Supporting Information

Carbocation Catalysis in Confined Space: Activation of Trityl Chloride Inside the Hexameric Resorcinarene Capsule

Margherita De Rosa,* Stefania Gambaro, Annunziata Soriente, Paolo Della Sala, Veronica Iuliano, Carmen Talotta, Carmine Gaeta, Antonio Rescifina,[†,]* and Placido Neri*

Laboratory of Supramolecular Chemistry, Dipartimento di Chimica e Biologia "A. Zambelli", Università di Salerno, Via Giovanni Paolo II, I-84084, Fisciano (SALERNO), Italy.

[†]Dipartimento di Scienze del Farmaco e della Salute, Università di Catania, viale Andrea Doria, 6, 95125 Catania, Italy

TABLE OF CONTENTS

1. General Remarks

Acrolein, crotonaldehyde, methacrolein, and methyl vinyl ketone were distilled prior to use. Cyclopentadiene was obtained by cracking the dimer dicyclopentadiene at 180°C prior to use and stored in freezer. $TrBF_4$ is commercially available and used as received. Other chemicals were reagent grade and were used without further purification. Solvents were purchased from Aldrich. Reaction temperatures were measured externally; reactions were monitored by ^1H NMR spectroscopy and by TLC on Merck silica gel plates (0.25 mm) and visualized by UV light. Flash chromatography was performed on Merck silica gel (60, 40-63 µm). NMR spectra were recorded on Bruker Avance-600 spectrometer [600.13 MHz (^1H) and 150.03 MHz (^{13}C)], Bruker Avance-400 spectrometer [400 (^1H) and 100.57 MHz (^{13}C)], Bruker Avance-300 spectrometer [300 (^1H) and 75.48 MHz (^{13}C)]; chemical shifts are reported relative to the residual solvent peak ($CHCl_3$: δ 7.26, $CDCl_3$: δ 77.23). DOSY experiments were performed on a Bruker Avance-600 spectrometer equipped with 5 mm PABBO BB|19F-1H\D Z-GRD Z114607/0109. The standard Bruker pulse program, ledbpgp2s, employing a double stimulated echo sequence and LED, bipolar gradient pulses for diffusion, and two spoil gradients were utilized. Diffusion times were 150 ms, eddy current delay was 5 ms, gradient recovery delays were 0.2 ms, and gradient pulse was 1400 ms. Individual rows of the quasi-2D diffusion databases were phased and baseline corrected. $CDCl_3$ used for experiments was passed through activated 3Å molecular sieves and alumina basic oxide to remove water and DCl traces and was preserved in a brown glass vial to keep out of the light. High-resolution mass spectra (HRMS) were acquired using a Bruker Solaris XR Fourier transform ion cyclotron resonance mass spectrometer equipped with a 7 T refrigerated actively-shielded superconducting magnet. The samples were ionized in positive ion mode using the ESI ion source (Bruker Daltonik GmbH, Bremen, Germany). The mass spectra were calibrated externally using a NaTFA solution in positive ion mode. Low resolution mass spectral analyses were carried out using an electrospray spectrometer Waters 4 micro quadrupole. A linear calibration was applied. HR MALDI mass spectra were recorded on a Bruker Solarix FT-ICR mass spectrometer equipped with a 7T magnet. The samples recorded in MALDI were prepared by mixing 10 µL of analyte in methanol (1 mg/mL) with 10 µL of solution of 2,5-dihydroxybenzoic acid (10 mg/mL in Methanol). The mass spectra were calibrated externally, and a linear calibration was applied. Elemental analysis was performed on a Flash EA 1112 Series with Thermal Conductivity Detector, for C, H, N, and S. Water saturated deuterated chloroform was prepared as reported in the literature. [1] Resorcinarene **1** was synthesized according to literature procedures. [1] The compounds **6a**-**6f**,[2,3,4] **6h**,[5] were previously described. The *endo: exo* ratio was determined by analogy to known compounds, and by NOESY experiments.

---

[1] a) T.M. Bruer, Q. Zhang, K. Tiefenbacher, *Angew. Chem. Int. Ed.* **2016**, *55*, 7698; b) Q. Zhang, K. Tiefenbacher, L. Catti, J. Pleiss, *J. Am. Chem. Soc.*, **2017**, *139*, 11482

[2] H.F.T. Klare, K. Bergander, M. Oestreich, *Angew. Chem., Int. Ed.* **2009**, *48*, 9077-9079.

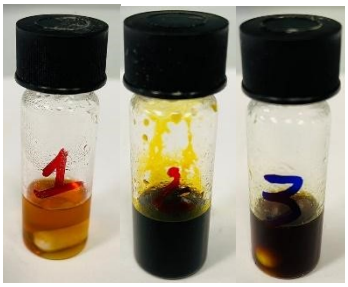
[3] Z. Zhu, J. H. Espenson, *J. Am. Chem. Soc.* **1997**, *119*, 3507–3512.

[4] E. Gould, T. Lebl, A. M. Z. Slawin, M. Reid, T. Daviesb, A. D. Smith, *Org. Biomol. Chem.*, **2013**, *11*, 7877-7892.

[5] R. K. Schmidt, K.Müther, C. Mück-Lichtenfeld, S. Grimme, M. Oestreich, *J. Am. Chem. Soc.* **2012**, *134,* 4421–4428.

2. Proofs of the formation and encapsulation of the trityl cation

For the encapsulation experiments, samples were prepared according to the following procedure: resorcinarene **1** (281.6 mg, 0.254 mmol) was weighed in a 4 mL vial and 1 mL of water saturated $CDCl_3$ was added. The mixture was warmed at 50°C until clarification (ca 5 min). To this solution, the appropriate guest Ph_3CX (0.0846 mmol, TrX, X= Cl or BF_4) was added and the mixture was stirred at 30 °C for 10 min before withdrawing the appropriate aliquot for analysis. Typical red-orange color of a tritylium ion in solution (Figure S1) was observed upon mixing of the hexameric capsule $\mathbf{C_6}$ and TrX.



(1) **(2)** **(3)**

Figure S1. Mixture of: (1) hexameric capsule $\mathbf{C_6}$ (42.3 mM), (2) capsule/TrCl (42.3 mM/84.6 mM), (3) capsule/$Tr^+BF_4^-$ (42.3 mM/84.6 mM).

3. UV-Vis experiments

All UV-Vis experiments were performed in a sealed cuvette and keeping the samples in the dark. The samples containing a solution of $\mathbf{C_6}$ and Ph_3CX (Tr-X) were prepared according to the following procedure: Resorcinarene **1** (281.6 mg, 0.254 mmol, 1 equiv) was weighed in a 4 mL vial. Then, 1 mL of water-saturated chloroform-d was added and the mixture was homogenized in an ultrasonic water bath at 40 °C for 10 min. Initial concentration of $\mathbf{C_6}$: 42.3 mM. To this clear yellow solution, Tr-X was added (2 equiv vs $\mathbf{C_6}$, for an initial concentration of 84.6 mM). When Tr-X was added, the solution turned red-orange instantly, indicating the formation of the trityl cation. After 2 h under stirring, the solution was diluted to the appropriate concentration and the UV-Vis spectra were recorded.

The UV-vis spectra of $TrBF_4$ solutions showed the characteristic twin absorption band at λ_{max}= 432 and 411 nm, indicating the presence of a free trityl cation.[6] In contrast, the solution containing Ph_3CCl did not show any absorption band in the region of interest.

[6] Shida, T. Electronic Absorption Spectra of radical Ions; Elsevier:Amsterdam, The Netherlands, 1988.

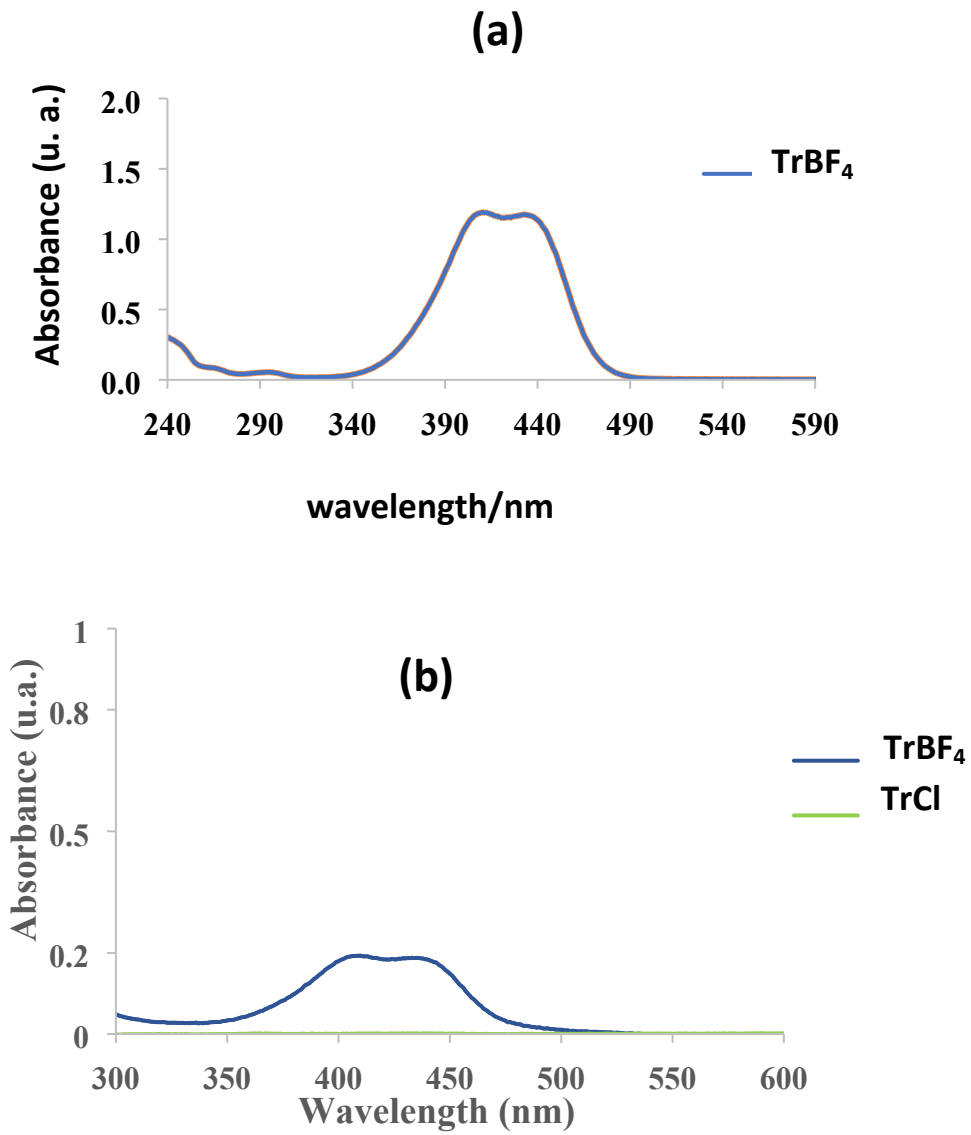


Figure S2. UV-vis absorption spectra of (a) $TrBF_4$ (0.08 mM) in CH_2Cl_2 at room temperature; (b) $TrBF_4$ (0.08 mM) in water-saturated $CDCl_3$ at room temperature (blue) and TrCl (0.08 mM) in water-saturated $CDCl_3$ (green) at room temperature

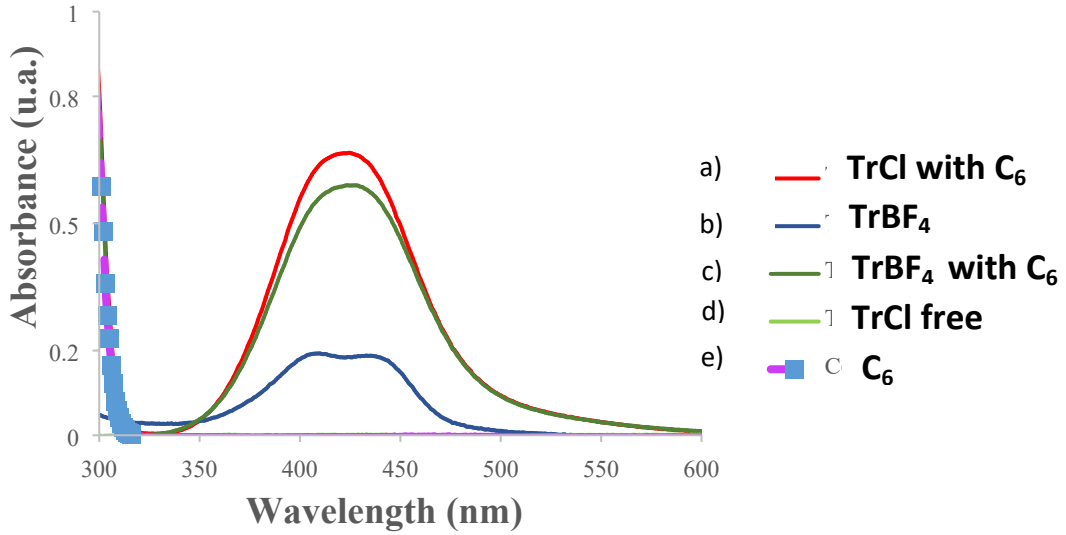


Figure S3. UV-Vis absorption spectra of a mixture of: (a) TrCl/C_6 (0.08mM/0.04mM), (b) $TrBF_4$ (0.08mM), (c) $TrBF_4/C_6$ (0.08mM/0.04mM), (d) TrCl (0.08mM), (e) C_6 (0.04mM) in water-saturated $CDCl_3$.

4. NMR experiments

4.1 ^{1}H and ^{13}C NMR of derivative 2a and Trityl cation ($TrBF_4$)

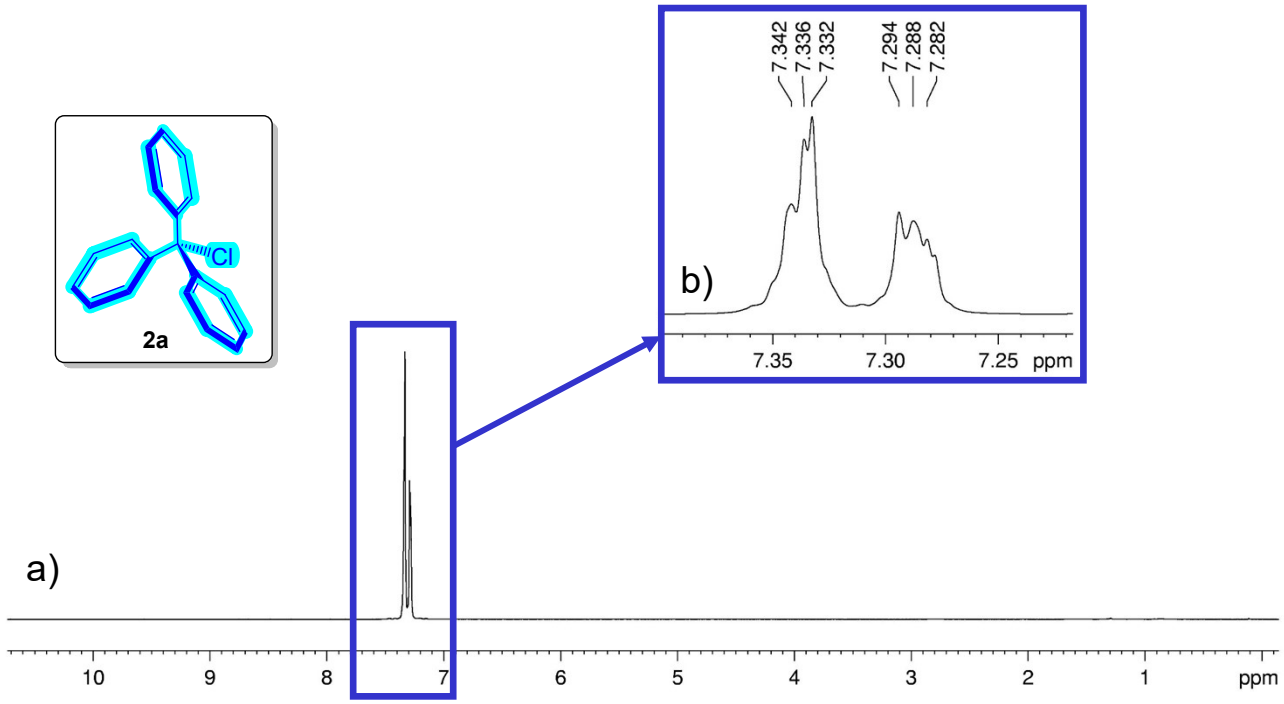


Figure S4. a) ^{1}H NMR and b) partial enlarged spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **2a**.

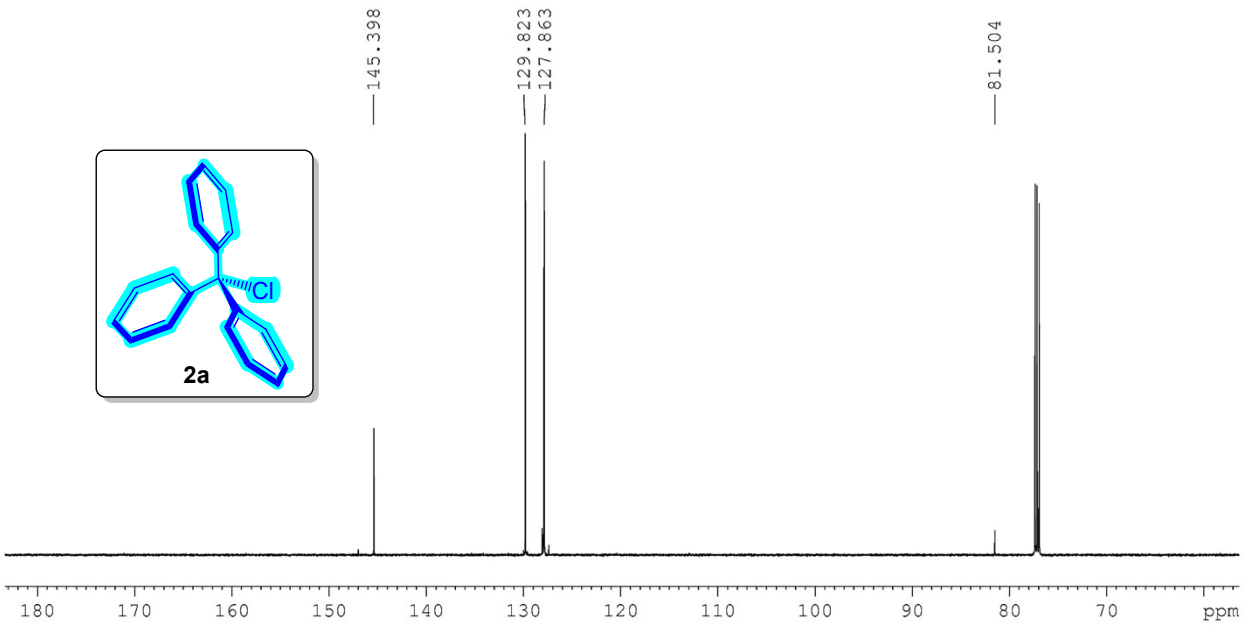


Figure S5. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 298 K) of **2a**.

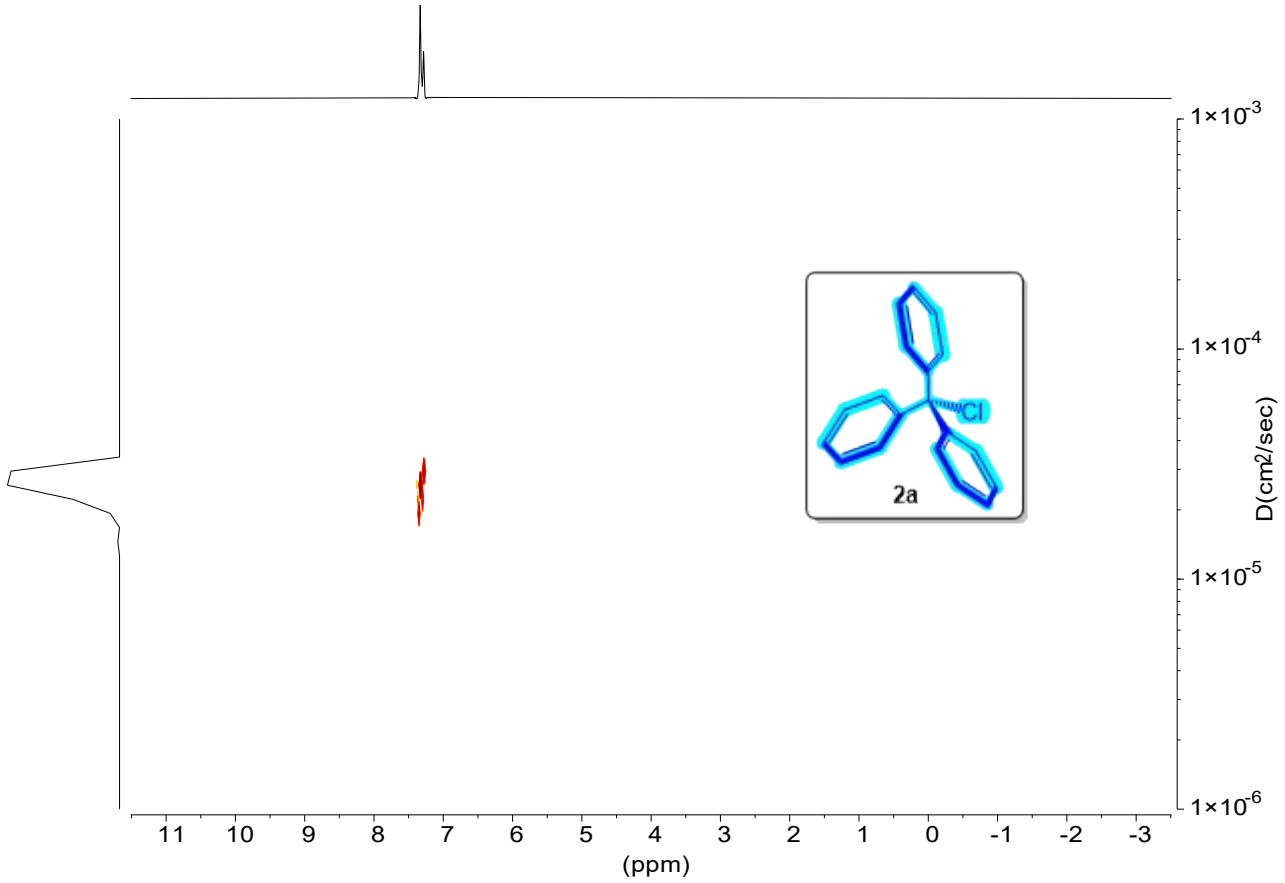


Figure S6. DOSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **2a** (17.0 mM) PulsePROG: ledbpgp2s, d20 = 0.15 sec, P30 = 1400 μs). Processing performed with MestreNova 14.0.0.

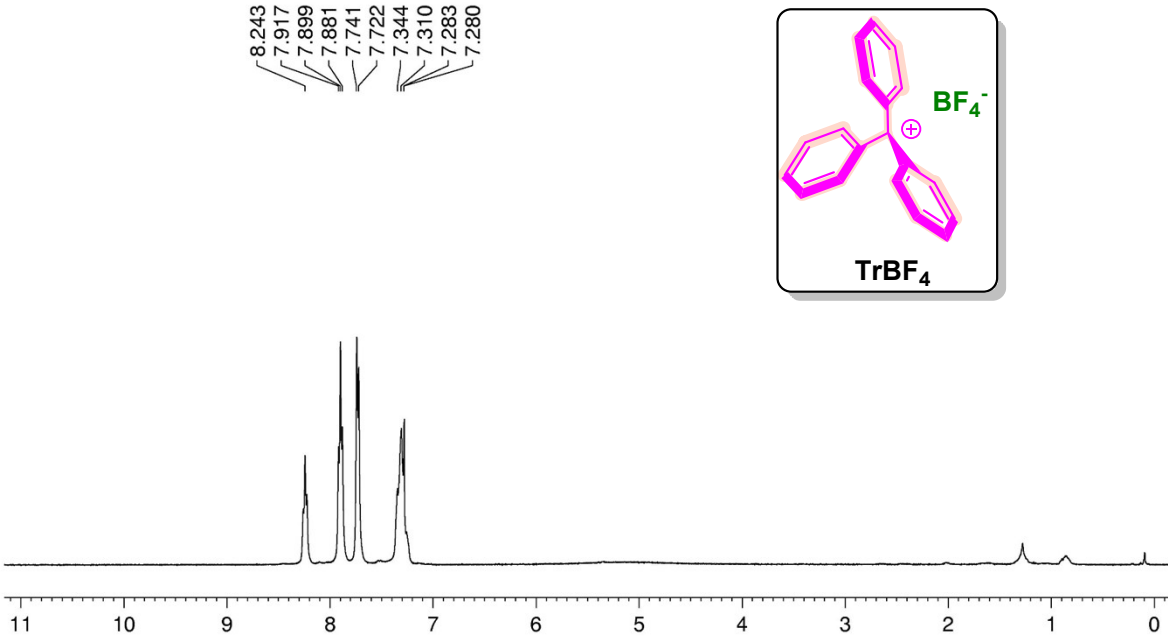


Figure S7. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **$TrBF_4$**.

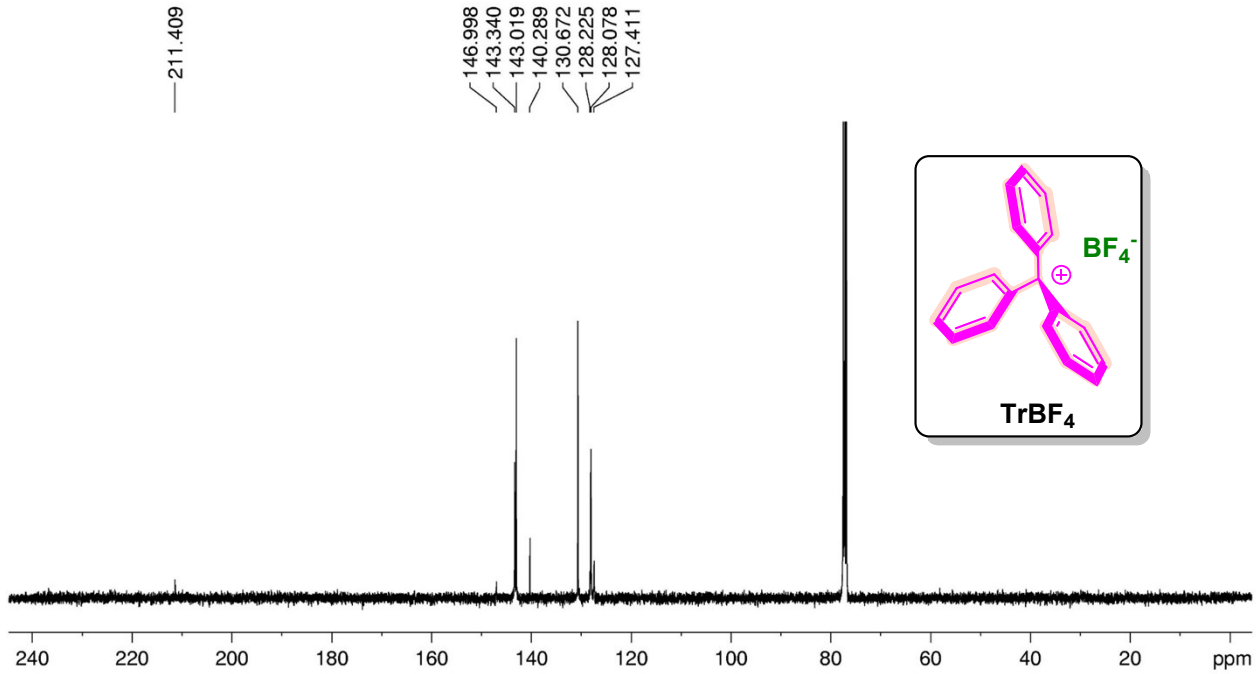


Figure S8. ^{13}C NMR spectrum (150 MHz, $CDCl_3$, 298 K) of **$TrBF_4$**.

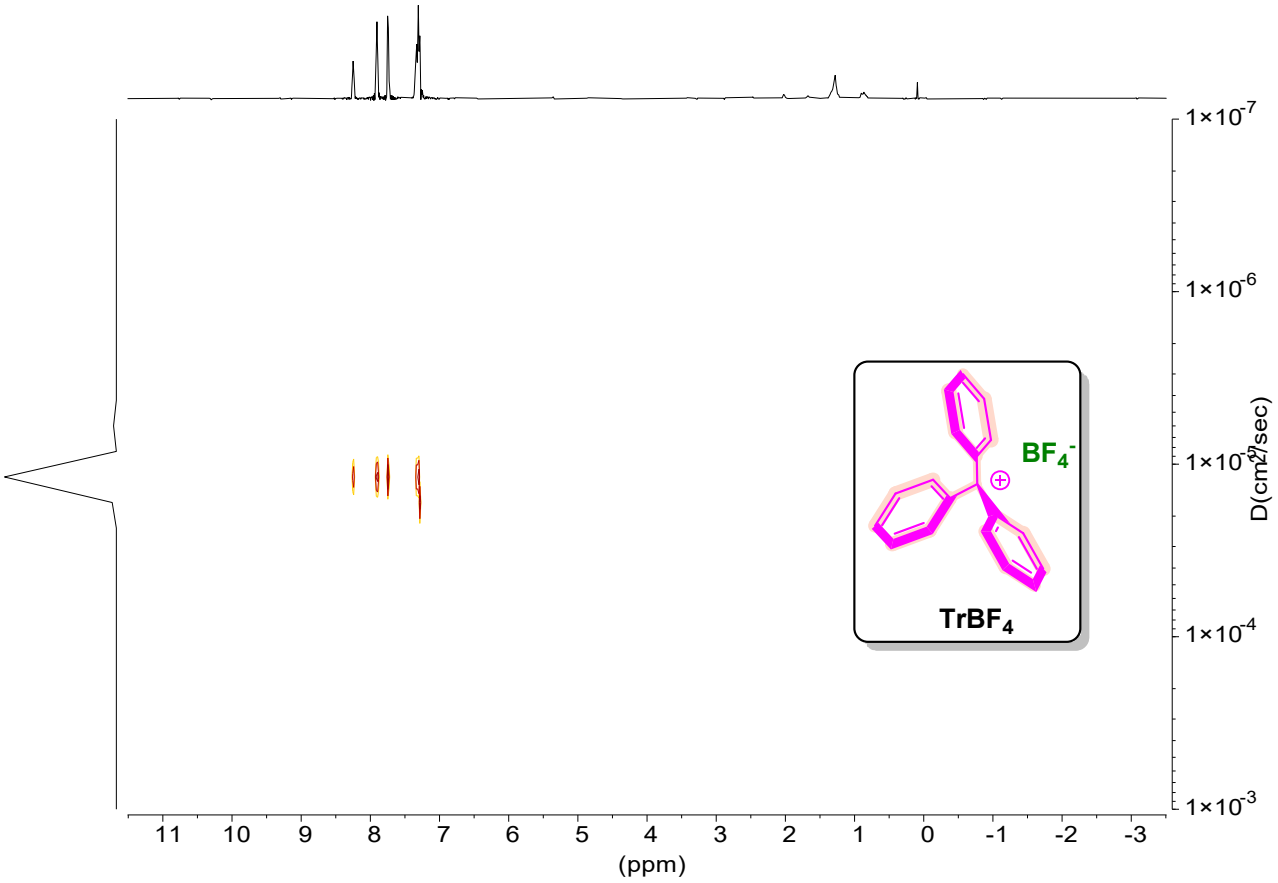


Figure S9. DOSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **$TrBF_4$** (17.2 mM) PulsePROG: ledbpgp2s, d20 = 0.15 sec, P30 = 500 μs). Processing performed with MestreNova 14.0.0.

4.2 1D and 2D NMR Studies of $[Tr@C_6]^+Cl^-$

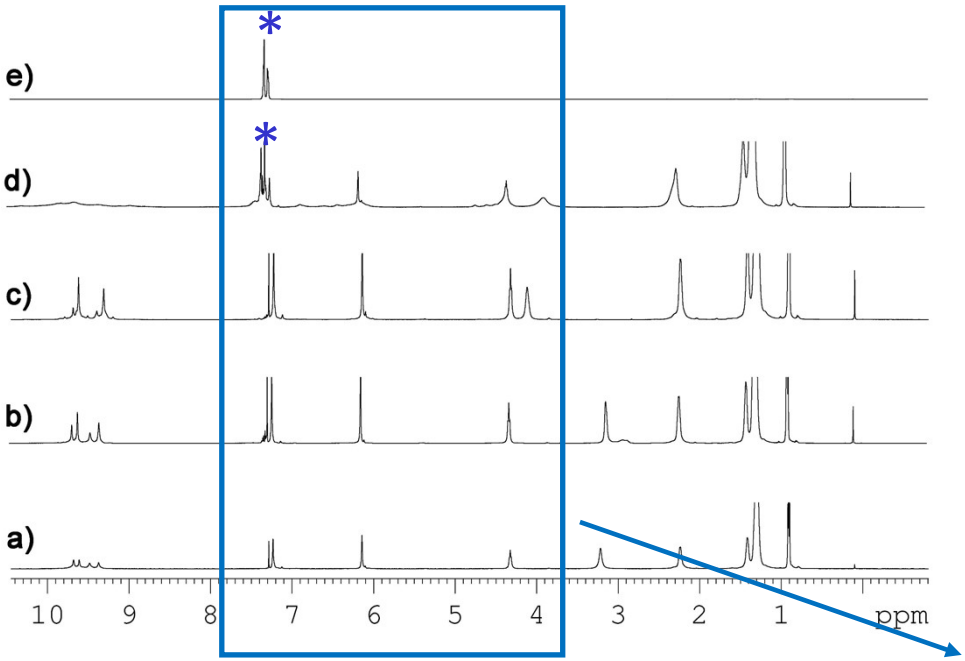
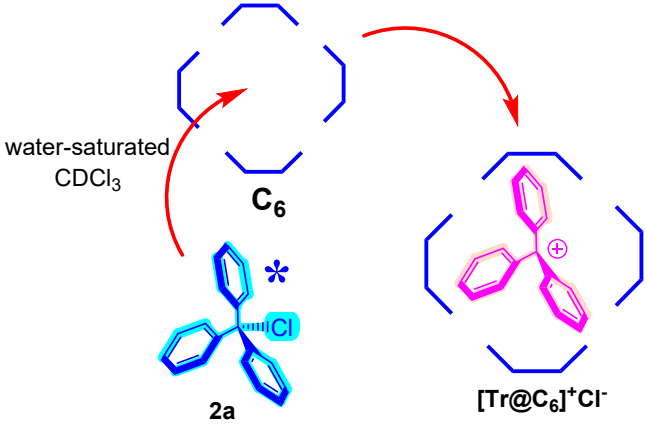


Figure S10. ^{1}H NMR spectra (600 MHz, $CDCl_3$, 298 K) of: a) hexamer $\mathbf{C_6}$ (3.4 mM); b) the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (1.7 mM); c) the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (3.4 mM); d) the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (17.0 mM); e) derivative **2a** (17.0 mM).



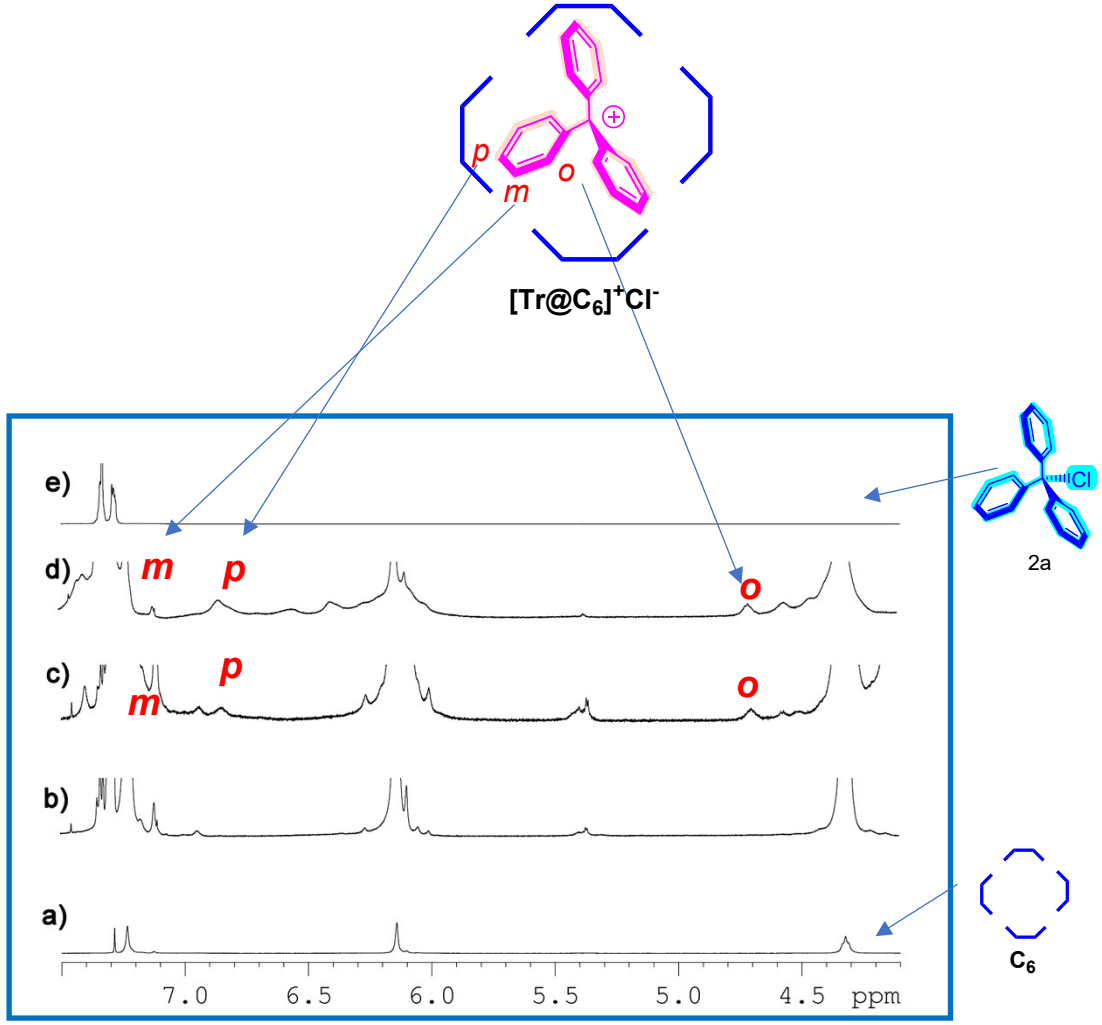


Figure S11. Expansion of ^{1}H NMR spectra (600 MHz, $CDCl_3$, 298 K) of: a) hexamer $\mathbf{C_6}$ (3.4 mM); b) the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (1.7 mM); c) the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (3.4 mM); d) the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (17.0 mM); e) derivative **2a** (17.0 mM).

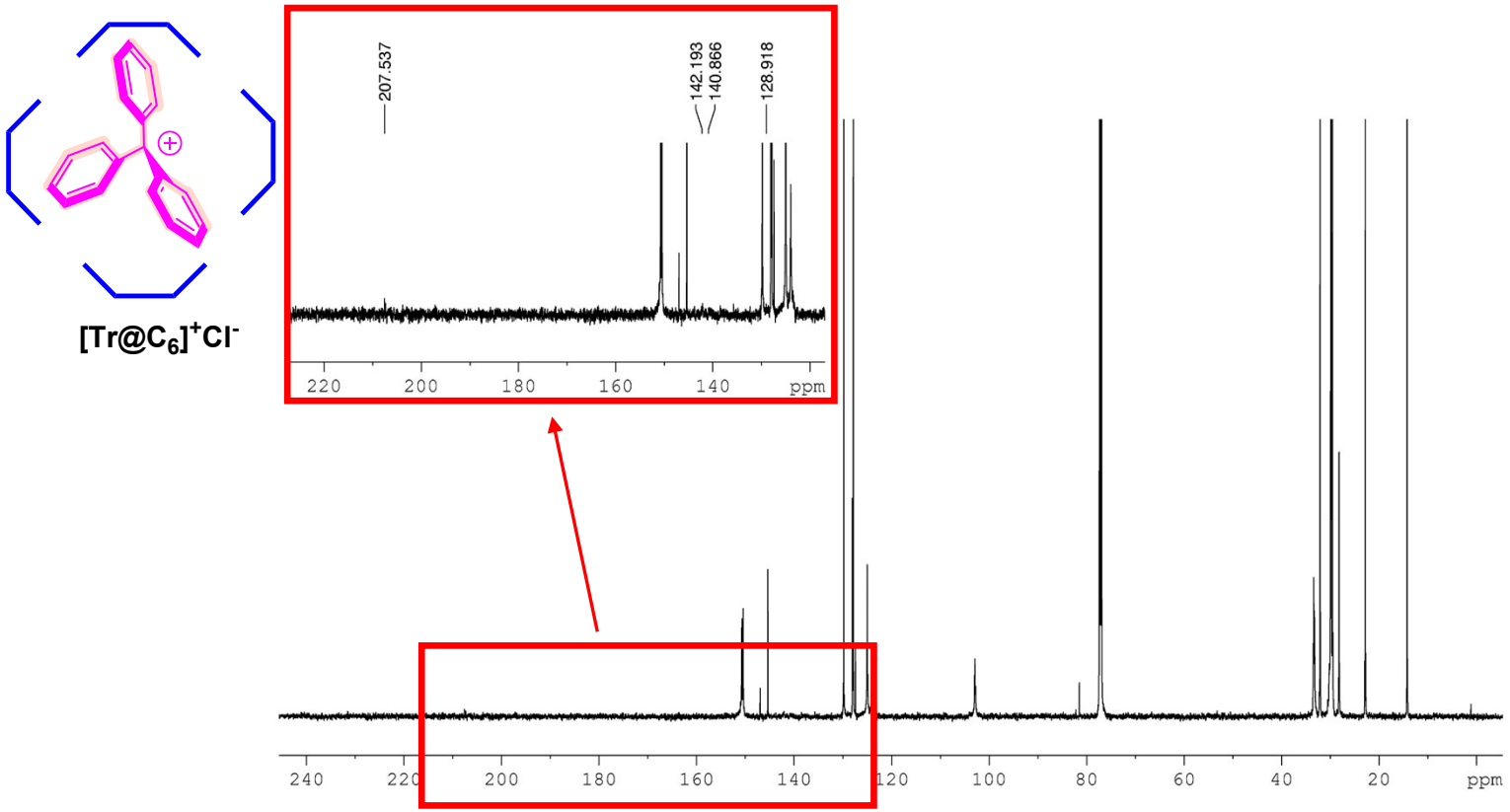


Figure S12. ^{13}C NMR spectrum (150 MHz, $CDCl_3$, 298 K) of the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (17 mM).

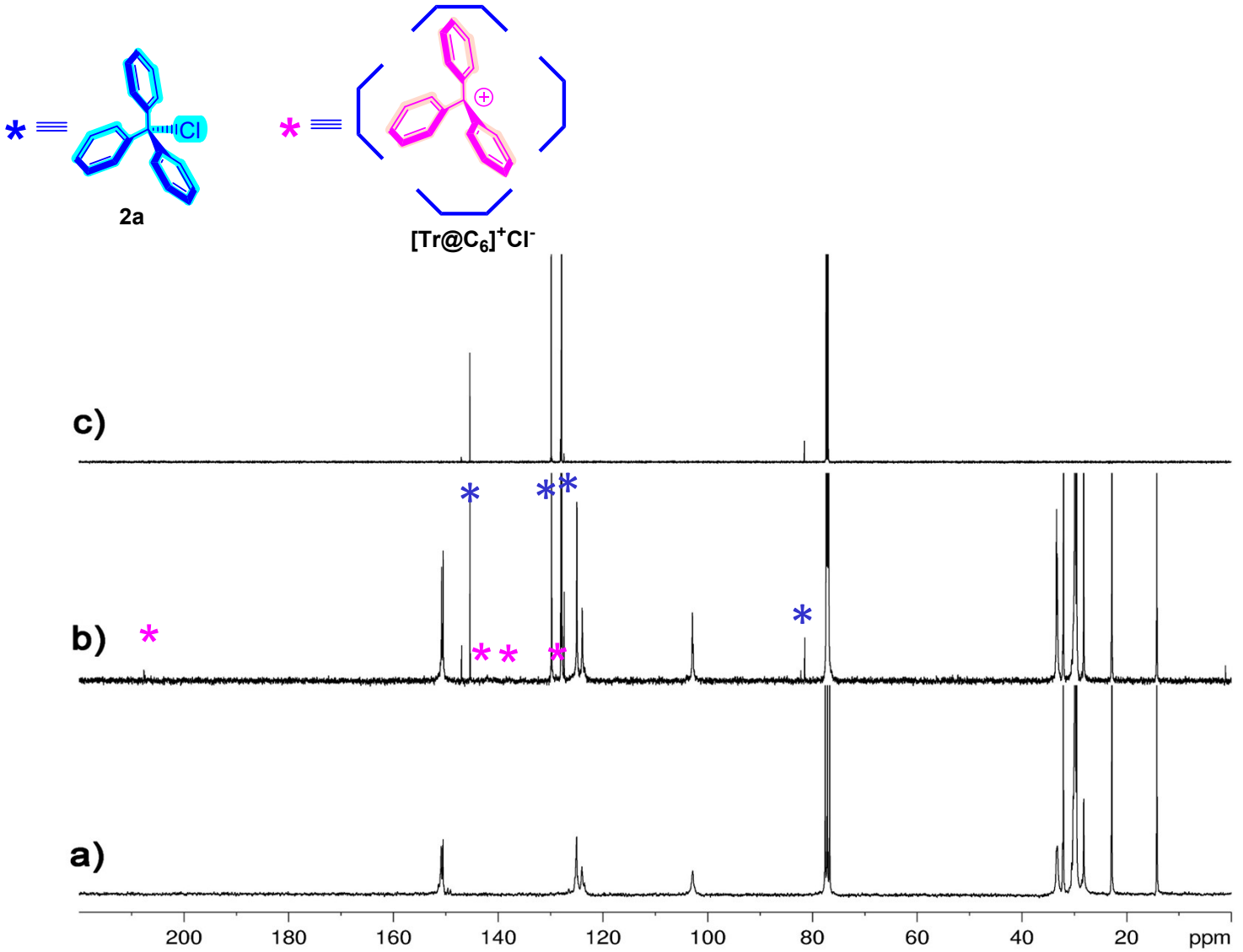


Figure S13. ^{13}C NMR spectra (150 MHz, $CDCl_3$, 298 K) of: a) hexamer $\mathbf{C_6}$ (3.4 mM); b) the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (17 mM); c) derivative **2a** (17.0 mM).

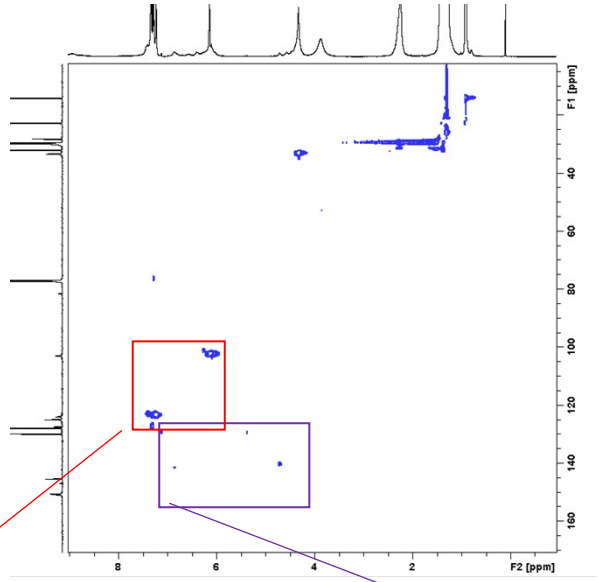


Figure S14. HSQC NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (17.0 mM).

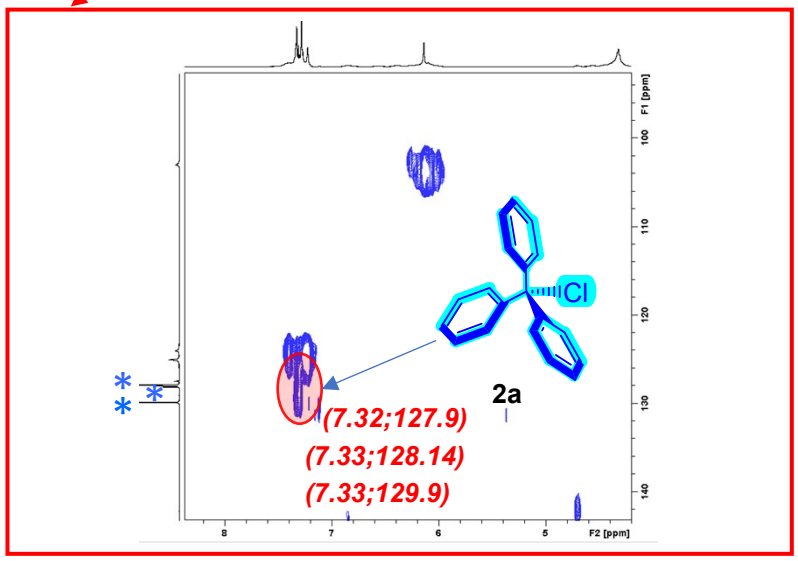
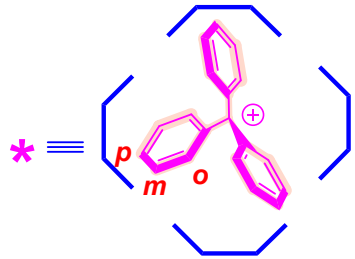


Figure S16. Expansion of the HSQC NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (17.0 mM). Marked the NMR signals of **TrCl** (**2a**).



$[Tr@C_6]^+Cl^-$

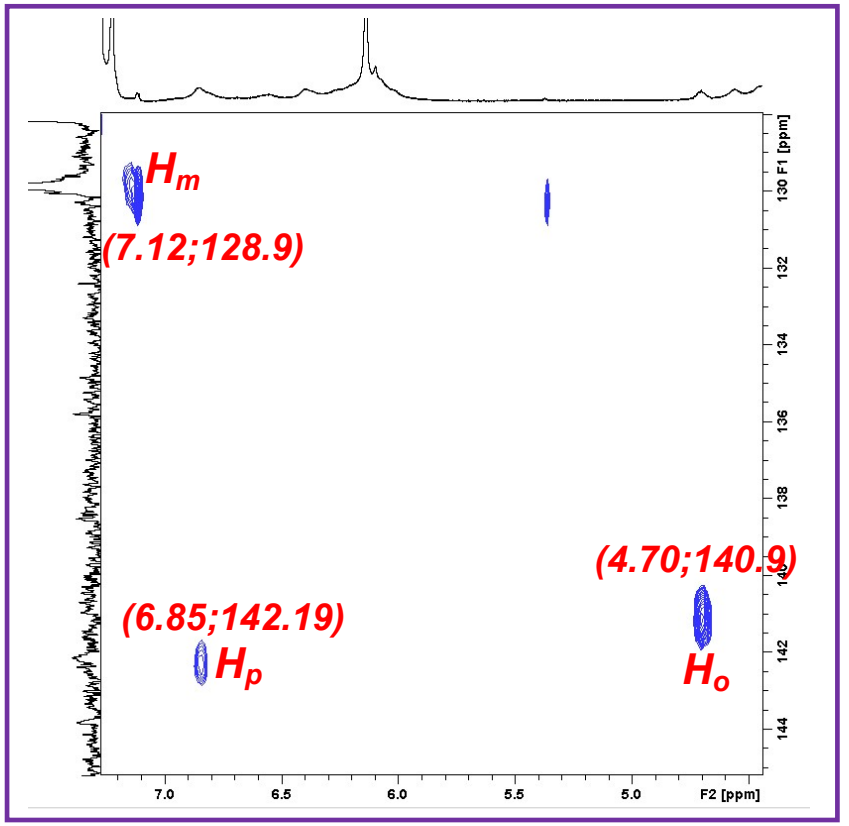


Figure S15. Expansion of the HSQC NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture $\mathbf{C_6}$ (3.4 mM) and **2a** (17.0 mM). Marked the NMR signals of $\mathbf{Tr^+}$ encapsulated inside the hexameric capsule $\mathbf{C_6}$ which show very similar values to the signals observed by mixing $TrBF_4$ salt with $\mathbf{C_6}$ (see *Figure S21*)

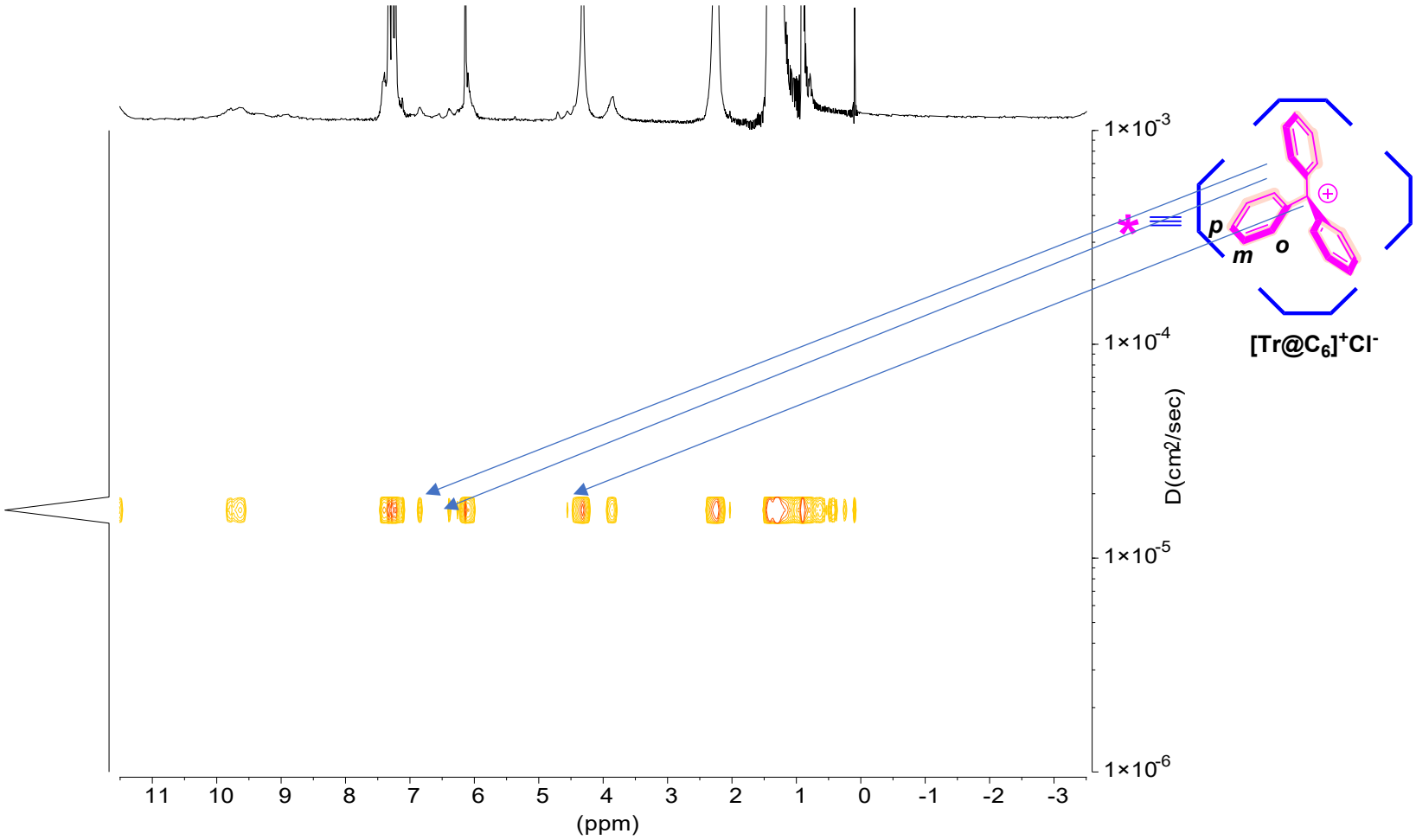


Figure S17. DOSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture of $\mathbf{C_6}$ (3.4 mM) and **2a** (17.0 mM). PulsePROG: ledbpgp2s, d20 = 0.15 sec, P30 = 500 μs). Processing performed with MestreNova 14.0.0.

4.3 1D and 2D NMR Studies of $[Tr@C_6]^+BF_4^-$

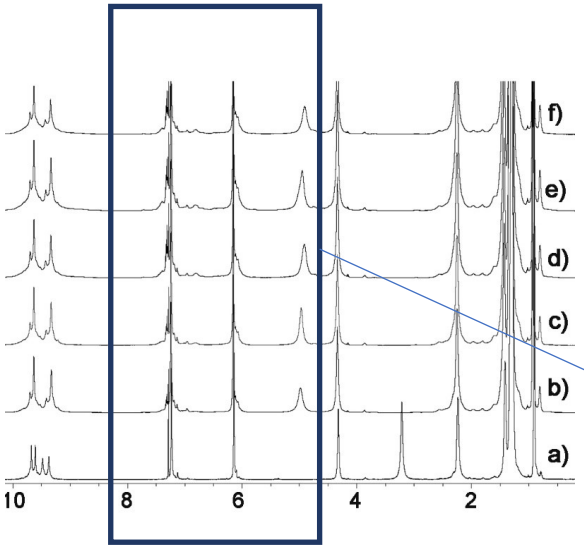
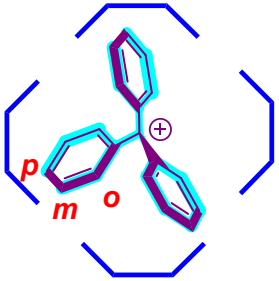


Figure S18. ^{1}H NMR spectra (600 MHz, $CDCl_3$, 298 K) of the mixture $\mathbf{C_6}$ (21.2 mM) and $TrBF_4$ in different ratio, in detail: a) $\mathbf{C_6}$ (21.2 mM), b) $\mathbf{C_6}$ (21.2 mM) and $TrBF_4$ (4.2 mM), c) $\mathbf{C_6}$ (21.2 mM) and $TrBF_4$ (8.5 mM), d) $\mathbf{C_6}$ (21.2 mM) and $TrBF_4$ (12.7 mM), e) $\mathbf{C_6}$ (21.2 mM) and $TrBF_4$ (17.0 mM), e) $\mathbf{C_6}$ (21.2 mM) and $TrBF_4$ (21.2 mM).



$[Tr@C_6]^+BF_4^-$

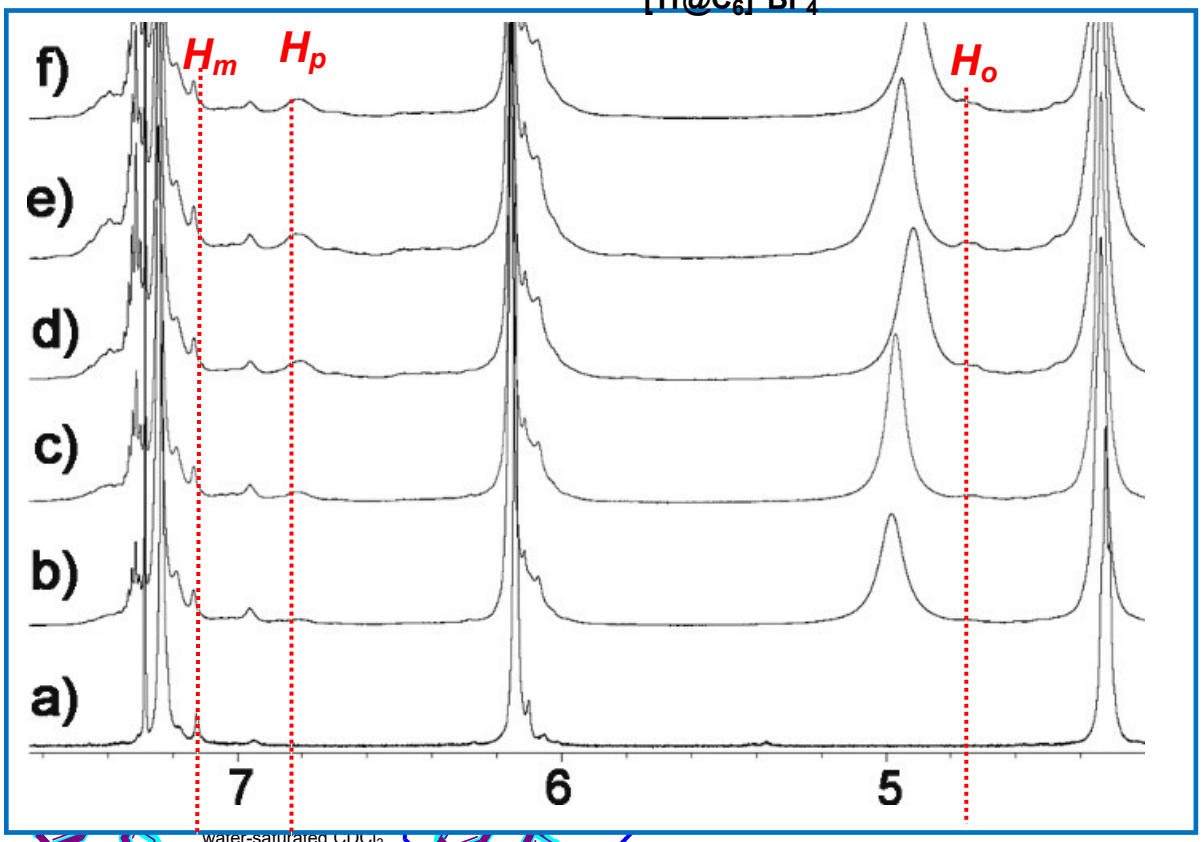


Figure S19. Significative regions of ^{1}H NMR spectra (600 MHz, $CDCl_3$, 298 K) of the mixture $\mathbf{C_6}$ (21.2 mM) and $TrBF_4$ in different ratio.

$[Tr@C_6]^+BF_4^-$

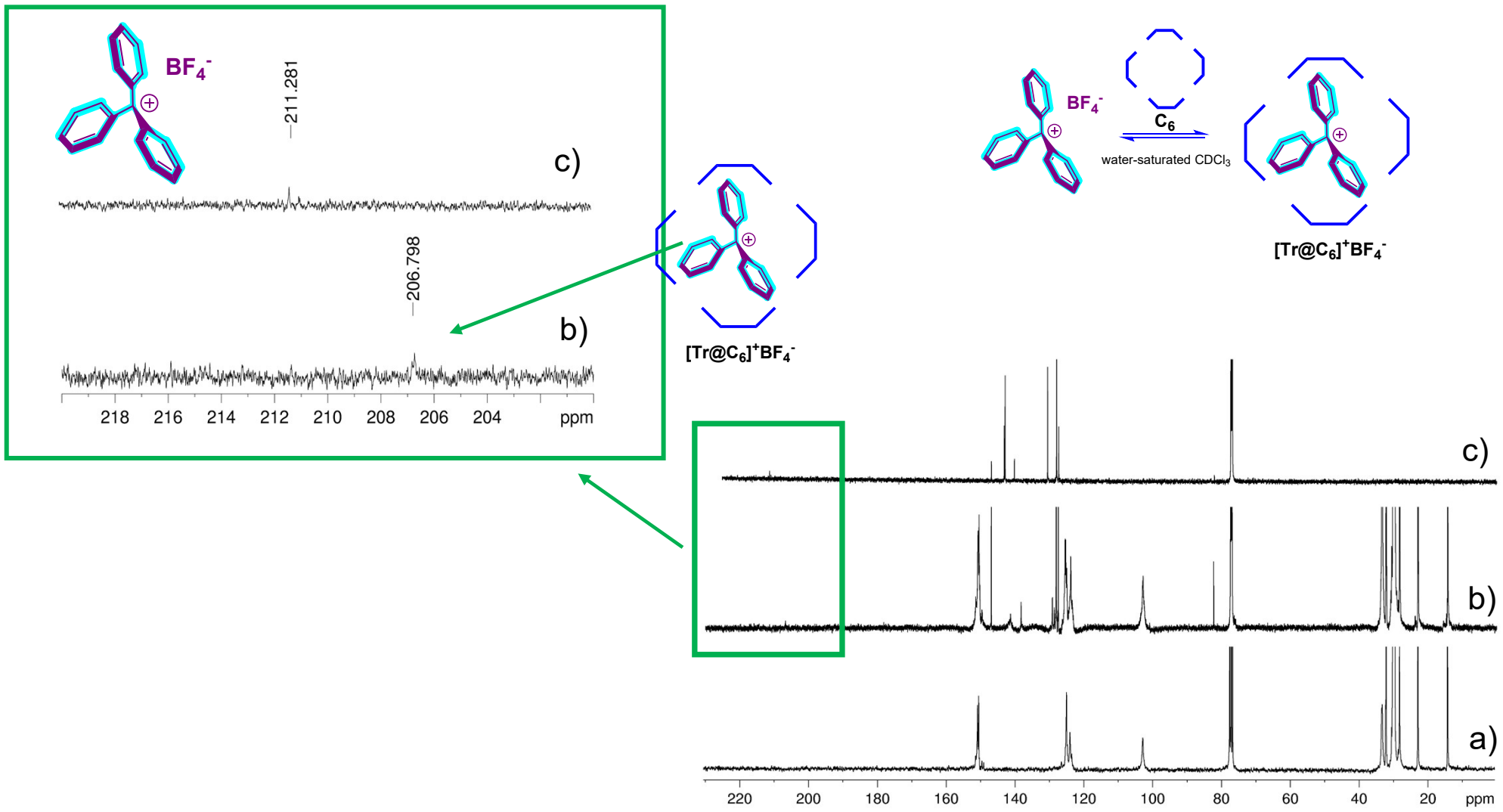


Figure S20. ^{13}C NMR spectra (150 MHz, $CDCl_3$, 298 K) of: a) hexamer $\mathbf{C_6}$ (3.4 mM); b) the mixture $\mathbf{C_6}$ (3.4 mM) and $\mathbf{TrBF_4}$ (17.0 mM); c) derivative $\mathbf{TrBF_4}$ (3.4 mM).

