chemical shift / ppm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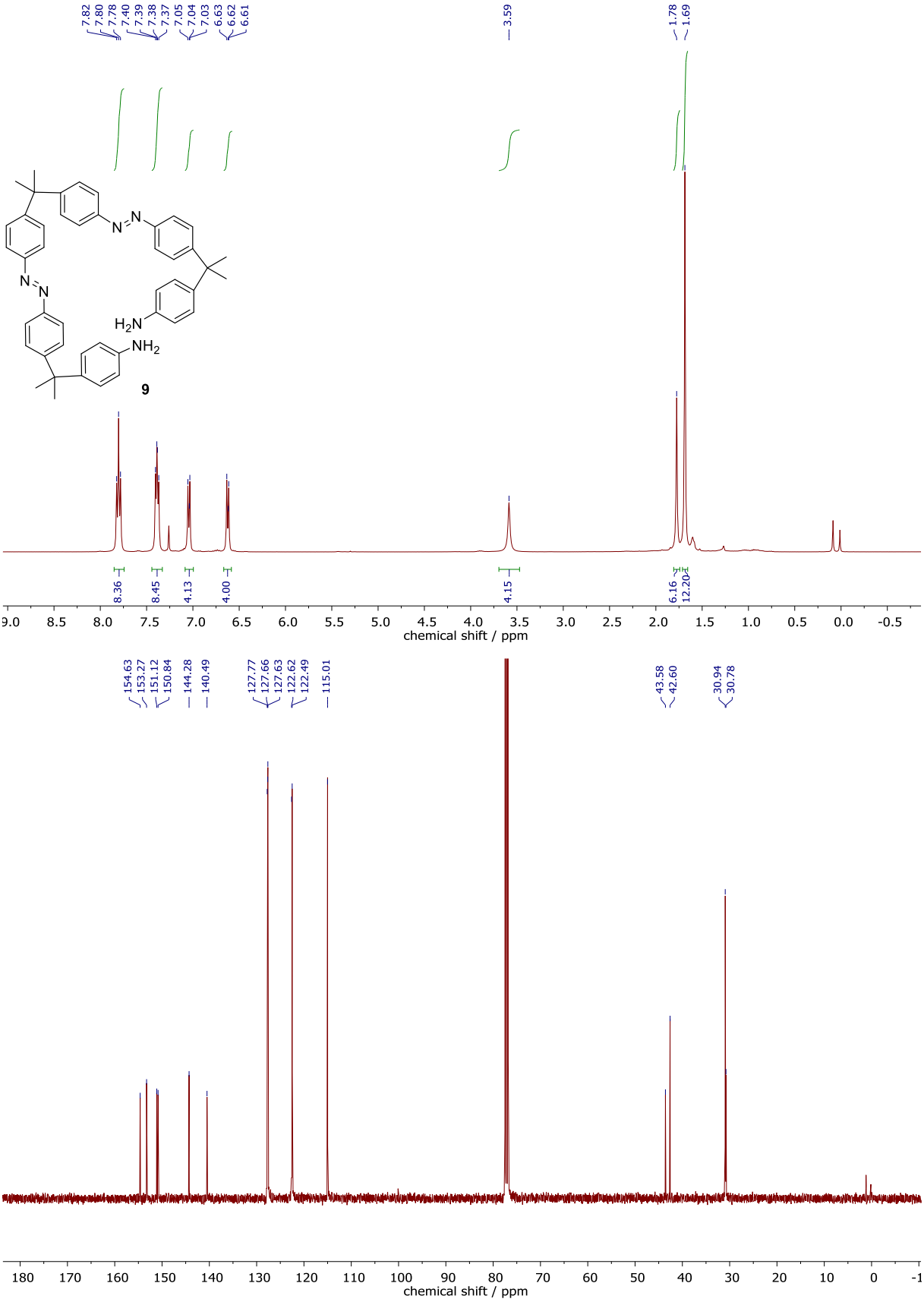
chemical shift / ppm

9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1.69
N
N
N
N
H2N
NH2
9
8.36
8.45
4.13
4.00
4.15
6.16
12.20
chemical shift / ppm
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153.27
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144.28
140.49
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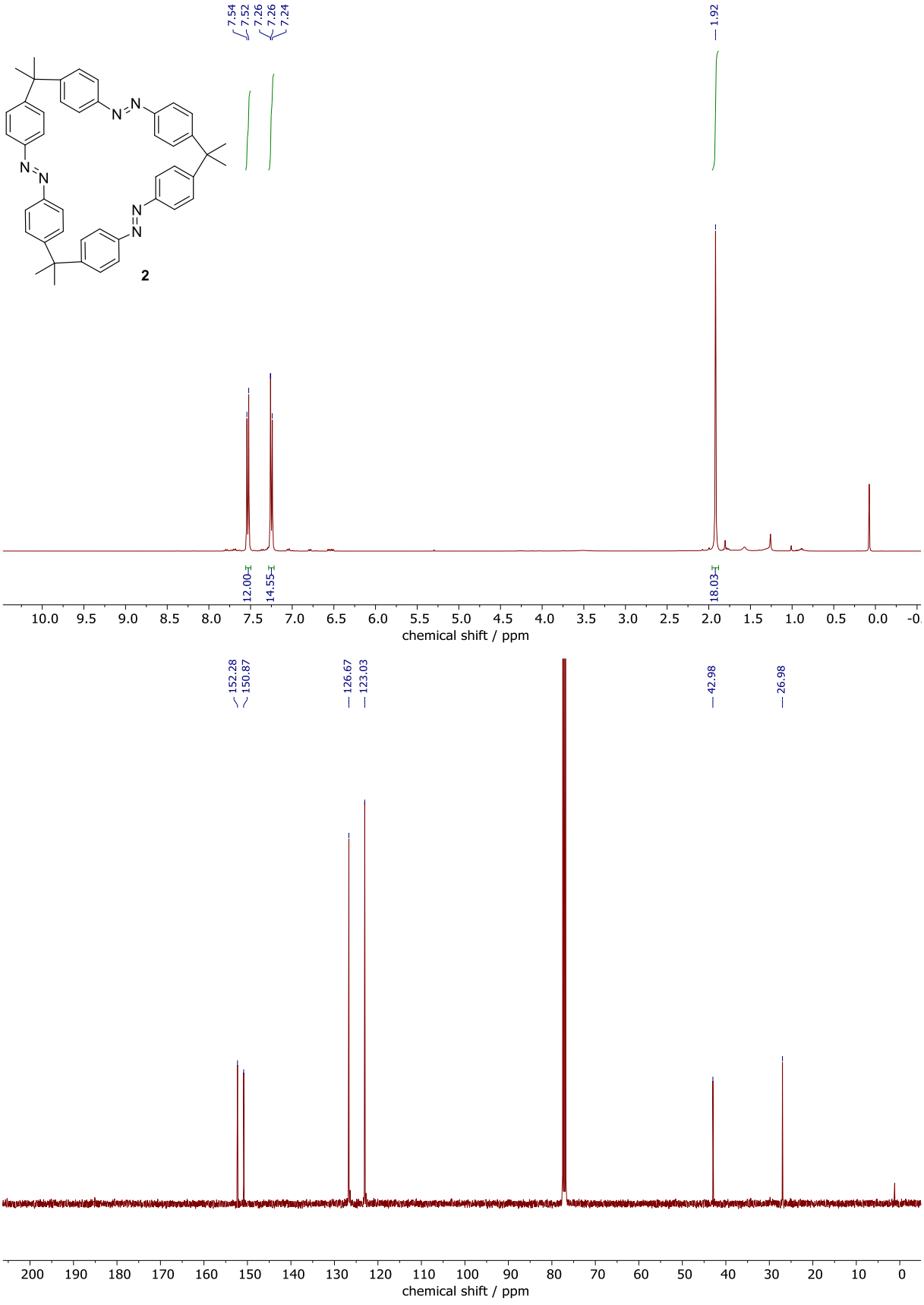
chemical shift / ppm

2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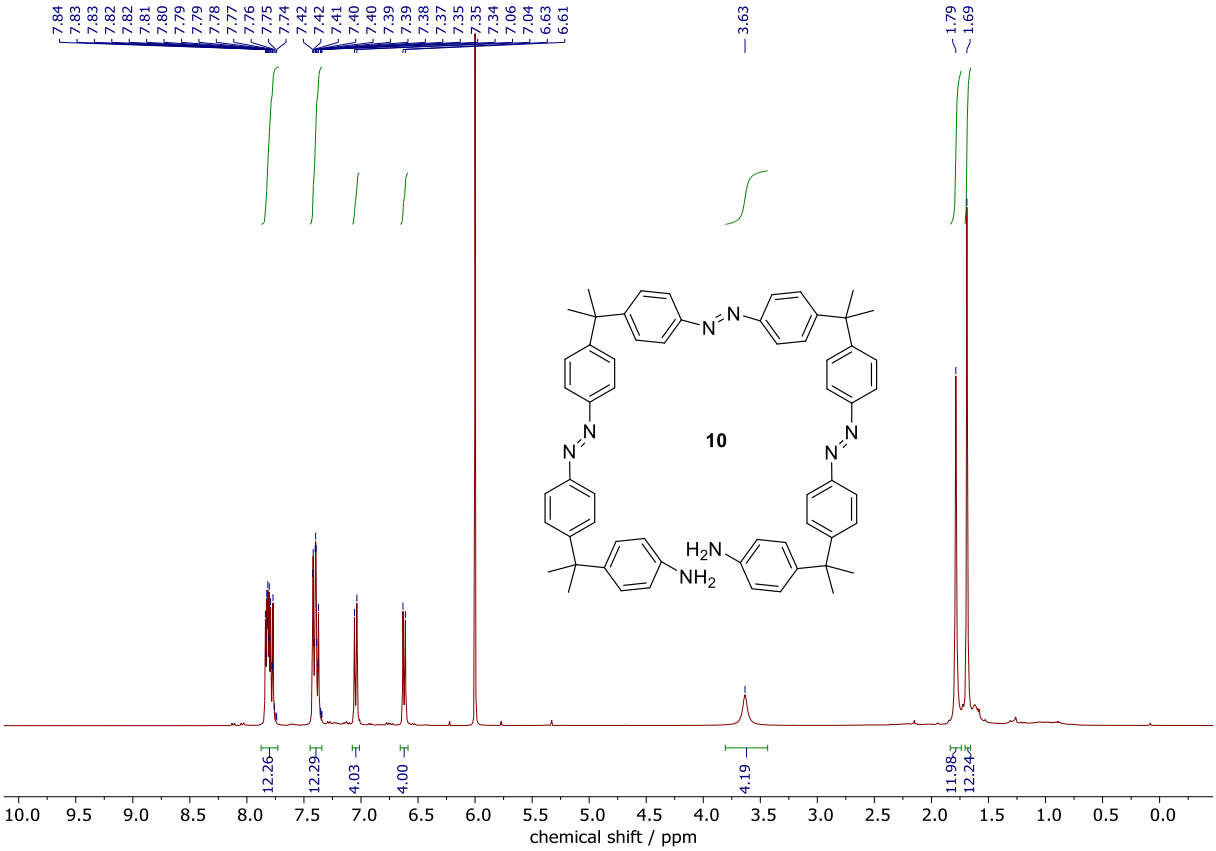
chemical shift / ppm

10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4.00
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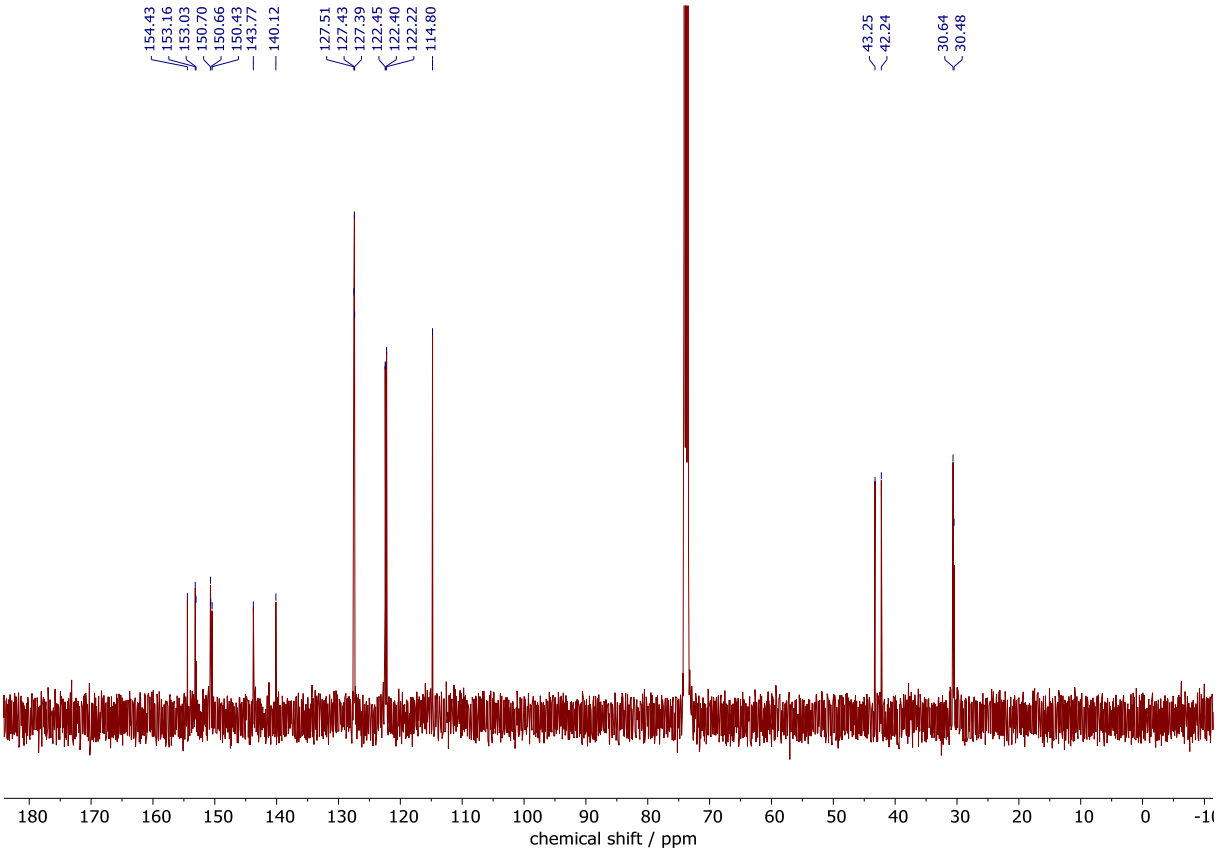
chemical shift / ppm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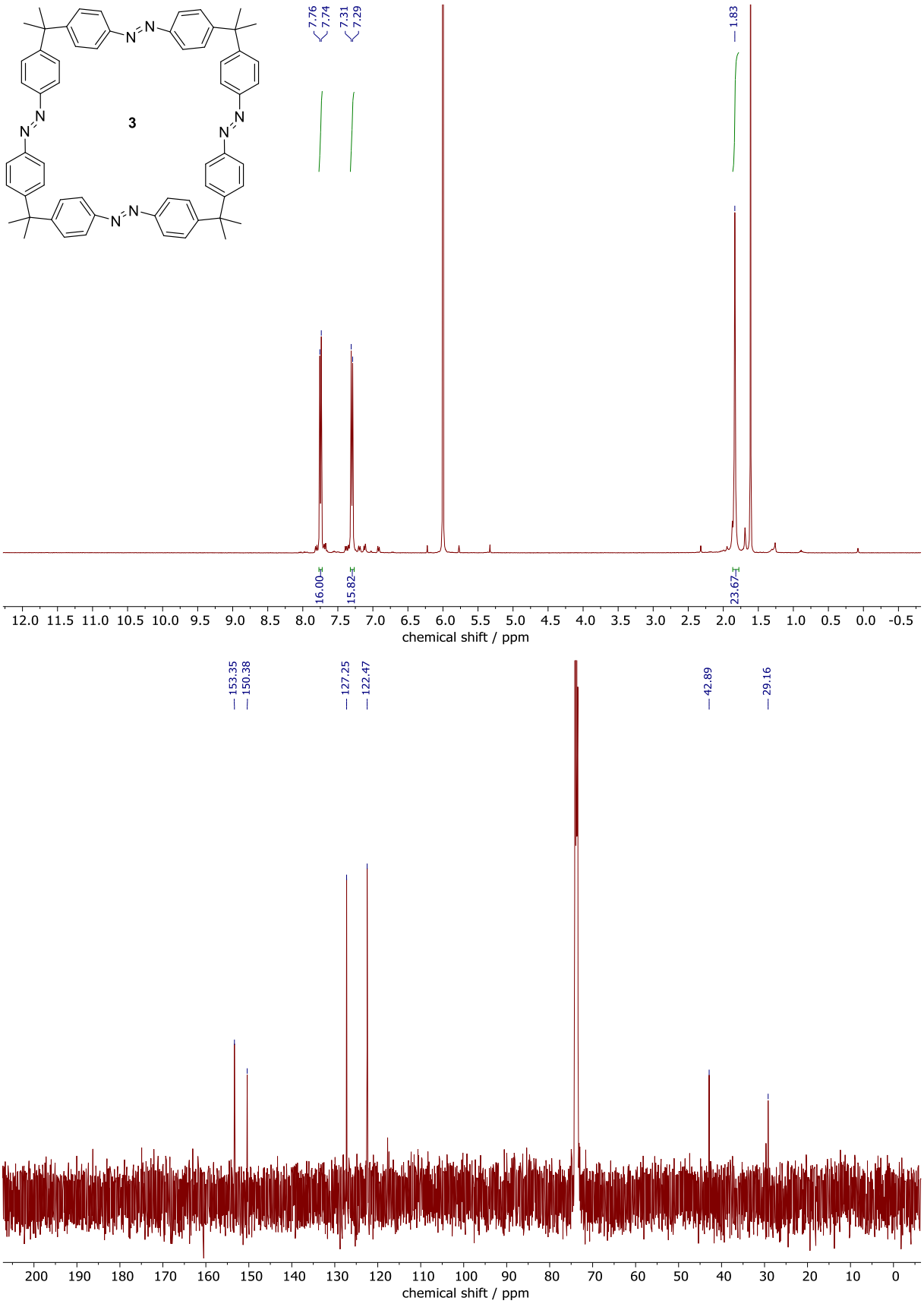
43.25
42.24
30.64
30.48
chemical shift / ppm

3


3
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7.74
7.31
7.29
1.83
16.00
15.82
23.67
chemical shift / ppm
153.35
150.38
127.25
122.47
42.89
29.16
chemical shift / ppm

NMR Isomerization Experiments

All thermal isomerization experiments were measured at a 600 MHz spectrometer. The samples were irradiated outside the spectrometer at 365 nm at rt (ca 1-1.5 h). The required irradiation time for reaching the PSS was determined previously. After irradiation, the NMR tube was immediately placed in the spectrometer and was equilibrated to constant temperature (~15 min) before start of the measurement. Isomerization during equilibration time was neglected due to the low overall rates.

Tetraazo Macrocycle 3

Assignment of the Isomers

Tetraazo macrocycle **3** showed complex ^{1}H NMR spectra due to the presence of six possible isomers. The all-*E*, all-*Z* and (*E,Z,E,Z*) isomers could be assigned considering chemical shifts, integral intensities and $^{3}J_{\text{H-H}}$ coupling (verified in ^{1}H-^{1}H COSY experiments). Then, thermal isomerizations were monitored and the rates of all signals were analyzed. The intensity of one set of signals increased and reached its maximum within the first few hours of the experiments and showed an exponential decay afterwards (Figure S4, yellow triangles). This set of six signals was assigned to the (*E,Z,Z,Z*) isomer, in consistency to its symmetry. Correlation was confirmed by ^{1}H-^{1}H COSY spectroscopy, however, some signals overlapped with signals of other isomers. Then, the rates of all other unassigned signals were compared. As a result, sets of signals with different rates were identified. Figure S4 shows the relative concentrations of all isomers as functions of time, where a representative signal from each data set is shown. It was still not possible to clearly assign the (*E,E,Z,Z*) and the (*E,E,E,Z*) isomers due to low signal intensities and overlap, but at least two different rates, one with quasistationary behavior, were obtained (Figure S4, blue rhombs and violet triangles). Due to the fact that computations predicted the lowest barrier for the (*E,E,E,Z*) → all-*E* isomerization, it is likely that the (*E,E,E,Z*) isomer shows the observed quasistationary behavior in the kinetic experiments. Furthermore, the thermal formation of the (*E,E,Z,Z*) isomer is unlikely, because the (*E,Z,Z,Z*) → (*E,Z,E,Z*) barrier was computed to be 5.5 kcal/mol lower in free energy. Thus, the photochemically generated concentrations of (*E,E,Z,Z*) should only decay and therefore not show accumulation at the beginning of the measurements.

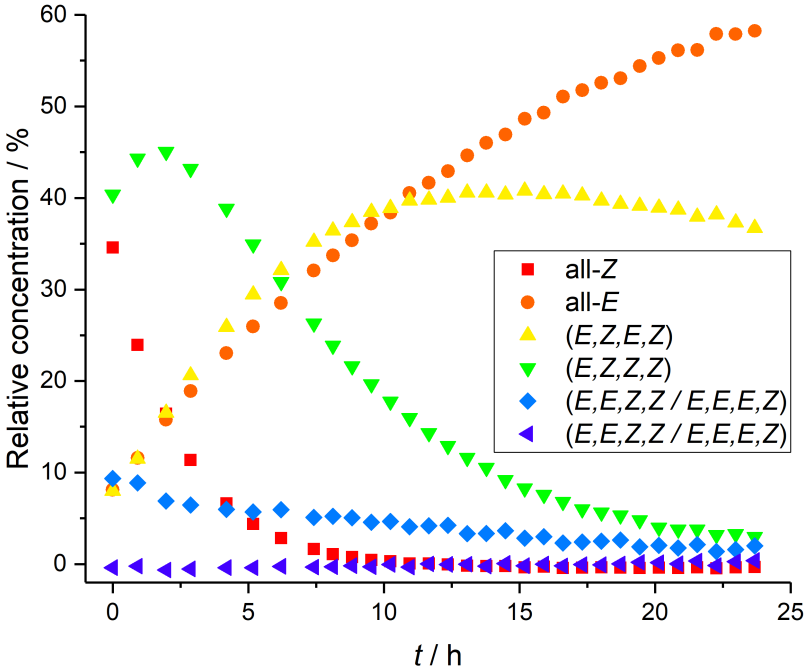


Figure S4: Relative concentrations of all isomers during thermal isomerization at 40 °C. Due to overlapping signals and low intensities, the (*E,E,Z,Z*) aswell as the (*E,E,E,Z*) isomers could not be clearly assigned.

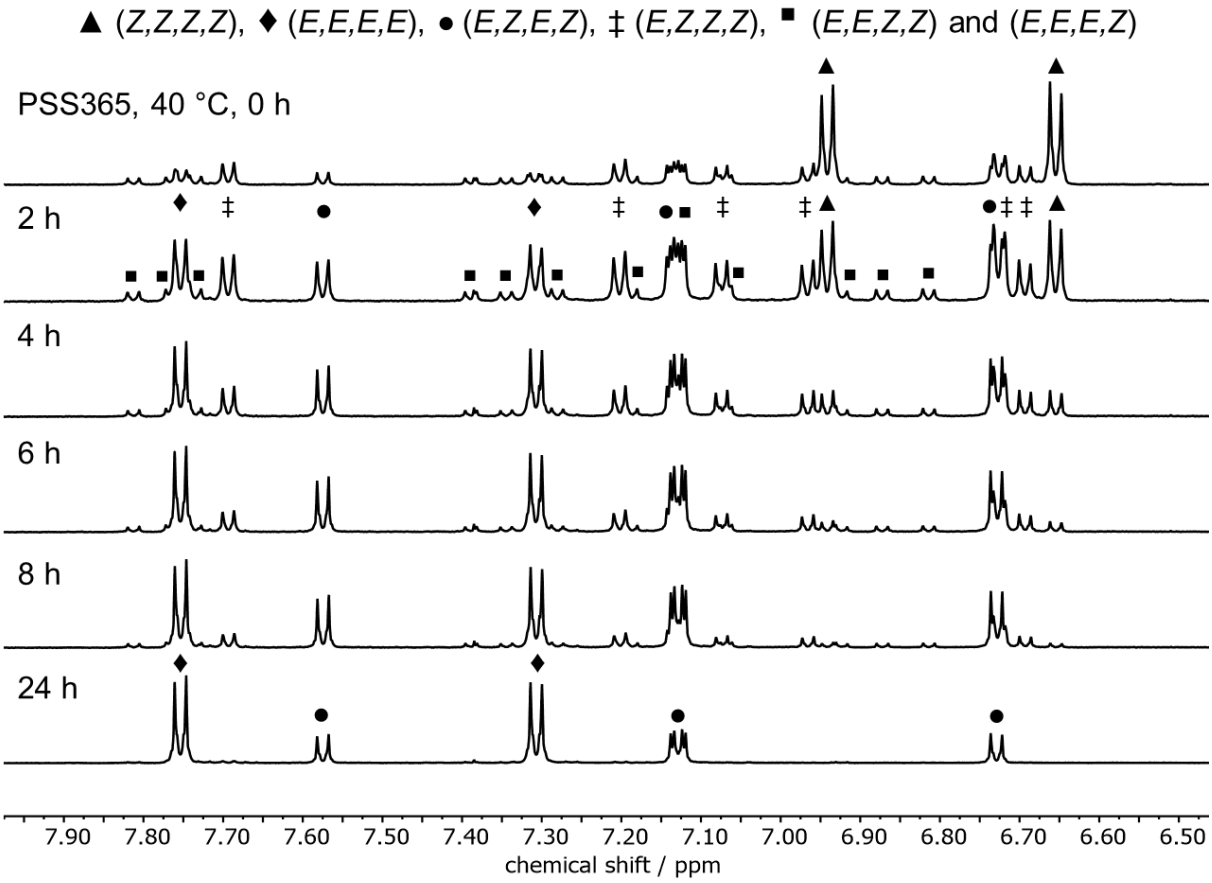


Figure S5: ^{1}H NMR-monitored (600 MHz) thermal isomerization of tetraazo macrocycle **3** from its PSS365 at 40 °C in 1,1,2,2-tetrachloroethane-d_2.

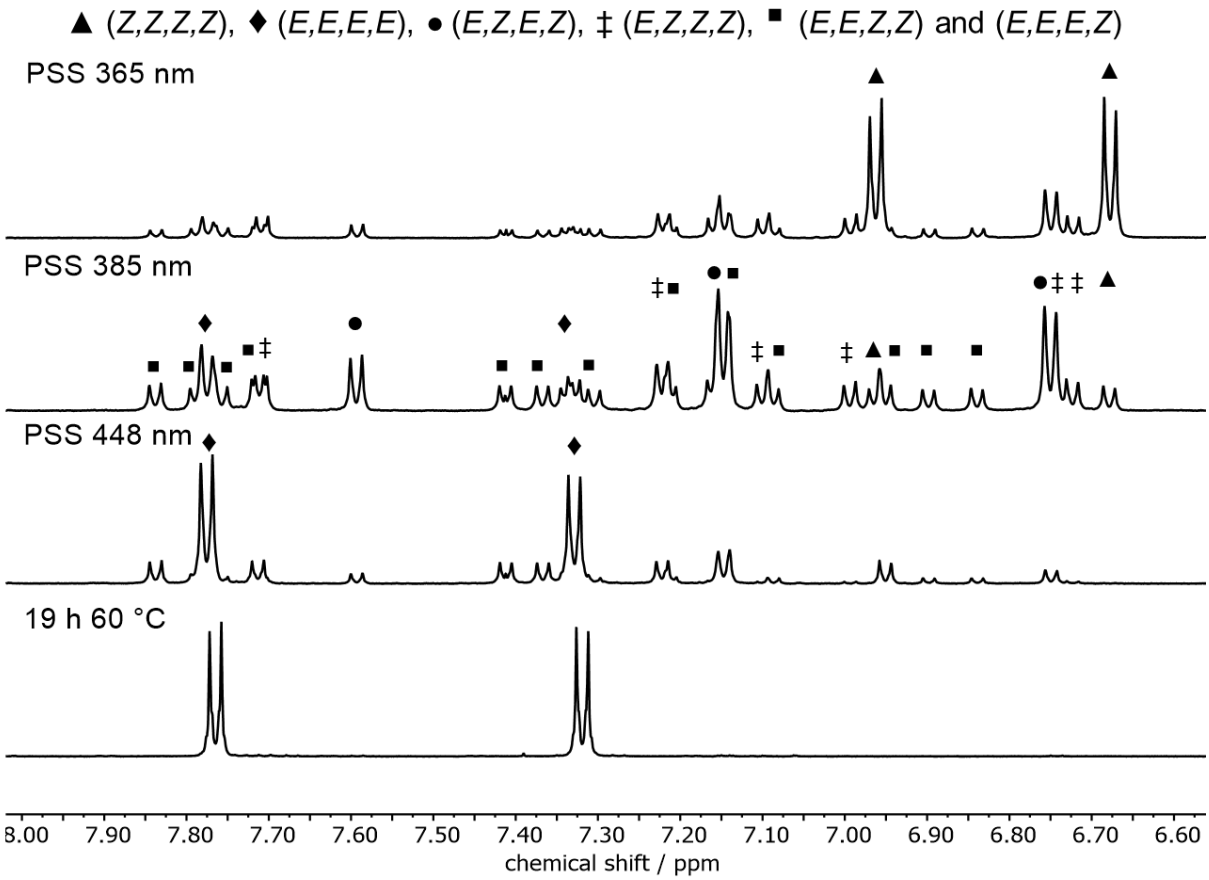


Figure S6: ^{1}H NMR spectra (600 MHz) of the different photostationary states of tetraazo macrocycle **3** in 1,1,2,2-tetrachloroethane-d_2.

UV-Vis Spectroscopy

Solvents for UV-Vis spectroscopy were purchased from Merck (Uvasol® quality). 1,1,2,2-Tetrachloroethane was purchased in reagent grade (98+%) from Alfa Aesar and was freshly distilled under nitrogen before use. The measurements were carried out with a SPECORD® 200 PLUS spectrophotometer equipped with two automatic eight-fold cell changers and a Peltier element thermostat system (0.1 °C accuracy) by Analytik Jena. The system was operated with the ASpect UV software by Analytik Jena. The sample solutions were measured in QS High Precision Cells made of Quartz Suprasil® with a light path of 10 mm by Hellma Analytics.

Photoisomerization of (*Z,Z*)-bisazo macrocycle 1

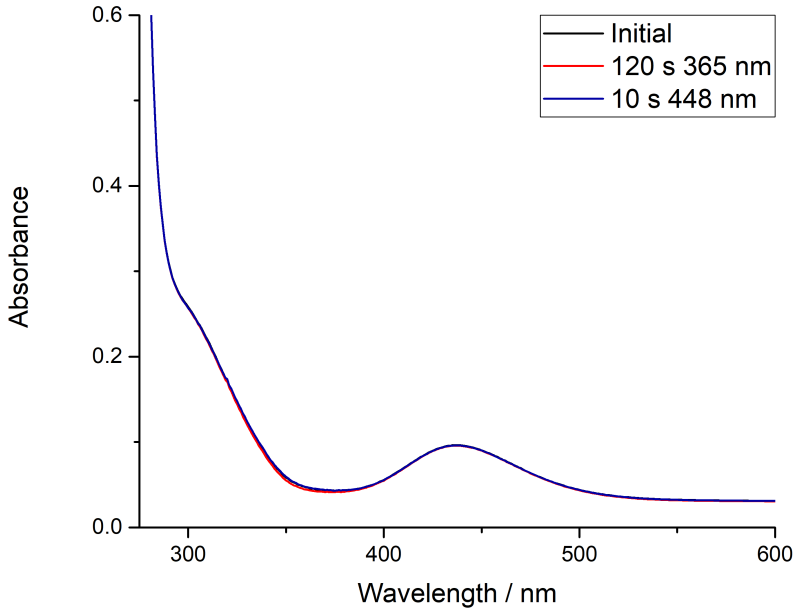


Figure S7: Irradiation of bisazo macrocycle **1** at 365 nm or 448 nm did not cause photoisomerization.

Trisazo macrocycle 2 in Acetonitrile

UV-Vis spectra of trisazo macrocycle **2** in different isomerization states were recorded to identify isosbestic wavelengths for UV-Vis detection in the HPLC switching experiments. An isosbestic point at 242 nm with maximum intensity was located, which was then used for UV-Vis detection.

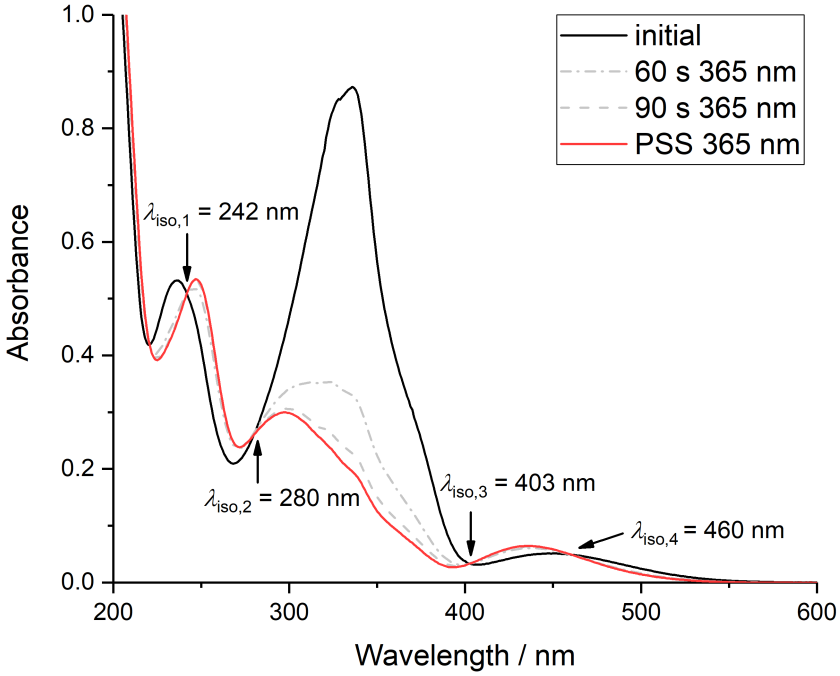


Figure S8: UV-Vis spectra of macrocycle **2**, $1.4 \cdot 10^{-5}$ mol/L in acetonitrile at different isomerization states. Four isosbestic points at wavelengths 242, 280, 403 and 460 nm were identified.

HPLC Isomerization Experiments

Relative isomer concentrations of trisazo macrocycle **2** were determined on a DIONEX UltiMate 3000 HPLC system using a Eurospher II 100-5 C18 column with acetonitrile/TBME (88:12) as isocratic eluent (0.636 colum volumes/min). Detection was carried out using an UltiMate 3000 UV-Vis detector at the previously determined isosbestic wavelength of 242 nm (see UV-Vis section). Irradiation and heating of the samples was carried out in 2 mL glass vials, from which aliquots of 5 µL ($2.5 - 3 \cdot 10^{-3}$ mol/L in TCE-d_2) were injected into the HPLC system for analysis. Table S3 shows the detailed conditions for the selective generation of the different isomers.

Table S2: Isomer ratios at the different photostationary states determined by HPLC.

	Peak area / %			
Conditions	(*Z,Z,Z*)	(*E,Z,Z*)	(*E,E,Z*)	(*E,E,E*)
10 min 365 nm	75.66	12.18	6.94	5.22
10 min 448 nm	3.96	21.38	26.21	48.41
10 min 385 nm	25.23	46.61	19.36	8.80

Table S3: detailed applied conditions for the selective generation of the isomers. After heating for 10 min, the samples were immediately cooled to rt water.