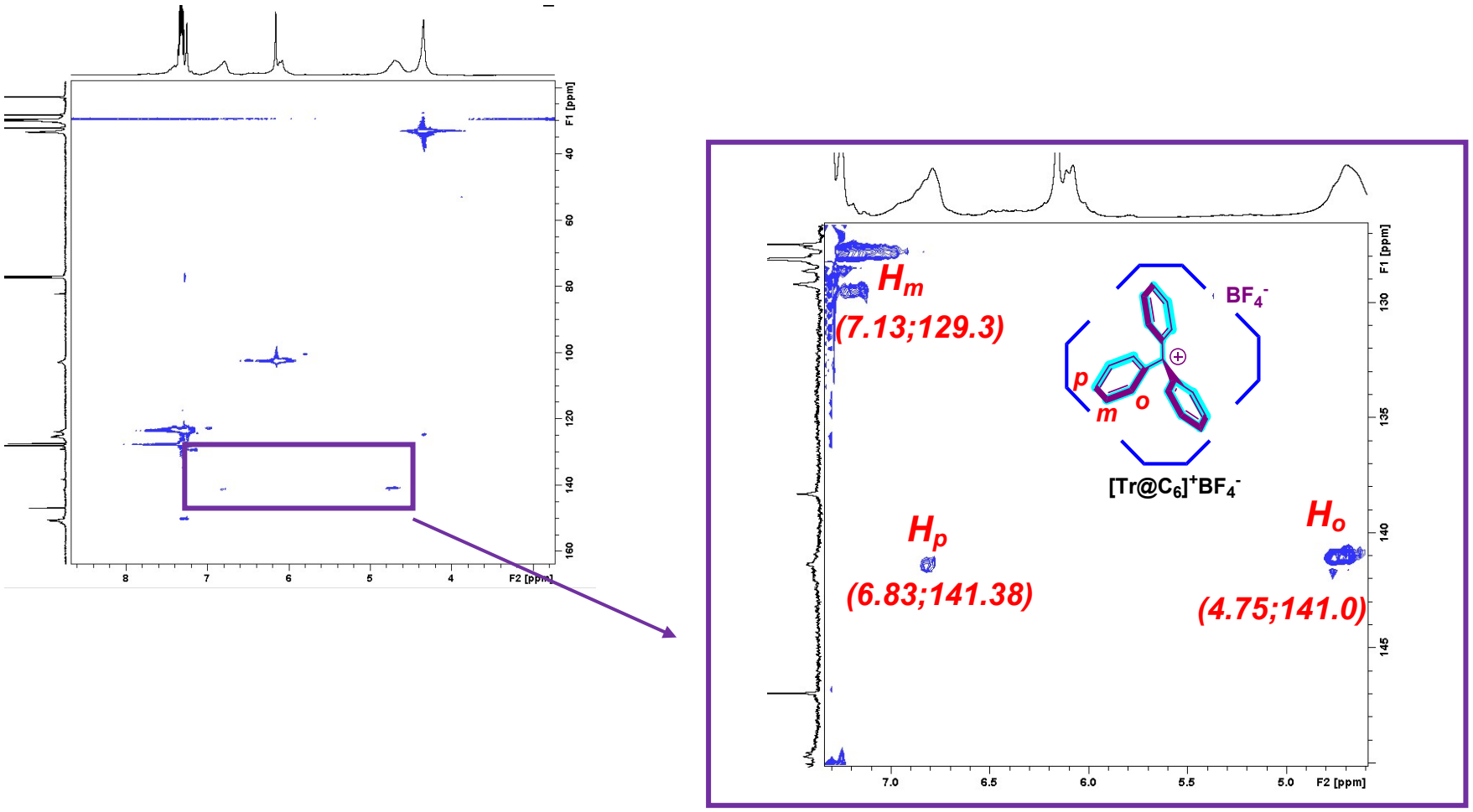


Figure S21. Significative portion of HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture $\mathbf{C_6}$ (3.4 mM) and $TrBF_4$ (3.4 mM). Marked the NMR signals of Tr^+ (o-, m-, and p-H) encapsulated inside the hexameric capsule $\mathbf{C_6}$ which show very similar values to the signals observed by mixing TrCl with $\mathbf{C_6}$ (see Figure S15).

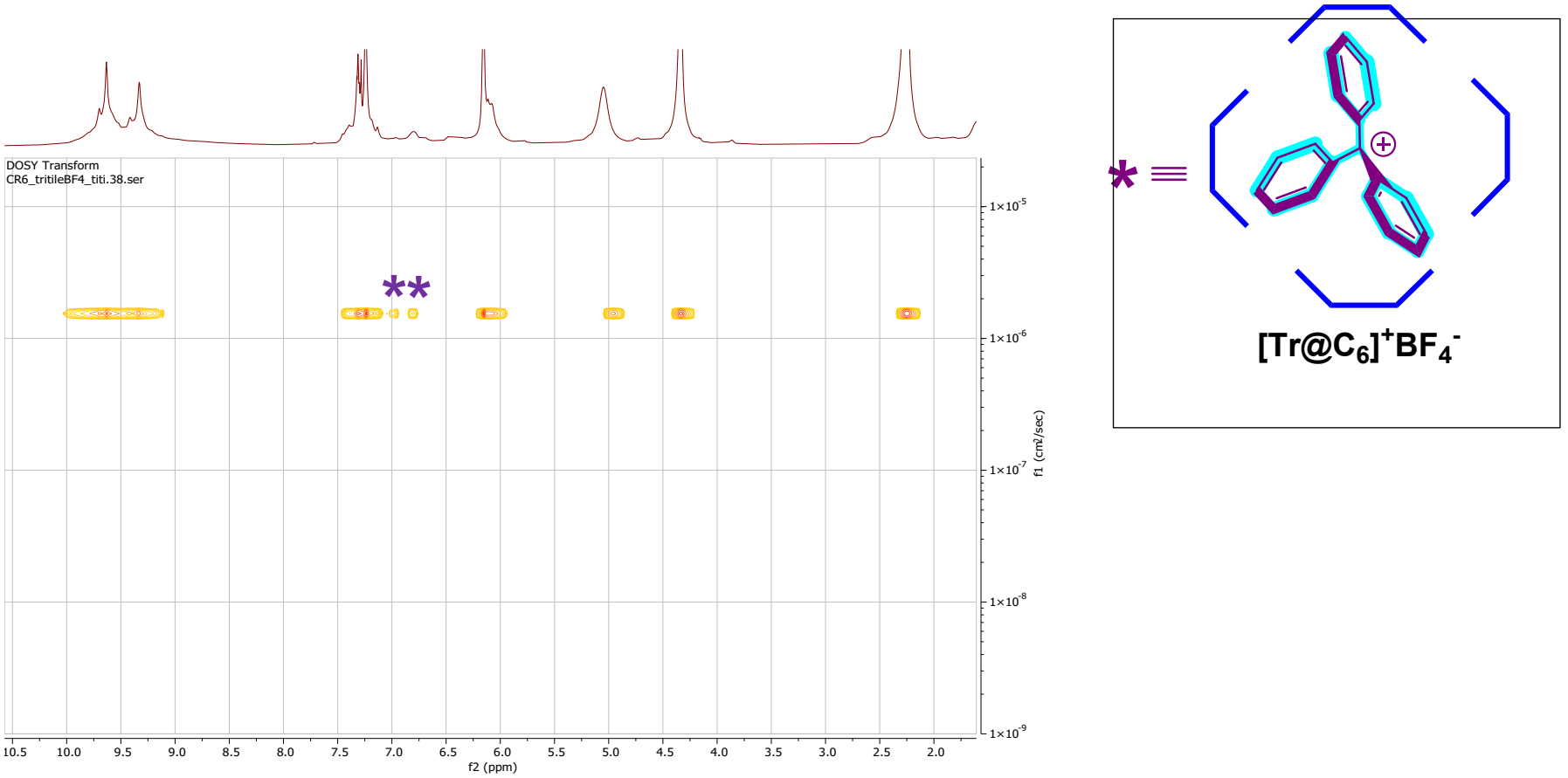


Figure S22. DOSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture of **C_6** (3.4 mM) and **$TrBF_4$** (3.4 mM). PulsePROG: ledbpgp2s, d20 = 0.15 sec, P30 = 500 μs). Processing performed with MestreNova 14.0.0.

4.4 Binding studies of the resorcin[4]arene capsule with 14

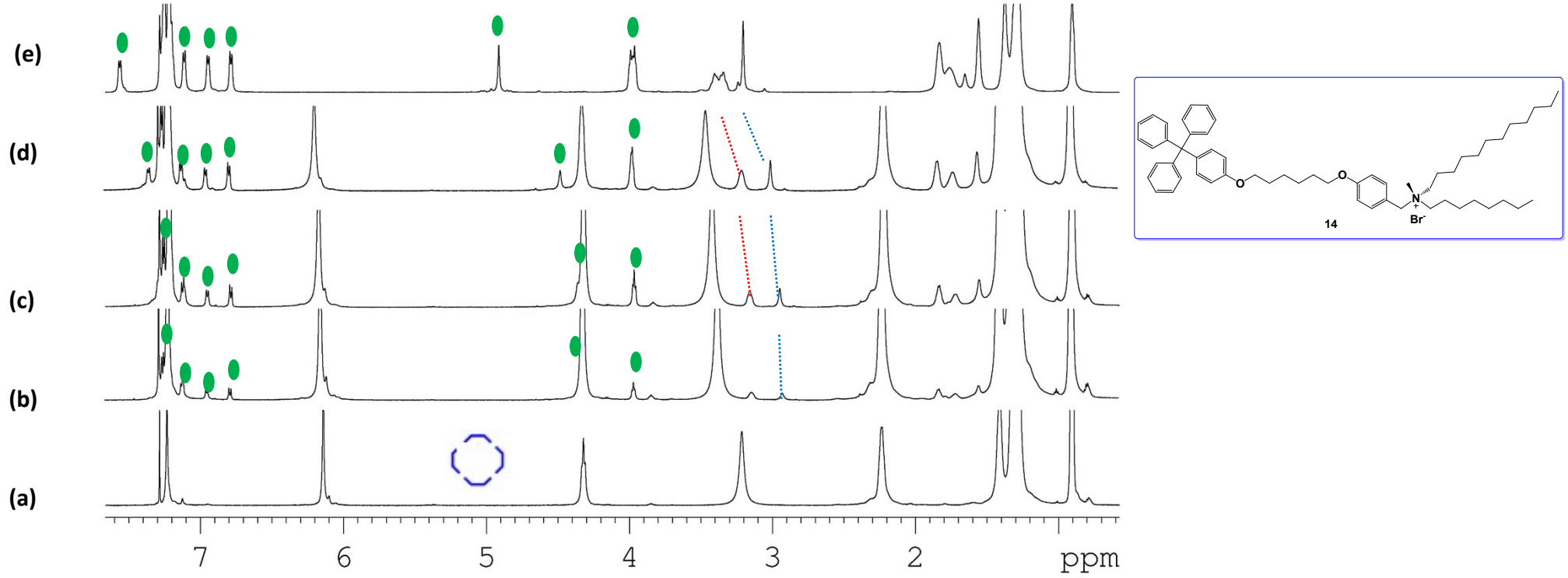


Figure S23. ^{1}H NMR spectra (600 MHz, water-saturated $CDCl_3$, 298 K) of: a) $\mathbf{C_6}$ (3.4 mM); b) $\mathbf{C_6}$ (3.4 mM) + **14** (1.7 mM); c) $\mathbf{C_6}$ (3.4 mM) + **14** (3.4 mM); d) $\mathbf{CR_6}$ (3.4 mM) + **14** (6.8 mM); e) **14** (3.4 mM). Marked with ● the ^{1}H NMR signals of **14.** Marked in blue the $^{+}$NMe singlet of **14** which is up-field shifted as the concentration of capsule increases in slow exchange in the NMR time scale upon external interaction with the aromatic walls of the hexameric capsule $\mathbf{C_6}$.

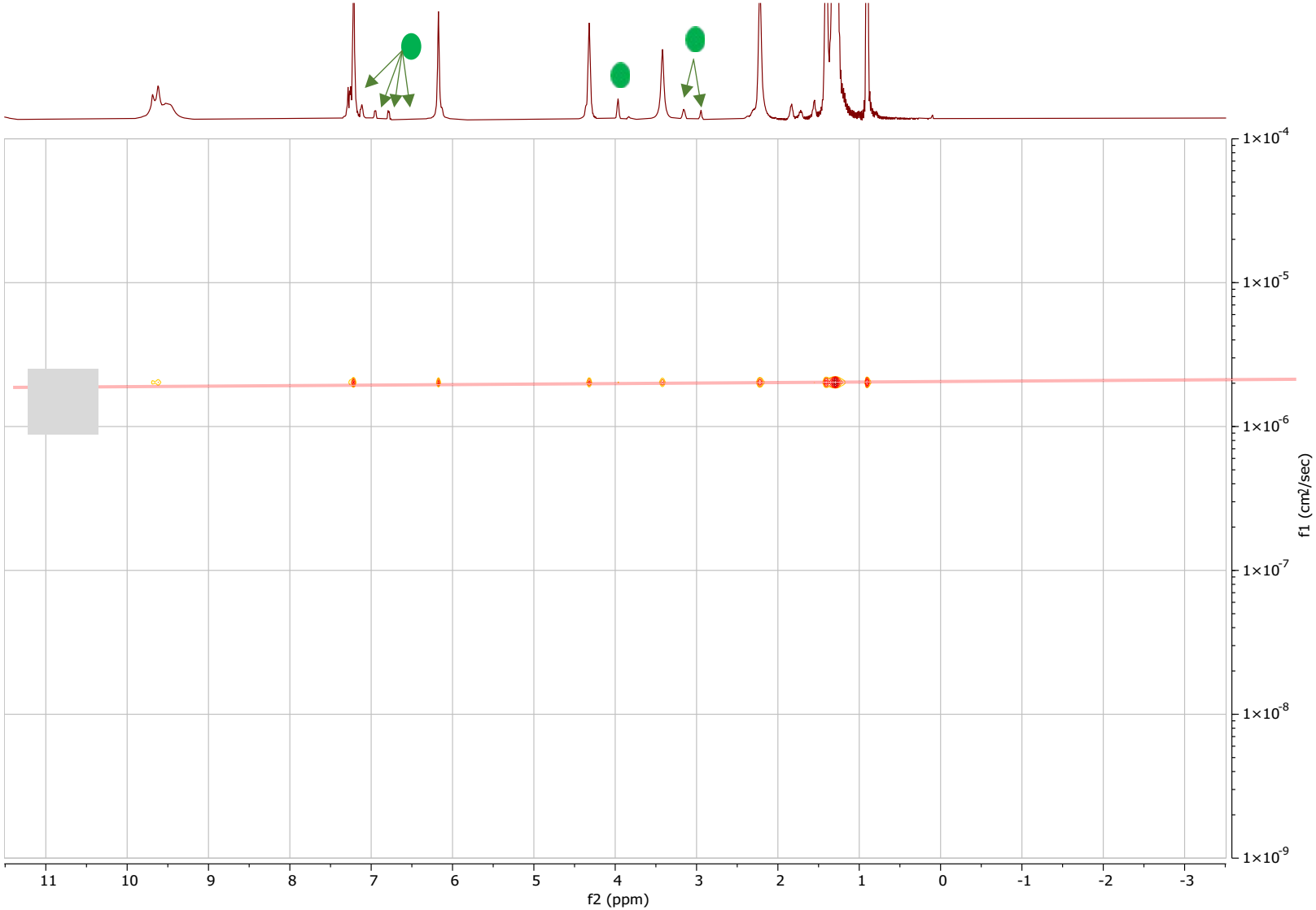


Figure S24. DOSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of a mixture **C_6** (3.4 mM) and **14** (3.4 mM). PulsePROG: ledbpgp2s, d20 = 0.15 sec, P30 = 500 ms). Processing performed with MestreNova 14.0.0.

5. Guest uptake

5.1 Degree of encapsulation of 5f in the presence of C_6

Resorcinarene **1** (140.5 mg, 0.127 mmol) was weighed in a 4 mL vial and 0.5 mL of water saturated $CDCl_3$ was added. The mixture was warmed at 50 °C until clarification (ca 5 min). To this solution aldehydes **5f** (0.0423 mmol, 2 equiv) was added and the mixture was kept at 30 °C under stirring for 1h before being subjected to NMR spectroscopy. ^{1}H-NMR spectrum showed the appearance of new upfield-shifted signals in the regions of 8.0-9.0 ppm and 5.0-7.2 0 ppm (see inserts in Figure S26). These signals indicate encapsulation of **5f** inside the cavity of **C_6**.

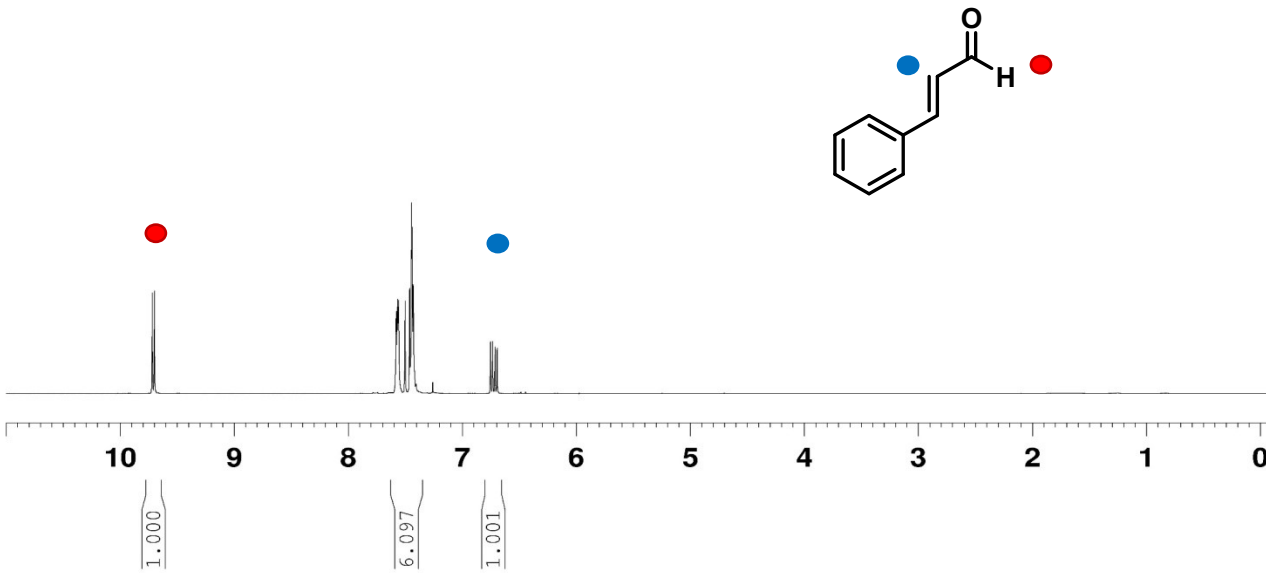


Figure S25. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of aldehyde **5f**.

The uptake of **5f** within **C_6** was measured by quantitative ^{1}H-NMR experiment. The amount of encapsulated aldehyde **5f** was calculated by the integration of proton signal H(●) of free aldehyde at 6.74 ppm (1H) with respect to the signal of 1,1,2,2-tetrachloroethane (TCE, 5.97 ppm, 2H) as an internal standard. In particular, the equation ($[G]_0 - [G]_t$)/ $[G]_0$ (as reported by Tiefenbacher et al. in *J. Am. Chem. Soc.* **2017,** *139*, 11482-11492) was used to determine the encapsulation degree of **5f**. The terms $[G]_0$ indicates the total concentration of **5f** and $[G]_t$ the remaining free **5f** after the sample was allowed to equilibrate for t=1h.

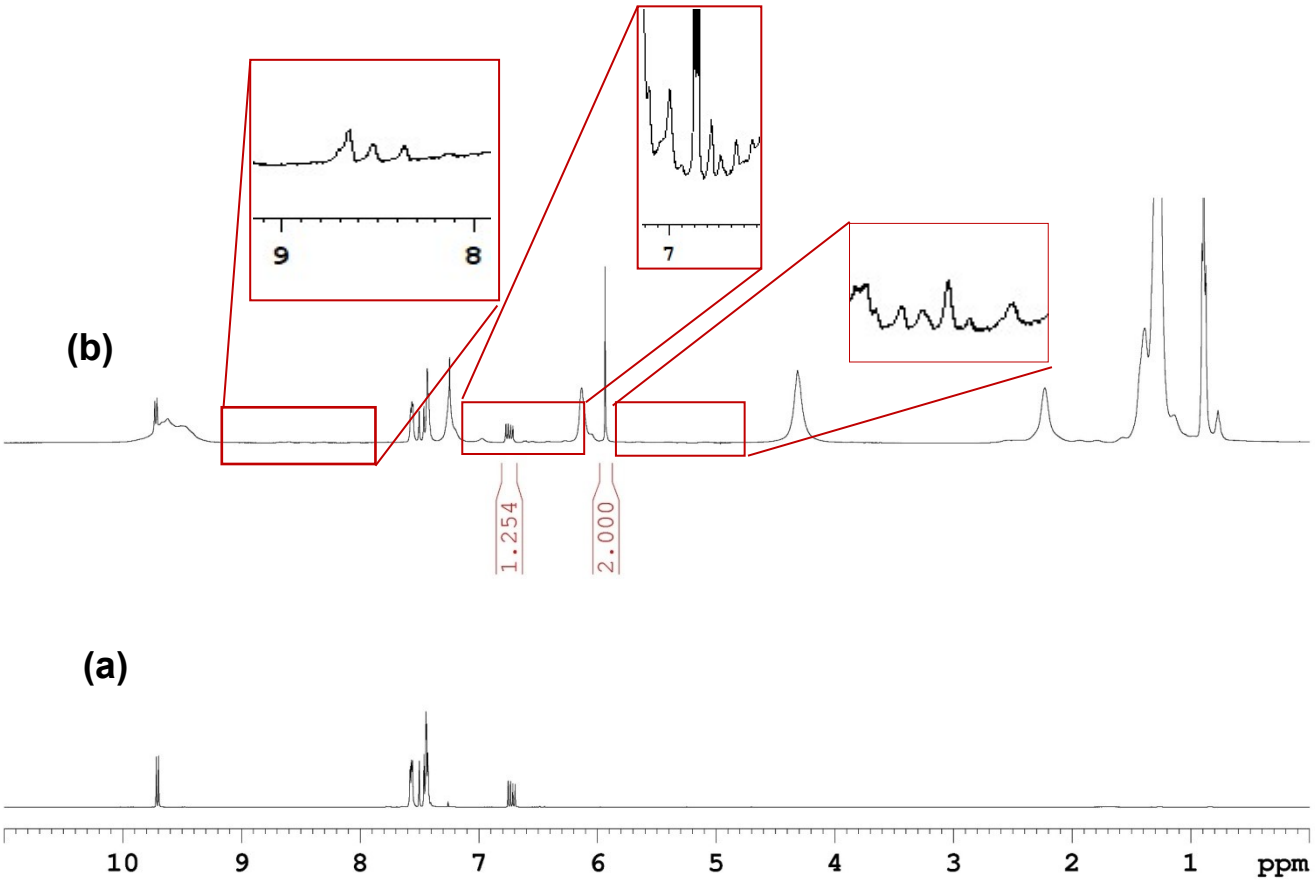


Figure S26. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of: (a) aldehyde **5f**; (b) the mixture of aldehyde **5f** (0.0423 mmol) and $\mathbf{C_6}$ (0.021 mmol) in $CDCl_3$ (0.5 mL). The signal of TCE (5.97 ppm, 2H, 27μmol) used as internal standard.

Table S1. Uptake of aldehyde **5f** inside $\mathbf{C_6}$

mmol of starting aldehyde	Integral of free aldehyde[a]	mmol of free aldehyde	mmol of encapsulated aldehyde	Uptake (%)
0.0423	1.254	0.0338	0.0084	20

[a] Integral of proton signal of free aldehyde at 6.74 ppm (1H) after the sample was allowed to equilibrate for t=1h

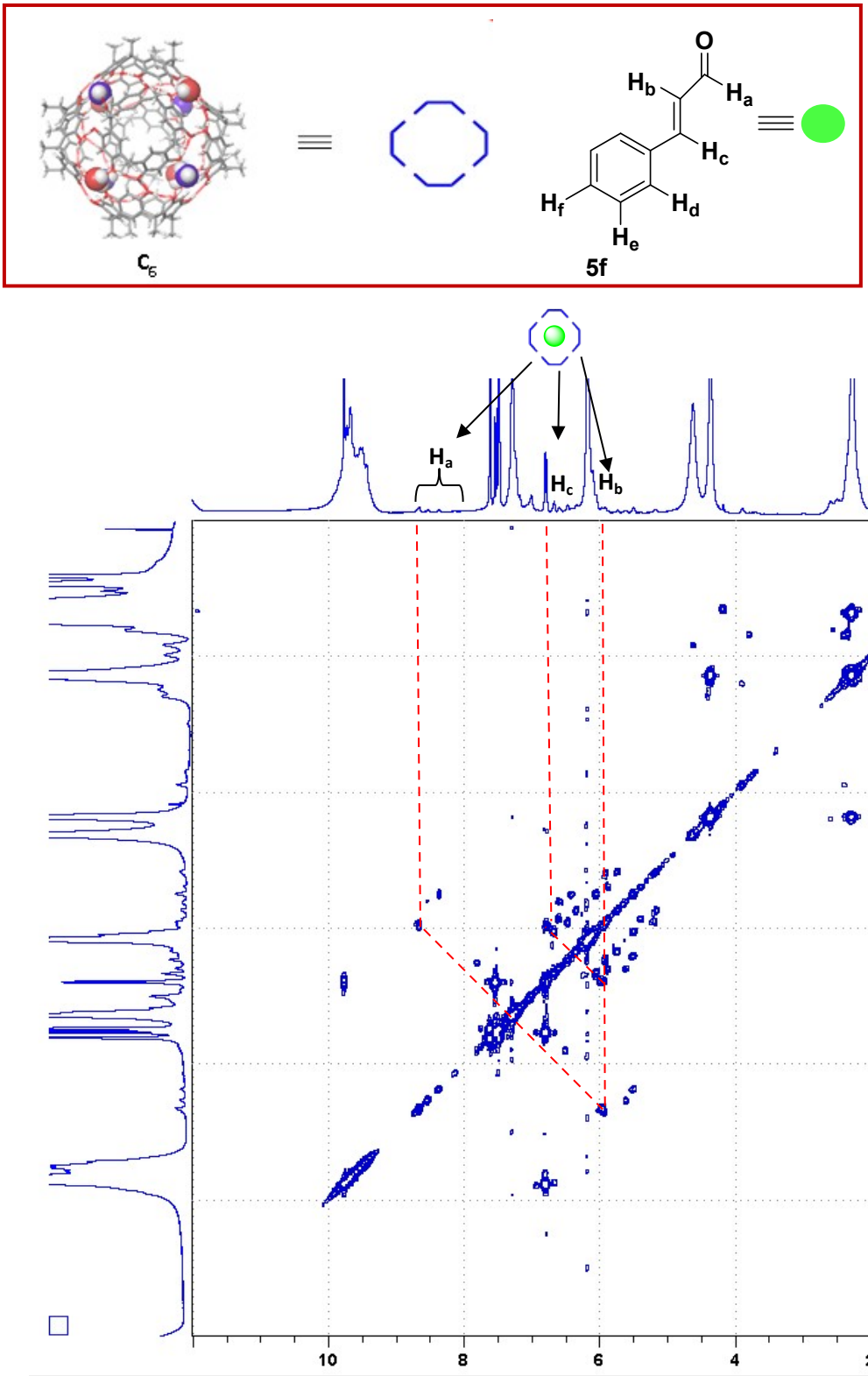


Figure S27. COSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture **5f** (42.3 mM) and $\mathbf{C_6}$ (21.2 mM).

The ^{1}H NMR signals of the encapsulated aldehyde **5f** are very complex, and in accord with the data previously reported by Cohen,[7] this indicates that the aromatic guest molecules are encapsulated in slightly different nanocontainers.

[7] L. Avram, Y. Cohen, *Org. Lett.* **2006**, *8*, 219-222.

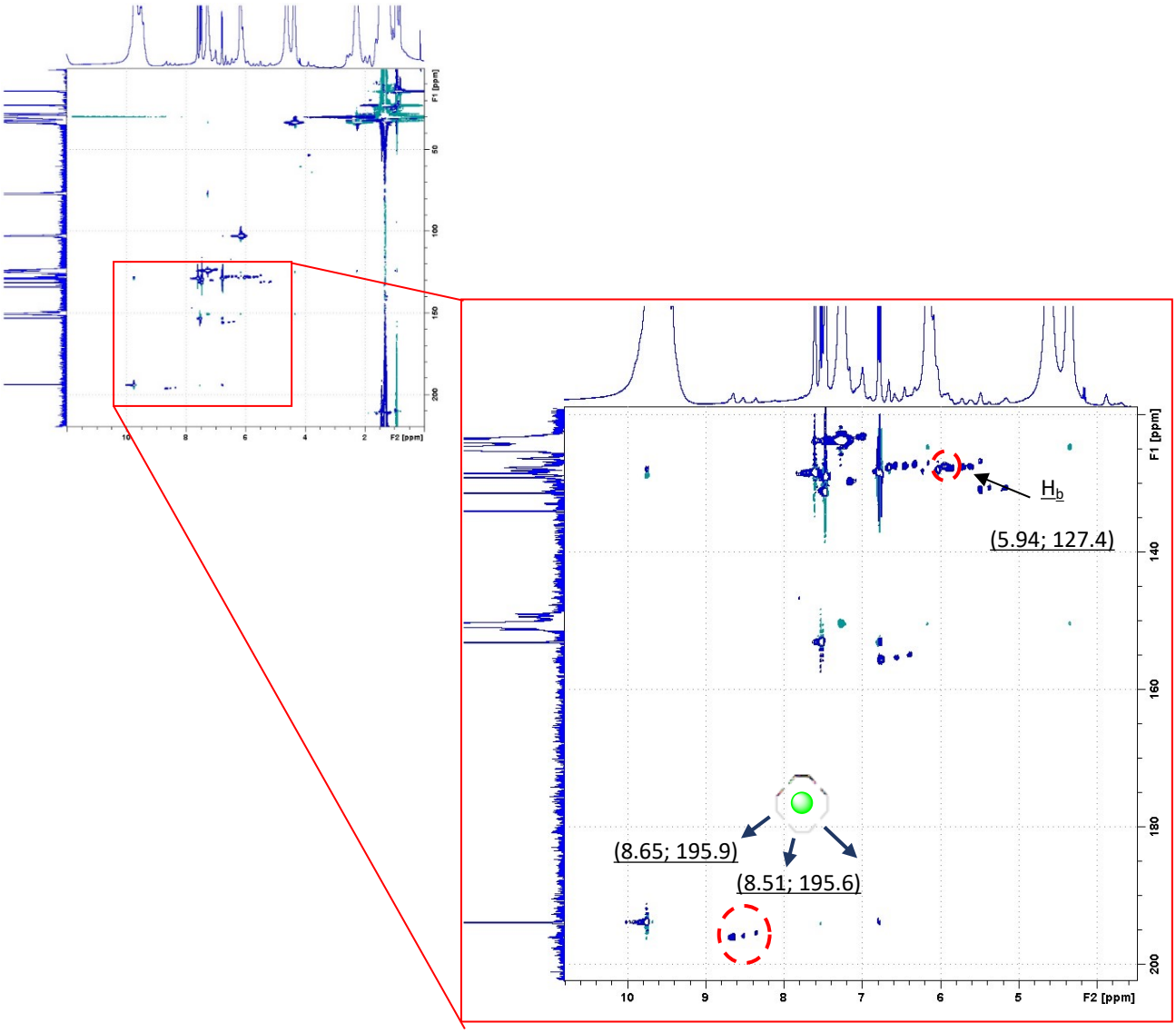


Figure S28. HSQC NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture **5f** (42.3 mM) and **C_6** (21.2 mM). Marked the NMR signals of **5f** encapsulated inside the hexameric capsule **C_6**

5.2 Degree of encapsulation of 5g in the presence of C_6

Resorcinarene **1** (140.5 mg, 127 µmol) was weighed in a 4 mL vial and 0.5 mL of water saturated $CDCl_3$ was added. The mixture was warmed at 50 °C until clarification (ca 5 min). To this solution aldehydes **5g** (0.0423 mmol, 2 equiv) was added and the mixture was kept at 30 °C under stirring for 1h before being subjected to NMR spectroscopy. ^{1}H-NMR spectrum showed the appearance of new upfield-shifted signals in the regions 8.0-9.0 and 5.0-7.2 ppm (see inserts in Figure S30). These signals indicate encapsulation of **5g** inside the cavity of **C_6**.

Figure S29. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of aldehyde **5g**.

The uptake of **5g** within **C_6** was measured by quantitative ^{1}H-NMR experiment. The amount of encapsulated aldehyde **5g** was calculated by the integration of proton signal of free aldehyde at 7.85 ppm (1H ●) with respect to the signal of 1,1,2,2-tetrachloroethane (TCE, 5.97 ppm, 2H, 5.35 μmol) as an internal standard. In particular, the equation $([G]_0 - [G]_t) / [G]_0$ (as reported by Tiefenbacher et al. in *J. Am. Chem. Soc.* **2017,** *139*, 11482-11492) was used to determine the encapsulation degree of **5g**. The terms $[G]_0$ indicates the total concentration of **5g** and $[G]_t$ the remaining free **5g** after the sample was allowed to equilibrate for t=1h.

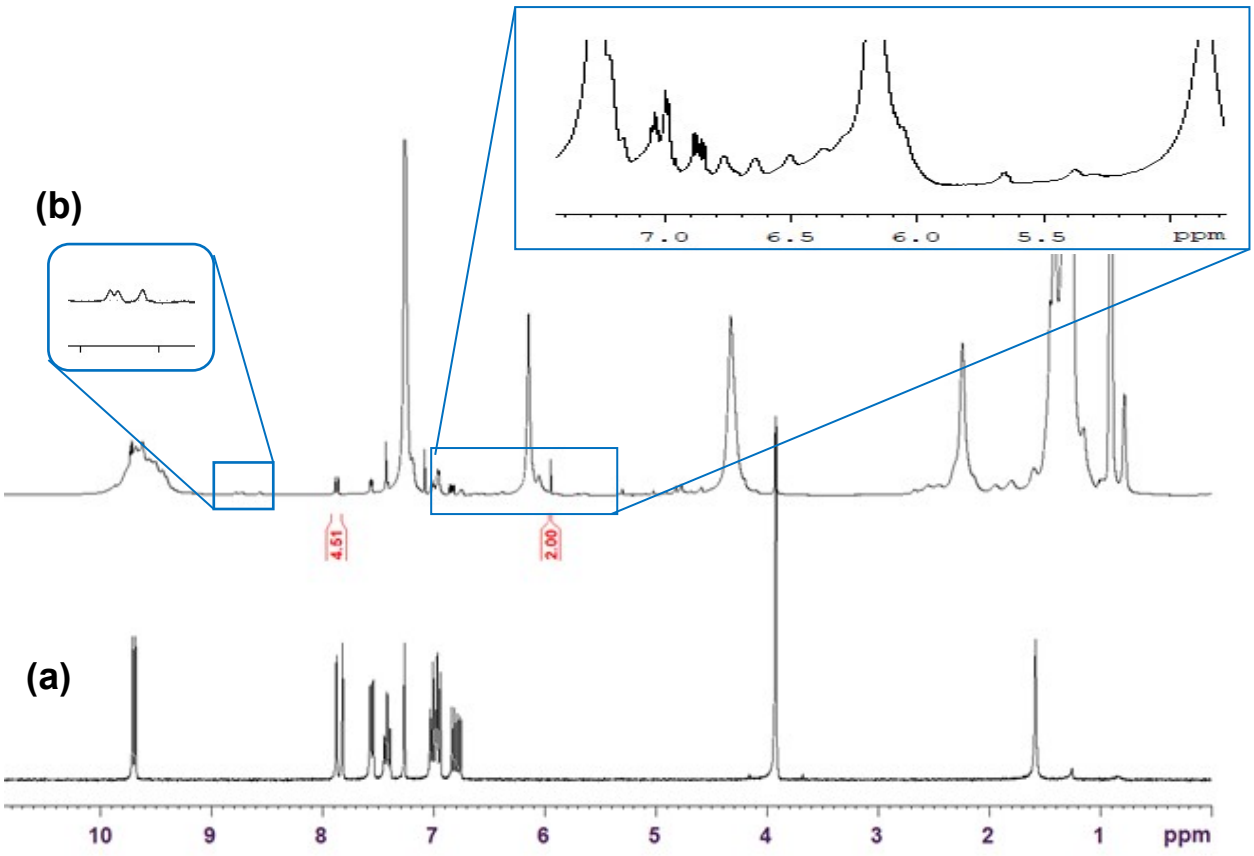


Figure S30. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of: (a) aldehyde **5g**; (b) the mixture of aldehyde **5g** (0.0423 mmol) and $\mathbf{C_6}$ (0.021 mmol) in $CDCl_3$ (0.5 mL). The signal of TCE (5.97 ppm, 2H, 5.35 μmol) used as internal standard.

Table S2. Uptake of aldehyde **5g** inside $\mathbf{C_6}$

mmol of starting aldehyde	Integral of free aldehyde[a]	mmol of free aldehyde	mmol of encapsulated aldehyde	Uptake (%)
0.0423	4.513	0.024	0.0183	43

[a] Integral of proton signal of free aldehyde at 7.85 ppm (1H) after the sample was allowed to equilibrate for t=1h

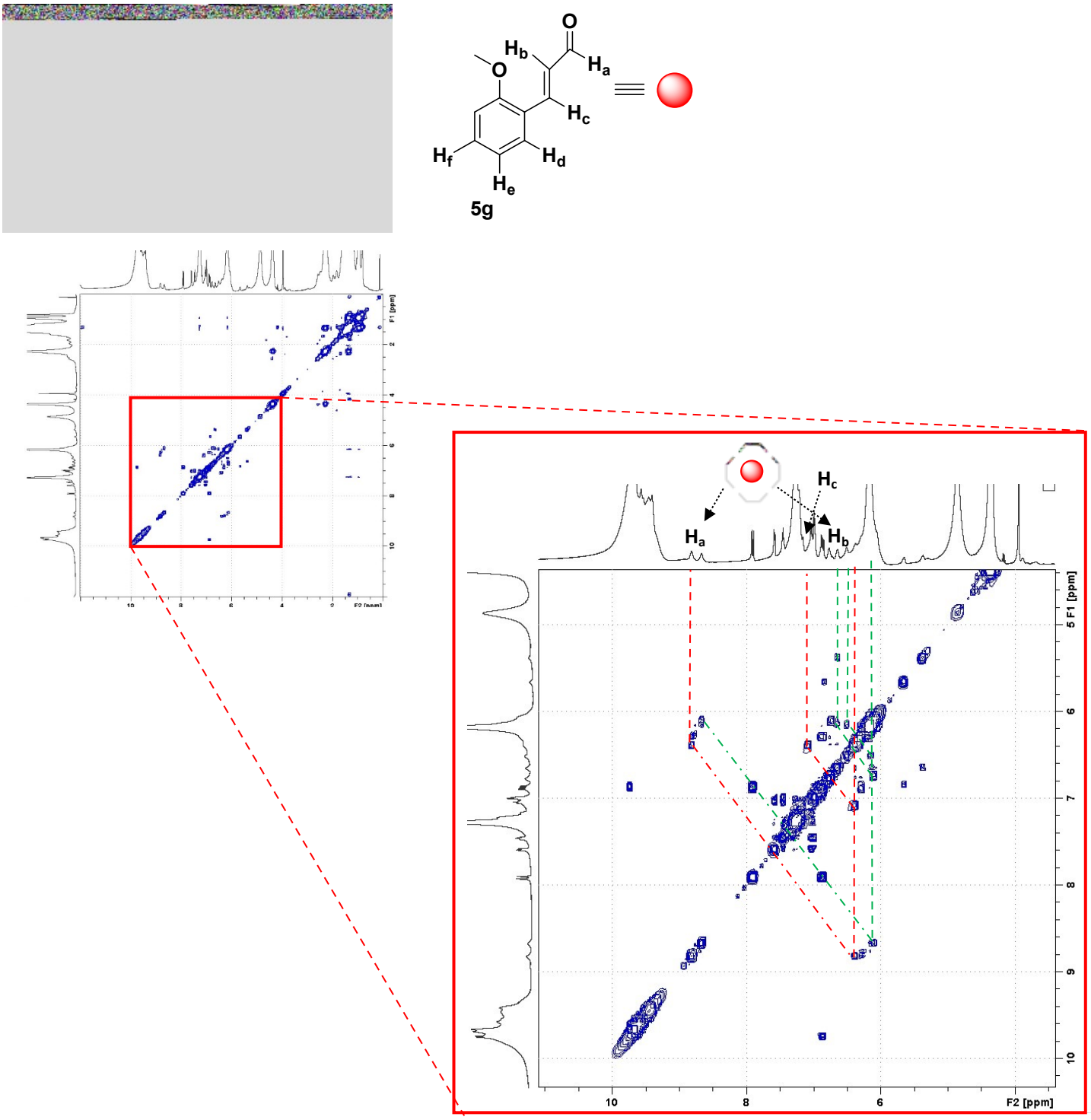


Figure S31. COSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture **5g** (42.3 mM) and $\mathbf{C_6}$ (21.2 mM)

The ^{1}H NMR signals of the encapsulated aldehyde **5g** are very complex, and in accord with the data previously reported by Cohen,[8] this indicates that the aromatic guest molecules are encapsulated in slightly different nanocontainers.

[8] L. Avram, Y. Cohen, *Org. Lett.* **2006**, *8*, 219-222.

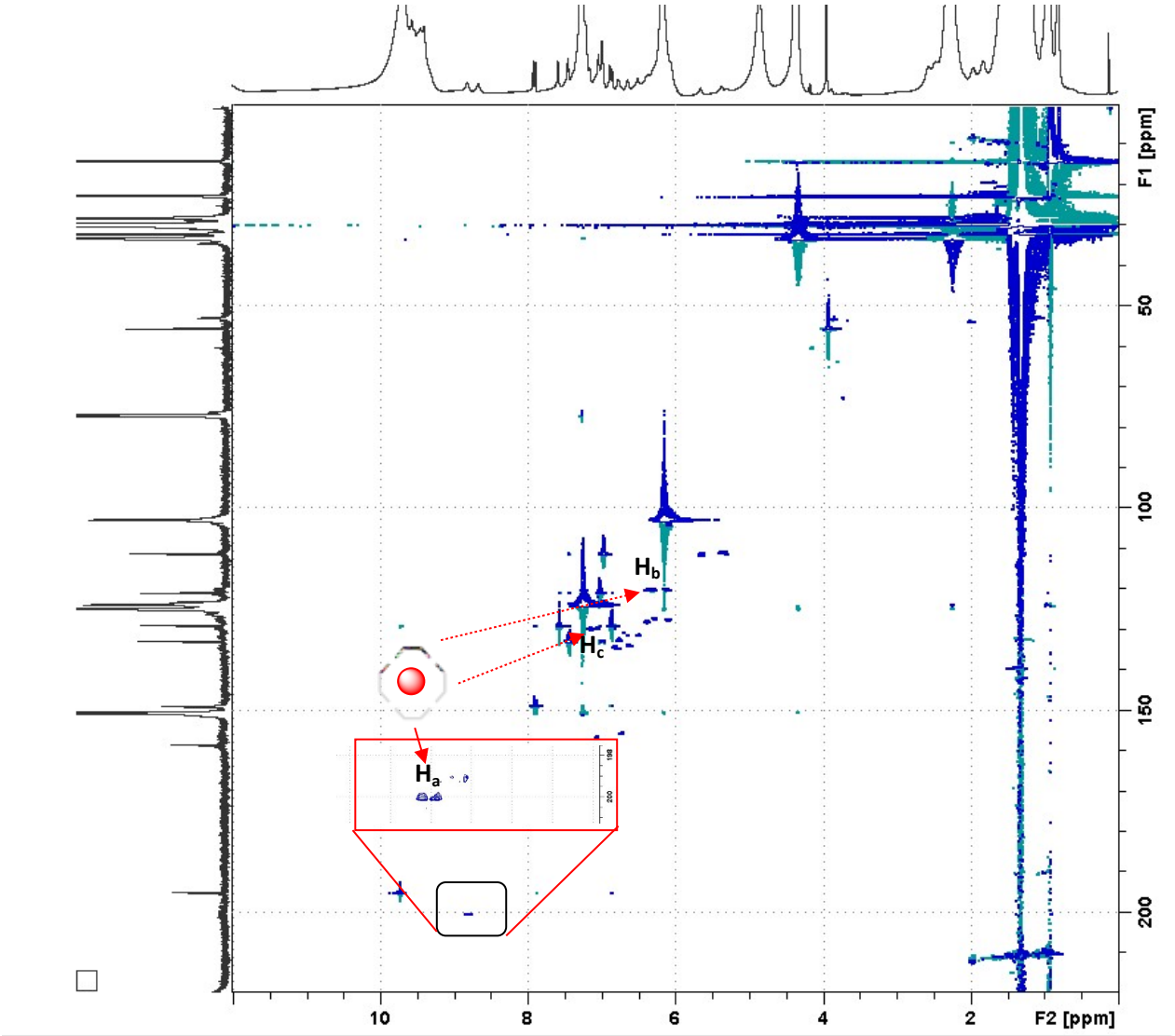
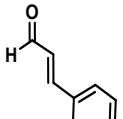
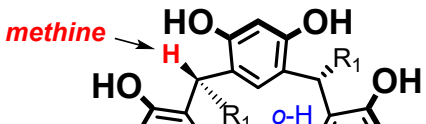


Figure S32. HSQC NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture **5g** (42.3 mM) and $\mathbf{C_6}$ (21.2 mM). Marked the NMR signals of **5g** encapsulated inside the hexameric capsule $\mathbf{C_6}$

5.3 Degree of encapsulation of large aldehyde 5k in the presence of C_6

Resorcinarene **1** (70 mg, 0.0635 mmol) was weighed in a 4 mL vial and 0.5 mL of water saturated $CDCl_3$ was added. The mixture was warmed at 50 °C until clarification (ca 5 min). To this solution aldehydes **5k** (0.021 mmol, 2 equiv respect to capsule $\mathbf{C_6}$) was added and the mixture was kept at 50 °C under stirring for 1h before being subjected to NMR spectroscopy to determine the total concentration of the free guest. For the





determination of the encapsulation ratio, the integral of the methine group (4.29 ppm, 24H) of capsule C_6 was used as reference.[9, 10, 11] For the guest integration, the signal of free guest **5k** (6.65 ppm, 1H) was used.

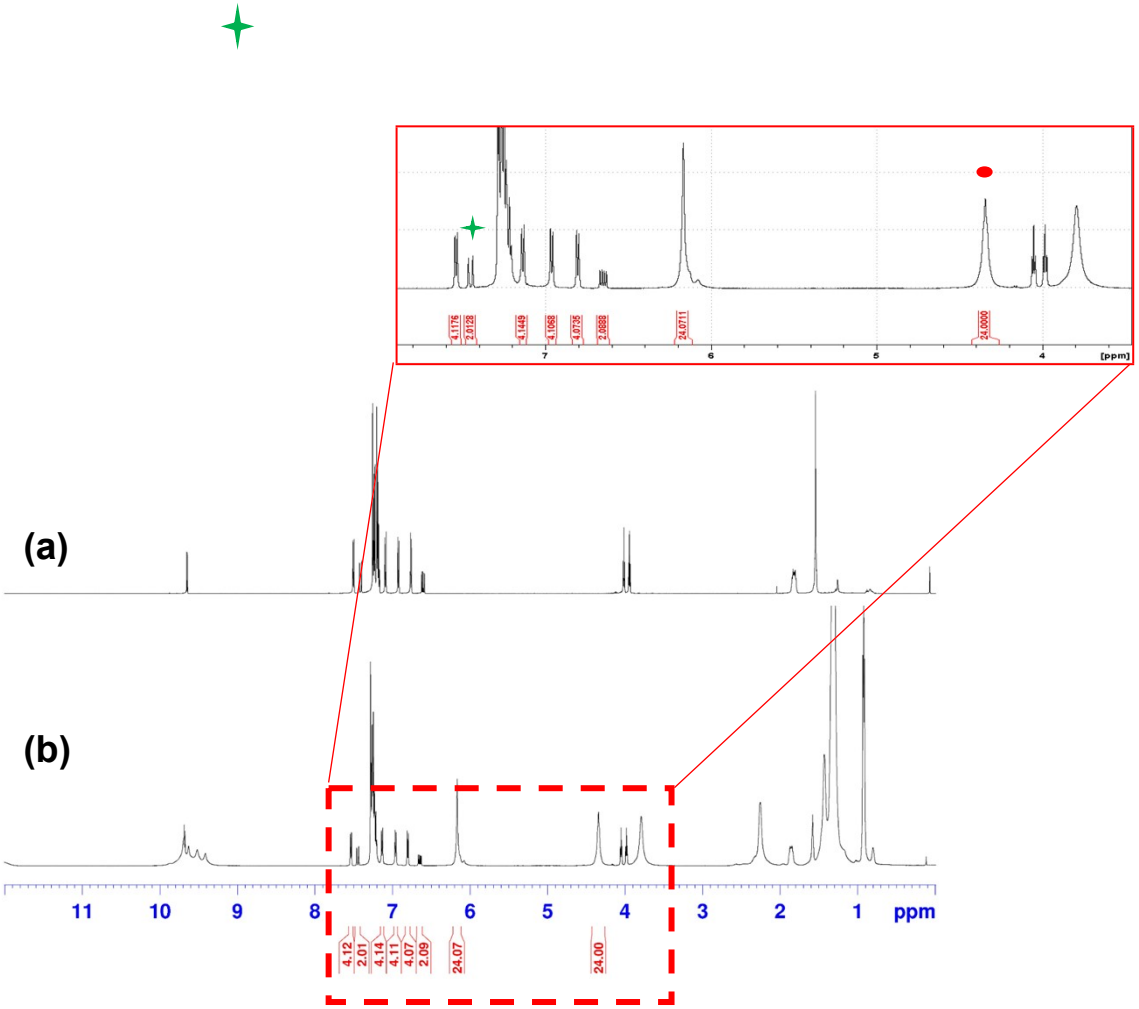


Figure S33. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of: (a) aldehyde **5k**; (b) the mixture of aldehyde **5k** (0.021 mmol) and **C_6** (0.011 mmol) in $CDCl_3$ (0.5 mL). Signals corresponding to free guest **5k** and **C_6** are highlighted by a star and a circle, respectively.

The encapsulation degree of the guest was determined by the equation $([G]_0 - [G]_t) / [G]_0$ (as reported by Tiefenbacher et al. in *J. Am. Chem. Soc.* **2017,** *139*, 11482-11492) was used to determine the encapsulation degree of **5k**. The terms $[G]_0$ indicates the total concentration of **5k**and $[G]_t$ the remaining free **5k** after the sample was allowed to equilibrate for t=1h.

[9] Q. Zhang, L. Catti, V. R. I. Kaila, K. Tiefenbacher, *Chem. Sci.* **2017,***8*, 1653-1657
[10] Q. Zhang, L. Catti, J. Pleiss, K. Tiefenbacher, *J. Am. Chem. Soc.* **2017,** *139*, 11482-11492
[11] S. Merget, L. Catti, G.M. Piccini, K. Tiefenbacher , *J. Am. Chem. Soc.* **2020,** *142*, 4400-4410

Table S3. Uptake of aldehyde **5k** inside C_6

mmol of starting aldehyde	Integral of free aldehyde[a]	mmol of free aldehyde	mmol of encapsulated aldehyde	Uptake (%)
0.021	2.09	0.021	0	0

[a] Integral of proton signal of free aldehyde at 6.65 ppm (1H) after the sample was allowed to equilibrate for t=1h

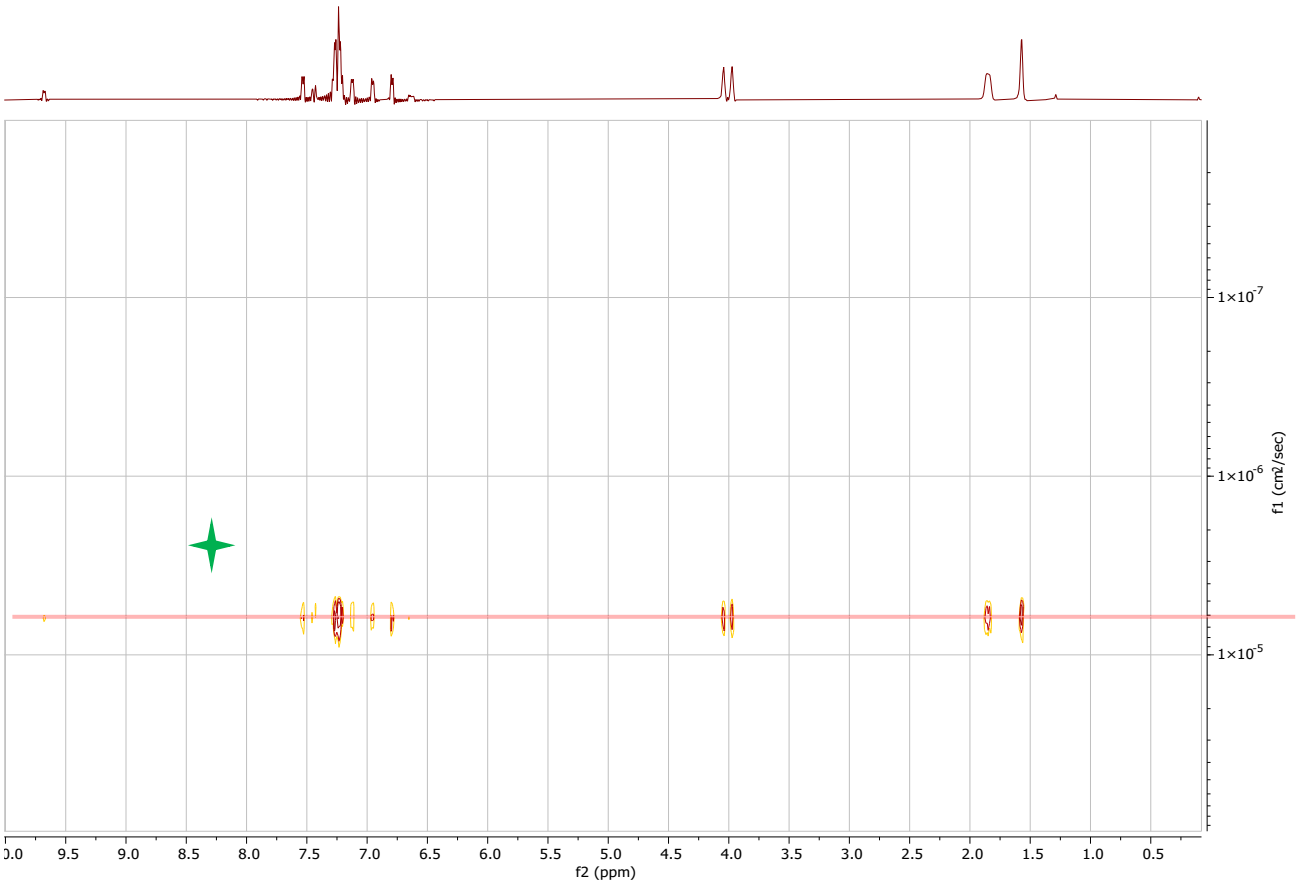


Figure S34. DOSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of aldehyde **5k** (42 mM). PulsePROG: ledbpgp2s, d20 = 0.15 sec, P30 = 1400 μs). Processing performed with MestreNova 14.0.0.

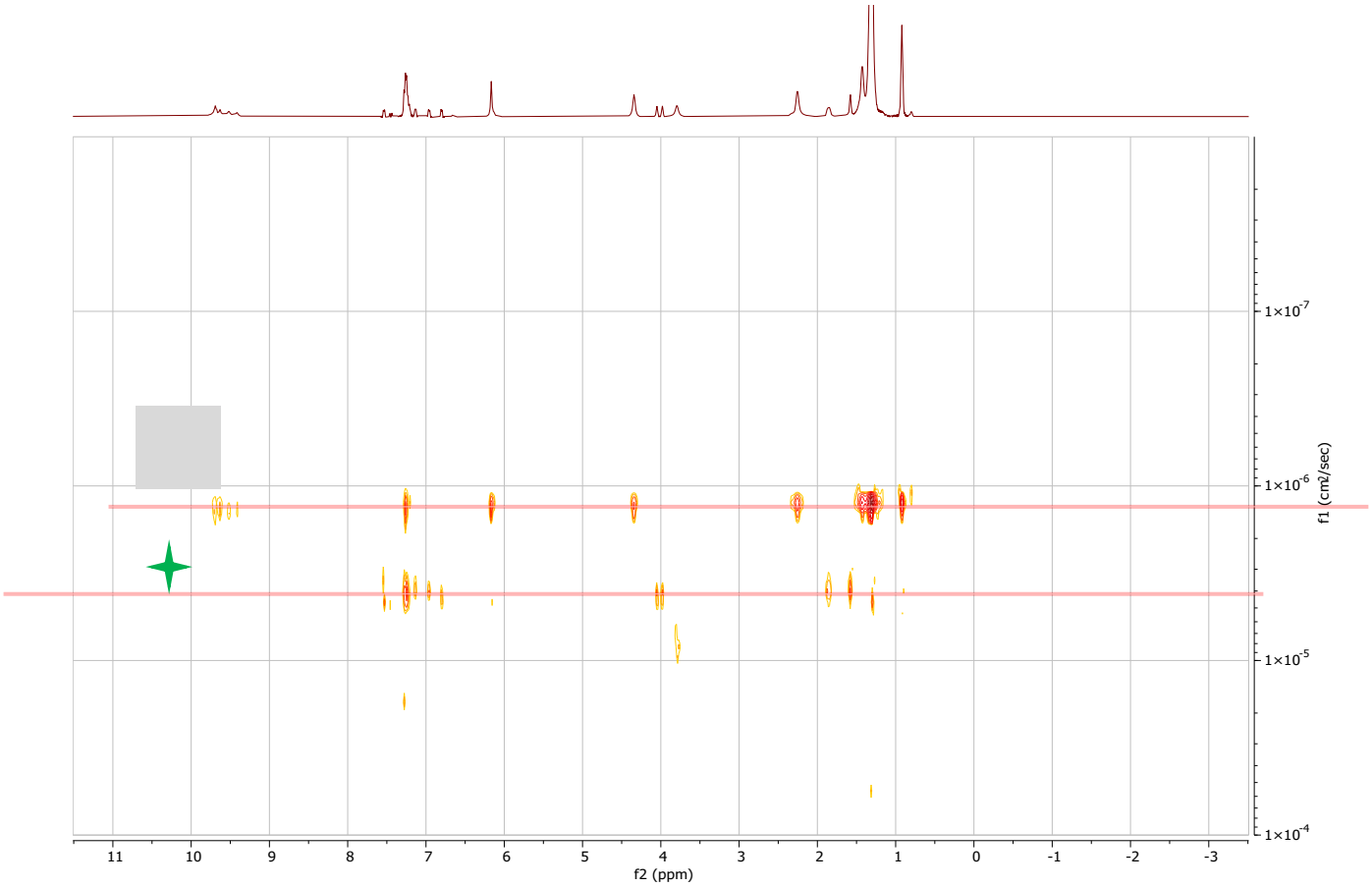


Figure S35. DOSY NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the mixture of **5k** (42 mM) and **C_6** (21.2 mM). PulsePROG: ledbpgp2s, d20 = 0.15 sec, P30 = 1400 µs). Processing performed with MestreNova 14.0.0.

6. General Procedures for the Diels-Alder reaction

6.1 General procedure in the presence of C_6 and Tr-X

Resorcinarene **1** (281.6 mg, 0.254 mmol, 1.56 equiv) was weighed in a 4 mL vial. Then, 1.1 mL of water-saturated chloroform was added, and the mixture was homogenized in an ultrasonic water bath at 40 °C for 10 min. To this clear yellow solution, Tr-X (0.1- 0.26 equiv) was added and, after 5 min under stirring, the dienophiles (0.163 mmol, 1 equiv.) followed by the diene (1 - 3 equiv.) were added. The solution was kept stirring at the appropriate temperature and time. The reaction was monitored by ^{1}H NMR analysis taking aliquots of the reaction mixture (30 µL) at various time intervals and diluting with chloroform-d. The reaction was stopped by adding 40 µL of DMSO and the mixture was purified by flash chromatography on silica gel to afford the desired title compounds. *Endo/exo* ratios were determined by ^{1}H NMR analysis via integration of proton signals of the title compounds in comparison with literature data[12].

6.2 General procedure in the presence of C_6

Resorcinarene **1** (281.6 mg, 0.254 mmol, 1.56 equiv.) was weighed in a 4 mL vial. Then, 1.1 mL of water-saturated chloroform was added, and the mixture was homogenized in an ultrasonic water bath at 40 °C for 10 min. To this clear yellow solution dienophile (0.163 mmol, 1 equiv.) followed by the diene (1 – 3 equiv.) were added. The solution was kept stirring at the appropriate temperature and time. The reaction was monitored by ^{1}H NMR analysis taking aliquots of the reaction mixture (30 µL) at various time intervals and diluting with chloroform-d. The reaction was stopped by adding 40 µL of DMSO and the mixture was directly subjected to NMR analysis. No conversion was observed.

6.3 Reaction in the presence of a competitive guest

6.3.1 Reaction in the presence of $Et_4N^+BF_4^-$ as a competitive guest

To a resorcinarene **1** (281.6 mg, 0.254 mmol, 1.56 equiv.) solution in water saturated chloroform-d (1.1 mL), tetraethylammonium tetrafluoroborate (10 equiv. or 1 equiv. relative to C_6) was added. Then, TrCl (0.042 mmol, 0.26 equiv.), dienophile (0.163 mmol, 1.0 equiv.) and the diene (0.489 mmol, 3 equiv.) were added to the solution in this order. The reaction system was kept under stirring (1400 rpm) at 50 °C for 16 h. No formation of product was observed.

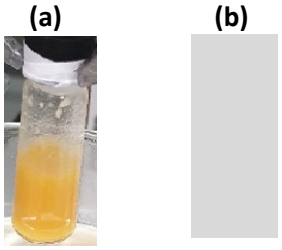
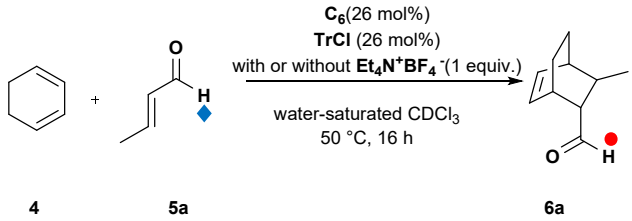


Figure S36. Mixture of: (a) hexameric capsule $\mathbf{C_6}$ (0.039M)/ $Et_4N^+BF_4^-$(1 equiv. relative to $\mathbf{C_6}$)/ TrCl (0.039 M), (b) hexameric capsule $\mathbf{C_6}$ (0.039M)/ TrCl (0.039 M)

[12] J. Bah, J. Franzén, *Chem. Eur. J.* **2014**, *20*, 1066-1072.



Scheme S1. DA reaction between **4** and **5a** in the presence of $\mathbf{C_6}$ and **TrCl** with and without competitive tetraethylammonium guest.

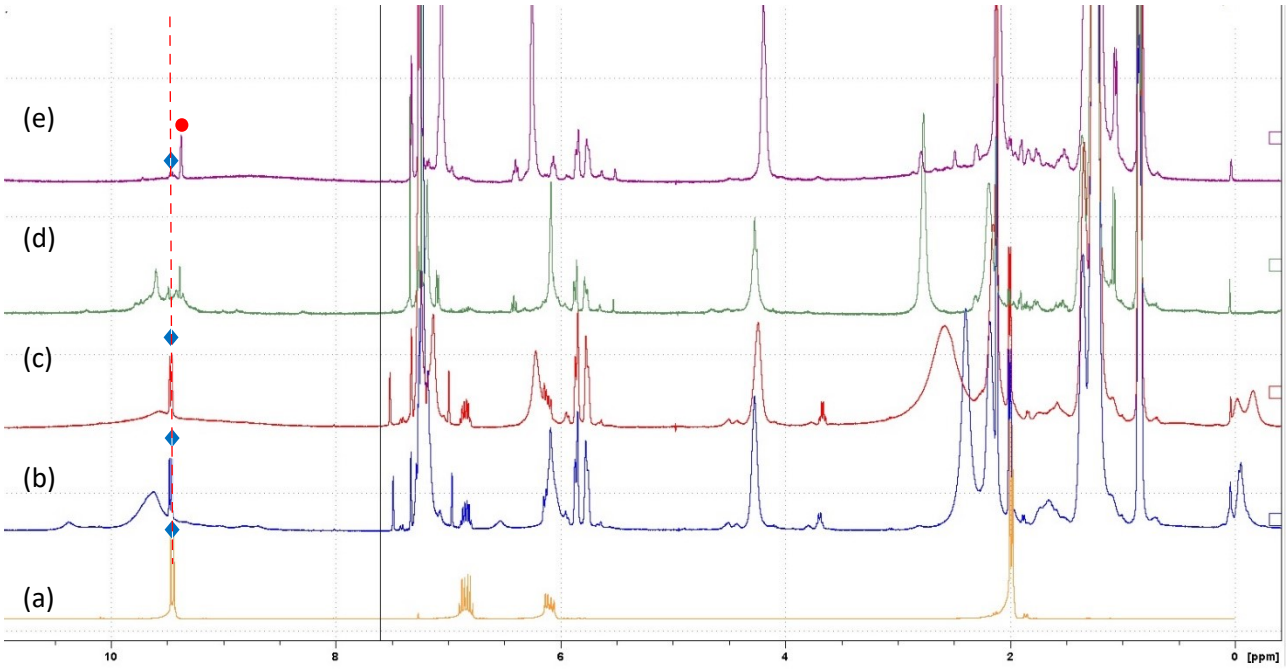


Figure S37. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of: (**a**) aldehyde **5a**; (**b**) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.039 M) in water-saturated $CDCl_3$ (1.1 mL) in the presence of tetraethylammonium tetrafluoroborate $Et_4N^+BF_4^-$(1 equiv. relative to $\mathbf{C_6}$) after 16h at 50°C; (**c**) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.039 M) in water-saturated $CDCl_3$ (1.1 mL) in the presence of tetraethylammonium tetrafluoroborate $Et_4N^+BF_4^-$ (1 equiv. relative to $\mathbf{C_6}$) after 16h at 50 °C and after addition of DMSO in order to disaggregate the capsule; (**d**) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.042 M) in water-saturated $CDCl_3$ (1.1 mL) after 16h at 50°C; (**e**) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.039 M) in water-saturated $CDCl_3$ (1.1 mL) after 16h at 50°C and after addition of DMSO in order to disaggregate the capsule.

6.3.2 Reaction in the presence of ammonium bromide 14 as a large competitive guest

To a solution of resorcinarene **1** (140 mg, 0.121 mmol) in water saturated chloroform-d (0.5 mL), ammonium

bromide **14** (19 mg, 0.023 mmol, 1 equiv. relative to C_6) was added. Then, TrCl (6 mg, 0.021 mmol, 1 equiv. relative to C_6), **5a** (0.163 mmol, 1.0 equiv.) and diene **4** (19.6 mg, 0.2445 mmol, 3 equiv.) were added to the solution in this order. The reaction system was kept under stirring (1400 rpm) at 50 °C for 16 h. ^{1}H-NMR of an aliquot of the reaction mixture revealed the formation of the product 6a (Figure S39) .

Figure S38. Mixture of: (a) hexameric capsule $\mathbf{C_6}$ (0.039M)/ **14** (1 equiv. relative to $\mathbf{C_6}$), (b) hexameric capsule $\mathbf{C_6}$ (0.039M)/ **14** (1 equiv. relative to $\mathbf{C_6}$)/**TrCl** (0.039 M).

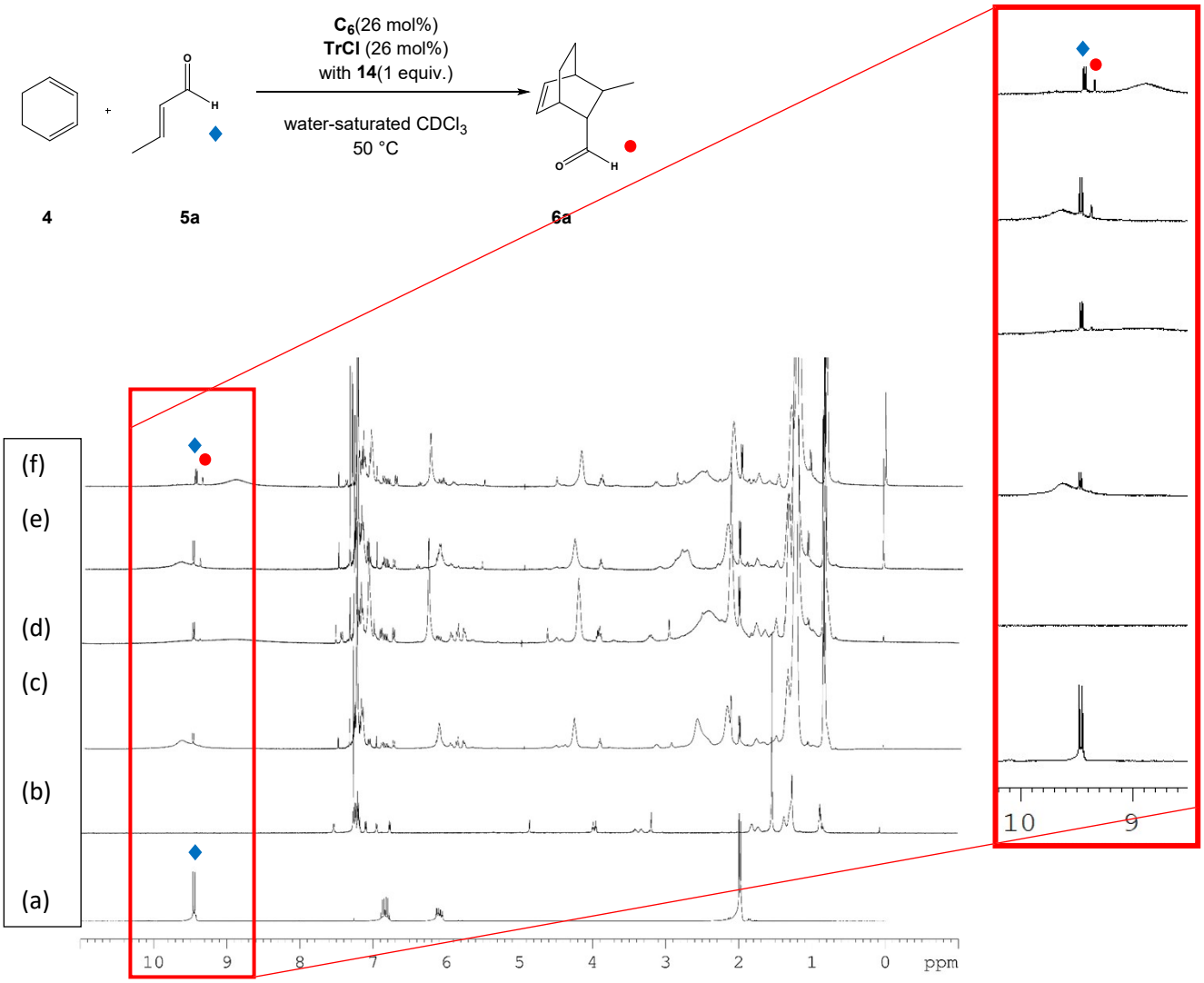


Figure S39. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of: (**a**) aldehyde **5a**; (**b**) ammonium bromide **14**; (c) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.039 M) in water-saturated $CDCl_3$ (1.1 mL) in the presence of ammonium bromide **14**(1 equiv. relative to $\mathbf{C_6}$) after 0.25h at

50°C; (d) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.039 M) in water-saturated $CDCl_3$ (1.1 mL) in the presence of ammonium bromide **14**(1 equiv. relative to $\mathbf{C_6}$) after 0.25h at 50°C and after addition of DMSO in order to disaggregate the capsule; (e) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.039 M) in water-saturated $CDCl_3$ (1.1 mL) in the presence of ammonium bromide **14**(1 equiv. relative to $\mathbf{C_6}$) after 1h at 50°C; (f) the reaction mixture of aldehyde **5a** (0.15 M) and cyclohexadiene **4** (0.45 M), $\mathbf{C_6}$ and **TrCl** (0.039 M) in water-saturated $CDCl_3$ (1.1 mL) in the presence of ammonium bromide **14**(1 equiv. relative to $\mathbf{C_6}$) after 1h at 50°C and after addition of DMSO in order to disaggregate the capsule;

6.4 Reaction in the presence of DMSO

To a resorcinarene **1** (281.6 mg, 0.254 mmol, 1.56 equiv.) solution in water saturated chloroform-d (1.1 mL), 90 µl of DMSO (1.27 mmol) were added. TrCl (0.042 mmol, 0.26 equiv.), dienophile (0.163 mmol, 1.0 equiv.) and the diene (0.489 mmol, 3 equiv.) were added to the solution in this order. The reaction system was kept under stirring (1400 rpm) at 50 °C for 16 h. No formation of product was observed.

6.5 General procedure in the presence of Tr-X and without C_6

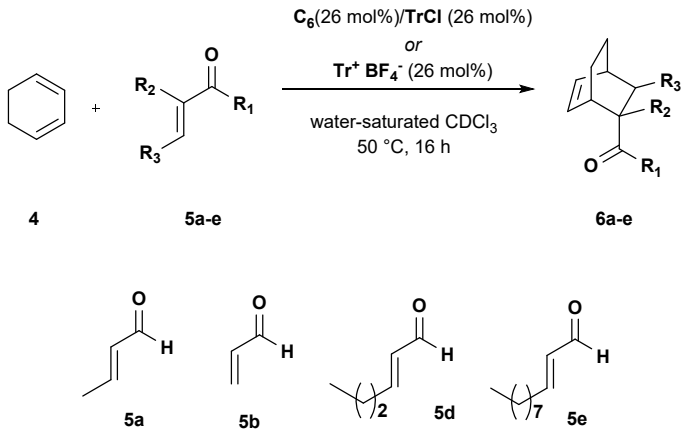
To a solution of water saturated chloroform (1.1 mL) Tr-X (0.042 mmol, 0.26 equiv.), dienophile (0.163 mmol, 1.0 equiv.) and the diene (0.489 mmol, 3 equiv.) were added in this order. The reaction mixture was vigorously stirred at 50°C for the appropriate time. The reaction was monitored by ^{1}H NMR analysis taking aliquots of the reaction mixture (30 µL) at various time intervals and diluting with chloroform-d.

6.6 General procedure in the absence of C_6 and Tr-X

To a solution of water saturated chloroform (1.1 mL) dienophile (0.163 mmol, 1.0 equiv.) and diene (0.489 mmol, 3 equiv.) were added in this order. The reaction mixture was vigorously stirred at 50°C for the appropriate time. The reaction was monitored by ^{1}H NMR analysis taking aliquots of the reaction mixture (30 µL) at various time intervals and diluting with chloroform-d. No formation of title compounds was observed.

6.7 Reaction progress for DA reactions

The DA reactions between cyclohexadiene **4** with aldehydes **5a, b, d, e** were performed at 50°C under standard reaction conditions in the presence of **TrCl** and $\mathbf{C_6}$ or of preformed trityl fluoroborate salt $\mathbf{3}^+$ $BF4^-$ without $\mathbf{C_6}$ and monitored as a function of time by quantitative ^{1}H-NMR (qNMR) spectroscopy using 1,1,2,2-tetrachloroethane (TCE) as an internal standard.



Scheme S2. DA reaction between **4** and aldehydes **5a-e** in the presence of $\mathbf{C_6}$ and **TrCl or** $\mathbf{Tr^+\ BF_4^-}$.

Table S4. Time-dependent conversion in **6a** of a mixture of **4** (0.489 mmol) and **5a** (0.163 mmol) in the presence of $\mathbf{TrCl/C_6}$ (0.042 mmol), in the presence of preformed trityl fluoroborate salt $\mathbf{3^+\ BF4^-}$ (0.042 mmol) without $\mathbf{C_6}$ or without $\mathbf{TrCl/C_6}$

Time (h)[a]	**6a (%)**[b] in the presence of $\mathbf{TrCl/C_6}$	**6a (%)**[c] in the presence of $\mathbf{3^+\ BF4^-}$	**6a (%)**[c] In the presence of only **TrCl**	**6a (%)**[c] In the presence of only $\mathbf{C_6}$	**6a (%)**[c] without $\mathbf{TrCl/C_6}$
0	0	0	0	0	0
0.08	5	0	0	0	0
0.17	7	0	0	0	0
0.25	13	15	0	0	0
0.50	24	35	0	0	0
1.0	41	39	0	0	0
3.0	60	46	0	0	0
6.0	87	50	0	0	0
16	99	55	0	0	0
24	99	55	0	0	0
32	99	55	0	0	0

(a) Time at which an aliquot (30 μL) of the reaction mixture was taken and monitored via ^{1}H-NMR spectrum. [(b)] Conversion was calculated after addition of DMSO (2 μL) to a reaction aliquot, in order to disaggregate the capsule. Conversion was calculated using TCE as internal standard. [(c)] Conversion was calculated using TCE as internal standard.

Table S5. Time-dependent conversion in **6b** of a mixture of **4** (0.489 mmol) and **5b** (0.163 mmol) in the presence of $\mathbf{TrCl/C_6}$ (0.042 mmol), in the presence of preformed trityl fluoroborate salt $\mathbf{3^+\ BF4^-}$ (0.042 mmol) without $\mathbf{C_6}$ or without $\mathbf{TrCl/C_6}$

Time (h)[a]	6b (%)[b] in the presence of **TrCl/C_6**	6b (%)[c] in the presence of **3^+ $BF4^-$**	6b (%)[c] In the presence of only **TrCl**	6b (%)[c] In the presence of only **C_6**	6a (%)[c] without **TrCl/C_6**
0	0	0	0	0	0
0.08	64	Quant.	0	0	0
0.17	95	Quant.	0	0	0
0.25	98		0	0	0
0.50	99		0	0	0
1.0	99		0	0	0
3.0	99		0	0	0
6.0	99		0	0	0
16	99		0	0	0
24	99		0	0	0
32	99		0	0	0

(a) Time at which an aliquot (30 μL) of the reaction mixture was taken and monitored via ^{1}H-NMR spectrum. [(b)] Conversion was calculated after addition of DMSO (2 μL) to a reaction aliquot, in order to disaggregate the capsule. Conversion was calculated using TCE as internal standard. [(c)] Conversion was calculated using TCE as internal standard.

Table S6. Time-dependent conversion in **6d** of a mixture of **4** (0.489 mmol) and **5d** (0.163 mmol) in the presence of **TrCl/C_6** (0.042 mmol), in the presence of preformed trityl fluoroborate salt **3^+ $BF4^-$** (0.042 mmol) without **C_6** or without **TrCl/C_6**

Time (h)[a]	6d (%)[b] in the presence of **TrCl/C_6**	6d (%)[c] in the presence of **3^+ $BF4^-$**	6d (%)[c] In the presence of only **TrCl**	6d (%)[c] In the presence of only **C_6**	6d (%)[c] without **TrCl/C_6**
0	0	0	0	0	0
0.08	0	0	0	0	0
0.17	0	0	0	0	0
0.25	0	12	0	0	0
0.50	6	24	0	0	0
1.0	12	28	0	0	0
3.0	29	40	0	0	0

6.0	53	46	0	0	0
16	78	53	0	0	0
24	80	53	0	0	0
32	80	53	0	0	0

[a] Time at which an aliquot (30 μL) of the reaction mixture was taken and monitored via ^{1}H-NMR spectrum. [b] Conversion was calculated after addition of DMSO (2 μL) to a reaction aliquot, in order to disaggregate the capsule. Conversion was calculated using TCE as internal standard. [c] Conversion was calculated using TCE as internal standard.

Table S7. Time-dependent conversion in **6e** of a mixture of **4** (0.489 mmol) and **5e** (0.163 mmol) in the presence of **TrCl/C_6** (0.042 mmol), in the presence of preformed trityl fluoroborate salt **3^+ $BF4^-$** (0.042 mmol) without **C_6** or without **TrCl/C_6**

Time (h)[a]	**6e (%)[b]** in the presence of **TrCl/C_6**	**6e (%)[c]** in the presence of **3^+ $BF4^-$**	**6e (%)[c]** In the presence of only **TrCl**	**6e (%)[c]** In the presence of only **C_6**	**6e (%)[c]** without **TrCl/C_6**
0	0	0	0	0	0
0.08	0	0	0	0	0
0.17	0	0	0	0	0
0.25	0	34	0	0	0
0.50	0	51	0	0	0
1.0	5	54	0	0	0
3.0	9	56	0	0	0
6.0	33	58	0	0	0
16	47	58	0	0	0
24	47	58	0	0	0
32	47	58	0	0	0

[a] Time at which an aliquot (30 μL) of the reaction mixture was taken and monitored via ^{1}H-NMR spectrum. [b] Conversion was calculated after addition of DMSO (2 μL) to a reaction aliquot, in order to disaggregate the capsule. Conversion was calculated using TCE as internal standard. [c] Conversion was calculated using TCE as internal standard.

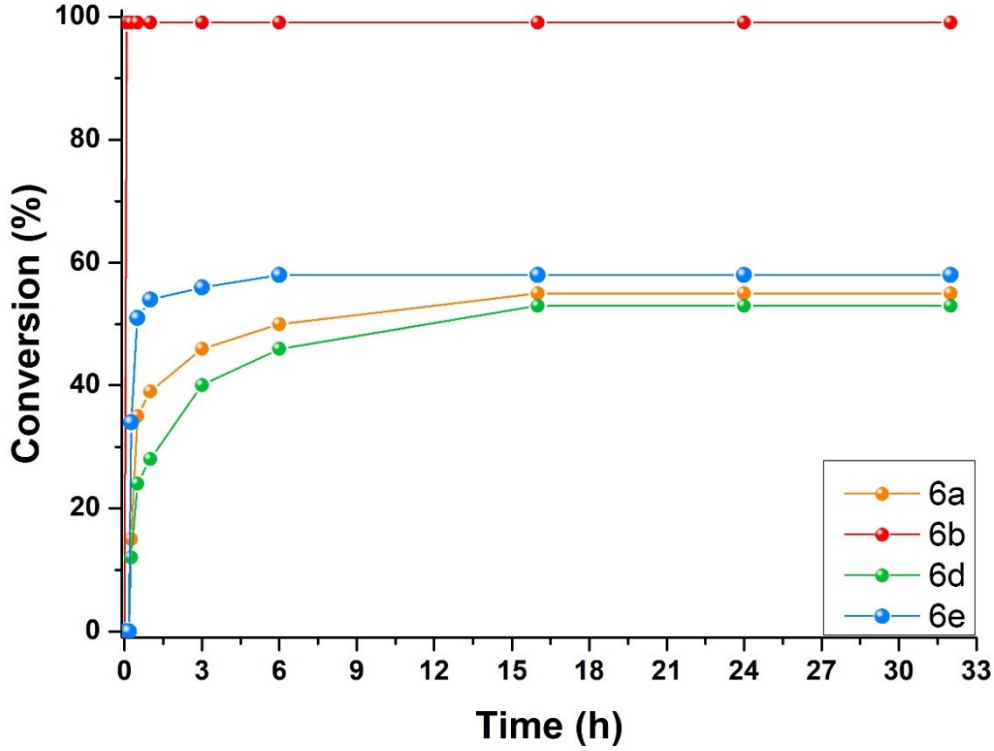


Figure S40. Reaction progress for DA reaction between **4** and aldehydes **5a-e** in the presence of **3**$^{+}$·**BF4**$^{-}$.

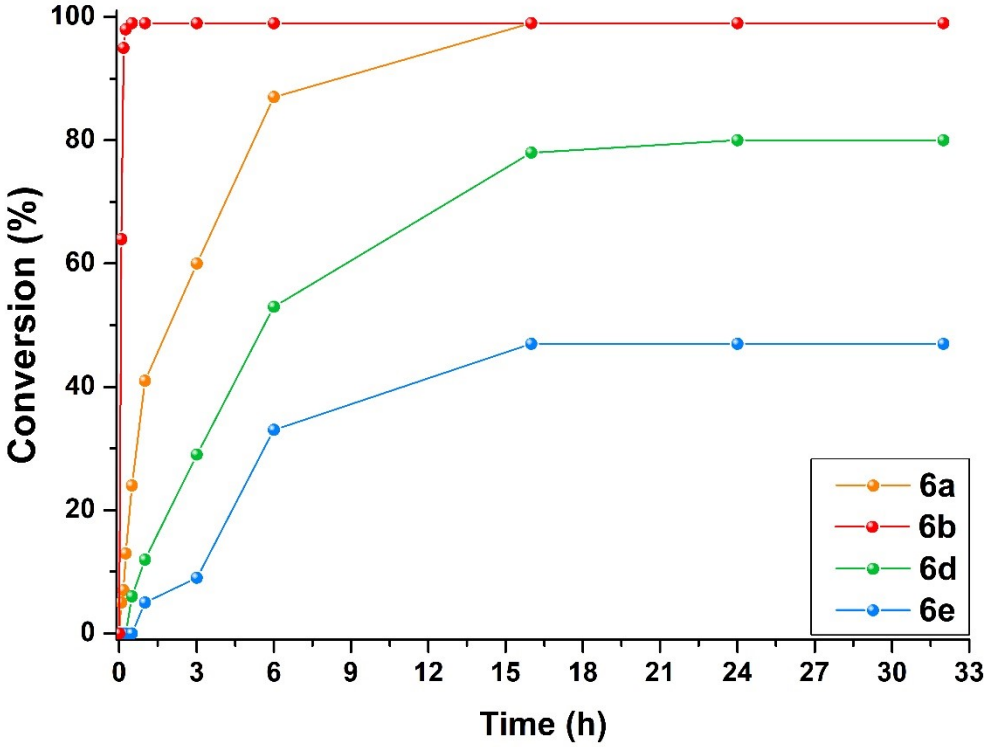
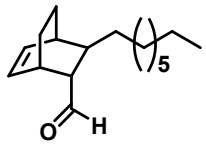


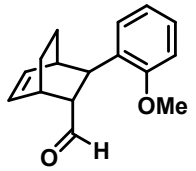
Figure S41. Reaction progress for DA reaction between **4** and aldehydes **5a-e** in the presence of **2a** (26 mol%) and **C$_6$** (26 mol %).

7. Characterization of novel compounds



3-octylbicyclo[2.2.2]oct-5-ene-2-carbaldehyde (6e). The title compound was prepared according to the general procedure *4.1* from *trans*-2-undecenal and 1,3-cyclohexadiene. Purification by flash column chromatography on silica gel (pentane: diethyl ether = 90:10) afforded **6e** as a slightly yellow oil in 46% yield in an *endo:exo* ratio of >99:1.^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 9.40 (d, J = 1.8 Hz, 1H), 6.41 (dd, J_1=J_2= 6.9 Hz, 1H), 6.11 (dd, J_1=J_2= 7.0 Hz, 1H), 2.85-2.78 (m, 1H), 2.43-2.50 (m, 1H), 1.95-2.00 (m, 2H), 1.80-1.69 (m, 3H), 1.62- 1.48 (m, 3H), 1.44-1.17 (m, 11H), 1.17- 1.01 (m, 1H), 0.87 (t, J= 7.2 Hz, 3 H).^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 204.3, 137.7, 130.8, 59.4, 37.4, 34.8, 33.3, 31.8, 31.3, 29.8, 29.5, 29.3, 27.9, 25.3, 22.6, 18.8, 14.1. Anal. calcd. for $C_{17}H_{28}O$: C, 82.20; H, 11.36. Found: C, 82.11; H, 11.45.

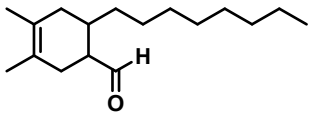
The *exo/endo* ratio was determined by ^{1} H NMR analysis on the crude reaction mixture: ^{1}H NMR ($CDCl_3$) δ 9.40 (1H, CHO- *endo*), 9.74 (1H, CHO -*exo*), in analogy with known compound **6d**[13]



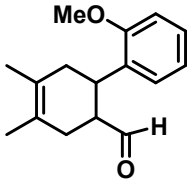
3-(2-methoxyphenyl)bicyclo[2.2.2]oct-5-ene-2-carbaldehyde (6g). The title compound was prepared according to the general procedure *4.1* from 2-methoxy-cinnamaldehyde and 1,3-cyclohexadiene. Purification by flash column chromatography on silica gel (pentane: diethyl ether = 95:5) afforded **6g** as a slightly yellow oil in 67% yield and in an *endo: exo* ratio of >99:1. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.42 (d, J = 1.8 Hz, 1H), 7.28-7.18 (m, 3H), 6.96 (dd, J_1=J_2= 7.6 Hz, 1H), 6.88 (d, J= 7.7 Hz, 1 H), 6.21 (dd, J_1=J_2= 7.6 Hz, 1H), 3.81 (s, 3H), 3.57-3.50 (m, 1H), 3.04-2.94 (m, 1H), 2.76-2.61 (m, 2H), 1.78-1.64 (m, 2H), 1.48-1.33 (m, 1H), 1.15- 0.99 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 204.0, 157.7, 137.3, 130.9, 130.0, 127.4, 127.1, 120.1, 110.6, 55.2, 55.1, 36.6, 34.0, 32.0, 25.7, 19.1. HRMS (ESI^+) *m/z*: [M^+] calcd for $C_{16}H_{18}O_2$ 242.13013, found: 242.10300, [M+ Na]$^+$ calcd. for $C_{16}H_{18}NaO_2$ 265.11990, found: 265.11976, [M+K]$^+$ calcd. for $C_{16}H_{18}KO_2$ 281.09384, found: 281.09368.

[13] (a) K. Ishihara, h. Kurihara, M. Matsumoto, H. Yamamoto, *J. Am. Chem. Soc.* **1998**, *120*, 6920-6930; (b) K. A. Ahrendt, C. J. Borths, D. W. C. MacMillan, *J. Am. Chem. Soc.* **2000**, *122*, 4243-4244.

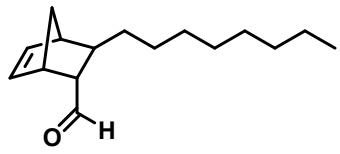
The *exo/endo* ratio was determined by [1] H-NMR analysis on the crude reaction mixture: ^{1}H-NMR ($CDCl_3$) δ 9.42 (1H, CHO- *endo*), 9.87 (1H, CHO -*exo*), in analogy with known compound **6f** [4]and confirmed by NOESY experiment (Figure S22)



3,4-dimethyl-6-octylcyclohex-3-ene-1-carbaldehyde (8e). The title compound was prepared according to the general procedure *4.1* from *trans*-2-undecenal and 2,3-dimethyl-1,3- butadiene. Purification by flash column chromatography on silica gel (pentane: diethyl ether = 95:5) afforded **8e** as a pale yellow oil in 5% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 9.58 (d, J = 3.2 Hz, 1H), 2.35- 1.85 (m, 6H), 1.73-1.47 (m, 8H), 1.45-1.16 (m, 12H), 0.87 (t, J= 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 205.5, 125.0, 122.5, 51.8, 35.6, 33.9, 33.4, 31.8, 29.8, 29.7, 29.5, 29.3, 26.8, 22.6, 19.1, 18.7, 14.7. Anal. calcd. for $C_{17}H_{30}O$: C, 81.54; H, 12.08. Found: C, 81.45; H, 12.16.



2'-methoxy-4,5-dimethyl-1,2,3,6-tetrahydro-[1,1'-biphenyl]-2-carbaldehyde (8g). The title compound was prepared according to the general procedure *4.1* from 2-methoxy-cinnamaldehyde and 2,3-dimethyl-1,3-butadiene. Purification by flash column chromatography on silica gel (pentane: diethyl ether = 95:5) afforded **8g** as a pale yellow oil in 60 % yield. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 9.44 (d, J = 2.9 Hz, 1H), 7.20-1.17 (m, 1H), 7.14 (dd, J= 1.6, 7.6 Hz, 1H), 6.91 (dd, J= 1.2, 7.5 Hz, 1H), 6.85 (d, J= 8.2 Hz, 1H), 3.81 (s, 3H), 3.55- 3.50 (m, 1H), 2.88 - 2.80 (m, 1H), 2.34- 2.26 (m, 1H), 2.22- 2.21 (m, 2H), 2.04- 2.01 (m, 1H), 1.68 (s, 3H), 1.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 204.9, 156.9, 131.3, 127.8, 127.5, 125.8, 123.3, 120.9, 110.5, 55.3, 51.0, 37.4, 34.2, 31.0, 18.8 (x2). HRMS (MALDI) *m/z*: [M+ Na] $^{+}$ calcd. for $C_{16}H_{20}NaO_2$ 267.13555, found: 267.13848.



3-octylbicyclo[2.2.1]hept-5-ene-2-carbaldehyde (10e). The title compound was prepared according to the general procedure *4.1* from *trans*-2-undecenal and 1,3-cyclopentadiene. Purification by flash column

chromatography on silica gel (pentane: diethyl ether = 90:10) afforded **10e** as a slightly yellow oil in 91% yield in an *endo:exo* ratio of 84:16.^{1}H NMR (600 MHz, $CDCl_3$): *endo* δ (ppm) 9.36 (d, J = 3.4 Hz, 1H), 6.27 (dd, J= 3.2, 5.8 Hz,1H), 6.5 (dd, J= 2.8, 5.6 Hz, 1H), 3.11 (bs, 1H), 2.66 (bs, 1H), 2.37 (dd, J= 3.5, 7.7 Hz,1H), 1.68- 1.64 (m, 1H), 1.56-1.21 (m, 16H), 0.88 (t, J= 6.8 Hz, 3 H).^{13}C NMR (150 MHz, $CDCl_3$): *endo* δ (ppm) 205.1, 138.8, 132.8, 60.1, 47.2, 46.5, 45.1, 42.2, 35.8, 31.9, 29.8, 29.5, 29.3, 28.4, 22.6, 14.1. Anal. calcd. for $C_{16}H_{26}O$: C, 81.99; H, 11.18. Found: C, 81.97; H, 11.20.

The *exo/endo* ratio was determined by ^{1} H NMR analysis on the crude reaction mixture: ^{1}H NMR ($CDCl_3$) δ 9.36 (1H, CHO- *endo*), 9.78 (1H, CHO -*exo*), in analogy with known compound **10d**[4, 14] and confirmed by NOESY experiment (Figure S32)

8. ^{1}H and ^{13}C NMR of novel compounds

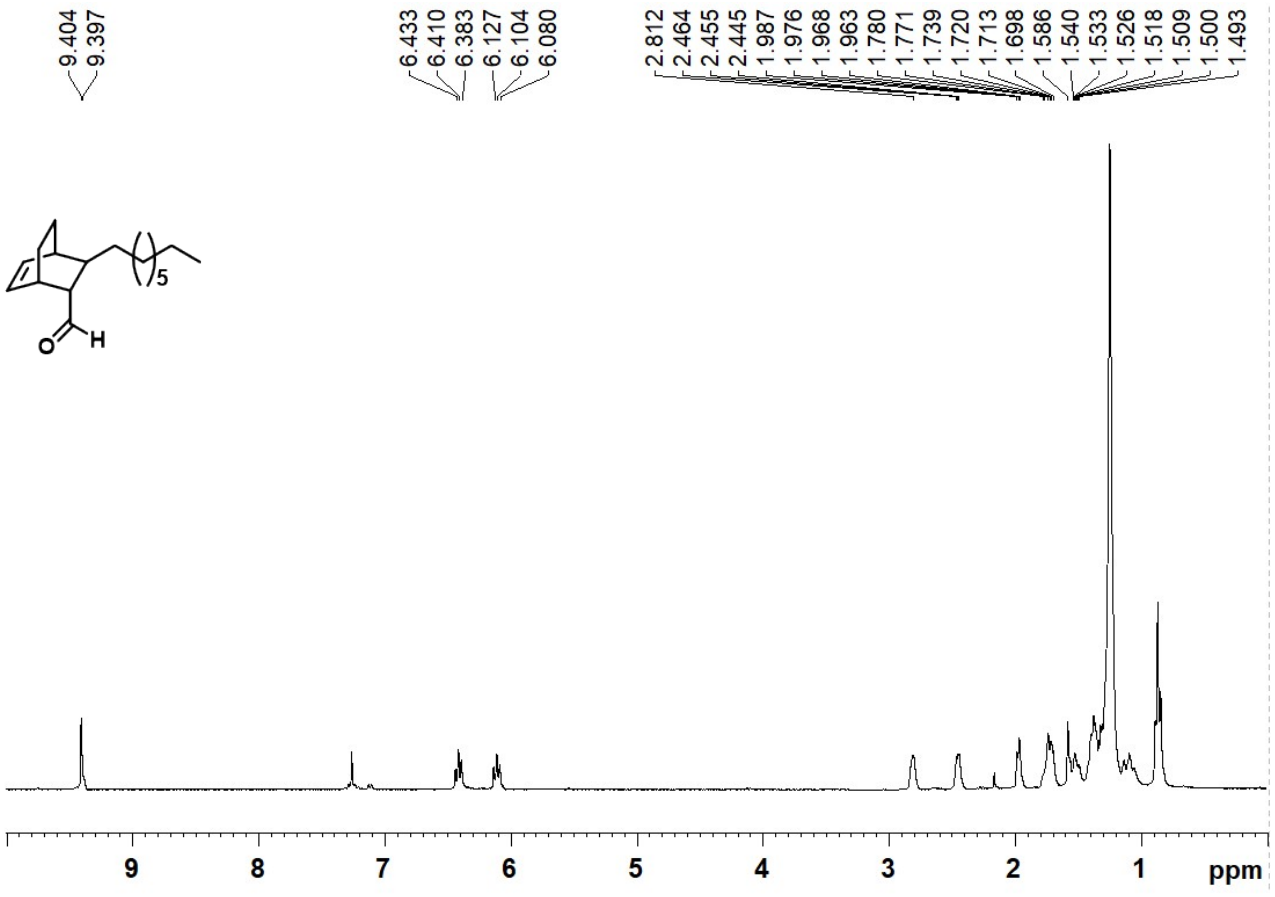


Figure S42. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of compound **6e.**

[14] a) K. Ishihara, H. Kurihara, M. Matsumoto, H. Yamamoto, *J. Am. Chem. Soc.* **1998**, *120*, 6920-6930; b) H. He, B.-J. Pei, H.-H. Chou, T. Tian, W.-H. Chan, A. W. M. Lee, *Org. Lett.* **2008**, *10*, 2421–2424.

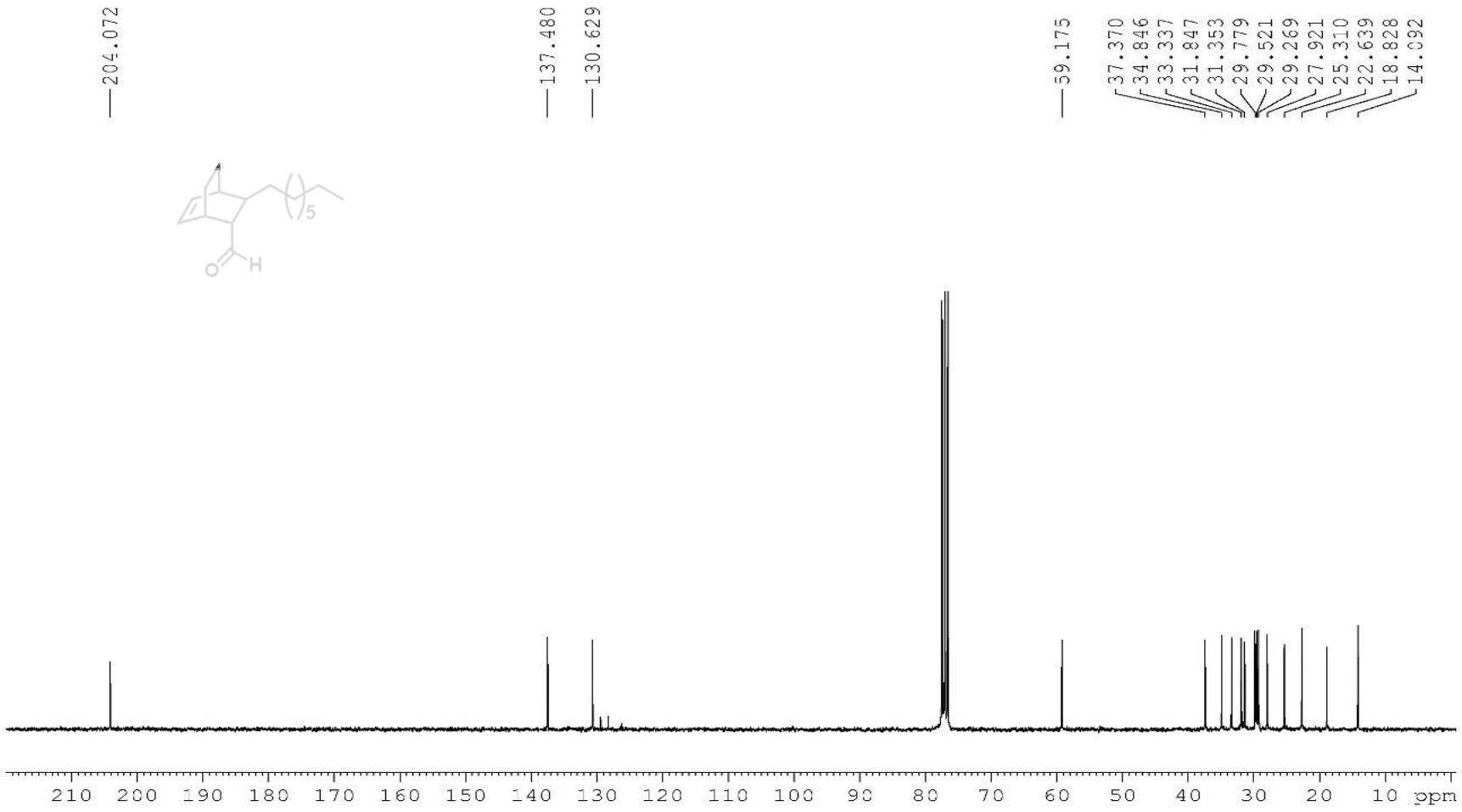


Figure S43. ^{13}C NMR spectrum (75 MHz, $CDCl_3$, 298 K) of compound **6e.**

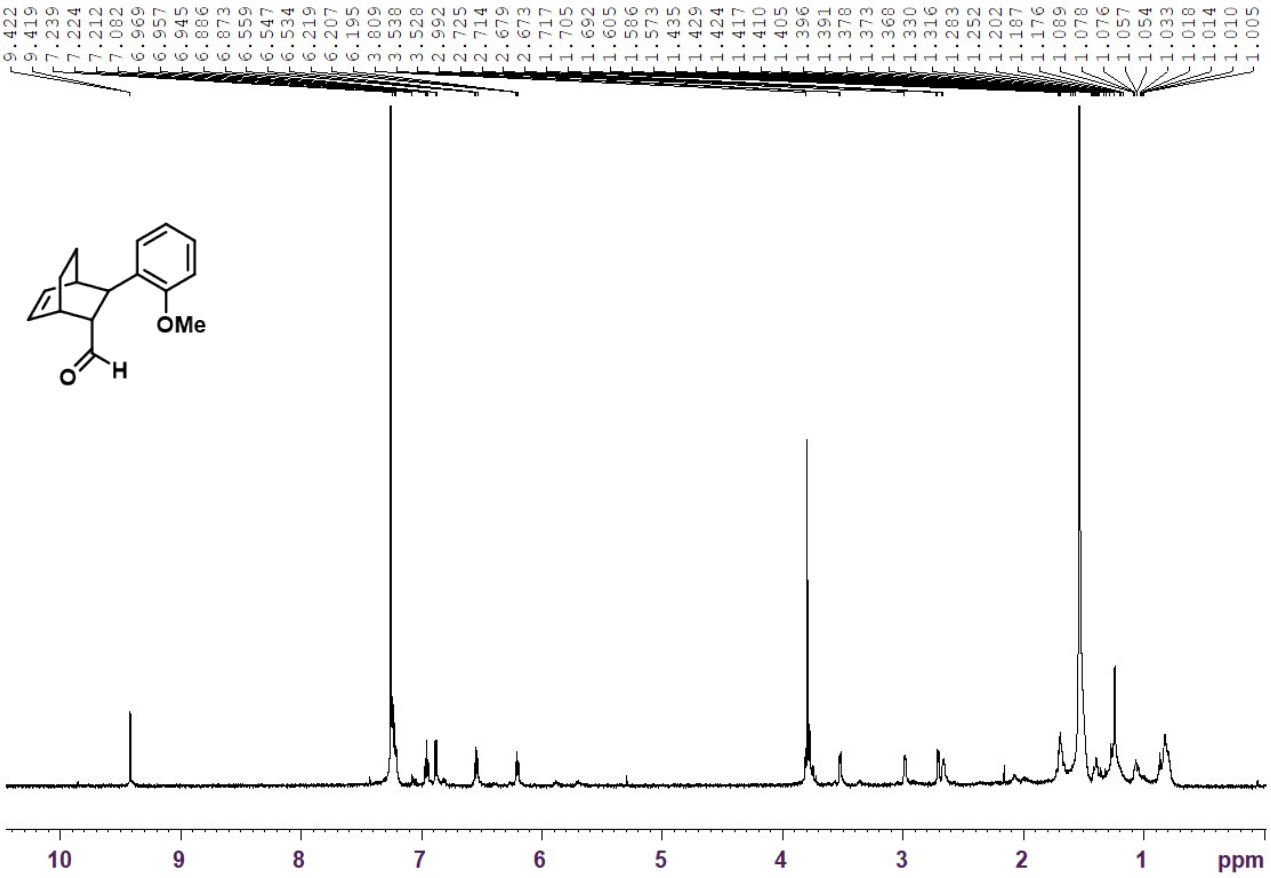


Figure S44. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of compound **6g.**

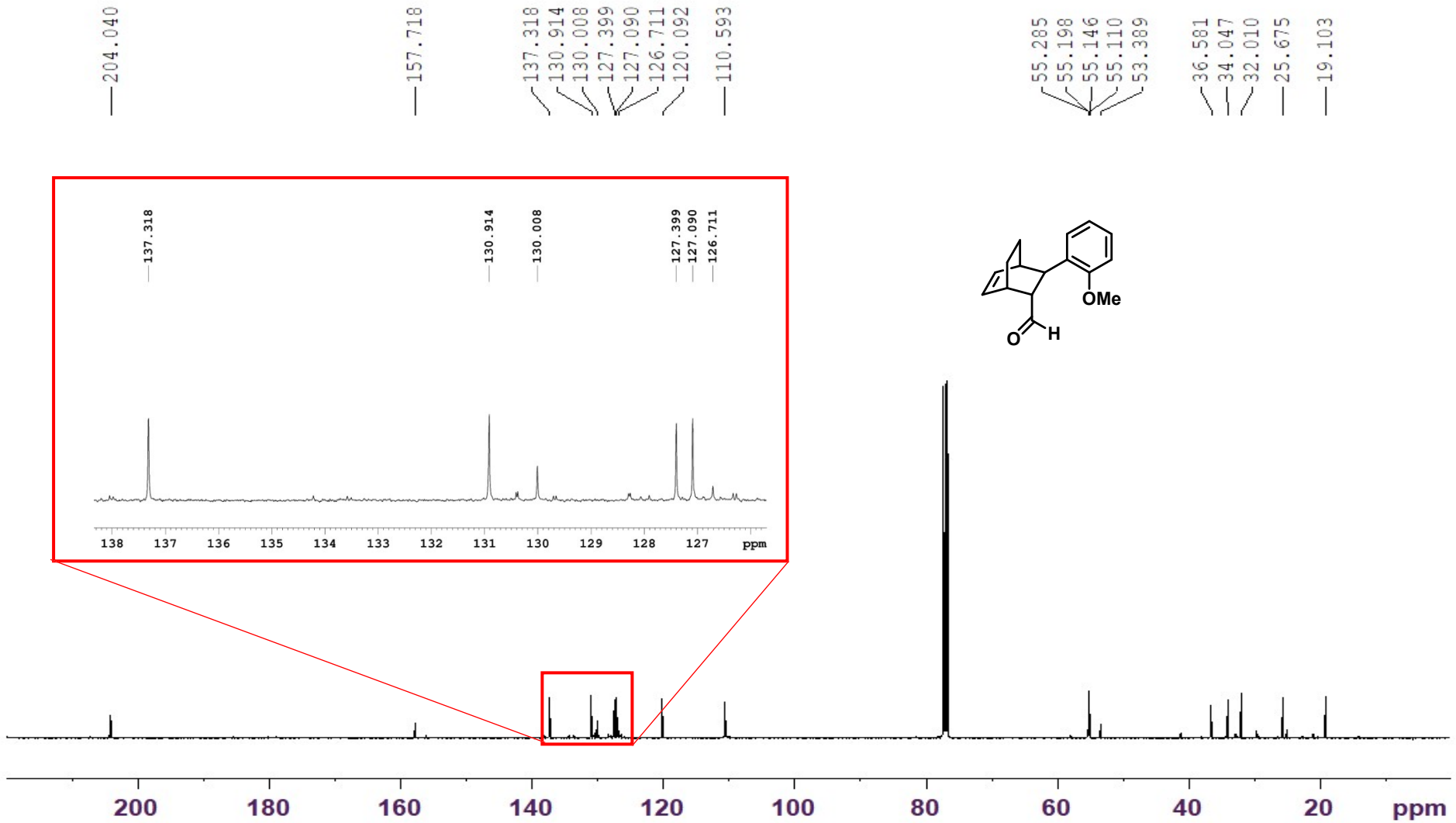


Figure S45. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of compound **6g**.

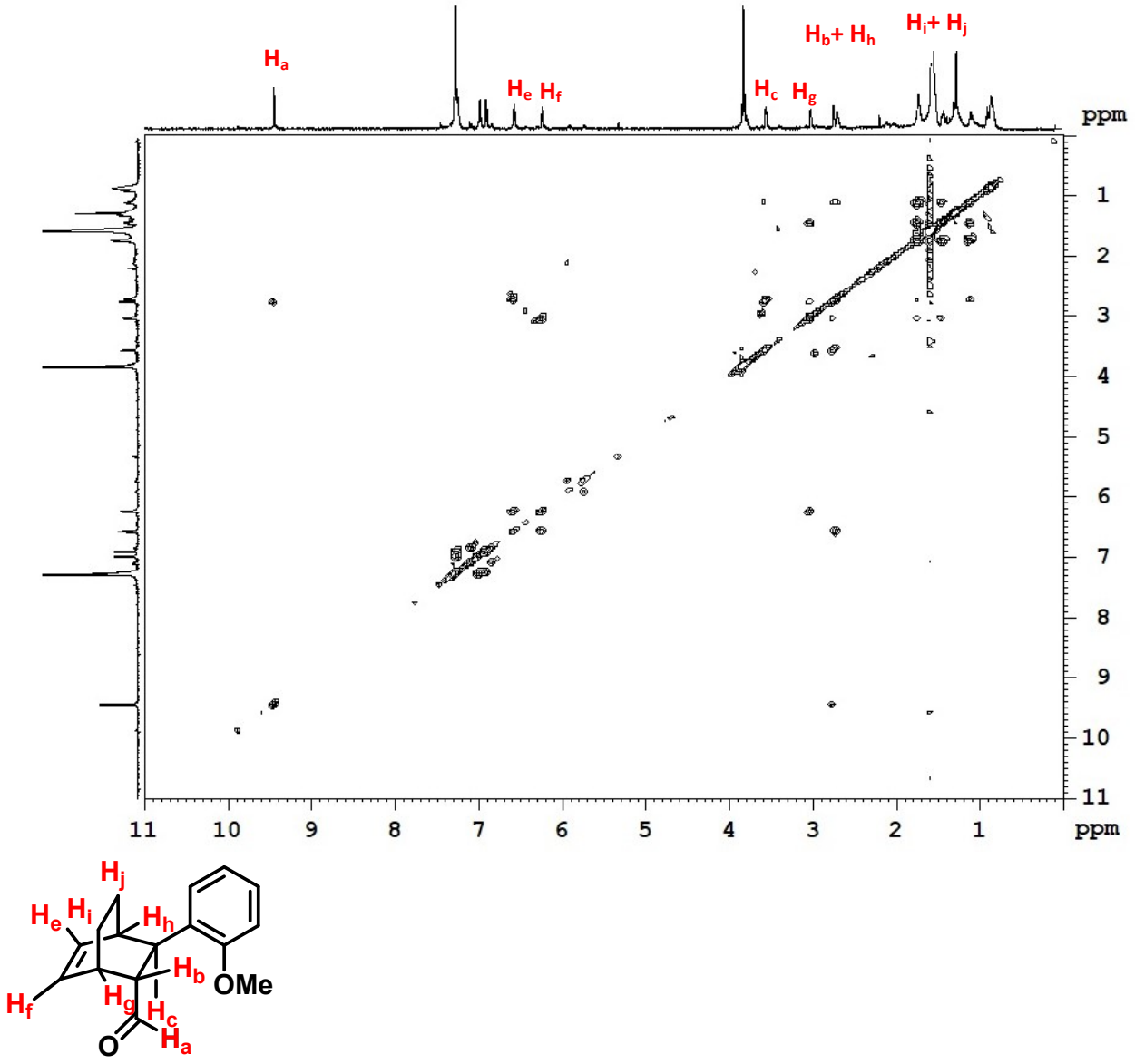


Figure S46. COSY spectrum (600 MHz, $CDCl_3$, 298 K) of compound **6g**.

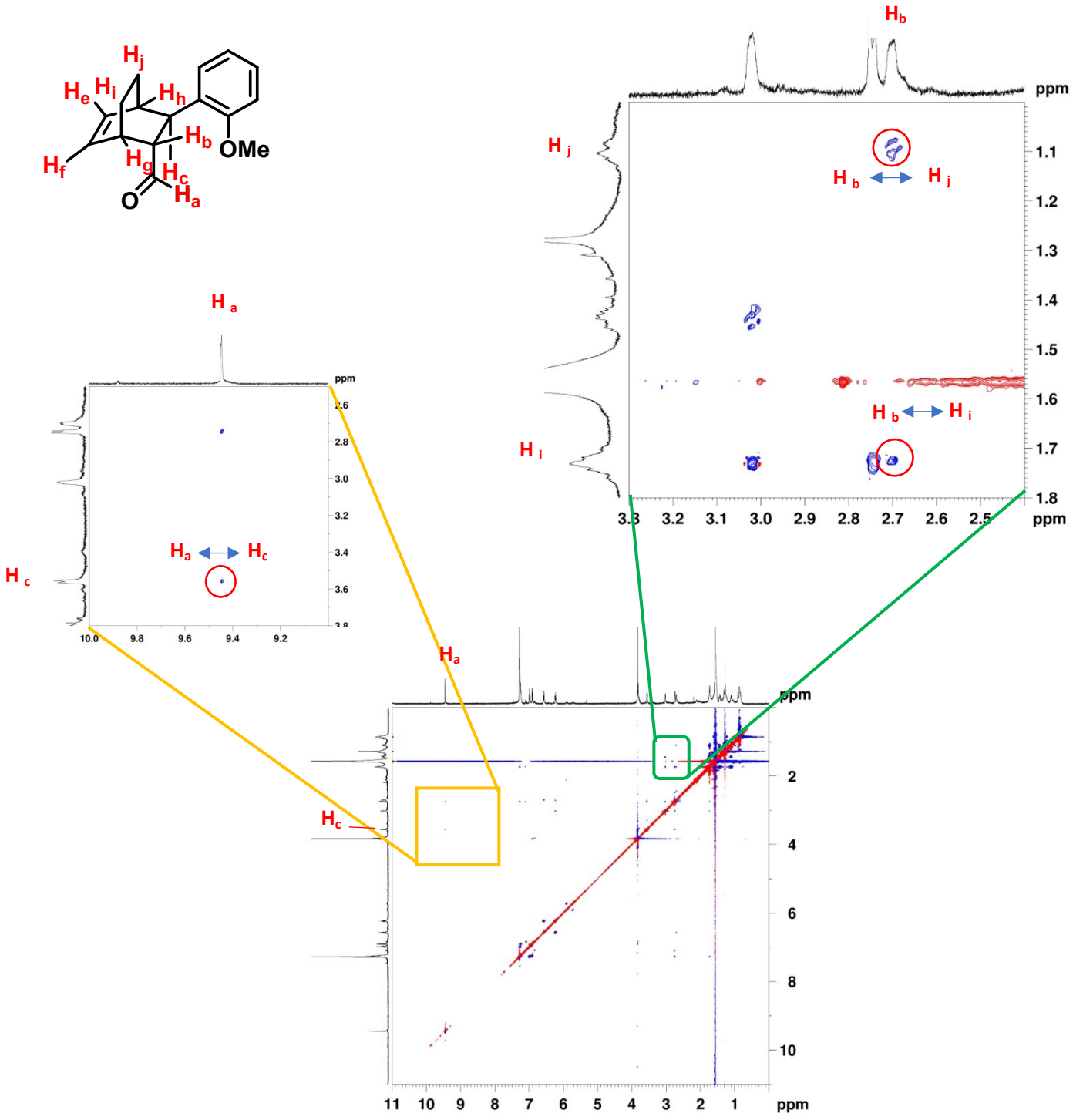


Figure S47. NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of compound **6g**. A d8 = 200 ms was used. In colored squares, relevant expansions of the NOESY spectrum are showed.

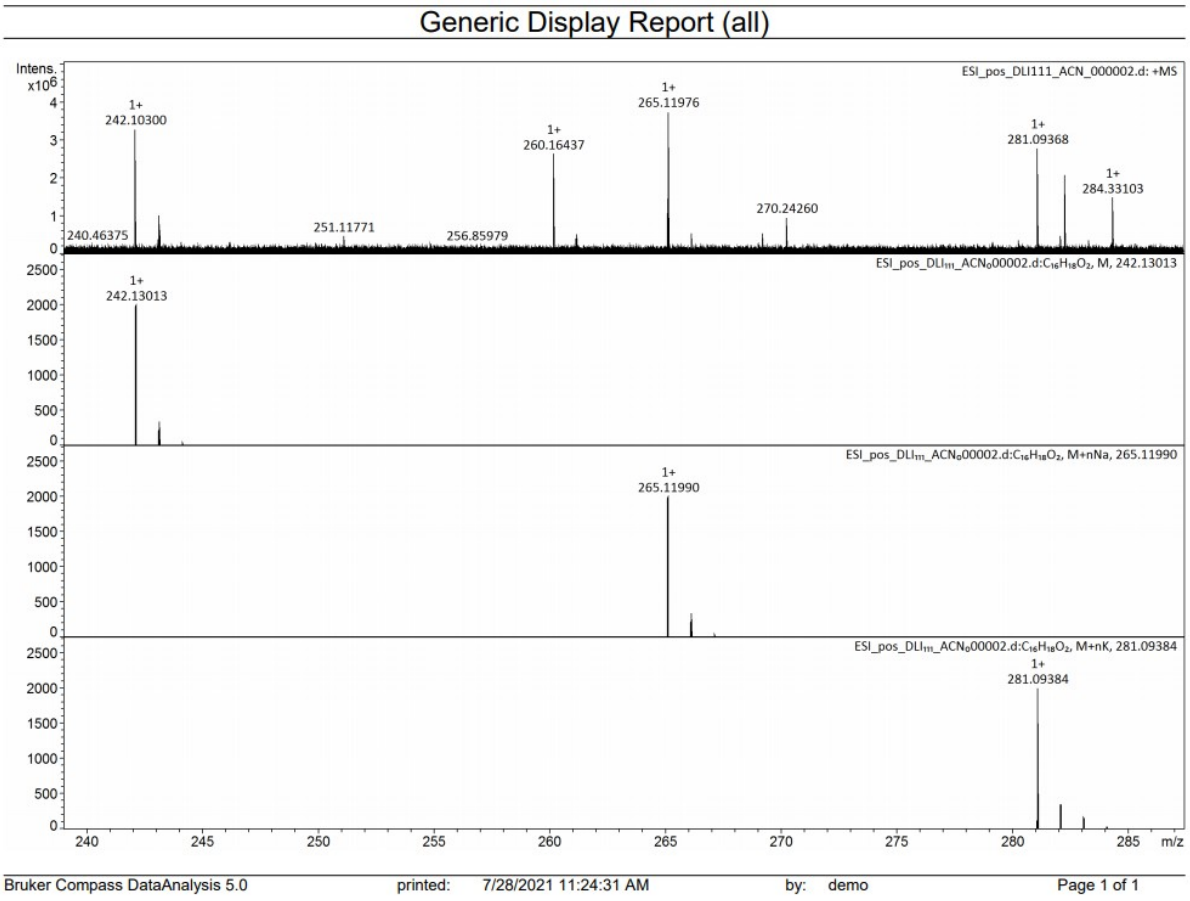


Figure S48. HRMS-ESI spectrum of compound **6g**. Top: experimental spectrum; down: calculated spectra.