Isomer	Conditions for generation
(*Z,Z,Z*)	10 min 365 nm
(*E,Z,Z*)	10 min 365 nm, then 10 min 80 °C in the dark
(*E,E,E*)	5 min 448 nm, then 10 min 80 °C

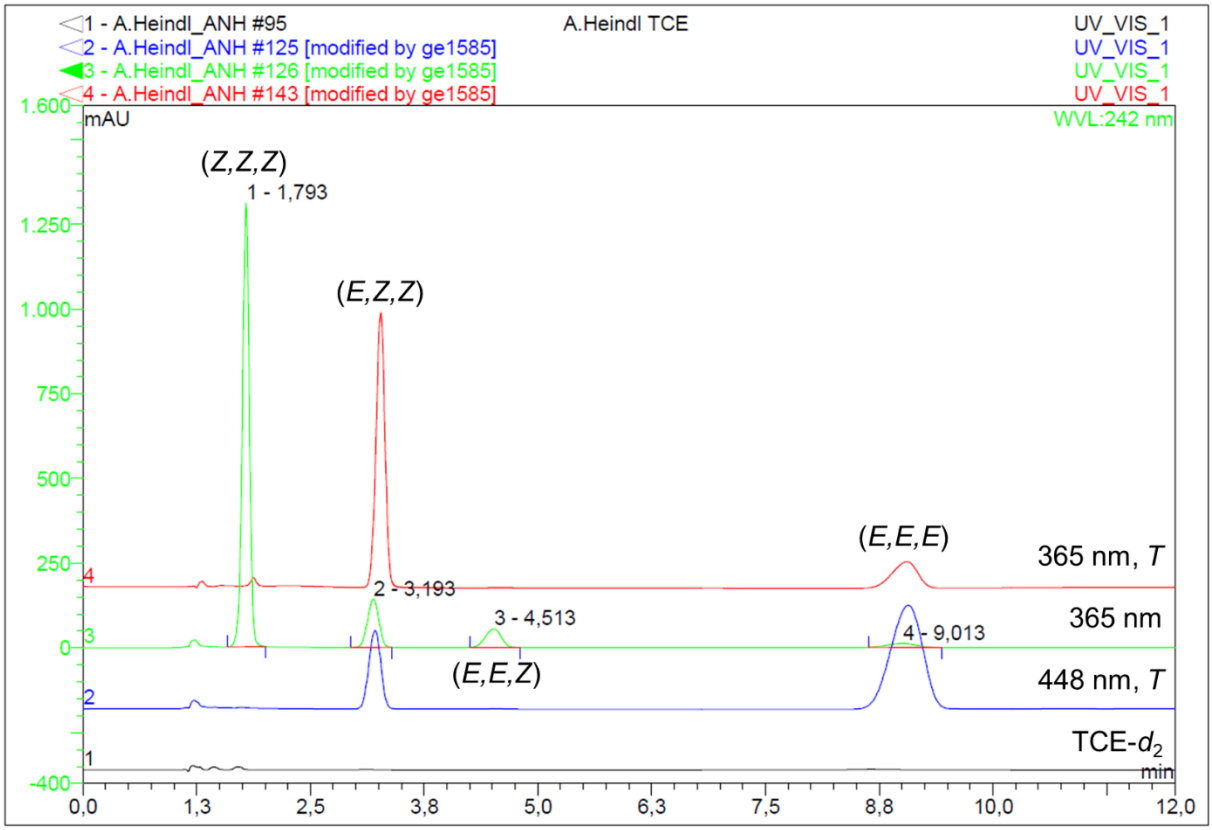


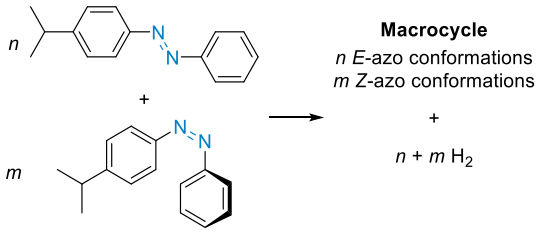
Figure S9: Chromatograms of the different isomer-enriched states of macrocycle **2**. Note the blank solvent chromatogram (bottom, black), which explains the origin of the impurities at ca 1.3 min.

Computational Data

All structures were optimized at the PBE0[7] density functional theory level with D3(BJ) dispersion correction[8] using the def2-SVP[9] basis set. Solvent effects of 1,1,2,2-tetrachloroethane were approximated by using the implicit SMD model[10] for dichloromethane. Thermodynamic quantities were obtained by frequency computations at the same level of theory. The absence of imaginary frequencies in ground state and the presence of one imaginary frequency in transition state computations was checked for every optimized geometry. Single point energies were computed at the PBE0-D3(BJ)/def2-TZVPP level of theory. For all computations, the Gaussian16 program package was used.[11] Computed structures were visualized with CYLview.[12]

Ring Strain

For the estimation of ring strain in the macrocyclic isomers, isodesmic equations in combination with the computed single point energies (PBE0-D3(BJ)/def2-TZVPP) on previously optimized structures were used.[13]



Scheme S1: General isodesmic equation used for estimation of ring strain.

According to Scheme S1, the ring strain energy for a macrocycle with *n* *E*-azo units and *m* Z-azo units is obtained according to (1):

$$\Delta E_{\text{strain}} = \left[E_{\text{el,macrocycle}} + (n+m)\, E_{\text{el,H}_2}\right] - \left[n\, E_{\text{el,}(E)-p-{}^{i}\text{PrAB}} + m\, E_{\text{el,}(Z)-p-{}^{i}\text{PrAB}}\right] \quad (1)$$

Table S4: Computed ring strain energies of bisazo macrocycle **1**.

1	ΔE_{strain} / kcal mol^{-1}	ΔE_{strain} per azo / kcal mol^{-1}
(*E*,*E*)	40.0	20.0
(*E*,*Z*)	53.8	26.9
(*Z*,*Z*)	26.1	13.1

Table S5: Computed ring strain energies of trisazo macrocycle **2**.

2	ΔE_{strain} / kcal mol^{-1}	ΔE_{strain} per azo / kcal mol^{-1}
(*E*,*E*,*E*)	52.5	17.5
(*E*,*E*,*Z*)	53.5	17.9
(*E*,*Z*,*Z*)	39.2	13.1
(*Z*,*Z*,*Z*)	40.5	13.5

Table S6: Computed ring strain energies of tetraazo macrocycle **3**.

3	ΔE_{strain} / kcal mol^{-1}	ΔE_{strain} per azo / kcal mol^{-1}
(*E*,*E*,*E*,*E*)	58.4	14.6
(*E*,*E*,*E*,*Z*)	58.3	14.6
(*E*,*E*,*Z*,*Z*)	59.5	14.9
(*E*,*Z*,*E*,*Z*)	53.4	13.3
(*E*,*Z*,*Z*,*Z*)	45.6	11.4
(*Z*,*Z*,*Z*,*Z*)	45.0	11.2

Thermal Isomerization Pathways of 1 and 3

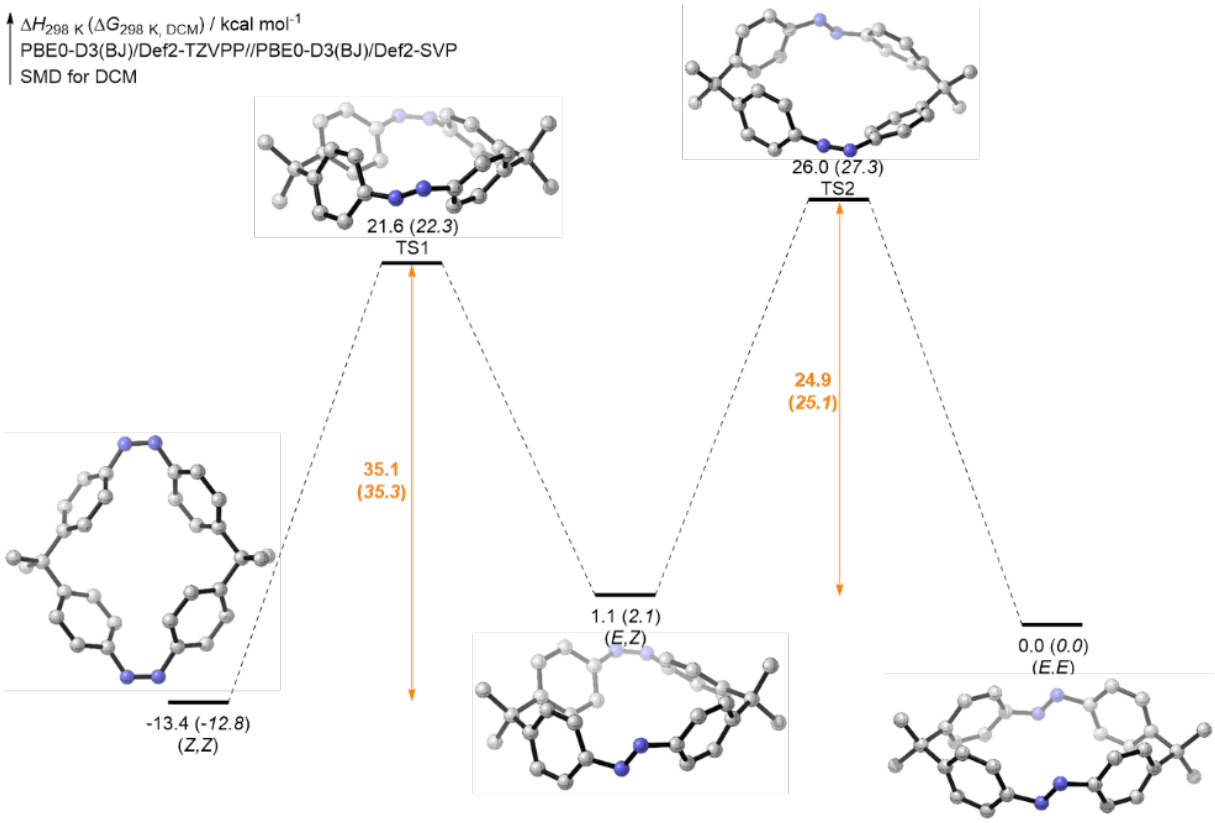


Figure S10: Thermal isomerization pathway of bisazo macrocycle **2**.

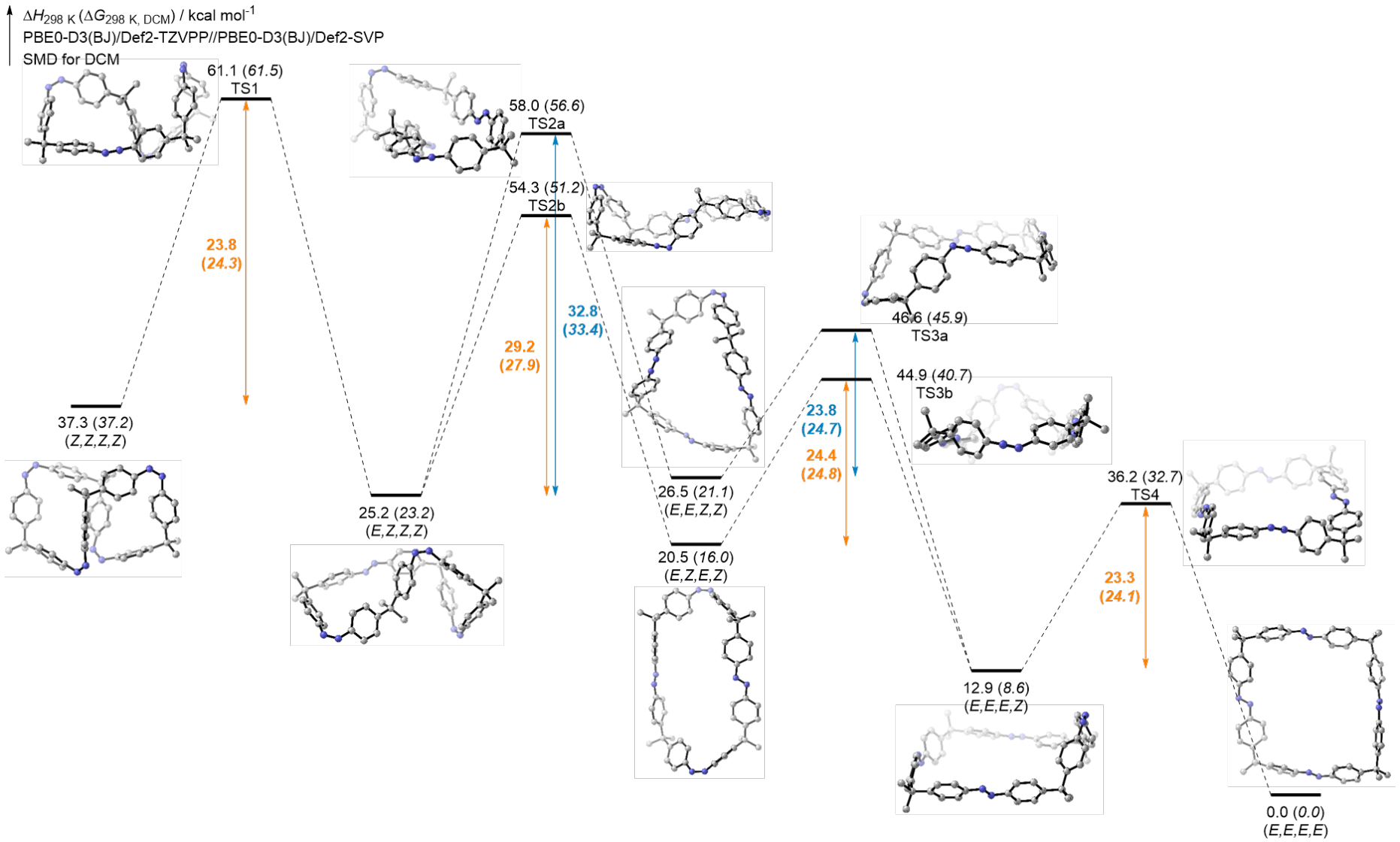


Figure S11: Thermal isomerization pathway of tetraazo macrocycle **3**.

Coordinates of Optimized Geometries

Bisazo macrocycle **1**

(*E*,*E*)-1

C	-2.2083654	2.18383152	1.06960954
C	-3.41591031	1.51878113	1.19667069
C	-4.18879968	1.17518218	0.07241791
C	-3.80125736	1.71464918	-1.161194
C	-2.58824675	2.38120574	-1.30243023
C	-1.73638643	2.5393001	-0.20398808
H	-1.55282364	2.33320779	1.92894192
H	-3.70642884	1.16336773	2.1863891
H	-4.39434126	1.521433	-2.05600964
H	-2.22823885	2.68990278	-2.28640925
C	-5.18253725	-0.00372124	0.15054779
C	-4.18862099	-1.17682473	0.01059064
C	-3.50387366	-1.67618355	1.13369311
C	-3.71330276	-1.55719279	-1.25113846
C	-2.28896228	-2.33166136	1.00847736
H	-3.87325628	-1.45964003	2.13728259
C	-2.5007914	-2.22255631	-1.39001395
H	-4.23265739	-1.23431002	-2.15424429
C	-1.72903227	-2.52624437	-0.26374509
H	-1.70121753	-2.60200735	1.88711184
H	-2.07109248	-2.40990607	-2.37641855
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C	2.58824675	2.38120574	1.30243023
C	2.2083654	2.18383152	-1.06960954
C	3.80125736	1.71464918	1.161194
H	2.22823885	2.68990278	2.28640925
C	3.41591031	1.51878113	-1.19667069
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C	3.71330276	-1.55719279	1.25113846
C	2.28896228	-2.33166136	-1.00847736
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H	4.23265739	-1.23431002	2.15424429
C	1.72903227	-2.52624437	0.26374509

H	1.70121753	-2.60200735	-1.88711184
H	2.07109248	-2.40990607	2.37641855
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N	-0.36350539	-2.75527809	-0.50743966
C	-6.22166648	0.02248054	-0.97197416
H	-5.78661289	0.02712021	-1.9787816
H	-6.87153285	-0.86210134	-0.90035911
H	-6.85081178	0.92040538	-0.88154769
C	-5.9552019	-0.03433763	1.47146539
H	-6.58084012	-0.93794481	1.52097514
H	-5.31373009	-0.03028885	2.36104622
H	-6.61335325	0.84441603	1.53942876
C	6.22166648	0.02248054	0.97197416
H	5.78661289	0.02712021	1.9787816
H	6.87153285	-0.86210134	0.90035911
H	6.85081178	0.92040538	0.88154769
C	5.9552019	-0.03433763	-1.47146539
H	6.58084012	-0.93794481	-1.52097514
H	5.31373009	-0.03028885	-2.36104622
H	6.61335325	0.84441603	-1.53942876

E(el) / Hartree :	-1376.42563		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-1376.46012		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-1377.87683		
Thermal corrections / Hartree:			
ZPVE:	0.512726	E(therm.):	0.540761
H(corr.):	0.541705	G(corr.):	0.456626
Imaginary Frequencies:	0		

(*E*,*Z*)-1

C	2.54109169	3.10351415	-1.02378259
C	3.5362992	2.12938383	-1.00758971
C	3.52022018	1.0973456	-0.06392941
C	2.4455251	1.06688102	0.84282335
C	1.42635813	2.00795059	0.81142589
C	1.46234989	3.04474661	-0.13437203
H	2.58941135	3.94120502	-1.72285088
H	4.34940521	2.20247228	-1.73128041
H	2.39401692	0.26611365	1.58444353
H	0.60988622	1.95391714	1.534067
C	4.6143796	0.0141225	0.02186222
C	3.84277928	-1.30568361	0.01808595
C	3.08281059	-1.6273631	-1.12107002
C	3.65071747	-2.07590538	1.17037983
C	2.03651862	-2.52436538	-1.05215796
H	3.23179559	-1.06355871	-2.04487365
C	2.58788128	-2.97247045	1.25746524

H	4.25968975	-1.89853634	2.05796498
C	1.71026246	-3.12509413	0.17839667
H	1.35208171	-2.65971205	-1.89112025
H	2.34295757	-3.46059472	2.20370355
N	0.60829647	4.1735494	-0.11284446
N	-0.60831546	4.17354673	0.1128483
C	-1.46236411	3.04474032	0.13437492
C	-1.426368	2.00794528	-0.81142391
C	-2.54110613	3.10350251	1.02378558
C	-2.44553098	1.06687142	-0.84282216
H	-0.60989589	1.95391592	-1.53406509
C	-3.53630952	2.129368	1.00759188
H	-2.58942931	3.94119256	1.7228546
C	-3.52022617	1.09733065	0.06393067
H	-2.39401944	0.26610491	-1.58444304
H	-4.34941581	2.20245237	1.73128266
C	-4.61438099	0.01410299	-0.02186186
C	-3.84277507	-1.30569985	-0.01808669
C	-3.08280501	-1.62737708	1.121069
C	-3.65071001	-2.07591985	-1.17038121
C	-2.03650924	-2.52437487	1.05215618
H	-3.23179239	-1.06357409	2.0448731
C	-2.58787002	-2.97248034	-1.25746739
H	-4.25968305	-1.89855264	-2.05796622
C	-1.71025054	-3.1251012	-0.17839896
H	-1.35207175	-2.65971934	1.89111836
H	-2.34294425	-3.46060278	-2.20370611
N	-0.39664236	-3.50582845	-0.4830243
N	0.39665589	-3.5058272	0.4830217
C	5.59431436	0.06939535	-1.15335184
H	6.31765931	-0.75462241	-1.06819734
H	5.09398126	-0.02290303	-2.12729412
H	6.15935565	1.01339271	-1.15217336
C	5.41145968	0.23031475	1.31350641
H	4.76504885	0.25072806	2.20185286
H	6.1653195	-0.56100583	1.44899034
H	5.93360222	1.19697785	1.26686219
C	-5.411462	0.23029294	-1.31350585
H	-4.76505127	0.25070973	-2.2018523
H	-6.16531846	-0.56103073	-1.44899044
H	-5.93360864	1.19695378	-1.26686082
C	-5.59431597	0.0693707	1.15335227
H	-6.31765744	-0.75465005	1.06819708
H	-5.09398247	-0.02292638	2.12729446
H	-6.15936125	1.01336567	1.15217459

E(el) / Hartree : -1376.42331

E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-1376.45701		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-1377.87491		
Thermal corrections / Hartree			
ZPVE:	0.512912	E(therm.):	0.540659
H(corr.):	0.541603	G(corr.):	0.457309
Imaginary frequencies:	0		

(*Z*,*Z*)-1

C	1.26356765	2.47814851	-0.93497835
C	2.11580758	1.38587809	-0.92737911
C	3.11701836	1.23747438	0.04603502
C	3.25915187	2.25349538	0.99461616
C	2.42861835	3.37253286	0.98013623
C	1.39909057	3.47322781	0.04436657
H	0.48533326	2.56307657	-1.69509186
H	1.98679619	0.60724073	-1.68374074
H	4.03442675	2.18871125	1.75911615
H	2.5556137	4.17655689	1.70816639
C	4.01573293	-4.125E-06	-1.5233E-06
C	3.117016	-1.23748096	-0.04603692
C	3.25914643	-2.25350223	-0.99461822
C	2.11580617	-1.38588279	0.92737847
C	2.42861085	-3.37253818	-0.98013722
H	4.03442046	-2.18871956	-1.7591192
C	1.26356422	-2.47815163	0.93497881
H	1.98679718	-0.60724519	1.68374026
C	1.39908407	-3.4732312	-0.04436626
H	2.5556038	-4.17656246	-1.70816753
H	0.48533063	-2.56307823	1.69509329
N	0.61648102	4.65684642	0.0604187
N	-0.61647261	4.6568474	-0.0604281
C	-1.39908434	3.47323027	-0.04437311
C	-2.42861229	3.37253495	-0.98014255
C	-1.26356327	2.47815309	0.93497423
C	-3.2591479	2.25349898	-0.99461977
H	-2.55560614	4.17655745	-1.70817467
C	-2.11580524	1.38588424	0.92737762
H	-0.48532873	2.56308156	1.69508753
C	-3.11701629	1.23748003	-0.04603615
H	-4.03442289	2.18871443	-1.75911961
H	-1.9867953	0.60724848	1.68374115
C	-4.01573317	3.3163E-06	3.4255E-06
C	-3.11701854	-1.23747507	0.04604195
C	-3.25915087	-2.25349372	0.99462579
C	-2.11580895	-1.38588118	-0.92737305
C	-2.42861735	-3.37253123	0.9801476

H	-4.0344248	-2.1887077	1.75912658
C	-1.26356902	-2.47815161	-0.93497063
H	-1.9867985	-0.6072457	-1.68373677
C	-1.39909073	-3.47322849	0.04437691
H	-2.5556118	-4.17655346	1.70817991
H	-0.48533556	-2.56308155	-1.69508488
N	0.61647231	-4.65684837	-0.06041735
N	-0.61648117	-4.65684707	0.060431
C	4.91724798	0.11608485	-1.23632668
H	5.62655908	-0.72358018	-1.29468425
H	4.33487998	0.14403247	-2.16862238
H	5.50105282	1.0462294	-1.17971921
C	4.91724934	-0.11609477	1.23632249
H	5.62656206	0.72356895	1.29467915
H	4.33488247	-0.14404132	2.16861892
H	5.50105239	-1.0462404	1.17971427
C	-4.91724973	-0.11608872	-1.23632034
H	-5.50105455	-1.04623309	-1.17970982
H	-5.62656086	0.7235762	-1.29467914
H	-4.33488286	-0.1440387	-2.16861667
C	-4.91724805	0.11609704	1.23632826
H	-5.50105121	1.0462425	1.17971842
H	-5.62656068	-0.72356656	1.29468791
H	-4.33488004	0.14404595	2.1686239

E(el) / Hartree :	-1376.44679		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-1376.48124		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-1377.89887		
Thermal corrections / Hartree			
ZPVE:	0.513817	E(therm.):	0.541388
H(corr.):	0.542332	G(corr.):	0.458285
Imaginary frequencies:	0		

TS (*E,Z*) → (*E,E*)

C	-2.36223575	2.69409987	1.18303304
C	-3.51356969	1.91219962	1.18502878
C	-3.941306	1.18875286	0.0660529
C	-3.18752987	1.36337659	-1.10612911
C	-2.04717808	2.13972901	-1.16157639
C	-1.56089579	2.77086734	0.01821423
H	-2.04802744	3.21741125	2.08724667
H	-4.07101042	1.84933916	2.12211758
H	-3.47128102	0.83243758	-2.01783578
H	-1.47138979	2.22355732	-2.08413494
C	-4.99379045	0.06581476	0.12725011
C	-4.10151072	-1.18167664	0.03884215
C	-3.27222085	-1.50502587	1.12949464

C	-3.85881593	-1.84099965	-1.17397642
C	-2.14210773	-2.28133789	0.96921312
H	-3.44723815	-1.03570762	2.09936903
C	-2.70869602	-2.60434873	-1.35500975
H	-4.51293089	-1.67000035	-2.03034761
C	-1.79429965	-2.76083938	-0.30716652
H	-1.43170215	-2.42193703	1.78542239
H	-2.44812615	-3.00176554	-2.33884408
N	-0.36416412	3.33546098	-0.01643334
N	0.72263065	3.78432306	-0.33581469
C	1.83317275	2.91775883	-0.07221391
C	1.77471038	1.88286384	0.86856666
C	2.97211971	3.08086158	-0.85655343
C	2.81986774	0.98367023	0.95536188
H	0.89013088	1.78062795	1.50130932
C	4.0011856	2.13763914	-0.79161639
H	3.00892518	3.91392984	-1.56210881
C	3.92781117	1.05336045	0.08768176
H	2.74483314	0.15634444	1.66395387
H	4.85236427	2.24262266	-1.46599301
C	4.93053158	-0.1179849	0.08956546
C	4.01855232	-1.34604901	-0.02855595
C	3.19966279	-1.45408811	-1.16726877
C	3.74270134	-2.1891823	1.05368556
C	2.03982049	-2.20474824	-1.14813595
H	3.40342875	-0.82691674	-2.03873387
C	2.56964712	-2.94089113	1.08922594
H	4.38369397	-2.17866802	1.93670031
C	1.65956911	-2.87557363	0.02838466
H	1.3300639	-2.17329706	-1.97656709
H	2.28232632	-3.48866685	1.98977271
N	0.32044866	-3.17870999	0.31414545
N	-0.47366851	-3.08031007	-0.64610677
C	-5.80779954	0.08965897	1.42218308
H	-6.53862443	-0.73263681	1.41957975
H	-5.19259459	-0.01999735	2.32480974
H	-6.35886342	1.03828159	1.50851334
C	-5.98423939	0.17171523	-1.03518586
H	-5.49253113	0.24752081	-2.01395701
H	-6.65428066	-0.70185587	-1.05968509
H	-6.59951496	1.07481505	-0.91171752
C	5.91707173	-0.05349449	-1.07810543
H	6.55955564	0.83707601	-1.00650711
H	6.56836067	-0.93933437	-1.05797937
H	5.41324344	-0.03069501	-2.05444639
C	5.72853158	-0.0920861	1.39720298
H	5.07708099	-0.08274636	2.28216768

H	6.39624334	-0.96467774	1.4675226
H	6.34782204	0.81596681	1.43473598

E(el) / Hartree :	-1376.38504		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-1376.4188		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-1377.83344		
Thermal corrections / Hartree			
ZPVE:	0.511181	E(therm.):	0.538826
H(corr.):	0.53977	G(corr.):	0.455947
Imaginary frequencies:	1		

TS (*Z*,*Z*) → (*E*,*Z*)

C	2.46421514	3.24204033	-0.89021132
C	3.39687786	2.2084617	-0.94019978
C	3.35563241	1.15453766	-0.02317244
C	2.33405378	1.17054718	0.94151376
C	1.37737616	2.17425975	0.97983478
C	1.42746414	3.22120869	0.04661301
H	2.52543613	4.08533913	-1.58136261
H	4.1763623	2.24631189	-1.70254281
H	2.27267061	0.35749984	1.66996112
H	0.59062781	2.15608947	1.73640565
C	4.37073276	0.00277614	-0.01914209
C	3.55848643	-1.29198938	0.00147731
C	2.55485469	-1.45131243	-0.97260349
C	3.70383414	-2.28752991	0.97077139
C	1.64962084	-2.48911466	-0.90275429
H	2.44518739	-0.69564493	-1.75427528
C	2.81116678	-3.360503	1.03592143
H	4.48869913	-2.21073814	1.72430512
C	1.74372033	-3.418025	0.14406283
H	0.8232959	-2.5687258	-1.6121828
H	2.87260096	-4.10529804	1.83260447
N	0.60382716	4.3708574	0.12134538
N	-0.62438612	4.36662809	0.27815216
C	-1.45784586	3.22530884	0.18523755
C	-1.31596229	2.20262009	-0.76742316
C	-2.59365535	3.23330707	0.9997076
C	-2.27820624	1.2094334	-0.85860813
H	-0.45778284	2.19492314	-1.44124014
C	-3.5373777	2.21191785	0.91832871
H	-2.7205192	4.0623147	1.69928326
C	-3.4034034	1.17992489	-0.01506687
H	-2.1439162	0.40937453	-1.59091736
H	-4.39858339	2.24085209	1.58721425
C	-4.41092363	0.02839654	-0.15620017
C	-3.58753726	-1.25619154	-0.0662819

C	-2.85242879	-1.50676719	1.10186218
C	-3.37934394	-2.13034431	-1.13930375
C	-1.89517341	-2.49855216	1.18018343
H	-2.99808004	-0.86857616	1.97799365
C	-2.39670891	-3.11379775	-1.12138243
H	-3.96302163	-2.01924534	-2.05532514
C	-1.56585043	-3.24921454	0.01462068
H	-1.29970683	-2.63965089	2.08333726
H	-2.21539456	-3.73414248	-2.00047103
N	-0.40346678	-3.88365446	0.01619699
N	0.65223999	-4.27508872	0.49625715
C	5.26413318	0.00079049	-1.26578799
H	5.93186193	-0.87269984	-1.24038187
H	4.67842463	-0.05150132	-2.19483717
H	5.89286208	0.90299263	-1.30495958
C	5.26782396	0.15268211	1.2151106
H	4.68845818	0.12311236	2.14912745
H	6.0323772	-0.63871703	1.25356662
H	5.78673645	1.12129705	1.17657791
C	-5.12143609	0.17384996	-1.50730144
H	-4.41378405	0.18737307	-2.34833698
H	-5.83283734	-0.65130418	-1.66717049
H	-5.68311833	1.1192057	-1.5328076
C	-5.48004738	0.04771107	0.94092868
H	-6.14878122	-0.81575842	0.81312085
H	-5.04565572	-0.01498436	1.94888844
H	-6.09315356	0.96075953	0.89045268

E(el) / Hartree :	-1376.39151		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-1377.84062		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-1376.39151		
Thermal corrections / Hartree			
ZPVE:	0.511414	E(therm.):	0.538985
H(corr.):	0.53993	G(corr.):	0.455767
Imaginary frequencies:	1		

Trisazo macrocycle **2**

(*E,E,E*)

C	-3.99095923	-2.8836305	-0.28260132
C	-2.66348193	-5.36383536	-0.08878481
C	-1.74107349	-6.58776013	-6.0062E-05
C	2.04437298	-4.47748591	0.28320207
C	-0.33491111	-5.97831493	0.08924623
N	-4.48612448	-1.58994612	-0.51168224
N	3.11464911	-3.59802154	0.51215332
N	-4.67616354	-0.89960102	0.50938004
C	-0.50103012	4.89896056	-0.28129365

C	-3.31269141	4.98850466	-0.08748036
C	-4.8337373	4.80102856	0.00090987
C	-4.90133507	0.46729646	0.28073892
C	-5.0090881	3.27844684	0.08889414
N	0.86702117	4.68171262	-0.51061947
N	1.5595412	4.49858361	0.51023336
N	3.61979631	-3.0907149	-0.50899821
C	4.4920014	-2.0144241	-0.28052806
C	5.97614389	0.37546726	-0.08868879
C	6.57533701	1.78613981	-0.00110185
C	2.85610077	4.01105128	0.28102575
C	5.34488183	2.69983107	0.08748828
C	4.5115042	-1.28788709	0.92086927
H	3.89706183	-1.64041927	1.75062743
C	5.23386353	-0.11183073	1.00230437
H	5.17058773	0.48150742	1.91726784
C	6.009609	-0.3973524	-1.25403598
H	6.58538156	-0.06412503	-2.11854402
C	5.26242127	-1.56907551	-1.35723181
H	5.23499419	-2.14199886	-2.28668263
C	4.98378228	3.38349637	1.2530604
H	5.64969164	3.38747292	2.11704559
C	3.74664197	4.01634553	1.35715429
H	3.43389392	4.49674609	2.28681688
C	4.45724713	2.74461031	-1.00282658
H	4.70220665	2.20054857	-1.91784326
C	3.23946447	3.39407199	-0.9206353
H	2.53057559	3.38753601	-1.7499369
C	-1.27281318	5.34303998	-1.35753738
H	-0.76369802	5.60568863	-2.28742724
C	-2.66108847	5.40391402	-1.25332654
H	-3.23830559	5.73561978	-2.11744894
C	-2.51867182	4.58993029	1.00308577
H	-3.00010527	4.23861129	1.91853261
C	-1.13902458	4.55284387	0.92068094
H	-0.52580298	4.19741608	1.75010277
C	-4.55502081	1.10863478	-0.91941531
H	-4.1925402	0.4985062	-1.74806117
C	-4.60104146	2.48804991	-1.00077104
H	-4.24952239	2.97278537	-1.91439168
C	-5.42381115	2.62317456	1.25288095
H	-5.76241455	3.19737132	2.11631928
C	-5.35401978	1.23520459	1.3561557
H	-5.61644326	0.72358816	2.28473347
C	-3.37455041	-3.26440725	0.92016283
H	-3.3748015	-2.55650368	1.75033774
C	-2.71715175	-4.477933	1.00254301

H	-2.17392223	-4.72017998	1.9187732
C	-3.98776448	-3.77297753	-1.35973428
H	-4.46795511	-3.46236433	-2.29022236
C	-3.34685849	-5.00592846	-1.25555951
H	-3.34422949	-5.6707912	-2.1203675
C	1.60327412	-5.2506947	1.35965552
H	2.17509153	-5.21921624	2.28965731
C	0.43692543	-6.00612747	1.25536548
H	0.10697348	-6.58419493	2.11957628
C	0.14806373	-5.23252846	-1.00124614
H	-0.44501791	-5.17333092	-1.9166337
C	1.31902329	-4.50207796	-0.91881841
H	1.668067	-3.88530295	-1.74831942
C	7.48584162	1.89423159	1.22602257
H	8.34611759	1.21961651	1.10628801
H	7.86905704	2.91997696	1.33790975
H	6.97932959	1.61662093	2.16000159
C	7.41392593	2.15312969	-1.22935261
H	6.83501565	2.13690715	-2.16236491
H	7.81563523	3.16993838	-1.11008068
H	8.26269093	1.46154207	-1.34265217
C	-5.57204248	5.343537	-1.2268051
H	-6.6532595	5.18195662	-1.10696366
H	-5.39864083	6.42460697	-1.33980061
H	-5.26870135	4.85086466	-2.16019869
C	-5.3824611	5.53471958	1.22855728
H	-4.88832298	5.23457835	2.16220836
H	-5.22887365	6.61716312	1.10924746
H	-6.46227688	5.35327278	1.34076401
C	-2.1031031	-7.43008635	1.22711791
H	-1.40568066	-8.27411206	1.34000552
H	-2.09165144	-6.85226799	2.1608808
H	-3.11698344	-7.83877997	1.10660319
C	-1.8415004	-7.4981413	-1.22794957
H	-2.86459141	-7.88796101	-1.34133971
H	-1.56605744	-6.98922275	-2.16125697
H	-1.16140146	-8.35404727	-1.10796179

E(el) / Hartree :	-2064.71141		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2064.7612		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2066.88759		
Thermal corrections / Hartree			
ZPVE:	0.771339	E(therm.):	0.814221
H(corr.):	0.815165	G(corr.):	0.696763
Imaginary frequencies:	0		

(*E,E,Z*)-2

H	-4.7491615	-4.42036705	-1.86494019
H	-5.87076352	-2.5093664	-2.97015346
H	4.16941295	-3.45962907	-2.18743528
H	6.33857135	-2.25831829	-2.35913273
H	5.65633966	0.52919172	-2.31615596
H	3.85108351	2.18460508	-1.96744757
C	-4.86465598	-3.4845452	-1.31735682
C	-5.48715332	-2.41606338	-1.95216658
H	-2.00983492	-4.3515391	2.9419231
H	-3.65020365	0.6988944	-1.63225449
C	4.58629702	-2.93538067	-1.32472885
C	5.80007038	-2.25518721	-1.41035233
C	5.64230464	1.11692952	-1.39609001
C	-1.50907073	-4.1892693	1.98690122
H	0.42491063	-3.85751943	2.91537884
H	-2.21039972	2.31367065	-0.47195364
C	4.62489483	2.03288062	-1.21365476
C	-0.14190682	-3.92094862	1.98411932
C	-3.73446284	-4.5404437	0.7340644
C	-4.10048792	1.56050488	-1.13577132
H	1.51210201	3.50462473	2.01189247
C	-4.42308704	-3.37996867	0.00581048
C	-2.2331822	-4.23686196	0.7921542
C	-3.28831393	2.48204703	-0.4796237
C	0.79211813	3.83404529	1.26119689
C	-5.66695174	-1.19222887	-1.29927251
C	3.83682074	-2.90154186	-0.14662099
N	2.53204619	-3.41970246	-0.20560099
H	-0.85346102	3.91644715	2.61847508
C	6.28145738	-1.51160049	-0.32848794
C	0.53920731	-3.72123505	0.78157965
C	7.39392825	-0.45855079	-0.47059606
N	-6.42478419	-0.25298376	-2.043953
C	-0.53906084	4.06305718	1.58505781
N	2.49386187	3.55192343	-0.49810084
C	6.57317383	0.83758693	-0.37797843
C	4.50475764	2.70598089	0.0130334
N	1.89972041	-3.38875992	0.86911294
C	1.22334375	3.95912228	-0.06443472
N	3.34832694	3.40356203	0.39812687
N	-6.40027896	0.97944592	-1.93016145
C	-1.53683677	-4.01414592	-0.41007725
C	-5.48797788	1.74521351	-1.16606357
C	-0.17507998	-3.77136431	-0.4265494
C	-1.47499344	4.43558262	0.61136076
C	-4.62995026	-2.15377061	0.6608931
C	-3.81889805	3.6130962	0.15738222