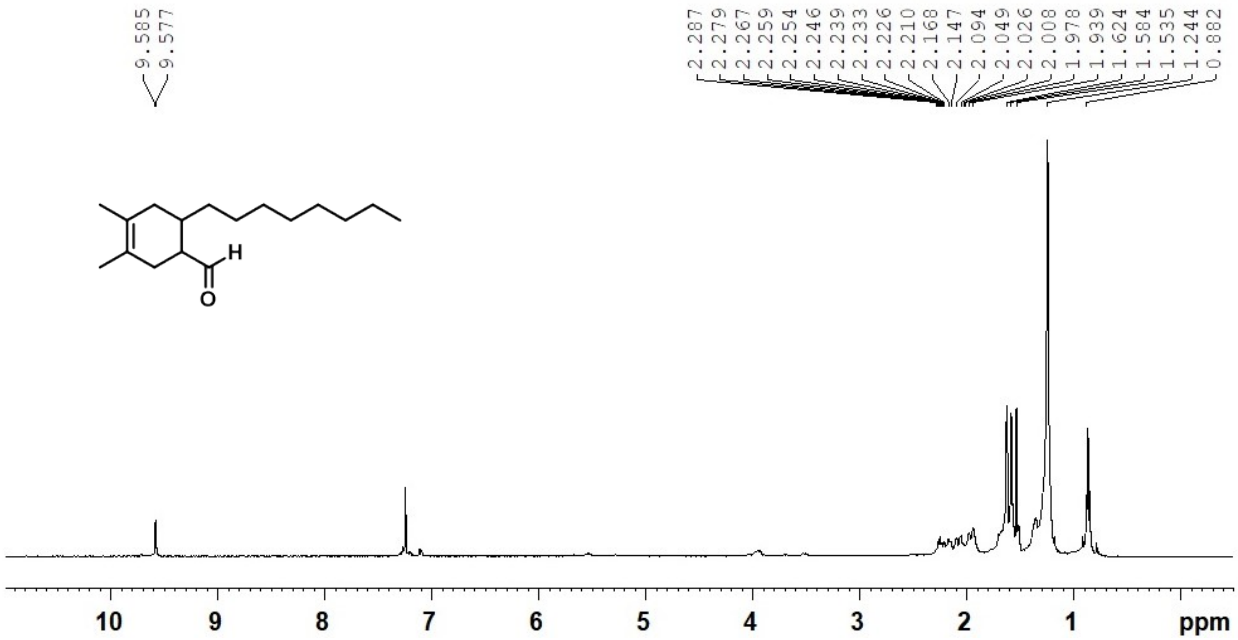


Figure S49. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of compound **8e.**

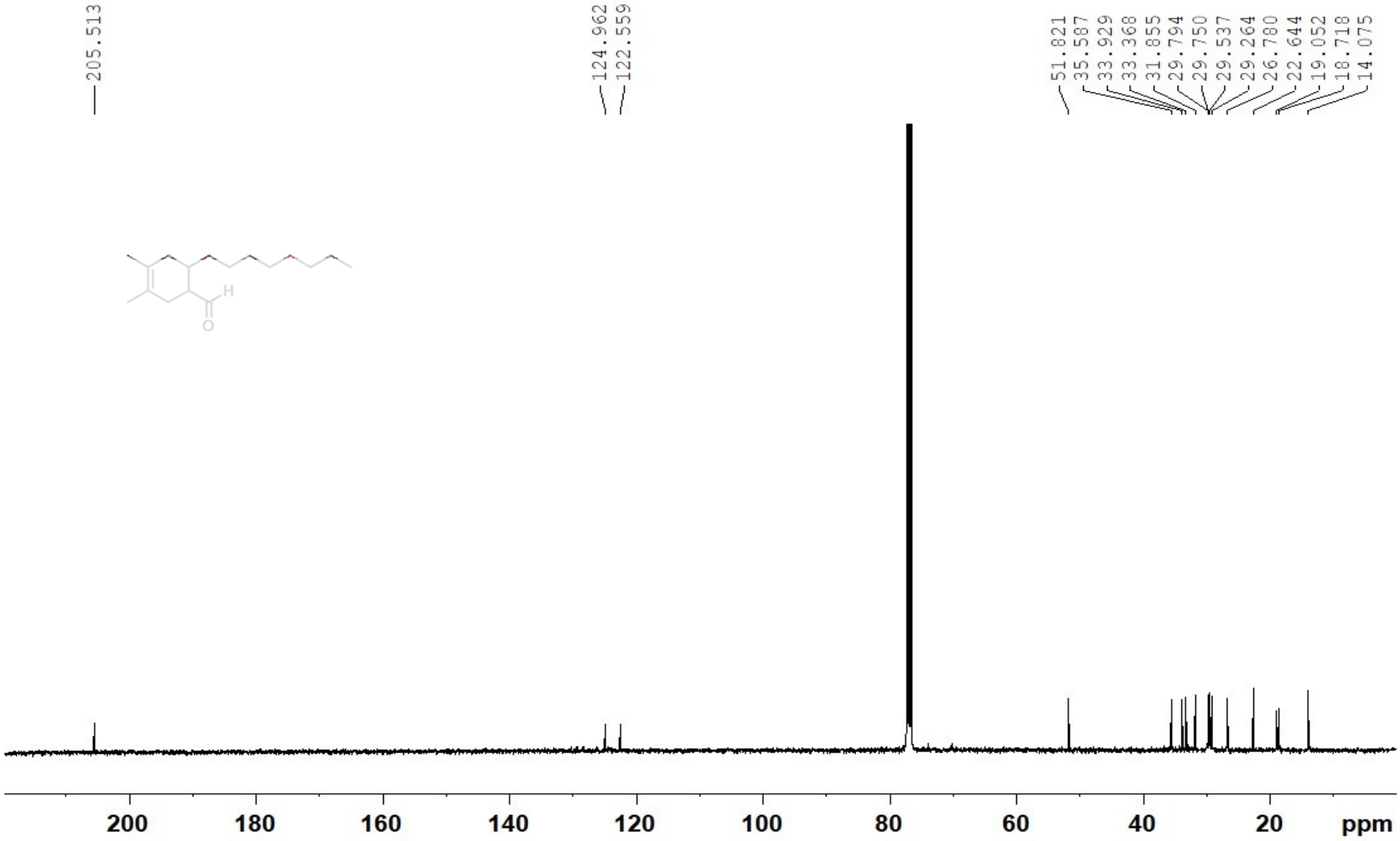


Figure S50. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of compound **8e.**

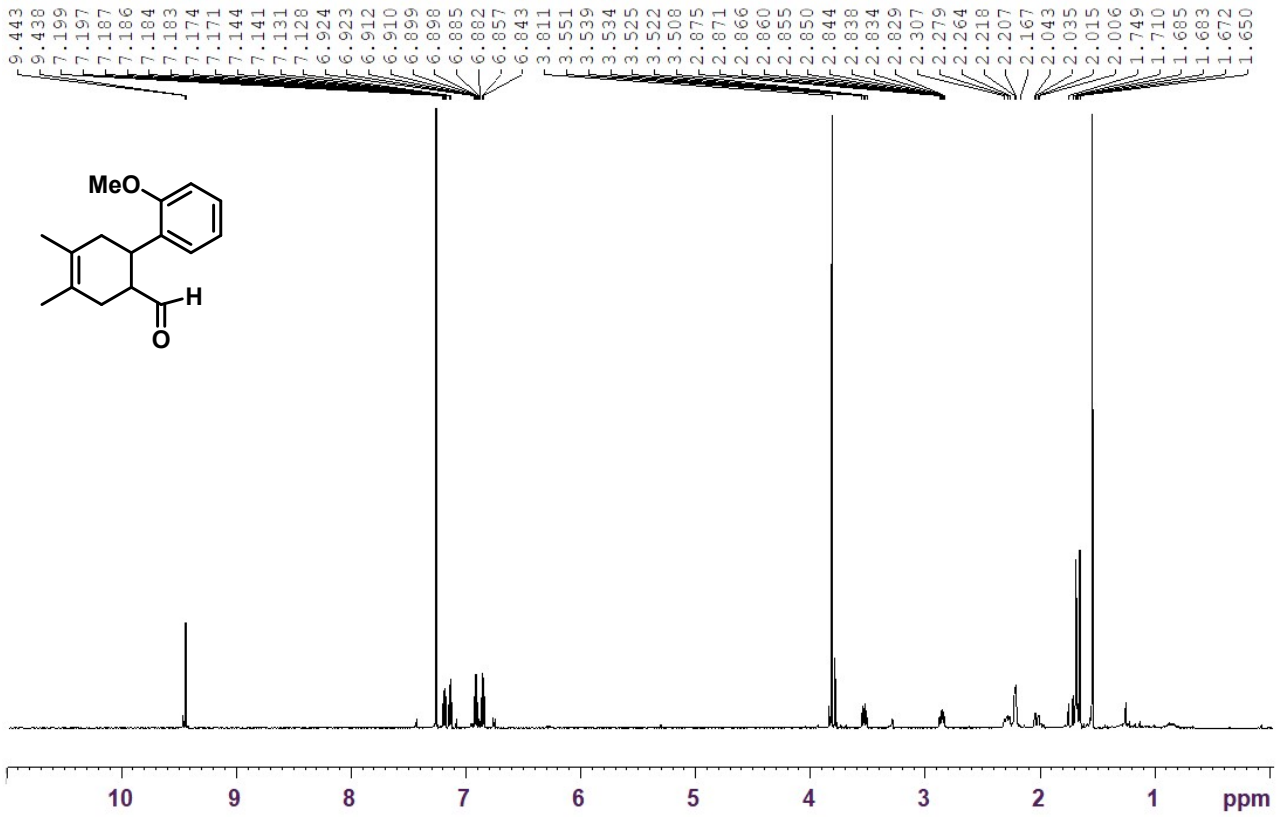


Figure S51. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of compound **8g.**

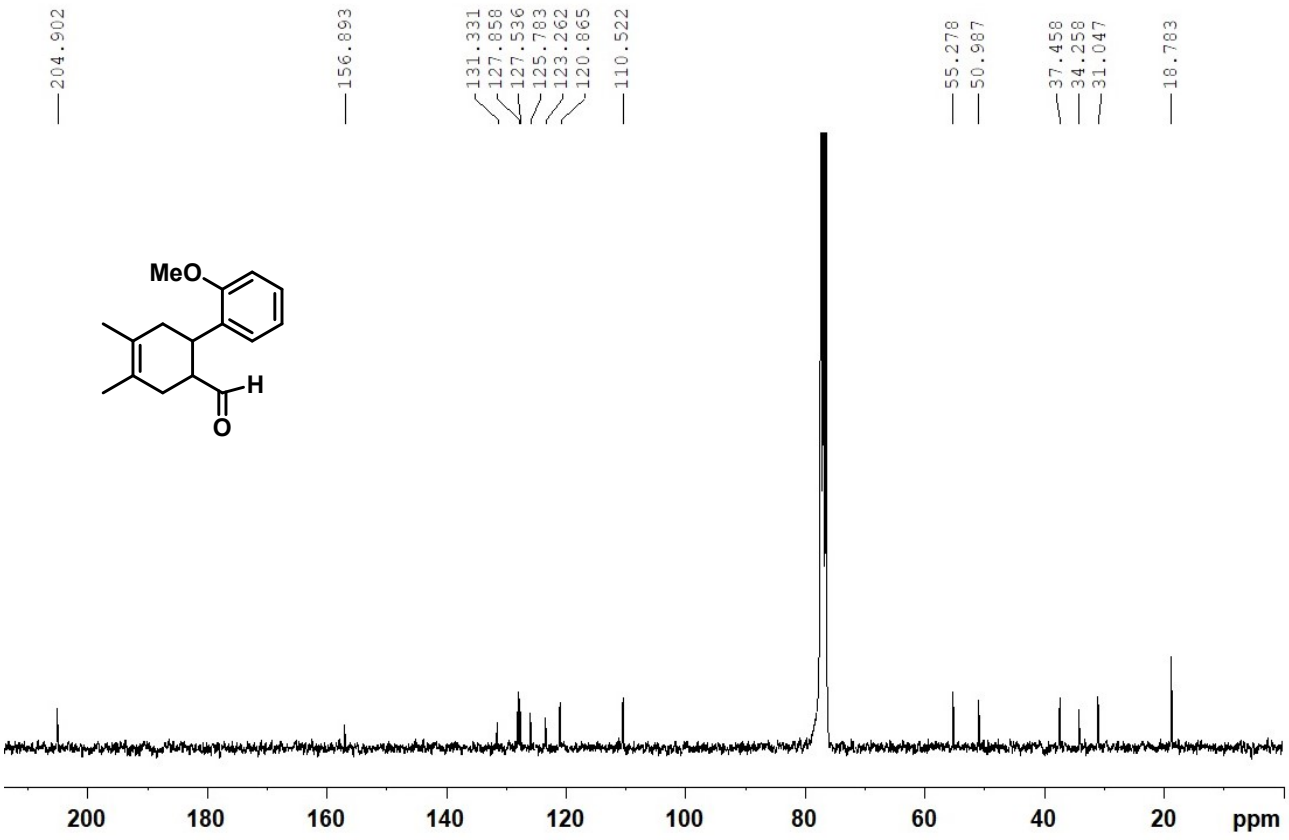


Figure S52.^{13}C NMR spectrum (75 MHz, $CDCl_3$, 298 K) of compound **8g.**

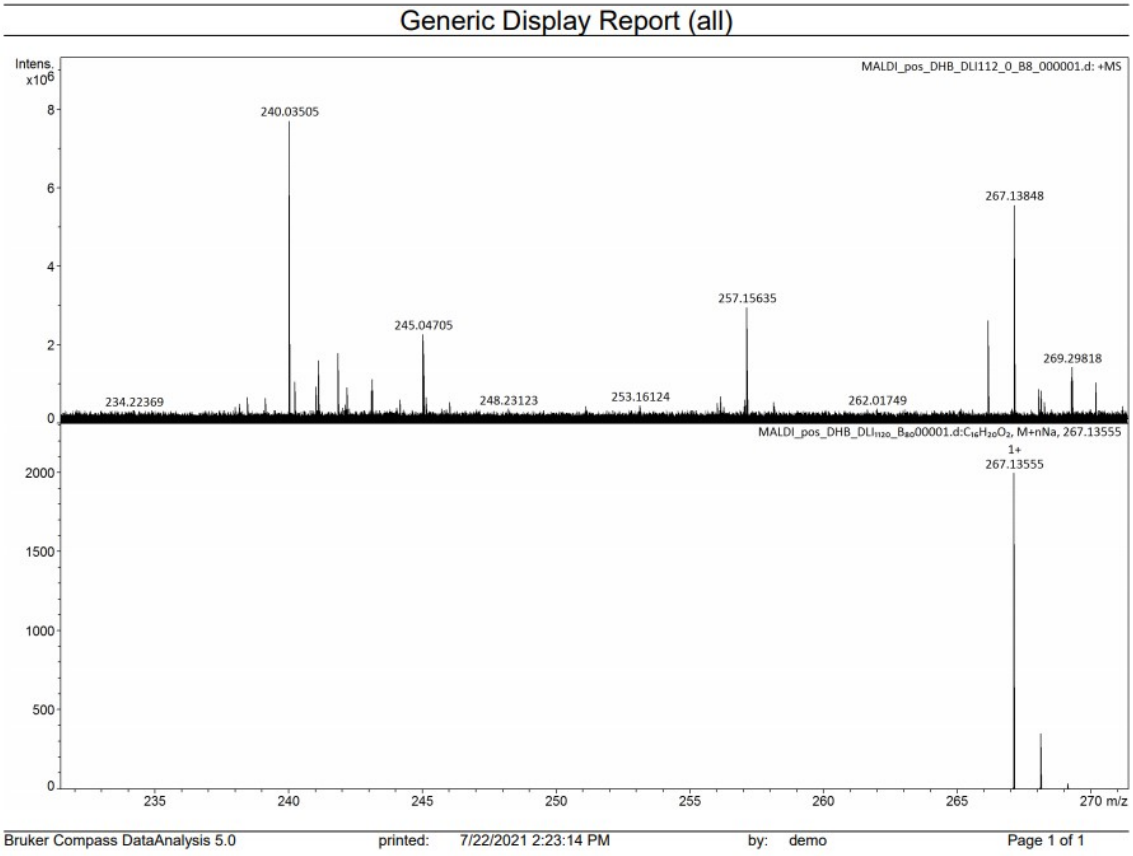


Figure S53. HRMS-MALDI spectrum of compound **8g**.

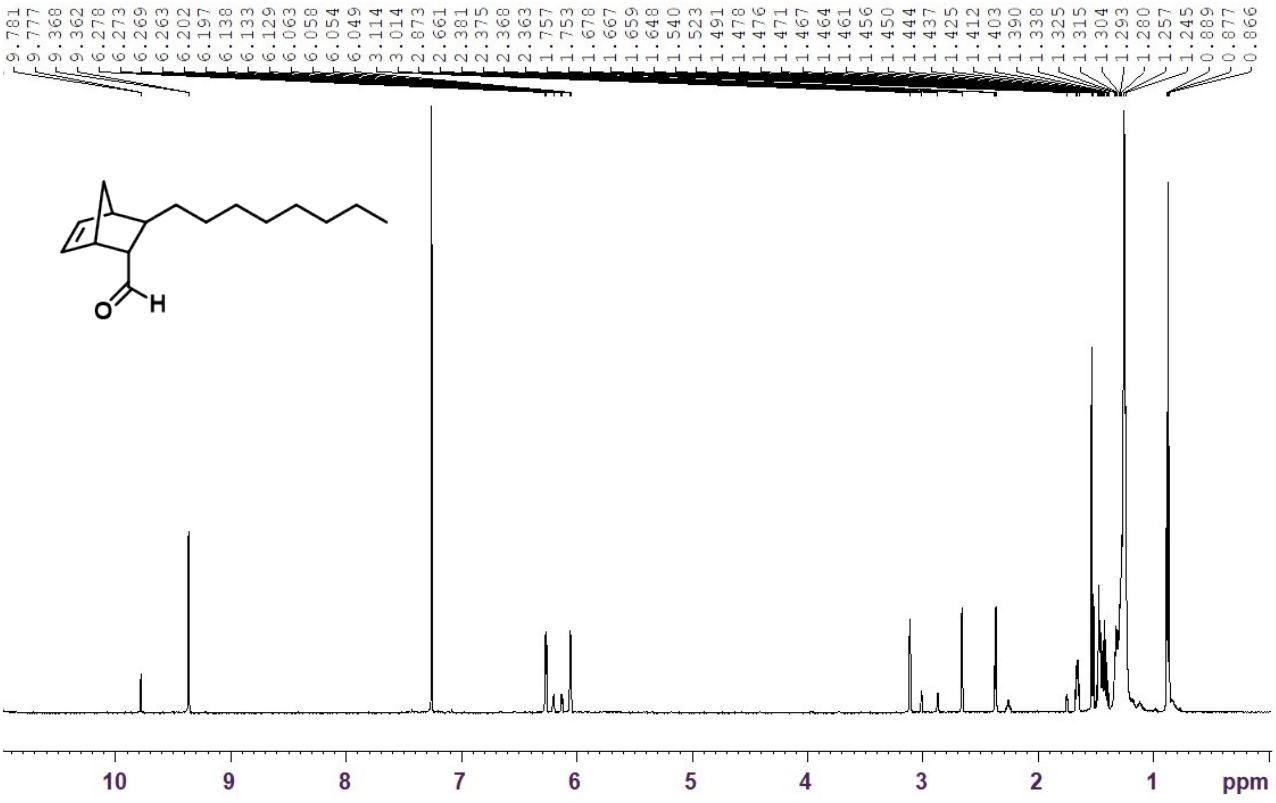


Figure S54. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of compound **10e.**

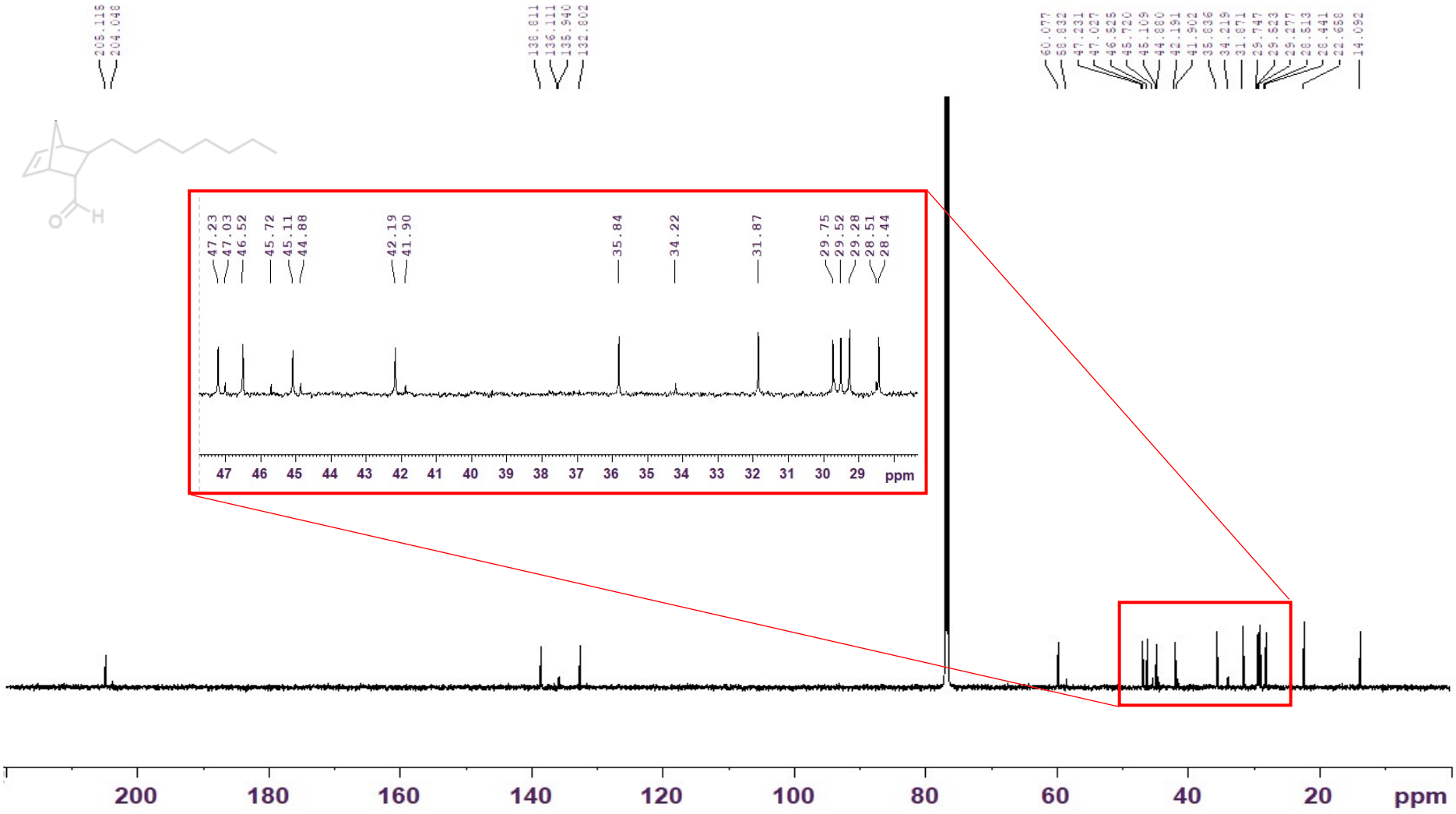


Figure S55. ^{13}C NMR spectrum (150 MHz, $CDCl_3$, 298 K) of compound **10e.**

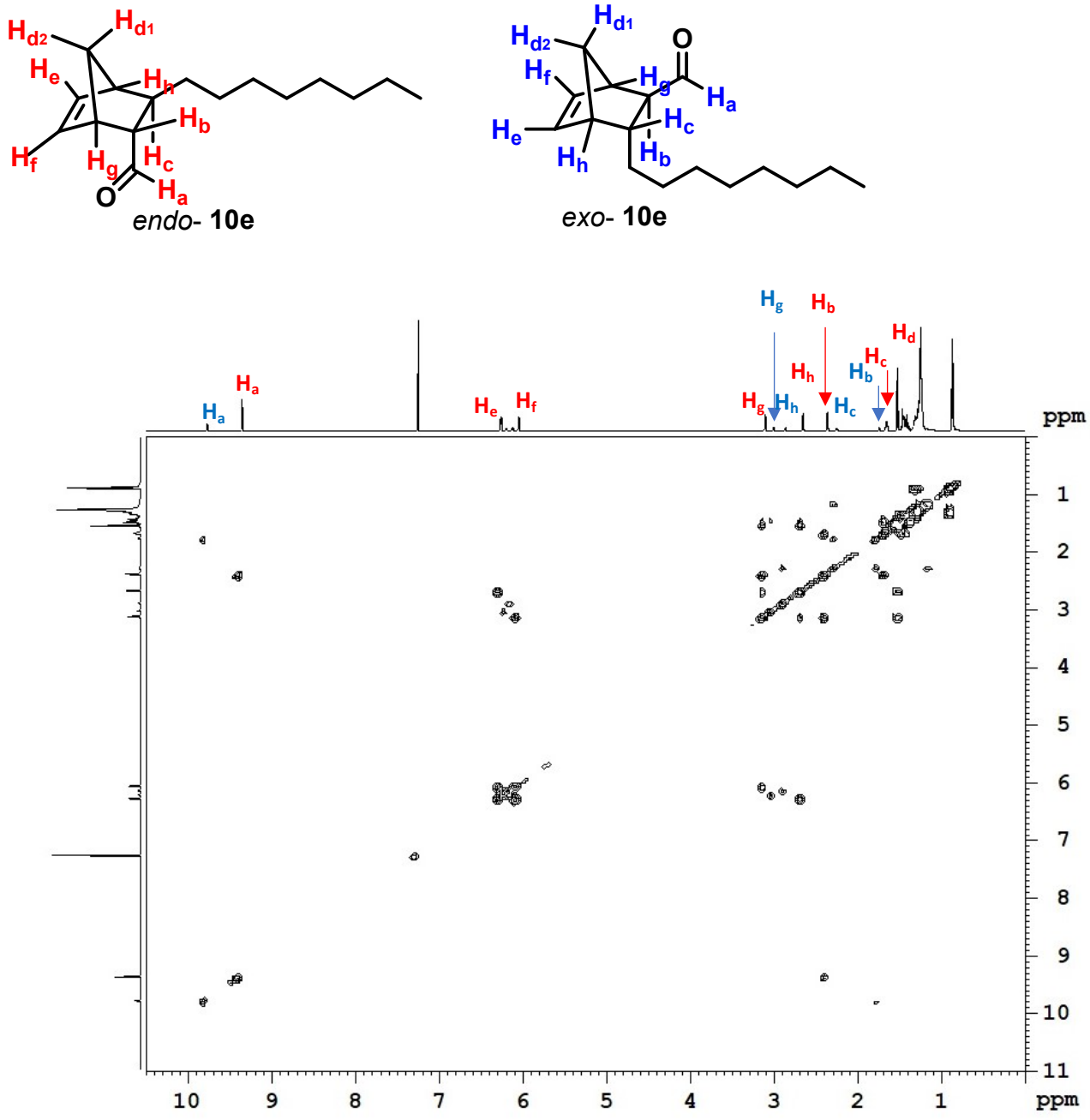


Figure S56. COSY spectrum (600 MHz, $CDCl_3$, 298 K) of compound **10e**.

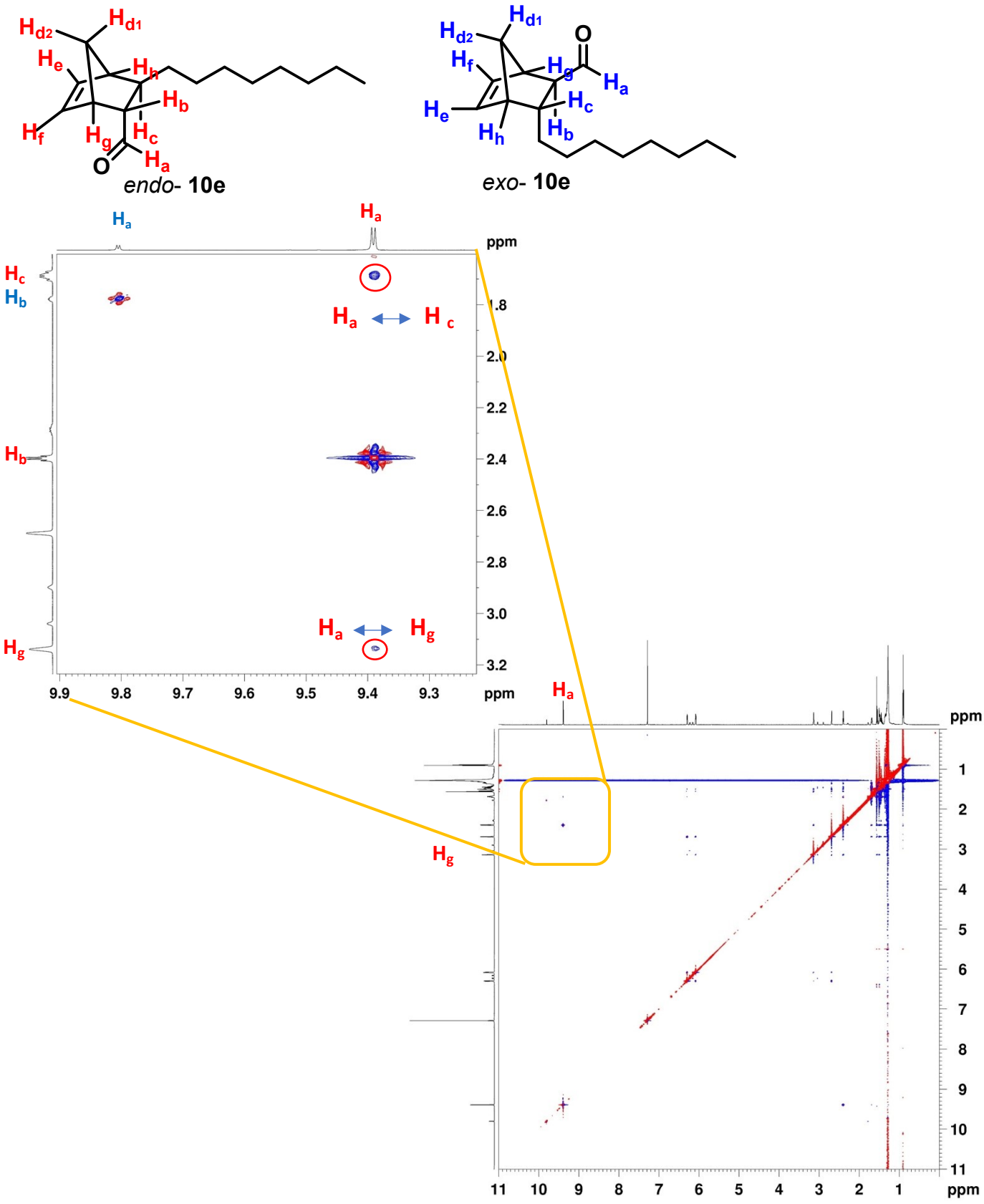
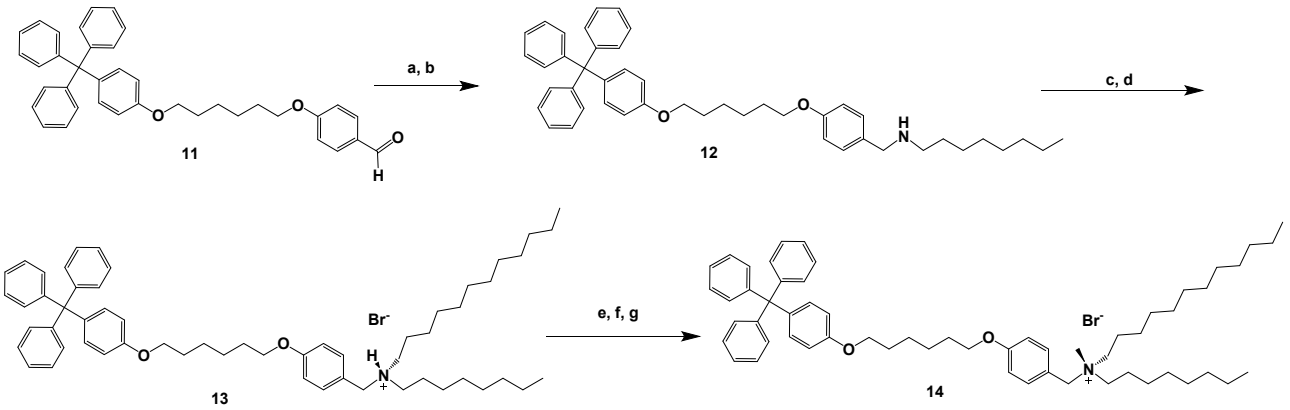


Figure S57. NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of compound **10e.** A d8 = 200 ms was used. In yellow square, relevant expansion of the NOESY spectrum is showed.

9. Synthesis and characterization of compound 14



Scheme S3: Synthesis of derivatives **12**-**14**, a) *n*-Octylamine, $CHCl_3$, 2 h, 25 °C; b) $NaBH_4$, CH_3OH, 2 h, 0 °C→25 °C for 2h; c) Dodecyl bromide, K_2CO_3, Acetone, overnight, 25 °C; d) HBr, 30 min, 25 °C; e) Methyl iodide, K_2CO_3, DMF, reflux, overnight; f) $AgNO_3$, 15 min, 25 °C; g) NaBr, 15 min, 25 °C .

Synthesis of derivative 12

A mixture of derivative **11**[15] (0.50 g, 0.92 mmol) and *n*-octylamine (0.12 g, 0.92 mmol) in $CHCl_3$ (5 mL) was stirred at room temperature for 2 h. The solvent was evaporated under reduced pressure to give the imine intermediate in a quantitative yield. The imine intermediate was used for the next step without further purification. The imine was dissolved in methanol (5 mL), and $NaBH_4$ (0.35 g, 9.20 mmol) was added at 0 °C and then the mixture was allowed to warm at room temperature. The solution was kept under stirring for 2 h. The solvent was removed under reduced pressure and subsequently the residue was diluted with ethyl acetate (50 mL). The mixture was washed with an aqueous saturated solution of $NaHCO_3$ (2 × 50 mL). The combined organic phases were dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo, to give derivative **12** as a white solid 92 % (0.54 g, 0.85 mmol). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): *δ* 7.30 (d, Ar*H*, 2H, *J*=8.5), 7.21 (overlapped, Ar*H*, 15H), 7.11 (d, Ar*H*, 2H, *J*=8.7), 6.87 (d, Ar*H*, 2H, *J*=8.5), 6.78 (d, Ar*H*, 2H, *J*=8.7), 3.96 (overlapped, OCH_2, 4H), 3.80 (s, ArCH_2N, 2H), 2.66 (t, NCH_2, 2H, *J*=7.4), 1.82 (overlapped, CH_2, 4H), 1.55 (overlapped, CH_2, 6H), 1.28 (overlapped, CH_2, 10H), 0.88 (t, CH_3, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ 157.2, 147.3, 138.9, 132.4, 131.3, 130.2, 127.5, 126.0, 114.7, 113.4, 68.0, 67.8, 64.5, 32.0, 29.6, 29.5, 29.4, 27.4, 26.1, 26.1, 22.8, 14.3. HR MS (MALDI): *m/z* calcd for $[M+H]^+$ $C_{46}H_{56}NO_2^+$ 654.4306, found 654.4276; calcd for $[M+Na]^+$ $C_{46}H_{55}NNaO_2^+$ 676.4125, found 676.4100.

Synthesis of derivative 13

A mixture of derivative **12** (0.50 g, 0.85 mmol) and K_2CO_3 (0.23 g, 1.70 mmol) in DMF (15 mL) was stirred at room temperature for 30 min. Subsequently, *n*-dodecyl bromide (0.42 g, 1.70 mmol) was added. After 12 h, the solvent was evaporated under reduced pressure and the residue was diluted with ethyl acetate (50 mL) and an aqueous solution of HBr 48 % (100 mL). The mixture was stirred for 30 min. After, the organic phase was separated, dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The raw was triturated by hexane. The precipitate was filtrated and dried under vacuum to give 0.75 g of brown solid (98 % , 0.83 mmol). ^{1}H NMR (600 MHz, $CDCl_3$, 298 K): δ 11.15 (s, N*H*, 1H), 7.52 (d, Ar*H*, 2H, J=8.5), 7.21 (overlapped, Ar*H*, 15H), 7.08 (d, Ar*H*, 2H, J=8.7), 6.93 (d, Ar*H*, 2H, J=8.5), 6.76 (d, Ar*H*, 2H, J=8.7), 4.11 (s, ArCH_2N, 2H), 3.95 (overlapped, OCH_2, 4H), 2.97 (bt, NCH_2, 2H), 2.85 (bt, NCH_2, 2H), 1.88 (overlapped, CH_2, 6H), 1.53 (overlapped, CH_2, 6H), 1.28 (overlapped, CH_2, 28H), 0.86 (overlapped, CH_3, 6H). ^{13}C NMR (150 MHz, $CDCl_3$, 298 K): δ 160.4, 157.0, 147.1, 138.8, 132.7, 132.2, 131.1, 127.4, 125.8, 119.7, 115.2, 113.2, 68.0, 67.6, 64.3, 56.3, 51.6, 31.9,

[15] P. La Manna, C. Talotta, C. Gaeta, A. Soriente, M. De Rosa, P. Neri, *J. Org. Chem.* 2017, **82**(17), 8973-8983.

31.6, 29.6, 29.6, 29.5, 29.4, 29.3, 29.3, 29.1, 29.0, 29.0, 28.9, 26.8, 25.9. HR MS (MALDI): *m/z,* calcd for $[M]^+$ $C_{58}H_{80}NO_2$ 822.6184, found 822.5994.

Synthesis of derivative 14

A suspension of derivative **13** (0.55 g, 0.61 mmol) and K_2CO_3 (0.17 g, 1.21 mmol) in DMF (15 mL) was stirred at room temperature for 30 min. Subsequently, Methyl Iodide (0.86 g, 6.10 mmol) was added. After 12 h, the solvent was evaporated under reduced pressure to give ammonium iodide that was used for the next step without further purification. The crude was diluted with ethyl acetate (50 mL) and an aqueous solution of HBr 48% (100 mL). The solution was stirred for 30 min. After, the organic phase was separated, and an excess of $AgNO_3$ was added. The mixture was stirred for 15 min. After this time, the mixture reaction was filtrated to remove the white solid. Subsequently, an excess of NaBr was added to filtrate solution and stirred for 15 min. Finally, solution was washed with water and the organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo to give 0.51 g of brown solid (92 %, 0.56 mmol). ^{1}H NMR (600 MHz, $CDCl_3$, 298 K): *δ* 7.52 (d, Ar*H*, 2H, *J* = 8.5), 7.21 (overlapped, Ar*H*, 15H), 7.09 (d, Ar*H*, 2H, *J*=8.7), 6.94 (d, Ar*H*, 2H, *J*=8.5), 6.76 (d, Ar*H*, 2H, *J*=8.7), 4.85 (s, ArCH_2N, 2H), 3.95 (overlapped, OCH_2, 4H), 3.42 (bt, NCH_2, 2H), 3.35 (bt, NCH_2, 2H), 3.19 (s, NCH_3, 3H), 1.78 (overlapped, CH_2, 8H), 1.53 (overlapped with H_2O, CH_2, 4H), 1.28 (overlapped, CH_2, 28H), 0.86 (overlapped, CH_3, 6H). ^{13}C NMR (150 MHz, $CDCl_3$, 298 K): *δ* 157.0, 147.1, 138.9, 134.5, 132.2, 131.1, 127.4, 125.8, 115.1, 113.2, 68.1, 67.6, 64.3, 59.9, 47.4, 31.9, 31.6, 29.6, 29.3, 29.1, 26.4, 26.0, 22.7, 22.6, 14.1. HR MS (MALDI): *m/z*, calcd for $[M]^+$ $C_{59}H_{82}NO_2^+$ 836.6341, found 836.6504.

Characterization of derivative 12

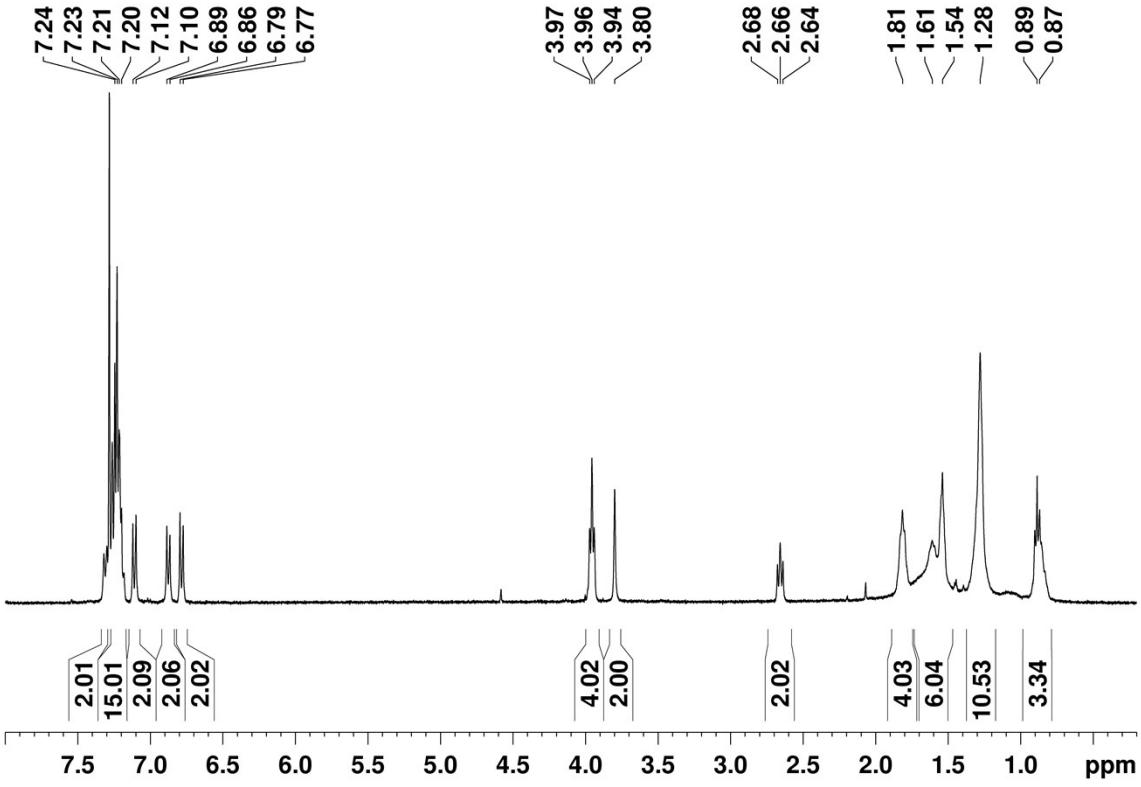


Figure S58. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of derivative **12**.

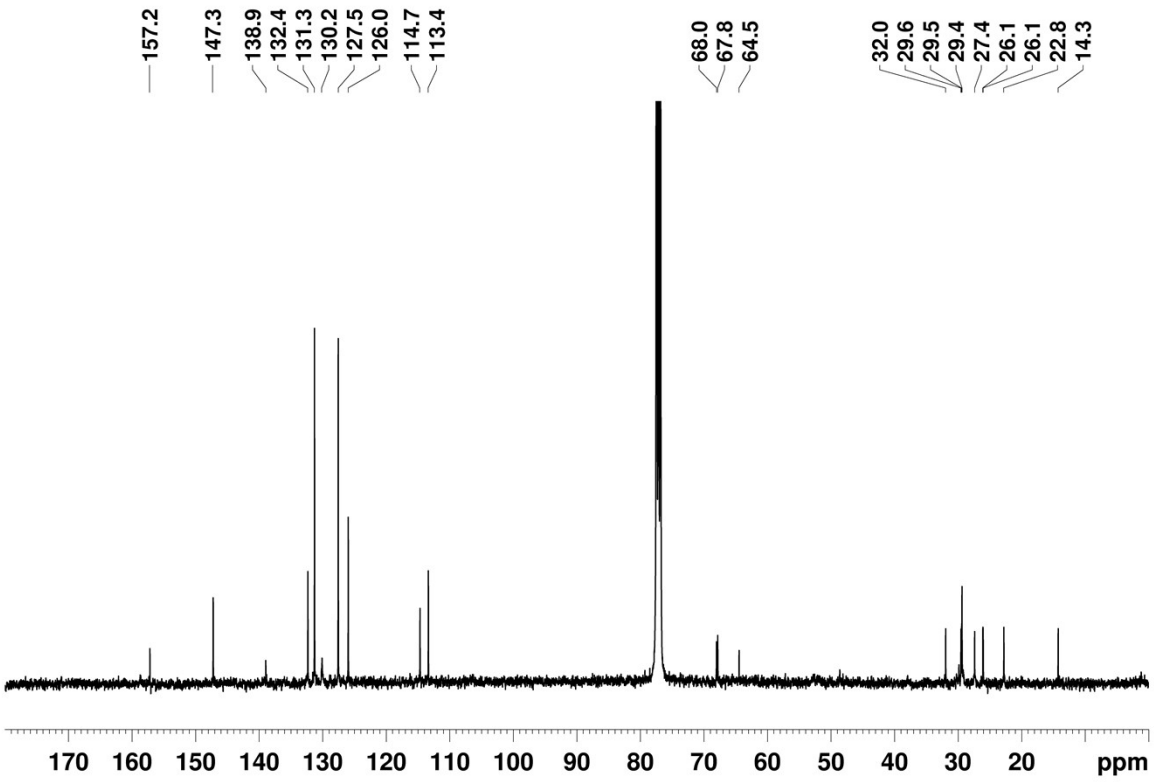


Figure S59. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of derivative **12**.

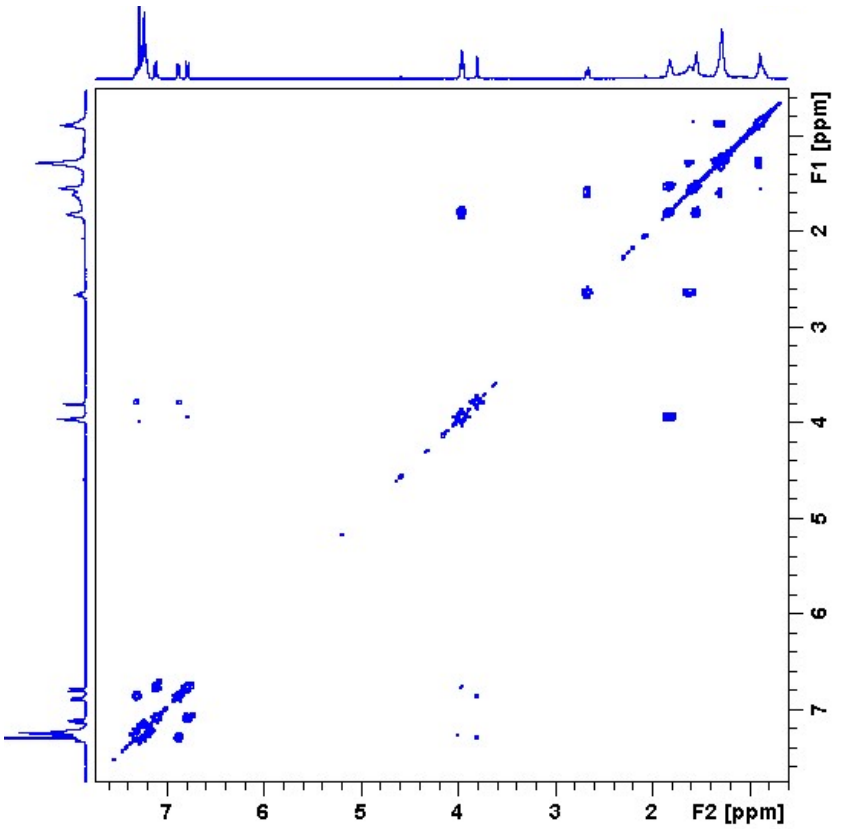


Figure S60. 2D COSY spectrum (400 MHz, $CDCl_3$, 298 K) of derivative **12**.

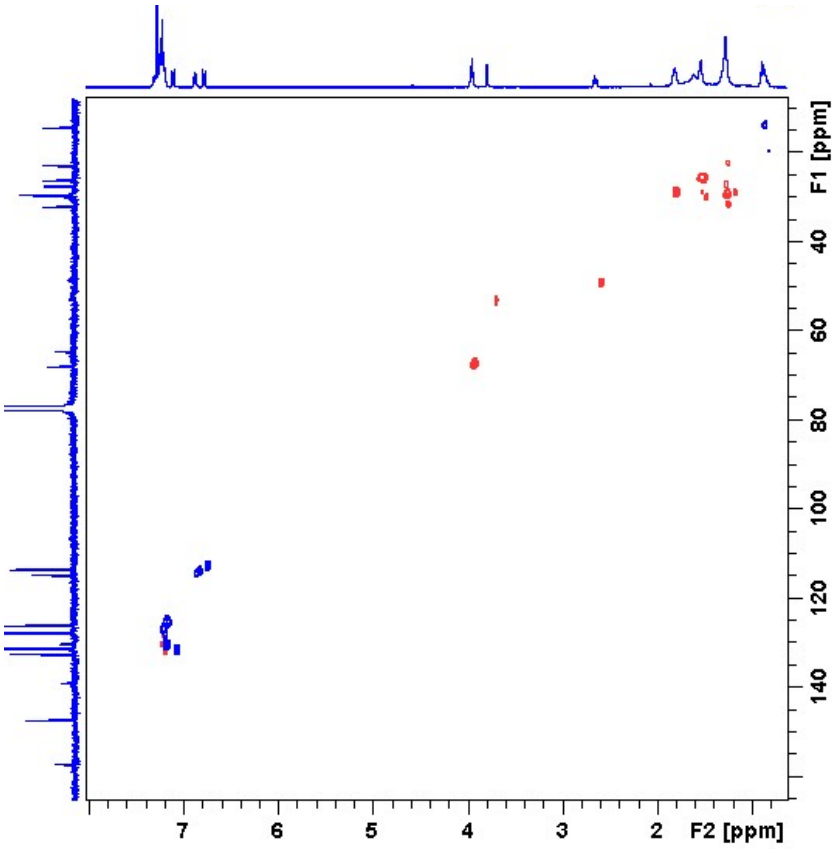


Figure S61. 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **12**.

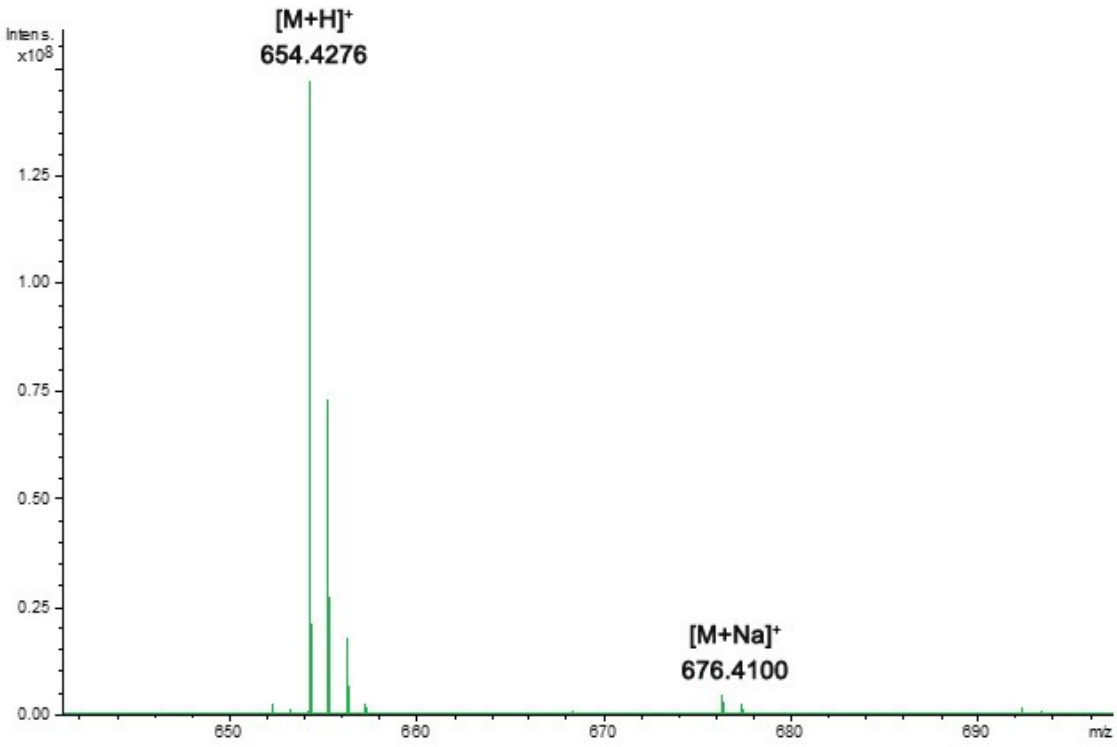


Figure S62. HR-MS of derivative **12**.

Characterization of derivative 13

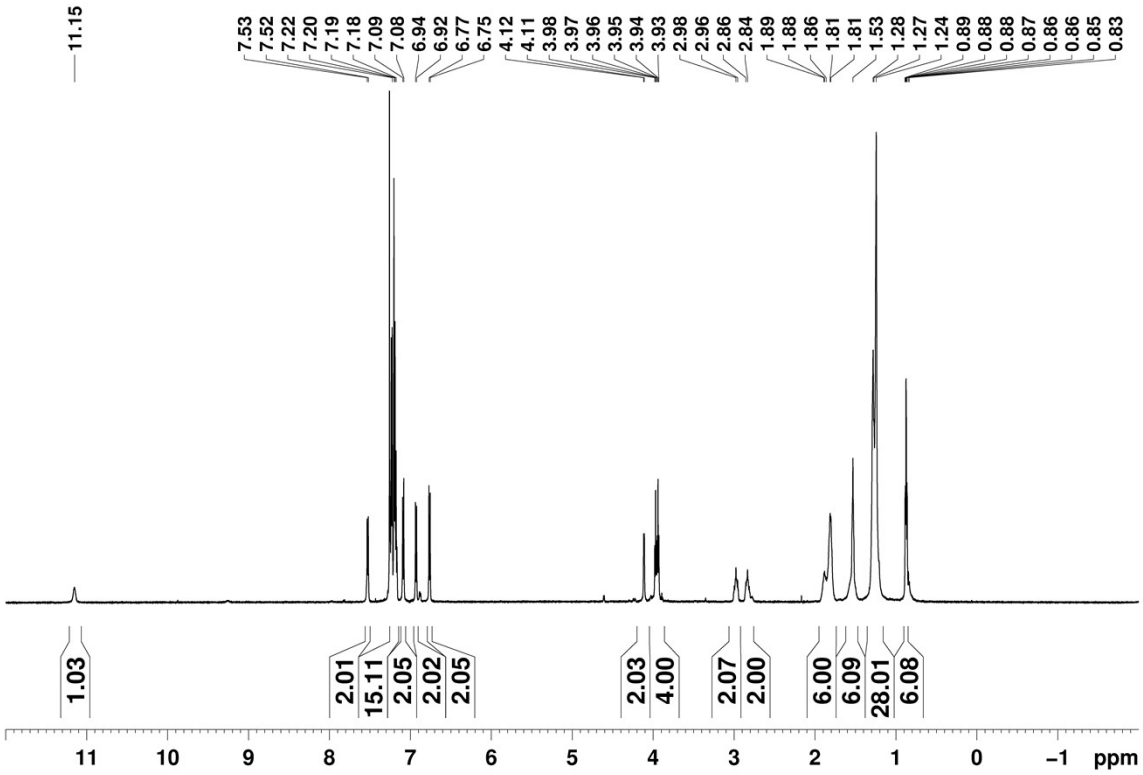


Figure S63. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **13**.

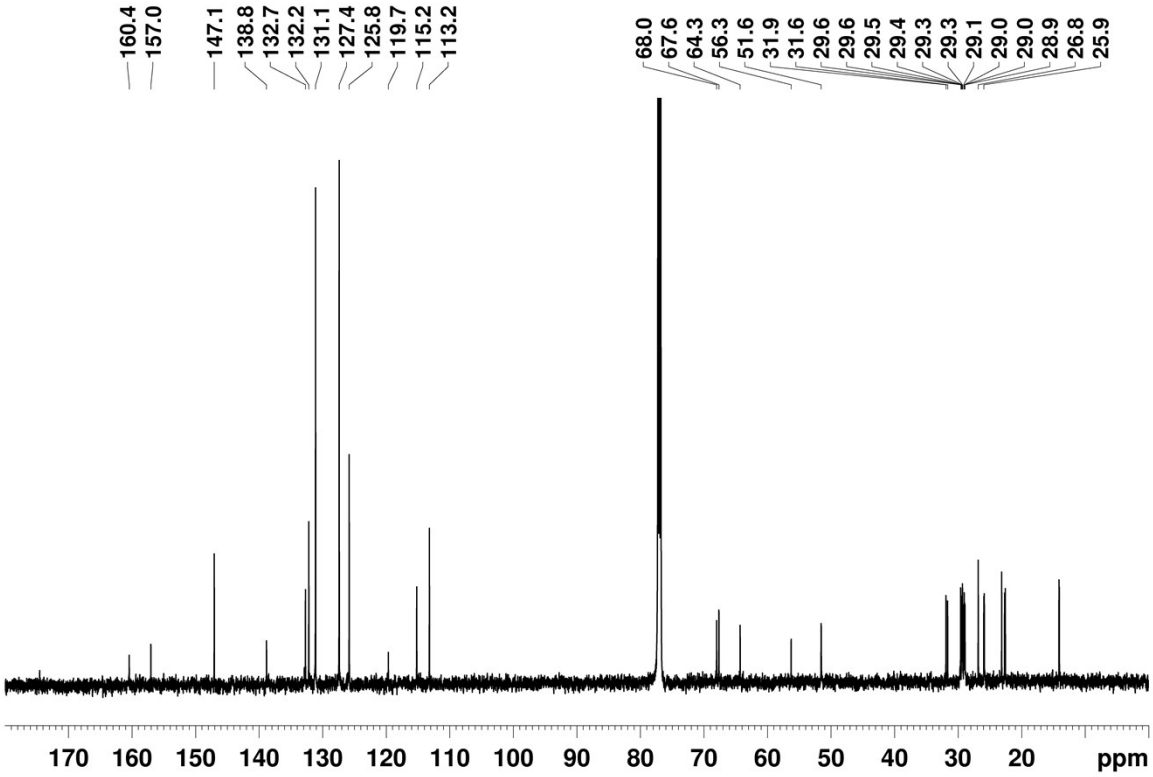


Figure S64. ^{13}C NMR spectrum (150 MHz, $CDCl_3$, 298 K) of derivative **13**.

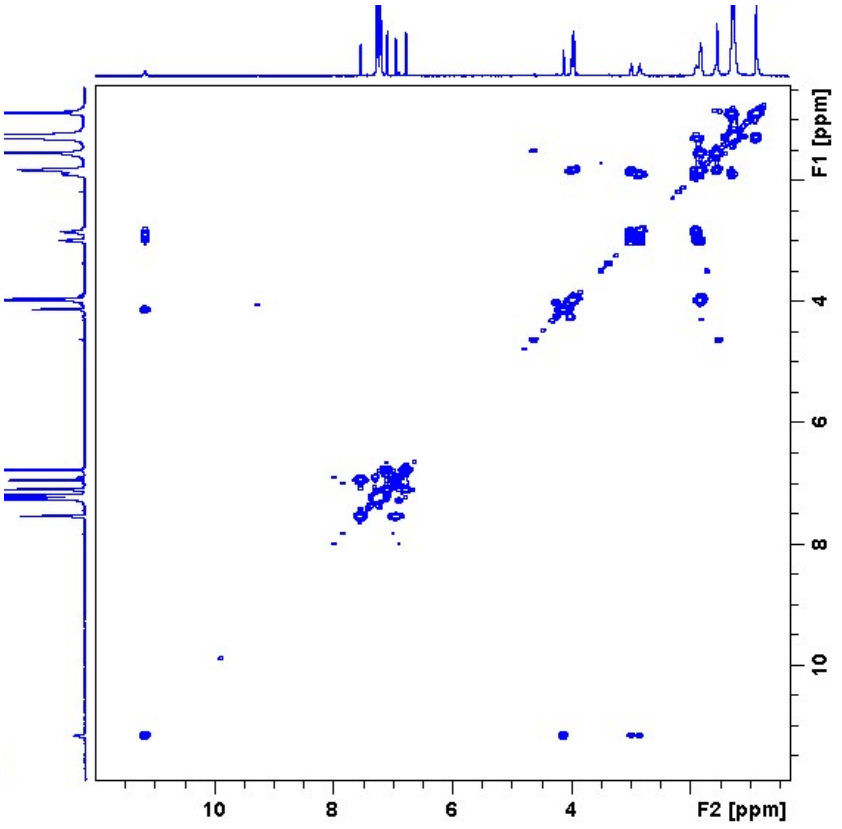


Figure S65. 2D COSY spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **13**.

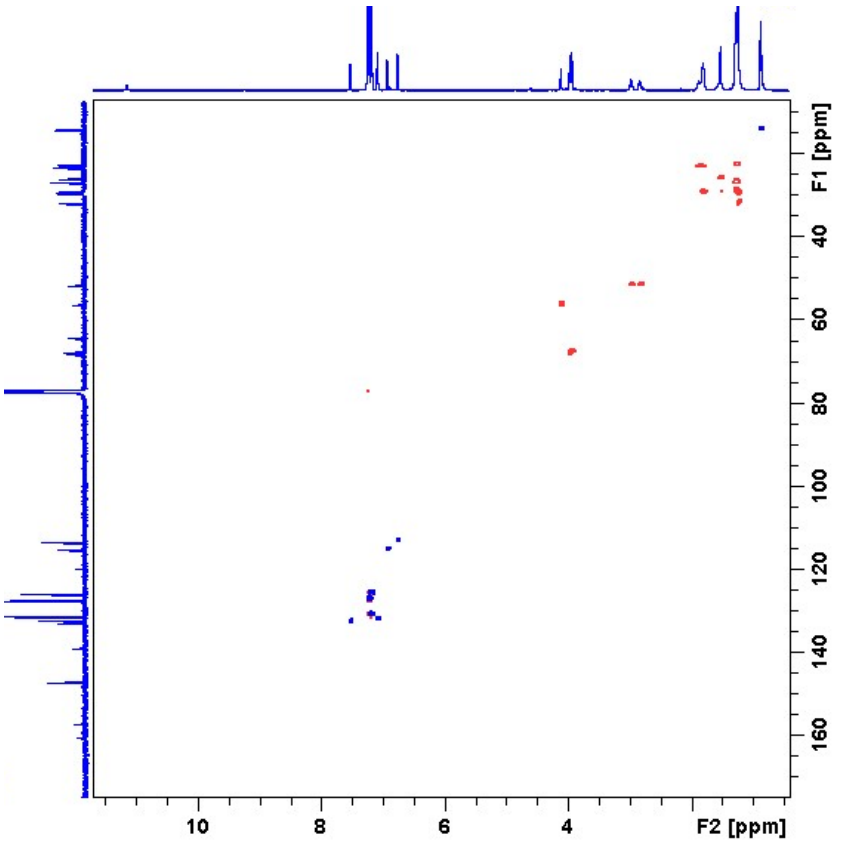


Figure S66. 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **13**.

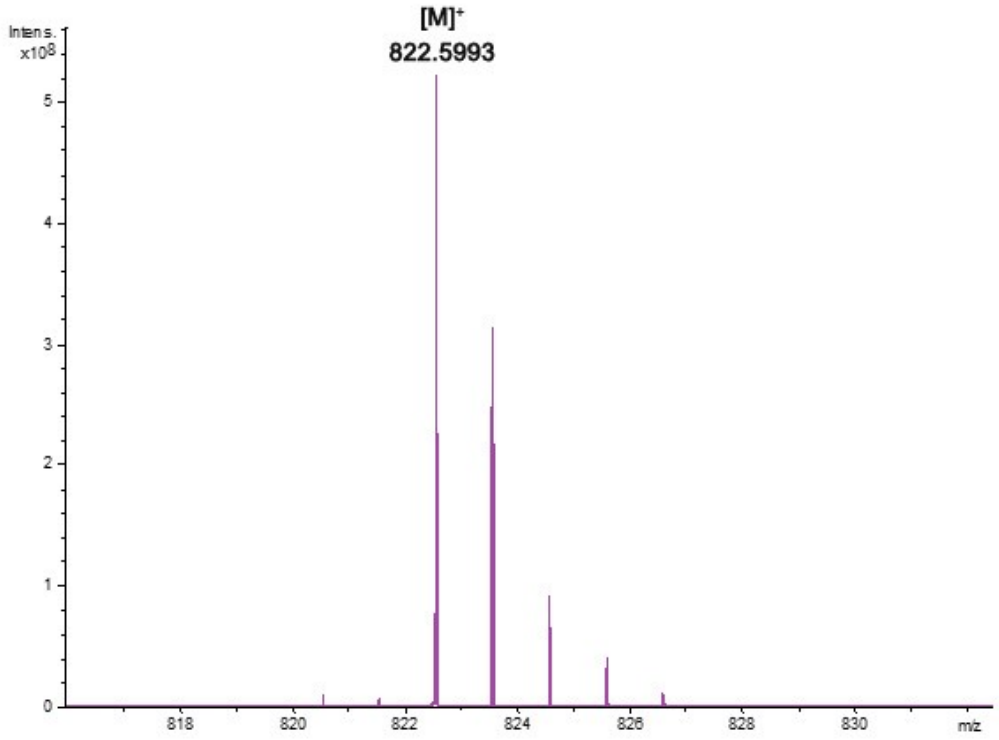


Figure S67. HR-MS of derivative **13**.

Characterization of derivative 14

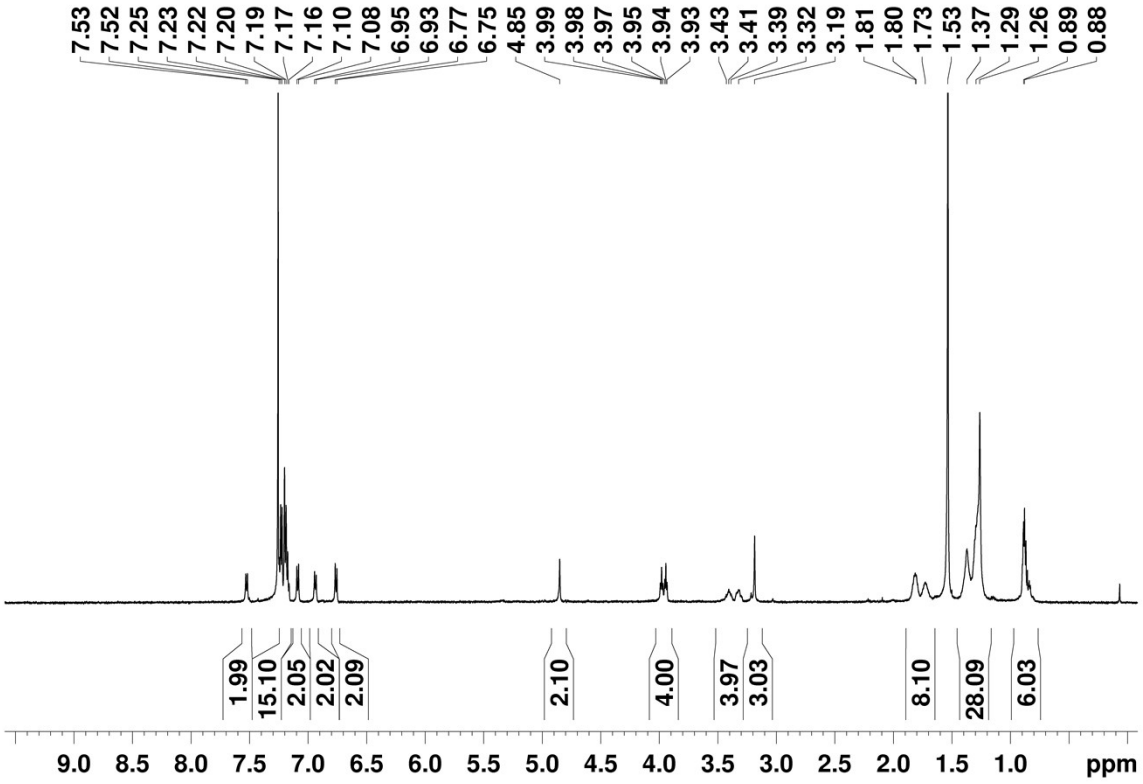


Figure S68. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **14**.

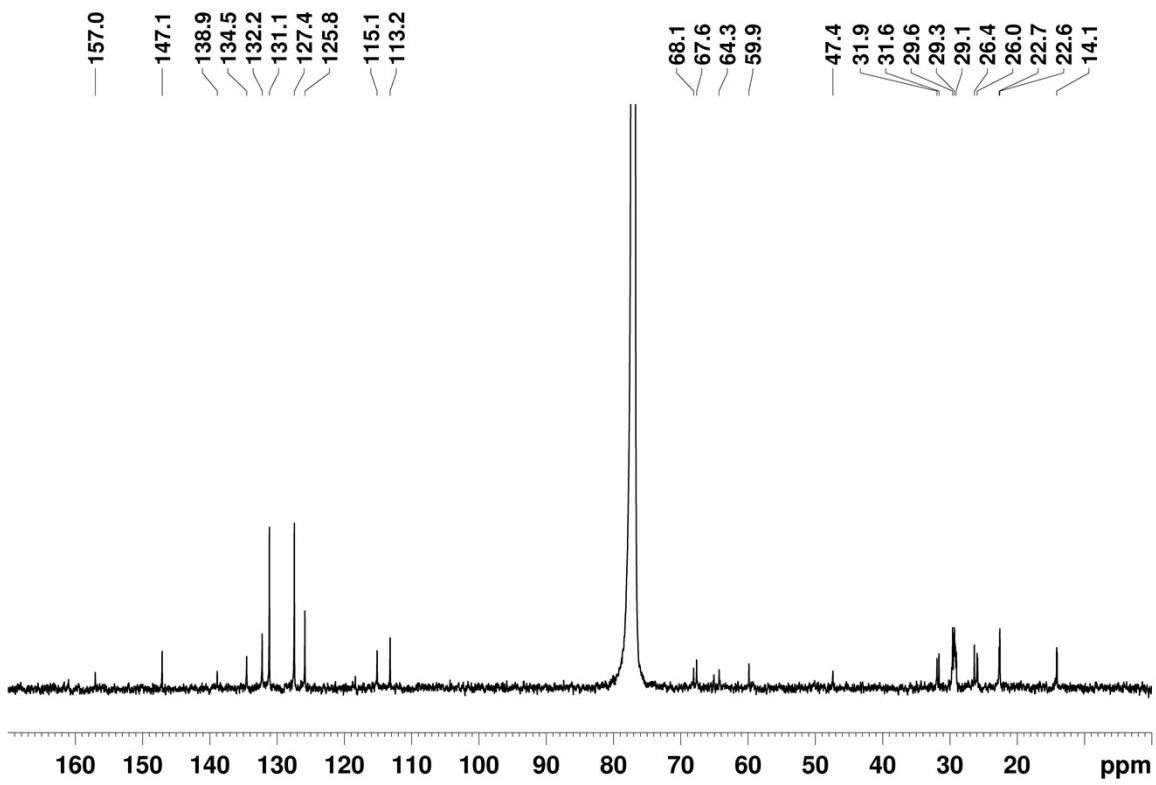


Figure S69. ^{13}C NMR spectrum (150 MHz, $CDCl_3$, 298 K) of derivative **14**.

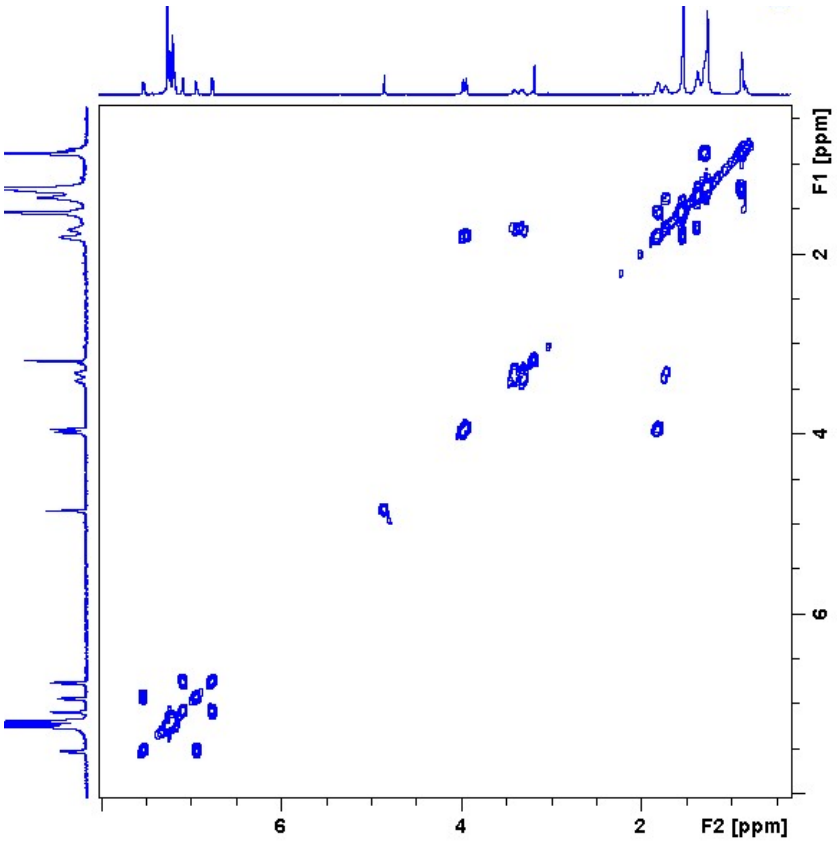


Figure S70. 2D COSY spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **14**.

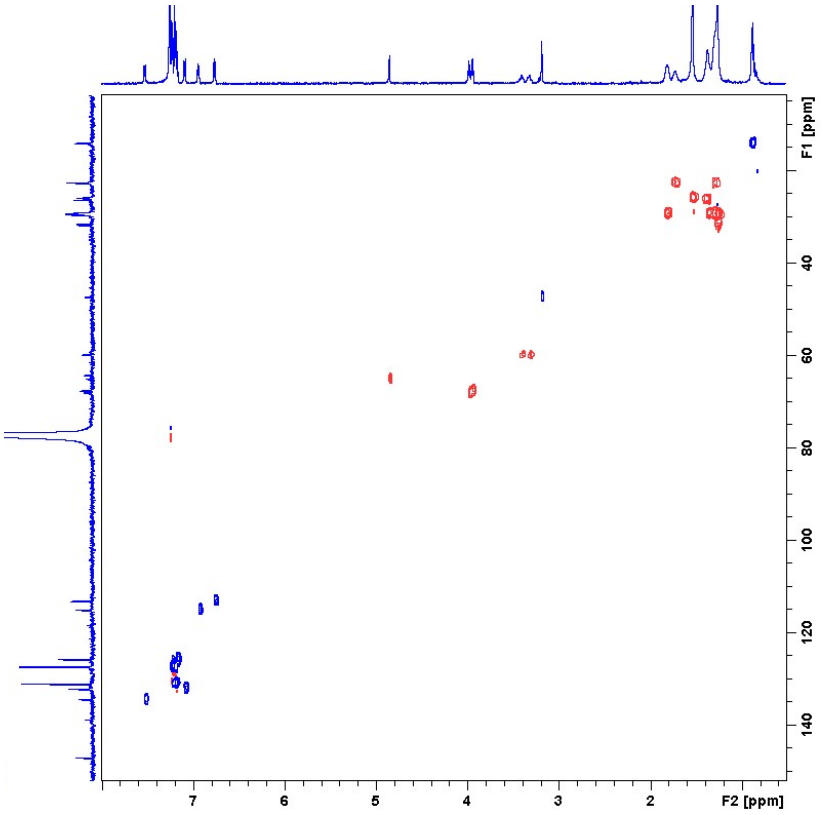


Figure S71. 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **14**.

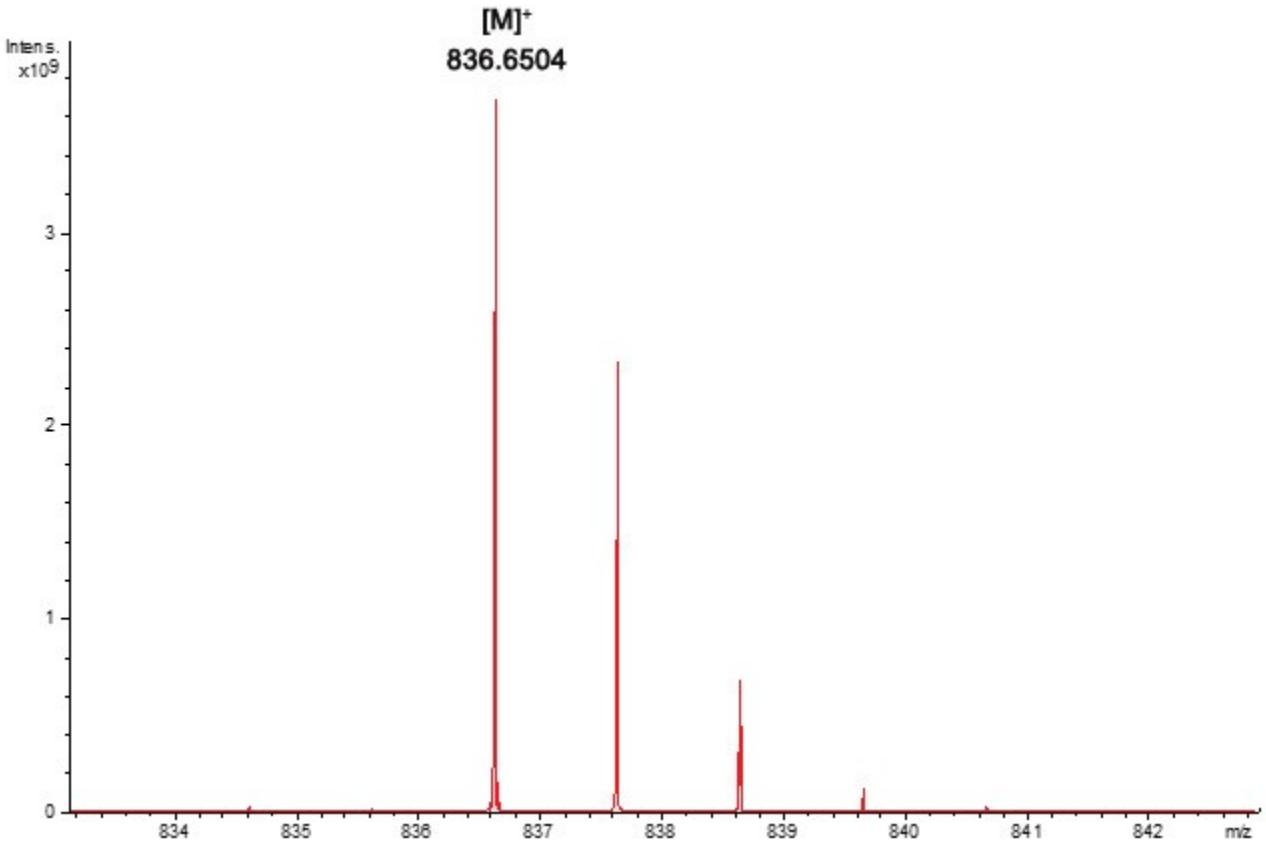
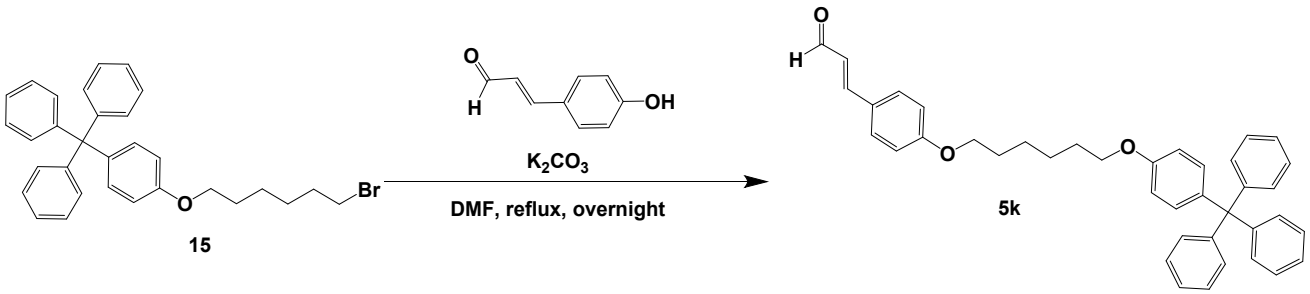


Figure S72. HR-MS of derivative **14**.

10. Synthesis and characterization of aldehyde 5k



A suspension of 4-hydroxycinnamaldehyde (0.15 g, 1.00 mmol) and K_2CO_3 (0.7 g, 5.0 mmol) in DMF (5 mL) was stirred at room temperature for 30 min. Then, derivative **15**[12] (0.61 g, 1.20 mmol) was added. After 12 h, the solvent was evaporated under reduced pressure and then the solid residue was dissolved in ethyl acetate (100 mL). The mixture was washed with HCl 1N (2 × 50 mL) and H_2O (2 × 50 mL). The combined organic phases were dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The crude product was purified through chromatography column on silica gel and using as solvent a mixture of petroleum ether/chloroform (1/4; *v*/*v*) as eluent. Derivative **5k** was isolated in 73 % of yield (0.13 g, 0.2 mmol). ^{1}H NMR (600 MHz, $CDCl_3$, 298 K): δ 9.65 (d, C*H*O, 1H, *J*=7.7), 7.50 (d, Ar*H*, 2H, *J*=9.1), 7.41 (d, C*H*, 1H, *J*=16.0), 7.20 (overlapped, Ar*H*, 15H), 7.08 (d, Ar*H*, 2H, *J*=8.8), 6.92 (d, Ar*H*, 2H, *J*=8.8), 6.76 (d, Ar*H*, 2H, *J*=9.1), 6.60 (dd, C*H*, 1H, J_1=16.0, J_2=7.7), 4.01 (t, OCH_2, 2H, *J*=6.4) 3.94 (t, OCH_2, 2H, *J*=6.4), 1.82 (overlapped, CH_2, 4H), 1.54 (overlapped with H_2O, CH_2, 4H). ^{13}C NMR (150 MHz, $CDCl_3$, 298 K): δ 193.7, 161.8, 157.0, 152.8, 147.1, 138.9, 132.2, 131.1, 130.4, 127.4, 126.6, 126.4, 125.8, 115.1, 113.2, 68.1, 67.6, 64.3, 29.3, 29.1, 25.9, 25.8. HRMS (MALDI): *m*/*z* calcd for $[M+Na]^+$ $C_{40}H_{38}NaO_3^+$ 589.2714, found 589.2811; calcd for $[M+K]^+$ $C_{40}H_{38}KO_3^+$ 605.2453, found 605.2491.

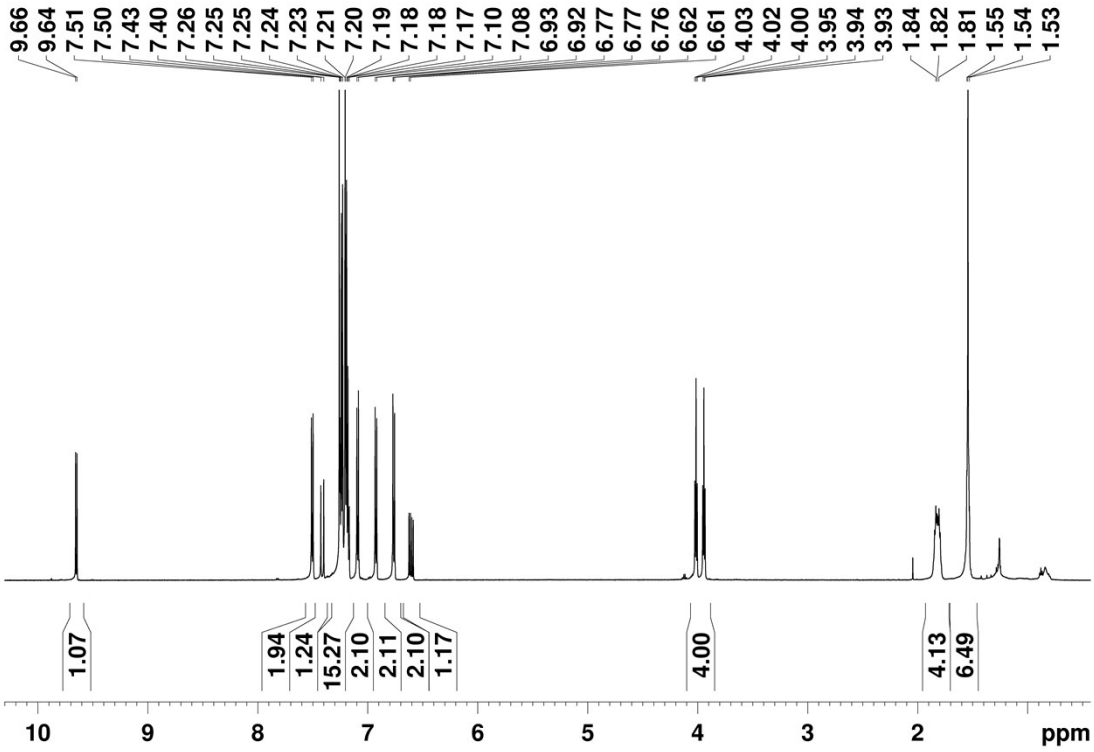


Figure S73. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5k**.

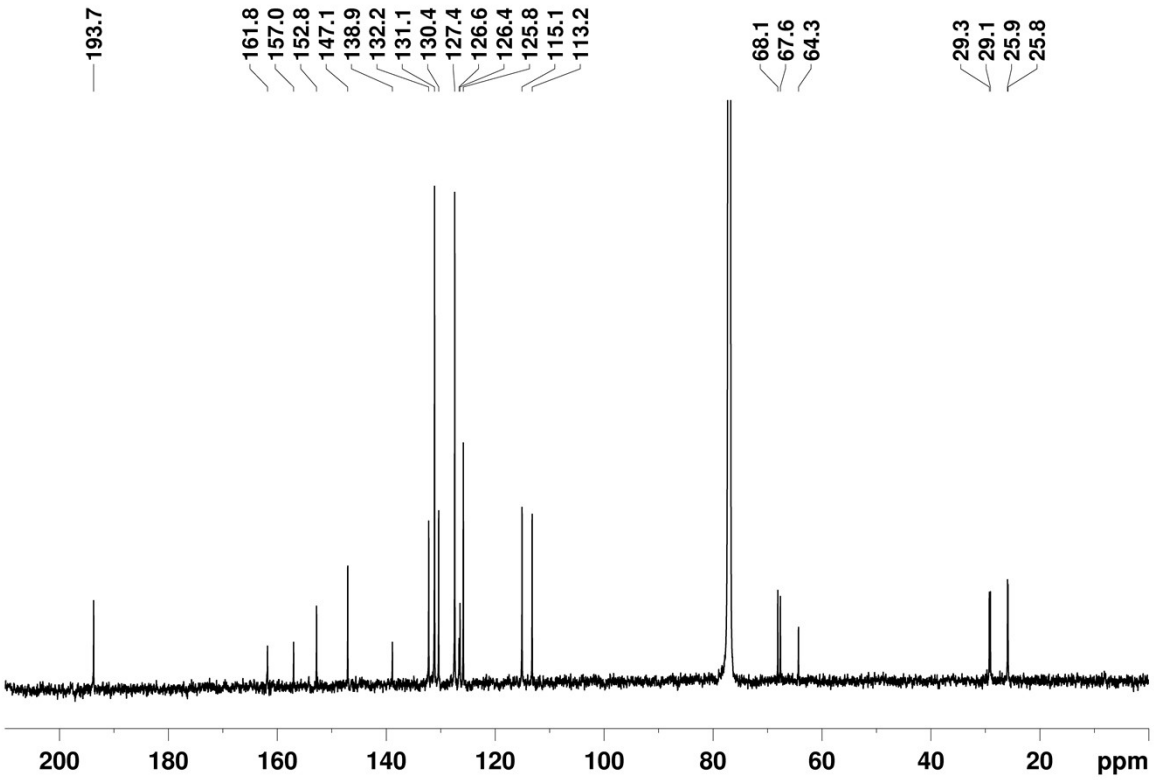


Figure S74. ^{13}C NMR spectrum (150 MHz, $CDCl_3$, 298 K) of derivative **5k**.

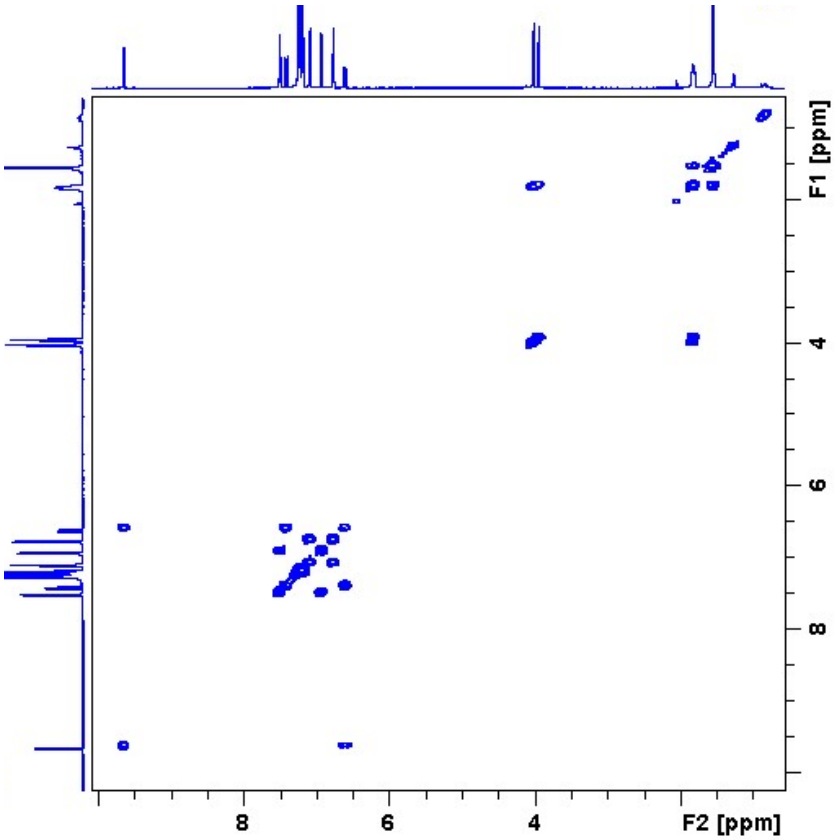


Figure S75. 2D COSY spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5k**.

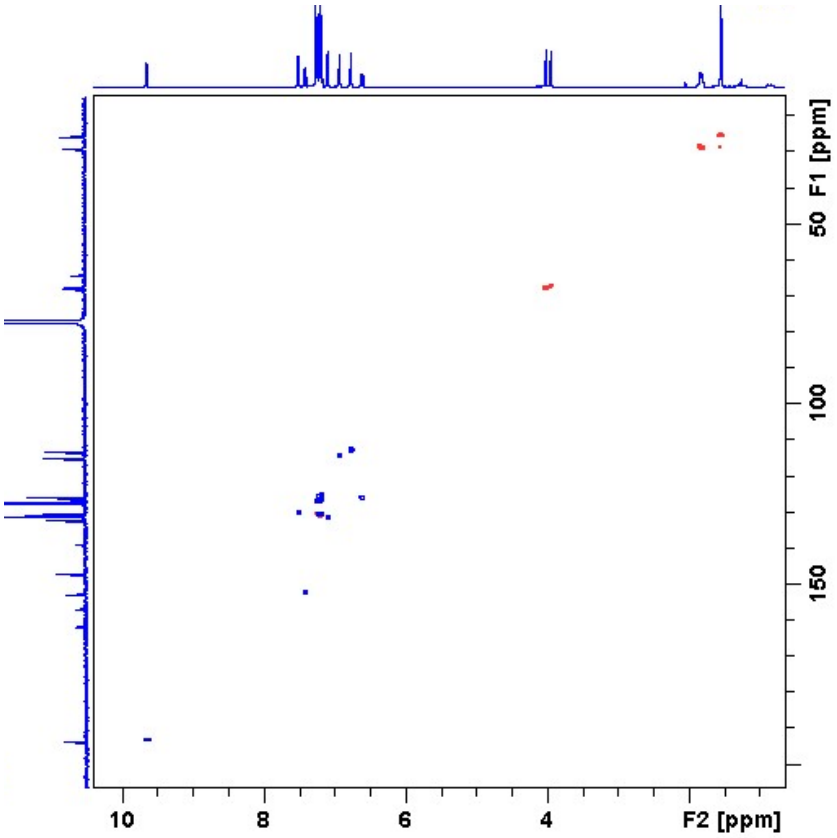


Figure S76. 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5k**.

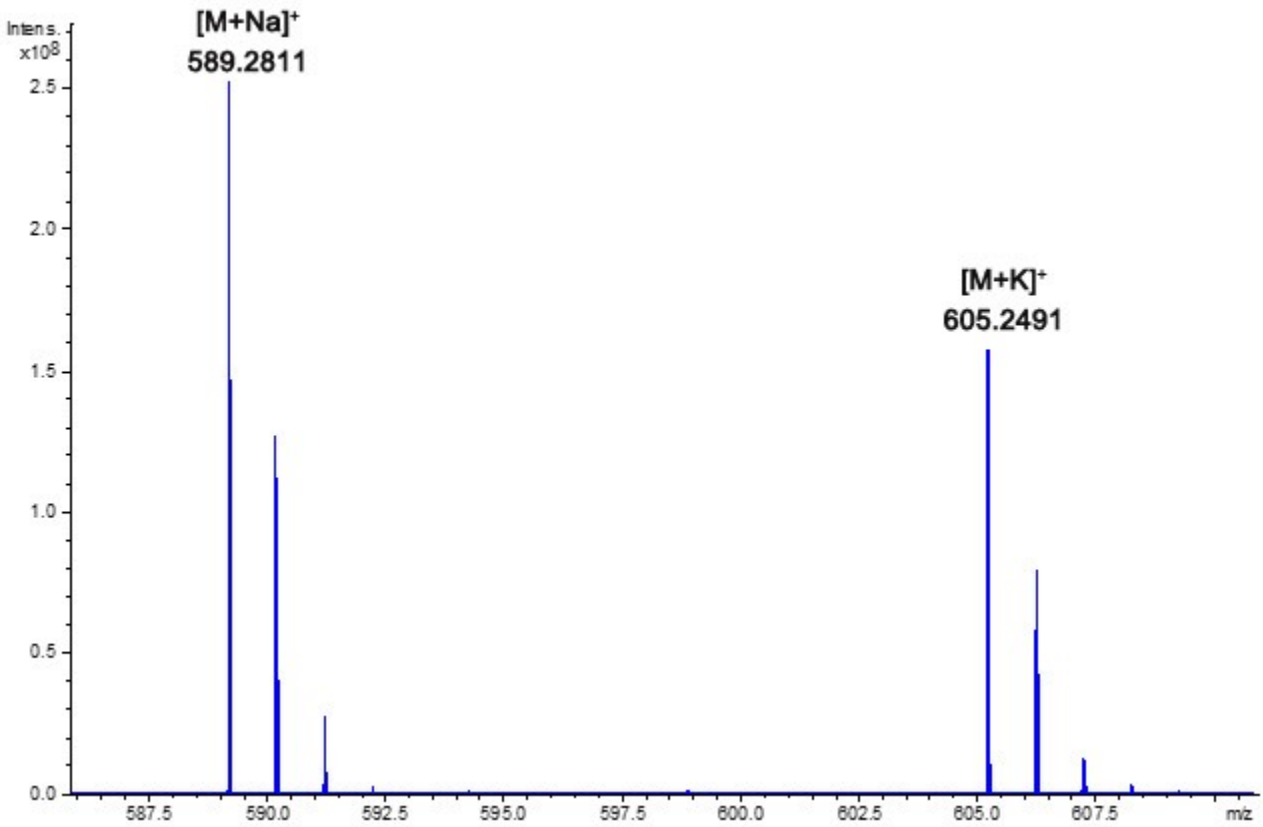


Figure S77. HR-MS of derivative **5k**.

11. Computational details

11.1 Quantum mechanical, ONIOM, and molecular dynamics calculations

Due to the high computational cost derived from the large number of atoms involved we choose to conduct an *in-silico* investigation using the ONIOM method upon a reduced model of **C**, namely $\mathbf{C_M}$ substituting the undecyl residues (the so-called "feet") present in the hexameric capsule with the methyl ones.

To deal with the multiple relevant minima due to the flexibility of the capsule and complexes we first conducted, on all compound@$\mathbf{C_M}$ complexes, a preliminary molecular dynamics (MD) study (10 ns) in chloroform, as explicit solvent, at 298 K utilizing the GAFF2 force field, and then full minimization of the structures saved every 100 ps of MD simulation has been performed at the GFN2-xTB level of theory, with the chloroform as implicit solvent, to locate the structure with the plausible lowest minima. These structures have been utilized as starting point for the other ones. Only in the case of TrX@$\mathbf{C_M}$ complexes, we performed a 2 μs of MD simulations.

The MD calculations have been performed with the YASARA Structure software, the semiempirical extended tight binding with the xTB program,[16] and the DFT and ONIOM ones with the Gaussian 16 suite of programs.[17]

In particular, a periodic simulation cell with boundaries extending 10 Å from the surface of the capsule was employed. The box was filled with chloroform, with a maximum sum of all bumps chloroform of 1.0 Å, and a density of 1.478 g mL^{-1} with explicit solvent. The final system dimensions were approximately 63 × 63 × 63 $Å^3$. The force field parameters were generated with the AutoSMILES utility, which employs semiempirical AM1 geometry optimization and assignment of charges, followed by the assignment of the AM1BCC atom and bond types with refinement using the RESP charges, and finally the assignments of general AMBER force field atom types. Optimization of the hydrogen bond network of the various was obtained using the method established by Hooft et al. A short MD was run on the solvent only. The entire system was then energy minimized using first a steepest descent minimization to remove conformational stress, followed by a simulated annealing minimization until convergence (<0.01 kcal/mol Å). The MD simulation was then initiated, using the NPT ensemble at 298 K, and integration time steps for intramolecular and intermolecular forces every 1.25 fs and 2.5 fs, respectively. Finally, 10 ns or 2 μs MD simulations without any restrictions were conducted, and the conformations of each system were recorded every 100 ps.

The QM/SE calculations have been performed using the ONIOM method incorporated in the Gaussian 16 package. The reactive species together with one of the four acidic molecules of water directly involved in the supramolecular assembly and the corresponding resorcinol hydroxyl with which it establishes a hydrogen bond were modeled using the M06-2X DFT functional, employing the aug-cc-pvdz basis set (in the case of

---

[16] Bannwarth, C., Caldeweyher, E., Ehlert, S., Hansen, A., Pracht, P., Seibert, J., *et al.* Extended tight-binding quantum chemistry methods. *WIREs Computational Molecular Science* **n/a**, e01493.

[17] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 16 revision A.03.

iodine, and only for it, we use the Def2SVPP basis set), while the semiempirical method PM6 was employed for all the other atoms.

All pure DFT calculations were performed at M06-2X/aug-cc-pvdz level.

In order to determine the activation energy barrier of each step and the reaction energy profile, reactant complex, transition state and product complex structures were fully optimized. All transition structures were characterized by only one imaginary frequency in normal mode analysis and further supported by Intrinsic Reaction Coordinate (IRC) calculations. Other stationary points (reactant complex, intermediates, and product complex) were characterized by all real frequencies and by IRC calculations. Thermodynamic corrections were calculated at 298.15 K and 1 atm for the optimized geometries. All the relative energies presented in the manuscript are referred to the sum of electronic and thermal free energies calculated at the ONIOM[M06-2X/aug-cc-pvdz:PM6] level (zero-point energy-corrected ONIOM values). The optimizations were carried out using the Berny analytical gradient optimization method. All calculations were carried out with the Gaussian 16 suite of programs. The global electrophilicity index ω, which measures the stabilization in energy when the system acquires an additional electronic charge ΔN from the environment was calculated as $\mu^2/2\eta$, where μ is the electronic chemical potential, calculated as $-(\epsilon_{HOMO} + \epsilon_{LUMO})/2$, and η is the chemical hardness, calculated as $\epsilon_{LUMO} - \epsilon_{HOMO}$.[18]

Table S8. Energies (in Hartree) and Number of Negative Frequencies of All Investigated Structures.

Structure	*E*(0)	*E*	*H*	*G*	Neg. Freq.
4	-233.213303	-233.208131	-233.207187	-233.241516	0
5_s-*cis*	-231.065098	-231.059244	-231.058299	-231.093942	0
5_s-*trans*	-231.068248	-231.062455	-231.061511	-231.096891	0
$\mathbf{C_M}$	-305.886893	-305.632198	-305.631254	-306.179087	0
TrF	-832.398889	-832.383188	-832.382244	-832.443890	0
TrCl	-1192.76453	-1192.74858	-1192.747636	-1192.809080	0
TrBr	-3306.753806	-3306.737549	-3306.736605	-3306.799283	0
TrI	-1030.197192	-1030.180734	-1030.179789	-1030.243590	0
$TrBF_4$	-1156.890938	-1156.870266	-1156.869321	-1156.941724	0
TrF@$\mathbf{C_M}$	-1138.294471	-1138.022373	-1138.021429	-1138.607338	0
TrCl@$\mathbf{C_M}$	-1498.673395	-1498.399996	-1498.399052	-1498.989985	0
TrBr@$\mathbf{C_M}$	-3612.666397	-3612.392629	-3612.391685	-3612.983475	0
TrI@$\mathbf{C_M}$	-1336.107528	-1335.833364	-1335.83242	-1336.426518	0
$TrBF_4$@$\mathbf{C_M}$	-1462.812803	-1462.535406	-1462.534462	-1463.134939	0
TS-*endo*@$\mathbf{C_M}$	-1962.973519	-1962.689695	-1962.688751	-1963.298552	1
TS-*exo*@$\mathbf{C_M}$	-1962.969247	-1962.68491	-1962.683966	-1963.294426	1
6-*endo*@$\mathbf{C_M}$	-1963.011532	-1962.728593	-1962.727649	-1963.336331	0
6-*exo*@$\mathbf{C_M}$	-1963.010733	-1962.727652	-1962.726708	-1963.336454	0
TS-*endo*	-1621.198824	-1621.167070	-1621.166126	-1621.258736	1
TS-*exo*	-1621.190475	-1621.158513	-1621.157569	-1621.254545	1

[18] Chattaraj P. K., Sarkar U., Roy D. R., Electrophylicity index, *Chem. Rev*. **2006**, *106*, 2065–2091.

11.2 Cartesian coordinates of all investigated structures

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.188198	0.718461	0.262877
2	6	0	-1.188198	-0.718461	-0.262877
3	6	0	0.107529	-1.419618	0.062506
4	6	0	1.254792	-0.725967	0.115810
5	6	0	1.254792	0.725967	-0.115810
6	6	0	0.107529	1.419618	-0.062506
7	1	0	-2.041292	1.270952	-0.148285
8	1	0	-1.312926	0.710367	1.359677
9	1	0	-2.041292	-1.270952	0.148285
10	1	0	-1.312926	-0.710366	-1.359677
11	1	0	0.107775	-2.501510	0.197485
12	1	0	2.201707	-1.229808	0.308779
13	1	0	2.201708	1.229807	-0.308779
14	1	0	0.107776	2.501510	-0.197485

5_s-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.314749	-0.121727	0.000081
2	6	0	-0.832891	-0.300382	-0.000124
3	6	0	0.063056	0.694782	-0.000031
4	6	0	1.519342	0.414319	-0.000281
5	1	0	2.182475	1.307341	0.000571
6	8	0	2.000563	-0.696670	0.000163
7	1	0	-2.755865	-0.606435	0.881615
8	1	0	-2.592379	0.937872	0.000244
9	1	0	-2.756098	-0.606232	-0.881446
10	1	0	-0.443225	-1.322172	-0.000378
11	1	0	-0.247960	1.741035	0.000218

5_s-*trans*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.423745	-0.164354	0.000031
2	6	0	1.038287	0.393640	0.000045
3	6	0	-0.088085	-0.330493	-0.000066
4	6	0	-1.402401	0.333647	-0.000020
5	1	0	-1.369382	1.447994	0.000178
6	8	0	-2.460978	-0.252105	-0.000025
7	1	0	2.976609	0.185108	0.882363
8	1	0	2.411072	-1.259368	-0.000220
9	1	0	2.976777	0.185524	-0.882030
10	1	0	0.946407	1.484885	0.000164
11	1	0	-0.082933	-1.421939	-0.000193

C_M

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.623027	-2.695889	6.163693
2	8	0	-3.513112	-6.550547	4.146384
3	6	0	-4.679836	-3.693750	6.135010
4	6	0	-4.610947	-4.602277	5.074558
5	6	0	-3.643825	-5.607053	5.163447
6	6	0	-2.769111	-5.737296	6.258304
7	6	0	-2.850330	-4.768937	7.268914
8	6	0	-3.795293	-3.739288	7.236131
9	6	0	-1.777108	-6.879929	6.305013
10	6	0	-1.800435	-7.601004	7.656368
11	1	0	-5.279767	-4.525792	4.221883
12	1	0	-2.148614	-4.818284	8.104084
13	1	0	-2.097887	-7.643194	5.531868
14	1	0	-1.532754	-6.944349	8.490201
15	1	0	-1.099701	-8.444701	7.662233
16	1	0	-2.801833	-7.998268	7.865585
17	8	0	4.810057	-3.526753	6.372173
18	8	0	2.756446	0.559464	7.925295

19	6	0	3.833611	-2.827355	7.038347
20	6	0	3.844508	-1.429894	7.091873
21	6	0	2.824933	-0.812901	7.823110
22	6	0	1.821775	-1.541038	8.496087
23	6	0	1.835387	-2.936213	8.370644
24	6	0	2.832069	-3.607976	7.656400
25	6	0	0.772953	-0.815424	9.311184
26	6	0	0.644340	-1.401627	10.721047
27	1	0	4.606471	-0.854932	6.573977
28	1	0	1.040153	-3.516299	8.843432
29	1	0	1.119161	0.254522	9.442758
30	1	0	0.344031	-2.454215	10.714579
31	1	0	-0.097727	-0.849012	11.309621
32	1	0	1.602633	-1.342770	11.252556
33	8	0	-0.865422	-6.774306	3.542693
34	8	0	3.377398	-5.171471	4.625532
35	6	0	-0.018960	-6.377404	4.553463
36	6	0	1.248430	-5.970792	4.126586
37	6	0	2.155033	-5.556728	5.110030
38	6	0	1.830500	-5.550474	6.486587
39	6	0	0.541709	-5.953711	6.850676
40	6	0	-0.398727	-6.394702	5.912227
41	6	0	2.859299	-5.114802	7.508434
42	6	0	2.712716	-5.823133	8.858984
43	1	0	1.509671	-5.941498	3.072323
44	1	0	0.261072	-5.934703	7.906425
45	1	0	3.876771	-5.406607	7.107147
46	1	0	2.761530	-6.912009	8.737545
47	1	0	1.768740	-5.587234	9.359973
48	1	0	3.522637	-5.528041	9.538256
49	8	0	0.133578	1.249595	7.361488
50	8	0	-4.139055	-0.386850	6.483343
51	6	0	-0.789028	0.264884	7.639129
52	6	0	-1.996825	0.392431	6.947682
53	6	0	-2.978312	-0.576930	7.186440
54	6	0	-2.781626	-1.649349	8.087008
55	6	0	-1.548351	-1.727742	8.742777
56	6	0	-0.541015	-0.772562	8.561834
57	6	0	-3.879203	-2.669649	8.305458
58	6	0	-3.885370	-3.266833	9.715759
59	1	0	-2.154277	1.187242	6.223556
60	1	0	-1.367757	-2.558240	9.429395

61	1	0	-4.868460	-2.133138	8.184235
62	1	0	-3.975401	-2.479583	10.474091
63	1	0	-2.978492	-3.838132	9.937479
64	1	0	-4.736607	-3.948113	9.841908
65	1	0	-6.202084	-2.686004	5.323076
66	1	0	-3.939104	-6.229491	3.307726
67	1	0	5.485400	-2.910973	5.920217
68	1	0	3.419150	1.028964	7.300832
69	1	0	-1.806414	-6.993630	3.888419
70	1	0	3.989370	-4.795087	5.349027
71	1	0	1.033539	1.080841	7.817905
72	1	0	-4.808487	-1.146640	6.610639
73	8	0	5.617647	3.490545	-5.799984
74	8	0	3.717824	-0.574572	-7.588455
75	6	0	4.713614	2.800129	-6.570401
76	6	0	4.724099	1.403159	-6.633307
77	6	0	3.784253	0.796758	-7.472563
78	6	0	2.863068	1.535169	-8.244304
79	6	0	2.868685	2.929156	-8.106493
80	6	0	3.785179	3.590227	-7.283116
81	6	0	1.904515	0.821532	-9.173203
82	6	0	1.937299	1.414503	-10.585772
83	1	0	5.423701	0.820159	-6.041977
84	1	0	2.130354	3.516782	-8.656087
85	1	0	2.254459	-0.250811	-9.270920
86	1	0	2.947681	1.348753	-11.008856
87	1	0	1.647365	2.469801	-10.607071
88	1	0	1.259560	0.871230	-11.255108
89	8	0	-4.830376	2.734495	-6.794650
90	8	0	-2.962828	6.536989	-4.473623
91	6	0	-3.890741	3.722284	-6.626347
92	6	0	-3.960981	4.623378	-5.559203
93	6	0	-2.975243	5.613111	-5.495910
94	6	0	-1.950988	5.731287	-6.458271
95	6	0	-1.903952	4.773521	-7.479492
96	6	0	-2.862423	3.762047	-7.593500
97	6	0	-0.943023	6.856268	-6.361920
98	6	0	-0.813100	7.615563	-7.686543
99	1	0	-4.740141	4.542879	-4.807260
100	1	0	-1.089785	4.816266	-8.205970
101	1	0	-1.332077	7.602889	-5.604903
102	1	0	-1.780552	8.038278	-7.985804

103	1	0	-0.473336	6.976294	-8.507569
104	1	0	-0.100914	8.444384	-7.595485
105	8	0	-0.355503	6.601307	-3.522531
106	8	0	3.993651	5.066492	-4.185988
107	6	0	0.601189	6.251914	-4.450785
108	6	0	1.814111	5.828681	-3.900440
109	6	0	2.829117	5.460156	-4.791529
110	6	0	2.659659	5.506955	-6.194885
111	6	0	1.420188	5.931516	-6.684790
112	6	0	0.379321	6.337133	-5.840772
113	6	0	3.793228	5.094892	-7.110549
114	6	0	3.787245	5.824408	-8.457454
115	1	0	1.951870	5.748503	-2.825511
116	1	0	1.260746	5.958579	-7.765339
117	1	0	4.761111	5.382277	-6.599201
118	1	0	4.664497	5.540221	-9.052650
119	1	0	3.820980	6.911237	-8.314822
120	1	0	2.901522	5.595621	-9.058316
121	8	0	1.036792	-1.246302	-7.317954
122	8	0	-3.296830	0.417837	-6.916403
123	6	0	0.157844	-0.252499	-7.690705
124	6	0	-1.120689	-0.374102	-7.139604
125	6	0	-2.062394	0.603949	-7.481359
126	6	0	-1.757420	1.679783	-8.347407
127	6	0	-0.458052	1.751622	-8.860260
128	6	0	0.515457	0.786940	-8.573987
129	6	0	-2.816407	2.709390	-8.681447
130	6	0	-2.647737	3.331170	-10.071180
131	1	0	-1.364003	-1.171075	-6.442046
132	1	0	-0.195011	2.584098	-9.517157
133	1	0	-3.814170	2.175313	-8.692629
134	1	0	-3.476625	4.016806	-10.288937
135	1	0	-2.643803	2.557838	-10.848770
136	1	0	-1.720475	3.904431	-10.168235
137	1	0	6.229053	2.868729	-5.271020
138	1	0	4.304149	-1.050988	-6.896645
139	1	0	-5.517428	2.721995	-6.040492
140	1	0	-3.634982	6.307726	-3.735776
141	1	0	-1.254658	6.825440	-3.955086
142	1	0	4.689611	4.723731	-4.848773
143	1	0	1.982995	-1.081192	-7.669145
144	1	0	-3.941791	1.184235	-7.110483

145	8	0	-0.049273	-3.801322	-7.384732
146	8	0	4.138270	-4.471527	-5.245139
147	6	0	0.840917	-4.603834	-6.718500
148	6	0	2.076610	-4.112447	-6.286375
149	6	0	2.941682	-5.018140	-5.661300
150	6	0	2.624778	-6.379633	-5.488390
151	6	0	1.350719	-6.803680	-5.893780
152	6	0	0.441782	-5.944797	-6.515775
153	6	0	3.637266	-7.336945	-4.894715
154	6	0	3.632412	-8.702539	-5.590086
155	1	0	2.344975	-3.068367	-6.414080
156	1	0	1.063368	-7.843836	-5.724539
157	1	0	4.665422	-6.896907	-5.069064
158	1	0	3.815043	-8.594445	-6.666014
159	1	0	2.683318	-9.234508	-5.470839
160	1	0	4.420364	-9.347287	-5.180805
161	8	0	0.343046	-8.265010	1.501717
162	8	0	-3.933251	-7.379755	-0.389983
163	6	0	-0.524791	-8.283161	0.439454
164	6	0	-1.822867	-7.775988	0.554510
165	6	0	-2.646662	-7.875920	-0.571349
166	6	0	-2.226331	-8.455309	-1.783199
167	6	0	-0.902676	-8.913000	-1.852369
168	6	0	-0.036633	-8.856891	-0.756953
169	6	0	-3.189289	-8.582683	-2.945363
170	6	0	-3.084679	-9.944394	-3.640382
171	1	0	-2.180618	-7.331534	1.478178
172	1	0	-0.540785	-9.337761	-2.791088
173	1	0	-4.240196	-8.519479	-2.527174
174	1	0	-3.261636	-10.760103	-2.928692
175	1	0	-2.103141	-10.113597	-4.093777
176	1	0	-3.832554	-10.030278	-4.438593
177	8	0	5.206917	-5.905075	-3.126216
178	8	0	2.951679	-7.476386	0.744039
179	6	0	4.233495	-6.674183	-2.530442
180	6	0	4.067081	-6.676435	-1.143940
181	6	0	3.087946	-7.529342	-0.619067
182	6	0	2.318085	-8.389385	-1.433308
183	6	0	2.485547	-8.295744	-2.820193
184	6	0	3.436968	-7.450217	-3.399912
185	6	0	1.377427	-9.392056	-0.801348
186	6	0	1.455013	-10.766713	-1.475448

187	1	0	4.656294	-6.031858	-0.496895
188	1	0	1.861388	-8.911845	-3.470579
189	1	0	1.714953	-9.545106	0.269581
190	1	0	1.135620	-10.743399	-2.521802
191	1	0	0.816184	-11.490826	-0.954806
192	1	0	2.481573	-11.152916	-1.455395
193	8	0	-4.836172	-6.351007	-2.836389
194	8	0	-2.644532	-4.088750	-6.382341
195	6	0	-3.859556	-6.298495	-3.801725
196	6	0	-3.730288	-5.179522	-4.628509
197	6	0	-2.736546	-5.220304	-5.613908
198	6	0	-1.908971	-6.348466	-5.808223
199	6	0	-2.047128	-7.416860	-4.913807
200	6	0	-3.015744	-7.426521	-3.904781
201	6	0	-0.933485	-6.387286	-6.965173
202	6	0	-0.908371	-7.751489	-7.663048
203	1	0	-4.361401	-4.303172	-4.504057
204	1	0	-1.383986	-8.278460	-5.015532
205	1	0	-1.293791	-5.641907	-7.738488
206	1	0	-0.559885	-8.555587	-7.007606
207	1	0	-0.244286	-7.729212	-8.535788
208	1	0	-1.910624	-8.027463	-8.013740
209	1	0	0.271890	-2.832596	-7.443543
210	1	0	4.651816	-5.102846	-4.621195
211	1	0	-0.047956	-7.785747	2.313893
212	1	0	-4.410844	-7.282826	-1.254560
213	1	0	5.763010	-5.394829	-2.439573
214	1	0	2.140552	-7.998154	1.073732
215	1	0	-5.446198	-5.537543	-2.869409
216	1	0	-1.826055	-4.096579	-6.989757
217	8	0	-0.925401	3.817728	7.298392
218	8	0	3.482642	4.456846	5.651208
219	6	0	0.041373	4.615273	6.742902
220	6	0	1.312201	4.113074	6.446086
221	6	0	2.252744	5.014312	5.933420
222	6	0	1.972854	6.381552	5.742158
223	6	0	0.665867	6.816824	6.005971
224	6	0	-0.317041	5.963265	6.512042
225	6	0	3.057947	7.333069	5.282762
226	6	0	2.975114	8.698234	5.974424
227	1	0	1.552531	3.064338	6.590556
228	1	0	0.411472	7.862439	5.818299

229	1	0	4.052552	6.885650	5.585488
230	1	0	3.814711	9.336260	5.670777
231	1	0	3.017265	8.588032	7.064675
232	1	0	2.054119	9.238730	5.734568
233	8	0	0.602891	8.155755	-1.429949
234	8	0	-3.794131	7.062350	-0.007110
235	6	0	-0.383935	8.161789	-0.478568
236	6	0	-1.627501	7.570001	-0.720826
237	6	0	-2.593183	7.674334	0.287201
238	6	0	-2.364621	8.365766	1.493051
239	6	0	-1.081572	8.892084	1.703161
240	6	0	-0.075401	8.813308	0.737708
241	6	0	-3.477654	8.537353	2.505736
242	6	0	-3.463422	9.919777	3.167318
243	1	0	-1.828134	7.036469	-1.644768
244	1	0	-0.865686	9.389741	2.651294
245	1	0	-4.459329	8.464918	1.947082
246	1	0	-4.321822	10.033941	3.841326
247	1	0	-3.522594	10.714803	2.414309
248	1	0	-2.560305	10.095763	3.760018
249	8	0	-5.180929	6.369398	2.299737
250	8	0	-3.438161	4.151495	6.117991
251	6	0	-4.310287	6.311238	3.364493
252	6	0	-4.304732	5.215534	4.229994
253	6	0	-3.416631	5.259935	5.312070
254	6	0	-2.579139	6.370330	5.559580
255	6	0	-2.587936	7.413093	4.625288
256	6	0	-3.445395	7.415924	3.520132
257	6	0	-1.728573	6.417627	6.811116
258	6	0	-1.771684	7.790427	7.490877
259	1	0	-4.946562	4.354029	4.065526
260	1	0	-1.910223	8.256964	4.769100
261	1	0	-2.170328	5.682335	7.551444
262	1	0	-2.803730	8.070750	7.735890
263	1	0	-1.359107	8.586335	6.863233
264	1	0	-1.198381	7.779548	8.425952
265	8	0	4.850769	5.918150	3.724312
266	8	0	3.123558	7.523109	-0.395580
267	6	0	3.962212	6.691557	3.011855
268	6	0	3.983554	6.710007	1.615863
269	6	0	3.073138	7.558645	0.973497
270	6	0	2.186948	8.397135	1.685839

271	6	0	2.172392	8.292122	3.081891
272	6	0	3.050773	7.452678	3.775065
273	6	0	1.310604	9.383447	0.943355
274	6	0	1.285116	10.759483	1.617473
275	1	0	4.662492	6.080814	1.046303
276	1	0	1.458678	8.892633	3.649408
277	1	0	1.766863	9.540200	-0.081896
278	1	0	2.300046	11.165605	1.710766
279	1	0	0.853175	10.730162	2.622545
280	1	0	0.694524	11.470777	1.027192
281	1	0	-0.623599	2.844941	7.383521
282	1	0	4.074640	5.088147	5.100619
283	1	0	0.338639	7.619585	-2.259220
284	1	0	-4.399137	6.985371	0.817271
285	1	0	-5.786550	5.549305	2.257613
286	1	0	-2.676204	4.150275	6.794999
287	1	0	5.489744	5.410186	3.111962
288	1	0	2.348902	8.027610	-0.824998
289	8	0	6.404140	4.491984	1.893592
290	8	0	6.482870	1.112941	5.219602
291	6	0	7.033827	3.385468	2.401767
292	6	0	6.413941	2.830999	3.529998
293	6	0	7.000249	1.689483	4.083382
294	6	0	8.149051	1.080641	3.532483
295	6	0	8.732336	1.687260	2.414922
296	6	0	8.222139	2.862590	1.850701
297	6	0	8.690861	-0.193153	4.142388
298	6	0	10.220757	-0.204039	4.224418
299	1	0	5.506718	3.266871	3.933225
300	1	0	9.621827	1.232621	1.972914
301	1	0	8.313912	-0.242631	5.209809
302	1	0	10.585482	0.648970	4.809391
303	1	0	10.696159	-0.152408	3.239781
304	1	0	10.577842	-1.120455	4.710250
305	8	0	6.545850	-4.503419	-1.123531
306	8	0	7.072416	-1.140137	-4.423786
307	6	0	7.247605	-3.407622	-1.554174
308	6	0	6.776565	-2.850259	-2.750895
309	6	0	7.438933	-1.717120	-3.230530
310	6	0	8.517183	-1.117956	-2.543105
311	6	0	8.954026	-1.728594	-1.362684
312	6	0	8.366629	-2.897523	-0.863969

313	6	0	9.139783	0.151447	-3.080913
314	6	0	10.668146	0.150927	-2.973964
315	1	0	5.920613	-3.277553	-3.261339
316	1	0	9.787927	-1.282363	-0.816112
317	1	0	8.897503	0.203712	-4.186497
318	1	0	11.018324	0.095627	-1.938339
319	1	0	11.089059	1.064750	-3.411144
320	1	0	11.095814	-0.704672	-3.510517
321	8	0	6.902799	1.599424	-4.230272
322	8	0	6.929920	4.845255	-0.766229
323	6	0	7.452404	2.040108	-3.048184
324	6	0	6.886971	3.214140	-2.538071
325	6	0	7.398088	3.695281	-1.327871
326	6	0	8.425503	3.021287	-0.621745
327	6	0	8.955652	1.859174	-1.185527
328	6	0	8.515010	1.361507	-2.419457
329	6	0	8.903651	3.575611	0.701532
330	6	0	10.431246	3.560198	0.824327
331	1	0	6.070504	3.711417	-3.053201
332	1	0	9.745033	1.324768	-0.653271
333	1	0	8.593044	4.664107	0.745254
334	1	0	10.751585	4.003795	1.774578
335	1	0	10.888883	4.141314	0.013779
336	1	0	10.849126	2.549946	0.775858
337	8	0	6.322776	-1.628499	5.011643
338	8	0	6.750532	-4.875136	1.575376
339	6	0	7.009102	-2.071826	3.904647
340	6	0	6.503116	-3.243171	3.329675
341	6	0	7.154180	-3.727705	2.190214
342	6	0	8.263566	-3.060018	1.614188
343	6	0	8.728009	-1.900509	2.238137
344	6	0	8.143736	-1.399509	3.409435
345	6	0	8.896194	-3.617167	0.358703
346	6	0	10.427338	-3.614180	0.424832
347	1	0	5.628850	-3.736778	3.742882
348	1	0	9.579161	-1.370948	1.805513
349	1	0	8.584629	-4.703045	0.274929
350	1	0	10.844205	-2.607492	0.526713
351	1	0	10.858612	-4.059221	-0.479789
352	1	0	10.777081	-4.200124	1.284188
353	1	0	6.790897	4.794793	0.990674
354	1	0	5.608884	1.554362	5.517251

355	1	0	6.822650	-4.815810	-0.184494
356	1	0	6.238101	-1.574806	-4.827309
357	1	0	7.245710	0.676268	-4.496446
358	1	0	6.202264	5.341442	-1.360986
359	1	0	6.636744	-0.707956	5.319271
360	1	0	5.950700	-5.364221	2.073632
361	8	0	-6.349058	-3.954908	-3.047072
362	8	0	-6.897274	-4.465163	1.640830
363	6	0	-7.073206	-3.630356	-1.930433
364	6	0	-6.592810	-4.199180	-0.742825
365	6	0	-7.286614	-3.898907	0.430824
366	6	0	-8.407016	-3.045293	0.464083
367	6	0	-8.847186	-2.512261	-0.753488
368	6	0	-8.223285	-2.813010	-1.969716
369	6	0	-9.068290	-2.724056	1.786159
370	6	0	-10.597132	-2.702046	1.691298
371	1	0	-5.715787	-4.837161	-0.749112
372	1	0	-9.711616	-1.844531	-0.753939
373	1	0	-8.805339	-3.559266	2.505613
374	1	0	-10.966461	-1.929804	1.009113
375	1	0	-11.045298	-2.509618	2.673921
376	1	0	-10.978800	-3.665854	1.332706
377	8	0	-6.637607	3.988420	2.252860
378	8	0	-6.641167	4.553655	-2.455819
379	6	0	-7.226118	3.684534	1.052515
380	6	0	-6.610245	4.269340	-0.062340
381	6	0	-7.155187	3.980086	-1.316374
382	6	0	-8.257246	3.113741	-1.486431
383	6	0	-8.839837	2.571735	-0.335726
384	6	0	-8.372943	2.870171	0.949945
385	6	0	-8.753464	2.790088	-2.878457
386	6	0	-10.282845	2.782526	-2.971137
387	1	0	-5.736568	4.900593	0.055336
388	1	0	-9.693868	1.899363	-0.444280
389	1	0	-8.396821	3.618398	-3.564389
390	1	0	-10.609392	2.587660	-4.000090
391	1	0	-10.696190	3.751681	-2.666604
392	1	0	-10.740013	2.017889	-2.335122
393	8	0	-6.857160	-2.659763	3.670206
394	8	0	-7.101934	2.058384	4.137376
395	6	0	-7.455499	-1.479324	3.293688
396	6	0	-6.950052	-0.336210	3.923455

397	6	0	-7.509493	0.893639	3.559947
398	6	0	-8.525851	0.999026	2.577868
399	6	0	-8.995303	-0.177291	1.990783
400	6	0	-8.505397	-1.438958	2.354811
401	6	0	-9.057555	2.363851	2.202254
402	6	0	-10.585438	2.385335	2.084825
403	1	0	-6.142619	-0.406577	4.646112
404	1	0	-9.775543	-0.114671	1.229525
405	1	0	-8.794062	3.073936	3.044675
406	1	0	-10.959022	1.715172	1.304490
407	1	0	-10.945440	3.394556	1.851845
408	1	0	-11.049138	2.075543	3.029874
409	8	0	-6.324504	2.699836	-4.464275
410	8	0	-6.555829	-2.014155	-4.966295
411	6	0	-6.976937	1.525297	-4.166116
412	6	0	-6.407222	0.377874	-4.729137
413	6	0	-7.021394	-0.846313	-4.443134
414	6	0	-8.156198	-0.940961	-3.599031
415	6	0	-8.684422	0.239902	-3.074016
416	6	0	-8.138443	1.496720	-3.369331
417	6	0	-8.743313	-2.301595	-3.297099
418	6	0	-10.273804	-2.309897	-3.371897
419	1	0	-5.512192	0.440722	-5.340950
420	1	0	-9.556451	0.184852	-2.419376
421	1	0	-8.382253	-3.013245	-4.101148
422	1	0	-10.612705	-1.996170	-4.367326
423	1	0	-10.736604	-1.636566	-2.643868
424	1	0	-10.668753	-3.316115	-3.187220
425	1	0	-6.623204	-3.409378	-3.873257
426	1	0	-6.004613	-4.898836	1.567490
427	1	0	-7.014128	3.438141	3.034646
428	1	0	-5.797202	5.102385	-2.269435
429	1	0	-7.175505	-3.451922	3.106726
430	1	0	-6.387487	1.920844	4.911720
431	1	0	-6.691343	3.492006	-3.936099
432	1	0	-5.745168	-1.883433	-5.642301
433	8	0	-4.318215	-5.552135	1.635346
434	1	0	-3.715409	-4.810778	1.494945
435	1	0	-4.149612	-6.172441	0.896185
436	8	0	4.865485	-2.196548	-5.704030
437	1	0	5.093896	-3.033527	-6.164102
438	1	0	4.151185	-2.457816	-5.081149

439	8	0	4.131127	2.178401	6.198315
440	1	0	3.508149	2.441962	5.485075
441	1	0	4.297799	3.014619	6.685847
442	8	0	-4.366668	6.091218	-2.162606
443	1	0	-4.578316	6.976840	-1.794729
444	1	0	-3.736239	5.710354	-1.511883
445	8	0	5.231194	6.384757	-2.001039
446	1	0	4.655097	6.787083	-1.323767
447	1	0	4.629920	5.973339	-2.654184
448	8	0	-5.462407	2.099278	6.157843
449	1	0	-4.832001	1.357241	6.253025
450	1	0	-4.917239	2.904524	6.074073
451	8	0	4.901322	-6.417314	2.570496
452	1	0	4.413980	-6.811442	1.822504
453	1	0	4.221699	-6.025644	3.154313
454	8	0	-4.657253	-2.072587	-6.742706
455	1	0	-4.127679	-2.873519	-6.563648
456	1	0	-4.021641	-1.328989	-6.758145

TrF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000254	0.000652	0.657975
2	6	0	-1.030298	1.036736	0.227765
3	6	0	-0.382239	-1.409723	0.227455
4	6	0	1.412753	0.374212	0.227021
5	6	0	2.037154	-0.228081	-0.865563
6	6	0	3.311149	0.184619	-1.261526
7	6	0	3.970257	1.192735	-0.562265
8	6	0	3.349447	1.792983	0.535260
9	6	0	2.074858	1.390608	0.923679
10	6	0	-1.221209	-1.650101	-0.860926
11	6	0	-1.499851	-2.960012	-1.256839
12	6	0	-0.950054	-4.034331	-0.561750
13	6	0	-0.114614	-3.796040	0.531630
14	6	0	0.173041	-2.490856	0.920046
15	6	0	-0.818162	1.887079	-0.857720
16	6	0	-1.814063	2.782855	-1.253015

17	6	0	-3.020695	2.839909	-0.560135
18	6	0	-3.232805	1.993767	0.530531
19	6	0	-2.245581	1.092535	0.918209
20	9	0	0.000556	0.000761	2.069112
21	1	0	1.532463	-1.023858	-1.410772
22	1	0	3.790429	-0.291100	-2.115755
23	1	0	4.966523	1.509369	-0.867571
24	1	0	3.860564	2.579788	1.088133
25	1	0	1.585206	1.859204	1.775469
26	1	0	-1.662450	-0.815526	-1.403156
27	1	0	-2.155451	-3.137769	-2.107900
28	1	0	-1.173016	-5.055611	-0.867132
29	1	0	0.316048	-4.631750	1.081251
30	1	0	0.827872	-2.300647	1.768512
31	1	0	0.126342	1.855155	-1.398127
32	1	0	-1.639622	3.442332	-2.101777
33	1	0	-3.794190	3.543331	-0.865006
34	1	0	-4.173003	2.035486	1.078438
35	1	0	-2.408779	0.427475	1.764387

TrCl

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000605	-0.000454	0.566228
2	6	0	0.327306	1.424234	0.119616
3	6	0	1.069397	-0.996117	0.118523
4	6	0	-1.398160	-0.428506	0.118889
5	6	0	1.110188	-2.276724	0.685790
6	6	0	2.021734	-3.223745	0.233339
7	6	0	2.907304	-2.909799	-0.800686
8	6	0	2.867601	-1.643285	-1.374260
9	6	0	1.953293	-0.689695	-0.918108
10	6	0	1.417325	2.097967	0.686460
11	6	0	1.783780	3.360276	0.234036
12	6	0	1.069760	3.971619	-0.799602
13	6	0	-0.008730	3.305975	-1.372630
14	6	0	-0.379481	2.037886	-0.916502
15	6	0	-2.526803	0.178617	0.685343

16	6	0	-3.803061	-0.135471	0.232684
17	6	0	-3.975119	-1.059996	-0.800578
18	6	0	-2.859234	-1.661312	-1.373098
19	6	0	-1.575857	-1.347959	-0.916839
20	1	0	0.421227	-2.527705	1.490093
21	1	0	2.043077	-4.212328	0.689527
22	1	0	3.623189	-3.650638	-1.153472
23	1	0	3.551150	-1.386547	-2.182042
24	1	0	1.932985	0.293417	-1.382750
25	1	0	1.978943	1.625537	1.490146
26	1	0	2.630499	3.871372	0.689772
27	1	0	1.355058	4.961484	-1.152546
28	1	0	-0.572356	3.770618	-2.180148
29	1	0	-1.221671	1.530132	-1.380980
30	1	0	-2.398827	0.901420	1.488909
31	1	0	-4.669209	0.342256	0.688086
32	1	0	-4.974901	-1.308184	-1.153592
33	1	0	-2.979541	-2.382251	-2.180202
34	1	0	-0.714911	-1.823626	-1.380857
35	17	0	-0.000503	-0.001531	2.421084

TrBr

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000301	0.000596	0.261331
2	6	0	-0.070166	-1.460307	-0.176047
3	6	0	-1.229684	0.791081	-0.177631
4	6	0	1.300257	0.669617	-0.177522
5	6	0	-1.480327	2.061286	0.360773
6	6	0	-2.543418	2.830153	-0.096788
7	6	0	-3.377250	2.346875	-1.108621
8	6	0	-3.130397	1.092617	-1.655594
9	6	0	-2.062225	0.317808	-1.194389
10	6	0	-1.046171	-2.310710	0.362720
11	6	0	-1.182671	-3.615669	-0.094467
12	6	0	-0.347866	-4.098034	-1.105988
13	6	0	0.616638	-3.259131	-1.652983
14	6	0	0.755515	-1.946657	-1.192451
15	6	0	2.524907	0.248794	0.360346

16	6	0	3.723270	0.782505	-0.097569
17	6	0	3.723246	1.746653	-1.109288
18	6	0	2.514234	2.163488	-1.655047
19	6	0	1.308076	1.628288	-1.193468
20	1	0	-0.834300	2.444910	1.148283
21	1	0	-2.724744	3.811627	0.338677
22	1	0	-4.212743	2.947578	-1.464795
23	1	0	-3.769487	0.705173	-2.447461
24	1	0	-1.880631	-0.655753	-1.643115
25	1	0	-1.701166	-1.941783	1.149851
26	1	0	-1.943149	-4.262063	0.341010
27	1	0	-0.452163	-5.121866	-1.461812
28	1	0	1.271248	-3.620283	-2.444619
29	1	0	1.508701	-1.303904	-1.641583
30	1	0	2.532905	-0.502780	1.147652
31	1	0	4.663466	0.446377	0.337050
32	1	0	4.661974	2.167707	-1.466098
33	1	0	2.499464	2.911039	-2.446638
34	1	0	0.374512	1.960150	-1.641388
35	35	0	0.000814	0.002238	2.292888

TrI

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000178	-0.000093	-0.038020
2	6	0	-1.439798	-0.258668	-0.469324
3	6	0	0.495925	1.376530	-0.466852
4	6	0	0.944643	-1.117118	-0.467934
5	6	0	1.696994	1.891216	0.044966
6	6	0	2.208329	3.099050	-0.411528
7	6	0	1.531021	3.822922	-1.397010
8	6	0	0.346003	3.317902	-1.919102
9	6	0	-0.168677	2.101738	-1.459880
10	6	0	-2.486609	0.524939	0.040211
11	6	0	-3.787706	0.363512	-0.417782
12	6	0	-4.074838	-0.586231	-1.402423
13	6	0	-3.044446	-1.360732	-1.922267
14	6	0	-1.734416	-1.197911	-1.461651