C	-5.24565054	-1.07779483	0.03588455
C	0.3066827	4.36061751	-1.04477089
C	-2.95678984	4.62610875	0.92698075
C	4.36734769	-2.25532243	0.98154831
C	5.5659862	-1.57605751	0.88240382
H	-2.0868937	-4.01359301	-1.35445859
C	-1.01481741	4.61053967	-0.70429049
C	6.52748049	1.61945083	0.78085537
C	5.49711387	2.53594688	0.98147488
H	0.36357089	-3.5889501	-1.35751535
H	0.65226031	4.44116122	-2.07756019
C	-6.0285189	2.88331647	-0.55398132
H	-4.29812384	-2.03111903	1.69378611
C	-5.21063945	3.78284607	0.11331488
H	-1.71992447	4.895698	-1.48853383
H	-5.40548408	-0.15269827	0.59024473
H	3.77962611	-2.24692605	1.90038584
H	5.9161082	-1.00689187	1.745906
H	7.25412382	1.46227997	1.57930104
H	5.40217258	3.08286892	1.92217316
H	-7.10569636	3.04678138	-0.62684938
H	-5.67175061	4.64960861	0.59139189
C	8.14014788	-0.54924824	-1.80340695
H	8.91641688	0.2287305	-1.84468681
H	8.6321526	-1.52833656	-1.90629949
H	7.48720523	-0.40656542	-2.67433404
C	8.42815427	-0.59688559	0.64907222
H	7.97981026	-0.60653453	1.65112766
H	8.97825848	-1.5414525	0.52780775
H	9.15449161	0.22917796	0.61023843
C	-3.33804797	6.06895406	0.54363347
H	-3.24330243	6.24243256	-0.53731872
H	-4.37314657	6.30188114	0.8319927
H	-2.67773656	6.77912086	1.06345058
C	-3.25199731	4.43411111	2.42158296
H	-4.32134553	4.5988954	2.61534253
H	-3.01014065	3.41445871	2.75478974
H	-2.68484013	5.15059975	3.03547175
C	-4.35363264	-4.71232607	2.12566817
H	-5.43460412	-4.89035282	2.02952908
H	-3.9130764	-5.57742857	2.64316227
H	-4.21620136	-3.83193136	2.7677552
C	-3.91578466	-5.87372643	-0.00748858
H	-3.45435513	-5.86847799	-1.00422057
H	-3.43511349	-6.67891845	0.56686734
H	-4.98330712	-6.11865765	-0.11968091
E(el) / Hartree :			-2064.68893

E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2064.73917		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2066.86578		
Thermal corrections / Hartree			
ZPVE:	0.771089	E(therm.):	0.814057
H(corr.):	0.815001	G(corr.):	0.695204
Imaginary frequencies:	0		

(*E*,*Z*,*Z*)-2

C	-0.70375033	1.46714324	3.16384664
H	-1.37851191	0.66673084	3.47860542
C	-1.68866763	5.23237182	0.12427596
H	-1.67653681	-4.31230109	2.06632441
H	-2.43520829	4.55542335	-0.29789377
H	-0.94959676	-7.58377579	1.68589959
N	-0.19568505	6.03211688	3.44649069
N	-0.00267483	4.98168365	4.07837451
C	-1.00795882	-3.50878896	2.37998969
H	-1.73777228	-2.14628463	0.90456305
C	-0.47839478	6.02457962	2.05231532
C	-1.03464075	-2.28228503	1.72684886
C	0.09473195	3.72849607	3.41404264
H	-2.69577474	3.80003563	-3.2319837
N	0.00267483	-4.98168365	4.07837451
C	-0.21433871	-6.9147938	1.23356975
C	-0.09473195	-3.72849607	3.41404264
N	0.19568505	-6.03211688	3.44649069
C	-0.92997351	6.04864405	-0.72980167
H	-0.59627434	-7.58191963	-0.76707089
C	0.14884713	1.25507236	2.0705276
C	-1.66665076	3.50492984	-3.02232314
C	0.21433871	6.9147938	1.23356975
H	-1.97477083	-2.38145397	-2.34708257
C	-0.14884713	-1.25507236	2.0705276
C	-1.1242216	5.9068634	-2.24369762
C	-0.0049667	-6.90731369	-0.14616857
H	-2.03639423	1.42388513	-3.5096515
C	0.47839478	-6.02457962	2.05231532
C	0.0049667	6.90731369	-0.14616857
C	0	0	1.21466221
H	-1.31086787	-4.74768432	-1.95852971
C	0.71379372	-2.67544589	3.85077828
C	-1.30876242	2.17170466	-3.19073053
C	1.00795882	3.50878896	2.37998969
C	-0.74340962	4.45657852	-2.56615635
C	0.70375033	-1.46714324	3.16384664
C	-0.95110324	-2.71463694	-2.53148089

H	0.94959676	7.58377579	1.68589959
C	-0.57384851	-4.03382843	-2.33300762
C	1.03464075	2.28228503	1.72684886
H	1.38368872	-2.83742671	4.69802036
N	-0.45007224	-0.43118059	-2.97447558
H	0.59627434	7.58191963	-0.76707089
H	1.67653681	4.31230109	2.06632441
C	0.92997351	-6.04864405	-0.72980167
C	0.00396224	1.7630409	-2.92933919
C	-0.00396224	-1.7630409	-2.92933919
C	1.47524849	-5.21364242	1.49113914
H	1.37851191	-0.66673084	3.47860542
C	0.57384851	4.03382843	-2.33300762
C	0.74340962	-4.45657852	-2.56615635
N	0.45007224	0.43118059	-2.97447558
H	1.73777228	2.14628463	0.90456305
C	1.1242216	-5.9068634	-2.24369762
C	0.95110324	2.71463694	-2.53148089
C	1.68866763	-5.23237182	0.12427596
H	2.05821205	-4.54563962	2.12613204
H	1.31086787	4.74768432	-1.95852971
C	1.30876242	-2.17170466	-3.19073053
C	1.66665076	-3.50492984	-3.02232314
H	1.97477083	2.38145397	-2.34708257
H	2.43520829	-4.55542335	-0.29789377
H	2.03639423	-1.42388513	-3.5096515
H	2.69577474	-3.80003563	-3.2319837
C	-0.71379372	2.67544589	3.85077828
H	-1.38368872	2.83742671	4.69802036
C	-1.47524849	5.21364242	1.49113914
H	-2.05821205	4.54563962	2.12613204
C	-1.22304496	0.24641507	0.31560365
H	-1.34214787	-0.54367112	-0.43909923
H	-2.1473915	0.31553918	0.90841564
H	-1.09593196	1.19510919	-0.22570653
C	1.22304496	-0.24641507	0.31560365
H	1.34214787	0.54367112	-0.43909923
H	2.1473915	-0.31553918	0.90841564
H	1.09593196	-1.19510919	-0.22570653
C	-2.57922175	6.23001654	-2.60146252
H	-3.29808531	5.60091048	-2.05893982
H	-2.79672192	7.27597797	-2.34091217
H	-2.7573376	6.10325152	-3.68034839
C	-0.22943551	6.85785085	-3.04596157
H	-0.47072903	7.9071231	-2.81777039
H	0.83974752	6.70286882	-2.84685774
H	-0.39208598	6.69817576	-4.12184366

C	0.22943551	-6.85785085	-3.04596157
H	0.47072903	-7.9071231	-2.81777039
H	-0.83974752	-6.70286882	-2.84685774
H	0.39208598	-6.69817576	-4.12184366
C	2.57922175	-6.23001654	-2.60146252
H	3.29808531	-5.60091048	-2.05893982
H	2.79672192	-7.27597797	-2.34091217
H	2.7573376	-6.10325152	-3.68034839

E(el) / Hartree :		-2064.69312	
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree		-2064.74202	
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree		-2066.8685	
Thermal corrections / Hartree			
ZPVE:		0.771441	E(therm.): 0.813942
H(corr.):		0.814886	G(corr.): 0.699048
Imaginary frequencies:		0	

(*Z*,*Z*,*Z*)-2

N	-1.91820426	-3.54091745	3.07041793
H	-2.55778801	-1.01615198	3.57649878
N	-0.89807447	-4.07995637	2.62209463
C	-3.03226272	-1.40960103	2.67467306
C	-2.74110615	-2.71202208	2.26091283
H	2.48119115	0.23906937	2.74340911
H	-0.29197711	-1.60434587	1.74730285
C	3.13074446	0.90786417	2.17703127
C	-3.89054116	-0.62159243	1.92024793
H	4.57388326	-0.6549413	1.82055024
C	-0.36509512	-3.7304748	1.35221658
H	-4.05500179	0.41204587	2.23064743
C	-0.05024745	-2.40007139	1.04109518
C	4.31723322	0.39340593	1.66018932
C	-3.37146794	-3.22703803	1.12676427
C	1.40239876	2.80903797	2.37807747
C	2.75608121	2.2346391	1.94896343
H	-3.16586409	-4.25206261	0.81276052
C	-4.54837376	-1.12344846	0.78640151
C	-0.00562544	-4.7429589	0.46430559
C	-4.27684114	-2.44418123	0.41642423
C	5.17216715	1.21494811	0.92330888
H	-0.21458418	-5.7811255	0.73144794
C	0.59550916	-2.10604365	-0.14727184
H	0.41479403	5.27792825	1.44533279
C	3.64834177	3.05259671	1.23888079
H	0.87934506	-1.07156698	-0.35401059
N	6.40664088	0.73614393	0.40373819
C	0.66057317	3.15930878	1.08442084

H	5.78870938	-2.76973442	-0.18612065
C	4.85682079	2.56688302	0.7617044
C	-5.49865495	-0.22351333	-0.01427602
C	0.24009179	4.45075224	0.75585307
H	-4.98859817	2.48784804	0.42398436
H	-4.77199024	-2.88555901	-0.44921712
C	0.59808804	-4.42585116	-0.75241337
C	5.05013717	-2.1803773	-0.73369521
H	3.70139262	-3.81827877	-1.01489073
H	3.3804574	4.09214613	1.03524906
C	0.91618418	-3.10495375	-1.07895954
C	3.88675912	-2.76065655	-1.21729009
N	6.44733115	-0.2321426	-0.36775212
C	0.4254847	2.13822318	0.15124694
C	-4.45520492	2.08746868	-0.43886555
H	0.7896589	1.12958729	0.35975702
C	-4.6187188	0.74938522	-0.81000409
H	5.54907362	3.2132855	0.2179961
C	5.25771746	-0.80759215	-0.89387862
C	-0.38036734	4.71902903	-0.46418399
H	0.84181471	-5.23633163	-1.4407752
C	2.93605781	-2.01617585	-1.93235413
H	-0.66986999	5.73731661	-0.73269351
C	-3.61120495	2.94006681	-1.14447824
C	1.63474371	-2.69643222	-2.36865883
H	-3.48956435	3.97814351	-0.82960199
C	-0.2351991	2.38014032	-1.04066035
C	4.34408219	-0.0565603	-1.63553775
C	-3.91689402	0.30172573	-1.9401608
C	-0.65328185	3.68131531	-1.35378873
C	3.20512666	-0.66373317	-2.15867252
H	-3.99685628	-0.74166259	-2.25120792
C	-2.93571522	2.4771026	-2.27508337
H	4.517316	1.00892752	-1.79473088
C	-3.12001021	1.15571846	-2.69011343
H	-0.4089886	1.56783506	-1.74797847
H	2.50745762	-0.04864999	-2.72869057
N	-1.20552015	3.98750609	-2.62661025
N	-2.17705458	3.36904692	-3.0803179
H	-2.6108451	0.80147678	-3.58926957
C	1.96162749	-3.89285689	-3.26832916
H	2.60719971	-4.62985779	-2.77088516
H	1.04302752	-4.4055798	-3.59224954
H	2.49022937	-3.54377048	-4.167193
C	0.71596882	-1.756641	-3.16016261
H	1.2021003	-1.41591711	-4.08703531
H	-0.20637633	-2.28947159	-3.4339318

H	0.42232866	-0.87065916	-2.57949807
C	-6.4510779	0.507558	0.94053261
H	-7.1130543	1.18461637	0.37983192
H	-7.07677319	-0.22653198	1.46885504
H	-5.93331386	1.10134743	1.7046652
C	-6.38468607	-1.02787702	-0.97405882
H	-5.81717568	-1.57839526	-1.735259
H	-6.9936793	-1.75560859	-0.41679756
H	-7.0639736	-0.34581217	-1.50590777
C	0.55710452	1.79891889	3.16482388
H	-0.40620091	2.25656666	3.43348668
H	0.3380775	0.89248717	2.5827858
H	1.06380806	1.49779551	4.09438601
C	1.62811926	4.02751083	3.27922435
H	0.66987559	4.46540227	3.59805855
H	2.177972	3.72144015	4.18101156
H	2.21564063	4.81367217	2.78510564

E(el) / Hartree :	-2064.66686		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2064.72019		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2066.84617		
Thermal corrections / Hartree			
ZPVE:	0.770474	E(therm.):	0.813448
H(corr.):	0.814392	G(corr.):	0.692555
Imaginary frequencies:	0		

TS (*E,E,Z*) → (*E,E,E*)

C	3.7081047	-3.24447377	-0.36603334
C	6.03306378	-1.65239007	-0.27033788
C	7.10791978	-0.55539205	-0.22089203
C	4.26286284	2.65960115	0.37462846
C	6.2630996	0.71442783	-0.03331699
N	2.45844189	-3.86624584	-0.52787737
N	3.14174711	3.44489866	0.68888165
N	1.8517339	-4.11076146	0.53369783
C	-5.54099907	-1.39422513	-0.64532392
C	-4.39713218	-3.88264587	-0.03463065
C	-3.77098742	-5.22221721	0.36725361
C	0.51368335	-4.5110246	0.3991684
C	-2.25205532	-5.04923109	0.39832086
N	-6.17693236	-0.17270285	-1.03930863
N	-5.6485175	0.86717585	-0.69725209
N	2.57085145	3.97227388	-0.28634408
C	1.30321397	4.51371758	-0.02780392
C	-1.36294545	5.40796275	0.18875243
C	-2.85290502	5.74814833	0.27886909
C	-5.01468309	1.99848611	-0.43492864

C	-3.62329131	4.43927358	0.07367082
C	0.5038417	4.10324313	1.05227727
H	0.92576693	3.40079777	1.77287187
C	-0.80754114	4.53382015	1.14063808
H	-1.44192584	4.14676969	1.9416503
C	-0.53747694	5.85296004	-0.84951028
H	-0.92623889	6.53777502	-1.6039855
C	0.77188184	5.39336041	-0.97299819
H	1.3999491	5.69238238	-1.81504059
C	-4.60759826	3.96161308	0.94273763
H	-4.8639772	4.52395676	1.84292611
C	-5.30108446	2.77749725	0.71290611
H	-6.06779029	2.43948335	1.4111804
C	-3.35124007	3.65284703	-1.05718696
H	-2.57138562	3.97096037	-1.75514003
C	-4.00762837	2.46667173	-1.32428357
H	-3.76153204	1.8779538	-2.20896294
C	-6.06578017	-2.55925545	-1.19885966
H	-6.92030422	-2.47231788	-1.87356229
C	-5.48978732	-3.79280018	-0.90269878
H	-5.90514104	-4.69203616	-1.35920767
C	-3.89676817	-2.694423	0.53083343
H	-3.04006493	-2.74616247	1.20714183
C	-4.4514502	-1.46164418	0.23056016
H	-4.04943717	-0.54236355	0.66347963
C	-0.232943	-4.36720809	-0.78197034
H	0.27441795	-4.00388445	-1.67700712
C	-1.59225618	-4.6277234	-0.7707203
H	-2.1741571	-4.45758461	-1.68055709
C	-1.48757031	-5.23751666	1.55283453
H	-1.95866778	-5.56972002	2.47839209
C	-0.12277923	-4.95985475	1.55804011
H	0.47189836	-5.05601603	2.46884434
C	4.13812515	-2.69188666	0.85115508
H	3.52005417	-2.84300294	1.73704375
C	5.2750139	-1.90832926	0.88718048
H	5.54346482	-1.42034567	1.82618303
C	4.48889136	-3.06021024	-1.50931845
H	4.1466948	-3.50185947	-2.44780907
C	5.64590169	-2.28465536	-1.45648748
H	6.21772937	-2.13187717	-2.37279331
C	5.11759255	2.29240731	1.41697589
H	4.95441794	2.73270483	2.40313362
C	6.11893074	1.34744337	1.206893
H	6.75381937	1.06136405	2.04667856
C	5.44078811	1.14607994	-1.08838805
H	5.51634421	0.66398625	-2.06513814

C	4.46470126	2.1076541	-0.89956699
H	3.7889134	2.40167928	-1.70419436
C	-3.13854054	6.38657274	1.64322652
H	-2.53347125	7.29746951	1.76239144
H	-4.19800925	6.67211148	1.72797052
H	-2.90052893	5.71402674	2.47926094
C	-3.28786922	6.74682397	-0.80118499
H	-3.13482401	6.35037007	-1.81506346
H	-4.36191121	6.95589943	-0.69192987
H	-2.7418838	7.69974813	-0.71370368
C	-4.1124827	-6.35024013	-0.61590047
H	-3.57804384	-7.26566136	-0.32340431
H	-5.18897849	-6.57755109	-0.60951922
H	-3.81862201	-6.10315807	-1.64609125
C	-4.3468435	-5.59362598	1.74107122
H	-4.11974148	-4.83068113	2.49961304
H	-5.44109439	-5.67711898	1.67160647
H	-3.95369812	-6.56157265	2.08809269
C	8.08056016	-0.80110018	0.93647214
H	8.78413551	0.03957087	1.0342646
H	7.57808713	-0.93511419	1.90314531
H	8.66226677	-1.713996	0.74186108
C	7.93922778	-0.47680398	-1.50396225
H	8.47067406	-1.42457276	-1.67889303
H	7.33893099	-0.25775214	-2.39644387
H	8.68834789	0.3227845	-1.4091493

E(el) / Hartree :	-2064.65893		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2064.70858		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2066.8322		
Thermal corrections / Hartree			
ZPVE:	0.769223	E(therm.):	0.812124
H(corr.):	0.813068	G(corr.):	0.693793
Imaginary frequencies:	1		

TS (*E,Z,Z*) → (*E,E,Z*)

C	-4.733184	3.56942545	1.39579029
C	-3.97286808	4.16393684	0.39257627
C	-2.87080662	3.50749685	-0.16434282
C	-4.44762609	2.2733644	1.82913723
C	-2.55695234	2.22955153	0.32687317
C	-3.33111155	1.60876245	1.29612122
H	-3.05833853	0.61479152	1.6524703
H	-1.67385625	1.71437562	-0.06009113
H	-5.5675956	4.09960163	1.85984662
H	-4.24071478	5.16720591	0.05963468
C	-2.0414719	4.10086664	-1.30432637

C	-0.5499171	3.97121786	-0.99478702
C	-0.04715115	4.37591278	0.25086466
C	0.38950914	3.53213445	-1.93300253
C	1.75092532	3.49055634	-1.66824045
C	-2.3484753	5.58827708	-1.53102286
C	-2.43445978	3.33633072	-2.57844547
C	2.2427659	3.9058807	-0.40310601
C	1.30334406	4.35302802	0.56159023
H	-0.74413026	4.71882588	1.02143166
H	2.45431436	3.13440153	-2.4219236
H	0.06547639	3.20288036	-2.92213223
H	1.6540891	4.67385546	1.54342926
C	-1.06625331	-4.50396195	-0.67951937
C	-2.45481361	-4.59008627	-0.67695585
C	-3.25265141	-3.504895	-1.06625451
C	-0.44453038	-3.32403946	-1.10205847
C	-2.61094067	-2.34246302	-1.51931306
C	-1.22916245	-2.25678202	-1.5569725
H	-0.72016797	-1.34886189	-1.88758165
H	-3.20698471	-1.47340984	-1.80724708
H	-0.44376285	-5.33193137	-0.33602661
H	-2.92135389	-5.51613586	-0.33763042
C	-4.77996613	-3.49566563	-0.93980819
C	-5.08862971	-2.40306769	0.09107207
C	-4.60152939	-2.54943817	1.39918133
C	-5.78023005	-1.22804819	-0.21687224
C	-5.93036774	-0.20829025	0.72099019
C	-5.34360684	-4.83391865	-0.45027384
C	-5.4007844	-3.20662886	-2.31102273
C	-5.40972343	-0.36175239	2.00756618
C	-4.7870553	-1.56486888	2.35697947
H	-4.04641519	-3.4506545	1.67028296
H	-6.44704919	0.71532692	0.4526347
H	-6.19631398	-1.08004906	-1.21447012
H	-4.41951259	-1.69345713	3.37722782
C	4.53918948	1.54030658	0.96463198
C	5.06118539	0.27774223	1.17482101
C	6.30051333	-0.10491728	0.62667187
C	5.276678	2.47150116	0.22501383
C	7.04974565	0.8612229	-0.04964859
C	6.55230288	2.15245193	-0.23139957
H	7.11587118	2.91002892	-0.78049922
H	8.02335545	0.60736527	-0.4711091
H	3.55148234	1.81369218	1.34302499
H	4.46976811	-0.45883057	1.72388781
C	6.72903745	-1.57303363	0.75206473
C	5.49003841	-2.3905994	0.37430167

C	4.89204527	-3.32316879	1.22389167
C	4.8468228	-2.09594688	-0.84242839
C	3.59636753	-2.60326862	-1.13934824
C	7.18388203	-1.82408649	2.19435143
C	7.88122693	-1.93220554	-0.19260532
C	2.95804713	-3.45404771	-0.22316899
C	3.64229944	-3.86558856	0.92051774
H	5.3712035	-3.60089183	2.16372221
H	3.06216327	-2.31168964	-2.04437986
H	5.30904014	-1.38523824	-1.53267726
H	3.14160405	-4.55299571	1.60556584
N	-5.23769056	1.78959174	2.90559657
N	-5.59703552	0.61030965	3.02173231
N	3.54282934	3.84623478	-0.1601837
N	4.7556642	3.74767284	-0.16232708
N	1.60753538	-3.83790063	-0.33107565
N	0.93405202	-3.07211461	-1.04854845
H	8.80005788	-1.38521065	0.06798056
H	7.63605931	-1.71527611	-1.24228663
H	8.09876987	-3.00727184	-0.1140804
H	-2.15723015	6.18263701	-0.62534436
H	-3.39238848	5.75109168	-1.84219369
H	-1.6962456	5.97606689	-2.32675359
H	-2.16636595	2.27147839	-2.51097974
H	-1.94615239	3.76226569	-3.46818144
H	-3.52198581	3.40196455	-2.73008765
H	-6.49843517	-3.16267692	-2.2423468
H	-5.13557802	-4.01108151	-3.01251488
H	-5.04715649	-2.26129917	-2.7447448
H	-4.95581502	-5.12053265	0.53680742
H	-5.10933017	-5.64314601	-1.15886951
H	-6.43765517	-4.76191525	-0.36539422
H	6.38712972	-1.60404008	2.91949639
H	8.03946534	-1.17478369	2.43062599
H	7.50325295	-2.86814123	2.33467895

E(el) / Hartree :	-2064.64213		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2064.69211		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2066.81638		
Thermal corrections / Hartree			
ZPVE:	0.769009	E(therm.):	0.81182
H(corr.):	0.812765	G(corr.):	0.693076
Imaginary frequencies:	1		

TS (*Z,Z,Z*) → (*E,Z,Z*)

N	4.54084982	2.53125488	3.00885958
N	3.75739405	3.40474201	2.61321875

C	4.85461721	1.4058123	2.20091234
C	5.43894377	1.5659124	0.94433894
C	4.66517269	0.11884344	2.71275989
C	4.95258677	-0.98413605	1.92162266
C	5.78153532	0.44735852	0.18930174
C	5.51036102	-0.84750816	0.64067444
H	6.2414841	0.60317844	-0.78715031
H	5.62461914	2.56953737	0.55738845
H	4.24564969	8.2989E-05	3.71422262
H	4.71849991	-1.98082867	2.30184054
C	2.9757459	3.2421217	1.43539004
C	2.10734672	2.1528283	1.27803012
C	2.95619047	4.26870439	0.49275635
C	1.25491626	2.09905973	0.1856355
C	2.13129819	4.17568077	-0.62705594
C	1.25859288	3.09674255	-0.80094093
H	2.16208197	4.98096343	-1.36189236
H	3.604468	5.13547997	0.63878041
H	2.09143896	1.35814282	2.02525264
H	0.56179745	1.25842915	0.1016031
C	-2.1888375	2.29335942	-1.92981395
C	-1.45456353	4.09268896	-0.52384608
C	5.71010952	-2.08809862	-0.23375329
C	4.31222019	-2.58856595	-0.61142463
C	6.47748747	-1.76867661	-1.52385153
C	6.51920152	-3.1371035	0.53674952
C	3.8912282	-3.91392012	-0.47863416
C	3.3808748	-1.68368869	-1.14542076
C	2.61833604	-4.33750296	-0.84850347
C	2.10790092	-2.05700066	-1.52892696
C	1.69277631	-3.4099895	-1.38168902
C	-3.49458801	2.46170282	-1.47577368
C	-2.75689037	4.29619498	-0.09203375
C	-3.78490554	3.4579605	-0.53819857
H	-3.00040674	5.09774384	0.60851958
H	-4.29271823	1.82014689	-1.85414034
H	2.3244531	-5.3811886	-0.72985721
H	4.56987889	-4.66592202	-0.07102843
H	1.40850269	-1.3254374	-1.9352155
H	3.65248372	-0.62927133	-1.24930759
N	0.46131584	-3.74238479	-1.73166312
N	-0.68199732	-3.85134458	-2.12972186
N	-5.09945347	3.77366299	-0.11167839
N	-5.92079079	2.94102328	0.29458853
C	-1.71621269	-3.61977452	-1.16740897
C	-2.98284684	-3.34011294	-1.68214582
C	-1.50647124	-3.63724413	0.21190599

C	-2.56409048	-3.35987912	1.07076403
C	-4.01844152	-3.02088325	-0.81679045
C	-3.83244603	-3.02858098	0.5743533
C	-5.00061022	-2.62840684	1.48154863
C	-4.67786012	-2.79598253	2.97097834
C	-6.20839069	-3.52202667	1.17573529
C	-5.2690278	-1.14932618	1.18278146
C	-6.44389368	-0.69293538	0.57955662
C	-4.28361471	-0.19924604	1.49810827
C	-6.62272887	0.65810733	0.29224212
C	-4.44196092	1.1446223	1.20168827
C	-5.61218087	1.58271941	0.56281491
H	-7.55153806	1.02160144	-0.15227525
H	-3.65718419	1.85563353	1.46247779
H	-3.35314238	-0.5227822	1.97050105
H	-7.24680388	-1.3900244	0.33655434
H	-4.99042627	-2.74243969	-1.22942993
H	-2.38876195	-3.39245735	2.14666492
H	-0.51303103	-3.87382122	0.60088423
H	-3.11845798	-3.34597926	-2.76584452
C	-1.14175365	3.09309803	-1.45700723
H	-0.65779029	4.73197556	-0.13585794
H	-1.99418254	1.51455864	-2.66878532
C	0.29347435	2.98199365	-1.98314448
C	0.49295614	4.11021625	-3.00510313
C	0.55078815	1.64798329	-2.69750452
H	6.71551861	-4.01907799	-0.09121172
H	6.00734266	-3.48023503	1.44670781
H	7.48992806	-2.71436359	0.83504489
H	-3.82767565	-2.18133368	3.29584033
H	-4.45180441	-3.84691695	3.20766937
H	-5.54850737	-2.49185171	3.56971388
H	-6.51927626	-3.47610827	0.12339591
H	-7.06975714	-3.23708967	1.79838304
H	-5.95791758	-4.56919441	1.3996694
H	-0.21993156	3.98630612	-3.83308723
H	1.51134677	4.09255191	-3.4237653
H	0.31215941	5.10050878	-2.56326802
H	-0.04356704	1.56636036	-3.61956005
H	0.30886535	0.78554828	-2.06020009
H	1.61195632	1.57508719	-2.97738339
H	6.60248383	-2.69060661	-2.11004534
H	7.47730807	-1.35895603	-1.30830521
H	5.93666021	-1.05285207	-2.15903117

E(el) / Hartree :	-2064.62764
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2064.67954
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2066.80287

Thermal corrections / Hartree

ZPVE:	0.768767	E(therm.):	0.811621
H(corr.):	0.812566	G(corr.):	0.692384
Imaginary frequencies:	1		

Tetraazo macrocycle **3**

(*E,E,E,E*)-3

H	7.87225031	-3.24250187	-1.37342285
H	0.83380745	-7.47790637	-3.27032698
H	3.02072949	-7.22291221	-2.56659946
H	1.65794209	-9.00514694	-2.84472086
H	9.19778988	-1.19618435	-0.88042889
H	4.78561479	-5.63759376	-1.83203466
C	0.78638378	-8.36842213	-2.62706998
H	9.4462796	1.11321633	-0.94305558
H	-0.11935177	-8.92823557	-2.9019455
C	7.59310248	-2.58125469	-0.55030322
C	2.99001495	-6.8241261	-1.55162361
C	8.32551799	-1.4284211	-0.26807377
C	3.98700317	-5.94047502	-1.15292154
H	10.5763459	0.28923861	0.16107062
C	9.78979245	1.05669989	0.09927785
H	7.20453848	1.39468682	-1.1196612
H	0.44700291	-5.36807421	-1.73127202
N	5.72516231	-4.03200402	-0.19806965
H	10.2425123	2.02629279	0.35298071
C	6.46541464	-2.90652127	0.20534262
C	0.72650171	-7.99430358	-1.14043701
C	1.93284901	-7.16314954	-0.69598734
C	6.93665953	2.03499596	-0.27532451
H	5.41416293	3.10230697	-1.38548939
C	-0.47132788	-5.77425544	-1.30110481
C	7.93549705	-0.5666611	0.76028266
C	3.94671627	-5.37325054	0.12654842
H	1.63530885	-9.83595301	-0.44970533
H	3.41601621	6.3819035	-2.58367004
C	8.6472847	0.75275538	1.0750938
C	5.93145253	2.97216118	-0.43377472
N	4.80398476	-4.35658226	0.57657572
C	-0.51992981	-7.12622505	-0.92762449
C	0.69015194	-9.28903749	-0.31862343
H	-1.49856836	-3.86726673	-1.31902242
C	-1.54593764	-4.93052259	-1.07546188
H	-0.12600051	-9.94943668	-0.64810806
C	7.58977632	1.85513265	0.9577628
C	6.08129691	-2.06334306	1.26150179

C	2.68669727	6.47235346	-1.77589314
H	1.3657651	7.75843942	-2.86972907
C	6.8041252	-0.91470275	1.5213877
C	1.94395307	-6.63853717	0.60512572
H	9.98367649	-0.1582687	2.51443938
C	2.93048854	-5.75435053	1.01212808
C	9.24680402	0.65746146	2.48339154
N	4.09491374	5.00273768	-0.52669333
C	1.53107451	7.23650371	-1.92651688
C	-1.71023033	-7.61438842	-0.37175722
H	-0.85952333	8.02370342	-3.23359301
C	5.5262926	3.75199058	0.66139998
C	-2.72515319	-5.42677933	-0.50711179
H	0.56055733	-9.0919229	0.75521497
H	9.76110769	1.59124669	2.75811197
C	2.93722091	5.79684683	-0.58028118
H	-1.06891949	5.79450517	-2.45796349
H	5.19011921	-2.32194571	1.83459413
C	7.19573755	2.65778289	2.03211477
C	-2.80866915	-6.78254748	-0.17121888
N	4.45236094	4.65695439	0.61632375
H	-0.10789934	9.49851837	-2.56756172
H	-1.78302117	-8.66007446	-0.06802181
C	-0.89543719	8.74632981	-2.40627782
H	1.12618466	-6.87972594	1.2886711
H	-2.85836241	4.06740703	-2.2641878
H	6.46616335	-0.24068478	2.31273647
N	-3.72426886	-4.47618417	-0.25120088
C	6.16304142	3.58315052	1.89213671
H	8.48616788	0.44405084	3.24734818
H	2.91740744	-5.30212778	2.00588676
C	-1.86963563	5.91943923	-1.7249087
C	0.58282069	7.3122403	-0.90244801
C	-2.85428278	4.94951261	-1.62075737
H	-1.86822837	9.25680079	-2.45584032
H	7.67651024	2.55039833	3.00516962
C	2.0040076	5.88281655	0.46547292
C	-0.74087731	8.07034873	-1.03804567
N	-4.88325876	-4.90455891	-0.09136849
H	-3.73124115	-7.15566269	0.27733291
C	0.84496943	6.61857346	0.29314048
C	-1.86509967	7.04107853	-0.88285431
H	5.8261302	4.18870409	2.73617945
H	-4.37886133	-2.62570718	1.24149997
H	-5.98657319	2.07029849	-1.48213111
C	-5.80469969	-3.8977729	0.25662266
C	-5.42312213	-2.73840391	0.94691231

H	2.20318237	5.33506424	1.3877703
C	-3.85776325	5.06269754	-0.65080986
H	-7.36448757	0.03173903	-1.10956535
H	0.06002889	9.85167079	-0.1032115
N	-4.76186729	3.99021349	-0.58026781
C	-0.78917994	9.16641172	0.03347109
C	-6.52856186	1.92023613	-0.54760236
C	-7.14254207	-4.07210346	-0.10091206
C	-6.36261896	-1.76249612	1.22874773
C	-7.30077745	0.79442915	-0.32893034
H	0.10114766	6.635146	1.09393013
H	-7.43064314	-4.99042052	-0.61701039
C	-2.89138801	7.15805134	0.06521569
H	-9.62595988	-0.75743621	-0.86793039
H	-6.05069038	-0.86031917	1.76045481
H	-1.71519508	9.75606432	-0.04488461
C	-3.87498841	6.18285415	0.18910755
C	-8.07193587	-3.0641709	0.15274639
C	-7.69790931	-1.88632969	0.80836026
H	-0.72685963	8.75838624	1.05202134
N	-5.5469847	4.00124223	0.38785498
C	-6.3953913	2.88203337	0.46797838
C	-9.91114523	-0.78287375	0.19374051
H	-2.9226859	8.02046995	0.73280136
C	-7.9532723	0.57403368	0.89914133
H	-9.10219227	-3.2057402	-0.17749951
H	-10.5211358	-1.68238661	0.36561487
C	-8.68349016	-0.75293882	1.11496964
H	-4.66262501	6.25958089	0.94034949
H	-10.5455491	0.09268598	0.39521848
C	-7.0952634	2.71252064	1.66312184
C	-7.85873505	1.56549729	1.87826782
C	-9.15900239	-0.92921598	2.56307455
H	-6.99171724	3.47819716	2.43482882
H	-9.63204025	-1.91532709	2.67734213
H	-8.32133476	-0.87703741	3.27378184
H	-8.35942229	1.44074378	2.83902478
H	-9.90147299	-0.16419529	2.8384417

E(el) / Hartree :	-2752.96792		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2753.03196		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.86872		
Thermal corrections / Hartree			
ZPVE:	1.028808	E(therm.):	1.087001
H(corr.):	1.087945	G(corr.):	0.933216
Imaginary frequencies:	0		

(*E*,*E*,*E*,*Z*)-3

H	8.20025577	2.11408971	-2.50769943
H	7.02889928	3.30732103	-3.10723775
H	9.10783783	3.60043743	-0.69529545
H	8.17385123	4.87809864	-1.5031561
C	7.18679002	2.51688607	-2.35919051
C	8.13814407	4.11896028	-0.70695936
H	6.46022453	1.71533667	-2.55763723
H	8.0650805	0.51104691	-1.07652678
C	7.01429285	3.10148694	-0.94948468
H	8.01961987	4.6312325	0.25904412
H	6.41578521	-3.94153541	-2.43256506
C	7.68404192	0.77120045	-0.08802947
H	6.27147751	5.8013967	-1.02638784
H	4.99755663	-4.40084627	-3.40292901
C	7.11844589	2.03070835	0.13893278
C	5.3163523	-3.93889769	-2.45588711
C	5.62614965	3.74110014	-0.88533519
C	5.42160762	5.12227207	-0.94849567
H	4.98553509	-2.89000022	-2.44755814
C	7.76180568	-0.18370865	0.92159703
H	8.19602951	-1.16263144	0.71279914
H	6.31571	-6.24946924	-1.5281483
C	4.49483851	2.90981711	-0.79460628
C	6.67879588	2.32444949	1.43834475
C	4.1358929	5.65918363	-0.90686041
H	4.73788306	-6.63485591	-2.24587642
C	5.22845663	-6.17591857	-1.37523147
H	4.63359994	1.82618423	-0.7502093
H	3.96973806	6.7375473	-0.95234171
C	4.77797552	-4.71326455	-1.243581
H	2.9148205	-3.75243048	-3.09413046
H	6.2439595	3.30480966	1.64869282
C	7.27641473	0.11067805	2.19993338
C	5.35065641	-4.03450129	0.00212239
C	3.21569834	3.43287321	-0.72769387
C	6.46597653	-4.53225157	0.68259744
C	6.77645648	1.39179884	2.46052194
H	6.91290089	-5.48201014	0.38599246
C	3.0267884	4.82374226	-0.76929271
C	4.79625029	-2.82511709	0.45116469
C	7.02261947	-3.84002014	1.75465339
C	2.45577945	-4.19838345	-2.21146955
H	4.96240007	-6.76798402	-0.4877036
H	3.89837591	-2.43589368	-0.03593006
C	5.36143625	-2.10882939	1.4963065