15	6	0	0.789767	-2.415652	0.041202
16	6	0	1.581501	-3.461071	-0.415926
17	6	0	2.548688	-3.233987	-1.399266
18	6	0	2.703954	-1.954165	-1.918682
19	6	0	1.906553	-0.901750	-1.458921
20	1	0	2.233155	1.335383	0.812489
21	1	0	3.139152	3.481050	0.004893
22	1	0	1.928404	4.772775	-1.751373
23	1	0	-0.189940	3.866691	-2.691949
24	1	0	-1.089217	1.720026	-1.894225
25	1	0	-2.274213	1.267986	0.807218
26	1	0	-4.584373	0.979244	-0.003125
27	1	0	-5.095730	-0.717326	-1.757826
28	1	0	-3.250896	-2.100286	-2.694364
29	1	0	-0.943227	-1.804952	-1.894305
30	1	0	0.039049	-2.603802	0.807052
31	1	0	1.446813	-4.459035	-0.001583
32	1	0	3.173774	-4.052032	-1.753916
33	1	0	3.448516	-1.762481	-2.689772
34	1	0	2.036567	0.087167	-1.891191
35	53	0	-0.002228	-0.001377	2.226285

$TrBF_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000562	0.000614	-0.783765
2	6	0	-1.354478	-0.498083	-0.797044
3	6	0	0.246478	1.423469	-0.795828
4	6	0	1.110087	-0.923657	-0.795949
5	6	0	1.361860	1.952777	-0.109352
6	6	0	1.581214	3.322201	-0.105035
7	6	0	0.715394	4.172580	-0.796062
8	6	0	-0.388125	3.660350	-1.484998
9	6	0	-0.634530	2.295917	-1.471532
10	6	0	-2.372189	0.203267	-0.112680
11	6	0	-3.667932	-0.291658	-0.110919
12	6	0	-3.969966	-1.467055	-0.802362
13	6	0	-2.972852	-2.166940	-1.488684

14	6	0	-1.668009	-1.697719	-1.472832
15	6	0	1.011675	-2.155100	-0.110361
16	6	0	2.088370	-3.029239	-0.107218
17	6	0	3.257556	-2.703380	-0.798319
18	6	0	3.364913	-1.490853	-1.486004
19	6	0	2.305898	-0.595881	-1.471761
20	5	0	-0.002763	-0.001819	2.526432
21	1	0	1.975026	1.283916	0.490153
22	1	0	2.415661	3.733474	0.458705
23	1	0	0.895619	5.247028	-0.791189
24	1	0	-1.052207	4.329061	-2.028729
25	1	0	-1.479952	1.885015	-2.019339
26	1	0	-2.101063	1.068581	0.487543
27	1	0	-4.442649	0.225745	0.450724
28	1	0	-4.990630	-1.848098	-0.800346
29	1	0	-3.218679	-3.077066	-2.032083
30	1	0	-0.888023	-2.225157	-2.018106
31	1	0	0.126618	-2.352734	0.490034
32	1	0	2.027985	-3.958058	0.455735
33	1	0	4.098156	-3.396414	-0.794653
34	1	0	4.276036	-1.248940	-2.029465
35	1	0	2.372514	0.342369	-2.018596
36	9	0	-0.002385	-0.002094	3.910189
37	9	0	-0.500949	1.230512	2.018150
38	9	0	-0.820714	-1.049268	2.017668
39	9	0	1.313363	-0.186849	2.017514

TrF@C_M

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.581424	2.693404	2.083286
2	8	0	-6.740966	4.762673	-2.104462
3	6	0	-7.829917	2.735502	0.731647
4	6	0	-7.155323	3.745264	0.037072
5	6	0	-7.345412	3.808713	-1.348520
6	6	0	-8.163720	2.877888	-2.038720
7	6	0	-8.819481	1.899085	-1.290803
8	6	0	-8.688591	1.812609	0.102539

9	6	0	-8.296808	2.975888	-3.543331
10	6	0	-9.751477	2.849745	-4.006786
11	1	0	-6.505797	4.443522	0.556714
12	1	0	-9.455488	1.175933	-1.806476
13	1	0	-7.955550	4.012866	-3.847296
14	1	0	-10.372308	3.629636	-3.547714
15	1	0	-10.197367	1.884801	-3.746461
16	1	0	-9.826283	2.963681	-5.095233
17	8	0	-5.145698	-3.236709	-5.861873
18	8	0	-5.503162	-4.923436	-1.352701
19	6	0	-5.773297	-3.328109	-4.641649
20	6	0	-5.249671	-4.122278	-3.618101
21	6	0	-5.973593	-4.194408	-2.424512
22	6	0	-7.210201	-3.527587	-2.255484
23	6	0	-7.650692	-2.693072	-3.285759
24	6	0	-6.945117	-2.558680	-4.488029
25	6	0	-8.015282	-3.755012	-0.998273
26	6	0	-9.491232	-4.036460	-1.304832
27	1	0	-4.319215	-4.674786	-3.747184
28	1	0	-8.575820	-2.129178	-3.152024
29	1	0	-7.612951	-4.690874	-0.503923
30	1	0	-9.984828	-3.204057	-1.815152
31	1	0	-10.051152	-4.239753	-0.384455
32	1	0	-9.587169	-4.916639	-1.953905
33	8	0	-5.536246	3.592299	-4.262710
34	8	0	-4.746810	-0.535918	-6.264136
35	6	0	-6.059949	2.360392	-4.560193
36	6	0	-5.181148	1.511527	-5.243269
37	6	0	-5.647156	0.235484	-5.577613
38	6	0	-6.944381	-0.209607	-5.233693
39	6	0	-7.778611	0.682668	-4.551636
40	6	0	-7.376179	1.981860	-4.220036
41	6	0	-7.379006	-1.616948	-5.590160
42	6	0	-8.873070	-1.730666	-5.903918
43	1	0	-4.174247	1.829448	-5.496387
44	1	0	-8.784611	0.357371	-4.275153
45	1	0	-6.831449	-1.913410	-6.535630
46	1	0	-9.506032	-1.488524	-5.044577
47	1	0	-9.123949	-2.754110	-6.211941
48	1	0	-9.154267	-1.058453	-6.723456
49	8	0	-5.896830	-3.687337	1.009267
50	8	0	-7.654985	0.223735	3.025209

51	6	0	-6.835269	-2.686587	0.968540
52	6	0	-6.744131	-1.762002	2.016395
53	6	0	-7.643611	-0.692654	2.003602
54	6	0	-8.575666	-0.495889	0.960438
55	6	0	-8.658610	-1.481201	-0.028595
56	6	0	-7.836165	-2.613809	-0.021723
57	6	0	-9.409931	0.765987	0.927071
58	6	0	-10.846102	0.525995	0.456099
59	1	0	-5.990271	-1.877833	2.789928
60	1	0	-9.395740	-1.368265	-0.826850
61	1	0	-9.481043	1.153944	1.989346
62	1	0	-11.353231	-0.197837	1.106286
63	1	0	-10.896564	0.136918	-0.566083
64	1	0	-11.425117	1.457620	0.478536
65	1	0	-8.029470	1.892008	2.538470
66	1	0	-6.166958	5.458233	-1.533944
67	1	0	-4.350217	-3.870401	-5.925799
68	1	0	-4.520240	-5.316007	-1.477990
69	1	0	-6.164309	4.165340	-3.689764
70	1	0	-5.069800	-1.495592	-6.398713
71	1	0	-5.843828	-4.229756	0.110191
72	1	0	-6.916182	0.032401	3.726489
73	8	0	7.197876	-2.988225	-0.983821
74	8	0	7.630696	1.414792	-2.661568
75	6	0	7.800668	-1.758667	-0.859409
76	6	0	7.373328	-0.810630	-1.796408
77	6	0	7.952292	0.461524	-1.737866
78	6	0	8.910556	0.806879	-0.754868
79	6	0	9.295895	-0.179759	0.156540
80	6	0	8.785573	-1.483564	0.110997
81	6	0	9.459980	2.214414	-0.714349
82	6	0	10.932674	2.276486	-0.296387
83	1	0	6.599591	-1.053045	-2.519716
84	1	0	10.028388	0.071175	0.926924
85	1	0	9.410210	2.622155	-1.769879
86	1	0	11.098648	1.907272	0.720539
87	1	0	11.305153	3.307255	-0.334467
88	1	0	11.552680	1.672226	-0.970195
89	8	0	5.169348	4.086372	4.458607
90	8	0	5.117460	-0.309712	6.216030
91	6	0	5.876129	2.927415	4.709769
92	6	0	5.115806	1.903900	5.285535

93	6	0	5.775511	0.708198	5.590186
94	6	0	7.150543	0.515061	5.305734
95	6	0	7.852584	1.569424	4.719935
96	6	0	7.251078	2.805039	4.436914
97	6	0	7.789615	-0.820114	5.617964
98	6	0	9.249747	-0.699313	6.066374
99	1	0	4.050683	2.030683	5.457365
100	1	0	8.909370	1.432018	4.480013
101	1	0	7.222007	-1.262485	6.493100
102	1	0	9.654037	-1.682948	6.336136
103	1	0	9.336523	-0.049270	6.944912
104	1	0	9.897330	-0.288293	5.285456
105	8	0	5.710019	-2.822793	5.482616
106	8	0	7.289296	-4.504210	1.322974
107	6	0	6.617280	-2.739857	4.453071
108	6	0	6.466598	-3.693847	3.440736
109	6	0	7.354130	-3.621247	2.361400
110	6	0	8.356744	-2.624998	2.271302
111	6	0	8.467440	-1.708844	3.319476
112	6	0	7.632291	-1.761801	4.442944
113	6	0	9.251729	-2.573907	1.052134
114	6	0	10.732056	-2.449527	1.428870
115	1	0	5.677256	-4.437534	3.485156
116	1	0	9.228832	-0.928671	3.263379
117	1	0	9.145595	-3.559932	0.506028
118	1	0	10.948393	-1.537684	1.993817
119	1	0	11.364329	-2.442727	0.533202
120	1	0	11.042706	-3.298499	2.050788
121	8	0	7.409594	3.952619	-1.787320
122	8	0	6.278810	5.674143	2.496018
123	6	0	7.621152	3.932297	-0.433868
124	6	0	6.833700	4.822980	0.306677
125	6	0	7.008085	4.820744	1.693384
126	6	0	7.916973	3.964831	2.348492
127	6	0	8.687096	3.104590	1.554811
128	6	0	8.584940	3.089686	0.160329
129	6	0	8.018094	3.975461	3.858933
130	6	0	9.471763	4.037395	4.338428
131	1	0	6.114454	5.468472	-0.183815
132	1	0	9.389234	2.424448	2.042080
133	1	0	7.520335	4.921686	4.229945
134	1	0	9.969390	4.934962	3.950681

135	1	0	10.060529	3.174251	4.011243
136	1	0	9.521707	4.073757	5.433291
137	1	0	7.447121	-3.633347	-0.226870
138	1	0	6.778309	1.144275	-3.245248
139	1	0	5.723940	4.777434	3.949422
140	1	0	4.059382	-0.202962	6.167763
141	1	0	5.695257	-1.968366	6.051334
142	1	0	6.557429	-5.255922	1.457280
143	1	0	7.757630	3.096985	-2.249941
144	1	0	5.564614	6.179430	1.970214
145	8	0	5.807647	5.999081	-2.787403
146	8	0	5.064034	2.754986	-6.173118
147	6	0	5.219152	5.607817	-3.968933
148	6	0	5.434202	4.329804	-4.488718
149	6	0	4.824436	4.025695	-5.712163
150	6	0	4.044002	4.963874	-6.423188
151	6	0	3.825203	6.212494	-5.829519
152	6	0	4.406064	6.568508	-4.607442
153	6	0	3.491630	4.612533	-7.788316
154	6	0	3.666216	5.753767	-8.796270
155	1	0	6.042332	3.594542	-3.967747
156	1	0	3.188331	6.936440	-6.341700
157	1	0	4.096620	3.741026	-8.186873
158	1	0	3.113801	6.655170	-8.513936
159	1	0	3.313030	5.451034	-9.789783
160	1	0	4.722894	6.033338	-8.888574
161	8	0	-3.599221	4.466735	-6.127700
162	8	0	-2.855367	7.258935	-2.362112
163	6	0	-2.902406	5.468855	-5.495540
164	6	0	-3.231813	5.864099	-4.196551
165	6	0	-2.502505	6.924695	-3.646001
166	6	0	-1.495668	7.605328	-4.364175
167	6	0	-1.169290	7.125666	-5.639428
168	6	0	-1.857090	6.064403	-6.235505
169	6	0	-0.821207	8.821288	-3.765684
170	6	0	-0.657587	9.955863	-4.782648
171	1	0	-4.006644	5.359243	-3.626126
172	1	0	-0.357195	7.603669	-6.191143
173	1	0	-1.498910	9.220405	-2.950303
174	1	0	-0.008691	9.682250	-5.620516
175	1	0	-0.223343	10.844276	-4.308160
176	1	0	-1.628846	10.243591	-5.204011

177	8	0	2.851179	1.921962	-7.697936
178	8	0	-1.822241	2.648274	-7.330734
179	6	0	1.773677	2.767774	-7.612009
180	6	0	0.474663	2.269914	-7.481500
181	6	0	-0.570333	3.201621	-7.452671
182	6	0	-0.353421	4.591206	-7.563713
183	6	0	0.973455	5.034959	-7.641089
184	6	0	2.055707	4.151048	-7.678565
185	6	0	-1.528565	5.544268	-7.617776
186	6	0	-1.320057	6.676423	-8.629636
187	1	0	0.279383	1.203566	-7.398337
188	1	0	1.168059	6.108521	-7.686271
189	1	0	-2.425450	4.955533	-7.981368
190	1	0	-1.122862	6.272896	-9.630418
191	1	0	-0.480224	7.327478	-8.368242
192	1	0	-2.214984	7.307499	-8.694735
193	8	0	-0.654848	8.355132	-1.047094
194	8	0	3.959268	7.222975	-1.130781
195	6	0	0.521464	8.166278	-1.727888
196	6	0	1.682300	7.752633	-1.066951
197	6	0	2.848515	7.642382	-1.833334
198	6	0	2.891163	7.956975	-3.205930
199	6	0	1.684930	8.312951	-3.826066
200	6	0	0.488333	8.433169	-3.115168
201	6	0	4.202495	7.921236	-3.962758
202	6	0	4.330588	9.069600	-4.969761
203	1	0	1.675477	7.508209	-0.009830
204	1	0	1.683582	8.512261	-4.900163
205	1	0	5.033987	8.068334	-3.208919
206	1	0	4.215931	10.040674	-4.473633
207	1	0	3.582963	9.017876	-5.767498
208	1	0	5.317773	9.053944	-5.448967
209	1	0	6.389652	5.260085	-2.388642
210	1	0	4.459540	2.513995	-6.959182
211	1	0	-4.356077	4.108241	-5.551188
212	1	0	-2.207427	7.927426	-1.946863
213	1	0	2.576476	0.941543	-7.638200
214	1	0	-2.540200	3.348715	-7.153467
215	1	0	-0.583370	8.077378	-0.068080
216	1	0	4.728127	6.951914	-1.755853
217	8	0	-5.887118	-4.975230	3.361686
218	8	0	-2.685495	-7.320220	0.602874

219	6	0	-4.795426	-5.798111	3.187580
220	6	0	-4.345913	-6.142330	1.909896
221	6	0	-3.229809	-6.979752	1.828493
222	6	0	-2.604464	-7.519468	2.976280
223	6	0	-3.071094	-7.108304	4.227682
224	6	0	-4.156541	-6.233140	4.366370
225	6	0	-1.470372	-8.508086	2.819117
226	6	0	-1.669235	-9.748930	3.696380
227	1	0	-4.839417	-5.778271	1.009979
228	1	0	-2.569999	-7.474516	5.125778
229	1	0	-1.482354	-8.873692	1.747357
230	1	0	-2.611318	-10.252308	3.443756
231	1	0	-1.704913	-9.512191	4.763989
232	1	0	-0.856619	-10.469570	3.544002
233	8	0	4.246765	-5.119184	5.902013
234	8	0	1.349667	-2.006790	8.030655
235	6	0	3.042974	-4.790693	6.471757
236	6	0	2.795837	-3.511505	6.974815
237	6	0	1.549681	-3.290286	7.573609
238	6	0	0.578317	-4.303480	7.708263
239	6	0	0.860329	-5.553531	7.139276
240	6	0	2.079768	-5.825921	6.515140
241	6	0	-0.697415	-4.032432	8.475877
242	6	0	-0.984456	-5.128920	9.507515
243	1	0	3.532680	-2.715791	6.901652
244	1	0	0.103974	-6.339185	7.188416
245	1	0	-0.544954	-3.073599	9.062771
246	1	0	-0.147799	-5.228745	10.210687
247	1	0	-1.137076	-6.110860	9.048683
248	1	0	-1.883348	-4.893764	10.089882
249	8	0	-1.454124	-1.472027	7.729798
250	8	0	-5.032077	-2.907957	4.972074
251	6	0	-2.209151	-2.476132	7.177283
252	6	0	-3.268940	-2.186703	6.312482
253	6	0	-4.018540	-3.266521	5.825690
254	6	0	-3.747799	-4.602020	6.190193
255	6	0	-2.643848	-4.833867	7.022590
256	6	0	-1.862785	-3.796844	7.540534
257	6	0	-4.640007	-5.728983	5.707904
258	6	0	-4.784951	-6.858414	6.732618
259	1	0	-3.500818	-1.168120	6.020738
260	1	0	-2.392486	-5.864065	7.288267

261	1	0	-5.676788	-5.299170	5.563167
262	1	0	-3.839635	-7.372800	6.932471
263	1	0	-5.493400	-7.615468	6.371521
264	1	0	-5.163985	-6.477201	7.688185
265	8	0	0.027267	-7.183620	0.698790
266	8	0	3.638382	-6.099309	3.424382
267	6	0	0.544404	-7.235483	1.967956
268	6	0	1.815252	-6.666161	2.099538
269	6	0	2.394045	-6.667944	3.373922
270	6	0	1.737680	-7.211479	4.502112
271	6	0	0.473211	-7.777454	4.307557
272	6	0	-0.138622	-7.829316	3.050516
273	6	0	2.394300	-7.157507	5.865344
274	6	0	2.032368	-8.342192	6.765522
275	1	0	2.322510	-6.222377	1.247426
276	1	0	-0.052001	-8.203960	5.165546
277	1	0	3.513679	-7.211255	5.705831
278	1	0	2.296254	-9.292736	6.285750
279	1	0	0.966022	-8.379689	7.008647
280	1	0	2.580576	-8.286253	7.714685
281	1	0	-6.224333	-4.607716	2.468029
282	1	0	-3.009328	-6.716305	-0.161144
283	1	0	4.875539	-4.315586	5.821937
284	1	0	0.381308	-1.854256	8.300974
285	1	0	-1.772706	-0.551816	7.444961
286	1	0	-5.514575	-3.716875	4.558905
287	1	0	-0.978916	-7.437690	0.663545
288	1	0	4.003834	-6.029476	4.377021
289	8	0	1.713867	-8.102828	-1.281611
290	8	0	-2.269832	-6.748708	-3.635612
291	6	0	1.038197	-7.771886	-2.430301
292	6	0	-0.305683	-7.390916	-2.390262
293	6	0	-0.940324	-7.130770	-3.609123
294	6	0	-0.271673	-7.242271	-4.848310
295	6	0	1.086770	-7.579760	-4.824969
296	6	0	1.770069	-7.852050	-3.634981
297	6	0	-1.026405	-7.006444	-6.137421
298	6	0	-0.650630	-8.011321	-7.231454
299	1	0	-0.846938	-7.317376	-1.449209
300	1	0	1.631823	-7.636723	-5.769707
301	1	0	-2.125115	-7.174451	-5.913689
302	1	0	-1.254793	-7.850338	-8.132540

303	1	0	-0.826787	-9.039314	-6.890691
304	1	0	0.400882	-7.941236	-7.526467
305	8	0	1.826327	-0.678586	-7.437199
306	8	0	5.772719	-1.754091	-5.209666
307	6	0	2.744273	-1.662111	-7.164445
308	6	0	3.792222	-1.260630	-6.329698
309	6	0	4.758276	-2.219392	-6.003532
310	6	0	4.695763	-3.550086	-6.477011
311	6	0	3.620607	-3.895140	-7.302261
312	6	0	2.641808	-2.969404	-7.684379
313	6	0	5.765034	-4.547260	-6.080456
314	6	0	6.115677	-5.526443	-7.205046
315	1	0	3.838239	-0.251807	-5.930640
316	1	0	3.545869	-4.921410	-7.669547
317	1	0	6.710110	-3.963973	-5.860947
318	1	0	6.933962	-6.189816	-6.897541
319	1	0	6.442137	-4.988936	-8.103478
320	1	0	5.272048	-6.162723	-7.490166
321	8	0	6.763799	-3.771163	-3.615534
322	8	0	4.210189	-6.925118	-1.157971
323	6	0	5.853680	-4.798992	-3.564579
324	6	0	5.462581	-5.354526	-2.344072
325	6	0	4.573677	-6.435579	-2.385880
326	6	0	4.101030	-6.980352	-3.600411
327	6	0	4.479987	-6.343932	-4.789040
328	6	0	5.355394	-5.253650	-4.805839
329	6	0	3.235795	-8.222944	-3.592269
330	6	0	3.622443	-9.210655	-4.698494
331	1	0	5.816902	-4.957463	-1.396426
332	1	0	4.084630	-6.716666	-5.736231
333	1	0	3.420230	-8.757887	-2.610739
334	1	0	3.474041	-8.800259	-5.702055
335	1	0	3.022505	-10.126326	-4.627423
336	1	0	4.678337	-9.495590	-4.614441
337	8	0	-2.949808	-4.935575	-5.495169
338	8	0	-0.619546	-1.633638	-7.960655
339	6	0	-1.861748	-4.625049	-6.265520
340	6	0	-1.817619	-3.297344	-6.706469
341	6	0	-0.722977	-2.914540	-7.487891
342	6	0	0.318180	-3.812439	-7.817217
343	6	0	0.217807	-5.129744	-7.356625
344	6	0	-0.870503	-5.572531	-6.596452

345	6	0	1.503811	-3.322188	-8.619451
346	6	0	1.916007	-4.305587	-9.718693
347	1	0	-2.593465	-2.590558	-6.427707
348	1	0	1.015592	-5.835381	-7.598434
349	1	0	1.189099	-2.369832	-9.145434
350	1	0	1.081689	-4.486618	-10.408057
351	1	0	2.225848	-5.277607	-9.322026
352	1	0	2.753088	-3.907861	-10.305190
353	1	0	1.152462	-7.930379	-0.445840
354	1	0	-2.614122	-6.458932	-2.720578
355	1	0	1.016918	-1.028888	-7.970302
356	1	0	6.346948	-2.505507	-4.820076
357	1	0	7.047193	-3.462173	-2.682022
358	1	0	3.468885	-7.624026	-1.223162
359	1	0	-2.856407	-5.849198	-5.021740
360	1	0	-1.286634	-0.977322	-7.467500
361	8	0	-0.197874	7.458364	1.538941
362	8	0	-4.617167	5.995546	1.702696
363	6	0	-1.330761	7.347304	2.311936
364	6	0	-2.410786	6.736149	1.667858
365	6	0	-3.597128	6.595151	2.396831
366	6	0	-3.723044	7.041166	3.732344
367	6	0	-2.604546	7.636567	4.326379
368	6	0	-1.401941	7.827618	3.636794
369	6	0	-5.032188	6.863479	4.471338
370	6	0	-5.290718	7.941539	5.528019
371	1	0	-2.322392	6.356919	0.653039
372	1	0	-2.675405	7.975032	5.362956
373	1	0	-5.864408	6.960745	3.709975
374	1	0	-6.280868	7.806648	5.982226
375	1	0	-5.265893	8.942868	5.080699
376	1	0	-4.557750	7.923321	6.340550
377	8	0	-2.584120	0.977508	6.754844
378	8	0	1.810565	2.524972	6.854494
379	6	0	-1.748519	2.034082	7.083955
380	6	0	-0.398903	1.803135	6.806533
381	6	0	0.503490	2.834973	7.098948
382	6	0	0.082885	4.079215	7.627717
383	6	0	-1.279977	4.248860	7.879657
384	6	0	-2.219892	3.233917	7.647182
385	6	0	1.097626	5.174730	7.883613
386	6	0	0.698422	6.130952	9.011046

387	1	0	-0.058434	0.871132	6.362069
388	1	0	-1.628894	5.204014	8.280968
389	1	0	2.057005	4.675614	8.216630
390	1	0	1.497089	6.861916	9.194445
391	1	0	0.527764	5.586598	9.947584
392	1	0	-0.209633	6.698355	8.784358
393	8	0	-6.604487	4.907899	3.343320
394	8	0	-5.249504	1.593237	6.595953
395	6	0	-5.903779	4.486499	4.442837
396	6	0	-5.976524	3.167827	4.906350
397	6	0	-5.248420	2.857522	6.060210
398	6	0	-4.447099	3.804558	6.730645
399	6	0	-4.376910	5.098441	6.198916
400	6	0	-5.099284	5.470021	5.062074
401	6	0	-3.688029	3.398116	7.975279
402	6	0	-3.952280	4.356484	9.139986
403	1	0	-6.585954	2.425348	4.399479
404	1	0	-3.734024	5.835995	6.684615
405	1	0	-4.073614	2.385568	8.304504
406	1	0	-3.649461	5.385086	8.919366
407	1	0	-3.416249	4.038048	10.042263
408	1	0	-5.022912	4.381825	9.382204
409	8	0	3.419753	4.738814	6.455008
410	8	0	2.152196	7.809958	2.953254
411	6	0	2.565148	5.644870	5.876713
412	6	0	2.865535	6.253228	4.654130
413	6	0	1.939716	7.173863	4.154875
414	6	0	0.747230	7.499971	4.835708
415	6	0	0.483458	6.837498	6.040722
416	6	0	1.375901	5.911087	6.589866
417	6	0	-0.205315	8.521316	4.252014
418	6	0	-0.587222	9.593154	5.277758
419	1	0	3.772173	6.004098	4.109632
420	1	0	-0.451781	7.046368	6.564195
421	1	0	0.336050	9.060423	3.416601
422	1	0	-1.092498	9.177781	6.155297
423	1	0	-1.254264	10.341944	4.833816
424	1	0	0.307104	10.117308	5.638760
425	1	0	0.595855	7.844750	2.056596
426	1	0	-5.454159	5.864986	2.268429
427	1	0	-3.558760	1.156789	7.032441
428	1	0	2.445792	3.322869	6.946305

429	1	0	-7.148736	4.161365	2.908880
430	1	0	-5.778001	0.910982	6.022830
431	1	0	4.221348	4.523148	5.849722
432	1	0	2.978946	7.444555	2.459432
433	8	0	-1.893441	-0.028957	-6.333966
434	1	0	-2.861677	-0.156589	-6.260534
435	1	0	-1.775748	0.909220	-6.604441
436	8	0	4.109227	6.926073	1.273377
437	1	0	4.333675	7.709843	0.724410
438	1	0	3.685286	6.308295	0.635070
439	8	0	5.602118	-6.507918	1.355931
440	1	0	5.271657	-6.617947	0.444196
441	1	0	4.813982	-6.408213	1.921787
442	8	0	2.503935	-0.166079	6.142152
443	1	0	2.225778	0.725278	6.426810
444	1	0	2.155114	-0.787855	6.815265
445	8	0	5.478073	0.853024	-4.031337
446	1	0	5.371424	1.498066	-4.761071
447	1	0	5.550777	-0.027121	-4.455864
448	8	0	-3.377226	0.786383	4.041593
449	1	0	-3.554097	1.734864	3.977129
450	1	0	-2.733325	0.711280	4.766346
451	8	0	-5.298912	6.631172	-1.003409
452	1	0	-4.850713	6.413096	-0.162650
453	1	0	-4.586624	6.838657	-1.641679
454	8	0	-5.690008	-0.212660	4.802973
455	1	0	-4.793860	-0.048793	4.361921
456	1	0	-5.668629	-1.153064	5.096587
457	6	0	-1.724568	-2.999104	0.469426
458	6	0	-0.345591	-3.231902	0.681611
459	6	0	0.101326	-3.733317	1.894756
460	6	0	-0.815869	-4.013845	2.908030
461	6	0	-2.183639	-3.798589	2.708769
462	6	0	-2.642084	-3.294848	1.504063
463	6	0	-2.168236	-2.382825	-0.758007
464	6	0	-1.437876	-2.601176	-1.980412
465	6	0	-3.309589	-1.494950	-0.749829
466	6	0	-4.145006	-1.409602	-1.886161
467	6	0	-5.221167	-0.538709	-1.896088
468	6	0	-5.458862	0.286675	-0.792719
469	6	0	-4.635194	0.223067	0.333879
470	6	0	-3.573670	-0.669853	0.366339

471	6	0	-1.303309	-1.545461	-2.915086
472	6	0	-0.496291	-1.700358	-4.031195
473	6	0	0.172328	-2.909765	-4.238281
474	6	0	0.009914	-3.977415	-3.347819
475	6	0	-0.781443	-3.831256	-2.222580
476	1	0	0.370386	-2.956713	-0.090212
477	1	0	1.166559	-3.890373	2.061233
478	1	0	-0.463719	-4.405652	3.862401
479	1	0	-2.887224	-4.033157	3.504944
480	1	0	-3.710020	-3.172271	1.327669
481	1	0	-3.962361	-2.070141	-2.730519
482	1	0	-5.879303	-0.496019	-2.763904
483	1	0	-6.296254	0.985633	-0.812598
484	1	0	-4.816739	0.879208	1.181773
485	1	0	-2.911233	-0.694250	1.228917
486	1	0	-1.783981	-0.588710	-2.718828
487	1	0	-0.384444	-0.876973	-4.740430
488	1	0	0.816976	-3.029281	-5.110857
489	1	0	0.512269	-4.923036	-3.542834
490	1	0	-0.957188	-4.667956	-1.552871
491	9	0	-3.276351	-5.908879	-1.420806

TrCl@C_M

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.454605	6.011789	3.054220
2	8	0	-2.154418	8.116007	-0.527794
3	6	0	-4.507388	6.562640	1.792192
4	6	0	-3.288163	7.050471	1.309746
5	6	0	-3.280714	7.583863	0.015804
6	6	0	-4.440258	7.592187	-0.802180
7	6	0	-5.630848	7.112131	-0.257181
8	6	0	-5.705236	6.624089	1.055686
9	6	0	-4.343579	8.102613	-2.223959
10	6	0	-5.508103	9.025392	-2.595419
11	1	0	-2.386094	6.999113	1.912823
12	1	0	-6.536111	7.122224	-0.867933
13	1	0	-3.403905	8.730996	-2.297714

14	1	0	-5.546966	9.889008	-1.919338
15	1	0	-6.479835	8.525066	-2.539449
16	1	0	-5.393012	9.408170	-3.616871
17	8	0	-5.592423	1.965165	-5.946290
18	8	0	-7.990610	0.186507	-2.157588
19	6	0	-6.377471	2.110946	-4.828926
20	6	0	-6.738527	1.008620	-4.051016
21	6	0	-7.574767	1.245095	-2.956224
22	6	0	-8.047624	2.528618	-2.615672
23	6	0	-7.618777	3.603313	-3.403837
24	6	0	-6.784820	3.426723	-4.514122
25	6	0	-8.981455	2.684700	-1.435743
26	6	0	-10.132703	3.652172	-1.731533
27	1	0	-6.391269	0.001452	-4.284624
28	1	0	-7.945231	4.612394	-3.144705
29	1	0	-9.458164	1.674624	-1.247388
30	1	0	-9.787923	4.667689	-1.948886
31	1	0	-10.820299	3.713330	-0.879202
32	1	0	-10.709984	3.311182	-2.600468
33	8	0	-1.750508	6.974107	-2.946050
34	8	0	-3.524612	3.796964	-5.849053
35	6	0	-2.897090	6.449302	-3.485580
36	6	0	-2.679925	5.396642	-4.381815
37	6	0	-3.805784	4.812696	-4.972104
38	6	0	-5.120138	5.248579	-4.691064
39	6	0	-5.275921	6.299785	-3.780479
40	6	0	-4.185440	6.935625	-3.176328
41	6	0	-6.300425	4.581173	-5.365155
42	6	0	-7.424464	5.560803	-5.714509
43	1	0	-1.677422	5.040163	-4.596319
44	1	0	-6.285019	6.642955	-3.540197
45	1	0	-5.934530	4.153488	-6.348019
46	1	0	-7.872035	6.025127	-4.830279
47	1	0	-8.230130	5.047518	-6.254903
48	1	0	-7.053517	6.367679	-6.358350
49	8	0	-7.934737	0.728630	0.472232
50	8	0	-6.367777	4.105984	3.409962
51	6	0	-7.775774	2.064134	0.713414
52	6	0	-7.154354	2.369557	1.932889
53	6	0	-6.946686	3.719856	2.227044
54	6	0	-7.311056	4.754479	1.337758
55	6	0	-7.939469	4.393659	0.141318

56	6	0	-8.214344	3.061940	-0.185981
57	6	0	-7.009242	6.192855	1.692024
58	6	0	-8.165632	7.139649	1.356357
59	1	0	-6.841600	1.578291	2.605883
60	1	0	-8.232893	5.180961	-0.557283
61	1	0	-6.873145	6.242283	2.816216
62	1	0	-9.081279	6.835440	1.878512
63	1	0	-8.394227	7.165035	0.286169
64	1	0	-7.931087	8.166345	1.663364
65	1	0	-5.349670	5.596151	3.330659
66	1	0	-1.329741	8.162599	0.151203
67	1	0	-5.346207	0.990161	-6.121590
68	1	0	-7.346757	-0.582626	-2.243349
69	1	0	-1.934219	7.679621	-2.223544
70	1	0	-4.361648	3.298591	-6.152957
71	1	0	-8.208372	0.526991	-0.508547
72	1	0	-6.033315	3.307000	3.971205
73	8	0	4.023098	-6.325972	-2.075663
74	8	0	7.169678	-2.858153	-2.762741
75	6	0	5.244702	-5.788186	-1.739192
76	6	0	5.547335	-4.589891	-2.395789
77	6	0	6.778737	-3.990315	-2.109457
78	6	0	7.681214	-4.540401	-1.166745
79	6	0	7.324348	-5.737762	-0.542186
80	6	0	6.127944	-6.407067	-0.832160
81	6	0	8.969025	-3.810939	-0.859315
82	6	0	10.140036	-4.749995	-0.553275
83	1	0	4.835320	-4.134065	-3.078708
84	1	0	8.005863	-6.173935	0.191520
85	1	0	9.256020	-3.235250	-1.791724
86	1	0	9.971520	-5.356788	0.341973
87	1	0	11.063584	-4.180794	-0.392291
88	1	0	10.313929	-5.438825	-1.389199
89	8	0	6.250209	-0.965115	4.866062
90	8	0	3.448703	-4.718729	5.558430
91	6	0	6.110621	-2.337040	4.804362
92	6	0	4.844197	-2.802887	5.173350
93	6	0	4.638119	-4.187063	5.156820
94	6	0	5.654736	-5.092799	4.762190
95	6	0	6.893223	-4.566214	4.392736
96	6	0	7.165368	-3.190279	4.430835
97	6	0	5.353225	-6.574810	4.734949

98	6	0	6.564870	-7.446516	5.080614
99	1	0	4.050192	-2.108502	5.431498
100	1	0	7.682757	-5.248858	4.070191
101	1	0	4.579313	-6.768830	5.539547
102	1	0	6.282225	-8.506401	5.109730
103	1	0	6.969994	-7.181627	6.064292
104	1	0	7.375139	-7.349798	4.351158
105	8	0	2.518387	-6.986697	4.378273
106	8	0	3.030880	-8.138539	-0.210785
107	6	0	3.353235	-7.162096	3.297961
108	6	0	2.728948	-7.574288	2.115603
109	6	0	3.546543	-7.755955	0.994598
110	6	0	4.944915	-7.538423	1.034918
111	6	0	5.511626	-7.130129	2.244692
112	6	0	4.743358	-6.958896	3.403421
113	6	0	5.771253	-7.742577	-0.216284
114	6	0	6.993244	-8.630168	0.044628
115	1	0	1.657265	-7.735901	2.073627
116	1	0	6.585618	-6.939884	2.289567
117	1	0	5.130133	-8.298920	-0.965457
118	1	0	7.673695	-8.203372	0.787779
119	1	0	7.565431	-8.789203	-0.876977
120	1	0	6.681007	-9.613732	0.417856
121	8	0	8.504375	-0.999105	-1.358277
122	8	0	8.274778	0.040674	3.273909
123	6	0	8.542503	-1.445504	-0.063510
124	6	0	8.394853	-0.453980	0.914527
125	6	0	8.412002	-0.871992	2.248088
126	6	0	8.560921	-2.222584	2.624431
127	6	0	8.716193	-3.168811	1.602911
128	6	0	8.742029	-2.806463	0.252647
129	6	0	8.522380	-2.614149	4.086390
130	6	0	9.683761	-3.539002	4.464098
131	1	0	8.257217	0.584518	0.636663
132	1	0	8.819011	-4.222592	1.871141
133	1	0	8.654321	-1.671782	4.698838
134	1	0	10.646570	-3.054078	4.260245
135	1	0	9.671509	-4.480614	3.905649
136	1	0	9.654529	-3.788604	5.531520
137	1	0	3.782550	-7.148273	-1.514087
138	1	0	6.371222	-2.408109	-3.315797
139	1	0	7.149098	-0.648069	4.498309

140	1	0	2.683707	-3.987185	5.638233
141	1	0	2.941896	-6.387514	5.092426
142	1	0	1.991185	-8.304183	-0.184662
143	1	0	8.303693	-1.760000	-2.026730
144	1	0	8.062433	0.977443	2.927904
145	8	0	8.594537	1.757218	-1.760746
146	8	0	6.306715	0.449473	-5.710552
147	6	0	7.979289	2.068028	-2.952964
148	6	0	7.422629	1.069638	-3.754829
149	6	0	6.846073	1.469863	-4.966635
150	6	0	6.841889	2.815433	-5.395612
151	6	0	7.371968	3.777319	-4.527705
152	6	0	7.955784	3.434851	-3.303063
153	6	0	6.293988	3.175593	-6.760492
154	6	0	7.196100	4.166451	-7.504235
155	1	0	7.427008	0.024990	-3.454262
156	1	0	7.337280	4.828710	-4.820018
157	1	0	6.280297	2.228725	-7.383074
158	1	0	7.278663	5.129610	-6.991423
159	1	0	6.807754	4.363872	-8.511055
160	1	0	8.211165	3.764648	-7.610770
161	8	0	0.442983	6.977232	-4.680824
162	8	0	2.419007	7.839727	-0.451895
163	6	0	1.548515	7.186379	-3.892244
164	6	0	1.423284	7.400491	-2.517420
165	6	0	2.598430	7.655595	-1.800408
166	6	0	3.863923	7.733014	-2.420597
167	6	0	3.934413	7.450024	-3.791160
168	6	0	2.795891	7.178586	-4.555309
169	6	0	5.084154	8.128499	-1.616668
170	6	0	5.977797	9.122922	-2.365445
171	1	0	0.460005	7.349879	-2.017390
172	1	0	4.910388	7.450862	-4.280770
173	1	0	4.721046	8.664647	-0.687138
174	1	0	6.394858	8.705366	-3.287234
175	1	0	6.820028	9.438648	-1.737848
176	1	0	5.412519	10.021550	-2.642307
177	8	0	4.158250	1.470558	-7.199827
178	8	0	0.850742	4.755586	-6.331165
179	6	0	3.804842	2.751532	-6.854425
180	6	0	2.462695	3.120005	-6.733195
181	6	0	2.188222	4.459652	-6.431924

182	6	0	3.205330	5.424432	-6.269337
183	6	0	4.533493	4.985369	-6.348973
184	6	0	4.866329	3.661192	-6.648894
185	6	0	2.850276	6.877790	-6.037123
186	6	0	3.776488	7.838122	-6.791365
187	1	0	1.660057	2.397029	-6.857963
188	1	0	5.337192	5.705807	-6.183024
189	1	0	1.811793	7.044095	-6.457269
190	1	0	3.768905	7.622303	-7.866811
191	1	0	4.815232	7.776911	-6.452577
192	1	0	3.449517	8.876610	-6.657110
193	8	0	4.712837	7.068337	0.909636
194	8	0	7.707331	3.439279	0.249915
195	6	0	5.589816	6.365638	0.122136
196	6	0	6.209436	5.202384	0.589416
197	6	0	7.134687	4.585755	-0.261132
198	6	0	7.471413	5.105975	-1.526277
199	6	0	6.777468	6.243297	-1.963863
200	6	0	5.839175	6.898486	-1.162740
201	6	0	8.554423	4.456474	-2.362266
202	6	0	9.424605	5.482179	-3.096995
203	1	0	5.969349	4.784134	1.561304
204	1	0	6.984952	6.635236	-2.962285
205	1	0	9.245220	3.905695	-1.654747
206	1	0	9.876012	6.190173	-2.391827
207	1	0	8.861305	6.065001	-3.832573
208	1	0	10.239476	4.981525	-3.635243
209	1	0	8.581126	0.753077	-1.576331
210	1	0	5.739817	0.800450	-6.483807
211	1	0	-0.421443	7.005700	-4.142653
212	1	0	3.303763	7.875483	0.053464
213	1	0	3.343761	0.871296	-7.330323
214	1	0	0.686833	5.693005	-5.965786
215	1	0	4.506340	6.585091	1.784668
216	1	0	8.212887	2.909425	-0.470232
217	8	0	-7.905387	-1.004390	2.714299
218	8	0	-6.968615	-4.353267	-0.632864
219	6	0	-7.598155	-2.291048	2.332093
220	6	0	-7.417194	-2.617968	0.986857
221	6	0	-7.146166	-3.955949	0.685787
222	6	0	-7.053013	-4.959112	1.673358
223	6	0	-7.198990	-4.566662	3.007677

224	6	0	-7.469685	-3.240123	3.368416
225	6	0	-6.788530	-6.390107	1.256323
226	6	0	-7.689457	-7.383442	1.997136
227	1	0	-7.483046	-1.868452	0.197639
228	1	0	-7.097126	-5.317344	3.793849
229	1	0	-7.053926	-6.479167	0.158863
230	1	0	-8.747477	-7.154908	1.816395
231	1	0	-7.534357	-7.370299	3.080264
232	1	0	-7.507248	-8.408302	1.650855
233	8	0	-0.165266	-7.563213	4.103108
234	8	0	-0.722662	-3.998297	7.190778
235	6	0	-0.958789	-6.770188	4.888980
236	6	0	-0.419556	-5.741574	5.664975
237	6	0	-1.308250	-5.001646	6.454231
238	6	0	-2.691726	-5.272205	6.500808
239	6	0	-3.183440	-6.287860	5.669201
240	6	0	-2.343805	-7.055745	4.858826
241	6	0	-3.583879	-4.499435	7.448264
242	6	0	-4.516996	-5.422109	8.239524
243	1	0	0.644329	-5.517672	5.658991
244	1	0	-4.256310	-6.489934	5.660157
245	1	0	-2.914236	-3.992945	8.210566
246	1	0	-3.940115	-6.165432	8.804412
247	1	0	-5.210617	-5.973541	7.597069
248	1	0	-5.116902	-4.849961	8.957432
249	8	0	-2.615926	-1.903364	7.359466
250	8	0	-6.194866	-0.242326	4.731469
251	6	0	-3.791802	-2.099902	6.679677
252	6	0	-4.414400	-1.045154	6.005168
253	6	0	-5.637249	-1.316705	5.378750
254	6	0	-6.248165	-2.586825	5.425419
255	6	0	-5.553408	-3.616997	6.073767
256	6	0	-4.330511	-3.405461	6.716977
257	6	0	-7.614926	-2.799204	4.807827
258	6	0	-8.493862	-3.752335	5.623557
259	1	0	-3.969102	-0.057482	5.958800
260	1	0	-5.990327	-4.618594	6.088646
261	1	0	-8.146682	-1.799554	4.808326
262	1	0	-8.086397	-4.767063	5.672861
263	1	0	-9.495550	-3.827292	5.180819
264	1	0	-8.611125	-3.393699	6.653251
265	8	0	-4.844522	-5.984231	-0.891717

266	8	0	-1.247986	-7.623474	1.570237
267	6	0	-4.437665	-6.507186	0.305786
268	6	0	-3.076961	-6.829497	0.366999
269	6	0	-2.591114	-7.355706	1.569104
270	6	0	-3.423297	-7.574327	2.690457
271	6	0	-4.774166	-7.230271	2.573823
272	6	0	-5.316354	-6.712504	1.393253
273	6	0	-2.851526	-8.164178	3.961268
274	6	0	-3.828753	-9.094177	4.687024
275	1	0	-2.416912	-6.656112	-0.478009
276	1	0	-5.431799	-7.379858	3.433561
277	1	0	-1.963826	-8.804135	3.668471
278	1	0	-4.157742	-9.906377	4.027124
279	1	0	-4.724180	-8.574748	5.041637
280	1	0	-3.349072	-9.550747	5.562126
281	1	0	-7.985545	-0.375782	1.915133
282	1	0	-6.698424	-3.563637	-1.194069
283	1	0	0.825546	-7.306575	4.159793
284	1	0	-1.416684	-3.381241	7.605221
285	1	0	-2.290042	-0.944508	7.288235
286	1	0	-7.021986	-0.494665	4.183594
287	1	0	-5.804280	-5.603022	-0.857277
288	1	0	-0.910184	-7.925097	2.485411
289	8	0	-3.412015	-6.837732	-3.187589
290	8	0	-5.625553	-2.984606	-5.061080
291	6	0	-3.648765	-5.952153	-4.209757
292	6	0	-4.512856	-4.867458	-4.039259
293	6	0	-4.739824	-4.050207	-5.150597
294	6	0	-4.122952	-4.266354	-6.399777
295	6	0	-3.230185	-5.339803	-6.500101
296	6	0	-2.979657	-6.204179	-5.428082
297	6	0	-4.446939	-3.347101	-7.557475
298	6	0	-4.594672	-4.103014	-8.882123
299	1	0	-5.002520	-4.667656	-3.086324
300	1	0	-2.717628	-5.513409	-7.448506
301	1	0	-5.457008	-2.881232	-7.343326
302	1	0	-4.876425	-3.418418	-9.691552
303	1	0	-5.376402	-4.869090	-8.806099
304	1	0	-3.672260	-4.606950	-9.186807
305	8	0	1.729994	0.083927	-7.421303
306	8	0	4.008539	-3.631059	-5.784205
307	6	0	1.840405	-1.283315	-7.450685

308	6	0	2.833991	-1.802720	-6.614899
309	6	0	2.994467	-3.192893	-6.593385
310	6	0	2.187058	-4.061513	-7.362928
311	6	0	1.205596	-3.484483	-8.175907
312	6	0	1.023835	-2.098913	-8.261953
313	6	0	2.394960	-5.559848	-7.281663
314	6	0	2.176333	-6.268429	-8.621882
315	1	0	3.436506	-1.153059	-5.986639
316	1	0	0.563842	-4.137085	-8.772412
317	1	0	3.476787	-5.738830	-7.000420
318	1	0	2.394530	-7.340105	-8.532039
319	1	0	2.838528	-5.857344	-9.393506
320	1	0	1.148652	-6.175804	-8.986807
321	8	0	3.440349	-6.122146	-4.777770
322	8	0	-0.704800	-7.514446	-2.935549
323	6	0	2.093737	-6.361122	-4.900095
324	6	0	1.340977	-6.813169	-3.813459
325	6	0	-0.012035	-7.091234	-4.041717
326	6	0	-0.608301	-6.955889	-5.314167
327	6	0	0.179966	-6.439554	-6.350803
328	6	0	1.532751	-6.133314	-6.177024
329	6	0	-2.042780	-7.387094	-5.530402
330	6	0	-2.225613	-8.165532	-6.837853
331	1	0	1.778067	-6.929286	-2.825188
332	1	0	-0.275715	-6.278438	-7.330007
333	1	0	-2.311805	-8.103332	-4.694081
334	1	0	-2.000196	-7.563326	-7.723371
335	1	0	-3.259277	-8.519260	-6.937550
336	1	0	-1.568194	-9.043257	-6.863793
337	8	0	-4.831653	-0.743498	-6.290884
338	8	0	-0.744299	0.949139	-7.984352
339	6	0	-3.699702	-0.981030	-7.023647
340	6	0	-2.824692	0.107841	-7.118699
341	6	0	-1.641960	-0.074275	-7.842858
342	6	0	-1.313693	-1.307142	-8.451979
343	6	0	-2.226270	-2.359376	-8.330414
344	6	0	-3.436664	-2.223181	-7.641344
345	6	0	0.003084	-1.460422	-9.180815
346	6	0	-0.144997	-2.199926	-10.513705
347	1	0	-3.053020	1.049493	-6.628898
348	1	0	-1.985558	-3.320879	-8.789674
349	1	0	0.375795	-0.420894	-9.432662

350	1	0	-0.846881	-1.672643	-11.172124
351	1	0	-0.519643	-3.221069	-10.391501
352	1	0	0.817977	-2.263028	-11.034757
353	1	0	-3.937785	-6.605307	-2.347291
354	1	0	-5.750015	-2.709881	-4.102745
355	1	0	0.920313	0.428217	-7.960362
356	1	0	3.983174	-4.640745	-5.626397
357	1	0	3.769127	-6.253135	-3.816617
358	1	0	-1.705129	-7.590602	-3.112632
359	1	0	-5.343684	-1.609744	-6.060147
360	1	0	-0.925396	1.732671	-7.294623
361	8	0	4.268050	5.504207	3.153257
362	8	0	-0.146242	6.986719	3.249303
363	6	0	3.228656	5.930003	3.948814
364	6	0	2.059303	6.243878	3.249902
365	6	0	0.964596	6.691398	3.998283
366	6	0	1.013386	6.829741	5.404103
367	6	0	2.207587	6.488366	6.048939
368	6	0	3.340970	6.058076	5.349511
369	6	0	-0.201453	7.327565	6.158122
370	6	0	0.143627	8.087915	7.441995
371	1	0	1.993266	6.113050	2.172632
372	1	0	2.261444	6.571146	7.137170
373	1	0	-0.735037	8.066221	5.486236
374	1	0	-0.765854	8.486287	7.910098
375	1	0	0.805070	8.936761	7.229437
376	1	0	0.640532	7.458533	8.186792
377	8	0	-2.000759	0.847900	6.920059
378	8	0	2.415377	-0.639859	7.042271
379	6	0	-0.724728	1.084023	7.407741
380	6	0	0.229358	0.152558	6.990347
381	6	0	1.543068	0.331630	7.443985
382	6	0	1.914985	1.418885	8.271071
383	6	0	0.915955	2.319113	8.648137
384	6	0	-0.421848	2.163711	8.257175
385	6	0	3.358143	1.581684	8.702217
386	6	0	3.521064	2.301293	10.044062
387	1	0	-0.027937	-0.668067	6.325751
388	1	0	1.182168	3.171541	9.278561
389	1	0	3.787020	0.544313	8.845170
390	1	0	4.579032	2.332511	10.336415
391	1	0	2.974010	1.780789	10.839287

392	1	0	3.165411	3.336025	10.016298
393	8	0	-2.529500	7.011350	4.712303
394	8	0	-3.727469	2.954922	7.045627
395	6	0	-2.317911	6.033305	5.649064
396	6	0	-3.206404	4.964540	5.809709
397	6	0	-2.916636	4.039155	6.817946
398	6	0	-1.772407	4.141436	7.635867
399	6	0	-0.894978	5.208459	7.404622
400	6	0	-1.144694	6.172777	6.424571
401	6	0	-1.517998	3.104832	8.708503
402	6	0	-1.250069	3.749015	10.071406
403	1	0	-4.090233	4.866408	5.185359
404	1	0	0.014683	5.284514	8.004501
405	1	0	-2.460955	2.488988	8.827976
406	1	0	-0.371966	4.402707	10.065491
407	1	0	-1.092539	2.986849	10.844065
408	1	0	-2.105620	4.363477	10.381417
409	8	0	5.065670	0.161616	7.060730
410	8	0	6.227963	4.059730	4.461114
411	6	0	4.986731	1.500818	6.766875
412	6	0	5.703657	2.057858	5.703477
413	6	0	5.566056	3.432861	5.492075
414	6	0	4.749695	4.250318	6.302745
415	6	0	4.033142	3.633950	7.335740
416	6	0	4.137404	2.263957	7.597441
417	6	0	4.653719	5.736614	6.031723
418	6	0	4.897153	6.561912	7.299101
419	1	0	6.325525	1.441653	5.060196
420	1	0	3.366587	4.241472	7.951446
421	1	0	5.482406	6.010457	5.310803
422	1	0	4.166716	6.352529	8.086879
423	1	0	4.853685	7.636195	7.082841
424	1	0	5.890067	6.346626	7.714596
425	1	0	5.084724	5.211742	3.695959
426	1	0	-0.940817	7.276626	3.818622
427	1	0	-2.686757	1.515904	7.300105
428	1	0	3.391468	-0.433756	7.272195
429	1	0	-3.365895	6.840234	4.149734
430	1	0	-4.508018	2.888165	6.359325
431	1	0	5.627258	-0.353096	6.371923
432	1	0	6.712695	3.391706	3.845250
433	8	0	-0.925589	2.532180	-5.924227

434	1	0	-1.777029	3.008148	-5.825960
435	1	0	-0.237755	3.233561	-5.972501
436	8	0	7.417979	2.580065	2.503131
437	1	0	8.118008	3.168199	2.142427
438	1	0	6.773271	2.504652	1.763212
439	8	0	0.464960	-8.625534	-0.545654
440	1	0	0.246457	-8.347916	-1.454247
441	1	0	-0.188020	-8.192116	0.032235
442	8	0	1.488363	-2.972684	5.660581
443	1	0	1.790868	-2.133834	6.057457
444	1	0	0.775072	-3.305545	6.244437
445	8	0	5.247895	-1.678255	-4.071137
446	1	0	5.631957	-0.966705	-4.626531
447	1	0	4.830701	-2.311698	-4.691971
448	8	0	-2.610079	1.760450	4.224896
449	1	0	-2.115969	2.590586	4.265254
450	1	0	-2.217599	1.212011	4.925051
451	8	0	-0.011677	8.510018	0.869309
452	1	0	0.158280	7.889097	1.606343
453	1	0	0.738035	8.400699	0.248810
454	8	0	-5.104174	2.296227	4.938402
455	1	0	-4.268305	2.010912	4.447472
456	1	0	-5.603334	1.459510	5.094770
457	6	0	-2.989224	-1.921389	-0.048188
458	6	0	-1.890240	-2.803112	0.033339
459	6	0	-1.834997	-3.756420	1.042060
460	6	0	-2.882078	-3.858928	1.959043
461	6	0	-3.987428	-3.003967	1.875187
462	6	0	-4.038129	-2.032383	0.891165
463	6	0	-3.017109	-0.879528	-1.050928
464	6	0	-2.415892	-1.096424	-2.341766
465	6	0	-3.575906	0.415824	-0.721921
466	6	0	-4.219328	1.187079	-1.714482
467	6	0	-4.687666	2.454238	-1.411329
468	6	0	-4.496407	2.982969	-0.129915
469	6	0	-3.867672	2.228691	0.862727
470	6	0	-3.420424	0.944981	0.576940
471	6	0	-1.779396	-0.030770	-3.020063
472	6	0	-1.138056	-0.254945	-4.229551
473	6	0	-1.136478	-1.536256	-4.786092
474	6	0	-1.787075	-2.594958	-4.140446
475	6	0	-2.412045	-2.385674	-2.924443

476	17	0	-5.889630	-1.985947	-2.200864
477	1	0	-1.061529	-2.695791	-0.664719
478	1	0	-0.973478	-4.418554	1.120138
479	1	0	-2.842053	-4.616954	2.742542
480	1	0	-4.809402	-3.108461	2.581827
481	1	0	-4.909078	-1.392103	0.785040
482	1	0	-4.392964	0.746626	-2.693372
483	1	0	-5.202103	3.041172	-2.171822
484	1	0	-4.849531	3.990732	0.096332
485	1	0	-3.710324	2.643705	1.854259
486	1	0	-2.896577	0.371461	1.339326
487	1	0	-1.745721	0.954866	-2.560215
488	1	0	-0.634328	0.569901	-4.739751
489	1	0	-0.632089	-1.712693	-5.737801
490	1	0	-1.805352	-3.582680	-4.599896
491	1	0	-2.963844	-3.185626	-2.438124

TrBr@C_M

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.358826	6.517225	3.271690
2	8	0	-1.119481	8.293681	-0.520798
3	6	0	-3.445792	7.058536	2.007317
4	6	0	-2.219553	7.389085	1.420671
5	6	0	-2.253211	7.906334	0.120759
6	6	0	-3.465917	8.046655	-0.603044
7	6	0	-4.657995	7.723639	0.044698
8	6	0	-4.683384	7.262178	1.369002
9	6	0	-3.422531	8.520052	-2.040357
10	6	0	-4.489715	9.576237	-2.341619
11	1	0	-1.284014	7.231366	1.950065
12	1	0	-5.602111	7.839371	-0.491647
13	1	0	-2.421405	9.023775	-2.204572
14	1	0	-4.364917	10.448194	-1.686869
15	1	0	-5.508257	9.203567	-2.195283
16	1	0	-4.412185	9.925919	-3.378360
17	8	0	-5.770240	2.533344	-5.495683
18	8	0	-8.233935	1.218060	-1.557161
19	6	0	-6.463632	2.819085	-4.344589

20	6	0	-6.962008	1.798950	-3.530525
21	6	0	-7.677969	2.181383	-2.393132
22	6	0	-7.895777	3.528261	-2.039938
23	6	0	-7.349153	4.509649	-2.875031
24	6	0	-6.634915	4.186651	-4.035174
25	6	0	-8.697304	3.844804	-0.795957
26	6	0	-9.691832	4.988316	-1.023542
27	1	0	-6.807857	0.749245	-3.777251
28	1	0	-7.484312	5.561237	-2.614672
29	1	0	-9.318924	2.930098	-0.551674
30	1	0	-9.201851	5.930112	-1.288811
31	1	0	-10.290539	5.170551	-0.122790
32	1	0	-10.384446	4.740888	-1.838247
33	8	0	-1.059029	7.040541	-2.908463
34	8	0	-3.445511	4.058861	-5.569819
35	6	0	-2.301644	6.662161	-3.348751
36	6	0	-2.291149	5.566858	-4.219974
37	6	0	-3.523603	5.128038	-4.714876
38	6	0	-4.743595	5.749610	-4.366995
39	6	0	-4.693406	6.832839	-3.482450
40	6	0	-3.488291	7.325854	-2.969760
41	6	0	-6.044559	5.239427	-4.948574
42	6	0	-7.040485	6.359420	-5.263846
43	1	0	-1.362725	5.070951	-4.485362
44	1	0	-5.628078	7.317155	-3.189827
45	1	0	-5.803708	4.740939	-5.936797
46	1	0	-7.365118	6.901938	-4.370539
47	1	0	-7.940950	5.952581	-5.741642
48	1	0	-6.600479	7.091255	-5.952330
49	8	0	-7.814857	1.747170	1.052622
50	8	0	-5.473329	4.836446	3.783946
51	6	0	-7.424255	3.041082	1.254110
52	6	0	-6.651940	3.245610	2.406853
53	6	0	-6.214540	4.547516	2.665825
54	6	0	-6.502846	5.628902	1.804679
55	6	0	-7.280775	5.369370	0.671615
56	6	0	-7.780941	4.095537	0.383186
57	6	0	-5.972002	7.008285	2.121079
58	6	0	-7.010488	8.109505	1.884941
59	1	0	-6.400429	2.414304	3.056801
60	1	0	-7.513303	6.194247	-0.006460
61	1	0	-5.730837	7.029919	3.228693

62	1	0	-7.910759	7.930833	2.485815
63	1	0	-7.325106	8.176386	0.838659
64	1	0	-6.609487	9.090883	2.166864
65	1	0	-4.270861	6.208613	3.620273
66	1	0	-0.241277	8.248900	0.089682
67	1	0	-5.680978	1.530143	-5.656953
68	1	0	-7.730801	0.356147	-1.657325
69	1	0	-1.093029	7.785971	-2.202902
70	1	0	-4.361246	3.672278	-5.799480
71	1	0	-8.214707	1.591513	0.108721
72	1	0	-5.224816	3.996046	4.327119
73	8	0	3.105250	-6.740221	-2.187999
74	8	0	6.588615	-3.707982	-3.221345
75	6	0	4.412230	-6.362454	-1.975804
76	6	0	4.801349	-5.215951	-2.677500
77	6	0	6.120206	-4.777135	-2.516122
78	6	0	7.029451	-5.433262	-1.650512
79	6	0	6.584204	-6.572996	-0.977140
80	6	0	5.290946	-7.085876	-1.145264
81	6	0	8.420760	-4.869666	-1.472511
82	6	0	9.487711	-5.944308	-1.241897
83	1	0	4.091784	-4.675771	-3.298925
84	1	0	7.270560	-7.089549	-0.302502
85	1	0	8.694812	-4.349011	-2.440527
86	1	0	9.324252	-6.510084	-0.319259
87	1	0	10.485541	-5.493915	-1.175424
88	1	0	9.500588	-6.663041	-2.070575
89	8	0	6.536344	-1.635154	4.366206
90	8	0	3.382322	-5.019766	5.379118
91	6	0	6.233720	-2.982344	4.355397
92	6	0	4.956167	-3.288473	4.836107
93	6	0	4.589281	-4.638636	4.873170
94	6	0	5.458306	-5.665204	4.424862
95	6	0	6.715763	-5.295547	3.945710
96	6	0	7.148476	-3.960902	3.924572
97	6	0	4.984208	-7.101165	4.462470
98	6	0	6.110623	-8.105922	4.725036
99	1	0	4.273002	-2.499702	5.137704
100	1	0	7.391986	-6.072473	3.581686
101	1	0	4.266904	-7.188736	5.335246
102	1	0	5.708666	-9.123717	4.806814
103	1	0	6.630227	-7.875734	5.662550

104	1	0	6.858238	-8.118903	3.925728
105	8	0	2.099273	-7.202965	4.366017
106	8	0	2.068146	-8.429004	-0.232536
107	6	0	2.810991	-7.477240	3.219041
108	6	0	2.041573	-7.824147	2.103142
109	6	0	2.730070	-8.104862	0.917897
110	6	0	4.142168	-8.051714	0.832940
111	6	0	4.856704	-7.700219	1.980759
112	6	0	4.218663	-7.430503	3.198340
113	6	0	4.827073	-8.363404	-0.480021
114	6	0	5.948160	-9.394194	-0.307489
115	1	0	0.959195	-7.867802	2.159379
116	1	0	5.945077	-7.633907	1.928112
117	1	0	4.061096	-8.840378	-1.163711
118	1	0	6.736106	-9.051076	0.369916
119	1	0	6.416605	-9.628112	-1.270754
120	1	0	5.549840	-10.329405	0.105998
121	8	0	8.294924	-2.029216	-2.003758
122	8	0	8.550006	-0.902265	2.607627
123	6	0	8.372557	-2.457657	-0.704256
124	6	0	8.428427	-1.441546	0.257852
125	6	0	8.494461	-1.839336	1.596082
126	6	0	8.500713	-3.192416	1.992444
127	6	0	8.452691	-4.165234	0.985328
128	6	0	8.417968	-3.828322	-0.371289
129	6	0	8.531885	-3.555897	3.461843
130	6	0	9.602726	-4.607548	3.769155
131	1	0	8.404255	-0.397951	-0.033786
132	1	0	8.440294	-5.219559	1.270337
133	1	0	8.822872	-2.627928	4.040214
134	1	0	10.596602	-4.243373	3.480480
135	1	0	9.435476	-5.548163	3.234471
136	1	0	9.629468	-4.837831	4.840967
137	1	0	2.817803	-7.527118	-1.598408
138	1	0	5.806488	-3.169042	-3.716184
139	1	0	7.428912	-1.432797	3.912463
140	1	0	2.718681	-4.201157	5.507028
141	1	0	2.645210	-6.638794	5.023120
142	1	0	1.022559	-8.456506	-0.115626
143	1	0	7.938568	-2.764376	-2.633971
144	1	0	8.431773	0.049188	2.256324
145	8	0	8.644643	0.694700	-2.471886

146	8	0	5.892849	-0.388951	-6.186101
147	6	0	7.973075	1.058947	-3.617508
148	6	0	7.235846	0.122635	-4.345226
149	6	0	6.610573	0.570611	-5.515444
150	6	0	6.729958	1.900003	-5.976899
151	6	0	7.442798	2.804130	-5.180689
152	6	0	8.083576	2.412783	-3.999959
153	6	0	6.113911	2.302638	-7.300273
154	6	0	7.058888	3.168662	-8.140334
155	1	0	7.141804	-0.910203	-4.019821
156	1	0	7.509052	3.847284	-5.496182
157	1	0	5.936606	1.355112	-7.896131
158	1	0	7.296625	4.122732	-7.660005
159	1	0	6.611872	3.395865	-9.116061
160	1	0	8.007320	2.648007	-8.320690
161	8	0	0.951569	6.794323	-4.827249
162	8	0	3.377182	7.482496	-0.806035
163	6	0	2.138817	6.884444	-4.141720
164	6	0	2.160588	7.130581	-2.766783
165	6	0	3.415822	7.258865	-2.159960
166	6	0	4.622178	7.180812	-2.888330
167	6	0	4.538728	6.872467	-4.252766
168	6	0	3.313790	6.723624	-4.909318
169	6	0	5.945747	7.442768	-2.201843
170	6	0	6.881072	8.310521	-3.050542
171	1	0	1.245934	7.196971	-2.184209
172	1	0	5.461414	6.753695	-4.824426
173	1	0	5.730231	8.034492	-1.260241
174	1	0	7.165211	7.829923	-3.991965
175	1	0	7.805578	8.535150	-2.504860
176	1	0	6.402774	9.264821	-3.303993
177	8	0	3.763214	0.856726	-7.519284
178	8	0	0.949663	4.519945	-6.449684
179	6	0	3.593427	2.175196	-7.175373
180	6	0	2.319190	2.701242	-6.949167
181	6	0	2.229720	4.067986	-6.658103
182	6	0	3.362603	4.908166	-6.607160
183	6	0	4.618554	4.314034	-6.788076
184	6	0	4.767592	2.955550	-7.082195
185	6	0	3.201668	6.396714	-6.382331
186	6	0	4.163592	7.228923	-7.237383
187	1	0	1.429956	2.076357	-6.987079

188	1	0	5.512079	4.936765	-6.708513
189	1	0	2.156806	6.678736	-6.715833
190	1	0	4.035844	6.999458	-8.302396
191	1	0	5.213889	7.049824	-6.987738
192	1	0	3.973493	8.300764	-7.101805
193	8	0	5.680520	6.481451	0.376888
194	8	0	8.151972	2.505915	-0.436937
195	6	0	6.393910	5.663987	-0.463313
196	6	0	6.910520	4.443010	-0.018613
197	6	0	7.676347	3.704315	-0.928242
198	6	0	7.958292	4.157778	-2.231907
199	6	0	7.367279	5.362196	-2.640093
200	6	0	6.588334	6.139673	-1.779726
201	6	0	8.878933	3.368588	-3.139165
202	6	0	9.798706	4.269915	-3.970329
203	1	0	6.710228	4.074157	0.981913
204	1	0	7.529501	5.708283	-3.663508
205	1	0	9.557503	2.748779	-2.478406
206	1	0	10.390952	4.928344	-3.323793
207	1	0	9.247586	4.905838	-4.670277
208	1	0	10.498072	3.666080	-4.562457
209	1	0	8.528509	-0.297919	-2.262219
210	1	0	5.308507	0.015505	-6.919338
211	1	0	0.146352	6.921765	-4.215920
212	1	0	4.300985	7.423962	-0.378538
213	1	0	2.875743	0.357256	-7.566236
214	1	0	0.928103	5.475354	-6.094613
215	1	0	5.498162	6.042680	1.280401
216	1	0	8.523442	1.906549	-1.183534
217	8	0	-7.683597	0.034645	3.344847
218	8	0	-7.670936	-3.553711	0.109526
219	6	0	-7.611835	-1.298626	3.003779
220	6	0	-7.674068	-1.702377	1.668537
221	6	0	-7.601367	-3.074211	1.412557
222	6	0	-7.470774	-4.038221	2.434295
223	6	0	-7.390371	-3.576255	3.751511
224	6	0	-7.461249	-2.212385	4.067478
225	6	0	-7.406750	-5.505084	2.062945
226	6	0	-8.303991	-6.365278	2.958391
227	1	0	-7.777684	-0.979069	0.860820
228	1	0	-7.265709	-4.299659	4.559510
229	1	0	-7.814870	-5.610158	1.011805

230	1	0	-9.347962	-6.033468	2.892036
231	1	0	-8.015870	-6.323157	4.013194
232	1	0	-8.270029	-7.417281	2.649065
233	8	0	-0.647296	-7.326018	4.234928
234	8	0	-0.515705	-3.743754	7.348240
235	6	0	-1.271160	-6.455784	5.088267
236	6	0	-0.551242	-5.502257	5.811563
237	6	0	-1.277154	-4.663437	6.665809
238	6	0	-2.675386	-4.762463	6.822835
239	6	0	-3.350594	-5.714640	6.046631
240	6	0	-2.677396	-6.578573	5.179961
241	6	0	-3.393277	-3.877823	7.819375
242	6	0	-4.369215	-4.670396	8.694782
243	1	0	0.527590	-5.406148	5.716757
244	1	0	-4.436903	-5.787896	6.127461
245	1	0	-2.612366	-3.447587	8.519979
246	1	0	-3.845234	-5.471635	9.231620
247	1	0	-5.169435	-5.141961	8.115696
248	1	0	-4.840928	-4.021671	9.442537
249	8	0	-2.102853	-1.444409	7.561262
250	8	0	-5.614930	0.615313	5.129179
251	6	0	-3.342579	-1.494911	6.978852
252	6	0	-3.866469	-0.389014	6.302561
253	6	0	-5.164442	-0.505397	5.789826
254	6	0	-5.944032	-1.666845	5.956903
255	6	0	-5.344795	-2.764706	6.592029
256	6	0	-4.051763	-2.710126	7.117119
257	6	0	-7.383218	-1.698632	5.487445
258	6	0	-8.299055	-2.480464	6.434972
259	1	0	-3.292840	0.522912	6.165636
260	1	0	-5.916326	-3.690977	6.691566
261	1	0	-7.764030	-0.632710	5.488718
262	1	0	-8.042471	-3.543046	6.491806
263	1	0	-9.342788	-2.418378	6.100378
264	1	0	-8.251013	-2.074303	7.452373
265	8	0	-5.696520	-5.361143	-0.315609
266	8	0	-1.997186	-7.237618	1.802277
267	6	0	-5.203957	-5.878682	0.851980
268	6	0	-3.876823	-6.318236	0.776406
269	6	0	-3.307854	-6.861154	1.933650
270	6	0	-4.029756	-6.990787	3.141817
271	6	0	-5.346886	-6.520881	3.164725

272	6	0	-5.967768	-5.973032	2.037655
273	6	0	-3.384301	-7.629805	4.351627
274	6	0	-4.363900	-8.458243	5.189271
275	1	0	-3.300906	-6.222874	-0.139781
276	1	0	-5.915078	-6.593849	4.095334
277	1	0	-2.600535	-8.355033	3.973160
278	1	0	-4.842793	-9.232611	4.577438
279	1	0	-5.158203	-7.852163	5.635253
280	1	0	-3.838549	-8.961725	6.010804
281	1	0	-7.796251	0.633241	2.527080
282	1	0	-7.379045	-2.835359	-0.524759
283	1	0	0.371538	-7.202343	4.223046
284	1	0	-1.092778	-3.045270	7.809370
285	1	0	-1.648836	-0.545294	7.420579
286	1	0	-6.498312	0.449301	4.637214
287	1	0	-6.612627	-4.903604	-0.193944
288	1	0	-1.592338	-7.555342	2.683600
289	8	0	-4.454287	-6.378992	-2.715074
290	8	0	-6.424521	-2.410152	-4.627585
291	6	0	-4.670762	-5.514101	-3.760182
292	6	0	-5.427389	-4.351860	-3.586721
293	6	0	-5.633498	-3.550202	-4.712562
294	6	0	-5.092179	-3.851616	-5.978682
295	6	0	-4.313076	-5.009169	-6.087126
296	6	0	-4.097021	-5.866657	-5.001492
297	6	0	-5.373772	-2.925768	-7.142803
298	6	0	-5.671653	-3.689613	-8.437234
299	1	0	-5.850424	-4.090477	-2.617947
300	1	0	-3.865440	-5.256406	-7.051822
301	1	0	-6.314236	-2.346033	-6.893368
302	1	0	-5.914401	-2.995947	-9.251578
303	1	0	-6.530338	-4.359257	-8.302791
304	1	0	-4.828724	-4.302936	-8.770310
305	8	0	1.172964	-0.222683	-7.495549
306	8	0	3.123154	-4.161473	-5.960303
307	6	0	1.118435	-1.593575	-7.500729
308	6	0	2.109040	-2.217037	-6.735821
309	6	0	2.103453	-3.615997	-6.693560
310	6	0	1.135530	-4.391583	-7.371922
311	6	0	0.167242	-3.711969	-8.118872
312	6	0	0.147331	-2.316231	-8.225181
313	6	0	1.163621	-5.902445	-7.265060

314	6	0	0.751099	-6.602847	-8.563137
315	1	0	2.834380	-1.636139	-6.173386
316	1	0	-0.595257	-4.290416	-8.645599
317	1	0	2.234238	-6.210309	-7.064106
318	1	0	0.841134	-7.691592	-8.460009
319	1	0	1.394710	-6.292892	-9.395411
320	1	0	-0.283131	-6.387993	-8.849701
321	8	0	2.330834	-6.527905	-4.832443
322	8	0	-1.790736	-7.342601	-2.626355
323	6	0	0.960112	-6.599356	-4.841140
324	6	0	0.248048	-6.922182	-3.683221
325	6	0	-1.142132	-7.040843	-3.797978
326	6	0	-1.816959	-6.875925	-5.026498
327	6	0	-1.058804	-6.488026	-6.139144
328	6	0	0.329769	-6.340923	-6.079581
329	6	0	-3.302366	-7.148098	-5.117250
330	6	0	-3.670816	-7.947786	-6.371953
331	1	0	0.745589	-7.057784	-2.726462
332	1	0	-1.568981	-6.303093	-7.086717
333	1	0	-3.582475	-7.798998	-4.232321
334	1	0	-3.452392	-7.406320	-7.297507
335	1	0	-4.741330	-8.187633	-6.378872
336	1	0	-3.116345	-8.893555	-6.408081
337	8	0	-5.378238	-0.279469	-5.889686
338	8	0	-1.233182	0.907916	-7.853834
339	6	0	-4.328503	-0.655209	-6.684921
340	6	0	-3.337108	0.321029	-6.844695
341	6	0	-2.233442	-0.000980	-7.641538
342	6	0	-2.093862	-1.264856	-8.259760
343	6	0	-3.112404	-2.202263	-8.066461
344	6	0	-4.251333	-1.922978	-7.302582
345	6	0	-0.858995	-1.571903	-9.077626
346	6	0	-1.184497	-2.299290	-10.385509
347	1	0	-3.422234	1.284744	-6.352456
348	1	0	-3.015992	-3.187023	-8.529663
349	1	0	-0.391085	-0.582806	-9.370857
350	1	0	-1.869222	-1.701418	-11.000182
351	1	0	-1.660094	-3.271396	-10.221795
352	1	0	-0.274641	-2.473348	-10.972597
353	1	0	-4.914561	-6.072646	-1.861538
354	1	0	-6.468725	-2.093568	-3.678376
355	1	0	0.362617	0.207132	-7.968555

356	1	0	2.990114	-5.157697	-5.774241
357	1	0	2.718841	-6.670318	-3.894594
358	1	0	-2.803318	-7.303788	-2.725240
359	1	0	-5.982796	-1.075047	-5.632185
360	1	0	-1.265616	1.706568	-7.158157
361	8	0	5.251779	5.017220	2.688870
362	8	0	1.060846	7.008521	3.093395
363	6	0	4.333159	5.568455	3.553290
364	6	0	3.157830	6.011562	2.939746
365	6	0	2.183320	6.589372	3.761514
366	6	0	2.355574	6.731245	5.157350
367	6	0	3.548730	6.258205	5.715183
368	6	0	4.567862	5.694343	4.938874
369	6	0	1.266768	7.370990	5.992835
370	6	0	1.792632	8.088861	7.239269
371	1	0	2.993556	5.880377	1.873044
372	1	0	3.695687	6.341897	6.794684
373	1	0	0.775030	8.165271	5.353441
374	1	0	0.973183	8.592265	7.768422
375	1	0	2.531057	8.853710	6.969212
376	1	0	2.266568	7.407277	7.952448
377	8	0	-1.181806	1.139862	6.946774
378	8	0	3.036780	-0.835609	6.803361
379	6	0	0.142815	1.235790	7.343357
380	6	0	0.956960	0.200237	6.878317
381	6	0	2.308986	0.232682	7.245317
382	6	0	2.853730	1.276028	8.031803
383	6	0	1.988018	2.284479	8.461744
384	6	0	0.618473	2.277320	8.160966
385	6	0	4.332227	1.280703	8.362206
386	6	0	4.667567	1.994659	9.674651
387	1	0	0.567074	-0.587721	6.239106
388	1	0	2.388417	3.104926	9.062876
389	1	0	4.652059	0.203790	8.496817
390	1	0	5.740507	1.911702	9.892900
391	1	0	4.123973	1.548363	10.515988
392	1	0	4.426855	3.062098	9.650172
393	8	0	-1.187124	7.328259	4.728843
394	8	0	-2.653660	3.417441	7.153468
395	6	0	-1.017114	6.329603	5.653129
396	6	0	-2.005773	5.366515	5.882782
397	6	0	-1.748305	4.411175	6.870980

398	6	0	-0.548101	4.388964	7.610830
399	6	0	0.425109	5.350463	7.309838
400	6	0	0.217424	6.335413	6.340587
401	6	0	-0.335988	3.333784	8.674376
402	6	0	0.091742	3.949207	10.009608
403	1	0	-2.936005	5.369379	5.321661
404	1	0	1.377464	5.323858	7.844074
405	1	0	-1.329961	2.825032	8.862860
406	1	0	1.033315	4.503088	9.937988
407	1	0	0.217588	3.176768	10.777814
408	1	0	-0.668910	4.654381	10.369647
409	8	0	5.746060	-0.343135	6.633279
410	8	0	7.130801	3.365159	3.869461
411	6	0	5.794466	0.992674	6.316867
412	6	0	6.485021	1.451607	5.191091
413	6	0	6.485972	2.830801	4.961720
414	6	0	5.832939	3.745596	5.815171
415	6	0	5.133148	3.227022	6.911511
416	6	0	5.101969	1.857275	7.192302
417	6	0	5.885017	5.230159	5.523454
418	6	0	6.320358	6.034999	6.752070
419	1	0	6.982824	0.761593	4.515886
420	1	0	4.588153	3.913677	7.562661
421	1	0	6.679869	5.399312	4.735362
422	1	0	5.635472	5.918898	7.597905
423	1	0	6.382133	7.104888	6.519193
424	1	0	7.312105	5.711433	7.093463
425	1	0	6.068422	4.636216	3.173178
426	1	0	0.350611	7.392605	3.715295
427	1	0	-1.759491	1.893947	7.347759
428	1	0	4.043533	-0.742476	6.967332
429	1	0	-2.078476	7.253502	4.235635
430	1	0	-3.470666	3.420940	6.504595
431	1	0	6.177350	-0.929110	5.907829
432	1	0	7.483893	2.638258	3.231582
433	8	0	-1.023750	2.514681	-5.820063
434	1	0	-1.803284	3.084842	-5.651904
435	1	0	-0.271935	3.133177	-5.961546
436	8	0	7.961381	1.718933	1.853966
437	1	0	8.694395	2.208277	1.419210
438	1	0	7.248442	1.716931	1.175285
439	8	0	-0.563691	-8.559796	-0.348759

440	1	0	-0.808142	-8.315141	-1.260237
441	1	0	-1.106294	-7.996761	0.231647
442	8	0	1.669562	-3.042636	5.609836
443	1	0	2.129022	-2.241336	5.927393
444	1	0	0.994387	-3.253865	6.288019
445	8	0	4.718203	-2.334285	-4.408767
446	1	0	5.137858	-1.684046	-5.011930
447	1	0	4.188661	-2.930659	-4.978861
448	8	0	-2.260440	1.939611	4.403937
449	1	0	-1.716151	2.734076	4.486120
450	1	0	-1.797625	1.276509	4.941080
451	8	0	1.162253	8.464048	0.679129
452	1	0	1.329836	7.839311	1.414067
453	1	0	1.837878	8.263500	-0.001040
454	8	0	-4.496224	2.863097	5.348245
455	1	0	-3.948267	2.216989	4.801083
456	1	0	-5.186676	2.303412	5.770079
457	6	0	-3.136745	-1.486004	0.319808
458	6	0	-2.172407	-2.515968	0.357213
459	6	0	-2.187760	-3.448096	1.387003
460	6	0	-3.174757	-3.379298	2.371647
461	6	0	-4.147760	-2.373559	2.334974
462	6	0	-4.125540	-1.425445	1.327256
463	6	0	-3.097435	-0.480351	-0.718992
464	6	0	-2.633653	-0.815393	-2.041461
465	6	0	-3.471532	0.884372	-0.410047
466	6	0	-4.093551	1.690712	-1.389582
467	6	0	-4.401960	3.010424	-1.105929
468	6	0	-4.070536	3.554181	0.140248
469	6	0	-3.462480	2.766394	1.119770
470	6	0	-3.174855	1.433584	0.855801
471	6	0	-1.925987	0.137338	-2.810963
472	6	0	-1.439584	-0.198274	-4.066034
473	6	0	-1.667616	-1.478008	-4.577837
474	6	0	-2.388444	-2.424062	-3.838352
475	6	0	-2.858327	-2.106126	-2.576673
476	1	0	-1.387170	-2.544793	-0.396625
477	1	0	-1.429472	-4.229339	1.427256
478	1	0	-3.192276	-4.121480	3.170969
479	1	0	-4.926678	-2.344435	3.095112
480	1	0	-4.904282	-0.671901	1.256268
481	1	0	-4.384032	1.241459	-2.336143

482	1	0	-4.902129	3.625419	-1.853458
483	1	0	-4.298409	4.600746	0.350642
484	1	0	-3.199364	3.191696	2.084708
485	1	0	-2.670384	0.830401	1.608217
486	1	0	-1.718480	1.119489	-2.390642
487	1	0	-0.880013	0.538554	-4.647698
488	1	0	-1.289319	-1.740593	-5.567291
489	1	0	-2.586446	-3.408247	-4.261342
490	1	0	-3.467082	-2.811083	-2.016985
491	35	0	-6.280740	-1.280369	-1.646919

TrI@C_M

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.714631	6.769041	3.345270
2	8	0	-0.606182	8.293610	-0.629106
3	6	0	-2.843679	7.279609	2.071696
4	6	0	-1.637426	7.518609	1.404707
5	6	0	-1.719365	7.997073	0.092259
6	6	0	-2.963034	8.186299	-0.564668
7	6	0	-4.131211	7.958629	0.162384
8	6	0	-4.103180	7.540789	1.500896
9	6	0	-2.978334	8.602102	-2.020417
10	6	0	-3.986020	9.720951	-2.298584
11	1	0	-0.682431	7.321051	1.883483
12	1	0	-5.097500	8.115064	-0.321451
13	1	0	-1.957414	9.025021	-2.267869
14	1	0	-3.756949	10.605515	-1.690419
15	1	0	-5.016360	9.429779	-2.071904
16	1	0	-3.952584	10.025033	-3.351898
17	8	0	-6.015202	2.697199	-5.110795
18	8	0	-8.510208	1.795714	-1.066635
19	6	0	-6.641330	3.090788	-3.951582
20	6	0	-7.237047	2.160032	-3.097364
21	6	0	-7.854537	2.653998	-1.945710
22	6	0	-7.871473	4.022287	-1.608862
23	6	0	-7.250109	4.910497	-2.493667
24	6	0	-6.641565	4.476559	-3.678174

25	6	0	-8.546524	4.454983	-0.324929
26	6	0	-9.422820	5.696242	-0.525308
27	1	0	-7.219417	1.091621	-3.315549
28	1	0	-7.239276	5.975571	-2.254695
29	1	0	-9.247041	3.623556	-0.009147
30	1	0	-8.852770	6.568674	-0.858957
31	1	0	-9.931439	5.970411	0.406937
32	1	0	-10.195410	5.504246	-1.280924
33	8	0	-0.788532	6.890207	-2.923671
34	8	0	-3.544787	3.991070	-5.303667
35	6	0	-2.079748	6.597540	-3.283891
36	6	0	-2.203068	5.461096	-4.091502
37	6	0	-3.489971	5.107035	-4.509486
38	6	0	-4.634316	5.852521	-4.148755
39	6	0	-4.451793	6.969363	-3.325878
40	6	0	-3.186848	7.378958	-2.889317
41	6	0	-5.996704	5.434136	-4.656873
42	6	0	-6.906035	6.622670	-4.983899
43	1	0	-1.333241	4.871042	-4.363069
44	1	0	-5.327462	7.548126	-3.022294
45	1	0	-5.840023	4.877216	-5.630763
46	1	0	-7.150792	7.224137	-4.102998
47	1	0	-7.854904	6.276192	-5.413274
48	1	0	-6.432561	7.287381	-5.716725
49	8	0	-7.713104	2.297393	1.495093
50	8	0	-4.888192	5.193884	3.968731
51	6	0	-7.193765	3.553270	1.636685
52	6	0	-6.311649	3.699803	2.717995
53	6	0	-5.744469	4.960648	2.922559
54	6	0	-6.013723	6.058217	2.075752
55	6	0	-6.898282	5.856750	1.011590
56	6	0	-7.525566	4.628307	0.780117
57	6	0	-5.355569	7.393113	2.337529
58	6	0	-6.315748	8.572857	2.154421
59	1	0	-6.082142	2.854765	3.357844
60	1	0	-7.114597	6.694316	0.343507
61	1	0	-5.041922	7.403483	3.427395
62	1	0	-7.188930	8.469885	2.810433
63	1	0	-6.687128	8.659914	1.128426
64	1	0	-5.821285	9.520331	2.401688
65	1	0	-3.621891	6.519524	3.749810
66	1	0	0.304374	8.222582	-0.068286

67	1	0	-6.016076	1.687330	-5.235960
68	1	0	-8.162799	0.868620	-1.191987
69	1	0	-0.723712	7.674688	-2.263122
70	1	0	-4.499733	3.674640	-5.474170
71	1	0	-8.197309	2.163100	0.591087
72	1	0	-4.660959	4.341587	4.500705
73	8	0	2.657357	-6.885203	-2.162870
74	8	0	6.231357	-4.087442	-3.499484
75	6	0	3.997878	-6.588638	-2.055094
76	6	0	4.402104	-5.475758	-2.800813
77	6	0	5.753699	-5.117840	-2.745277
78	6	0	6.683599	-5.819726	-1.939230
79	6	0	6.221894	-6.923419	-1.218712
80	6	0	4.890890	-7.357499	-1.282949
81	6	0	8.115136	-5.338994	-1.871551
82	6	0	9.130823	-6.470595	-1.687204
83	1	0	3.681813	-4.898379	-3.374796
84	1	0	6.924303	-7.474814	-0.589697
85	1	0	8.350748	-4.856257	-2.868924
86	1	0	9.000288	-7.004706	-0.740745
87	1	0	10.155510	-6.079657	-1.701741
88	1	0	9.043292	-7.206987	-2.495588
89	8	0	6.786099	-1.886852	3.981678
90	8	0	3.531520	-5.074837	5.277675
91	6	0	6.414350	-3.216329	4.026592
92	6	0	5.155238	-3.442429	4.592581
93	6	0	4.722440	-4.769969	4.689431
94	6	0	5.508307	-5.851840	4.217788
95	6	0	6.750709	-5.561167	3.652920
96	6	0	7.249158	-4.252109	3.568273
97	6	0	4.963544	-7.259040	4.324259
98	6	0	6.050641	-8.317780	4.534927
99	1	0	4.533674	-2.610895	4.912835
100	1	0	7.362314	-6.381468	3.270236
101	1	0	4.304608	-7.288328	5.245601
102	1	0	5.601938	-9.310064	4.670007
103	1	0	6.645718	-8.095988	5.428565
104	1	0	6.738962	-8.389187	3.686917
105	8	0	2.076112	-7.218026	4.428436
106	8	0	1.664343	-8.508646	-0.133453
107	6	0	2.693040	-7.547300	3.241573
108	6	0	1.831420	-7.871538	2.187877

109	6	0	2.420728	-8.205552	0.963881
110	6	0	3.824347	-8.229604	0.782128
111	6	0	4.633852	-7.897420	1.871232
112	6	0	4.096325	-7.573370	3.123556
113	6	0	4.400877	-8.597716	-0.567777
114	6	0	5.470077	-9.689647	-0.451603
115	1	0	0.754669	-7.859754	2.319667
116	1	0	5.717934	-7.889272	1.742915
117	1	0	3.565196	-9.038145	-1.191591
118	1	0	6.319277	-9.384363	0.167386
119	1	0	5.859698	-9.962964	-1.439289
120	1	0	5.047013	-10.594680	0.002537
121	8	0	8.146573	-2.509825	-2.466809
122	8	0	8.739492	-1.302686	2.094106
123	6	0	8.272320	-2.913642	-1.162612
124	6	0	8.448547	-1.882873	-0.231238
125	6	0	8.569575	-2.255621	1.110394
126	6	0	8.517954	-3.597864	1.539028
127	6	0	8.347443	-4.586762	0.561268
128	6	0	8.250073	-4.276841	-0.798744
129	6	0	8.620403	-3.932467	3.012107
130	6	0	9.651248	-5.034413	3.277389
131	1	0	8.472968	-0.846298	-0.546984
132	1	0	8.286521	-5.631894	0.872705
133	1	0	8.995875	-3.010485	3.549786
134	1	0	10.643133	-4.730157	2.920510
135	1	0	9.401808	-5.974728	2.775205
136	1	0	9.732335	-5.244980	4.350518
137	1	0	2.368529	-7.653786	-1.550096
138	1	0	5.448274	-3.517058	-3.956133
139	1	0	7.654594	-1.742682	3.464050
140	1	0	2.918572	-4.219751	5.422415
141	1	0	2.692627	-6.668987	5.033684
142	1	0	0.630232	-8.466266	0.052385
143	1	0	7.697863	-3.229756	-3.052776
144	1	0	8.658629	-0.353322	1.727180
145	8	0	8.558108	0.186879	-3.011458
146	8	0	5.509960	-0.823117	-6.507504
147	6	0	7.833931	0.562621	-4.120350
148	6	0	6.998266	-0.346206	-4.772709
149	6	0	6.323272	0.109256	-5.912074
150	6	0	6.486891	1.417971	-6.417018

151	6	0	7.301128	2.297651	-5.693967
152	6	0	7.995628	1.898073	-4.546865
153	6	0	5.808713	1.823692	-7.708682
154	6	0	6.739004	2.623920	-8.626812
155	1	0	6.868225	-1.363978	-4.414148
156	1	0	7.405799	3.327167	-6.042223
157	1	0	5.548265	0.874068	-8.269516
158	1	0	7.051176	3.575673	-8.186161
159	1	0	6.242570	2.851213	-9.578353
160	1	0	7.648419	2.053750	-8.852560
161	8	0	1.054630	6.576362	-4.981450
162	8	0	3.788393	7.224067	-1.157563
163	6	0	2.291058	6.628186	-4.385368
164	6	0	2.422186	6.889469	-3.019343
165	6	0	3.722125	6.979949	-2.507094
166	6	0	4.868583	6.847708	-3.319212
167	6	0	4.674543	6.526804	-4.669623
168	6	0	3.400650	6.415853	-5.233736
169	6	0	6.247618	7.064956	-2.733665
170	6	0	7.160191	7.866632	-3.667735
171	1	0	1.555934	6.993952	-2.372003
172	1	0	5.548300	6.367311	-5.304821
173	1	0	6.125332	7.688870	-1.796305
174	1	0	7.357987	7.349461	-4.611889
175	1	0	8.128932	8.061913	-3.191884
176	1	0	6.708752	8.835368	-3.915532
177	8	0	3.377741	0.498216	-7.764459
178	8	0	0.823801	4.317542	-6.594824
179	6	0	3.296561	1.828845	-7.434273
180	6	0	2.066586	2.423364	-7.142721
181	6	0	2.064393	3.796663	-6.869882
182	6	0	3.239810	4.577415	-6.899201
183	6	0	4.450842	3.916472	-7.143287
184	6	0	4.512527	2.548127	-7.423028
185	6	0	3.169015	6.075206	-6.689597
186	6	0	4.108166	6.844617	-7.624940
187	1	0	1.145850	1.844886	-7.117104
188	1	0	5.378156	4.492860	-7.126082
189	1	0	2.118445	6.405475	-6.953655
190	1	0	3.892290	6.607908	-8.674068
191	1	0	5.163136	6.613602	-7.448250
192	1	0	3.983769	7.926641	-7.494500

193	8	0	6.137480	6.187045	-0.113857
194	8	0	8.338233	2.068811	-0.994964
195	6	0	6.743229	5.312396	-0.981069
196	6	0	7.231478	4.078356	-0.540536
197	6	0	7.887567	3.278102	-1.483190
198	6	0	8.091249	3.683286	-2.817020
199	6	0	7.530455	4.905331	-3.215129
200	6	0	6.858477	5.743295	-2.321855
201	6	0	8.900568	2.825331	-3.766981
202	6	0	9.806765	3.657496	-4.681036
203	1	0	7.090858	3.746214	0.482728
204	1	0	7.630189	5.216047	-4.257689
205	1	0	9.589494	2.181656	-3.140492
206	1	0	10.478655	4.293801	-4.092822
207	1	0	9.242838	4.310149	-5.354891
208	1	0	10.428115	3.004233	-5.306734
209	1	0	8.402714	-0.793183	-2.769241
210	1	0	4.904237	-0.405093	-7.215376
211	1	0	0.299839	6.722258	-4.311311
212	1	0	4.738514	7.142777	-0.795829
213	1	0	2.464149	0.046377	-7.752068
214	1	0	0.873763	5.274798	-6.247045
215	1	0	6.000376	5.779936	0.812333
216	1	0	8.620103	1.433157	-1.750686
217	8	0	-7.406803	0.491737	3.761883
218	8	0	-8.050051	-3.273892	0.792114
219	6	0	-7.475016	-0.860517	3.501004
220	6	0	-7.740938	-1.333530	2.214883
221	6	0	-7.771345	-2.718669	2.037274
222	6	0	-7.534835	-3.631797	3.086075
223	6	0	-7.272258	-3.104053	4.353645
224	6	0	-7.249211	-1.722911	4.594082
225	6	0	-7.553308	-5.117024	2.788334
226	6	0	-8.376619	-5.897513	3.817850
227	1	0	-7.904180	-0.651978	1.377875
228	1	0	-7.075918	-3.787621	5.181655
229	1	0	-8.072034	-5.263954	1.793034
230	1	0	-9.412200	-5.534725	3.838279
231	1	0	-7.980830	-5.807148	4.834014
232	1	0	-8.404329	-6.965162	3.567269
233	8	0	-0.677803	-7.163405	4.433050
234	8	0	-0.145411	-3.545488	7.461979

235	6	0	-1.194026	-6.250213	5.313017
236	6	0	-0.377030	-5.327145	5.969509
237	6	0	-0.999416	-4.431375	6.847224
238	6	0	-2.388769	-4.443818	7.089700
239	6	0	-3.163711	-5.374058	6.383151
240	6	0	-2.595506	-6.293885	5.499174
241	6	0	-2.994763	-3.488710	8.095572
242	6	0	-3.953874	-4.196667	9.057370
243	1	0	0.697356	-5.295362	5.805961
244	1	0	-4.245100	-5.383542	6.532986
245	1	0	-2.150153	-3.077218	8.730445
246	1	0	-3.439109	-5.005230	9.592248
247	1	0	-4.810797	-4.645869	8.545410
248	1	0	-4.345219	-3.498161	9.806599
249	8	0	-1.576900	-1.164388	7.620739
250	8	0	-5.120477	1.008904	5.335059
251	6	0	-2.856312	-1.157919	7.130609
252	6	0	-3.355041	-0.054288	6.431763
253	6	0	-4.693699	-0.104997	6.024104
254	6	0	-5.534379	-1.196046	6.317667
255	6	0	-4.962737	-2.301013	6.966131
256	6	0	-3.631573	-2.312332	7.387553
257	6	0	-7.005929	-1.141725	5.968298
258	6	0	-7.891760	-1.799345	7.032123
259	1	0	-2.732389	0.804310	6.197977
260	1	0	-5.586462	-3.177105	7.160799
261	1	0	-7.306599	-0.050726	5.938099
262	1	0	-7.713488	-2.875225	7.125846
263	1	0	-8.953130	-1.669738	6.783280
264	1	0	-7.723448	-1.349094	8.017574
265	8	0	-6.058466	-5.083370	0.252877
266	8	0	-2.225628	-6.984223	2.093004
267	6	0	-5.478592	-5.579992	1.388768
268	6	0	-4.170727	-6.048469	1.210809
269	6	0	-3.515470	-6.582923	2.325394
270	6	0	-4.135763	-6.680085	3.591416
271	6	0	-5.433712	-6.175032	3.718156
272	6	0	-6.136906	-5.629599	2.639293
273	6	0	-3.410024	-7.326487	4.750351
274	6	0	-4.340920	-8.106100	5.685181
275	1	0	-3.674151	-5.984203	0.246695
276	1	0	-5.920338	-6.218091	4.695847

277	1	0	-2.690542	-8.086174	4.316187
278	1	0	-4.903683	-8.866953	5.130533
279	1	0	-5.066221	-7.463692	6.193450
280	1	0	-3.762575	-8.621670	6.462445
281	1	0	-7.569045	1.054255	2.929594
282	1	0	-7.865898	-2.597521	0.083432
283	1	0	0.344720	-7.105765	4.363702
284	1	0	-0.652567	-2.802735	7.935675
285	1	0	-1.077499	-0.305394	7.402889
286	1	0	-6.046766	0.877223	4.918670
287	1	0	-6.947460	-4.599550	0.435458
288	1	0	-1.757922	-7.302697	2.941406
289	8	0	-4.940042	-6.093116	-2.257235
290	8	0	-6.939914	-2.209972	-4.320906
291	6	0	-5.191171	-5.285504	-3.340319
292	6	0	-5.926404	-4.104983	-3.203999
293	6	0	-6.156728	-3.359131	-4.362480
294	6	0	-5.647341	-3.723295	-5.625124
295	6	0	-4.898716	-4.903026	-5.700745
296	6	0	-4.673401	-5.715146	-4.582115
297	6	0	-5.928488	-2.832862	-6.817089
298	6	0	-6.290127	-3.636099	-8.070837
299	1	0	-6.309650	-3.780779	-2.235607
300	1	0	-4.483964	-5.205285	-6.664338
301	1	0	-6.839567	-2.208430	-6.568192
302	1	0	-6.526421	-2.967041	-8.907344
303	1	0	-7.171084	-4.263783	-7.887078
304	1	0	-5.481563	-4.297024	-8.398027
305	8	0	0.734809	-0.435073	-7.556784
306	8	0	2.577505	-4.425334	-6.018676
307	6	0	0.612211	-1.800982	-7.513860
308	6	0	1.616733	-2.453170	-6.792388
309	6	0	1.541531	-3.847961	-6.703279
310	6	0	0.492371	-4.590515	-7.291924
311	6	0	-0.483944	-3.883077	-8.001773
312	6	0	-0.437212	-2.492464	-8.154583
313	6	0	0.444439	-6.096085	-7.130842
314	6	0	-0.086600	-6.815626	-8.374126
315	1	0	2.405683	-1.895550	-6.296164
316	1	0	-1.307227	-4.435160	-8.460858
317	1	0	1.506945	-6.457693	-6.983620
318	1	0	-0.050925	-7.903565	-8.235674

319	1	0	0.520039	-6.571994	-9.254849
320	1	0	-1.123100	-6.551117	-8.605750
321	8	0	1.726189	-6.692377	-4.751052
322	8	0	-2.286327	-7.181997	-2.263858
323	6	0	0.356263	-6.685320	-4.672216
324	6	0	-0.297305	-6.917981	-3.459337
325	6	0	-1.696034	-6.966772	-3.485134
326	6	0	-2.436441	-6.822345	-4.677605
327	6	0	-1.731240	-6.521179	-5.850459
328	6	0	-0.336227	-6.444076	-5.880738
329	6	0	-3.934223	-7.031465	-4.666347
330	6	0	-4.408424	-7.883821	-5.849201
331	1	0	0.251691	-7.036613	-2.528726
332	1	0	-2.289826	-6.350818	-6.773072
333	1	0	-4.186907	-7.619255	-3.730114
334	1	0	-4.225831	-7.404066	-6.815615
335	1	0	-5.485878	-8.078463	-5.780116
336	1	0	-3.894060	-8.852505	-5.862770
337	8	0	-5.768757	-0.152399	-5.629455
338	8	0	-1.650451	0.790136	-7.779018
339	6	0	-4.768429	-0.596858	-6.452105
340	6	0	-3.736821	0.325629	-6.670531
341	6	0	-2.683617	-0.063826	-7.504746
342	6	0	-2.630715	-1.343351	-8.103606
343	6	0	-3.681865	-2.227588	-7.846752
344	6	0	-4.773632	-1.880487	-7.043016
345	6	0	-1.452087	-1.721819	-8.972508
346	6	0	-1.871936	-2.461822	-10.246133
347	1	0	-3.758955	1.302413	-6.198132
348	1	0	-3.650347	-3.224784	-8.292272
349	1	0	-0.957635	-0.760299	-9.310857
350	1	0	-2.561071	-1.848515	-10.840260
351	1	0	-2.378262	-3.409420	-10.037231
352	1	0	-1.000210	-2.686554	-10.872519
353	1	0	-5.361086	-5.737547	-1.404152
354	1	0	-6.983792	-1.866484	-3.384660
355	1	0	-0.088164	0.021119	-7.980660
356	1	0	2.404743	-5.406552	-5.790890
357	1	0	2.165415	-6.822790	-3.833846
358	1	0	-3.299456	-7.092892	-2.305885
359	1	0	-6.398756	-0.911814	-5.330511
360	1	0	-1.604680	1.596447	-7.095885

361	8	0	5.785460	4.791304	2.250557
362	8	0	1.731799	7.001791	2.862241
363	6	0	4.949900	5.404954	3.156300
364	6	0	3.762915	5.896010	2.604888
365	6	0	2.870945	6.538889	3.470858
366	6	0	3.135133	6.698556	4.850273
367	6	0	4.335017	6.175473	5.345642
368	6	0	5.275073	5.545102	4.522095
369	6	0	2.132554	7.409623	5.734744
370	6	0	2.767149	8.116575	6.935941
371	1	0	3.527446	5.753240	1.552977
372	1	0	4.551911	6.272133	6.412199
373	1	0	1.647988	8.219651	5.109805
374	1	0	2.007675	8.671931	7.501404
375	1	0	3.528716	8.835848	6.610622
376	1	0	3.243954	7.420989	7.633532
377	8	0	-0.559022	1.344873	6.896405
378	8	0	3.537550	-0.849865	6.570255
379	6	0	0.786309	1.374346	7.229316
380	6	0	1.522437	0.295525	6.733882
381	6	0	2.890372	0.259131	7.035889
382	6	0	3.526225	1.278150	7.785071
383	6	0	2.735122	2.331584	8.249503
384	6	0	1.353759	2.393112	8.016300
385	6	0	5.018556	1.210829	8.037548
386	6	0	5.461368	1.928681	9.315432
387	1	0	1.062646	-0.473803	6.118469
388	1	0	3.205856	3.133589	8.823971
389	1	0	5.289377	0.121176	8.176188
390	1	0	6.539159	1.794094	9.476766
391	1	0	4.943248	1.525405	10.193744
392	1	0	5.274185	3.006592	9.282828
393	8	0	-0.393684	7.487122	4.621206
394	8	0	-1.915839	3.685332	7.180775
395	6	0	-0.221169	6.491483	5.548581
396	6	0	-1.243576	5.584963	5.849401
397	6	0	-0.978611	4.628014	6.833834
398	6	0	0.260170	4.551334	7.503136
399	6	0	1.263339	5.455445	7.131252
400	6	0	1.051140	6.438272	6.160738
401	6	0	0.480092	3.499003	8.567876
402	6	0	1.009251	4.108339	9.869073

403	1	0	-2.204267	5.631156	5.343917
404	1	0	2.243023	5.383880	7.608994
405	1	0	-0.524632	3.040244	8.817238
406	1	0	1.970059	4.616500	9.738355
407	1	0	1.141179	3.339542	10.639897
408	1	0	0.303257	4.852635	10.260411
409	8	0	6.252162	-0.513302	6.268251
410	8	0	7.652171	3.069113	3.350074
411	6	0	6.348416	0.812437	5.921371
412	6	0	6.993958	1.215352	4.748489
413	6	0	7.048803	2.588375	4.490089
414	6	0	6.493422	3.550343	5.360558
415	6	0	5.834287	3.087747	6.506109
416	6	0	5.751149	1.726636	6.816380
417	6	0	6.600942	5.025049	5.035824
418	6	0	7.149825	5.827949	6.219383
419	1	0	7.417452	0.489243	4.060682
420	1	0	5.362841	3.812759	7.172931
421	1	0	7.353533	5.139983	4.198064
422	1	0	6.513089	5.761170	7.107140
423	1	0	7.250094	6.889171	5.961589
424	1	0	8.143392	5.460577	6.506962
425	1	0	6.609793	4.377581	2.693246
426	1	0	1.085062	7.441812	3.515016
427	1	0	-1.080376	2.123217	7.326978
428	1	0	4.554486	-0.813917	6.689985
429	1	0	-1.319547	7.460193	4.192039
430	1	0	-2.766288	3.723845	6.578214
431	1	0	6.601181	-1.134311	5.527225
432	1	0	7.927768	2.313454	2.707537
433	8	0	-1.192445	2.408146	-5.800052
434	1	0	-1.932383	3.003447	-5.560948
435	1	0	-0.437931	2.998634	-6.021971
436	8	0	8.260679	1.337801	1.322441
437	1	0	8.989714	1.774551	0.829280
438	1	0	7.504943	1.365097	0.692285
439	8	0	-0.977348	-8.457293	-0.082049
440	1	0	-1.263319	-8.233557	-0.986493
441	1	0	-1.450210	-7.839818	0.503870
442	8	0	1.947330	-3.002172	5.564348
443	1	0	2.478061	-2.227086	5.832315
444	1	0	1.309040	-3.158173	6.291835

445	8	0	4.352563	-2.654143	-4.603193
446	1	0	4.760402	-2.037208	-5.248046
447	1	0	3.761925	-3.238382	-5.123980
448	8	0	-1.748501	2.187753	4.396087
449	1	0	-1.175652	2.966183	4.394274
450	1	0	-1.265047	1.536574	4.929739
451	8	0	1.749745	8.391965	0.416174
452	1	0	1.941393	7.771365	1.149194
453	1	0	2.364132	8.147269	-0.306941
454	8	0	-3.886240	3.204999	5.485103
455	1	0	-3.397050	2.542068	4.905297
456	1	0	-4.567568	2.668126	5.950032
457	6	0	-3.060015	-1.229279	0.603242
458	6	0	-2.179440	-2.333491	0.608493
459	6	0	-2.219764	-3.252372	1.648419
460	6	0	-3.151454	-3.096665	2.677173
461	6	0	-4.040036	-2.015434	2.676183
462	6	0	-3.989306	-1.079322	1.657523
463	6	0	-3.015558	-0.258925	-0.467466
464	6	0	-2.679675	-0.669275	-1.806810
465	6	0	-3.304145	1.132310	-0.190343
466	6	0	-3.955846	1.927491	-1.160722
467	6	0	-4.215904	3.263101	-0.901696
468	6	0	-3.803640	3.832656	0.307753
469	6	0	-3.161282	3.057661	1.276798
470	6	0	-2.922690	1.710840	1.040138
471	6	0	-1.983605	0.208701	-2.671349
472	6	0	-1.645489	-0.194723	-3.954192
473	6	0	-2.015044	-1.466556	-4.400887
474	6	0	-2.724216	-2.338186	-3.565988
475	6	0	-3.043160	-1.954878	-2.274953
476	1	0	-1.438886	-2.433379	-0.183703
477	1	0	-1.527045	-4.093274	1.661955
478	1	0	-3.191668	-3.830298	3.483504
479	1	0	-4.778257	-1.918741	3.470540
480	1	0	-4.709423	-0.268028	1.615128
481	1	0	-4.311060	1.460477	-2.075530
482	1	0	-4.741958	3.868436	-1.639141
483	1	0	-3.994175	4.890304	0.499530
484	1	0	-2.835831	3.506094	2.211778
485	1	0	-2.396141	1.116661	1.784656
486	1	0	-1.670667	1.184889	-2.305486

487	1	0	-1.092031	0.482287	-4.609975
488	1	0	-1.756218	-1.780057	-5.413691
489	1	0	-3.033116	-3.314905	-3.936080
490	1	0	-3.642150	-2.600409	-1.638872
491	53	0	-6.573172	-0.954955	-1.198683

$TrBF_4@C_M$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.629383	-7.712915	-0.651759
2	8	0	-0.165513	-7.861101	3.402461
3	6	0	-2.645409	-7.754237	0.722587
4	6	0	-1.385300	-7.804369	1.328969
5	6	0	-1.343690	-7.801803	2.729173
6	6	0	-2.521555	-7.713433	3.515215
7	6	0	-3.750795	-7.683763	2.853844
8	6	0	-3.847970	-7.729178	1.456188
9	6	0	-2.410438	-7.664571	5.024191
10	6	0	-3.420018	-8.588484	5.712435
11	1	0	-0.478800	-7.837787	0.731129
12	1	0	-4.667859	-7.627049	3.444832
13	1	0	-1.382685	-8.056264	5.298915
14	1	0	-3.284068	-9.625820	5.380828
15	1	0	-4.458404	-8.313779	5.502697
16	1	0	-3.288876	-8.568679	6.801466
17	8	0	-4.737150	-0.891586	6.363744
18	8	0	-6.439547	-1.066903	1.846674
19	6	0	-5.326268	-1.547772	5.308182
20	6	0	-5.613407	-0.873289	4.117500
21	6	0	-6.249540	-1.604974	3.111635
22	6	0	-6.678696	-2.937393	3.296496
23	6	0	-6.282309	-3.587441	4.469296
24	6	0	-5.577457	-2.925673	5.481935
25	6	0	-7.602007	-3.562562	2.277244
26	6	0	-8.703849	-4.408072	2.924180
27	1	0	-5.395527	0.189683	4.006550
28	1	0	-6.542793	-4.638374	4.607775
29	1	0	-8.127559	-2.703495	1.749429
30	1	0	-8.312456	-5.274139	3.465569

31	1	0	-9.404194	-4.782933	2.168039
32	1	0	-9.281817	-3.806993	3.639606
33	8	0	-0.071925	-5.955251	5.352237
34	8	0	-2.480423	-2.356374	7.069360
35	6	0	-1.313709	-5.479574	5.681696
36	6	0	-1.312182	-4.178526	6.199864
37	6	0	-2.547062	-3.623763	6.549827
38	6	0	-3.764469	-4.320290	6.376514
39	6	0	-3.705380	-5.619172	5.859323
40	6	0	-2.494681	-6.235595	5.520336
41	6	0	-5.072806	-3.636310	6.718970
42	6	0	-6.108620	-4.583159	7.327999
43	1	0	-0.387263	-3.621919	6.324067
44	1	0	-4.636547	-6.173801	5.720543
45	1	0	-4.855925	-2.849105	7.504515
46	1	0	-6.406485	-5.383569	6.643513
47	1	0	-7.019832	-4.034130	7.600519
48	1	0	-5.720417	-5.055379	8.238710
49	8	0	-7.040787	-2.504096	-0.362193
50	8	0	-4.870331	-6.496925	-1.742822
51	6	0	-6.613736	-3.770662	-0.037995
52	6	0	-5.959604	-4.458342	-1.065783
53	6	0	-5.508883	-5.752237	-0.780895
54	6	0	-5.680779	-6.361074	0.481074
55	6	0	-6.334143	-5.622572	1.473500
56	6	0	-6.831636	-4.337603	1.234404
57	6	0	-5.173091	-7.764964	0.725954
58	6	0	-6.211223	-8.642887	1.431656
59	1	0	-5.809709	-3.996950	-2.037006
60	1	0	-6.467783	-6.065548	2.462852
61	1	0	-4.989630	-8.239999	-0.286697
62	1	0	-7.135130	-8.702229	0.842626
63	1	0	-6.482697	-8.264260	2.422155
64	1	0	-5.834256	-9.664554	1.564112
65	1	0	-3.563227	-7.585070	-1.049727
66	1	0	0.686339	-7.950171	2.765338
67	1	0	-4.782362	0.118396	6.249208
68	1	0	-6.466686	-0.072154	1.874071
69	1	0	-0.102211	-6.875235	4.900906
70	1	0	-3.402602	-1.938068	7.193543
71	1	0	-7.321379	-1.974262	0.478868
72	1	0	-4.725754	-5.955287	-2.607543

73	8	0	2.502009	7.249020	-0.426207
74	8	0	6.398870	5.169379	1.265034
75	6	0	3.845872	6.999887	-0.594488
76	6	0	4.407711	6.193189	0.400942
77	6	0	5.770094	5.893004	0.295514
78	6	0	6.555698	6.344979	-0.793349
79	6	0	5.941018	7.153147	-1.752396
80	6	0	4.594485	7.531666	-1.662834
81	6	0	8.001737	5.915081	-0.888578
82	6	0	8.908806	6.957037	-1.549534
83	1	0	3.795083	5.791731	1.204607
84	1	0	6.532000	7.510920	-2.598473
85	1	0	8.380435	5.785627	0.171142
86	1	0	8.637086	7.152791	-2.591652
87	1	0	9.953567	6.622884	-1.543263
88	1	0	8.860977	7.911846	-1.011544
89	8	0	6.221853	0.731775	-5.118336
90	8	0	2.613257	3.225376	-6.898993
91	6	0	5.752645	1.963297	-5.528855
92	6	0	4.422324	1.954524	-5.961815
93	6	0	3.885103	3.164882	-6.414956
94	6	0	4.640667	4.364784	-6.422745
95	6	0	5.958708	4.311793	-5.967490
96	6	0	6.557796	3.117001	-5.539457
97	6	0	3.986012	5.642498	-6.899497
98	6	0	4.959443	6.603478	-7.589254
99	1	0	3.830997	1.045065	-5.918915
100	1	0	6.549827	5.230349	-5.951985
101	1	0	3.218212	5.348639	-7.679335
102	1	0	4.426776	7.482725	-7.973273
103	1	0	5.455328	6.116963	-8.437416
104	1	0	5.739285	6.969698	-6.914219
105	8	0	1.110591	5.485254	-6.571939
106	8	0	1.175017	8.171122	-2.651670
107	6	0	1.851337	6.204649	-5.659717
108	6	0	1.106295	6.829851	-4.653668
109	6	0	1.816317	7.556266	-3.693427
110	6	0	3.225675	7.678599	-3.726840
111	6	0	3.915646	7.037422	-4.759100
112	6	0	3.252566	6.308404	-5.754656
113	6	0	3.939489	8.470559	-2.652828
114	6	0	4.910415	9.494422	-3.250692

115	1	0	0.023019	6.753032	-4.626754
116	1	0	5.004959	7.103305	-4.788775
117	1	0	3.160731	9.065729	-2.087028
118	1	0	5.695654	9.028770	-3.854180
119	1	0	5.399020	10.078450	-2.461898
120	1	0	4.374856	10.196408	-3.902495
121	8	0	8.331242	3.431520	0.554999
122	8	0	8.415170	0.838500	-3.431762
123	6	0	8.255826	3.396742	-0.814890
124	6	0	8.383610	2.126804	-1.390478
125	6	0	8.305719	2.052272	-2.784214
126	6	0	8.107565	3.184644	-3.600893
127	6	0	7.990793	4.429500	-2.969007
128	6	0	8.086857	4.569315	-1.580905
129	6	0	8.005242	3.033742	-5.104029
130	6	0	8.914656	4.022681	-5.840316
131	1	0	8.526134	1.247681	-0.772731
132	1	0	7.816181	5.317618	-3.580450
133	1	0	8.378125	1.999333	-5.371940
134	1	0	9.961666	3.878831	-5.545503
135	1	0	8.660308	5.066486	-5.629705
136	1	0	8.850821	3.880195	-6.925781
137	1	0	2.096405	7.801571	-1.189806
138	1	0	5.714351	4.773340	1.984458
139	1	0	7.164099	0.783703	-4.726675
140	1	0	2.061348	2.340172	-6.701941
141	1	0	1.685572	4.795153	-7.062032
142	1	0	0.137566	7.993329	-2.650590
143	1	0	7.898515	4.282076	0.941281
144	1	0	8.427745	0.054811	-2.778662
145	8	0	8.817418	1.036713	1.869467
146	8	0	6.185986	3.083148	5.250186
147	6	0	8.258021	1.028328	3.126883
148	6	0	7.470359	2.093358	3.569047
149	6	0	6.960249	2.014110	4.870870
150	6	0	7.239379	0.928484	5.729570
151	6	0	7.999805	-0.128921	5.216421
152	6	0	8.531784	-0.104715	3.922690
153	6	0	6.734567	0.939355	7.157124
154	6	0	7.806451	0.488450	8.155054
155	1	0	7.254013	2.948529	2.934520
156	1	0	8.191630	-0.997415	5.849729

157	1	0	6.483588	2.012243	7.422492
158	1	0	8.124728	-0.546202	7.994620
159	1	0	7.433338	0.560521	9.184169
160	1	0	8.699794	1.120471	8.078956
161	8	0	1.984015	-4.625266	6.793316
162	8	0	4.276130	-6.451590	3.057706
163	6	0	3.138125	-4.830468	6.074296
164	6	0	3.123089	-5.557220	4.881248
165	6	0	4.350118	-5.750446	4.235400
166	6	0	5.568835	-5.274477	4.766046
167	6	0	5.513346	-4.503212	5.934167
168	6	0	4.314969	-4.268375	6.615191
169	6	0	6.880056	-5.619661	4.092857
170	6	0	7.950714	-6.054236	5.099495
171	1	0	2.198566	-5.941977	4.459864
172	1	0	6.437830	-4.080069	6.332188
173	1	0	6.694085	-6.512707	3.420668
174	1	0	8.214495	-5.260317	5.805175
175	1	0	8.871059	-6.354541	4.584034
176	1	0	7.604047	-6.911492	5.689987
177	8	0	4.256480	2.165170	7.061299
178	8	0	1.804983	-1.874429	7.464565
179	6	0	4.212119	0.798804	7.185716
180	6	0	2.992608	0.119000	7.238518
181	6	0	3.037295	-1.268161	7.425251
182	6	0	4.249507	-1.973876	7.580073
183	6	0	5.441905	-1.247583	7.460823
184	6	0	5.457764	0.137195	7.271683
185	6	0	4.237146	-3.455695	7.888841
186	6	0	5.321295	-3.856859	8.895506
187	1	0	2.045058	0.641436	7.134080
188	1	0	6.392535	-1.780485	7.531267
189	1	0	3.244962	-3.689111	8.382877
190	1	0	5.224644	-3.279888	9.823355
191	1	0	6.333781	-3.695600	8.513012
192	1	0	5.235470	-4.919757	9.153273
193	8	0	6.350176	-5.605905	1.383583
194	8	0	8.412423	-1.395045	0.605763
195	6	0	7.016655	-4.495719	1.834878
196	6	0	7.367326	-3.457041	0.966350
197	6	0	8.097744	-2.392224	1.506378
198	6	0	8.502196	-2.351571	2.855270

199	6	0	8.075247	-3.393809	3.690753
200	6	0	7.340757	-4.480543	3.210633
201	6	0	9.378573	-1.225038	3.361290
202	6	0	10.437588	-1.706674	4.359155
203	1	0	7.068953	-3.465557	-0.076879
204	1	0	8.335619	-3.359008	4.751115
205	1	0	9.946414	-0.811568	2.473630
206	1	0	11.062267	-2.492905	3.918738
207	1	0	10.000487	-2.110407	5.277819
208	1	0	11.097688	-0.879702	4.650309
209	1	0	8.592251	1.891936	1.356138
210	1	0	5.689330	2.901744	6.123431
211	1	0	1.192297	-5.110441	6.383126
212	1	0	5.156036	-6.430811	2.543735
213	1	0	3.325355	2.575837	7.014256
214	1	0	1.873318	-2.889803	7.473497
215	1	0	6.087632	-5.526806	0.400458
216	1	0	8.753487	-0.548823	1.076454
217	8	0	-8.073415	-2.065693	-2.948413
218	8	0	-8.604188	2.264671	-0.861206
219	6	0	-8.157576	-0.686404	-2.996210
220	6	0	-8.365906	0.054009	-1.830551
221	6	0	-8.389990	1.445683	-1.954499
222	6	0	-8.188725	2.104920	-3.189384
223	6	0	-7.999299	1.312889	-4.323405
224	6	0	-8.000078	-0.089607	-4.261909
225	6	0	-8.195920	3.619013	-3.220570
226	6	0	-9.124522	4.160785	-4.312827
227	1	0	-8.506427	-0.433139	-0.869483
228	1	0	-7.846951	1.797572	-5.289464
229	1	0	-8.621399	3.983048	-2.236034
230	1	0	-10.153865	3.817006	-4.148691
231	1	0	-8.831035	3.840799	-5.316909
232	1	0	-9.136995	5.257710	-4.305490
233	8	0	-1.530416	5.194385	-5.919222
234	8	0	-1.138057	0.944582	-7.996271
235	6	0	-2.091027	4.089704	-6.499104
236	6	0	-1.302217	3.039351	-6.974114
237	6	0	-1.964497	1.951839	-7.554810
238	6	0	-3.367401	1.899109	-7.686655
239	6	0	-4.112031	2.965889	-7.162501
240	6	0	-3.504361	4.075183	-6.571676

241	6	0	-4.018910	0.732117	-8.395681
242	6	0	-5.041114	1.190088	-9.440387
243	1	0	-0.217778	3.054696	-6.889844
244	1	0	-5.201136	2.931247	-7.226316
245	1	0	-3.208528	0.176865	-8.962230
246	1	0	-4.566469	1.841187	-10.186087
247	1	0	-5.868889	1.756870	-9.002591
248	1	0	-5.471023	0.333103	-9.972381
249	8	0	-2.568376	-1.440757	-7.484736
250	8	0	-5.932995	-2.925059	-4.485420
251	6	0	-3.810160	-1.314027	-6.925604
252	6	0	-4.261524	-2.212882	-5.953306
253	6	0	-5.565627	-2.037915	-5.471683
254	6	0	-6.420654	-1.026320	-5.948816
255	6	0	-5.896486	-0.120341	-6.882964
256	6	0	-4.600419	-0.235677	-7.388060
257	6	0	-7.860877	-0.962903	-5.487683
258	6	0	-8.821649	-0.536070	-6.602588
259	1	0	-3.641816	-3.033810	-5.606461
260	1	0	-6.530890	0.697174	-7.236047
261	1	0	-8.164480	-2.014380	-5.194589
262	1	0	-8.645916	0.489095	-6.943730
263	1	0	-9.861701	-0.583412	-6.253542
264	1	0	-8.733089	-1.195351	-7.474164
265	8	0	-6.512831	4.301976	-0.891071
266	8	0	-2.893214	5.655327	-3.477430
267	6	0	-6.034900	4.448898	-2.167243
268	6	0	-4.730360	4.956269	-2.229248
269	6	0	-4.176211	5.180632	-3.494566
270	6	0	-4.892637	4.922465	-4.686730
271	6	0	-6.177372	4.385321	-4.566643
272	6	0	-6.783118	4.148862	-3.326755
273	6	0	-4.283447	5.254617	-6.031039
274	6	0	-5.312723	5.769225	-7.043536
275	1	0	-4.161762	5.165098	-1.326694
276	1	0	-6.737952	4.156221	-5.476381
277	1	0	-3.551065	6.103776	-5.866874
278	1	0	-5.845740	6.642836	-6.648544
279	1	0	-6.061734	5.016506	-7.306521
280	1	0	-4.817886	6.075351	-7.974038
281	1	0	-8.010566	-2.401248	-1.991334
282	1	0	-8.791579	1.725115	-0.047061

283	1	0	-0.505284	5.189649	-5.983109
284	1	0	-1.660129	0.109450	-8.240417
285	1	0	-2.048574	-2.231602	-7.104895
286	1	0	-6.881956	-2.746469	-4.131067
287	1	0	-7.370514	3.753408	-0.846579
288	1	0	-2.496321	5.736794	-4.412110
289	8	0	-5.211295	6.511383	0.749157
290	8	0	-6.902899	3.682717	4.292471
291	6	0	-5.297509	6.126989	2.067053
292	6	0	-6.101743	5.049088	2.449551
293	6	0	-6.113012	4.709907	3.804426
294	6	0	-5.303805	5.359531	4.762165
295	6	0	-4.528690	6.438717	4.327665
296	6	0	-4.535650	6.869970	2.994236
297	6	0	-5.334249	4.876809	6.196591
298	6	0	-5.558387	6.031608	7.179355
299	1	0	-6.699043	4.504255	1.719203
300	1	0	-3.906285	6.968923	5.050750
301	1	0	-6.226579	4.188985	6.311869
302	1	0	-5.605761	5.664051	8.211438
303	1	0	-6.507944	6.538733	6.964188
304	1	0	-4.769549	6.788173	7.131459
305	8	0	1.572484	2.960760	6.894700
306	8	0	3.005674	6.318180	3.999973
307	6	0	1.354791	4.235081	6.432038
308	6	0	2.255462	4.663264	5.452713
309	6	0	2.067210	5.946349	4.925361
310	6	0	1.006840	6.787465	5.334218
311	6	0	0.142699	6.307225	6.324201
312	6	0	0.307374	5.048089	6.912697
313	6	0	0.822599	8.147964	4.693700
314	6	0	0.355888	9.217020	5.685901
315	1	0	3.048289	4.014377	5.092832
316	1	0	-0.685754	6.937902	6.654484
317	1	0	1.833534	8.486583	4.312871
318	1	0	0.287893	10.196516	5.196154
319	1	0	1.062549	9.310086	6.519679
320	1	0	-0.627677	8.997418	6.113069
321	8	0	1.828450	7.899845	2.134251
322	8	0	-2.426273	7.417564	0.079965
323	6	0	0.461786	7.830794	2.211824
324	6	0	-0.317232	7.606880	1.073012

325	6	0	-1.707172	7.644319	1.232330
326	6	0	-2.319474	7.924844	2.471070
327	6	0	-1.490184	8.063835	3.592861
328	6	0	-0.097189	8.020591	3.496935
329	6	0	-3.816588	8.119374	2.541086
330	6	0	-4.201456	9.329283	3.402297
331	1	0	0.131633	7.390084	0.106685
332	1	0	-1.948390	8.225501	4.570730
333	1	0	-4.173986	8.351469	1.490044
334	1	0	-3.935150	9.198394	4.455503
335	1	0	-5.283934	9.504460	3.361903
336	1	0	-3.702127	10.238321	3.046634
337	8	0	-5.079004	1.966547	5.682334
338	8	0	-0.748260	1.792810	7.549047
339	6	0	-4.058903	2.676605	6.255780
340	6	0	-2.947144	1.883355	6.581122
341	6	0	-1.847860	2.509570	7.174420
342	6	0	-1.824520	3.903155	7.419951
343	6	0	-2.953083	4.646760	7.069788
344	6	0	-4.096688	4.063403	6.506963
345	6	0	-0.590129	4.537841	8.020142
346	6	0	-0.917254	5.616003	9.057192
347	1	0	-2.948028	0.817444	6.368634
348	1	0	-2.945862	5.725436	7.246661
349	1	0	-0.026468	3.723984	8.571526
350	1	0	-1.525895	5.200640	9.870132
351	1	0	-1.472964	6.457577	8.631560
352	1	0	0.000238	6.021733	9.500664
353	1	0	-5.765184	5.913584	0.148470
354	1	0	-7.555429	3.376953	3.608487
355	1	0	0.812669	2.633467	7.506847
356	1	0	2.733684	7.153736	3.477650
357	1	0	2.175940	7.700996	1.188378
358	1	0	-3.423478	7.334509	0.263518
359	1	0	-5.863845	2.542205	5.374525
360	1	0	-0.740526	0.813373	7.141997
361	8	0	5.707173	-5.088043	-1.259167
362	8	0	1.822465	-7.595764	-0.687845
363	6	0	4.847681	-5.999900	-1.829314
364	6	0	3.765829	-6.357054	-1.018724
365	6	0	2.852019	-7.281060	-1.538175
366	6	0	2.993825	-7.843043	-2.827935