C	6.50690759	-2.60097382	2.13790301
H	7.87809609	-4.24213372	2.30143562
C	3.2510465	-4.70742037	-1.18177654
N	7.37870695	-0.76746812	3.3096484
N	7.10885775	-1.97528253	3.25998973
H	2.33853492	2.79120944	-0.63379312
N	1.76505574	5.44067836	-0.67735759
H	4.91732189	-1.16548408	1.81923478
H	6.45051757	1.62838894	3.47551
C	1.06675491	-4.24232949	-2.1282018
H	0.43646089	-3.83665943	-2.92217356
C	2.60619571	-5.26455961	-0.06102952
H	-0.08548502	7.00942634	-1.3489975
N	0.86877601	4.7049849	-0.22109427
H	3.2122855	-5.64444171	0.76603182
C	0.43932652	-4.80978268	-1.01772763
C	-0.81930542	6.44993169	-0.76630874
C	1.22556203	-5.32472533	0.02662192
C	-0.41699778	5.26184348	-0.14330394
N	-0.96338061	-4.78526242	-1.03025513
C	-2.13652342	6.88236955	-0.649687
H	-2.43285024	7.80104588	-1.15887573
H	0.72372222	-5.75329055	0.89550159
C	-1.34880856	4.5292892	0.60048985
H	-3.09522405	-3.94977492	-1.79195434
N	-1.5347102	-5.37841485	-0.09425201
H	-1.01773982	3.60048368	1.06925136
C	-3.07874605	6.1573019	0.09453144
H	-4.88917986	5.10184151	-1.96412673
H	-4.80505049	7.29635016	-1.80551838
C	-2.65348646	4.97850359	0.72547062
C	-3.65330781	-4.49457237	-1.02978114
H	-4.40621991	8.5872947	-0.64897081
C	-2.93859901	-5.27970763	-0.10992587
C	-4.96267485	7.64686115	-0.77586784
H	-6.00677788	2.88795792	-2.18176965
C	-5.41540887	4.67558446	-1.1070955
C	-4.53711947	6.60629181	0.26667083
C	-6.02639238	3.43706356	-1.23819857
C	-5.02784858	-4.40239355	-0.93234276
H	-5.56475953	-3.75134955	-1.62650652
H	-3.36912359	4.38625638	1.29967478
C	-5.39980993	5.35040747	0.1220126
H	-6.03211602	7.87379102	-0.655737
C	-3.63776816	-5.97769553	0.87601948
H	-4.01372293	8.1336315	1.71064975
C	-4.66190011	7.24701057	1.65574257

H	-7.48592245	-4.92620681	-2.0334312
H	-3.06705244	-6.58338275	1.58323429
C	-6.6057412	2.81925847	-0.12426042
C	-5.74632679	-5.08541617	0.06734551
N	-7.00277623	1.48055567	-0.29556966
H	-4.34643262	6.56081113	2.454371
C	-5.02763303	-5.88503747	0.95946271
C	-6.08291637	4.76860834	1.1992949
H	-8.19334123	-0.47412517	-1.36632173
C	-7.91592482	-5.38070822	-1.13048822
H	-8.33490534	-2.94210392	-1.58672924
C	-7.86146836	-1.12711341	-0.5574895
C	-7.92453937	-2.51146066	-0.67208844
H	-7.76492027	-6.46728035	-1.2075279
C	-6.66758477	3.51209448	1.08951745
H	-5.69690211	7.56632255	1.85488959
C	-7.26220928	-4.86305064	0.15635777
N	-7.0614254	0.82207512	0.7611679
C	-7.32153733	-0.54891201	0.59660475
C	-7.42677492	-3.3496531	0.33631249
H	-6.12183449	5.27998035	2.16200579
H	-8.99934077	-5.18487705	-1.12716531
H	-5.54502474	-6.4341769	1.74733871
C	-6.94761665	-2.75197812	1.51073617
C	-6.91449851	-1.3732843	1.65154017
H	-7.14131689	3.02947511	1.94573486
H	-6.54378432	-3.37646162	2.31040709
H	-6.51168873	-0.90033244	2.54939834
C	-7.90331954	-5.6046371	1.3330585
H	-7.78285457	-6.69288018	1.22230801
H	-7.47630472	-5.31349525	2.30235283
H	-8.98044622	-5.38478496	1.36477697

E(el) / Hartree :	-2752.94683		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2753.01199		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.84859		
Thermal corrections / Hartree			
ZPVE:	1.028529	E(therm.):	1.086705
H(corr.):	1.087649	G(corr.):	0.93254
Imaginary frequencies:	0		

(*E,E,Z,Z*)-3

H	2.58726154	3.29854426	-4.00082873
H	4.33930319	3.2375342	-3.71474885
C	3.35662766	3.2166031	-3.21960173
H	2.88541074	5.79608915	-3.85991348
H	3.23305241	2.23908417	-2.73028195

H	4.56182069	5.69434783	-3.27827039
C	3.50932149	5.68706129	-2.95980232
C	3.20485253	4.37538738	-2.2229183
H	5.49433506	2.78974543	-1.93445904
H	1.02360382	6.05699592	-2.73902643
C	0.78355831	5.24241708	-2.05417073
C	1.77639159	4.32620644	-1.67879058
H	3.34847777	6.56346944	-2.31516858
C	5.29528486	3.42016704	-1.0666253
H	3.98842063	-0.59826902	-2.356452
C	-0.51581863	5.13992591	-1.57030405
C	1.42637305	3.29976764	-0.7895448
C	4.18105882	4.26557561	-1.0507493
H	5.22581699	-0.29750669	-0.22606296
H	-1.29239423	5.84768525	-1.8647965
H	2.18774408	2.58302474	-0.47096334
H	7.71625216	-2.87183103	0.67560893
C	0.13579639	3.19294923	-0.29500996
C	-0.85013224	4.10790035	-0.6856552
C	4.12994508	-1.43877416	-1.67303987
H	-5.26624401	5.48086319	-1.57024113
C	6.16821918	3.35034293	0.01552204
H	7.0258202	2.67719675	-0.0209685
C	4.8295352	-1.28162392	-0.48001131
H	6.79753842	-4.20584939	1.39051656
C	7.09932742	-3.15998399	1.53885209
N	-2.12788491	3.88754687	-0.1497978
H	-0.14805495	2.39875135	0.39843942
C	3.99288199	5.0799151	0.07610019
C	-5.42944814	4.8170574	-0.71849234
H	7.71951373	-3.11779621	2.44708651
N	2.99151096	-2.74933601	-3.31291104
H	-7.56789764	4.81001928	-0.90497402
H	1.31679365	-5.94238289	-3.92239309
N	-3.04764706	4.60399881	-0.59230153
C	3.59662043	-2.67926314	-2.032084
N	2.0350691	-3.4820624	-3.59931539
C	-6.71618629	4.4333059	-0.33666563
H	3.13350261	5.75428363	0.1121558
C	5.94821604	4.14771035	1.14342992
C	5.05161416	-2.36647439	0.37627214
H	-9.21525055	3.21707832	-0.90414447
C	-4.31357323	4.30353732	-0.05605113
C	5.86084873	-2.26236718	1.67796199
C	4.87454846	5.04538987	1.14611419
H	-7.793311	1.67570279	-1.31117175
C	0.92735468	-5.52243203	-2.99258797

C	6.25634124	-0.81494645	1.96984439
C	7.58411545	-0.37628743	1.93152367
H	8.38680451	-1.07379106	1.6933022
H	-9.5578689	4.48879967	0.29071618
C	-9.40276244	3.40695159	0.16131365
C	1.27283487	-4.21268899	-2.65422645
C	5.27433095	0.13344223	2.30179468
C	7.92226501	0.94576185	2.20750832
C	3.83640579	-3.7830071	-1.20002896
H	-6.86268332	-0.59475816	-1.69864765
N	6.83570106	4.21041358	2.24911114
H	4.2260325	-0.1692559	2.35310417
H	8.96490858	1.27044135	2.20277506
C	4.55092012	-3.617419	-0.02324618
C	6.92538448	1.88484009	2.46779057
C	5.59053464	1.46443878	2.53471335
C	-7.6976049	0.98349125	-0.47211398
C	-6.91249746	3.54571553	0.72403
H	-0.13221288	-7.29942385	-2.44227958
C	0.10374938	-6.27337774	-2.15692996
C	5.01959233	-2.79004594	2.85626047
C	-4.50205743	3.47478546	1.06186627
H	-10.3388753	2.89583393	0.42969265
C	-7.16735928	-0.27649774	-0.69967896
H	4.76978355	-3.85205343	2.71808674
N	7.32754319	3.20809919	2.78405715
H	4.7414049	5.69893079	2.01077889
H	4.80469746	2.18476826	2.77000207
C	-8.26952832	2.90882433	1.06121809
H	5.5834728	-2.69257649	3.7961947
C	-5.77959039	3.11382738	1.43981202
H	3.47421677	-4.77285552	-1.48000343
C	0.72536185	-3.63904959	-1.49724075
C	-8.00725695	1.41504511	0.82555636
H	-2.98831513	-5.30011943	-1.82576487
H	-4.88499576	-3.74079775	-1.41427968
H	-3.62315887	3.0958806	1.58429411
H	4.72739609	-4.49734683	0.59942377
H	-2.39404577	-7.64426229	-1.60960208
H	4.07487703	-2.23971129	2.96466547
H	0.95257677	-2.60201748	-1.24306977
C	-0.44025448	-5.72146706	-0.9939532
C	-6.90928485	-1.13617599	0.37439885
C	-3.29650445	-5.07676876	-0.80082728
H	-8.81663514	4.30950036	2.61704726
C	-4.3509205	-4.20893967	-0.58654136
C	-8.64738539	3.22802702	2.51111421

C	-0.12004716	-4.38722264	-0.69214011
N	-6.13342768	-2.26531447	0.06948862
C	-1.85756395	-7.81573938	-0.66521819
H	-5.90486719	2.42211359	2.2759172
H	-1.028032	-8.51270149	-0.85901731
C	-7.8689424	0.4935595	1.87471356
H	-9.57357188	2.70719665	2.79913263
C	-1.35423428	-6.50494808	-0.04617677
C	-7.31623992	-0.76375809	1.66183139
N	-5.64984763	-2.86565727	1.04946349
C	-2.56853049	-5.63078008	0.26905636
C	-4.71478991	-3.86539887	0.72653651
H	-7.86037362	2.94895287	3.22470816
H	-2.55246558	-8.30787704	0.03067326
H	-0.56330501	-3.91842738	0.19025546
H	-8.14034176	0.78053608	2.89199243
C	-0.53799289	-6.84848141	1.20697196
H	0.34705007	-7.43469729	0.91963445
H	-7.13479311	-1.45237001	2.48856742
C	-4.04045764	-4.4538988	1.79722965
C	-2.97741199	-5.32677619	1.56941284
H	-0.1864947	-5.94425166	1.72495627
H	-1.12563535	-7.4511994	1.91643957
H	-4.33913795	-4.17522936	2.80998638
H	-2.44732731	-5.74438699	2.42619817

E(el) / Hartree :	-2752.92396		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.99015		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.8265		
Thermal corrections / Hartree			
ZPVE:	1.028152	E(therm.):	1.086277
H(corr.):	1.087222	G(corr.):	0.931548
Imaginary frequencies:	0		

(*E,Z,E,Z*)-3

H	5.65891911	4.11675965	-3.51455816
H	7.23937601	3.37079264	-3.1973359
C	6.20046018	3.43729995	-2.84045295
H	5.74024632	2.4420681	-2.92442322
H	6.5292151	6.01725244	-2.1024914
H	-6.81794507	2.87308646	-2.95360044
C	6.90805335	5.30266917	-1.35569104
H	7.9692837	5.11670768	-1.57567027
C	6.13541964	3.97738177	-1.40439161
C	4.05395433	5.39748524	-0.89104617
H	5.58031989	-4.15277143	-3.31225995
C	4.65940815	4.14770439	-1.04140805

H	4.63734635	6.31065803	-1.01275219
C	-6.98452125	2.73269037	-1.88354677
N	-8.61627167	1.06077352	-2.46840121
C	2.70065133	5.50192977	-0.57695863
H	7.88527806	1.8315943	-1.82288018
C	3.86039623	3.00072916	-0.87012498
N	-8.73020011	-0.1728784	-2.47263742
H	2.22000768	6.47439871	-0.45189115
H	5.56670418	-2.52212094	-2.57949169
C	6.00400898	-3.52904747	-2.51026723
H	-5.50549992	4.16496607	-1.28195027
C	1.92061797	4.35698822	-0.40684655
H	7.08474965	-3.43748339	-2.69140827
C	2.51492973	3.09274395	-0.55986083
H	3.52257816	-3.7284665	-2.73669435
H	4.32153243	2.01387642	-0.96715175
N	0.57097714	4.57134578	-0.08180287
C	-6.26605375	3.45660078	-0.94330604
C	-7.91089262	1.77160277	-1.46493075
H	6.8509087	5.77121839	-0.36240257
H	-6.11762333	-0.03315381	-1.55250267
H	1.89533657	2.20547126	-0.42153616
C	7.65411425	1.9988454	-0.76992916
C	6.78355762	3.0278131	-0.39503123
H	1.13397418	-3.89256906	-2.08483574
C	3.26815378	-4.0057579	-1.71302284
H	-6.07829274	6.00867436	0.35280808
C	-8.04301068	-1.0320977	-1.57397046
C	-6.69910995	-0.88559284	-1.1996809
H	-1.3959985	5.91682816	0.44433565
C	-2.03388638	5.04126869	0.57277334
C	1.92665427	-4.09357074	-1.36262758
H	-3.79863167	6.16408167	1.01503356
N	-0.11747349	3.54429775	0.07597674
C	-3.38033066	5.164209	0.89171222
H	5.73329803	-6.20539231	-1.82486473
C	5.76787746	-4.15276741	-1.12661675
C	-1.46630379	3.77221138	0.40432308
H	7.3704541	-5.60653015	-1.49194301
C	-6.48667376	3.29003581	0.43209138
C	8.23017254	1.1559934	0.17601091
C	-8.17734533	1.62350238	-0.10155236
C	6.32815486	-5.58353543	-1.14013422
C	-6.21192515	5.57065146	1.35259611
H	8.89014388	0.34607659	-0.14013793
H	-2.68131788	-4.78719321	-1.97812697
C	4.28309279	-4.2453485	-0.77685298

C	6.54901622	3.22036024	0.97443582
C	-8.74073084	-2.16822558	-1.157576
C	-4.19866388	4.03684001	1.04844001
C	-6.10249237	-1.83394651	-0.38193314
C	-2.27118616	2.63739563	0.56362594
H	-7.28847374	5.57409714	1.5768213
H	-9.76838169	-2.30093676	-1.5022493
C	6.48202567	-3.25793138	-0.11073418
C	-5.67983795	4.13256474	1.42150988
C	-7.47371437	2.38250759	0.82956807
H	-5.05323612	-1.70702825	-0.10572555
C	-3.61632819	2.77188718	0.87790637
H	5.88054653	4.02321402	1.29585142
N	-0.63527875	-4.43001287	-0.47112588
C	-2.97147354	-4.54797089	-0.95296746
H	-8.92541129	0.90115849	0.23057951
H	-5.71284536	6.2202547	2.0878309
H	8.30195803	-4.42362025	0.00660884
C	7.78279832	-3.52051442	0.33046868
H	-5.08304895	-4.56449637	-1.34012554
C	1.56680457	-4.41690372	-0.04920171
H	-1.8122852	1.65598172	0.42628047
C	5.85414063	-2.09471261	0.3628898
H	4.82572807	-1.88124203	0.06198206
C	-4.30384391	-4.4263193	-0.58629395
C	-1.95887469	-4.35000472	-0.00620248
C	7.95051441	1.33732817	1.53337983
H	6.28793484	-6.04498692	-0.14276322
C	-8.13741878	-3.10171875	-0.3202086
C	7.14243524	2.40817952	1.92996214
H	-4.23809653	1.87819306	0.97746012
C	-6.80802895	-2.95269869	0.08871736
N	0.2409945	-4.45212659	0.41468457
C	3.90677023	-4.59306567	0.52934264
C	8.43466184	-2.65315628	1.20229159
C	6.50130903	-1.21105612	1.21368361
C	2.57047048	-4.66621539	0.89484424
H	-7.69647506	2.24192211	1.88815825
C	7.81811127	-1.47209326	1.62065816
H	9.43816537	-2.8741456	1.57191402
C	-5.82661778	3.63782559	2.86741729
C	-4.66671111	-4.07938008	0.72404303
C	-2.30613888	-4.02998693	1.31131572
H	5.98195406	-0.3195963	1.56771685
H	-8.71867372	-3.96656073	0.00291301
N	8.54084835	0.55453516	2.55745828
H	4.68006986	-4.77260827	1.2805521

C	-6.14634343	-3.92220056	1.07181076
H	-6.76670305	-5.74331972	0.01363475
H	6.96953366	2.56969432	2.9960158
H	-6.86100574	3.75030931	3.2263648
C	-3.64330726	-3.89320052	1.6630199
H	-5.17696598	4.2308254	3.52745352
N	8.54224	-0.68424846	2.5541611
H	-5.5355242	2.58234497	2.96993468
H	-1.50634248	-3.87000145	2.03594293
C	-6.78289204	-5.32048918	1.02857766
H	2.27081732	-4.90672959	1.91696042
H	-5.87334848	-2.35716275	2.58364413
C	-6.35655983	-3.33954877	2.47727043
H	-3.8865676	-3.61870463	2.69010476
H	-7.82542899	-5.30163172	1.37953173
H	-6.22378726	-6.00026415	1.68797317
H	-7.43221556	-3.20403066	2.66091995
H	-5.9640088	-4.01168361	3.2557301

E(el) / Hartree :	-2752.93449		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.99978		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.83628		
Thermal corrections / Hartree			
ZPVE:	1.028371	E(therm.):	1.086482
H(corr.):	1.087426	G(corr.):	0.93208
Imaginary frequencies:	0		

(*E,Z,Z,Z*)-3

H	-8.46153375	-1.66442911	-2.26411095
H	-5.27801038	-0.15121587	-0.93512463
H	-3.38865973	0.17246194	-2.48588222
H	-7.98827658	-3.98171493	-1.62477293
C	-8.15522636	-1.32925982	-1.26263352
C	-5.05961158	-0.92154062	-1.67952183
C	-3.99171534	-0.73580229	-2.54271006
H	-4.02889193	4.58707655	-2.08135745
H	-9.03506092	-1.37887337	-0.6022725
H	7.74218631	-4.02266827	-1.13793818
C	-7.55240455	-3.66217014	-0.66643889
H	-7.84080519	-0.27929864	-1.34940562
H	-8.34349841	-3.71992959	0.09531866
H	-2.00954751	3.73570137	-2.50439073
H	-0.15682481	0.83410528	-3.27398006
H	4.5355558	-3.17355546	-0.87267635
C	-4.17849421	3.9131058	-1.22416309
N	5.06175038	-4.88204812	1.19480721
N	6.24455894	-4.65229351	0.90112604

H	-4.00989339	2.88048662	-1.56299673
H	0.40856561	3.30700098	-2.8827871
C	-7.0211712	-2.22576536	-0.74761538
H	-5.22990745	3.99354887	-0.9120289
C	-5.84346715	-2.08643383	-1.71828054
C	3.86345995	-3.08055571	-0.018384
C	7.51727705	-3.16048301	-0.50650957
C	-1.31330902	3.83160372	-1.6703979
H	0.89494098	1.03128838	-1.050111
C	-0.27409635	0.03747725	-2.53675231
C	-3.68640869	-1.71828792	-3.4952674
C	0.04081452	3.59458983	-1.89538873
C	4.04779879	-3.89023199	1.11156269
N	-2.67814559	-1.53708279	-4.47535555
H	-6.76768995	-4.38152065	-0.39221706
C	6.71501296	-3.34261089	0.61912158
C	0.32102379	0.1352847	-1.28156904
H	2.69636532	-1.53616464	-0.93216613
C	2.83050034	-2.15827154	-0.04388148
N	-1.53011337	-1.16424481	-4.19956631
H	-3.26491783	6.3988741	-0.54606689
H	8.56431083	-1.76617082	-1.75245091
C	7.97821775	-1.88694749	-0.84028103
C	-5.53713017	-3.04715198	-2.68607632
C	-3.26477588	4.29058002	-0.05118539
C	-1.03538809	-1.0818471	-2.87194864
H	2.46880889	0.60353177	0.48322383
C	-1.78094866	4.13656803	-0.38971138
C	-4.48979019	-2.85531245	-3.58465404
C	-3.52840438	5.7580062	0.30779671
C	-6.52095224	-1.79714686	0.63193109
H	-4.59092843	5.92636813	0.54101289
C	3.13880222	-3.8035917	2.16623022
H	-7.83717752	-0.09931732	0.88558481
C	0.95724759	3.67346642	-0.8452274
C	1.95986718	-1.99661476	1.04593477
C	-7.00790269	-0.67211644	1.30198265
N	2.26239282	3.22468115	-1.10782138
H	3.25595068	-4.47804876	3.01717355
C	1.68070831	0.44683478	1.23250536
C	0.22611221	-0.90602754	-0.35438631
C	6.47527516	-2.25749876	1.47398122
C	2.12411486	-2.84776468	2.14236567
H	-5.07564412	-3.40127965	0.7336405
C	-5.47859942	-2.51804218	1.23519586
H	8.12308559	0.39123192	-2.56302221
H	-6.1283433	-3.9610208	-2.76032461

C	-3.56252783	3.33699669	1.1095442
H	-4.27100985	-3.59415857	-4.35856376
H	-2.74011503	1.63215584	0.05739684
C	0.92440871	-0.86989069	1.00563475
C	7.69335324	-0.78297597	-0.03306937
C	-0.83917591	4.26449728	0.64780345
C	-1.14071525	-2.13705183	-1.95334398
H	2.16746697	0.42572772	2.21823346
C	-3.22903784	1.97949907	0.97194767
H	-2.92822133	6.08666827	1.1683427
C	0.50899274	4.04390414	0.43304161
H	5.88336096	-2.39775843	2.37977405
C	4.56654477	1.75636491	-1.26809267
H	0.99576567	1.30828748	1.2068865
H	3.75652658	1.44798675	-1.93115555
C	8.77406964	0.75620692	-1.75616116
C	-4.12826706	3.74935827	2.3187464
C	5.78366545	1.10029594	-1.260944
C	6.96284354	-1.00440342	1.14561782
C	-0.50375609	-2.04692142	-0.72466166
N	3.09854302	3.44691523	-0.20984348
H	-4.38714259	4.79724698	2.47606617
C	4.3407909	2.81456403	-0.37098395
H	5.92873226	0.24089167	-1.92040929
H	1.45224517	-2.77717662	2.99900539
C	-6.42224734	-0.22567546	2.48326985
C	6.82155079	1.47866099	-0.38855518
H	9.71346905	0.18358473	-1.78644398
C	8.10958789	0.65029739	-0.37852498
C	5.36478742	3.20860245	0.49207009
C	-4.91963284	-2.11507366	2.43926871
C	6.59683236	2.55780621	0.4702301
H	-1.18833041	4.49128479	1.65856992
H	-1.700561	-3.0357182	-2.21780045
C	-3.48174475	1.06399469	1.9808263
H	-6.78399812	0.68210529	2.96969075
H	9.01291012	1.80801956	-1.97078961
H	5.16668519	4.02450719	1.19029312
C	-5.34895216	-0.92538087	3.03487051
C	-4.34231311	2.84643327	3.35950487
H	1.23590468	4.09789049	1.24482974
C	-0.13587835	-0.99640903	2.10623673
H	7.37639296	2.88450104	1.15936856
H	-3.21874774	0.01563145	1.83862861
C	-4.05376373	1.49288026	3.18888439
H	-4.10702318	-2.67923346	2.90219307
H	-0.55695809	-2.89620569	-0.03868424

H	6.73230371	-0.16065099	1.80096779
H	0.31614805	-0.92562514	3.10665205
H	-0.69060047	-1.94422531	2.04681436
H	-4.74359592	3.18129791	4.31847014
H	-0.85702283	-0.17195382	2.01385436
C	9.11681203	1.13706656	0.66970728
N	-4.72263553	-0.48890467	4.2310956
H	10.0076376	0.49272661	0.64904556
N	-4.21261173	0.6371881	4.31448239
H	8.70697719	1.10078188	1.68893039
H	9.43923392	2.16906858	0.4623304

E(el) / Hartree :	-2752.92783		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.99242		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.82851		
Thermal corrections / Hartree			
ZPVE:	1.02858	E(therm.):	1.086239
H(corr.):	1.087183	G(corr.):	0.935186
Imaginary frequencies:	0		

(*Z*,*Z*,*Z*,*Z*)-3

H	-4.01223672	2.11192916	0.83515622
H	-2.51353816	4.83807371	-1.2283318
H	-4.11725321	-0.18923335	1.72303359
H	-7.70952636	-1.5992055	2.49169438
H	-0.40818719	3.90423886	-2.14466305
C	-4.81990836	1.44322624	0.53105984
C	-4.88931988	0.15003989	1.02861885
H	1.20107664	3.28089517	-3.46969762
C	-2.50512551	3.85605386	-1.7060528
H	-6.16701691	-1.25098055	3.28358373
C	-6.68661825	-1.97450715	2.6396675
N	5.01563902	4.3418808	0.47746093
H	7.27694931	1.96576	-1.20071917
C	-1.32940661	3.32635051	-2.23497078
N	5.83368445	3.4892027	0.10340096
H	-6.74559688	-2.93894935	3.16817637
C	1.19891522	2.21503718	-3.19699452
H	1.37198078	2.13439447	-2.11558962
H	2.98506615	3.20952307	-0.87988276
N	-4.87219526	3.81676688	-1.3357862
N	-5.83284644	3.25061649	-0.79709615
C	-5.79941171	1.90473642	-0.35645413
C	6.6061199	1.37741253	-0.57145138
H	-0.37878115	2.85176347	-5.3131644
C	3.72713525	4.03855043	0.97057763
C	-3.70507005	3.14506552	-1.78413431

C	2.74427928	3.46394737	0.15429785
H	2.04851432	1.73690142	-3.70558219
H	-7.89682602	-2.79923245	0.42402238
C	-5.91481871	-0.73072852	0.64991395
C	5.68612306	2.07789654	0.21679803
C	-5.99623748	-2.13056351	1.27594149
C	-1.33279784	2.09915045	-2.90527026
H	-1.25852172	3.41840273	0.72732502
C	-0.29974821	1.77163906	-5.12285281
C	-6.83833694	-3.09727485	0.43285966
C	3.40426869	4.40900888	2.27571238
C	-0.10527051	1.5281799	-3.61967423
H	7.42173615	-0.51104067	-1.1649571
C	1.49633911	3.17779343	0.68444304
C	6.68291771	-0.01128771	-0.53774297
H	-4.35621887	-3.0794376	-0.70304023
H	4.16004389	4.90494896	2.88805687
H	-6.78260483	-4.10809284	0.86246948
H	0.55375106	1.38474248	-5.70084143
H	0.75189921	2.68816611	0.05098918
H	-1.2522916	4.72275202	1.92719453
C	-6.85592363	1.06083912	-0.7035386
C	-1.30224306	3.63124221	1.80349099
C	-6.89186177	-0.24764143	-0.22803673
C	-3.71998403	1.90875444	-2.44914076
C	-3.86335986	-3.08111916	0.27122753
H	-1.76785306	1.3011007	1.00782307
C	2.15086626	4.09589247	2.79999648
C	-4.57276131	-2.67354404	1.41195684
C	-2.5514956	1.40802337	-2.99954316
C	1.18317492	3.45195219	2.02565871
C	4.84387605	1.33771255	1.07125147
H	-1.21960732	1.30263839	-5.5002903
H	0.24744622	0.42728591	-1.15987741
H	-6.49704747	-3.15171994	-0.61030619
H	-2.28061049	3.29343745	2.17944886
H	6.92920379	-2.66374229	-1.49632877
C	-0.00073995	0.04192223	-3.27797856
H	8.03853517	-2.48845975	-0.11160845
H	4.12948351	1.82836464	1.72846836
C	5.85120395	-0.75320957	0.30537001
C	-1.0168243	0.76118525	1.58551235
H	1.94184699	4.35512094	3.83881753
C	0.19036108	-0.33608647	-1.93970113
C	-0.16007031	2.97408012	2.58480464
H	-7.63919985	1.43877275	-1.3641651
C	7.05655564	-2.87452157	-0.42556972

H	-1.63564061	-1.1010529	0.73900855
H	-4.65076491	1.35028682	-2.55145472
C	4.92875477	-0.04609465	1.09491922
C	-2.52828345	-3.46150341	0.33650477
H	-7.71601828	-0.89132628	-0.53929179
C	-3.90228134	-2.71123301	2.63917907
H	-1.9837036	-3.77246759	-0.55848279
C	-0.94466562	-0.62008752	1.42842252
H	-2.57962565	0.44599992	-3.51729688
H	-4.42343604	-2.44435851	3.55891498
C	-0.14634758	1.4499372	2.43497025
C	-0.11738708	-0.97335432	-4.23153606
C	5.93075754	-2.27718443	0.42902676
H	-0.34522114	4.41985052	4.20838388
H	-0.28124441	-0.726133	-5.28108677
H	7.06533527	-3.96743508	-0.30508544
C	-0.34478651	3.32880025	4.06433968
C	0.3041554	-1.66610642	-1.57092535
C	-1.85073102	-3.35926397	1.55526814
H	4.04985883	-3.85545128	1.79642582
C	-2.55092872	-3.03195668	2.71583781
H	4.24801792	-0.59790305	1.74795276
C	4.60013102	-2.86530844	-0.04876834
C	3.77726414	-3.65263874	0.76041703
H	0.48579952	-1.9348996	-0.53136872
C	0.031979	-1.35786404	2.11390939
H	7.18604988	-2.16245866	2.19145494
H	-1.31100682	2.94025221	4.41781345
C	0.82846047	0.70183962	3.11406497
C	6.23513503	-2.62663494	1.89175278
H	0.43854778	2.89924049	4.70398069
C	-0.05796704	-2.31694892	-3.86545718
C	4.19578332	-2.64067593	-1.37522746
C	0.18990363	-2.67134877	-2.53999357
C	2.5990464	-4.20641617	0.26644938
N	-0.45914229	-3.61448151	1.60124019
H	-2.02567869	-2.99758294	3.6725233
H	4.81766418	-2.02589826	-2.03084126
H	1.95406066	-4.82234176	0.8946823
C	0.93077935	-0.66894369	2.9413749
N	0.35087996	-2.73177098	1.92423794
H	6.33180764	-3.7150316	2.02159788
H	1.55355372	1.21322852	3.75165973
C	3.0163319	-3.16828903	-1.87449857
H	5.45861712	-2.26832576	2.58137017
C	2.19503098	-3.94521212	-1.04264238
H	-0.18825747	-3.10786188	-4.60723886

N	0.16509986	-4.05036944	-2.20552698
H	2.73044112	-2.98148893	-2.91041105
N	1.00999502	-4.5912319	-1.47792491
H	1.72096745	-1.24449962	3.428388

E(el) / Hartree :	-2752.90955		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.97379		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.80926		
Thermal corrections / Hartree			
ZPVE:	1.02893	E(therm.):	1.086331
H(corr.):	1.087275	G(corr.):	0.937866
Imaginary frequencies:	0		

TS (*E,E,E,Z*) → (*E,E,E,E*)

H	-7.97896657	4.29401859	3.04036124
H	-6.73010365	5.55610336	3.12376686
H	-8.87415441	5.06317761	0.80377562
H	-7.84431582	6.48459281	1.0767117
C	-6.95379791	4.55251272	2.73336797
C	-7.87581845	5.48468815	0.61698043
H	-6.25755771	3.84425736	3.20636189
H	-7.89233266	2.23437496	2.36986738
C	-6.80933335	4.54704974	1.20378873
H	-7.75703142	5.59855911	-0.47071231
H	-6.57330266	-6.75591352	1.24516466
C	-7.60606717	2.09890799	1.32523546
H	-5.89659044	7.0982604	0.52764654
H	-5.06871428	-7.59236752	1.68278373
C	-7.03016381	3.15484798	0.6128604
C	-5.4809703	-6.6444775	1.30567701
C	-5.38959587	5.02607968	0.89146041
C	-5.09507585	6.36124258	0.59240794
H	-5.26319282	-5.85348492	2.03803622
C	-7.81793673	0.8452496	0.76517156
H	-8.25607242	0.03987153	1.35655268
H	-6.2075889	-7.82826429	-0.99800454
C	-4.31835986	4.11899364	0.9718551
C	-6.68981602	2.89800075	-0.72505414
C	-3.78359204	6.77814826	0.37837126
H	-4.55048055	-8.36370789	-0.64676609
C	-5.15246525	-7.51494032	-1.0018144
H	-4.52804835	3.073992	1.21280513
H	-3.54911378	7.82055543	0.15219187
C	-4.92037	-6.30492435	-0.08434926
H	-3.04866169	-6.87975136	1.90517157
H	-6.22756794	3.69099954	-1.32003987
C	-7.48418679	0.60691811	-0.59263001

C	-5.66211252	-5.05762003	-0.56539881
C	-3.01422514	4.51545263	0.73001773
C	-6.68172918	-5.11399602	-1.5201527
C	-6.91227238	1.67604189	-1.33441858
H	-6.92922129	-6.05809665	-2.00604693
C	-2.73644027	5.85578486	0.42018947
C	-5.37137952	-3.81319653	0.02553325
C	-7.40758042	-3.97414872	-1.85661398
C	-2.60135669	-6.43532887	1.0150213
H	-4.85254856	-7.30274377	-2.03838948
H	-4.56397703	-3.74918999	0.75976544
C	-6.08429485	-2.67200214	-0.30537532
C	-7.11794772	-2.75672973	-1.24699262
H	-8.21707306	-4.00403302	-2.58921358
C	-3.41367379	-6.04585903	-0.05991927
N	-7.71595335	-0.56883243	-1.15308194
N	-7.95744418	-1.66180592	-1.62985335
H	-2.18404895	3.80907478	0.77618045
N	-1.43882718	6.33549594	0.16929777
H	-5.85974639	-1.71098087	0.16416091
H	-6.64616758	1.51594546	-2.38002413
C	-1.2228786	-6.27197984	0.97547691
H	-0.5878362	-6.57683568	1.80847933
C	-2.79558286	-5.46679093	-1.1772214
H	0.58019644	7.72776033	0.73246239
N	-0.62545743	5.45724981	-0.17707736
H	-3.4084574	-5.14057962	-2.0215676
C	-0.61743882	-5.70325618	-0.15207578
C	1.24206062	7.05131952	0.18877431
C	-1.41886974	-5.29245596	-1.22383082
C	0.70492665	5.87313526	-0.34259995
N	0.76648344	-5.49599172	-0.28996522
C	2.60131782	7.31842022	0.05178138
H	3.00485807	8.22611635	0.50368644
H	-0.93021651	-4.83942583	-2.08886271
C	1.54078087	4.9907513	-1.03718163
H	2.79636525	-4.59365117	-1.32186835
N	1.47026779	-5.95560351	0.6306776
H	1.10422733	4.07253899	-1.43522425
C	3.45061395	6.4340917	-0.62624779
H	4.73385765	5.29836028	1.56434897
H	5.25229395	7.52730768	1.23400442
C	2.88703475	5.2784682	-1.18905413
C	3.44119744	-5.00004838	-0.54162849
H	5.07065333	8.7258801	-0.07160874
C	2.85105406	-5.72668086	0.50613642
C	5.49004934	7.74067967	0.18212327

H	5.52097542	2.99829059	2.11175116
C	5.35055941	4.75015244	0.84803439
C	4.96295907	6.65298173	-0.76126364
C	5.77587134	3.46876328	1.15998181
C	4.80883594	-4.7981559	-0.55015747
H	5.2556623	-4.20262935	-1.3506711
H	3.53005579	4.56765221	-1.71344974
C	5.6246141	5.31937667	-0.40434018
H	6.5840099	7.80922714	0.09152014
C	3.66210401	-6.24921053	1.5151678
H	4.72521815	8.02848552	-2.4164436
C	5.25230907	7.08712272	-2.20355348
H	7.47995802	-4.97253123	2.57463311
H	3.18430723	-6.81052007	2.32086733
C	6.49117297	2.7145075	0.22122454
C	5.63773898	-5.30807769	0.46767417
N	6.7130599	1.37034281	0.55902903
H	4.90561684	6.34153852	-2.93339161
C	5.04085937	-6.04375625	1.49410401
C	6.40880341	4.58497162	-1.3047978
H	6.18009788	-0.64536601	1.79241928
C	7.88146998	-5.45595789	1.67262703
H	6.12166364	-3.12254057	2.02923883
C	6.69208656	-1.29217806	1.07899433
C	6.67215894	-2.66846244	1.20102389
H	7.82471863	-6.54658254	1.80994154
C	6.83692942	3.29681498	-1.00448426
H	6.32871381	7.2572343	-2.3613929
C	7.14025963	-5.01693938	0.40399828
N	7.28695391	0.67758775	-0.30395879
C	7.33793754	-0.69833132	-0.01860191
C	7.29253196	-3.50192494	0.25168278
H	6.65655653	5.00425634	-2.28104946
H	8.94328469	-5.18151721	1.59155308
H	5.64723827	-6.45595881	2.3015821
C	7.97279087	-2.89833587	-0.80849968
C	7.99113651	-1.51082647	-0.94658342
H	7.40041935	2.70095132	-1.72420366
H	8.47292117	-3.50865736	-1.56149275
H	8.48526572	-1.03183761	-1.79454053
C	7.72692408	-5.79116309	-0.78293212
H	7.55529115	-6.86811556	-0.64120929
H	7.26002267	-5.50230183	-1.73536504
H	8.81269814	-5.62938724	-0.86512083

E(el) / Hartree :	-2752.91198
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.97572
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.80953

Thermal corrections / Hartree

ZPVE:	1.026636	E(therm.):	1.084814
H(corr.):	1.085758	G(corr.):	0.930503
Imaginary frequencies:	1		

TS (*E,E,Z,Z*) → (*E,E,E,Z*)

H	3.30935706	-3.48759953	4.02320361
H	5.03701111	-3.11759949	3.84134794
C	4.08032102	-3.18244293	3.30099226
H	4.03617638	-5.86129271	3.59168914
H	3.81721419	-2.17986172	2.93316023
H	5.68323666	-5.4197096	3.09099386
C	4.64910202	-5.53851676	2.73646128
C	4.14821818	-4.20682216	2.15807497
H	6.18487302	-2.2946097	2.21640517
H	2.26051486	-6.25633722	2.40505309
C	1.89966199	-5.41181619	1.81633269
C	2.74157018	-4.3178426	1.56893783
H	4.64375151	-6.33774247	1.98098336
C	6.12162747	-2.82361755	1.26458035
H	4.04543261	2.04423549	2.53966212
C	0.59817653	-5.44768239	1.33065929
C	2.23968865	-3.26083561	0.7961932
C	5.13205181	-3.79190734	1.06347338
H	6.12154146	1.99645369	1.13499157
H	-0.06281976	-6.29241665	1.53061518
H	2.88270894	-2.40471769	0.57604162
H	7.90349571	3.76228619	0.62413894
C	0.94418723	-3.28956768	0.30076249
C	0.10629891	-4.37808924	0.57292389
C	4.12668098	2.63365167	1.62366089
H	-3.95151953	-6.64640555	1.19970242
C	7.04550783	-2.51071545	0.27169567
H	7.80973998	-1.75508327	0.45890983
C	5.27277438	2.61872752	0.84053402
H	7.24919348	5.21671951	-0.16095525
C	7.6671622	4.21707923	-0.34893692
N	-1.2004294	-4.28964198	0.06597075
H	0.5423876	-2.46894364	-0.29705092
C	5.11036871	-4.45922687	-0.1705556
C	-4.26903273	-5.89074174	0.47800276
H	8.60450026	4.34796459	-0.91018413
N	1.88292298	3.33999522	2.09135012
H	-6.35469753	-6.38098512	0.6093413
H	-0.04837237	6.20996527	2.9681377
N	-1.98489786	-5.19326264	0.41657424

C	3.03258947	3.41108983	1.23941389
N	0.92496313	4.02922341	1.7936121
C	-5.61373855	-5.7321291	0.14021489
H	4.34841333	-5.22097894	-0.35428147
C	7.00731955	-3.18258214	-0.9548115
C	5.35271427	3.37473853	-0.33852468
H	-8.31273006	-5.08414082	0.8488276
C	-3.29824378	-5.04766634	-0.06514228
C	6.65451512	3.37472539	-1.14001059
C	6.04730901	-4.18236837	-1.15472059
H	-7.15053782	-3.24055427	1.33833997
C	-0.61630931	5.8406131	2.11335343
C	7.1318917	1.93693891	-1.35119895
C	8.46968621	1.55929796	-1.20039354
H	9.21150773	2.28368234	-0.86177169
H	-8.36821962	-6.30913196	-0.4426287
C	-8.4622601	-5.23341376	-0.22959992
C	-0.15764816	4.69257112	1.42082797
C	6.22502741	0.96487173	-1.80179872
C	8.89296163	0.26885692	-1.50611167
C	3.09101705	4.17198212	0.07045221
H	-6.97472461	-0.81558	1.86870038
N	7.99356357	-3.04214295	-1.96384639
H	5.17373209	1.23416136	-1.93491027
H	9.9458279	-0.00998166	-1.42638701
C	4.24238787	4.14815081	-0.70718562
C	7.97124133	-0.6965798	-1.91428155
C	6.62542891	-0.33625126	-2.07069943
C	-7.35683033	-2.50051199	0.56159946
C	-6.012525	-4.73790446	-0.75592289
H	-2.09929414	7.35521816	2.27900445
C	-1.7847465	6.47767846	1.71028938
C	6.4871313	4.00688379	-2.52968476
C	-3.68055741	-4.08113013	-1.01010675
H	-9.4923555	-4.93112021	-0.46842887
C	-7.24813225	-1.15339505	0.86707384
H	6.23160552	5.07529352	-2.46086151
N	8.47712155	-1.9586825	-2.31479296
H	6.05590761	-4.73185128	-2.0984013
H	5.90101344	-1.07673182	-2.41531116
C	-7.47915751	-4.41696897	-1.07386605
H	7.43253537	3.9242333	-3.08481934
C	-5.01288761	-3.93956753	-1.34475253
H	2.22642277	4.77138525	-0.22532814
C	-0.91428075	4.24246053	0.30331995
C	-7.62780981	-2.92676737	-0.74668207
H	-4.62597027	4.80419598	2.01684994

H	-5.98990572	2.74975828	1.68865667
H	-2.91172082	-3.43510294	-1.43530215
H	4.26947763	4.74262393	-1.62101128
H	-4.58972148	7.11700146	2.23746087
H	5.70945778	3.4973673	-3.11726564
H	-0.57695791	3.36499803	-0.25059475
C	-2.56539248	6.01461297	0.64688274
C	-7.3979581	-0.18798018	-0.13614528
C	-5.11186901	4.62217206	1.05486799
H	-7.60306955	-5.80575295	-2.72973103
C	-5.86226842	3.47522738	0.88439637
C	-7.74678157	-4.73030302	-2.55020435
C	-2.08890202	4.88546716	-0.03862762
N	-7.03110141	1.11868184	0.22262463
C	-4.44755263	7.61513375	1.26766538
H	-5.30288771	-3.15218605	-2.04493222
H	-3.78031086	8.47710899	1.41977503
C	-7.87836091	-1.94822073	-1.7192258
H	-8.78076636	-4.47361696	-2.82795783
C	-3.88485531	6.65970224	0.20761335
C	-7.76050132	-0.59402475	-1.42660307
N	-7.00127628	1.95000851	-0.70650137
C	-4.88270144	5.51961351	-0.00602771
C	-6.41386668	3.18318576	-0.3756623
H	-7.0643293	-4.18990786	-3.22099439
H	-5.42367483	8.00204377	0.9397341
H	-2.66862179	4.48230912	-0.87369381
H	-8.11938456	-2.24361757	-2.74166071
C	-3.6342743	7.46254365	-1.074753
H	-2.8886212	8.24579758	-0.87500578
H	-7.88651134	0.16819877	-2.19720627
C	-6.26225944	4.10287437	-1.41434916
C	-5.50734864	5.26095209	-1.22844101
H	-3.23843035	6.82735872	-1.88062434
H	-4.55333425	7.95175625	-1.43488791
H	-6.70246673	3.86260805	-2.38458164
H	-5.37011912	5.93974872	-2.07100261

E(el) / Hartree :	-2752.88796		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.95311		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.78655		
Thermal corrections / Hartree			
ZPVE:	1.026224	E(therm.):	1.08433
H(corr.):	1.085274	G(corr.):	0.929991
Imaginary frequencies:	1		

TS (*E,Z,E,Z*) → (*E,E,E,Z*)

H	-5.23734731	6.83604879	2.33377542
H	-6.82107198	6.04414304	2.49824215
C	-5.78190992	5.89518328	2.16662748
H	-5.32092313	5.12299556	2.79986872
H	-6.07245768	7.61167659	0.10696103
H	6.68579712	2.5988745	3.28963616
C	-6.45744143	6.60489261	-0.11808783
H	-7.52512476	6.5882536	0.14434065
C	-5.72199784	5.51778503	0.67877051
C	-3.56830301	6.4484746	-0.37346863
H	-5.97341372	-6.63493852	2.41037346
C	-4.24132674	5.42656065	0.30327805
H	-4.1077259	7.33710045	-0.70316843
C	6.94151609	2.42967315	2.24155475
N	8.25342737	0.55333436	2.98532821
C	-2.20289999	6.35747972	-0.63195087
H	-7.35463769	3.92372695	2.32324435
C	-3.49782264	4.3002564	0.70403739
N	8.24077136	-0.68554035	2.96280869
H	-1.66850407	7.15507626	-1.15244072
H	-6.01614639	-4.87421186	2.70219471
C	-6.41067836	-5.68369319	2.07111026
H	5.74048588	4.04502	1.49940211
C	-1.47980024	5.23097258	-0.23443796
H	-7.49699581	-5.73587824	2.23388994
C	-2.14311631	4.19367125	0.44213468
H	-3.90896746	-5.86773057	2.24553945
H	-4.01262739	3.48819973	1.22396959
N	-0.10733562	5.23387461	-0.52955348
C	6.42972275	3.23826712	1.23703923
C	7.7667877	1.34819434	1.91544269
H	-6.37692342	6.43674601	-1.20220316
H	5.73615414	-0.33107171	1.88778892
H	-1.56609831	3.32076564	0.75104242
C	-7.20293014	3.50675336	1.32587144
C	-6.40109956	4.17807621	0.39880214
H	-1.51004973	-5.56512066	1.68003146
C	-3.63485931	-5.54166147	1.2412444
H	6.70809716	5.78640253	-0.0892665
C	7.59846282	-1.43682693	1.94282603
C	6.29672625	-1.17826687	1.48959269
H	2.08224437	6.31426215	-0.77314998
C	2.61221847	5.36061897	-0.77510116
C	-2.28845985	-5.37767855	0.93895821
H	4.54092731	6.22326903	-1.10448561

N	0.48968444	4.15799457	-0.32854614
C	3.98782358	5.29404093	-0.960308
H	-6.0523698	-7.54242877	0.06710068
C	-6.1244237	-5.44037373	0.58255247
C	1.87539732	4.18846953	-0.56688699
H	-7.69255716	-6.86175975	0.01581088
C	6.76455937	3.03091791	-0.1095231
C	-7.82523064	2.29723939	1.04243683
C	8.15423787	1.15888707	0.58620291
C	-6.63565097	-6.65200554	-0.20853223
C	6.88906352	5.31028785	-1.06395762
H	-8.43603988	1.79684796	1.79499888
H	2.32063797	-5.40450312	1.62050486
C	-4.63116416	-5.28293966	0.28973001
C	-6.26006352	3.5758923	-0.86095476
C	8.27258164	-2.56252268	1.46805519
C	4.66612888	4.06761197	-0.9516627
C	5.72450176	-2.00126689	0.53160075
C	2.54089187	2.95666082	-0.55489009
H	7.97390682	5.16397397	-1.16921327
H	9.26212073	-2.78790861	1.87124117
C	-6.83036622	-4.14163205	0.18867704
C	6.17592424	3.95543487	-1.17622401
C	7.65948806	1.99835251	-0.40749696
H	4.7069295	-1.79209476	0.19186974
C	3.91315111	2.90040605	-0.75402658
H	-5.63321264	4.05865396	-1.61661949
N	0.29133694	-4.94734141	0.12609246
C	2.61650586	-4.9717619	0.66262134
H	8.83120196	0.34313772	0.32679093
H	6.5656532	6.00304799	-1.85568469
H	-8.4497113	-5.04148892	-0.92878045
C	-8.00585818	-4.11356552	-0.56659264
H	4.71794859	-4.93046268	1.10703493
C	-1.90575696	-4.94682221	-0.33720095
H	1.95145875	2.05387621	-0.38123083
C	-6.29345813	-2.91884495	0.63407703
H	-5.36874631	-2.92443925	1.21671153
C	3.94648383	-4.71019535	0.36478404
C	1.61298453	-4.6728542	-0.26693069
C	-7.67019732	1.70220308	-0.23475826
H	-6.53185345	-6.50660073	-1.29351697
C	7.6979516	-3.36444482	0.48496549
C	-6.87023974	2.38010909	-1.19489697
H	4.4216565	1.93295018	-0.72930674
C	6.41914979	-3.09421825	-0.01101551
N	-0.57850263	-4.71174067	-0.73464649

C	-4.23204047	-4.8657539	-0.98829929
C	-8.62771279	-2.9040237	-0.87250479
C	-6.89757049	-1.71212869	0.32883412
C	-2.89097909	-4.6986805	-1.30042952
H	7.97032959	1.82110612	-1.43793407
C	-8.0717691	-1.70605449	-0.43419435
H	-9.54611214	-2.86402675	-1.46233347
C	6.38954055	3.4162026	-2.59794942
C	4.31521725	-4.14109279	-0.86297423
C	1.9668403	-4.10861218	-1.49864772
H	-6.47128807	-0.76572747	0.67012808
H	8.26364312	-4.21939093	0.11214265
N	-8.23841953	0.54431235	-0.52437348
H	-4.99102841	-4.64379033	-1.74288573
C	5.7944075	-3.89267295	-1.15659376
H	6.4337792	-5.86292235	-0.42858951
H	-6.73567306	1.9400234	-2.18375209
H	7.45825228	3.38199794	-2.85944931
C	3.30052674	-3.84888921	-1.78528635
H	5.88913372	4.07672835	-3.32084449
N	-8.76778369	-0.51136191	-0.81106984
H	5.96818104	2.40733571	-2.71748066
H	1.17414392	-3.87467377	-2.21056721
C	6.46203962	-5.2625412	-1.34944986
H	-2.57196641	-4.3600313	-2.28820287
H	5.49734959	-2.0978372	-2.38343539
C	6.00657727	-3.0713331	-2.43717616
H	3.54955951	-3.40140138	-2.7482463
H	7.51117509	-5.15822808	-1.66466056
H	5.93312645	-5.82300692	-2.13398676
H	7.08054148	-2.87922327	-2.57481036
H	5.64417636	-3.60913673	-3.32665545

E(el) / Hartree :	-2752.89719		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.96181		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.79548		
Thermal corrections / Hartree			
ZPVE:	1.026466	E(therm.):	1.084583
H(corr.):	1.085528	G(corr.):	0.930067
Imaginary frequencies:	1		

TS (*E,Z,Z,Z*) → (*E,E,Z,Z*)

H	8.45131328	-3.6591516	2.1526977
H	6.97447731	-0.73724914	1.53866994
H	5.37309327	0.57957379	2.89348858
H	6.65343022	-5.35040657	1.60402012
C	8.29331136	-3.20630424	1.16303704

C	6.1252217	-1.24266889	2.00429
C	5.22416191	-0.49176527	2.74452552
H	3.33469774	3.92109244	2.81321762
H	8.94388497	-3.73001346	0.44657187
H	-7.87770756	-2.35722179	0.72644888
C	6.48899529	-4.82894631	0.64825231
H	8.62267952	-2.15916353	1.21752966
H	7.1401414	-5.29012538	-0.10841847
H	1.51957862	1.94214881	2.30810856
H	2.92801934	0.19252399	1.01520899
H	-4.26647596	-1.06591812	-0.99035047
C	3.71052068	3.27637459	2.00562479
N	-5.59432968	-3.34879519	-1.73754757
N	-6.30144477	-2.41590039	-1.40694899
H	3.55407471	2.23341551	2.31221673
H	-0.92492404	1.77163445	2.51000512
C	6.81982588	-3.33686781	0.76717106
H	4.79396375	3.44438934	1.92859425
C	5.93367131	-2.61576105	1.78719654
C	-3.61572363	-1.91303285	-1.22098117
C	-7.87458367	-1.45327086	0.1163203
C	0.9019177	2.6329584	1.73688396
H	2.06147392	-0.68773586	-1.07505659
C	2.10397926	-0.5212579	1.04423517
C	4.06052567	-1.09564694	3.22816361
C	-0.47675816	2.53319701	1.86866843
C	-4.18120833	-3.1384268	-1.59986843
N	3.08965948	-0.29086219	3.88209995
H	5.44969274	-4.99909203	0.33350664
C	-7.11828701	-1.43066509	-1.08252941
C	1.61037076	-1.03808939	-0.14713859
H	-1.80031157	-0.83170635	-0.85915795
C	-2.23841	-1.7884109	-1.15608705
N	1.91657281	-0.27203259	3.48077581
H	3.16584086	5.78253476	0.99443338
H	-9.03765848	-0.34402221	1.50928409
C	-8.52772625	-0.30322502	0.54435211
C	4.83871023	-3.22538347	2.40496218
C	2.99943495	3.62252056	0.6882957
C	1.5270821	-0.89640632	2.26050243
H	0.00617108	-0.7866581	-2.61610852
C	1.48400951	3.59024277	0.89675097
C	3.89715029	-2.47570156	3.10439809
C	3.47402487	5.02310629	0.25914888
C	6.5007239	-2.65242078	-0.56845125
H	4.57119646	5.03621668	0.1839421
C	-3.36106599	-4.2234398	-1.8918754

H	8.53226156	-2.25259015	-1.19407898
C	-1.32108618	3.40235741	1.17155784
C	-1.39006297	-2.87113818	-1.45656201
C	7.47289938	-2.12979765	-1.4250307
N	-2.69741479	3.17814164	1.32498304
H	-3.82976474	-5.16591942	-2.18342781
C	0.43928573	-1.79409553	-2.69761747
C	0.56995084	-1.97252454	-0.16294341
C	-7.19870862	-0.26895982	-1.89943235
C	-1.97559183	-4.08951671	-1.8137143
H	4.36713896	-2.89881231	-0.29020169
C	5.15353223	-2.49609067	-0.93332767
H	-9.11002932	1.61055063	2.50132973
H	4.6734804	-4.29830437	2.29940463
C	3.39963128	2.65905919	-0.44131311
H	3.01563755	-2.95822155	3.52983246
H	1.48031275	2.67257696	-1.43329344
C	0.12201199	-2.65040575	-1.4591695
C	-8.5218198	0.88386226	-0.19480536
C	0.62288915	4.47469745	0.22312537
C	0.44072042	-1.77464996	2.26138031
H	0.02393549	-2.27297851	-3.59600324
C	2.51601013	2.33172035	-1.47970413
H	3.08155559	5.30824967	-0.72650086
C	-0.7565548	4.38934511	0.35186048
H	-6.66912537	-0.24740966	-2.85314992
C	-5.31865725	2.60726663	1.62479564
H	1.52343704	-1.69012737	-2.85200983
H	-4.62428033	2.07811344	2.2782638
C	-9.68193738	2.119518	1.71395768
C	4.71484079	2.18133251	-0.5430005
C	-6.64816783	2.25005207	1.53990753
C	-7.88657853	0.8388439	-1.44742395
C	-0.00102532	-2.33205807	1.06656466
N	-3.45428182	3.95447527	0.70736033
H	5.44237697	2.41601788	0.23590112
C	-4.81865177	3.63573827	0.80730191
H	-7.00268314	1.40316598	2.13107321
H	-1.35107194	-4.9521879	-2.0471271
C	7.11802391	-1.4263979	-2.57725162
C	-7.53241371	2.88617699	0.64592342
H	-10.6177376	1.56101606	1.5583691
C	-8.9063448	2.24455164	0.39933623
C	-5.70103375	4.34003265	-0.01340902
C	4.78854035	-1.77014342	-2.05202885
C	-7.04364269	3.96773302	-0.09231254
H	1.03588607	5.24370452	-0.43113596

H	-0.03759379	-2.03071989	3.20924357
C	2.94022753	1.61173454	-2.59220881
H	7.88137247	-1.01182396	-3.23914233
H	-9.93791476	3.12062382	2.0912115
H	-5.30173987	5.15274585	-0.62423514
C	5.77388095	-1.18617867	-2.85650154
C	5.13909373	1.42441083	-1.62848867
H	-1.42338403	5.06715785	-0.18331239
C	0.90578975	-3.96674933	-1.56873997
H	-7.69968979	4.50676174	-0.77737238
H	2.25795436	1.41447842	-3.4223335
C	4.25246239	1.13559442	-2.67535605
H	3.73638123	-1.62684144	-2.3004461
H	-0.82873991	-3.04532694	1.08714093
H	-7.85889498	1.73484341	-2.07237622
H	0.70909008	-4.47871845	-2.52305003
H	0.66099893	-4.65189641	-0.74362827
H	6.17347569	1.08270488	-1.6768067
H	1.98439647	-3.75679978	-1.52111454
C	-9.77269352	3.04941544	-0.57130627
N	5.4163797	-0.4225356	-3.9945484
H	-10.7348267	2.53661812	-0.71555678
N	4.65735415	0.55332469	-3.90906019
H	-9.31126286	3.16522364	-1.56131096
H	-9.9773023	4.05600711	-0.17491122

E(el) / Hartree :	-2752.87713		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.94052		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.77414		
Thermal corrections / Hartree			
ZPVE:	1.026287	E(therm.):	1.08413
H(corr.):	1.085074	G(corr.):	0.932851
Imaginary frequencies:	1		

TS (*E,Z,Z,Z*) → (*E,Z,E,Z*)

H	-8.79653462	-2.68699509	-2.81157241
H	-6.24598363	-0.67907157	-1.57090544
H	-3.90216313	-0.84646711	-2.27415921
H	-8.68618051	-4.62570484	-1.33702494
C	-8.79762548	-2.00401114	-1.94971316
C	-5.78592499	-1.67025477	-1.62289345
C	-4.45950642	-1.74563757	-2.00696239
H	-4.05703533	2.4931652	-3.18251979
H	-9.84326411	-1.82897232	-1.65122602
H	9.80378994	-0.88908292	-1.98101854
C	-8.65557657	-3.96472236	-0.45756461
H	-8.3730613	-1.04963042	-2.29105246

H	-9.69009901	-3.78829932	-0.12811803
H	-2.14150233	1.51333465	-2.58662617
H	-1.6411441	-1.3969841	-0.75515403
H	6.46106361	-1.60691547	-1.53138833
C	-4.50660415	2.29648859	-2.19730438
N	7.94496642	-3.54109078	-0.28521003
N	8.8982888	-2.7612816	-0.4308959
H	-4.40912076	1.22496736	-1.97561408
H	0.31059118	1.24602511	-2.27604175
C	-7.98975986	-2.62887263	-0.80532937
H	-5.58056763	2.52273441	-2.26441747
C	-6.53530677	-2.7998095	-1.25614456
C	5.96331686	-2.09853028	-0.69382576
C	9.30889013	-0.48546702	-1.09520368
C	-1.64573892	2.04366685	-1.77238243
H	0.12523486	-0.74829602	0.84319042
C	-0.66028869	-1.87688908	-0.79158393
C	-3.80463851	-3.00568098	-2.06497294
C	-0.26965026	1.8877814	-1.6099123
C	6.63330153	-3.09398555	0.0321648
N	-2.53718026	-3.10329925	-2.42511082
H	-8.13820733	-4.50073677	0.34993798
C	8.78011419	-1.37282325	-0.15942899
C	0.33708408	-1.52307832	0.10406324
H	4.17412106	-0.94642131	-0.90688807
C	4.67806545	-1.72606855	-0.33101625
N	-1.36998717	-3.27407687	-2.72540738
H	-3.43984848	4.80887575	-2.44857621
H	9.52194641	1.55949132	-1.69887182
C	9.14757574	0.88908682	-0.92419025
C	-5.87483407	-4.0314132	-1.30274585
C	-3.86851068	3.16343009	-1.10427075
C	-0.39901228	-2.84529475	-1.76677949
H	2.90422647	0.24933805	0.47703118
C	-2.37727701	2.87789921	-0.92278478
C	-4.55309667	-4.15721634	-1.71079568
C	-4.01072145	4.63270277	-1.52533818
C	-7.95627217	-1.73482594	0.4379655
H	-5.06256474	4.88717808	-1.72588943
C	5.96314832	-3.74975734	1.06325074
H	-8.93367878	-0.01513192	-0.43754895
C	0.40539258	2.57681911	-0.60037426
C	4.01921949	-2.31590753	0.76098663
C	-8.43342803	-0.42092178	0.4425818
N	1.80225494	2.43214731	-0.56977423
H	6.47146695	-4.56026323	1.58987519
C	2.71771767	-0.30467456	1.40602854

C	1.59790658	-2.1454324	0.07868324
C	8.21407607	-0.8703084	1.02081498
C	4.6834927	-3.34380061	1.43669004
H	-6.97179131	-3.23354054	1.64530771
C	-7.36136539	-2.21349925	1.61595483
H	8.24277639	3.42215638	-1.7624317
H	-6.40245746	-4.94635179	-1.02660583
C	-4.59131925	2.85618586	0.20734486
H	-4.07257145	-5.13550281	-1.7496624
H	-3.71468042	0.88427767	0.34452353
C	2.63062994	-1.82241787	1.16375531
C	8.4977367	1.40336069	0.2005328
C	-1.69095845	3.52227741	0.12417166
C	0.85954809	-3.43687548	-1.84381667
H	3.53493767	-0.08242402	2.1078711
C	-4.41219886	1.59497563	0.79561491
H	-3.62738537	5.3210888	-0.75868875
C	-0.32428558	3.38756836	0.28564666
H	7.84676075	-1.55509632	1.78626088
C	4.5243148	2.36436394	-0.73804775
H	1.78791615	0.0892149	1.84108542
H	3.97804685	1.89426181	-1.55730652
C	8.65436715	3.74333682	-0.79520007
C	-5.45388795	3.75512056	0.84017634
C	5.90461282	2.33444033	-0.67580737
C	8.07892917	0.49678241	1.18737793
C	1.83755784	-3.10799924	-0.91002304
N	2.39486925	3.11827936	0.28700859
H	-5.60310164	4.75547161	0.43152174
C	3.79551699	3.02060653	0.26820593
H	6.46220568	1.80571931	-1.45304999
H	4.20233806	-3.85349707	2.27154905
C	-8.24842638	0.41328159	1.54199467
C	6.61164265	2.95237377	0.37354099
H	9.75318324	3.71194119	-0.85674485
C	8.14314733	2.88196047	0.36658873
C	4.48281628	3.64467426	1.3107435
C	-7.22429173	-1.41280468	2.7405012
C	5.87566038	3.60620149	1.36440715
H	-2.25451425	4.14692985	0.82236587
H	1.04340679	-4.17476421	-2.62775275
C	-5.11035215	1.219397	1.93098124
H	-8.5849924	1.45112714	1.50843486
H	8.35169709	4.78893922	-0.63929247
H	3.89986312	4.15791312	2.07831785
C	-7.60994335	-0.07067014	2.68387013
C	-6.13548053	3.40212901	2.00445562

H	0.21341336	3.90721559	1.07981647
C	2.1421609	-2.49157822	2.45733363
H	6.38434695	4.09793929	2.19456961
H	-4.96754972	0.22529631	2.35544255
C	-6.00795176	2.11659225	2.52725406
H	-6.76173824	-1.79605084	3.65275696
H	2.80793747	-3.60467555	-0.95563408
H	7.58247088	0.87015262	2.08617577
H	2.83463982	-2.29252797	3.28967592
H	2.03334689	-3.57951841	2.33980006
H	-6.79718837	4.11272174	2.50439336
H	1.15674461	-2.09106919	2.73454861
C	8.76738463	3.41636753	1.66008696
N	-7.387648	0.75948221	3.81666632
H	9.85947109	3.29383998	1.61953517
N	-6.71553535	1.79688661	3.72019472
H	8.40449878	2.88551596	2.55136989
H	8.55387396	4.48799666	1.79017583

E(el) / Hartree :	-2752.88195		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.947		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.78007		
Thermal corrections / Hartree			
ZPVE:	1.026405	E(therm.):	1.084265
H(corr.):	1.085209	G(corr.):	0.931728
Imaginary frequencies:	1		

TS (*Z,Z,Z,Z*) → (*E,Z,Z,Z*)

H	-8.34535587	-1.43647863	-2.93353699
H	-5.49464251	0.1025883	-1.27578415
H	-3.43554886	0.75242561	-2.45363691
H	-7.70955368	-3.78089719	-2.73220601
C	-8.09668113	-1.25880947	-1.87717834
C	-5.07820353	-0.57107401	-2.02856531
C	-3.91097436	-0.20426123	-2.67390024
H	-3.27200291	4.57245295	-1.9795882
H	-8.99752078	-1.45542906	-1.2752549
H	6.54584689	-4.61733971	-1.22405696
C	-7.39100417	-3.62621914	-1.69036632
H	-7.83716203	-0.19561761	-1.77724041
H	-8.24773619	-3.8544357	-1.03968576
H	-1.12811621	4.2160874	-2.14590922
H	0.01805425	1.58760341	-2.43105742
H	3.81941762	-3.35939573	-0.43331524
C	-3.4741353	3.76454076	-1.26106916
N	4.48728095	-4.94152182	1.71880469
N	5.6141869	-4.86323475	1.20745506

H	-3.11362011	2.82501203	-1.7029956
H	1.31040043	4.3474816	-2.2164773
C	-6.94319372	-2.17971504	-1.46094981
H	-4.56499464	3.68963283	-1.14117453
C	-5.7005203	-1.80554985	-2.27874517
C	3.27377883	-3.15015314	0.48683344
C	6.57486168	-3.67833634	-0.66724246
C	-0.58637743	4.1707042	-1.19902204
H	0.74547219	1.53563131	-0.08483066
C	-0.20459186	0.71587487	-1.81336282
C	-3.33169644	-1.06907905	-3.61139723
C	0.8004022	4.24344388	-1.2577953
C	3.54276338	-3.88217782	1.65130199
N	-2.16830777	-0.70787211	-4.33185007
H	-6.59862591	-4.35422339	-1.46734963
C	6.10284095	-3.65520545	0.64423585
C	0.22504822	0.66676258	-0.48906943
H	2.11851191	-1.59268574	-0.41453804
C	2.31110498	-2.15302637	0.50263265
N	-1.14000398	-0.29717087	-3.77689453
H	-2.91908247	6.19096068	-0.21465832
H	7.33219912	-2.53827857	-2.31199307
C	7.0162478	-2.50197645	-1.26863447
C	-5.13640577	-2.63516555	-3.25109431
C	-2.81528402	4.05153978	0.09493722
C	-0.91016748	-0.34984604	-2.37509711
H	2.30386811	0.7455375	1.41096143
C	-1.28637353	4.0361837	0.00389985
C	-3.97835125	-2.26191851	-3.93317057
C	-3.24708743	5.45742432	0.5358942
C	-6.52973578	-1.98143152	-0.00054628
H	-4.34181898	5.53256779	0.63577753
C	2.77707437	-3.64243119	2.79388679
H	-7.81628954	-0.29372743	0.41997481
C	1.56508519	4.21805967	-0.06249353
C	1.58475481	-1.84818136	1.66400477
C	-7.01064888	-0.93131768	0.78612625
N	2.87820418	4.36251744	-0.0777944
H	2.95275685	-4.25688946	3.67941492
C	1.46638256	0.56984865	2.10208067
C	0.02438995	-0.47530072	0.29214511
C	6.18822088	-2.47095669	1.38711686
C	1.82857957	-2.6235334	2.80356508
H	-5.13039149	-3.62972351	-0.04533673
C	-5.52642614	-2.79865534	0.54272053
H	6.62659628	-0.30629145	-3.1358458
H	-5.59837288	-3.59381782	-3.49168898

C	-3.26050765	2.97840897	1.09035465
H	-3.54628097	-2.90668856	-4.70141624
H	-2.57923157	1.34587271	-0.15904641
C	0.63070806	-0.6490028	1.68542178
C	7.05722668	-1.29734891	-0.56037213
C	-0.51379127	3.98022821	1.17374652
C	-1.17127553	-1.48091014	-1.58351705
H	1.89254851	0.39861806	3.1011955
C	-3.0637751	1.62370285	0.77900149
H	-2.78700816	5.74481746	1.49222428
C	0.86715986	4.07465722	1.16863054
H	5.85183931	-2.45701897	2.42547574
C	4.36197206	2.0419345	-0.70055054
H	0.84885217	1.47887757	2.13971676
H	3.28333216	1.90662713	-0.81486561
C	7.61000121	-0.05539509	-2.71200165
C	-3.82256095	3.27954689	2.33580689
C	5.23862715	0.99510717	-0.94203416
C	6.66958341	-1.3169235	0.78802142
C	-0.69780389	-1.53571579	-0.2803902
N	4.08917731	4.45907838	-0.07491636
H	-3.98728384	4.31740419	2.6269653
C	4.8734272	3.2902163	-0.32123596
H	4.84101299	0.01994681	-1.23475667
H	1.26887544	-2.43999816	3.72183642
C	-6.43752594	-0.63232527	2.01896366
C	6.63198328	1.15684067	-0.80916228
H	8.34180014	-0.7980455	-3.06356503
C	7.56837838	0.00402345	-1.17676605
C	6.24741861	3.46830741	-0.18137428
C	-4.98417626	-2.54695405	1.79424695
C	7.11699918	2.40761003	-0.41548714
H	-1.01405044	3.86042453	2.13909593
H	-1.70773915	-2.33255343	-2.00423755
C	-3.44175876	0.61286195	1.64928264
H	-6.78472449	0.22658118	2.5964496
H	7.91052239	0.92367662	-3.11246855
H	6.61081995	4.4551494	0.11312324
C	-5.3883593	-1.41296019	2.50438163
C	-4.141366	2.27558354	3.24774729
H	1.43304682	4.04661401	2.10057744
C	-0.4969342	-0.82112076	2.71140525
H	8.18849074	2.56948461	-0.29687773
H	-3.27725917	-0.42557771	1.36285293
C	-3.98316949	0.93235195	2.90516164
H	-4.19682326	-3.18130477	2.20728835
H	-0.85583206	-2.44961479	0.2983069

H	6.71342027	-0.39425931	1.37293599
H	-0.1031448	-0.89157547	3.73531338
H	-1.10183833	-1.71932223	2.51788072
H	-4.52081792	2.5211288	4.24207608
H	-1.16121856	0.05221364	2.6783618
C	8.99903376	0.22555628	-0.66388007
N	-4.76136518	-1.11645063	3.74047345
H	9.60921407	-0.65936695	-0.89472142
N	-4.20580486	-0.0257774	3.93358525
H	9.02156158	0.3721762	0.42600443
H	9.47522969	1.09334035	-1.14504069

E(el) / Hartree :	-2752.87161		
E(el) SMD-PBE0-D3(BJ)/def2-SVP / Hartree	-2752.93315		
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree	-2755.76908		
Thermal corrections / Hartree			
ZPVE:	1.026554	E(therm.):	1.084056
H(corr.):	1.085001	G(corr.):	0.933752
Imaginary frequencies:	1		

p-^{i}Propylazobenzene

(*E*)-^{i}Pr-AB

C	4.97141687	-1.30373584	-9.6561E-06
C	3.59643257	-1.11415147	-8.7986E-06
C	-2.68196624	-1.0939077	-1.2056E-05
C	-3.22392313	0.19804076	-1.1413E-06
C	-1.30654969	-1.28959404	-1.2894E-05
C	-2.33920419	1.28738474	8.9493E-06
C	-0.43596703	-0.19382582	-2.785E-06
C	-0.96399484	1.1051459	8.225E-06
C	5.83729599	-0.20493151	8.973E-07
C	3.07616772	0.18955854	2.7171E-06
C	5.32163738	1.09028666	1.2356E-05
C	3.94358521	1.28736844	1.3248E-05
N	0.93746061	-0.49257883	-4.5081E-06
N	1.70113907	0.49167351	4.5207E-06
H	5.37998094	-2.31738001	-1.8637E-05
H	2.89693228	-1.95124539	-1.6866E-05
H	-3.3454893	-1.96256781	-2.0034E-05
H	-0.87120013	-2.29108375	-2.1353E-05
H	6.91847525	-0.3629561	1.447E-07
H	-2.74866969	2.30179586	1.7552E-05
H	-0.27167292	1.9482589	1.603E-05
H	5.99639966	1.94940189	2.061E-05
H	3.50487864	2.28729477	2.2045E-05
C	-4.72069971	0.41920419	-1.029E-07
C	-5.37204751	-0.14355355	1.26327873

H	-4.91915587	0.283123	2.17056015
H	-6.45007401	0.08072442	1.27918315
H	-5.25945283	-1.23813702	1.31655215
C	-5.37204629	-0.1435327	-1.26328885
H	-6.45007273	0.08074571	-1.27919068
H	-4.91915366	0.28315871	-2.17056279
H	-5.25945175	-1.23811531	-1.31658015
H	-4.88064567	1.51097282	8.8311E-06

E(el) / Hartree : -689.427819

E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree -690.15884

Thermal corrections / Hartree

ZPVE:	0.276935	E(therm.):	0.292104
H(corr.):	0.293048	G(corr.):	0.232505

Imaginary frequencies: 0

(*Z*)-^{i}Pr-AB

H	2.26419582	-2.13255056	-2.06944821
H	1.49956045	0.2142539	-1.79412526
C	2.59724909	-1.55144381	-1.20619235
C	2.16687719	-0.23738201	-1.05803189
C	3.44349478	-2.12999063	-0.25910866
H	-0.82194992	2.79032805	-1.51949422
C	2.60083515	0.51386464	0.04229697
C	-1.00644237	1.92769464	-0.87567644
H	-2.95665779	1.50634783	-1.68012635
C	-2.19659637	1.21139518	-0.95122178
N	2.29545262	1.89272201	0.18969226
N	1.14937523	2.35121024	0.09690731
C	-0.01259845	1.53944312	0.02602036
C	3.88759716	-1.37406019	0.82614123
C	-2.4515035	0.13433544	-0.09578296
C	3.49094909	-0.04744042	0.96381314
C	-0.25831722	0.47506254	0.90435072
C	-1.46678945	-0.20506449	0.84344136
H	4.5636756	-1.81619009	1.5617797
H	0.49621245	0.18983125	1.63923522
H	3.85362293	0.57291839	1.786168
H	-1.64425676	-1.02599688	1.54328795
H	3.76968841	-3.165801	-0.3762862
C	-3.75723231	-0.62679639	-0.1704318
H	-4.34538907	-0.16875088	-0.98404659
C	-3.53145757	-2.09456241	-0.53269232
H	-2.95653303	-2.6148603	0.24995552
H	-4.4917845	-2.62169957	-0.64487537
H	-2.97407991	-2.19196429	-1.47625155
C	-4.56564991	-0.48711234	1.11928397

H	-5.53940349	-0.99307222	1.02691639
H	-4.03613294	-0.93942962	1.97297009
H	-4.74949841	0.56983688	1.36288877

E(el) / Hartree :		-689.406316	
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree		-690.138635	
Thermal corrections / Hartree			
ZPVE:		0.276589	E(therm.): 0.291669
H(corr.):		0.292613	G(corr.): 0.232629
Imaginary frequencies:		0	

$\underline{H_2}$

H	-1.11552619	-0.34260138	-3.09595984
H	-1.4449105	0.34260138	-3.12423146

E(el) / Hartree :		-1.1638278	
E(el) PBE0-D3(BJ)/def2-TZVPP / Hartree		-1.16840206	
Thermal corrections / Hartree			
ZPVE:		0.009988	E(therm.): 0.012348
H(corr.):		0.013292	G(corr.): -0.001545
Imaginary frequencies:		0	

X-Ray Crystallography

Single crystals were obtained by diffusion of *n*-pentane into a concentrated solution of compounds **1**,**2** in CH_2Cl_2 or $CHCl_3$ at −20 °C. For tetraazo-macrocycle **3**, single crystals were obtained by slow evaporation of a solution in CS_2/CH_2Cl_2, 1:1.

Diffraction data for all samples were collected at low temperatures (100K) using φ- and ω-scans on a BRUKER D8 Venture system equipped with dual IμS microfocus sources, a PHOTON100 detector and an OXFORD CRYOSYSTEMS 700 low temperature system. Mo-Kα radiation with wavelength 0.71073 Å and a collimating Quazar multilayer mirror were used. Semi-empirical absorption correction from equivalents was applied using SADABS-2016/2[14] and the structure was solved by direct methods using SHELXT2014/5.[15]
Refinement was performed against F^2 on all data by full-matrix least squares using SHELXL2016/6.[15] All non-hydrogen atoms were refined anisotropically and C-H hydrogen atoms were positioned at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2x or 1.5x (CH_3 hydrogens) the U_{eq} value of the atoms they are linked to. The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as CCDC No. 1902881 – 1902883 and can be obtained free of charge.[https://www.ccdc.cam.ac.uk/structures/]

Bisazo macrocycle 1

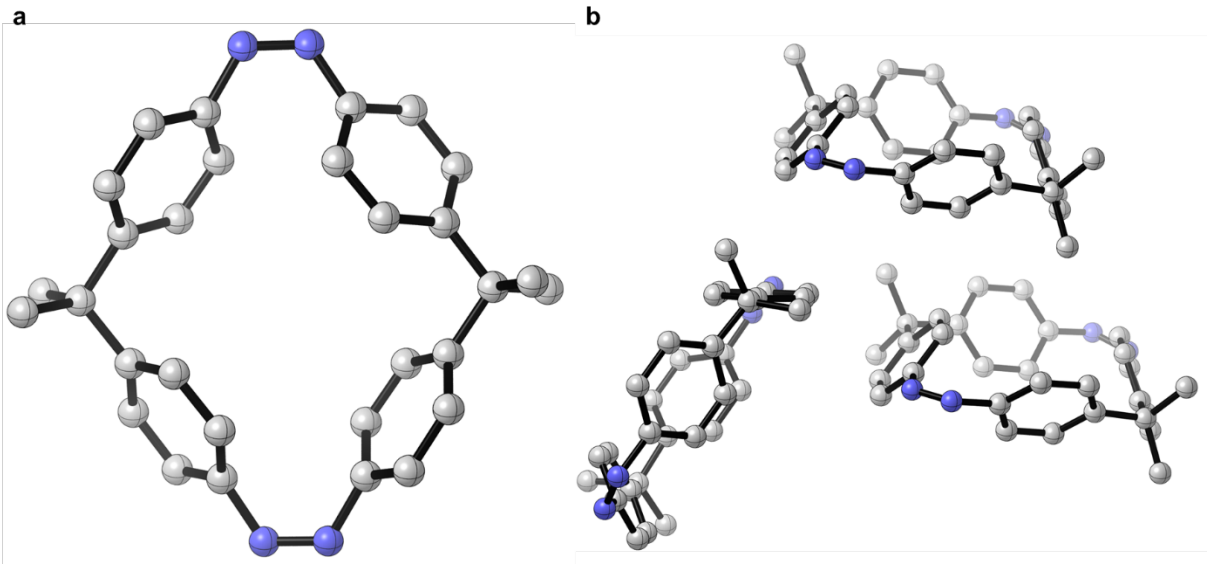

Figure S12a: Single crystal structure of bisazo macrocycle **1**. **b:** Crystal packing of bisazo macrocycle **1** (grey: carbon, blue: nitrogen; hydrogens omitted).

The unit cell was determined using 9672 reflections and the structure was solved in the monoclinic space group $P2_1$. The asymmetric unit contains one Bisazo macrocycle **1** molecule.

Crystal data and structure refinement for Bisazo macrocycle **1**.

CCDC No	1902881	
Empirical formula	$C_{30}\ H_{28}\ N_4$	
Formula weight	444.56	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.7996(6) Å	α= 90°.
	b = 6.7102(4) Å	β= 98.2079(17)°.
	c = 15.2460(8) Å	γ = 90°.
Volume	1194.78(11) $Å^3$	
Z	2	
Density (calculated)	1.236 Mg/m^3	
Absorption coefficient	0.570 mm^{-1}	
F(000)	472	
Crystal size	0.844 x 0.533 x 0.300 mm^3	
Theta range for data collection	2.928 to 74.460°.	

Index ranges	-14<=h<=14, -8<=k<=8, -19<=l<=19
Reflections collected	66300
Independent reflections	4876 [R(int) = 0.0356]
Completeness to theta = 67.679°	99.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4876 / 1 / 312
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0281, wR2 = 0.0743
R indices (all data)	R1 = 0.0284, wR2 = 0.0745
Absolute structure parameter	0.01(10)
Extinction coefficient	0.0169(11)
Largest diff. peak and hole	0.291 and -0.139 e.Å^{-3}

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

	x	y	z	U(eq)
N(1)	2077(1)	3857(2)	5509(1)	21(1)
N(2)	3030(1)	3015(2)	5536(1)	20(1)
N(3)	2886(1)	5857(2)	-533(1)	22(1)
N(4)	2051(1)	7010(2)	-519(1)	23(1)
C(1)	3588(1)	2818(2)	4758(1)	17(1)
C(2)	3045(1)	1940(3)	3978(1)	18(1)
C(3)	3647(1)	1682(2)	3274(1)	18(1)
C(4)	4791(1)	2291(2)	3316(1)	16(1)
C(5)	5318(1)	3145(2)	4104(1)	17(1)
C(6)	4731(1)	3358(2)	4829(1)	18(1)
C(7)	5416(1)	1943(3)	2512(1)	17(1)
C(8)	5523(1)	-301(3)	2391(1)	20(1)
C(9)	6623(1)	2848(3)	2638(1)	21(1)
C(10)	4717(1)	2925(3)	1698(1)	16(1)
C(11)	4413(1)	4929(3)	1754(1)	20(1)
C(12)	3791(1)	5917(3)	1052(1)	21(1)
C(13)	3455(1)	4901(3)	255(1)	19(1)
C(14)	3792(1)	2934(3)	170(1)	20(1)
C(15)	4402(1)	1947(3)	893(1)	18(1)
C(21)	1513(1)	7256(3)	268(1)	20(1)
C(22)	1328(2)	9171(3)	550(1)	23(1)
C(23)	763(1)	9473(3)	1281(1)	21(1)
C(24)	336(1)	7878(3)	1714(1)	17(1)
C(25)	497(1)	5955(3)	1397(1)	21(1)
C(26)	1081(2)	5631(3)	686(1)	22(1)
C(27)	-323(1)	8123(3)	2508(1)	18(1)
C(28)	-1559(1)	7399(3)	2230(1)	22(1)
C(29)	-373(2)	10312(3)	2801(1)	21(1)
C(30)	303(1)	6916(2)	3287(1)	16(1)
C(31)	1472(1)	7275(3)	3556(1)	18(1)
C(32)	2083(1)	6280(3)	4264(1)	19(1)
C(33)	1526(1)	4870(3)	4726(1)	18(1)
C(34)	359(1)	4540(3)	4488(1)	19(1)
C(35)	-242(1)	5532(3)	3761(1)	18(1)

Bond lengths [Å] and angles [°] for Bisazo macrocycle **1**.

N(1)-N(2)	1.254(2)	C(15)-H(15)	0.9500
N(1)-C(33)	1.446(2)	C(21)-C(22)	1.382(3)
N(2)-C(1)	1.442(2)	C(21)-C(26)	1.394(3)
N(3)-N(4)	1.255(2)	C(22)-C(23)	1.393(2)
N(3)-C(13)	1.441(2)	C(22)-H(22)	0.9500
N(4)-C(21)	1.446(2)	C(23)-C(24)	1.389(2)
C(1)-C(6)	1.386(2)	C(23)-H(23)	0.9500
C(1)-C(2)	1.397(2)	C(24)-C(25)	1.401(2)
C(2)-C(3)	1.379(2)	C(24)-C(27)	1.538(2)
C(2)-H(2)	0.9500	C(25)-C(26)	1.383(2)
C(3)-C(4)	1.403(2)	C(25)-H(25)	0.9500
C(3)-H(3)	0.9500	C(26)-H(26)	0.9500
C(4)-C(5)	1.395(2)	C(27)-C(30)	1.537(2)
C(4)-C(7)	1.535(2)	C(27)-C(28)	1.538(2)
C(5)-C(6)	1.393(2)	C(27)-C(29)	1.539(2)
C(5)-H(5)	0.9500	C(28)-H(28A)	0.9800
C(6)-H(6)	0.9500	C(28)-H(28B)	0.9800
C(7)-C(8)	1.524(2)	C(28)-H(28C)	0.9800
C(7)-C(9)	1.536(2)	C(29)-H(29A)	0.9800
C(7)-C(10)	1.536(2)	C(29)-H(29B)	0.9800
C(8)-H(8A)	0.9800	C(29)-H(29C)	0.9800
C(8)-H(8B)	0.9800	C(30)-C(35)	1.389(2)
C(8)-H(8C)	0.9800	C(30)-C(31)	1.403(2)
C(9)-H(9A)	0.9800	C(31)-C(32)	1.382(2)
C(9)-H(9B)	0.9800	C(31)-H(31)	0.9500
C(9)-H(9C)	0.9800	C(32)-C(33)	1.397(2)
C(10)-C(15)	1.395(2)	C(32)-H(32)	0.9500
C(10)-C(11)	1.397(2)	C(33)-C(34)	1.391(2)
C(11)-C(12)	1.377(2)	C(34)-C(35)	1.397(2)
C(11)-H(11)	0.9500	C(34)-H(34)	0.9500
C(12)-C(13)	1.401(2)	C(35)-H(35)	0.9500
C(12)-H(12)	0.9500		
C(13)-C(14)	1.390(3)	N(2)-N(1)-C(33)	122.23(13)
C(14)-C(15)	1.394(2)	N(1)-N(2)-C(1)	121.85(14)
C(14)-H(14)	0.9500	N(4)-N(3)-C(13)	122.26(14)

N(3)-N(4)-C(21)	121.55(14)	C(11)-C(10)-C(7)	118.46(14)
C(6)-C(1)-C(2)	120.03(15)	C(12)-C(11)-C(10)	121.92(15)
C(6)-C(1)-N(2)	117.66(14)	C(12)-C(11)-H(11)	119.0
C(2)-C(1)-N(2)	122.03(15)	C(10)-C(11)-H(11)	119.0
C(3)-C(2)-C(1)	119.33(14)	C(11)-C(12)-C(13)	119.55(16)
C(3)-C(2)-H(2)	120.3	C(11)-C(12)-H(12)	120.2
C(1)-C(2)-H(2)	120.3	C(13)-C(12)-H(12)	120.2
C(2)-C(3)-C(4)	121.83(15)	C(14)-C(13)-C(12)	119.57(15)
C(2)-C(3)-H(3)	119.1	C(14)-C(13)-N(3)	116.79(15)
C(4)-C(3)-H(3)	119.1	C(12)-C(13)-N(3)	123.21(16)
C(5)-C(4)-C(3)	117.74(14)	C(13)-C(14)-C(15)	120.01(15)
C(5)-C(4)-C(7)	122.99(14)	C(13)-C(14)-H(14)	120.0
C(3)-C(4)-C(7)	119.25(14)	C(15)-C(14)-H(14)	120.0
C(6)-C(5)-C(4)	121.02(14)	C(14)-C(15)-C(10)	120.94(15)
C(6)-C(5)-H(5)	119.5	C(14)-C(15)-H(15)	119.5
C(4)-C(5)-H(5)	119.5	C(10)-C(15)-H(15)	119.5
C(1)-C(6)-C(5)	119.92(14)	C(22)-C(21)-C(26)	120.07(15)
C(1)-C(6)-H(6)	120.0	C(22)-C(21)-N(4)	118.12(16)
C(5)-C(6)-H(6)	120.0	C(26)-C(21)-N(4)	121.48(16)
C(8)-C(7)-C(4)	107.71(13)	C(21)-C(22)-C(23)	119.89(16)
C(8)-C(7)-C(9)	108.29(14)	C(21)-C(22)-H(22)	120.1
C(4)-C(7)-C(9)	112.50(13)	C(23)-C(22)-H(22)	120.1
C(8)-C(7)-C(10)	111.74(13)	C(24)-C(23)-C(22)	121.07(16)
C(4)-C(7)-C(10)	108.41(13)	C(24)-C(23)-H(23)	119.5
C(9)-C(7)-C(10)	108.23(13)	C(22)-C(23)-H(23)	119.5
C(7)-C(8)-H(8A)	109.5	C(23)-C(24)-C(25)	117.97(15)
C(7)-C(8)-H(8B)	109.5	C(23)-C(24)-C(27)	123.40(15)
H(8A)-C(8)-H(8B)	109.5	C(25)-C(24)-C(27)	118.61(15)
C(7)-C(8)-H(8C)	109.5	C(26)-C(25)-C(24)	121.52(16)
H(8A)-C(8)-H(8C)	109.5	C(26)-C(25)-H(25)	119.2
H(8B)-C(8)-H(8C)	109.5	C(24)-C(25)-H(25)	119.2
C(7)-C(9)-H(9A)	109.5	C(25)-C(26)-C(21)	119.39(17)
C(7)-C(9)-H(9B)	109.5	C(25)-C(26)-H(26)	120.3
H(9A)-C(9)-H(9B)	109.5	C(21)-C(26)-H(26)	120.3
C(7)-C(9)-H(9C)	109.5	C(30)-C(27)-C(24)	108.11(13)
H(9A)-C(9)-H(9C)	109.5	C(30)-C(27)-C(28)	112.27(14)
H(9B)-C(9)-H(9C)	109.5	C(24)-C(27)-C(28)	108.37(13)
C(15)-C(10)-C(11)	117.90(15)	C(30)-C(27)-C(29)	108.21(13)
C(15)-C(10)-C(7)	123.61(14)	C(24)-C(27)-C(29)	112.02(14)

C(28)-C(27)-C(29)	107.92(14)	C(32)-C(31)-C(30)	121.72(15)
C(27)-C(28)-H(28A)	109.5	C(32)-C(31)-H(31)	119.1
C(27)-C(28)-H(28B)	109.5	C(30)-C(31)-H(31)	119.1
H(28A)-C(28)-H(28B)	109.5	C(31)-C(32)-C(33)	119.37(15)
C(27)-C(28)-H(28C)	109.5	C(31)-C(32)-H(32)	120.3
H(28A)-C(28)-H(28C)	109.5	C(33)-C(32)-H(32)	120.3
H(28B)-C(28)-H(28C)	109.5	C(34)-C(33)-C(32)	119.78(15)
C(27)-C(29)-H(29A)	109.5	C(34)-C(33)-N(1)	116.84(14)
C(27)-C(29)-H(29B)	109.5	C(32)-C(33)-N(1)	123.07(14)
H(29A)-C(29)-H(29B)	109.5	C(33)-C(34)-C(35)	120.10(15)
C(27)-C(29)-H(29C)	109.5	C(33)-C(34)-H(34)	119.9
H(29A)-C(29)-H(29C)	109.5	C(35)-C(34)-H(34)	119.9
H(29B)-C(29)-H(29C)	109.5	C(30)-C(35)-C(34)	120.74(15)
C(35)-C(30)-C(31)	118.20(15)	C(30)-C(35)-H(35)	119.6
C(35)-C(30)-C(27)	123.13(14)	C(34)-C(35)-H(35)	119.6
C(31)-C(30)-C(27)	118.63(14)		

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Bisazo macrocycle **1**. 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)	20(1)	26(1)	16(1)	1(1)	4(1)	2(1)
N(2)	21(1)	24(1)	17(1)	0(1)	3(1)	2(1)
N(3)	22(1)	27(1)	17(1)	2(1)	3(1)	1(1)
N(4)	23(1)	29(1)	16(1)	2(1)	4(1)	2(1)
C(1)	19(1)	18(1)	14(1)	1(1)	2(1)	4(1)
C(2)	15(1)	21(1)	19(1)	0(1)	2(1)	-1(1)
C(3)	17(1)	19(1)	17(1)	-1(1)	0(1)	-2(1)
C(4)	16(1)	15(1)	16(1)	1(1)	2(1)	2(1)
C(5)	15(1)	16(1)	19(1)	0(1)	0(1)	-1(1)
C(6)	20(1)	17(1)	15(1)	-2(1)	-2(1)	2(1)
C(7)	17(1)	19(1)	16(1)	-1(1)	3(1)	0(1)
C(8)	21(1)	23(1)	15(1)	-1(1)	2(1)	4(1)
C(9)	16(1)	29(1)	20(1)	0(1)	3(1)	-1(1)
C(10)	14(1)	20(1)	16(1)	0(1)	4(1)	-2(1)
C(11)	23(1)	20(1)	16(1)	-2(1)	2(1)	-3(1)
C(12)	21(1)	20(1)	20(1)	0(1)	3(1)	-1(1)

C(13)	17(1)	26(1)	15(1)	3(1)	5(1)	-1(1)
C(14)	20(1)	26(1)	14(1)	-3(1)	5(1)	0(1)
C(15)	18(1)	20(1)	18(1)	-3(1)	4(1)	1(1)
C(21)	16(1)	29(1)	14(1)	1(1)	1(1)	2(1)
C(22)	23(1)	24(1)	22(1)	8(1)	6(1)	3(1)
C(23)	22(1)	20(1)	21(1)	2(1)	4(1)	3(1)
C(24)	14(1)	23(1)	14(1)	1(1)	0(1)	1(1)
C(25)	21(1)	22(1)	21(1)	0(1)	4(1)	-3(1)
C(26)	22(1)	24(1)	21(1)	-4(1)	3(1)	-1(1)
C(27)	14(1)	22(1)	17(1)	1(1)	3(1)	2(1)
C(28)	16(1)	30(1)	20(1)	4(1)	2(1)	1(1)
C(29)	21(1)	22(1)	20(1)	0(1)	6(1)	4(1)
C(30)	16(1)	18(1)	14(1)	-3(1)	3(1)	2(1)
C(31)	17(1)	18(1)	19(1)	0(1)	4(1)	-2(1)
C(32)	15(1)	22(1)	19(1)	-2(1)	2(1)	-1(1)
C(33)	20(1)	20(1)	14(1)	-2(1)	4(1)	2(1)
C(34)	18(1)	21(1)	19(1)	2(1)	7(1)	1(1)
C(35)	15(1)	20(1)	20(1)	-2(1)	6(1)	0(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)
for Bisazo macrocycle **1**.

	x	y	z	U(eq)
H(2)	2269	1526	3933	22
H(3)	3276	1074	2747	22
H(5)	6088	3589	4147	21
H(6)	5115	3872	5372	21
H(8A)	4758	-897	2283	29
H(8B)	5953	-880	2928	29
H(8C)	5927	-567	1885	29
H(9A)	6970	2654	2097	32
H(9B)	7095	2191	3136	32
H(9C)	6576	4277	2761	32
H(11)	4641	5631	2291	24
H(12)	3592	7278	1109	25
H(14)	3606	2262	-380	24

H(15)	4606	588	836	22
H(22)	1586	10280	245	27
H(23)	667	10791	1486	25
H(25)	198	4847	1677	25
H(26)	1187	4315	483	27
H(28A)	-1924	8206	1733	33
H(28B)	-1990	7530	2731	33
H(28C)	-1550	5998	2049	33
H(29A)	-797	11097	2321	31
H(29B)	407	10837	2942	31
H(29C)	-760	10394	3327	31
H(31)	1855	8227	3242	22
H(32)	2873	6552	4437	23
H(34)	-31	3638	4822	23
H(35)	-1032	5256	3587	21

Trisazo macrocycle 2

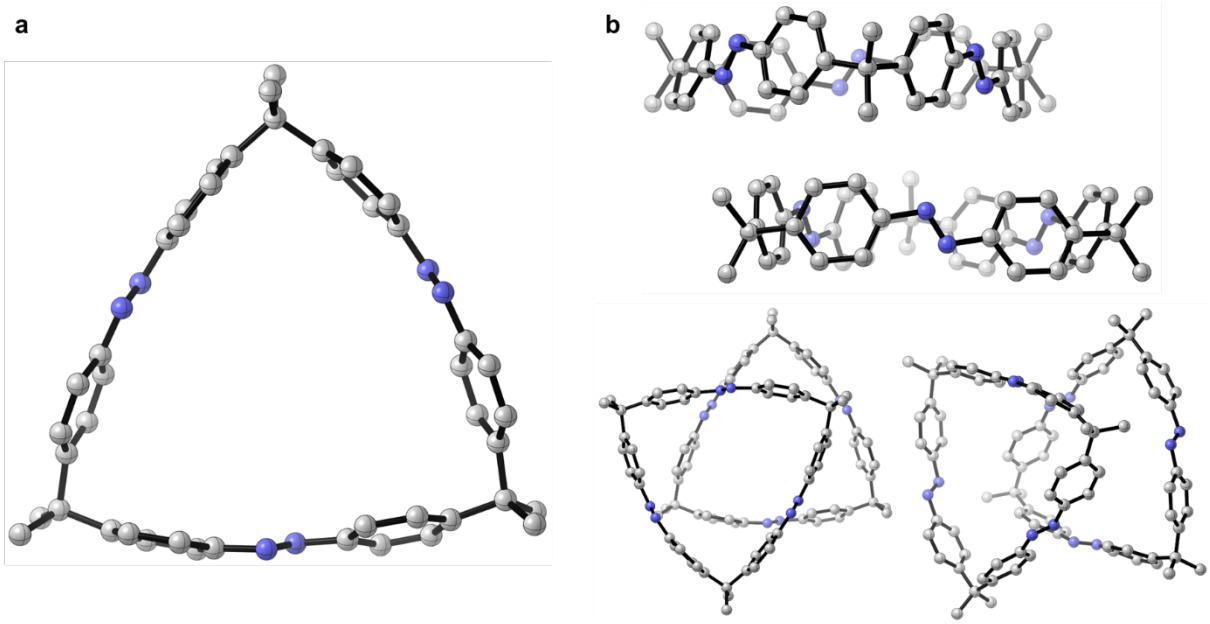

Figure S13a: Single crystal structure of trisazo macrocycle **2**. **b:** Crystal packing of trisazo macrocycle **2** (grey: carbon, blue: nitrogen; hydrogens omitted).

The unit cell of Trisazo macrocycle **2** was determined using 9869 reflections and the structure was solved in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of Trisazo macrocycle **2**, half of a pentane molecule and other, heavily disordered solvent

molecules. One of the three diphenyl-azo parts of the molecule was found to be disordered over two positions. The disorder was modeled with the help of similarity restraints on anisotropic displacement parameters, advanced rigid bond restraints[16] and same distance restraints on 1,2 and 1,3 distances.[17] The disorder ratio was allowed to refine freely and converged to 0.554(6). The pentane molecule was found to be disordered over the inversion center and was modeled using the SHELX negative PART instruction to suppress the binding to its symmetry equivalent. The full molecule was refined half occupied over two positions using the restraints already mentioned. Additionally all anisotropic displacement parameters for the pentane molecule were set to the same parameters. This disorder ratio was also allowed to refine freely and converged to 0.64(2). It was not possible to find a reasonable disorder model for the other, heavily disordered solvent molecules. SQUEEZE[18] as implemented in PLATON[19] was used to include a model for these solvent molecules. The obtained model was added as .fab-file to the refinement using SHELXL. SQUEEZE found one independent void with disordered solvent, located at 0.0 0.5 0.5, with a volume of 354 $Å^3$. The equivalent of 90 electrons were identified in the void. This could e.g. correspond to about two molecules of CH_2Cl_2 in the unit cell.

Crystal data and structure refinement for Trisazo macrocycle **2**.

CCDC No	1902882	
Empirical formula	$C_{47.5}H_{48}N_6$	
Formula weight	702.92	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.3008(6) Å	α= 111.0170(19)°.
	b = 14.1002(7) Å	β= 100.7420(19)°.
	c = 15.7086(8) Å	γ = 102.7284(19)°.
Volume	2180.2(2) $Å^3$	
Z	2	
Density (calculated)	1.071 Mg/m^3	
Absorption coefficient	0.064 mm^{-1}	
F(000)	750	
Crystal size	0.208 x 0.157 x 0.155 mm^3	
Theta range for data collection	2.487 to 28.699°.	
Index ranges	-15<=h<=15, -19<=k<=19, -21<=l<=21	
Reflections collected	97608	

Independent reflections	11267 [R(int) = 0.0633]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11267 / 1550 / 634
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1355
R indices (all data)	R1 = 0.0811, wR2 = 0.1474
Largest diff. peak and hole	0.312 and -0.370 e.Å^{-3}

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

	x	y	z	U(eq)
N(1)	7827(1)	6138(1)	3239(1)	21(1)
N(2)	6650(1)	5971(1)	3110(1)	22(1)
N(3)	10074(1)	6596(1)	8651(1)	22(1)
N(4)	10916(1)	6681(1)	8243(1)	24(1)
C(1)	8594(1)	7129(1)	4021(1)	19(1)
C(2)	8132(1)	7810(1)	4663(1)	27(1)
C(3)	8967(1)	8684(1)	5457(1)	26(1)
C(4)	10279(1)	8906(1)	5643(1)	18(1)
C(5)	10720(1)	8246(1)	4969(1)	24(1)
C(6)	9891(1)	7363(1)	4169(1)	24(1)
C(7)	11182(1)	9748(1)	6620(1)	18(1)
C(8)	10647(2)	10660(1)	7052(1)	25(1)
C(9)	12491(1)	10265(1)	6549(1)	23(1)
C(10)	11292(1)	9098(1)	7223(1)	18(1)
C(11)	11957(2)	8358(1)	7032(1)	26(1)
C(12)	11878(2)	7619(1)	7424(1)	28(1)
C(13)	11130(1)	7600(1)	8028(1)	22(1)
C(14)	10557(1)	8392(1)	8298(1)	24(1)
C(15)	10635(1)	9131(1)	7896(1)	22(1)
C(21)	9722(1)	5594(1)	8727(1)	19(1)
C(22)	8901(1)	5508(1)	9272(1)	19(1)
C(23)	8355(1)	4528(1)	9280(1)	18(1)
C(24)	8604(1)	3613(1)	8735(1)	16(1)

C(25)	9495(1)	3726(1)	8233(1)	19(1)
C(26)	10052(1)	4700(1)	8227(1)	21(1)
C(27)	7822(1)	2480(1)	8560(1)	16(1)
C(28)	7001(1)	2487(1)	9238(1)	23(1)
C(29)	8690(1)	1814(1)	8698(1)	23(1)
C(41)	5892(1)	4931(1)	2408(1)	20(1)
C(42)	6379(1)	4120(1)	1960(1)	22(1)
C(43)	5560(1)	3099(1)	1377(1)	20(1)
C(44)	4244(1)	2854(1)	1217(1)	17(1)
C(45)	3776(1)	3691(1)	1628(1)	22(1)
C(46)	4590(1)	4717(1)	2224(1)	24(1)
C(47)	3390(1)	1677(1)	743(1)	18(1)
C(48)	3820(2)	985(1)	-68(1)	27(1)
C(49)	2000(1)	1559(1)	309(1)	25(1)
N(5)	5364(3)	1202(2)	4597(3)	18(1)
N(6)	4380(3)	1449(2)	4377(2)	20(1)
C(30)	7022(14)	1999(14)	7498(5)	14(1)
C(31)	7292(8)	1236(7)	6778(5)	11(1)
C(32)	6674(6)	958(5)	5829(4)	14(1)
C(33)	5801(4)	1432(4)	5587(3)	14(1)
C(34)	5476(6)	2159(5)	6299(4)	19(1)
C(35)	6078(12)	2426(11)	7241(5)	21(1)
C(50)	3472(17)	1405(14)	1620(8)	16(1)
C(51)	4277(7)	847(5)	1831(4)	19(1)
C(52)	4556(4)	792(3)	2717(3)	17(1)
C(53)	4027(4)	1314(3)	3405(2)	16(1)
C(54)	3147(4)	1801(3)	3182(2)	21(1)
C(55)	2876(6)	1840(7)	2302(4)	20(1)
N(5A)	4755(4)	1537(3)	4811(3)	20(1)
N(6A)	5116(3)	1064(2)	4106(3)	19(1)
C(30A)	6914(19)	2076(18)	7549(7)	16(2)
C(31A)	7080(11)	1360(10)	6735(7)	18(2)
C(32A)	6382(7)	1144(6)	5815(5)	18(1)
C(33A)	5481(6)	1639(5)	5708(4)	15(1)
C(34A)	5260(7)	2326(7)	6508(5)	20(1)
C(35A)	5992(14)	2559(13)	7410(6)	17(2)
C(50A)	3620(20)	1291(19)	1549(11)	18(2)
C(51A)	4382(9)	647(7)	1597(5)	17(1)
C(52A)	4788(5)	538(4)	2434(4)	18(1)

C(53A)	4452(5)	1072(4)	3238(3)	16(1)
C(54A)	3608(6)	1643(4)	3180(3)	20(1)
C(55A)	3204(8)	1743(8)	2334(6)	23(1)
C(1S)	6496(11)	6983(9)	1413(8)	23(1)
C(2S)	6203(14)	5893(10)	658(9)	23(1)
C(3S)	4850(15)	5315(10)	132(12)	23(1)
C(4S)	4608(13)	4120(12)	-497(11)	23(1)
C(5S)	3207(11)	3525(10)	-925(10)	23(1)
C(1T)	6999(7)	6374(6)	1037(5)	23(1)
C(2T)	5537(8)	5970(7)	622(6)	23(1)
C(3T)	5154(8)	4839(6)	-126(6)	23(1)
C(4T)	3724(6)	4332(5)	-507(5)	23(1)
C(5T)	3301(7)	3237(6)	-1231(5)	23(1)

Bond lengths [Å] and angles [°] for Trisazo macrocycle **2**.

N(1)-N(2)	1.2621(17)	C(8)-H(8AC)	0.9800
N(1)-C(1)	1.4313(18)	C(9)-H(9A)	0.9800
N(2)-C(41)	1.4265(18)	C(9)-H(9AB)	0.9800
N(3)-N(4)	1.2506(17)	C(9)-H(9AC)	0.9800
N(3)-C(21)	1.4344(18)	C(10)-C(15)	1.394(2)
N(4)-C(13)	1.4352(19)	C(10)-C(11)	1.397(2)
C(1)-C(6)	1.384(2)	C(11)-C(12)	1.383(2)
C(1)-C(2)	1.392(2)	C(11)-H(11)	0.9500
C(2)-C(3)	1.383(2)	C(12)-C(13)	1.386(2)
C(2)-H(2)	0.9500	C(12)-H(12)	0.9500
C(3)-C(4)	1.396(2)	C(13)-C(14)	1.389(2)
C(3)-H(3)	0.9500	C(14)-C(15)	1.394(2)
C(4)-C(5)	1.389(2)	C(14)-H(14)	0.9500
C(4)-C(7)	1.5431(19)	C(15)-H(15)	0.9500
C(5)-C(6)	1.390(2)	C(21)-C(22)	1.388(2)
C(5)-H(5)	0.9500	C(21)-C(26)	1.398(2)
C(6)-H(6)	0.9500	C(22)-C(23)	1.3887(19)
C(7)-C(8)	1.534(2)	C(22)-H(22)	0.9500
C(7)-C(9)	1.541(2)	C(23)-C(24)	1.391(2)
C(7)-C(10)	1.5425(18)	C(23)-H(23)	0.9500
C(8)-H(8A)	0.9800	C(24)-C(25)	1.4063(19)
C(8)-H(8AB)	0.9800	C(24)-C(27)	1.5430(18)

C(25)-C(26)	1.383(2)	C(31)-C(32)	1.391(6)
C(25)-H(25)	0.9500	C(31)-H(31)	0.9500
C(26)-H(26)	0.9500	C(32)-C(33)	1.378(4)
C(27)-C(28)	1.5365(19)	C(32)-H(32)	0.9500
C(27)-C(29)	1.5372(19)	C(33)-C(34)	1.390(5)
C(27)-C(30A)	1.544(9)	C(34)-C(35)	1.381(7)
C(27)-C(30)	1.554(6)	C(34)-H(34)	0.9500
C(28)-H(28A)	0.9800	C(35)-H(35)	0.9500
C(28)-H(28B)	0.9800	C(50)-C(51)	1.395(7)
C(28)-H(28C)	0.9800	C(50)-C(55)	1.399(7)
C(29)-H(29A)	0.9800	C(51)-C(52)	1.402(6)
C(29)-H(29B)	0.9800	C(51)-H(51)	0.9500
C(29)-H(29C)	0.9800	C(52)-C(53)	1.389(5)
C(41)-C(46)	1.387(2)	C(52)-H(52)	0.9500
C(41)-C(42)	1.396(2)	C(53)-C(54)	1.388(5)
C(42)-C(43)	1.386(2)	C(54)-C(55)	1.383(6)
C(42)-H(42)	0.9500	C(54)-H(54)	0.9500
C(43)-C(44)	1.4018(19)	C(55)-H(55)	0.9500
C(43)-H(43)	0.9500	N(5A)-N(6A)	1.263(6)
C(44)-C(45)	1.395(2)	N(5A)-C(33A)	1.432(7)
C(44)-C(47)	1.5426(19)	N(6A)-C(53A)	1.434(6)
C(45)-C(46)	1.392(2)	C(30A)-C(35A)	1.389(10)
C(45)-H(45)	0.9500	C(30A)-C(31A)	1.392(10)
C(46)-H(46)	0.9500	C(31A)-C(32A)	1.399(9)
C(47)-C(48)	1.535(2)	C(31A)-H(31A)	0.9500
C(47)-C(49)	1.5369(19)	C(32A)-C(33A)	1.372(6)
C(47)-C(50A)	1.550(9)	C(32A)-H(32A)	0.9500
C(47)-C(50)	1.550(7)	C(33A)-C(34A)	1.389(6)
C(48)-H(48A)	0.9800	C(34A)-C(35A)	1.382(9)
C(48)-H(48B)	0.9800	C(34A)-H(34A)	0.9500
C(48)-H(48C)	0.9800	C(35A)-H(35A)	0.9500
C(49)-H(49A)	0.9800	C(50A)-C(51A)	1.391(9)
C(49)-H(49B)	0.9800	C(50A)-C(55A)	1.393(9)
C(49)-H(49C)	0.9800	C(51A)-C(52A)	1.384(8)
N(5)-N(6)	1.262(4)	C(51A)-H(51A)	0.9500
N(5)-C(33)	1.431(5)	C(52A)-C(53A)	1.388(6)
N(6)-C(53)	1.435(5)	C(52A)-H(52A)	0.9500
C(30)-C(31)	1.389(8)	C(53A)-C(54A)	1.387(6)
C(30)-C(35)	1.400(8)	C(54A)-C(55A)	1.389(8)

C(54A)-H(54A)	0.9500	C(6)-C(1)-C(2)	119.15(13)
C(55A)-H(55A)	0.9500	C(6)-C(1)-N(1)	116.04(13)
C(1S)-C(2S)	1.483(10)	C(2)-C(1)-N(1)	124.63(13)
C(1S)-H(1SA)	0.9800	C(3)-C(2)-C(1)	119.93(14)
C(1S)-H(1SB)	0.9800	C(3)-C(2)-H(2)	120.0
C(1S)-H(1SC)	0.9800	C(1)-C(2)-H(2)	120.0
C(2S)-C(3S)	1.477(12)	C(2)-C(3)-C(4)	121.75(14)
C(2S)-H(2SA)	0.9900	C(2)-C(3)-H(3)	119.1
C(2S)-H(2SB)	0.9900	C(4)-C(3)-H(3)	119.1
C(3S)-C(4S)	1.546(12)	C(5)-C(4)-C(3)	117.32(13)
C(3S)-H(3SA)	0.9900	C(5)-C(4)-C(7)	121.46(12)
C(3S)-H(3SB)	0.9900	C(3)-C(4)-C(7)	120.67(13)
C(4S)-C(5S)	1.509(11)	C(4)-C(5)-C(6)	121.43(13)
C(4S)-H(4SA)	0.9900	C(4)-C(5)-H(5)	119.3
C(4S)-H(4SB)	0.9900	C(6)-C(5)-H(5)	119.3
C(5S)-H(5SA)	0.9800	C(1)-C(6)-C(5)	120.28(14)
C(5S)-H(5SB)	0.9800	C(1)-C(6)-H(6)	119.9
C(5S)-H(5SC)	0.9800	C(5)-C(6)-H(6)	119.9
C(1T)-C(2T)	1.549(8)	C(8)-C(7)-C(9)	106.70(12)
C(1T)-H(1TA)	0.9800	C(8)-C(7)-C(10)	112.09(12)
C(1T)-H(1TB)	0.9800	C(9)-C(7)-C(10)	111.09(11)
C(1T)-H(1TC)	0.9800	C(8)-C(7)-C(4)	111.46(11)
C(2T)-C(3T)	1.508(7)	C(9)-C(7)-C(4)	112.22(11)
C(2T)-H(2TA)	0.9900	C(10)-C(7)-C(4)	103.41(11)
C(2T)-H(2TB)	0.9900	C(7)-C(8)-H(8A)	109.5
C(3T)-C(4T)	1.518(8)	C(7)-C(8)-H(8AB)	109.5
C(3T)-H(3TA)	0.9900	H(8A)-C(8)-H(8AB)	109.5
C(3T)-H(3TB)	0.9900	C(7)-C(8)-H(8AC)	109.5
C(4T)-C(5T)	1.455(7)	H(8A)-C(8)-H(8AC)	109.5
C(4T)-H(4TA)	0.9900	H(8AB)-C(8)-H(8AC)	109.5
C(4T)-H(4TB)	0.9900	C(7)-C(9)-H(9A)	109.5
C(5T)-H(5TA)	0.9800	C(7)-C(9)-H(9AB)	109.5
C(5T)-H(5TB)	0.9800	H(9A)-C(9)-H(9AB)	109.5
C(5T)-H(5TC)	0.9800	C(7)-C(9)-H(9AC)	109.5
		H(9A)-C(9)-H(9AC)	109.5
N(2)-N(1)-C(1)	114.04(12)	H(9AB)-C(9)-H(9AC)	109.5
N(1)-N(2)-C(41)	113.90(12)	C(15)-C(10)-C(11)	117.16(13)
N(4)-N(3)-C(21)	113.52(12)	C(15)-C(10)-C(7)	122.50(12)
N(3)-N(4)-C(13)	113.81(12)	C(11)-C(10)-C(7)	119.97(12)

C(12)-C(11)-C(10)	121.74(14)	C(28)-C(27)-C(30)	112.8(7)
C(12)-C(11)-H(11)	119.1	C(29)-C(27)-C(30)	110.0(4)
C(10)-C(11)-H(11)	119.1	C(24)-C(27)-C(30)	103.2(8)
C(11)-C(12)-C(13)	120.23(14)	C(27)-C(28)-H(28A)	109.5
C(11)-C(12)-H(12)	119.9	C(27)-C(28)-H(28B)	109.5
C(13)-C(12)-H(12)	119.9	H(28A)-C(28)-H(28B)	109.5
C(12)-C(13)-C(14)	118.93(14)	C(27)-C(28)-H(28C)	109.5
C(12)-C(13)-N(4)	115.49(14)	H(28A)-C(28)-H(28C)	109.5
C(14)-C(13)-N(4)	125.28(13)	H(28B)-C(28)-H(28C)	109.5
C(13)-C(14)-C(15)	120.22(14)	C(27)-C(29)-H(29A)	109.5
C(13)-C(14)-H(14)	119.9	C(27)-C(29)-H(29B)	109.5
C(15)-C(14)-H(14)	119.9	H(29A)-C(29)-H(29B)	109.5
C(10)-C(15)-C(14)	121.20(14)	C(27)-C(29)-H(29C)	109.5
C(10)-C(15)-H(15)	119.4	H(29A)-C(29)-H(29C)	109.5
C(14)-C(15)-H(15)	119.4	H(29B)-C(29)-H(29C)	109.5
C(22)-C(21)-C(26)	119.48(13)	C(46)-C(41)-C(42)	119.51(13)
C(22)-C(21)-N(3)	115.81(13)	C(46)-C(41)-N(2)	116.05(13)
C(26)-C(21)-N(3)	124.43(13)	C(42)-C(41)-N(2)	124.28(13)
C(21)-C(22)-C(23)	120.50(13)	C(43)-C(42)-C(41)	119.64(13)
C(21)-C(22)-H(22)	119.8	C(43)-C(42)-H(42)	120.2
C(23)-C(22)-H(22)	119.8	C(41)-C(42)-H(42)	120.2
C(22)-C(23)-C(24)	120.86(13)	C(42)-C(43)-C(44)	121.70(13)
C(22)-C(23)-H(23)	119.6	C(42)-C(43)-H(43)	119.1
C(24)-C(23)-H(23)	119.6	C(44)-C(43)-H(43)	119.1
C(23)-C(24)-C(25)	117.87(12)	C(45)-C(44)-C(43)	117.55(13)
C(23)-C(24)-C(27)	122.48(12)	C(45)-C(44)-C(47)	121.60(12)
C(25)-C(24)-C(27)	119.16(12)	C(43)-C(44)-C(47)	120.12(12)
C(26)-C(25)-C(24)	121.56(13)	C(46)-C(45)-C(44)	121.17(13)
C(26)-C(25)-H(25)	119.2	C(46)-C(45)-H(45)	119.4
C(24)-C(25)-H(25)	119.2	C(44)-C(45)-H(45)	119.4
C(25)-C(26)-C(21)	119.48(13)	C(41)-C(46)-C(45)	120.26(14)
C(25)-C(26)-H(26)	120.3	C(41)-C(46)-H(46)	119.9
C(21)-C(26)-H(26)	120.3	C(45)-C(46)-H(46)	119.9
C(28)-C(27)-C(29)	106.83(11)	C(48)-C(47)-C(49)	106.70(11)
C(28)-C(27)-C(24)	112.97(11)	C(48)-C(47)-C(44)	111.99(11)
C(29)-C(27)-C(24)	111.10(11)	C(49)-C(47)-C(44)	112.30(12)
C(28)-C(27)-C(30A)	107.3(9)	C(48)-C(47)-C(50A)	107.0(4)
C(29)-C(27)-C(30A)	116.6(5)	C(49)-C(47)-C(50A)	115.3(8)
C(24)-C(27)-C(30A)	102.1(10)	C(44)-C(47)-C(50A)	103.6(10)

C(48)-C(47)-C(50)	116.7(4)	C(50)-C(51)-H(51)	119.2
C(49)-C(47)-C(50)	108.3(6)	C(52)-C(51)-H(51)	119.2
C(44)-C(47)-C(50)	100.9(8)	C(53)-C(52)-C(51)	119.2(3)
C(47)-C(48)-H(48A)	109.5	C(53)-C(52)-H(52)	120.4
C(47)-C(48)-H(48B)	109.5	C(51)-C(52)-H(52)	120.4
H(48A)-C(48)-H(48B)	109.5	C(54)-C(53)-C(52)	119.9(3)
C(47)-C(48)-H(48C)	109.5	C(54)-C(53)-N(6)	115.6(4)
H(48A)-C(48)-H(48C)	109.5	C(52)-C(53)-N(6)	124.4(4)
H(48B)-C(48)-H(48C)	109.5	C(55)-C(54)-C(53)	119.9(3)
C(47)-C(49)-H(49A)	109.5	C(55)-C(54)-H(54)	120.1
C(47)-C(49)-H(49B)	109.5	C(53)-C(54)-H(54)	120.1
H(49A)-C(49)-H(49B)	109.5	C(54)-C(55)-C(50)	121.8(5)
C(47)-C(49)-H(49C)	109.5	C(54)-C(55)-H(55)	119.1
H(49A)-C(49)-H(49C)	109.5	C(50)-C(55)-H(55)	119.1
H(49B)-C(49)-H(49C)	109.5	N(6A)-N(5A)-C(33A)	114.7(5)
N(6)-N(5)-C(33)	113.9(4)	N(5A)-N(6A)-C(53A)	113.2(5)
N(5)-N(6)-C(53)	113.2(4)	C(35A)-C(30A)-C(31A)	116.7(8)
C(31)-C(30)-C(35)	118.3(6)	C(35A)-C(30A)-C(27)	119.2(8)
C(31)-C(30)-C(27)	122.5(6)	C(31A)-C(30A)-C(27)	123.4(9)
C(35)-C(30)-C(27)	118.9(7)	C(30A)-C(31A)-C(32A)	122.5(7)
C(30)-C(31)-C(32)	119.8(5)	C(30A)-C(31A)-H(31A)	118.8
C(30)-C(31)-H(31)	120.1	C(32A)-C(31A)-H(31A)	118.8
C(32)-C(31)-H(31)	120.1	C(33A)-C(32A)-C(31A)	118.9(6)
C(33)-C(32)-C(31)	121.1(4)	C(33A)-C(32A)-H(32A)	120.5
C(33)-C(32)-H(32)	119.5	C(31A)-C(32A)-H(32A)	120.5
C(31)-C(32)-H(32)	119.5	C(32A)-C(33A)-C(34A)	119.9(5)
C(32)-C(33)-C(34)	119.8(4)	C(32A)-C(33A)-N(5A)	124.6(5)
C(32)-C(33)-N(5)	116.2(4)	C(34A)-C(33A)-N(5A)	115.5(5)
C(34)-C(33)-N(5)	123.8(4)	C(35A)-C(34A)-C(33A)	120.2(6)
C(35)-C(34)-C(33)	119.0(5)	C(35A)-C(34A)-H(34A)	119.9
C(35)-C(34)-H(34)	120.5	C(33A)-C(34A)-H(34A)	119.9
C(33)-C(34)-H(34)	120.5	C(34A)-C(35A)-C(30A)	121.7(7)
C(34)-C(35)-C(30)	121.8(6)	C(34A)-C(35A)-H(35A)	119.2
C(34)-C(35)-H(35)	119.1	C(30A)-C(35A)-H(35A)	119.2
C(30)-C(35)-H(35)	119.1	C(51A)-C(50A)-C(55A)	118.1(7)
C(51)-C(50)-C(55)	117.2(5)	C(51A)-C(50A)-C(47)	123.6(7)
C(51)-C(50)-C(47)	121.6(6)	C(55A)-C(50A)-C(47)	117.6(8)
C(55)-C(50)-C(47)	120.7(6)	C(52A)-C(51A)-C(50A)	120.3(6)
C(50)-C(51)-C(52)	121.7(5)	C(52A)-C(51A)-H(51A)	119.9

C(50A)-C(51A)-H(51A)	119.9	C(4S)-C(5S)-H(5SA)	109.5
C(51A)-C(52A)-C(53A)	120.7(4)	C(4S)-C(5S)-H(5SB)	109.5
C(51A)-C(52A)-H(52A)	119.7	H(5SA)-C(5S)-H(5SB)	109.5
C(53A)-C(52A)-H(52A)	119.7	C(4S)-C(5S)-H(5SC)	109.5
C(54A)-C(53A)-C(52A)	119.8(4)	H(5SA)-C(5S)-H(5SC)	109.5
C(54A)-C(53A)-N(6A)	124.4(5)	H(5SB)-C(5S)-H(5SC)	109.5
C(52A)-C(53A)-N(6A)	115.6(5)	C(2T)-C(1T)-H(1TA)	109.5
C(53A)-C(54A)-C(55A)	118.7(4)	C(2T)-C(1T)-H(1TB)	109.5
C(53A)-C(54A)-H(54A)	120.6	H(1TA)-C(1T)-H(1TB)	109.5
C(55A)-C(54A)-H(54A)	120.6	C(2T)-C(1T)-H(1TC)	109.5
C(54A)-C(55A)-C(50A)	121.9(6)	H(1TA)-C(1T)-H(1TC)	109.5
C(54A)-C(55A)-H(55A)	119.0	H(1TB)-C(1T)-H(1TC)	109.5
C(50A)-C(55A)-H(55A)	119.0	C(3T)-C(2T)-C(1T)	108.1(7)
C(2S)-C(1S)-H(1SA)	109.5	C(3T)-C(2T)-H(2TA)	110.1
C(2S)-C(1S)-H(1SB)	109.5	C(1T)-C(2T)-H(2TA)	110.1
H(1SA)-C(1S)-H(1SB)	109.5	C(3T)-C(2T)-H(2TB)	110.1
C(2S)-C(1S)-H(1SC)	109.5	C(1T)-C(2T)-H(2TB)	110.1
H(1SA)-C(1S)-H(1SC)	109.5	H(2TA)-C(2T)-H(2TB)	108.4
H(1SB)-C(1S)-H(1SC)	109.5	C(2T)-C(3T)-C(4T)	112.1(5)
C(3S)-C(2S)-C(1S)	116.3(9)	C(2T)-C(3T)-H(3TA)	109.2
C(3S)-C(2S)-H(2SA)	108.2	C(4T)-C(3T)-H(3TA)	109.2
C(1S)-C(2S)-H(2SA)	108.2	C(2T)-C(3T)-H(3TB)	109.2
C(3S)-C(2S)-H(2SB)	108.2	C(4T)-C(3T)-H(3TB)	109.2
C(1S)-C(2S)-H(2SB)	108.2	H(3TA)-C(3T)-H(3TB)	107.9
H(2SA)-C(2S)-H(2SB)	107.4	C(5T)-C(4T)-C(3T)	114.4(5)
C(2S)-C(3S)-C(4S)	112.7(10)	C(5T)-C(4T)-H(4TA)	108.7
C(2S)-C(3S)-H(3SA)	109.1	C(3T)-C(4T)-H(4TA)	108.7
C(4S)-C(3S)-H(3SA)	109.1	C(5T)-C(4T)-H(4TB)	108.7
C(2S)-C(3S)-H(3SB)	109.1	C(3T)-C(4T)-H(4TB)	108.7
C(4S)-C(3S)-H(3SB)	109.1	H(4TA)-C(4T)-H(4TB)	107.6
H(3SA)-C(3S)-H(3SB)	107.8	C(4T)-C(5T)-H(5TA)	109.5
C(5S)-C(4S)-C(3S)	111.2(13)	C(4T)-C(5T)-H(5TB)	109.5
C(5S)-C(4S)-H(4SA)	109.4	H(5TA)-C(5T)-H(5TB)	109.5
C(3S)-C(4S)-H(4SA)	109.4	C(4T)-C(5T)-H(5TC)	109.5
C(5S)-C(4S)-H(4SB)	109.4	H(5TA)-C(5T)-H(5TC)	109.5
C(3S)-C(4S)-H(4SB)	109.4	H(5TB)-C(5T)-H(5TC)	109.5
H(4SA)-C(4S)-H(4SB)	108.0		

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Trisazo macrocycle **2**. 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)	21(1)	23(1)	18(1)	9(1)	4(1)	5(1)
N(2)	21(1)	22(1)	22(1)	10(1)	2(1)	7(1)
N(3)	21(1)	25(1)	15(1)	7(1)	1(1)	3(1)
N(4)	21(1)	29(1)	23(1)	14(1)	6(1)	8(1)
C(1)	23(1)	20(1)	16(1)	9(1)	4(1)	5(1)
C(2)	17(1)	34(1)	24(1)	6(1)	1(1)	10(1)
C(3)	23(1)	30(1)	22(1)	4(1)	4(1)	14(1)
C(4)	21(1)	17(1)	17(1)	9(1)	5(1)	6(1)
C(5)	19(1)	25(1)	24(1)	7(1)	9(1)	2(1)
C(6)	23(1)	23(1)	21(1)	4(1)	10(1)	4(1)
C(7)	21(1)	15(1)	17(1)	7(1)	5(1)	6(1)
C(8)	30(1)	19(1)	26(1)	7(1)	7(1)	11(1)
C(9)	24(1)	18(1)	25(1)	10(1)	6(1)	3(1)
C(10)	17(1)	16(1)	15(1)	6(1)	1(1)	2(1)
C(11)	28(1)	29(1)	33(1)	19(1)	16(1)	14(1)
C(12)	27(1)	31(1)	39(1)	22(1)	14(1)	14(1)
C(13)	19(1)	25(1)	21(1)	12(1)	1(1)	3(1)
C(14)	23(1)	30(1)	17(1)	10(1)	6(1)	3(1)
C(15)	23(1)	21(1)	19(1)	5(1)	5(1)	6(1)
C(21)	20(1)	20(1)	13(1)	7(1)	-2(1)	2(1)
C(22)	19(1)	18(1)	16(1)	5(1)	1(1)	6(1)
C(23)	15(1)	23(1)	14(1)	7(1)	3(1)	6(1)
C(24)	16(1)	19(1)	10(1)	7(1)	0(1)	4(1)
C(25)	22(1)	20(1)	14(1)	5(1)	6(1)	6(1)
C(26)	19(1)	25(1)	14(1)	7(1)	5(1)	2(1)
C(27)	16(1)	19(1)	12(1)	6(1)	3(1)	4(1)
C(28)	26(1)	25(1)	19(1)	11(1)	9(1)	5(1)
C(29)	23(1)	24(1)	23(1)	12(1)	4(1)	9(1)
C(41)	21(1)	21(1)	19(1)	10(1)	3(1)	6(1)
C(42)	16(1)	26(1)	24(1)	11(1)	5(1)	7(1)
C(43)	21(1)	22(1)	21(1)	10(1)	8(1)	9(1)
C(44)	18(1)	22(1)	13(1)	10(1)	2(1)	5(1)
C(45)	16(1)	26(1)	26(1)	13(1)	3(1)	9(1)
C(46)	22(1)	24(1)	27(1)	11(1)	5(1)	12(1)

C(47)	18(1)	22(1)	12(1)	8(1)	2(1)	4(1)
C(48)	27(1)	26(1)	22(1)	5(1)	6(1)	6(1)
C(49)	20(1)	30(1)	19(1)	7(1)	-1(1)	5(1)
N(5)	19(1)	16(1)	18(2)	9(1)	1(1)	1(1)
N(6)	18(1)	22(1)	18(2)	10(1)	0(1)	3(1)
C(30)	8(2)	19(4)	13(2)	8(2)	0(2)	1(2)
C(31)	11(3)	11(2)	10(2)	3(1)	2(1)	4(2)
C(32)	17(2)	8(2)	15(2)	5(1)	4(1)	3(1)
C(33)	16(2)	11(2)	13(2)	4(1)	1(1)	3(1)
C(34)	20(2)	19(3)	18(2)	6(2)	3(2)	11(1)
C(35)	25(2)	17(3)	16(2)	-1(2)	7(2)	9(2)
C(50)	14(4)	14(3)	14(2)	5(2)	-1(2)	1(2)
C(51)	19(2)	16(3)	17(2)	3(2)	5(2)	4(2)
C(52)	19(2)	15(2)	17(2)	5(2)	2(2)	7(1)
C(53)	16(2)	17(2)	14(1)	7(1)	4(1)	5(1)
C(54)	21(2)	28(2)	20(1)	14(1)	7(1)	13(1)
C(55)	18(3)	32(2)	15(2)	14(1)	4(2)	12(2)
N(5A)	19(2)	18(2)	17(2)	7(1)	1(2)	2(1)
N(6A)	22(2)	16(1)	18(2)	9(1)	3(1)	3(1)
C(30A)	22(5)	12(3)	14(3)	5(2)	10(2)	3(3)
C(31A)	14(3)	19(3)	29(3)	15(2)	7(2)	11(2)
C(32A)	25(4)	11(3)	17(2)	4(2)	8(2)	6(2)
C(33A)	17(2)	10(2)	17(2)	6(2)	5(2)	6(2)
C(34A)	23(3)	18(3)	14(2)	2(2)	2(2)	10(2)
C(35A)	19(3)	18(4)	9(3)	1(3)	-1(2)	9(2)
C(50A)	15(4)	20(5)	14(3)	7(3)	2(2)	-1(2)
C(51A)	22(2)	14(3)	11(2)	2(2)	3(2)	5(2)
C(52A)	22(2)	12(2)	15(2)	2(2)	3(2)	5(1)
C(53A)	20(2)	12(2)	13(2)	3(2)	4(2)	6(1)
C(54A)	27(3)	24(2)	18(2)	11(2)	10(2)	17(2)
C(55A)	22(4)	24(2)	26(2)	11(2)	5(2)	12(2)
C(1S)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(2S)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(3S)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(4S)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(5S)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(1T)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(2T)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(3T)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)

C(4T)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)
C(5T)	36(1)	25(1)	24(1)	16(1)	20(1)	22(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Trisazo macrocycle **2**.

	x	y	z	U(eq)
H(2)	7243	7675	4555	33
H(3)	8639	9146	5889	32
H(5)	11607	8403	5056	29
H(6)	10217	6918	3723	29
H(8A)	10575	11041	6641	38
H(8AB)	11216	11158	7687	38
H(8AC)	9807	10365	7105	38
H(9A)	12877	9710	6287	34
H(9AB)	13038	10781	7185	34
H(9AC)	12389	10634	6130	34
H(11)	12477	8361	6622	31
H(12)	12338	7122	7280	34
H(14)	10110	8432	8759	29
H(15)	10234	9666	8083	27
H(22)	8712	6123	9642	23
H(23)	7804	4483	9662	21
H(25)	9720	3120	7890	23
H(26)	10655	4760	7885	25
H(28A)	6394	2867	9143	34
H(28B)	7545	2849	9899	34
H(28C)	6539	1749	9103	34
H(29A)	8173	1072	8498	34
H(29B)	9175	2112	9371	34
H(29C)	9276	1833	8311	34
H(42)	7267	4267	2055	26
H(43)	5898	2550	1077	24
H(45)	2885	3558	1499	27
H(46)	4252	5273	2507	29
H(48A)	3290	238	-321	40
H(48B)	4708	1042	177	40

H(48C)	3736	1235	-577	40
H(49A)	1940	1789	-212	38
H(49B)	1692	2004	801	38
H(49C)	1482	809	63	38
H(31)	7896	905	6933	13
H(32)	6858	433	5339	16
H(34)	4848	2467	6140	23
H(35)	5846	2912	7728	25
H(51)	4645	496	1363	23
H(52)	5100	402	2845	21
H(54)	2733	2107	3633	25
H(55)	2268	2171	2156	24
H(31A)	7689	1005	6807	22
H(32A)	6530	663	5272	21
H(34A)	4603	2636	6434	24
H(35A)	5862	3062	7948	20
H(51A)	4623	282	1053	20
H(52A)	5301	92	2459	22
H(54A)	3312	1959	3708	24
H(55A)	2624	2132	2291	28
H(1SA)	6077	7401	1153	34
H(1SB)	7415	7336	1642	34
H(1SC)	6188	6933	1944	34
H(2SA)	6666	5949	192	27
H(2SB)	6539	5457	953	27
H(3SA)	4550	5660	-277	27
H(3SB)	4352	5371	593	27
H(4SA)	5010	4059	-1015	27
H(4SB)	5001	3792	-107	27
H(5SA)	2860	3716	-1438	34
H(5SB)	2776	3719	-432	34
H(5SC)	3074	2753	-1183	34
H(1TA)	7383	6610	608	34
H(1TB)	7294	5793	1102	34
H(1TC)	7246	6975	1664	34
H(2TA)	5135	5990	1134	27
H(2TB)	5257	6434	334	27
H(3TA)	5525	4405	153	27
H(3TB)	5501	4840	-660	27

H(4TA)	3385	4341	32	27
H(4TB)	3361	4774	-779	27
H(5TA)	2374	2957	-1418	34
H(5TB)	3667	2793	-973	34
H(5TC)	3579	3225	-1789	34

Tetraazo macrocycle 3

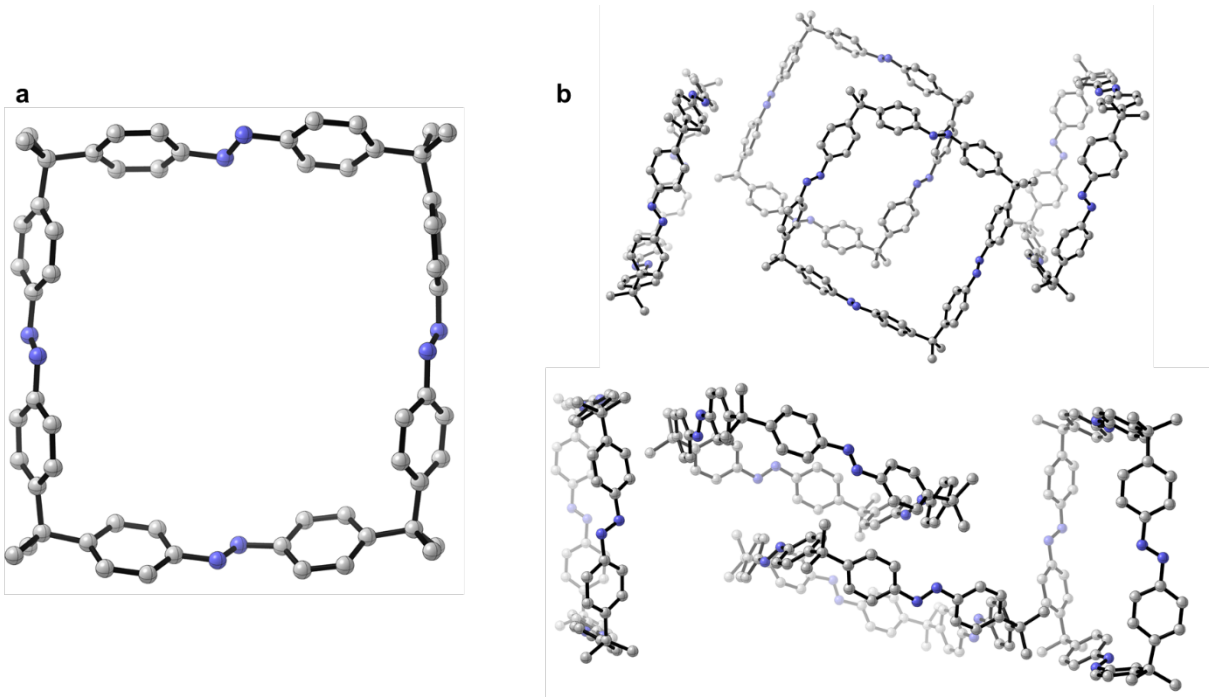

Figure S14a: Single crystal structure of tetraazo macrocycle **3**. **b:** Crystal packing of tetraazo macrocycle **3** (grey: carbon, blue: nitrogen; hydrogens omitted).

The unit cell of Tetraazo macrocycle **3** was determined using 9769 reflections and the structure was solved in the monoclinic space group $P2_1/n$. The asymmetric unit contains one molecule of Tetraazo macrocycle **3**, two disordered CH_2Cl_2 molecules and other, heavily disordered solvent molecules. One of the four diphenyl-azo parts of the molecule was found to be disordered over two positions. The disorder was modeled with the help of similarity restraints (with s.u. set to 50% of the standard value) on anisotropic displacement parameters, advanced rigid bond restraints and same distance restraints on 1,2 and 1,3 distances. The anisotropic displacement parameters of some of the atoms in the disordered part were set to the same values. The disorder ratio was allowed to refine freely and converged to 0.612(13). Both disordered CH_2Cl_2 molecules were modeled over two positions with the restraints mentioned before. Their disorder rations were refined and converged to 0.911(3) and 0.658(17). It was not possible to find a reasonable disorder model for the other, heavily disordered solvent molecules. SQUEEZE was used to include a model for these solvent molecules. The obtained model was added as .fab-file to the refinement using SHELXL. SQUEEZE found four independent voids with disordered solvent, located at 0.10 0.09 0.16, -0.10 0.91 0.84, 0.40 0.59 0.34 and 0.60 0.41 0.66 with a combined volume of 332 $Å^3$. The equivalent of 72 electrons were identified in the void.

Crystal data and structure refinement for Tetraazo macrocycle **3** .

CCDC No	1902883	
Empirical formula	$C_{62}\ H_{60}\ Cl_4\ N_8$	
Formula weight	1058.98	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 16.6359(7) Å	α= 90°.
	b = 20.2232(9) Å	β= 100.2158(13)°.
	c = 17.4545(8) Å	γ = 90°.
Volume	5779.1(4) $Å^3$	
Z	4	
Density (calculated)	1.217 Mg/m^3	
Absorption coefficient	0.251 mm^{-1}	
F(000)	2224	
Crystal size	0.169 x 0.166 x 0.126 mm^3	
Theta range for data collection	2.367 to 26.372°.	
Index ranges	-20<=h<=20, -25<=k<=25, -21<=l<=21	
Reflections collected	181053	
Independent reflections	11826 [R(int) = 0.0749]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11826 / 1918 / 822	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0675, wR2 = 0.1604	
R indices (all data)	R1 = 0.0941, wR2 = 0.1755	
Largest diff. peak and hole	0.686 and -0.543 $e.Å^{-3}$	

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

	x	y	z	U(eq)
N(1)	9101(1)	4504(1)	4292(1)	23(1)
N(2)	8914(1)	5106(1)	4199(1)	26(1)
N(3)	4298(1)	6605(1)	5416(2)	38(1)
N(4)	4014(1)	7144(1)	5144(1)	30(1)
N(5)	1025(9)	5172(4)	970(6)	29(1)
N(6)	1630(4)	5309(3)	657(4)	29(1)
N(5A)	1073(15)	5114(7)	1046(9)	29(1)
N(6A)	1423(6)	5332(6)	526(6)	29(1)
N(7)	5813(1)	3379(1)	-582(1)	24(1)
N(8)	6007(1)	3045(1)	30(1)	23(1)
C(1)	6862(1)	3032(1)	329(1)	21(1)
C(2)	7085(2)	2780(2)	1076(2)	29(1)
C(3)	7893(2)	2778(2)	1435(2)	29(1)
C(4)	8506(1)	3024(1)	1057(1)	21(1)
C(5)	8275(2)	3248(1)	298(1)	22(1)
C(6)	7464(2)	3255(1)	-66(1)	22(1)
C(7)	9385(1)	3049(1)	1507(1)	21(1)
C(8)	9963(1)	3410(1)	1051(1)	26(1)
C(9)	9697(2)	2337(1)	1649(2)	26(1)
C(10)	9359(1)	3433(1)	2262(1)	20(1)
C(11)	9571(2)	3168(1)	3004(1)	23(1)
C(12)	9494(2)	3535(1)	3660(1)	24(1)
C(13)	9213(1)	4178(1)	3592(1)	22(1)
C(14)	9001(2)	4451(1)	2850(2)	30(1)
C(15)	9068(2)	4080(1)	2205(2)	29(1)
C(21)	8713(2)	5420(1)	4873(1)	25(1)
C(22)	8879(2)	5169(1)	5623(2)	25(1)
C(23)	8580(2)	5486(1)	6218(1)	25(1)
C(24)	8108(1)	6055(1)	6080(1)	23(1)
C(25)	7988(2)	6320(2)	5332(2)	30(1)
C(26)	8289(2)	6013(1)	4737(2)	31(1)
C(27)	7729(2)	6405(1)	6712(1)	26(1)
C(28)	8175(2)	7062(1)	6905(2)	30(1)

C(29)	7825(2)	5998(2)	7467(2)	32(1)
C(30)	6815(2)	6499(1)	6387(2)	27(1)
C(31)	6336(2)	5938(2)	6182(2)	47(1)
C(32)	5514(2)	5993(2)	5871(2)	50(1)
C(33)	5158(2)	6612(2)	5752(2)	36(1)
C(34)	5618(2)	7171(2)	5933(2)	31(1)
C(35)	6446(2)	7107(2)	6250(2)	30(1)
C(41)	3163(2)	7100(1)	4805(2)	26(1)
C(42)	2849(2)	7612(1)	4322(2)	28(1)
C(43)	2046(2)	7586(1)	3928(1)	25(1)
C(44)	1544(1)	7050(1)	4007(1)	21(1)
C(45)	1858(2)	6558(1)	4536(2)	31(1)
C(46)	2656(2)	6575(2)	4926(2)	34(1)
C(47)	703(2)	6957(1)	3493(1)	23(1)
C(48)	378(2)	7608(1)	3086(2)	31(1)
C(49)	72(2)	6714(1)	3975(2)	26(1)
C(50)	765(7)	6438(7)	2858(8)	22(2)
C(51)	284(4)	5881(3)	2692(3)	20(1)
C(52)	381(4)	5462(3)	2087(4)	22(1)
C(53)	933(6)	5599(7)	1614(8)	26(1)
C(54)	1432(6)	6156(4)	1777(4)	41(2)
C(55)	1341(6)	6561(4)	2387(4)	40(2)
C(61)	1701(8)	4879(7)	9(8)	26(2)
C(62)	1295(6)	4283(6)	-132(6)	26(2)
C(63)	1486(8)	3858(7)	-703(7)	22(2)
C(64)	2060(20)	4029(13)	-1160(20)	20(2)
C(65)	2414(9)	4660(6)	-1042(8)	23(2)
C(66)	2237(9)	5080(6)	-471(8)	28(2)
C(50A)	890(10)	6487(11)	2831(13)	24(3)
C(51A)	267(7)	6076(7)	2473(8)	40(3)
C(52A)	354(7)	5648(7)	1878(8)	42(3)
C(53A)	1088(10)	5625(11)	1627(13)	26(1)
C(54A)	1741(7)	6000(5)	2000(6)	35(2)
C(55A)	1651(7)	6408(6)	2614(7)	36(2)
C(61A)	1556(12)	4841(11)	-39(12)	26(2)
C(62A)	1134(11)	4277(10)	-259(11)	26(2)
C(63A)	1358(12)	3871(11)	-831(12)	23(3)
C(64A)	2040(30)	4010(20)	-1150(40)	20(3)
C(65A)	2480(15)	4590(9)	-920(12)	24(3)

C(66A)	2253(14)	4990(9)	-358(12)	29(3)
C(67)	2356(1)	3561(1)	-1740(1)	20(1)
C(68)	2157(2)	3865(1)	-2562(1)	25(1)
C(69)	1955(2)	2875(1)	-1768(2)	25(1)
C(70)	3280(1)	3490(1)	-1466(1)	19(1)
C(71)	3859(2)	3723(1)	-1881(1)	22(1)
C(72)	4689(2)	3683(1)	-1578(1)	24(1)
C(73)	4953(1)	3399(1)	-853(1)	22(1)
C(74)	4376(2)	3167(1)	-424(1)	23(1)
C(75)	3557(1)	3211(1)	-731(1)	22(1)
Cl(1S)	6917(1)	4109(1)	2631(1)	114(1)
Cl(2S)	6466(2)	5053(1)	3742(1)	110(1)
C(1S)	6138(3)	4408(3)	3084(3)	75(1)
Cl(1T)	6256(19)	4027(15)	2086(13)	176(9)
Cl(2T)	6828(7)	4753(8)	3446(10)	77(4)
C(1T)	6740(30)	3950(13)	3058(16)	75(1)
Cl(3S)	6180(3)	5427(2)	8397(3)	92(1)
Cl(4S)	4716(1)	5509(1)	9052(1)	35(1)
C(2S)	5740(3)	5258(5)	9221(4)	40(2)
Cl(3T)	6355(7)	5554(6)	8664(10)	122(4)
Cl(4T)	4764(8)	5478(6)	9055(7)	175(7)
C(2T)	5792(11)	5299(17)	9365(14)	108(6)

Bond lengths [Å] and angles [°] for Tetraazo macrocycle **3** .

N(1)-N(2)	1.259(3)	N(7)-C(73)	1.425(3)
N(1)-C(13)	1.429(3)	N(8)-C(1)	1.426(3)
N(2)-C(21)	1.428(3)	C(1)-C(2)	1.388(3)
N(3)-N(4)	1.247(3)	C(1)-C(6)	1.389(3)
N(3)-C(33)	1.446(4)	C(2)-C(3)	1.379(4)
N(4)-C(41)	1.438(3)	C(2)-H(2)	0.9500
N(5)-N(6)	1.259(9)	C(3)-C(4)	1.399(3)
N(5)-C(53)	1.446(7)	C(3)-H(3)	0.9500
N(6)-C(61)	1.448(7)	C(4)-C(5)	1.389(3)
N(5A)-N(6A)	1.241(13)	C(4)-C(7)	1.534(3)
N(5A)-C(53A)	1.446(11)	C(5)-C(6)	1.386(3)
N(6A)-C(61A)	1.445(11)	C(5)-H(5)	0.9500
N(7)-N(8)	1.256(3)	C(6)-H(6)	0.9500

C(7)-C(9)	1.536(4)	C(30)-C(35)	1.377(4)
C(7)-C(10)	1.536(3)	C(30)-C(31)	1.394(4)
C(7)-C(8)	1.538(3)	C(31)-C(32)	1.384(4)
C(8)-H(8A)	0.9800	C(31)-H(31)	0.9500
C(8)-H(8B)	0.9800	C(32)-C(33)	1.385(5)
C(8)-H(8C)	0.9800	C(32)-H(32)	0.9500
C(9)-H(9A)	0.9800	C(33)-C(34)	1.371(4)
C(9)-H(9B)	0.9800	C(34)-C(35)	1.397(4)
C(9)-H(9C)	0.9800	C(34)-H(34)	0.9500
C(10)-C(11)	1.389(3)	C(35)-H(35)	0.9500
C(10)-C(15)	1.393(4)	C(41)-C(42)	1.379(4)
C(11)-C(12)	1.389(4)	C(41)-C(46)	1.395(4)
C(11)-H(11)	0.9500	C(42)-C(43)	1.390(4)
C(12)-C(13)	1.380(4)	C(42)-H(42)	0.9500
C(12)-H(12)	0.9500	C(43)-C(44)	1.391(3)
C(13)-C(14)	1.394(4)	C(43)-H(43)	0.9500
C(14)-C(15)	1.374(4)	C(44)-C(45)	1.394(4)
C(14)-H(14)	0.9500	C(44)-C(47)	1.534(3)
C(15)-H(15)	0.9500	C(45)-C(46)	1.381(4)
C(21)-C(22)	1.384(4)	C(45)-H(45)	0.9500
C(21)-C(26)	1.391(4)	C(46)-H(46)	0.9500
C(22)-C(23)	1.386(4)	C(47)-C(49)	1.539(4)
C(22)-H(22)	0.9500	C(47)-C(50)	1.543(7)
C(23)-C(24)	1.391(4)	C(47)-C(48)	1.546(4)
C(23)-H(23)	0.9500	C(47)-C(50A)	1.569(10)
C(24)-C(25)	1.392(4)	C(48)-H(48A)	0.9800
C(24)-C(27)	1.537(3)	C(48)-H(48B)	0.9800
C(25)-C(26)	1.378(4)	C(48)-H(48C)	0.9800
C(25)-H(25)	0.9500	C(49)-H(49A)	0.9800
C(26)-H(26)	0.9500	C(49)-H(49B)	0.9800
C(27)-C(28)	1.530(4)	C(49)-H(49C)	0.9800
C(27)-C(29)	1.537(4)	C(50)-C(51)	1.382(8)
C(27)-C(30)	1.538(3)	C(50)-C(55)	1.391(9)
C(28)-H(28A)	0.9800	C(51)-C(52)	1.386(7)
C(28)-H(28B)	0.9800	C(51)-H(51)	0.9500
C(28)-H(28C)	0.9800	C(52)-C(53)	1.367(8)
C(29)-H(29A)	0.9800	C(52)-H(52)	0.9500
C(29)-H(29B)	0.9800	C(53)-C(54)	1.399(9)
C(29)-H(29C)	0.9800	C(54)-C(55)	1.373(7)

C(54)-H(54)	0.9500	C(68)-H(68C)	0.9800
C(55)-H(55)	0.9500	C(69)-H(69A)	0.9800
C(61)-C(62)	1.382(8)	C(69)-H(69B)	0.9800
C(61)-C(66)	1.389(9)	C(69)-H(69C)	0.9800
C(62)-C(63)	1.395(8)	C(70)-C(71)	1.387(3)
C(62)-H(62)	0.9500	C(70)-C(75)	1.401(3)
C(63)-C(64)	1.391(10)	C(71)-C(72)	1.391(3)
C(63)-H(63)	0.9500	C(71)-H(71)	0.9500
C(64)-C(65)	1.402(10)	C(72)-C(73)	1.388(3)
C(64)-C(67)	1.535(8)	C(72)-H(72)	0.9500
C(65)-C(66)	1.380(8)	C(73)-C(74)	1.399(3)
C(65)-H(65)	0.9500	C(74)-C(75)	1.375(3)
C(66)-H(66)	0.9500	C(74)-H(74)	0.9500
C(50A)-C(51A)	1.387(11)	C(75)-H(75)	0.9500
C(50A)-C(55A)	1.395(12)	Cl(1S)-C(1S)	1.742(5)
C(51A)-C(52A)	1.379(10)	Cl(2S)-C(1S)	1.760(5)
C(51A)-H(51A)	0.9500	C(1S)-H(1SA)	0.9900
C(52A)-C(53A)	1.370(12)	C(1S)-H(1SB)	0.9900
C(52A)-H(52A)	0.9500	Cl(1T)-C(1T)	1.749(15)
C(53A)-C(54A)	1.388(11)	Cl(2T)-C(1T)	1.755(16)
C(54A)-C(55A)	1.382(10)	C(1T)-H(1TA)	0.9900
C(54A)-H(54A)	0.9500	C(1T)-H(1TB)	0.9900
C(55A)-H(55A)	0.9500	Cl(3S)-C(2S)	1.760(5)
C(61A)-C(62A)	1.358(11)	Cl(4S)-C(2S)	1.752(6)
C(61A)-C(66A)	1.404(12)	C(2S)-H(2SA)	0.9900
C(62A)-C(63A)	1.394(11)	C(2S)-H(2SB)	0.9900
C(62A)-H(62A)	0.9500	Cl(3T)-C(2T)	1.746(14)
C(63A)-C(64A)	1.382(12)	Cl(4T)-C(2T)	1.737(14)
C(63A)-H(63A)	0.9500	C(2T)-H(2TA)	0.9900
C(64A)-C(65A)	1.400(13)	C(2T)-H(2TB)	0.9900
C(64A)-C(67)	1.533(11)		
C(65A)-C(66A)	1.376(11)	N(2)-N(1)-C(13)	113.8(2)
C(65A)-H(65A)	0.9500	N(1)-N(2)-C(21)	114.3(2)
C(66A)-H(66A)	0.9500	N(4)-N(3)-C(33)	115.2(2)
C(67)-C(70)	1.533(3)	N(3)-N(4)-C(41)	112.4(2)
C(67)-C(69)	1.536(3)	N(6)-N(5)-C(53)	114.1(8)
C(67)-C(68)	1.542(3)	N(5)-N(6)-C(61)	112.9(7)
C(68)-H(68A)	0.9800	N(6A)-N(5A)-C(53A)	107.9(13)
C(68)-H(68B)	0.9800	N(5A)-N(6A)-C(61A)	113.9(13)

N(8)-N(7)-C(73)	113.0(2)	C(11)-C(10)-C(7)	124.3(2)
N(7)-N(8)-C(1)	114.2(2)	C(15)-C(10)-C(7)	118.4(2)
C(2)-C(1)-C(6)	119.4(2)	C(12)-C(11)-C(10)	121.2(2)
C(2)-C(1)-N(8)	115.7(2)	C(12)-C(11)-H(11)	119.4
C(6)-C(1)-N(8)	124.9(2)	C(10)-C(11)-H(11)	119.4
C(3)-C(2)-C(1)	120.2(2)	C(13)-C(12)-C(11)	120.8(2)
C(3)-C(2)-H(2)	119.9	C(13)-C(12)-H(12)	119.6
C(1)-C(2)-H(2)	119.9	C(11)-C(12)-H(12)	119.6
C(2)-C(3)-C(4)	121.2(2)	C(12)-C(13)-C(14)	118.6(2)
C(2)-C(3)-H(3)	119.4	C(12)-C(13)-N(1)	117.1(2)
C(4)-C(3)-H(3)	119.4	C(14)-C(13)-N(1)	124.1(2)
C(5)-C(4)-C(3)	117.7(2)	C(15)-C(14)-C(13)	120.1(3)
C(5)-C(4)-C(7)	123.7(2)	C(15)-C(14)-H(14)	120.0
C(3)-C(4)-C(7)	118.5(2)	C(13)-C(14)-H(14)	120.0
C(6)-C(5)-C(4)	121.5(2)	C(14)-C(15)-C(10)	122.1(2)
C(6)-C(5)-H(5)	119.3	C(14)-C(15)-H(15)	118.9
C(4)-C(5)-H(5)	119.3	C(10)-C(15)-H(15)	118.9
C(5)-C(6)-C(1)	119.9(2)	C(22)-C(21)-C(26)	119.2(2)
C(5)-C(6)-H(6)	120.1	C(22)-C(21)-N(2)	125.4(2)
C(1)-C(6)-H(6)	120.1	C(26)-C(21)-N(2)	115.4(2)
C(4)-C(7)-C(9)	108.4(2)	C(21)-C(22)-C(23)	120.1(2)
C(4)-C(7)-C(10)	106.69(18)	C(21)-C(22)-H(22)	120.0
C(9)-C(7)-C(10)	113.4(2)	C(23)-C(22)-H(22)	120.0
C(4)-C(7)-C(8)	112.2(2)	C(22)-C(23)-C(24)	121.3(2)
C(9)-C(7)-C(8)	107.6(2)	C(22)-C(23)-H(23)	119.3
C(10)-C(7)-C(8)	108.7(2)	C(24)-C(23)-H(23)	119.3
C(7)-C(8)-H(8A)	109.5	C(23)-C(24)-C(25)	117.6(2)
C(7)-C(8)-H(8B)	109.5	C(23)-C(24)-C(27)	123.2(2)
H(8A)-C(8)-H(8B)	109.5	C(25)-C(24)-C(27)	119.2(2)
C(7)-C(8)-H(8C)	109.5	C(26)-C(25)-C(24)	121.5(3)
H(8A)-C(8)-H(8C)	109.5	C(26)-C(25)-H(25)	119.2
H(8B)-C(8)-H(8C)	109.5	C(24)-C(25)-H(25)	119.2
C(7)-C(9)-H(9A)	109.5	C(25)-C(26)-C(21)	120.1(2)
C(7)-C(9)-H(9B)	109.5	C(25)-C(26)-H(26)	119.9
H(9A)-C(9)-H(9B)	109.5	C(21)-C(26)-H(26)	120.0
C(7)-C(9)-H(9C)	109.5	C(28)-C(27)-C(29)	107.7(2)
H(9A)-C(9)-H(9C)	109.5	C(28)-C(27)-C(24)	108.2(2)
H(9B)-C(9)-H(9C)	109.5	C(29)-C(27)-C(24)	112.1(2)
C(11)-C(10)-C(15)	117.2(2)	C(28)-C(27)-C(30)	112.6(2)

C(29)-C(27)-C(30)	109.2(2)	C(42)-C(43)-H(43)	119.3
C(24)-C(27)-C(30)	107.2(2)	C(44)-C(43)-H(43)	119.3
C(27)-C(28)-H(28A)	109.5	C(43)-C(44)-C(45)	117.4(2)
C(27)-C(28)-H(28B)	109.5	C(43)-C(44)-C(47)	122.6(2)
H(28A)-C(28)-H(28B)	109.5	C(45)-C(44)-C(47)	119.7(2)
C(27)-C(28)-H(28C)	109.5	C(46)-C(45)-C(44)	121.6(2)
H(28A)-C(28)-H(28C)	109.5	C(46)-C(45)-H(45)	119.2
H(28B)-C(28)-H(28C)	109.5	C(44)-C(45)-H(45)	119.2
C(27)-C(29)-H(29A)	109.5	C(45)-C(46)-C(41)	119.9(3)
C(27)-C(29)-H(29B)	109.5	C(45)-C(46)-H(46)	120.1
H(29A)-C(29)-H(29B)	109.5	C(41)-C(46)-H(46)	120.1
C(27)-C(29)-H(29C)	109.5	C(44)-C(47)-C(49)	111.00(19)
H(29A)-C(29)-H(29C)	109.5	C(44)-C(47)-C(50)	109.5(6)
H(29B)-C(29)-H(29C)	109.5	C(49)-C(47)-C(50)	108.3(4)
C(35)-C(30)-C(31)	117.7(2)	C(44)-C(47)-C(48)	111.9(2)
C(35)-C(30)-C(27)	123.7(2)	C(49)-C(47)-C(48)	107.9(2)
C(31)-C(30)-C(27)	118.4(3)	C(50)-C(47)-C(48)	108.2(8)
C(32)-C(31)-C(30)	121.0(3)	C(44)-C(47)-C(50A)	103.1(8)
C(32)-C(31)-H(31)	119.5	C(49)-C(47)-C(50A)	116.9(7)
C(30)-C(31)-H(31)	119.5	C(48)-C(47)-C(50A)	106.1(12)
C(31)-C(32)-C(33)	119.9(3)	C(47)-C(48)-H(48A)	109.5
C(31)-C(32)-H(32)	120.0	C(47)-C(48)-H(48B)	109.5
C(33)-C(32)-H(32)	120.0	H(48A)-C(48)-H(48B)	109.5
C(34)-C(33)-C(32)	120.3(3)	C(47)-C(48)-H(48C)	109.5
C(34)-C(33)-N(3)	124.9(3)	H(48A)-C(48)-H(48C)	109.5
C(32)-C(33)-N(3)	114.7(3)	H(48B)-C(48)-H(48C)	109.5
C(33)-C(34)-C(35)	119.0(3)	C(47)-C(49)-H(49A)	109.5
C(33)-C(34)-H(34)	120.5	C(47)-C(49)-H(49B)	109.5
C(35)-C(34)-H(34)	120.5	H(49A)-C(49)-H(49B)	109.5
C(30)-C(35)-C(34)	122.0(3)	C(47)-C(49)-H(49C)	109.5
C(30)-C(35)-H(35)	119.0	H(49A)-C(49)-H(49C)	109.5
C(34)-C(35)-H(35)	119.0	H(49B)-C(49)-H(49C)	109.5
C(42)-C(41)-C(46)	119.4(2)	C(51)-C(50)-C(55)	117.1(6)
C(42)-C(41)-N(4)	116.4(2)	C(51)-C(50)-C(47)	126.5(6)
C(46)-C(41)-N(4)	124.2(2)	C(55)-C(50)-C(47)	116.3(7)
C(41)-C(42)-C(43)	120.1(2)	C(50)-C(51)-C(52)	121.1(5)
C(41)-C(42)-H(42)	120.0	C(50)-C(51)-H(51)	119.5
C(43)-C(42)-H(42)	120.0	C(52)-C(51)-H(51)	119.5
C(42)-C(43)-C(44)	121.4(2)	C(53)-C(52)-C(51)	121.3(6)

C(53)-C(52)-H(52)	119.4	C(52A)-C(53A)-N(5A)	110.0(11)
C(51)-C(52)-H(52)	119.4	C(54A)-C(53A)-N(5A)	129.4(13)
C(52)-C(53)-C(54)	118.5(6)	C(55A)-C(54A)-C(53A)	120.5(9)
C(52)-C(53)-N(5)	121.6(7)	C(55A)-C(54A)-H(54A)	119.8
C(54)-C(53)-N(5)	119.9(7)	C(53A)-C(54A)-H(54A)	119.8
C(55)-C(54)-C(53)	119.7(6)	C(54A)-C(55A)-C(50A)	120.5(9)
C(55)-C(54)-H(54)	120.2	C(54A)-C(55A)-H(55A)	119.8
C(53)-C(54)-H(54)	120.2	C(50A)-C(55A)-H(55A)	119.8
C(54)-C(55)-C(50)	122.3(5)	C(62A)-C(61A)-C(66A)	119.4(10)
C(54)-C(55)-H(55)	118.8	C(62A)-C(61A)-N(6A)	129.4(12)
C(50)-C(55)-H(55)	118.8	C(66A)-C(61A)-N(6A)	111.1(11)
C(62)-C(61)-C(66)	119.6(7)	C(61A)-C(62A)-C(63A)	120.4(13)
C(62)-C(61)-N(6)	124.0(8)	C(61A)-C(62A)-H(62A)	119.8
C(66)-C(61)-N(6)	116.4(7)	C(63A)-C(62A)-H(62A)	119.8
C(61)-C(62)-C(63)	120.0(8)	C(64A)-C(63A)-C(62A)	120.9(13)
C(61)-C(62)-H(62)	120.0	C(64A)-C(63A)-H(63A)	119.6
C(63)-C(62)-H(62)	120.0	C(62A)-C(63A)-H(63A)	119.6
C(64)-C(63)-C(62)	121.3(8)	C(63A)-C(64A)-C(65A)	118.5(11)
C(64)-C(63)-H(63)	119.4	C(63A)-C(64A)-C(67)	123.6(13)
C(62)-C(63)-H(63)	119.4	C(65A)-C(64A)-C(67)	117.9(13)
C(63)-C(64)-C(65)	117.3(7)	C(66A)-C(65A)-C(64A)	120.2(13)
C(63)-C(64)-C(67)	123.9(10)	C(66A)-C(65A)-H(65A)	119.9
C(65)-C(64)-C(67)	118.8(9)	C(64A)-C(65A)-H(65A)	119.9
C(66)-C(65)-C(64)	121.7(9)	C(65A)-C(66A)-C(61A)	120.4(13)
C(66)-C(65)-H(65)	119.1	C(65A)-C(66A)-H(66A)	119.8
C(64)-C(65)-H(65)	119.1	C(61A)-C(66A)-H(66A)	119.8
C(65)-C(66)-C(61)	119.8(8)	C(70)-C(67)-C(64A)	107(3)
C(65)-C(66)-H(66)	120.1	C(70)-C(67)-C(64)	105.7(16)
C(61)-C(66)-H(66)	120.1	C(70)-C(67)-C(69)	109.3(2)
C(51A)-C(50A)-C(55A)	116.8(9)	C(64A)-C(67)-C(69)	111.1(10)
C(51A)-C(50A)-C(47)	117.7(9)	C(64)-C(67)-C(69)	113.0(6)
C(55A)-C(50A)-C(47)	125.3(9)	C(70)-C(67)-C(68)	111.53(19)
C(52A)-C(51A)-C(50A)	123.1(10)	C(64A)-C(67)-C(68)	110(3)
C(52A)-C(51A)-H(51A)	118.5	C(64)-C(67)-C(68)	109.4(19)
C(50A)-C(51A)-H(51A)	118.5	C(69)-C(67)-C(68)	108.1(2)
C(53A)-C(52A)-C(51A)	118.7(10)	C(67)-C(68)-H(68A)	109.5
C(53A)-C(52A)-H(52A)	120.6	C(67)-C(68)-H(68B)	109.5
C(51A)-C(52A)-H(52A)	120.6	H(68A)-C(68)-H(68B)	109.5
C(52A)-C(53A)-C(54A)	120.0(10)	C(67)-C(68)-H(68C)	109.5

H(68A)-C(68)-H(68C)	109.5	C(70)-C(75)-H(75)	119.2
H(68B)-C(68)-H(68C)	109.5	Cl(1S)-C(1S)-Cl(2S)	112.6(3)
C(67)-C(69)-H(69A)	109.5	Cl(1S)-C(1S)-H(1SA)	109.1
C(67)-C(69)-H(69B)	109.5	Cl(2S)-C(1S)-H(1SA)	109.1
H(69A)-C(69)-H(69B)	109.5	Cl(1S)-C(1S)-H(1SB)	109.1
C(67)-C(69)-H(69C)	109.5	Cl(2S)-C(1S)-H(1SB)	109.1
H(69A)-C(69)-H(69C)	109.5	H(1SA)-C(1S)-H(1SB)	107.8
H(69B)-C(69)-H(69C)	109.5	Cl(1T)-C(1T)-Cl(2T)	106.6(16)
C(71)-C(70)-C(75)	117.9(2)	Cl(1T)-C(1T)-H(1TA)	110.4
C(71)-C(70)-C(67)	123.7(2)	Cl(2T)-C(1T)-H(1TA)	110.4
C(75)-C(70)-C(67)	118.2(2)	Cl(1T)-C(1T)-H(1TB)	110.4
C(70)-C(71)-C(72)	121.1(2)	Cl(2T)-C(1T)-H(1TB)	110.4
C(70)-C(71)-H(71)	119.5	H(1TA)-C(1T)-H(1TB)	108.6
C(72)-C(71)-H(71)	119.5	Cl(4S)-C(2S)-Cl(3S)	109.8(4)
C(73)-C(72)-C(71)	120.2(2)	Cl(4S)-C(2S)-H(2SA)	109.7
C(73)-C(72)-H(72)	119.9	Cl(3S)-C(2S)-H(2SA)	109.7
C(71)-C(72)-H(72)	119.9	Cl(4S)-C(2S)-H(2SB)	109.7
C(72)-C(73)-C(74)	119.3(2)	Cl(3S)-C(2S)-H(2SB)	109.7
C(72)-C(73)-N(7)	116.8(2)	H(2SA)-C(2S)-H(2SB)	108.2
C(74)-C(73)-N(7)	123.8(2)	Cl(4T)-C(2T)-Cl(3T)	109.9(12)
C(75)-C(74)-C(73)	119.8(2)	Cl(4T)-C(2T)-H(2TA)	109.7
C(75)-C(74)-H(74)	120.1	Cl(3T)-C(2T)-H(2TA)	109.7
C(73)-C(74)-H(74)	120.1	Cl(4T)-C(2T)-H(2TB)	109.7
C(74)-C(75)-C(70)	121.7(2)	Cl(3T)-C(2T)-H(2TB)	109.7
C(74)-C(75)-H(75)	119.2	H(2TA)-C(2T)-H(2TB)	108.2

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Tetraazo macrocycle **3**. 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)	19(1)	31(1)	20(1)	-1(1)	6(1)	-2(1)
N(2)	26(1)	33(1)	22(1)	-2(1)	8(1)	1(1)
N(3)	23(1)	46(2)	44(2)	3(1)	4(1)	-9(1)
N(4)	24(1)	40(1)	26(1)	1(1)	7(1)	-6(1)
N(5)	35(2)	26(1)	24(2)	6(1)	4(2)	5(2)
N(6)	35(2)	26(1)	24(2)	6(1)	4(2)	5(2)
N(5A)	35(2)	26(1)	24(2)	6(1)	4(2)	5(2)
N(6A)	35(2)	26(1)	24(2)	6(1)	4(2)	5(2)
N(7)	19(1)	34(1)	17(1)	0(1)	0(1)	0(1)
N(8)	19(1)	30(1)	20(1)	1(1)	0(1)	-1(1)
C(1)	17(1)	26(1)	19(1)	-2(1)	-1(1)	-2(1)
C(2)	18(1)	46(2)	22(1)	7(1)	4(1)	-5(1)
C(3)	20(1)	48(2)	18(1)	7(1)	2(1)	-3(1)
C(4)	18(1)	27(1)	18(1)	-1(1)	3(1)	0(1)
C(5)	20(1)	28(1)	18(1)	0(1)	6(1)	-2(1)
C(6)	22(1)	27(1)	15(1)	0(1)	2(1)	-1(1)
C(7)	14(1)	31(1)	17(1)	-2(1)	2(1)	-1(1)
C(8)	14(1)	43(2)	21(1)	-4(1)	4(1)	-4(1)
C(9)	21(1)	35(1)	22(1)	-4(1)	2(1)	2(1)
C(10)	10(1)	31(1)	20(1)	-1(1)	4(1)	-2(1)
C(11)	20(1)	28(1)	21(1)	0(1)	2(1)	-1(1)
C(12)	22(1)	31(1)	18(1)	3(1)	2(1)	-3(1)
C(13)	15(1)	32(1)	20(1)	-1(1)	4(1)	-1(1)
C(14)	33(2)	32(2)	24(1)	2(1)	6(1)	9(1)
C(15)	32(1)	39(2)	16(1)	4(1)	2(1)	8(1)
C(21)	22(1)	33(1)	21(1)	-2(1)	8(1)	-2(1)
C(22)	23(1)	27(1)	24(1)	-2(1)	3(1)	-2(1)
C(23)	23(1)	35(1)	18(1)	-2(1)	2(1)	-4(1)
C(24)	16(1)	35(1)	20(1)	-4(1)	5(1)	-4(1)
C(25)	28(1)	37(2)	25(1)	-1(1)	6(1)	5(1)
C(26)	34(2)	39(2)	21(1)	4(1)	8(1)	5(1)
C(27)	18(1)	38(2)	21(1)	-5(1)	4(1)	-3(1)
C(28)	18(1)	42(2)	29(1)	-9(1)	2(1)	-1(1)
C(29)	27(1)	51(2)	21(1)	-4(1)	9(1)	1(1)

C(30)	16(1)	45(2)	23(1)	-5(1)	8(1)	-3(1)
C(31)	24(2)	48(2)	68(2)	-6(2)	4(1)	-4(1)
C(32)	25(2)	48(2)	75(2)	-4(2)	3(2)	-8(1)
C(33)	19(1)	51(2)	36(2)	2(1)	6(1)	-9(1)
C(34)	25(1)	42(2)	26(1)	3(1)	6(1)	-2(1)
C(35)	22(1)	41(2)	27(1)	1(1)	3(1)	-7(1)
C(41)	18(1)	40(2)	22(1)	-2(1)	6(1)	-6(1)
C(42)	24(1)	33(1)	30(1)	-2(1)	12(1)	-7(1)
C(43)	26(1)	29(1)	22(1)	3(1)	9(1)	-1(1)
C(44)	20(1)	28(1)	15(1)	-2(1)	5(1)	-1(1)
C(45)	23(1)	38(2)	31(1)	10(1)	1(1)	-9(1)
C(46)	26(1)	45(2)	30(2)	12(1)	-1(1)	-4(1)
C(47)	27(1)	26(1)	15(1)	-3(1)	-2(1)	2(1)
C(48)	38(2)	27(1)	24(1)	-4(1)	-6(1)	4(1)
C(49)	18(1)	32(1)	25(1)	-5(1)	-1(1)	2(1)
C(50)	27(3)	23(3)	16(3)	3(2)	5(3)	-4(2)
C(51)	13(2)	26(3)	20(3)	2(2)	3(2)	-2(2)
C(52)	16(2)	21(3)	27(3)	4(2)	4(2)	-3(2)
C(53)	36(4)	25(2)	16(1)	1(1)	2(2)	2(2)
C(54)	59(4)	46(4)	26(3)	-5(3)	27(3)	-26(3)
C(55)	60(4)	35(3)	30(3)	-13(3)	24(3)	-32(3)
C(61)	39(5)	22(3)	17(3)	-1(2)	2(3)	-6(3)
C(62)	27(4)	32(2)	19(4)	2(2)	7(3)	-2(2)
C(63)	25(4)	24(3)	16(4)	0(3)	-3(3)	-4(3)
C(64)	20(4)	25(3)	14(3)	2(3)	-1(3)	3(3)
C(65)	29(4)	24(3)	16(4)	7(3)	4(3)	0(3)
C(66)	43(3)	22(3)	20(4)	7(3)	8(3)	-6(3)
C(50A)	34(5)	20(5)	16(5)	-2(4)	-2(4)	2(4)
C(51A)	22(4)	44(6)	51(6)	-23(5)	-7(4)	15(4)
C(52A)	31(4)	46(6)	43(6)	-25(5)	-8(4)	10(4)
C(53A)	36(4)	25(2)	16(1)	1(1)	2(2)	2(2)
C(54A)	47(5)	31(4)	32(5)	1(3)	22(4)	-2(4)
C(55A)	39(5)	40(5)	32(5)	-5(4)	16(4)	-4(4)
C(61A)	34(5)	29(5)	15(4)	5(3)	8(4)	11(4)
C(62A)	27(4)	32(2)	19(4)	2(2)	7(3)	-2(2)
C(63A)	19(5)	27(4)	23(6)	2(4)	1(5)	4(4)
C(64A)	21(5)	23(5)	15(5)	1(5)	-1(4)	4(4)
C(65A)	29(5)	26(5)	19(6)	1(5)	5(5)	4(4)
C(66A)	41(5)	23(6)	22(6)	-3(5)	5(4)	3(4)

C(67)	17(1)	27(1)	16(1)	0(1)	-1(1)	2(1)
C(68)	21(1)	36(2)	16(1)	-1(1)	-1(1)	6(1)
C(69)	21(1)	28(1)	26(1)	-7(1)	2(1)	-2(1)
C(70)	19(1)	21(1)	17(1)	-1(1)	0(1)	2(1)
C(71)	23(1)	28(1)	15(1)	1(1)	0(1)	-1(1)
C(72)	22(1)	31(1)	19(1)	3(1)	4(1)	-2(1)
C(73)	19(1)	28(1)	18(1)	-2(1)	-1(1)	1(1)
C(74)	21(1)	30(1)	16(1)	4(1)	-1(1)	4(1)
C(75)	19(1)	29(1)	19(1)	3(1)	4(1)	-1(1)
Cl(1S)	65(1)	130(1)	157(2)	85(1)	52(1)	32(1)
Cl(2S)	137(2)	111(1)	75(1)	35(1)	3(1)	-63(1)
C(1S)	45(2)	116(4)	63(3)	35(3)	9(2)	-14(2)
Cl(1T)	158(17)	219(19)	136(11)	6(13)	-17(12)	-1(16)
Cl(2T)	43(6)	94(7)	101(9)	64(6)	29(6)	14(6)
C(1T)	45(2)	116(4)	63(3)	35(3)	9(2)	-14(2)
Cl(3S)	101(2)	95(2)	105(2)	14(2)	83(2)	-1(2)
Cl(4S)	35(1)	43(1)	26(1)	-4(1)	4(1)	-9(1)
C(2S)	42(3)	42(3)	40(3)	-8(3)	17(2)	-17(2)
Cl(3T)	155(6)	76(4)	140(7)	61(5)	41(6)	15(4)
Cl(4T)	176(9)	156(9)	189(12)	-12(7)	21(7)	-10(7)
C(2T)	129(10)	87(11)	110(11)	0(10)	25(9)	-22(10)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)
for Tetraazo macrocycle **3** .

	x	y	z	U(eq)
H(2)	6679	2607	1342	35
H(3)	8037	2608	1948	35
H(5)	8683	3399	21	26
H(6)	7320	3413	-585	26
H(8A)	9999	3162	576	39
H(8B)	10507	3443	1374	39
H(8C)	9752	3854	912	39
H(9A)	9706	2121	1148	39
H(9B)	9334	2092	1932	39
H(9C)	10250	2344	1956	39
H(11)	9773	2728	3065	28

H(12)	9636	3341	4161	28
H(14)	8809	4894	2791	36
H(15)	8911	4271	1703	35
H(22)	9198	4779	5729	30
H(23)	8701	5311	6730	30
H(25)	7692	6721	5229	36
H(26)	8206	6206	4234	37
H(28A)	8143	7325	6429	45
H(28B)	8749	6976	7127	45
H(28C)	7919	7306	7284	45
H(29A)	7572	5563	7355	49
H(29B)	7557	6229	7846	49
H(29C)	8406	5943	7681	49
H(31)	6579	5512	6258	56
H(32)	5195	5607	5739	60
H(34)	5377	7597	5843	37
H(35)	6764	7495	6374	36
H(42)	3181	7982	4258	34
H(43)	1836	7943	3598	30
H(45)	1514	6203	4631	37
H(46)	2859	6229	5277	41
H(48A)	747	7754	2740	47
H(48B)	350	7948	3480	47
H(48C)	-168	7533	2782	47
H(49A)	-458	6655	3634	39
H(49B)	20	7040	4379	39
H(49C)	252	6290	4221	39
H(51)	-119	5783	2999	24
H(52)	58	5073	1998	26
H(54)	1832	6254	1467	49
H(55)	1682	6939	2490	48
H(62)	886	4164	159	31
H(63)	1216	3443	-784	27
H(65)	2783	4801	-1366	28
H(66)	2481	5506	-408	34
H(51A)	-244	6091	2645	48
H(52A)	-87	5374	1647	50
H(54A)	2253	5976	1831	42
H(55A)	2112	6636	2891	43

H(62A)	683	4159	-21	31
H(63A)	1039	3491	-1000	28
H(65A)	2937	4705	-1150	29
H(66A)	2569	5370	-183	35
H(68A)	2381	3583	-2930	37
H(68B)	2399	4307	-2556	37
H(68C)	1563	3898	-2723	37
H(69A)	1364	2920	-1942	37
H(69B)	2062	2677	-1248	37
H(69C)	2181	2592	-2132	37
H(71)	3686	3914	-2380	27
H(72)	5077	3850	-1868	29
H(74)	4548	2980	77	28
H(75)	3169	3048	-438	26
H(1SA)	5925	4042	3366	90
H(1SB)	5685	4570	2682	90
H(1TA)	7283	3747	3089	90
H(1TB)	6408	3670	3349	90
H(2SA)	5774	4778	9336	48
H(2SB)	6044	5496	9678	48
H(2TA)	5863	4818	9454	130
H(2TB)	5993	5529	9863	130

References

[1] a) R. Salvio, L. Mandolini, C. Savelli, *J. Org. Chem.* **2013**, *78*, 7259; b) Y. Yano, JP 2012140345, **2012**.

[2] C. Zhang, N. Jiao, *Angew. Chem. Int. Ed.* **2010**, *49*, 6174.

[3] A. Heindl, L. Schweighauser, C. Logemann, H. Wegner, *Synthesis* **2017**, *49*, 2632.

[4] B. Priewisch, K. Rück-Braun, *J. Org. Chem.* **2005**, *70*, 2350.

[5] S. Bellotto, R. Reuter, C. Heinis, H. A. Wegner, *J. Org. Chem.* **2011**, *76*, 9826.

[6] R. Reuter, H. A. Wegner, *Chem. Eur. J.* **2011**, *17*, 2987.

[7] a) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1996**, *77*, 3865; b) C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, *110*, 6158.

[8] a) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104; b) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456.

[9] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

[10] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378.

[11] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji et al., *Gaussian 16 Rev. A.03*, Wallingford, CT, **2016**.

[12] C. Y. Legault, *CYLview*, Université de Sherbrooke, **2009**.

[13] a) S. E. Wheeler, K. N. Houk, P. v. R. Schleyer, W. D. Allen, *J. Am. Chem. Soc.* **2009**, *131*, 2547; b) M. Hammerich, C. Schütt, C. Stähler, P. Lentes, F. Röhricht, R. Höppner, R. Herges, *J. Am. Chem. Soc.* **2016**, *138*, 13111.

[14] L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Cryst.* **2015**, *48*, 3.

[15] G. M. Sheldrick, *Acta Cryst. A* **2015**, *71*, 3.

[16] A. Thorn, B. Dittrich, G. M. Sheldrick, *Acta Cryst. A* **2012**, *68*, 448.

[17] P. Müller, *Cryst. Rev.* **2009**, *15*, 57.

[18] A. L. Spek, *Acta Cryst. C* **2015**, *71*, 9.

[19] A. L. Spek, *Acta Cryst. D* **2009**, *65*, 148.