367	6	0	4.093273	-7.441071	-3.594299
368	6	0	5.053242	-6.541911	-3.115240
369	6	0	1.970008	-8.834096	-3.340029
370	6	0	2.542374	-9.849606	-4.333405
371	1	0	3.621363	-5.909182	-0.039198
372	1	0	4.213887	-7.851824	-4.599644
373	1	0	1.605445	-9.431840	-2.450792
374	1	0	1.777461	-10.583948	-4.617093
375	1	0	3.382028	-10.400072	-3.891794
376	1	0	2.899990	-9.383454	-5.256801
377	8	0	-1.297107	-3.501011	-6.077068
378	8	0	2.648321	-1.164328	-6.925646
379	6	0	0.015205	-3.590201	-6.511622
380	6	0	0.707293	-2.375810	-6.495639
381	6	0	2.041846	-2.390786	-6.921436
382	6	0	2.690236	-3.577580	-7.336627
383	6	0	1.944865	-4.759027	-7.330348
384	6	0	0.594383	-4.794044	-6.956056
385	6	0	4.146442	-3.542487	-7.751886
386	6	0	4.517191	-4.613769	-8.781440
387	1	0	0.236555	-1.460506	-6.148462
388	1	0	2.427699	-5.689928	-7.639122
389	1	0	4.331660	-2.544664	-8.252437
390	1	0	5.563786	-4.500244	-9.093292
391	1	0	3.893564	-4.529222	-9.679485
392	1	0	4.406419	-5.631094	-8.393179
393	8	0	-0.422564	-8.666408	-1.981574
394	8	0	-2.448848	-5.906028	-5.399062
395	6	0	-0.415264	-8.000040	-3.182608
396	6	0	-1.528832	-7.280419	-3.630374
397	6	0	-1.420167	-6.655017	-4.875951
398	6	0	-0.258524	-6.737208	-5.671845
399	6	0	0.837767	-7.440136	-5.157974
400	6	0	0.786759	-8.086078	-3.918902
401	6	0	-0.228803	-6.061934	-7.025527
402	6	0	0.226444	-7.024008	-8.127495
403	1	0	-2.428855	-7.204408	-3.028674
404	1	0	1.761656	-7.478756	-5.738895
405	1	0	-1.287659	-5.760337	-7.288063
406	1	0	1.234786	-7.414980	-7.957835
407	1	0	0.220987	-6.532003	-9.107487
408	1	0	-0.447620	-7.888505	-8.186117

409	8	0	5.412658	-1.303469	-6.754325
410	8	0	7.338579	-3.721408	-3.047123
411	6	0	5.634134	-2.446139	-6.025176
412	6	0	6.416324	-2.431980	-4.866433
413	6	0	6.594512	-3.649327	-4.202312
414	6	0	6.027541	-4.857514	-4.661142
415	6	0	5.228063	-4.806449	-5.809584
416	6	0	5.019936	-3.618109	-6.517273
417	6	0	6.278990	-6.148339	-3.911520
418	6	0	6.776570	-7.256847	-4.844796
419	1	0	6.850191	-1.509512	-4.491100
420	1	0	4.747140	-5.722404	-6.159105
421	1	0	7.113432	-5.959680	-3.170076
422	1	0	6.056828	-7.500739	-5.632493
423	1	0	6.982451	-8.177819	-4.286171
424	1	0	7.707473	-6.954009	-5.341209
425	1	0	6.452622	-4.797855	-1.895574
426	1	0	1.136197	-8.216767	-1.114143
427	1	0	-1.759179	-4.421349	-6.066639
428	1	0	3.655121	-1.209882	-7.105439
429	1	0	-1.292810	-8.536373	-1.469411
430	1	0	-3.233894	-5.783395	-4.739655
431	1	0	5.818569	-0.474637	-6.305790
432	1	0	7.640291	-2.791956	-2.720478
433	8	0	-0.441828	-0.485213	6.298851
434	1	0	-1.093064	-1.179948	6.535104
435	1	0	0.427923	-0.844235	6.584737
436	8	0	8.097921	-1.415585	-1.800639
437	1	0	8.878335	-1.689961	-1.269955
438	1	0	7.409191	-1.230649	-1.122168
439	8	0	-1.440834	7.898985	-2.317378
440	1	0	-1.634110	8.288988	-1.446981
441	1	0	-1.841048	7.011142	-2.295865
442	8	0	1.171878	1.115502	-6.292542
443	1	0	1.741154	0.321845	-6.246638
444	1	0	0.515512	0.933840	-6.997468
445	8	0	4.727911	4.210763	3.032188
446	1	0	5.228949	3.838158	3.788391
447	1	0	4.192092	4.946262	3.396864
448	8	0	-2.737881	-2.771593	-3.299262
449	1	0	-1.997190	-2.816707	-3.923105
450	1	0	-3.132934	-1.897410	-3.434311

451	8	0	2.095628	-8.092873	2.124258
452	1	0	2.133757	-7.765629	1.203930
453	1	0	2.760363	-7.575835	2.621401
454	8	0	-4.331237	-4.892707	-3.870623
455	1	0	-3.894054	-4.045233	-3.548785
456	1	0	-5.098740	-4.598037	-4.405319
457	6	0	-3.685111	0.090165	-0.427221
458	6	0	-3.272551	1.295634	-1.037761
459	6	0	-3.710430	1.619211	-2.314754
460	6	0	-4.569331	0.753007	-2.993750
461	6	0	-4.998247	-0.435976	-2.391777
462	6	0	-4.563721	-0.769977	-1.120052
463	6	0	-3.150577	-0.291128	0.863606
464	6	0	-2.817499	0.723350	1.832678
465	6	0	-2.917477	-1.681952	1.158145
466	6	0	-3.019696	-2.146016	2.491045
467	6	0	-2.813143	-3.482783	2.781292
468	6	0	-2.465831	-4.368940	1.757789
469	6	0	-2.343487	-3.926366	0.437872
470	6	0	-2.576744	-2.594897	0.131973
471	6	0	-1.692439	0.551286	2.674954
472	6	0	-1.320740	1.554902	3.556148
473	6	0	-2.075712	2.728447	3.626439
474	6	0	-3.209167	2.898054	2.822440
475	6	0	-3.576242	1.914879	1.920421
476	1	0	-2.565718	1.944498	-0.523814
477	1	0	-3.375657	2.542776	-2.786643
478	1	0	-4.917415	1.007945	-3.995234
479	1	0	-5.681543	-1.099255	-2.918375
480	1	0	-4.942917	-1.661191	-0.625425
481	1	0	-3.319016	-1.453499	3.274729
482	1	0	-2.925526	-3.844121	3.802699
483	1	0	-2.288815	-5.417401	1.995806
484	1	0	-2.055643	-4.621594	-0.347800
485	1	0	-2.449860	-2.250665	-0.891870
486	1	0	-1.085963	-0.348432	2.585534
487	1	0	-0.440880	1.425945	4.187119
488	1	0	-1.785774	3.516708	4.322338
489	1	0	-3.801328	3.805719	2.906173
490	1	0	-4.478119	2.027329	1.325423
491	9	0	-9.055275	0.782697	1.400772
492	5	0	-8.243846	1.485215	2.314746

493	9	0	-8.189021	0.856181	3.543619
494	9	0	-6.920758	1.550753	1.750490
495	9	0	-8.712695	2.807316	2.438506

TS-*endo*@C_M

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.801264	2.509471	4.927381
2	8	0	-4.501569	6.526397	2.762907
3	6	0	-6.123120	3.515349	4.046348
4	6	0	-5.132567	4.491316	3.883582
5	6	0	-5.387656	5.512880	2.962211
6	6	0	-6.571008	5.545841	2.181512
7	6	0	-7.531733	4.559237	2.406351
8	6	0	-7.353686	3.549357	3.363020
9	6	0	-6.743670	6.628939	1.138698
10	6	0	-8.149915	7.235876	1.150550
11	1	0	-4.205879	4.446405	4.447580
12	1	0	-8.455709	4.576553	1.824065
13	1	0	-6.031638	7.470136	1.401239
14	1	0	-8.378732	7.662025	2.135544
15	1	0	-8.929770	6.501759	0.924924
16	1	0	-8.233980	8.041959	0.411520
17	8	0	-6.403720	2.629630	-4.893009
18	8	0	-7.809550	-1.232566	-2.373881
19	6	0	-7.106630	2.038504	-3.869756
20	6	0	-7.036087	0.660888	-3.654558
21	6	0	-7.822636	0.132747	-2.627470
22	6	0	-8.658371	0.927988	-1.816473
23	6	0	-8.652707	2.309352	-2.045466
24	6	0	-7.891697	2.893957	-3.064533
25	6	0	-9.510336	0.265768	-0.755733
26	6	0	-10.921615	0.859095	-0.687713
27	1	0	-6.389939	0.016988	-4.253123
28	1	0	-9.264005	2.952139	-1.409199
29	1	0	-9.636581	-0.819198	-1.056917
30	1	0	-10.922591	1.919158	-0.416492
31	1	0	-11.532130	0.329420	0.053735
32	1	0	-11.425383	0.770063	-1.658597

33	8	0	-4.016318	6.782794	0.110273
34	8	0	-5.072398	4.861985	-4.001637
35	6	0	-5.007798	6.230064	-0.662769
36	6	0	-4.582900	5.813169	-1.929441
37	6	0	-5.539693	5.226124	-2.764085
38	6	0	-6.884029	5.044868	-2.368539
39	6	0	-7.249297	5.481221	-1.090638
40	6	0	-6.341780	6.102232	-0.223290
41	6	0	-7.867686	4.386717	-3.314054
42	6	0	-9.263036	5.014984	-3.254683
43	1	0	-3.550081	5.925296	-2.242063
44	1	0	-8.281282	5.340881	-0.760712
45	1	0	-7.489165	4.550201	-4.369037
46	1	0	-9.736815	4.901447	-2.274597
47	1	0	-9.928124	4.549072	-3.993033
48	1	0	-9.218463	6.088039	-3.476810
49	8	0	-7.815284	-1.913951	0.211609
50	8	0	-7.089143	0.194802	4.388847
51	6	0	-8.040320	-0.824470	1.004580
52	6	0	-7.441255	-0.891880	2.269734
53	6	0	-7.616046	0.199960	3.123913
54	6	0	-8.330482	1.356327	2.737174
55	6	0	-8.913493	1.367318	1.465934
56	6	0	-8.811094	0.283405	0.587113
57	6	0	-8.427722	2.531034	3.683961
58	6	0	-9.829408	3.147812	3.718073
59	1	0	-6.857048	-1.762583	2.562493
60	1	0	-9.472342	2.251446	1.150109
61	1	0	-8.225874	2.141119	4.728476
62	1	0	-10.575071	2.398976	4.013492
63	1	0	-10.138673	3.549076	2.747818
64	1	0	-9.876981	3.970210	4.442230
65	1	0	-6.515547	1.769904	4.955729
66	1	0	-3.683195	6.515519	3.440904
67	1	0	-5.888081	1.947773	-5.449090
68	1	0	-6.964248	-1.643666	-2.738012
69	1	0	-4.328537	7.003608	1.061312
70	1	0	-5.732937	4.268495	-4.507788
71	1	0	-8.111337	-1.765188	-0.769453
72	1	0	-6.476030	-0.633355	4.565766
73	8	0	5.601296	-3.450843	-4.425519
74	8	0	7.661158	0.676053	-3.353476

75	6	0	6.619819	-2.803918	-3.772976
76	6	0	6.588814	-1.408559	-3.889232
77	6	0	7.594909	-0.685932	-3.239835
78	6	0	8.593056	-1.313694	-2.459814
79	6	0	8.578237	-2.710175	-2.385329
80	6	0	7.627473	-3.485901	-3.058956
81	6	0	9.620828	-0.469129	-1.742030
82	6	0	11.017642	-1.098596	-1.741434
83	1	0	5.800354	-0.917063	-4.450808
84	1	0	9.341635	-3.214436	-1.788444
85	1	0	9.711007	0.505399	-2.312580
86	1	0	11.050136	-2.055643	-1.211303
87	1	0	11.745351	-0.433587	-1.260744
88	1	0	11.360516	-1.281620	-2.767608
89	8	0	6.547134	-1.146997	4.558770
90	8	0	4.846717	-5.415668	3.408573
91	6	0	6.747269	-2.338520	3.889119
92	6	0	5.673989	-3.232038	3.966958
93	6	0	5.820118	-4.468191	3.326658
94	6	0	6.991478	-4.803700	2.600229
95	6	0	8.021877	-3.865488	2.548037
96	6	0	7.943376	-2.629280	3.208130
97	6	0	7.068750	-6.141912	1.898661
98	6	0	8.471186	-6.757706	1.935854
99	1	0	4.759799	-2.964296	4.490129
100	1	0	8.924926	-4.102316	1.980940
101	1	0	6.392634	-6.853380	2.465516
102	1	0	8.471285	-7.748994	1.465427
103	1	0	8.817384	-6.878404	2.969258
104	1	0	9.212853	-6.150153	1.408024
105	8	0	4.344082	-6.820326	1.190993
106	8	0	5.081059	-5.949317	-3.418976
107	6	0	5.206270	-6.410620	0.203925
108	6	0	4.674033	-6.417006	-1.090322
109	6	0	5.506514	-5.975192	-2.123868
110	6	0	6.826176	-5.517546	-1.887290
111	6	0	7.308485	-5.551213	-0.577155
112	6	0	6.532585	-6.025939	0.487850
113	6	0	7.653436	-4.999905	-3.042744
114	6	0	9.074867	-5.572150	-3.043458
115	1	0	3.649777	-6.729871	-1.271198
116	1	0	8.322749	-5.201232	-0.376648

117	1	0	7.167036	-5.358157	-4.000576
118	1	0	9.636422	-5.310849	-2.141427
119	1	0	9.643969	-5.205833	-3.906057
120	1	0	9.047532	-6.667740	-3.102884
121	8	0	8.297361	2.024568	-1.072043
122	8	0	8.059842	0.932616	3.547112
123	6	0	8.539633	1.107282	-0.080565
124	6	0	8.160623	1.513519	1.205892
125	6	0	8.378773	0.607134	2.247408
126	6	0	8.926810	-0.676170	2.039502
127	6	0	9.295711	-1.022345	0.733947
128	6	0	9.146270	-0.138676	-0.341019
129	6	0	9.080424	-1.630430	3.205037
130	6	0	10.461020	-2.293162	3.231811
131	1	0	7.729659	2.493838	1.372880
132	1	0	9.716887	-2.013468	0.549760
133	1	0	9.000255	-1.023225	4.157475
134	1	0	11.253721	-1.537542	3.296026
135	1	0	10.657919	-2.894835	2.338544
136	1	0	10.559768	-2.955564	4.100592
137	1	0	5.578731	-4.460714	-4.234403
138	1	0	6.832898	1.077599	-3.868251
139	1	0	7.315592	-0.491959	4.412905
140	1	0	3.909832	-5.021070	3.751480
141	1	0	4.707159	-6.618590	2.131090
142	1	0	4.114410	-6.369158	-3.552970
143	1	0	8.323442	1.602073	-2.011923
144	1	0	7.600825	1.840038	3.621158
145	8	0	6.964328	4.276388	-0.326545
146	8	0	4.804133	4.366607	-4.540643
147	6	0	6.309290	4.961773	-1.320509
148	6	0	5.872654	4.304648	-2.472323
149	6	0	5.227127	5.075413	-3.448591
150	6	0	5.040151	6.469170	-3.308213
151	6	0	5.454919	7.063319	-2.111122
152	6	0	6.097365	6.339815	-1.100645
153	6	0	4.423121	7.274505	-4.432306
154	6	0	5.059334	8.659473	-4.590043
155	1	0	6.012530	3.234704	-2.616608
156	1	0	5.282796	8.132252	-1.965563
157	1	0	4.628684	6.720564	-5.398252
158	1	0	4.902131	9.300058	-3.716882

159	1	0	4.634711	9.182113	-5.456731
160	1	0	6.141398	8.577251	-4.748754
161	8	0	-1.979698	8.081470	-1.292866
162	8	0	0.002744	7.368152	2.957998
163	6	0	-0.921910	8.202754	-0.429251
164	6	0	-0.986684	7.690807	0.869409
165	6	0	0.116852	7.912507	1.702417
166	6	0	1.247767	8.645438	1.284089
167	6	0	1.283831	9.078247	-0.048826
168	6	0	0.217156	8.876249	-0.927860
169	6	0	2.351713	8.971178	2.266418
170	6	0	2.906164	10.387856	2.081249
171	1	0	-1.852224	7.133729	1.219441
172	1	0	2.171045	9.603816	-0.408618
173	1	0	1.898836	8.942028	3.304515
174	1	0	3.391743	10.529419	1.110734
175	1	0	3.648698	10.619040	2.854952
176	1	0	2.104198	11.132970	2.156978
177	8	0	2.736759	5.616849	-5.852709
178	8	0	-1.231522	7.311250	-3.869526
179	6	0	2.095063	6.462909	-4.982027
180	6	0	0.705654	6.443558	-4.841282
181	6	0	0.137057	7.375287	-3.963478
182	6	0	0.909953	8.313655	-3.246649
183	6	0	2.301879	8.256268	-3.392966
184	6	0	2.922513	7.348974	-4.256344
185	6	0	0.233445	9.343489	-2.366772
186	6	0	0.844901	10.739102	-2.526862
187	1	0	0.083370	5.737675	-5.385133
188	1	0	2.922080	8.947062	-2.818363
189	1	0	-0.844722	9.427371	-2.706354
190	1	0	0.798223	11.066312	-3.573134
191	1	0	1.894649	10.778961	-2.220483
192	1	0	0.298551	11.474463	-1.923391
193	8	0	2.504173	6.967245	4.161952
194	8	0	6.341646	4.915387	2.239449
195	6	0	3.474790	6.904653	3.195808
196	6	0	4.439232	5.891123	3.199704
197	6	0	5.411764	5.935786	2.195024
198	6	0	5.453757	6.946539	1.216377
199	6	0	4.436884	7.911940	1.234988
200	6	0	3.442572	7.923234	2.216008

201	6	0	6.568071	6.968449	0.190812
202	6	0	7.149200	8.371825	-0.003988
203	1	0	4.430926	5.104069	3.946186
204	1	0	4.426462	8.682184	0.460414
205	1	0	7.412768	6.324046	0.587174
206	1	0	7.525947	8.775046	0.943869
207	1	0	6.413395	9.084391	-0.390420
208	1	0	7.986208	8.350760	-0.713495
209	1	0	7.262472	3.345589	-0.626180
210	1	0	4.242870	4.930750	-5.186964
211	1	0	-2.786229	7.634349	-0.856335
212	1	0	0.852712	7.478126	3.508786
213	1	0	2.100218	4.923337	-6.263405
214	1	0	-1.590839	7.885714	-3.108245
215	1	0	2.536525	6.166760	4.797757
216	1	0	6.905448	4.887687	1.382007
217	8	0	-7.028297	-4.299341	1.587945
218	8	0	-5.344219	-5.342256	-2.814752
219	6	0	-6.389192	-5.127379	0.694695
220	6	0	-6.181668	-4.732879	-0.629590
221	6	0	-5.566253	-5.654304	-1.481045
222	6	0	-5.150007	-6.932531	-1.052275
223	6	0	-5.338665	-7.255531	0.295303
224	6	0	-5.957820	-6.375698	1.192523
225	6	0	-4.520111	-7.880488	-2.050320
226	6	0	-5.086234	-9.299732	-1.932333
227	1	0	-6.482825	-3.749075	-0.990241
228	1	0	-4.993495	-8.225136	0.659243
229	1	0	-4.794403	-7.516056	-3.086699
230	1	0	-6.172534	-9.295768	-2.087279
231	1	0	-4.899091	-9.750067	-0.952790
232	1	0	-4.644505	-9.959630	-2.688852
233	8	0	2.291323	-8.531307	0.529398
234	8	0	0.879396	-6.864744	4.752624
235	6	0	1.333731	-8.365996	1.498820
236	6	0	1.598180	-7.657493	2.673312
237	6	0	0.571605	-7.590341	3.622809
238	6	0	-0.673491	-8.226602	3.444723
239	6	0	-0.903271	-8.873729	2.221960
240	6	0	0.079055	-8.961390	1.232927
241	6	0	-1.688477	-8.231702	4.566862
242	6	0	-2.283257	-9.626440	4.793753

243	1	0	2.555213	-7.172688	2.844395
244	1	0	-1.879041	-9.328321	2.040023
245	1	0	-1.139105	-7.961507	5.521649
246	1	0	-1.492334	-10.356972	5.004211
247	1	0	-2.840756	-9.993687	3.926496
248	1	0	-2.970904	-9.622725	5.648166
249	8	0	-1.522473	-5.746986	5.779047
250	8	0	-5.659949	-4.198629	4.038702
251	6	0	-2.639101	-5.929444	5.001757
252	6	0	-3.601852	-4.923071	4.875555
253	6	0	-4.729550	-5.205739	4.095319
254	6	0	-4.906469	-6.444128	3.440523
255	6	0	-3.890851	-7.398953	3.569601
256	6	0	-2.755238	-7.180467	4.356628
257	6	0	-6.171154	-6.712627	2.651473
258	6	0	-6.698816	-8.137057	2.851186
259	1	0	-3.488932	-3.960532	5.365065
260	1	0	-3.995859	-8.354425	3.050279
261	1	0	-6.973687	-6.018234	3.047881
262	1	0	-6.005800	-8.900300	2.483721
263	1	0	-7.647496	-8.275804	2.317207
264	1	0	-6.880654	-8.341429	3.913177
265	8	0	-2.842513	-6.020877	-3.569061
266	8	0	1.157481	-7.664743	-1.840900
267	6	0	-2.264136	-6.923712	-2.718204
268	6	0	-0.865298	-6.879572	-2.687562
269	6	0	-0.210014	-7.767124	-1.826899
270	6	0	-0.907152	-8.691851	-1.016974
271	6	0	-2.304433	-8.687930	-1.085537
272	6	0	-3.011709	-7.835650	-1.939660
273	6	0	-0.152180	-9.633938	-0.104107
274	6	0	-0.824185	-11.002504	0.043681
275	1	0	-0.313081	-6.161213	-3.284691
276	1	0	-2.864311	-9.383135	-0.455409
277	1	0	0.858932	-9.826502	-0.575105
278	1	0	-0.955745	-11.480053	-0.935007
279	1	0	-1.810071	-10.940918	0.514838
280	1	0	-0.209312	-11.669989	0.660216
281	1	0	-7.344225	-3.438110	1.148207
282	1	0	-5.370645	-4.343864	-2.954049
283	1	0	3.154053	-8.031220	0.747482
284	1	0	0.058170	-6.711563	5.336342

285	1	0	-1.497787	-4.822550	6.205017
286	1	0	-6.354453	-4.354843	3.305843
287	1	0	-3.864708	-5.942064	-3.438460
288	1	0	1.600823	-8.241365	-1.125366
289	8	0	-1.520378	-5.393223	-5.989584
290	8	0	-4.865983	-1.930962	-6.237052
291	6	0	-2.083068	-4.289886	-6.584821
292	6	0	-3.202289	-3.665605	-6.030868
293	6	0	-3.736666	-2.574639	-6.722598
294	6	0	-3.187996	-2.090875	-7.928926
295	6	0	-2.043936	-2.731316	-8.418727
296	6	0	-1.472983	-3.835852	-7.775529
297	6	0	-3.846305	-0.918921	-8.623128
298	6	0	-3.829518	-1.048498	-10.149865
299	1	0	-3.637049	-3.995122	-5.086142
300	1	0	-1.583559	-2.360642	-9.336529
301	1	0	-4.936362	-0.918782	-8.315228
302	1	0	-4.361909	-0.210978	-10.616970
303	1	0	-4.323965	-1.975677	-10.465373
304	1	0	-2.815872	-1.061510	-10.561830
305	8	0	1.010360	3.605248	-6.409245
306	8	0	4.457505	0.463869	-6.536237
307	6	0	1.548819	2.531126	-7.080524
308	6	0	2.720326	2.021952	-6.509604
309	6	0	3.291413	0.898443	-7.116766
310	6	0	2.724401	0.276794	-8.251860
311	6	0	1.565771	0.845872	-8.791023
312	6	0	0.973679	1.994129	-8.250321
313	6	0	3.358233	-0.972660	-8.829447
314	6	0	3.247680	-1.054206	-10.354529
315	1	0	3.151451	2.471124	-5.619306
316	1	0	1.110891	0.383602	-9.670435
317	1	0	4.464309	-0.935575	-8.591906
318	1	0	3.767143	-1.944348	-10.731756
319	1	0	3.703922	-0.176530	-10.827866
320	1	0	2.210844	-1.113810	-10.700670
321	8	0	4.712791	-2.251004	-6.777528
322	8	0	1.246025	-5.384216	-5.937322
323	6	0	3.476300	-2.782144	-7.064595
324	6	0	2.961943	-3.848427	-6.323312
325	6	0	1.720517	-4.362467	-6.717949
326	6	0	1.018851	-3.868301	-7.840170

327	6	0	1.553387	-2.757978	-8.504337
328	6	0	2.779352	-2.190298	-8.140344
329	6	0	-0.250453	-4.552308	-8.302889
330	6	0	-0.286620	-4.733841	-9.824369
331	1	0	3.489889	-4.256642	-5.465922
332	1	0	0.998129	-2.324138	-9.338549
333	1	0	-0.255409	-5.595058	-7.858232
334	1	0	-0.291122	-3.781397	-10.363215
335	1	0	-1.185608	-5.284982	-10.127337
336	1	0	0.585768	-5.301424	-10.170265
337	8	0	-5.020737	0.734646	-6.524247
338	8	0	-1.630646	4.028380	-6.894400
339	6	0	-3.871968	1.144223	-7.144686
340	6	0	-3.372710	2.377123	-6.703239
341	6	0	-2.188787	2.838356	-7.286276
342	6	0	-1.507193	2.113686	-8.289419
343	6	0	-2.049225	0.888974	-8.692212
344	6	0	-3.237757	0.385248	-8.152130
345	6	0	-0.229011	2.664788	-8.880809
346	6	0	-0.219889	2.585302	-10.411242
347	1	0	-3.887583	2.941503	-5.932426
348	1	0	-1.526798	0.306044	-9.453995
349	1	0	-0.177716	3.764956	-8.621584
350	1	0	-1.068196	3.141422	-10.830396
351	1	0	-0.292954	1.558027	-10.781910
352	1	0	0.699226	3.020337	-10.821213
353	1	0	-1.997584	-5.653813	-5.126670
354	1	0	-4.974738	-2.114979	-5.253896
355	1	0	0.059827	3.847208	-6.745296
356	1	0	4.732438	-0.468382	-6.858501
357	1	0	5.146461	-2.702495	-5.971391
358	1	0	0.287686	-5.642617	-6.179301
359	1	0	-5.192417	-0.276697	-6.645971
360	1	0	-2.058683	4.389063	-5.990650
361	8	0	2.700194	4.567570	5.502136
362	8	0	-1.946444	4.530883	5.854885
363	6	0	1.619310	4.303893	6.319819
364	6	0	0.376316	4.534213	5.723906
365	6	0	-0.762718	4.282502	6.498806
366	6	0	-0.682666	3.819779	7.833068
367	6	0	0.589766	3.600964	8.369865
368	6	0	1.762809	3.856381	7.647952

369	6	0	-1.947795	3.565823	8.626626
370	6	0	-1.777515	3.779228	10.133593
371	1	0	0.294116	4.868701	4.693758
372	1	0	0.673948	3.226384	9.393149
373	1	0	-2.717912	4.321735	8.285215
374	1	0	-2.737203	3.647674	10.650498
375	1	0	-1.421668	4.793715	10.349660
376	1	0	-1.070848	3.075300	10.584109
377	8	0	-1.629828	-3.087735	6.664193
378	8	0	3.023905	-3.079844	6.578651
379	6	0	-0.483447	-2.639584	7.276303
380	6	0	0.699893	-3.037918	6.647355
381	6	0	1.905911	-2.619924	7.222665
382	6	0	1.954730	-1.811851	8.380610
383	6	0	0.737488	-1.437275	8.960744
384	6	0	-0.496371	-1.857986	8.451068
385	6	0	3.292121	-1.381287	8.944181
386	6	0	3.286816	-1.222417	10.467572
387	1	0	0.681926	-3.624510	5.732855
388	1	0	0.750134	-0.804133	9.851098
389	1	0	4.036246	-2.202502	8.713437
390	1	0	4.291745	-0.976823	10.833923
391	1	0	2.973876	-2.153006	10.956869
392	1	0	2.615219	-0.428252	10.808308
393	8	0	-4.118256	3.213618	6.966169
394	8	0	-3.877410	-1.601274	7.244133
395	6	0	-3.568984	2.040909	7.425301
396	6	0	-4.066519	0.795244	7.031591
397	6	0	-3.458848	-0.338069	7.582884
398	6	0	-2.394587	-0.255121	8.507328
399	6	0	-1.906680	1.016890	8.828115
400	6	0	-2.474885	2.183378	8.305805
401	6	0	-1.814928	-1.516218	9.110362
402	6	0	-1.718709	-1.425434	10.636811
403	1	0	-4.888369	0.710964	6.325583
404	1	0	-1.053687	1.100586	9.504604
405	1	0	-2.531953	-2.364168	8.887831
406	1	0	-1.070447	-0.609988	10.972161
407	1	0	-1.325977	-2.357281	11.061194
408	1	0	-2.709591	-1.251891	11.075988
409	8	0	5.244823	-1.455130	6.978359
410	8	0	5.051829	3.310555	6.244247

411	6	0	4.746411	-0.202763	7.237071
412	6	0	5.202486	0.918391	6.535439
413	6	0	4.657291	2.156525	6.886603
414	6	0	3.683357	2.302394	7.895173
415	6	0	3.239867	1.141615	8.542822
416	6	0	3.760677	-0.121355	8.245692
417	6	0	3.144235	3.674201	8.239421
418	6	0	3.197414	3.944661	9.746210
419	1	0	5.942150	0.823442	5.746087
420	1	0	2.459240	1.227165	9.302042
421	1	0	3.820903	4.441803	7.755021
422	1	0	2.598658	3.233746	10.324651
423	1	0	2.830760	4.951874	9.978273
424	1	0	4.228469	3.872611	10.115582
425	1	0	3.589255	4.325155	5.947051
426	1	0	-2.764016	4.270994	6.412873
427	1	0	-2.480382	-2.709388	7.095121
428	1	0	3.888028	-2.666347	6.926734
429	1	0	-4.889402	3.052606	6.315365
430	1	0	-4.549338	-1.595223	6.457354
431	1	0	5.878753	-1.459442	6.174850
432	1	0	5.704440	3.123896	5.477272
433	8	0	-2.268205	4.690591	-4.464186
434	1	0	-3.226394	4.712422	-4.253231
435	1	0	-1.933018	5.591326	-4.267284
436	8	0	6.528390	3.208381	3.943796
437	1	0	7.020003	4.057223	3.918604
438	1	0	5.876675	3.295137	3.212603
439	8	0	2.801477	-7.013166	-4.110665
440	1	0	2.388648	-6.439324	-4.782999
441	1	0	2.124540	-7.156363	-3.420916
442	8	0	2.513186	-4.593700	4.208146
443	1	0	2.631274	-4.216526	5.104851
444	1	0	1.979011	-5.412952	4.329121
445	8	0	5.417008	1.673400	-4.258984
446	1	0	5.479761	2.540348	-4.704897
447	1	0	4.935269	1.087008	-4.885261
448	8	0	-4.487844	-1.670365	2.528995
449	1	0	-4.700295	-1.044607	1.820406
450	1	0	-3.837937	-2.274668	2.141709
451	8	0	-2.446081	6.878957	4.317869
452	1	0	-2.086120	6.097322	4.781507

453	1	0	-1.723100	7.212633	3.751115
454	8	0	-5.121226	-1.501233	4.861769
455	1	0	-4.451216	-1.087163	4.255960
456	1	0	-5.264255	-2.404811	4.458718
457	6	0	-1.867279	-1.973190	0.224177
458	6	0	-1.035169	-2.179444	1.324416
459	6	0	-1.119165	-3.366446	2.056612
460	6	0	-2.034810	-4.349988	1.692603
461	6	0	-2.872723	-4.139860	0.594078
462	6	0	-2.798269	-2.956820	-0.135664
463	6	0	-1.866622	-0.660852	-0.554334
464	6	0	-1.838290	-0.854223	-2.065908
465	6	0	-3.024162	0.184505	-0.015717
466	6	0	-4.287240	0.093279	-0.607984
467	6	0	-5.357671	0.803177	-0.065339
468	6	0	-5.180898	1.601852	1.064781
469	6	0	-3.929566	1.667470	1.674635
470	6	0	-2.857925	0.952465	1.142792
471	6	0	-2.265149	0.165255	-2.921580
472	6	0	-2.096246	0.048287	-4.298637
473	6	0	-1.503270	-1.091260	-4.837632
474	6	0	-1.088978	-2.119245	-3.991703
475	6	0	-1.250156	-1.998842	-2.613415
476	17	0	-5.139698	-2.367522	-3.239900
477	1	0	-0.315890	-1.419134	1.622545
478	1	0	-0.457249	-3.520113	2.908657
479	1	0	-2.095316	-5.280181	2.257506
480	1	0	-3.583993	-4.908091	0.298431
481	1	0	-3.454603	-2.807063	-0.992820
482	1	0	-4.445524	-0.528793	-1.487169
483	1	0	-6.334954	0.731703	-0.536382
484	1	0	-6.019555	2.166636	1.473672
485	1	0	-3.787952	2.273200	2.569716
486	1	0	-1.894527	0.989930	1.651478
487	1	0	-2.749287	1.054815	-2.522070
488	1	0	-2.430068	0.852436	-4.950569
489	1	0	-1.370678	-1.179698	-5.915328
490	1	0	-0.629811	-3.015062	-4.404946
491	1	0	-0.912933	-2.804016	-1.964301
492	6	0	1.310150	0.304277	-2.757147
493	6	0	1.969721	-0.404953	-1.691699
494	6	0	3.026755	0.160563	-1.028179

495	6	0	1.750759	1.214131	0.581882
496	6	0	0.724299	1.913457	-0.060909
497	6	0	1.674746	1.575146	-3.058095
498	6	0	2.854236	2.263779	-2.438017
499	6	0	3.771760	1.306265	-1.666186
500	6	0	-0.428985	1.270263	-0.464373
501	1	0	-1.235631	1.796102	-0.974657
502	8	0	-0.584641	0.002577	-0.202932
503	6	0	2.871719	1.942476	1.254161
504	1	0	0.473305	-0.158113	-3.271327
505	1	0	1.560882	-1.362295	-1.369060
506	1	0	3.544155	-0.425483	-0.268184
507	1	0	1.509836	0.224931	0.965910
508	1	0	0.824928	2.970112	-0.296937
509	1	0	1.096347	2.131313	-3.799978
510	1	0	3.435035	2.761466	-3.229833
511	1	0	2.493722	3.083539	-1.799340
512	1	0	4.369549	1.853806	-0.930902
513	1	0	4.494101	0.860169	-2.369885
514	1	0	3.765799	1.321386	1.362025
515	1	0	3.122373	2.871250	0.729936
516	1	0	2.524873	2.204540	2.264544

Only one negative frequency: -246.94

TS-*exo*@$\mathbf{C_M}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.113809	5.993591	1.944527
2	8	0	-3.421383	7.311667	-2.287983
3	6	0	-5.346697	6.179283	0.602899
4	6	0	-4.249727	6.657115	-0.124129
5	6	0	-4.419734	6.820315	-1.503173
6	6	0	-5.627446	6.475577	-2.160781
7	6	0	-6.693392	6.026689	-1.379515
8	6	0	-6.596002	5.903545	0.013742
9	6	0	-5.714885	6.597316	-3.666764
10	6	0	-7.023100	7.249012	-4.125319
11	1	0	-3.308526	6.882933	0.367912
12	1	0	-7.636028	5.768425	-1.867027

13	1	0	-4.881490	7.287902	-4.001172
14	1	0	-7.130032	8.249688	-3.687659
15	1	0	-7.907315	6.672282	-3.836212
16	1	0	-7.044206	7.358963	-5.216307
17	8	0	-6.331391	-0.393107	-5.544523
18	8	0	-8.052153	-1.365655	-1.147485
19	6	0	-7.030313	-0.048765	-4.410195
20	6	0	-7.134334	-0.933603	-3.336127
21	6	0	-7.901822	-0.524607	-2.242012
22	6	0	-8.559329	0.721950	-2.189799
23	6	0	-8.379500	1.589129	-3.274267
24	6	0	-7.624010	1.232948	-4.398020
25	6	0	-9.420375	1.057593	-0.991045
26	6	0	-10.732248	1.740869	-1.391934
27	1	0	-6.632903	-1.902402	-3.336266
28	1	0	-8.845629	2.575746	-3.243920
29	1	0	-9.709905	0.077121	-0.502421
30	1	0	-10.573685	2.701025	-1.892168
31	1	0	-11.359223	1.928127	-0.511653
32	1	0	-11.304756	1.105226	-2.079280
33	8	0	-3.056332	5.626572	-4.382476
34	8	0	-4.616598	1.642441	-6.236121
35	6	0	-4.160739	4.852944	-4.649376
36	6	0	-3.873783	3.644999	-5.295626
37	6	0	-4.952307	2.801958	-5.582911
38	6	0	-6.284302	3.131341	-5.244507
39	6	0	-6.508260	4.351947	-4.599263
40	6	0	-5.471392	5.248252	-4.311112
41	6	0	-7.407705	2.168064	-5.568301
42	6	0	-8.695540	2.874529	-6.001146
43	1	0	-2.855046	3.367940	-5.545783
44	1	0	-7.529445	4.620028	-4.318134
45	1	0	-7.076089	1.540742	-6.451107
46	1	0	-9.120489	3.501104	-5.210665
47	1	0	-9.462534	2.141096	-6.281284
48	1	0	-8.515876	3.517582	-6.871100
49	8	0	-7.959754	-0.154509	1.234132
50	8	0	-6.675061	4.050549	2.989956
51	6	0	-7.988563	1.204764	1.100849
52	6	0	-7.310908	1.902874	2.109507
53	6	0	-7.287463	3.297482	2.023415
54	6	0	-7.882249	3.999021	0.950059

55	6	0	-8.546580	3.252319	-0.028155
56	6	0	-8.640573	1.857470	0.030792
57	6	0	-7.770533	5.505298	0.882941
58	6	0	-9.075813	6.177104	0.445633
59	1	0	-6.816100	1.369042	2.918581
60	1	0	-9.012325	3.777088	-0.865686
61	1	0	-7.558134	5.874637	1.933065
62	1	0	-9.893896	5.916249	1.128748
63	1	0	-9.386438	5.882000	-0.561560
64	1	0	-8.973175	7.269113	0.448981
65	1	0	-5.908621	5.550876	2.423061
66	1	0	-2.576851	7.651620	-1.738196
67	1	0	-5.975197	-1.346576	-5.503008
68	1	0	-7.303738	-2.041127	-1.128998
69	1	0	-3.280789	6.463369	-3.832637
70	1	0	-5.393082	0.978671	-6.270584
71	1	0	-8.304717	-0.649835	0.393766
72	1	0	-6.151063	3.467937	3.681933
73	8	0	4.700006	-6.265078	-0.846673
74	8	0	7.232566	-2.757843	-2.771271
75	6	0	5.827217	-5.484965	-0.781721
76	6	0	5.920690	-4.519338	-1.791930
77	6	0	7.041332	-3.683424	-1.779422
78	6	0	8.032562	-3.762412	-0.775103
79	6	0	7.891528	-4.751724	0.203238
80	6	0	6.819329	-5.651670	0.206922
81	6	0	9.182788	-2.781710	-0.783988
82	6	0	10.515616	-3.422363	-0.384168
83	1	0	5.141611	-4.424009	-2.542147
84	1	0	8.647886	-4.829818	0.987508
85	1	0	9.309738	-2.422141	-1.850565
86	1	0	10.505528	-3.817240	0.636800
87	1	0	11.333967	-2.695042	-0.445905
88	1	0	10.759908	-4.256969	-1.053579
89	8	0	6.703216	1.225993	4.463095
90	8	0	4.456808	-2.482702	6.368708
91	6	0	6.710279	-0.129278	4.727344
92	6	0	5.561530	-0.598626	5.372078
93	6	0	5.513390	-1.961704	5.686994
94	6	0	6.567692	-2.848337	5.348372
95	6	0	7.680627	-2.322909	4.692058
96	6	0	7.796688	-0.957249	4.389473

97	6	0	6.437645	-4.316192	5.691307
98	6	0	7.764774	-4.947659	6.125106
99	1	0	4.733767	0.068911	5.597236
100	1	0	8.493996	-2.994838	4.409405
101	1	0	5.743596	-4.387909	6.584426
102	1	0	7.617828	-5.994865	6.417707
103	1	0	8.186382	-4.416218	6.986614
104	1	0	8.516889	-4.936785	5.330240
105	8	0	3.602923	-4.907009	5.594872
106	8	0	4.020270	-7.369605	1.555316
107	6	0	4.412644	-5.360711	4.584148
108	6	0	3.770852	-6.136744	3.611790
109	6	0	4.551426	-6.598748	2.547407
110	6	0	5.927692	-6.285749	2.428914
111	6	0	6.517135	-5.520781	3.438087
112	6	0	5.792627	-5.071870	4.549104
113	6	0	6.699677	-6.769310	1.221828
114	6	0	8.053751	-7.378437	1.600063
115	1	0	2.706890	-6.345354	3.676950
116	1	0	7.576552	-5.269241	3.361875
117	1	0	6.100382	-7.601754	0.742110
118	1	0	8.713514	-6.664072	2.101819
119	1	0	8.579262	-7.747578	0.711458
120	1	0	7.915564	-8.226986	2.282403
121	8	0	7.959713	-0.368283	-1.854639
122	8	0	8.249948	1.900011	2.304474
123	6	0	8.311748	-0.415558	-0.530966
124	6	0	8.101443	0.776480	0.175208
125	6	0	8.391088	0.762512	1.542649
126	6	0	8.836872	-0.394777	2.216311
127	6	0	9.060618	-1.545461	1.451662
128	6	0	8.848868	-1.573596	0.068119
129	6	0	9.021139	-0.370787	3.719166
130	6	0	10.325383	-1.041763	4.158994
131	1	0	7.724313	1.659503	-0.326521
132	1	0	9.414133	-2.450620	1.951270
133	1	0	9.096501	0.713237	4.037433
134	1	0	11.190895	-0.549333	3.699030
135	1	0	10.369022	-2.100632	3.883836
136	1	0	10.446808	-0.982547	5.247721
137	1	0	4.595362	-6.887082	-0.032687
138	1	0	6.366069	-2.625419	-3.368927

139	1	0	7.520779	1.517140	3.928300
140	1	0	3.604866	-1.830388	6.373624
141	1	0	4.060061	-4.184048	6.164913
142	1	0	3.003713	-7.629127	1.718357
143	1	0	7.984537	-1.301681	-2.306739
144	1	0	7.872426	2.682438	1.767798
145	8	0	7.925330	2.115361	-3.032072
146	8	0	5.483932	-0.429577	-6.217486
147	6	0	7.166217	2.027064	-4.175302
148	6	0	6.665049	0.800250	-4.617559
149	6	0	5.946045	0.799485	-5.819479
150	6	0	5.729005	1.973539	-6.573354
151	6	0	6.203942	3.181734	-6.050612
152	6	0	6.932351	3.240323	-4.857570
153	6	0	5.026166	1.893811	-7.911972
154	6	0	5.738631	2.717835	-8.989428
155	1	0	6.832106	-0.121236	-4.065014
156	1	0	6.009811	4.106890	-6.597495
157	1	0	5.069503	0.814099	-8.256451
158	1	0	5.754583	3.788251	-8.762632
159	1	0	5.243028	2.597352	-9.961056
160	1	0	6.780018	2.392739	-9.104603
161	8	0	-1.038087	5.512486	-6.276533
162	8	0	1.137900	7.580359	-2.600727
163	6	0	0.087351	6.022590	-5.681262
164	6	0	0.047361	6.548125	-4.387407
165	6	0	1.231058	7.101012	-3.883352
166	6	0	2.420193	7.166646	-4.640537
167	6	0	2.417791	6.566484	-5.907081
168	6	0	1.270223	5.987785	-6.454889
169	6	0	3.633241	7.887963	-4.094044
170	6	0	4.327369	8.749749	-5.153838
171	1	0	-0.858566	6.519072	-3.787386
172	1	0	3.341504	6.559744	-6.489375
173	1	0	3.271754	8.601600	-3.291449
174	1	0	4.729954	8.159641	-5.982936
175	1	0	5.161576	9.310719	-4.714929
176	1	0	3.626790	9.477292	-5.583093
177	8	0	3.082459	-0.048672	-7.594872
178	8	0	-0.514920	3.033855	-7.397247
179	6	0	2.605480	1.237629	-7.607301
180	6	0	1.240994	1.501853	-7.465052

181	6	0	0.835853	2.841783	-7.521325
182	6	0	1.748774	3.902866	-7.710550
183	6	0	3.107687	3.580705	-7.804552
184	6	0	3.566453	2.259939	-7.769881
185	6	0	1.249015	5.328536	-7.816780
186	6	0	2.002299	6.142240	-8.873777
187	1	0	0.515028	0.705161	-7.317294
188	1	0	3.834138	4.387746	-7.922308
189	1	0	0.169866	5.286304	-8.158653
190	1	0	1.937304	5.659496	-9.856788
191	1	0	3.064002	6.263426	-8.638204
192	1	0	1.571822	7.147185	-8.967876
193	8	0	3.636542	7.516171	-1.356701
194	8	0	7.020800	4.183017	-1.418586
195	6	0	4.525840	6.725603	-2.033972
196	6	0	5.336873	5.804124	-1.363546
197	6	0	6.256100	5.082371	-2.134390
198	6	0	6.398757	5.267202	-3.522360
199	6	0	5.520485	6.163910	-4.149913
200	6	0	4.581004	6.909134	-3.435428
201	6	0	7.477323	4.531878	-4.289768
202	6	0	8.136857	5.406003	-5.361423
203	1	0	5.254272	5.654694	-0.291880
204	1	0	5.581694	6.289702	-5.233576
205	1	0	8.294990	4.263089	-3.553943
206	1	0	8.555674	6.318619	-4.920203
207	1	0	7.439041	5.712586	-6.147050
208	1	0	8.957768	4.865519	-5.849981
209	1	0	8.097088	1.200626	-2.610342
210	1	0	4.831943	-0.358826	-7.000915
211	1	0	-1.858598	5.569221	-5.668818
212	1	0	2.040047	7.873926	-2.230217
213	1	0	2.333361	-0.740567	-7.527964
214	1	0	-0.763758	4.017221	-7.285464
215	1	0	3.607421	7.303587	-0.355501
216	1	0	7.557806	3.561552	-2.033365
217	8	0	-7.344744	-1.140401	3.843055
218	8	0	-6.141784	-5.048820	1.275694
219	6	0	-6.882430	-2.431380	3.736348
220	6	0	-6.728725	-3.040104	2.488086
221	6	0	-6.299322	-4.369850	2.475781
222	6	0	-6.014491	-5.092846	3.653286

223	6	0	-6.139565	-4.418570	4.872381
224	6	0	-6.575402	-3.089642	4.946698
225	6	0	-5.584127	-6.540361	3.549565
226	6	0	-6.313763	-7.431632	4.560497
227	1	0	-6.930303	-2.506342	1.559347
228	1	0	-5.890962	-4.945771	5.795370
229	1	0	-5.885672	-6.913474	2.524006
230	1	0	-7.399352	-7.375559	4.410808
231	1	0	-6.113503	-7.146605	5.597821
232	1	0	-6.014983	-8.480247	4.442559
233	8	0	1.266129	-6.294954	6.115109
234	8	0	0.386719	-2.101653	8.176520
235	6	0	0.408649	-5.403607	6.711795
236	6	0	0.846336	-4.149474	7.144162
237	6	0	-0.092406	-3.332102	7.784699
238	6	0	-1.419764	-3.741666	8.025618
239	6	0	-1.817886	-4.986960	7.519087
240	6	0	-0.927610	-5.839785	6.862001
241	6	0	-2.346653	-2.865308	8.839533
242	6	0	-3.099329	-3.666513	9.908218
243	1	0	1.867876	-3.815533	6.985055
244	1	0	-2.855094	-5.302499	7.647502
245	1	0	-1.702628	-2.117274	9.398046
246	1	0	-2.396608	-4.182111	10.574376
247	1	0	-3.756976	-4.428677	9.478778
248	1	0	-3.721177	-3.005993	10.524537
249	8	0	-1.770405	-0.256701	8.110472
250	8	0	-5.781243	0.343514	5.641564
251	6	0	-2.953251	-0.741267	7.609764
252	6	0	-3.780940	0.058421	6.815497
253	6	0	-4.990223	-0.498420	6.382025
254	6	0	-5.376773	-1.816641	6.709066
255	6	0	-4.488748	-2.584875	7.471291
256	6	0	-3.279748	-2.071810	7.952567
257	6	0	-6.720739	-2.349029	6.257455
258	6	0	-7.411402	-3.194924	7.332211
259	1	0	-3.505967	1.073547	6.545678
260	1	0	-4.756378	-3.616247	7.712508
261	1	0	-7.395292	-1.457903	6.072978
262	1	0	-6.852172	-4.102455	7.580149
263	1	0	-8.407408	-3.509047	6.995243
264	1	0	-7.537627	-2.622403	8.258972

265	8	0	-3.803731	-6.396385	1.229889
266	8	0	0.076524	-7.038698	3.726711
267	6	0	-3.280990	-6.588655	2.480433
268	6	0	-1.888932	-6.731970	2.514032
269	6	0	-1.289248	-6.915321	3.764843
270	6	0	-2.035330	-6.972806	4.963371
271	6	0	-3.422719	-6.819003	4.869683
272	6	0	-4.077926	-6.648643	3.645831
273	6	0	-1.338544	-7.180700	6.290841
274	6	0	-2.163169	-8.005023	7.284440
275	1	0	-1.296234	-6.666658	1.607358
276	1	0	-4.017951	-6.842148	5.785627
277	1	0	-0.396491	-7.775455	6.090573
278	1	0	-2.424996	-8.981328	6.858631
279	1	0	-3.096159	-7.510478	7.572093
280	1	0	-1.592545	-8.184552	8.204151
281	1	0	-7.579503	-0.744387	2.936039
282	1	0	-6.060927	-4.400248	0.507677
283	1	0	2.199750	-5.904965	5.986110
284	1	0	-0.365841	-1.484918	8.479839
285	1	0	-1.594633	0.702517	7.818522
286	1	0	-6.541838	-0.153032	5.173964
287	1	0	-4.794666	-6.102270	1.248338
288	1	0	0.494613	-7.055261	4.657281
289	8	0	-2.646820	-7.726643	-0.974046
290	8	0	-5.526146	-4.864019	-3.575155
291	6	0	-3.108695	-7.233805	-2.169849
292	6	0	-4.095781	-6.247529	-2.211038
293	6	0	-4.538034	-5.832304	-3.470910
294	6	0	-4.025962	-6.363178	-4.673930
295	6	0	-3.012308	-7.323602	-4.573594
296	6	0	-2.536812	-7.782808	-3.340008
297	6	0	-4.581491	-5.877740	-5.994640
298	6	0	-4.695957	-6.995831	-7.036243
299	1	0	-4.497041	-5.795903	-1.302381
300	1	0	-2.580332	-7.731981	-5.489230
301	1	0	-5.636999	-5.516186	-5.797449
302	1	0	-5.156018	-6.622094	-7.959139
303	1	0	-5.322273	-7.813957	-6.659104
304	1	0	-3.725538	-7.423823	-7.305259
305	8	0	0.920399	-1.759859	-7.209853
306	8	0	3.896896	-4.581698	-5.010771

307	6	0	1.279481	-3.065880	-6.974965
308	6	0	2.400631	-3.213232	-6.150937
309	6	0	2.789304	-4.515175	-5.816368
310	6	0	2.096090	-5.654706	-6.281516
311	6	0	0.996629	-5.445748	-7.121473
312	6	0	0.580271	-4.166397	-7.510746
313	6	0	2.537026	-7.040106	-5.854974
314	6	0	2.328217	-8.100598	-6.939717
315	1	0	2.938149	-2.348597	-5.773228
316	1	0	0.445108	-6.313287	-7.492889
317	1	0	3.651306	-6.998540	-5.661260
318	1	0	2.714242	-9.072781	-6.607056
319	1	0	2.858274	-7.829568	-7.860599
320	1	0	1.273287	-8.242622	-7.195207
321	8	0	3.853535	-6.821830	-3.430702
322	8	0	0.089258	-8.106888	-0.840196
323	6	0	2.544400	-7.233931	-3.333541
324	6	0	1.951903	-7.463299	-2.089832
325	6	0	0.630968	-7.928946	-2.085440
326	6	0	-0.079479	-8.199524	-3.276751
327	6	0	0.543881	-7.889453	-4.490930
328	6	0	1.854707	-7.403320	-4.553243
329	6	0	-1.454602	-8.831029	-3.213556
330	6	0	-1.613854	-9.967247	-4.229805
331	1	0	2.483507	-7.280004	-1.160072
332	1	0	-0.008452	-8.037861	-5.421164
333	1	0	-1.564386	-9.303437	-2.188916
334	1	0	-1.529892	-9.622859	-5.265065
335	1	0	-2.594728	-10.447219	-4.123367
336	1	0	-0.847313	-10.736792	-4.077720
337	8	0	-5.400377	-3.103572	-5.617016
338	8	0	-1.654362	-1.422397	-7.989536
339	6	0	-4.255945	-3.381877	-6.314966
340	6	0	-3.582539	-2.257433	-6.811784
341	6	0	-2.384598	-2.475864	-7.497998
342	6	0	-1.862786	-3.770285	-7.716140
343	6	0	-2.578268	-4.857539	-7.203269
344	6	0	-3.783893	-4.697942	-6.510813
345	6	0	-0.565174	-3.939352	-8.474754
346	6	0	-0.663888	-5.025244	-9.551208
347	1	0	-3.980555	-1.259343	-6.660744
348	1	0	-2.181326	-5.864947	-7.346557

349	1	0	-0.358689	-2.969732	-9.021153
350	1	0	-1.460051	-4.785445	-10.267757
351	1	0	-0.890678	-6.012562	-9.136596
352	1	0	0.274614	-5.109086	-10.111861
353	1	0	-3.074877	-7.264860	-0.170565
354	1	0	-5.586453	-4.337028	-2.720245
355	1	0	0.031115	-1.677505	-7.735837
356	1	0	4.061980	-5.522604	-4.641922
357	1	0	4.287046	-6.703883	-2.513582
358	1	0	-0.911153	-8.313186	-0.879427
359	1	0	-5.698713	-3.896030	-5.026383
360	1	0	-1.958652	-0.503386	-7.568758
361	8	0	3.647738	6.614679	1.247713
362	8	0	-0.923957	7.503418	1.408187
363	6	0	2.608410	7.117616	2.004889
364	6	0	1.362940	7.078561	1.372019
365	6	0	0.263800	7.567488	2.088835
366	6	0	0.385217	8.088374	3.398232
367	6	0	1.657103	8.095150	3.979011
368	6	0	2.794862	7.640662	3.299751
369	6	0	-0.839018	8.599383	4.129745
370	6	0	-0.531518	9.714246	5.133712
371	1	0	1.244246	6.658097	0.377544
372	1	0	1.770976	8.477411	4.996551
373	1	0	-1.530280	9.051924	3.356345
374	1	0	-1.459078	10.090516	5.584845
375	1	0	-0.035267	10.559983	4.642964
376	1	0	0.111974	9.380232	5.953626
377	8	0	-1.483135	2.310981	7.020912
378	8	0	3.119205	1.621428	7.139495
379	6	0	-0.252961	2.887609	7.229905
380	6	0	0.828246	2.016117	7.068266
381	6	0	2.111044	2.539617	7.269081
382	6	0	2.334634	3.894936	7.600659
383	6	0	1.213532	4.720262	7.743534
384	6	0	-0.093208	4.240936	7.596038
385	6	0	3.748688	4.404526	7.781133
386	6	0	3.862456	5.528230	8.815679
387	1	0	0.679066	0.982276	6.768923
388	1	0	1.362040	5.773759	7.991916
389	1	0	4.370119	3.545053	8.176543
390	1	0	4.911487	5.816735	8.959080

391	1	0	3.471328	5.205243	9.788324
392	1	0	3.315653	6.430067	8.523161
393	8	0	-3.155915	7.571190	3.048881
394	8	0	-3.488072	4.108765	6.398453
395	6	0	-2.723155	6.912609	4.175031
396	6	0	-3.397274	5.794381	4.673959
397	6	0	-2.896244	5.217558	5.846161
398	6	0	-1.769307	5.732916	6.523784
399	6	0	-1.104841	6.822873	5.950094
400	6	0	-1.558729	7.435479	4.777325
401	6	0	-1.314165	5.105350	7.823263
402	6	0	-1.110717	6.155078	8.920899
403	1	0	-4.270735	5.388528	4.170380
404	1	0	-0.202151	7.204545	6.431400
405	1	0	-2.144626	4.425422	8.185007
406	1	0	-0.345805	6.893949	8.662887
407	1	0	-0.810914	5.682915	9.864193
408	1	0	-2.042290	6.705275	9.105727
409	8	0	5.535308	2.783990	6.418878
410	8	0	5.868422	5.841935	2.697338
411	6	0	5.211771	3.946153	5.764473
412	6	0	5.747273	4.244809	4.506725
413	6	0	5.385495	5.467141	3.933672
414	6	0	4.518138	6.379880	4.567085
415	6	0	3.983621	6.013093	5.809440
416	6	0	4.320256	4.810680	6.438125
417	6	0	4.182843	7.696959	3.900864
418	6	0	4.382713	8.881844	4.851001
419	1	0	6.405861	3.547324	3.998268
420	1	0	3.278271	6.687758	6.299694
421	1	0	4.912116	7.847439	3.048112
422	1	0	3.744624	8.823871	5.738709
423	1	0	4.163608	9.831101	4.347435
424	1	0	5.421360	8.923740	5.203211
425	1	0	4.531989	6.604589	1.762749
426	1	0	-1.723404	7.794995	1.976181
427	1	0	-2.249278	2.991621	7.059473
428	1	0	4.048049	2.040738	7.149115
429	1	0	-3.992130	7.144641	2.648016
430	1	0	-4.204043	3.694035	5.776002
431	1	0	6.102666	2.158873	5.840354
432	1	0	6.410536	5.100623	2.250780

433	8	0	-1.948542	0.696611	-6.508699
434	1	0	-2.857662	0.979451	-6.274493
435	1	0	-1.519574	1.490330	-6.889018
436	8	0	7.063775	4.041555	1.007727
437	1	0	7.672966	4.552065	0.432662
438	1	0	6.367189	3.727952	0.392450
439	8	0	1.589381	-8.300151	1.657923
440	1	0	1.202389	-8.250835	0.764664
441	1	0	0.946968	-7.871266	2.257522
442	8	0	2.309281	-1.014994	6.369133
443	1	0	2.516656	-0.150926	6.779839
444	1	0	1.665682	-1.454268	6.970754
445	8	0	5.022592	-2.152584	-4.009295
446	1	0	5.207561	-1.700419	-4.861982
447	1	0	4.487652	-2.945213	-4.240149
448	8	0	-4.399735	1.086780	2.863882
449	1	0	-3.819511	0.319792	2.978859
450	1	0	-4.600681	1.108589	1.916506
451	8	0	-1.264691	8.351302	-1.275851
452	1	0	-0.952429	8.003737	-0.416234
453	1	0	-0.548586	8.169692	-1.914773
454	8	0	-4.880245	2.820183	4.489337
455	1	0	-4.214196	2.655582	3.769617
456	1	0	-5.144164	1.897289	4.768682
457	6	0	-2.072994	-1.038634	1.326438
458	6	0	-1.225160	-0.533186	2.313207
459	6	0	-1.393652	-0.915115	3.645820
460	6	0	-2.410866	-1.799847	3.997595
461	6	0	-3.261226	-2.301425	3.009486
462	6	0	-3.100738	-1.922060	1.679036
463	6	0	-1.981224	-0.552251	-0.117439
464	6	0	-2.148567	-1.666385	-1.148457
465	6	0	-2.969241	0.609300	-0.255671
466	6	0	-4.307440	0.343415	-0.568021
467	6	0	-5.221845	1.391540	-0.642112
468	6	0	-4.820295	2.703995	-0.387924
469	6	0	-3.498333	2.964162	-0.036135
470	6	0	-2.577075	1.919162	0.035464
471	6	0	-2.675893	-1.407978	-2.416741
472	6	0	-2.723508	-2.412890	-3.379567
473	6	0	-2.226322	-3.680994	-3.094760
474	6	0	-1.691173	-3.945328	-1.834523

475	6	0	-1.653753	-2.944166	-0.867016
476	17	0	-5.630392	-3.178307	-1.029290
477	1	0	-0.429934	0.162641	2.051004
478	1	0	-0.720979	-0.521312	4.407250
479	1	0	-2.540041	-2.102010	5.036801
480	1	0	-4.052388	-2.999075	3.275554
481	1	0	-3.771527	-2.320502	0.918633
482	1	0	-4.641183	-0.674564	-0.763228
483	1	0	-6.253446	1.175754	-0.909186
484	1	0	-5.539475	3.520395	-0.460781
485	1	0	-3.180037	3.983671	0.181217
486	1	0	-1.550059	2.137434	0.328673
487	1	0	-3.073496	-0.424872	-2.659440
488	1	0	-3.148420	-2.196087	-4.355506
489	1	0	-2.252872	-4.460049	-3.855795
490	1	0	-1.300743	-4.934939	-1.603189
491	1	0	-1.239063	-3.160069	0.116477
492	6	0	2.872945	-1.202139	-1.735309
493	6	0	2.102376	0.682463	-0.901619
494	6	0	0.959238	1.021653	-1.673499
495	6	0	1.333957	-0.975277	-4.097507
496	6	0	2.514187	-0.317919	-3.999022
497	6	0	3.333981	-0.511346	-2.836739
498	6	0	-0.310463	0.606315	-1.378727
499	1	0	-1.140977	0.868466	-2.034976
500	8	0	-0.602080	-0.049676	-0.277017
501	6	0	3.267593	1.622029	-0.813939
502	1	0	3.566332	-1.378426	-0.911746
503	1	0	1.908075	0.080089	-0.011550
504	1	0	1.071856	1.652397	-2.552222
505	1	0	0.690087	-0.797404	-4.964262
506	1	0	2.829964	0.385373	-4.768265
507	1	0	4.311483	-0.027637	-2.791651
508	1	0	4.181776	1.109279	-0.497013
509	1	0	3.439447	2.136302	-1.765625
510	1	0	3.022137	2.379097	-0.056391
511	6	0	1.647000	-2.080422	-1.798945
512	1	0	0.965641	-1.820378	-0.981738
513	1	0	1.974712	-3.104544	-1.583511
514	6	0	0.900200	-2.046281	-3.148341
515	1	0	-0.177758	-1.966185	-2.987042
516	1	0	1.029012	-2.996997	-3.689711

Only one negative frequency: -227.89

6-*endo*@$\mathbf{C_M}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.705477	8.167936	1.545473
2	8	0	-0.900608	8.051564	-2.852819
3	6	0	-2.932490	8.079506	0.194734
4	6	0	-1.827672	8.151181	-0.642125
5	6	0	-1.973524	8.032850	-2.013983
6	6	0	-3.243250	7.828656	-2.565085
7	6	0	-4.325967	7.751688	-1.708392
8	6	0	-4.213033	7.906602	-0.334717
9	6	0	-3.409558	7.672466	-4.064318
10	6	0	-4.469707	8.626661	-4.615472
11	1	0	-0.846518	8.293703	-0.216314
12	1	0	-5.299548	7.555934	-2.128117
13	1	0	-2.463658	7.964122	-4.536533
14	1	0	-4.149115	9.652018	-4.445109
15	1	0	-5.433193	8.496245	-4.132406
16	1	0	-4.589975	8.473057	-5.685605
17	8	0	-6.653646	1.097274	-5.262730
18	8	0	-8.258449	1.155377	-0.760076
19	6	0	-7.114775	1.780198	-4.171061
20	6	0	-7.516967	1.109394	-3.029299
21	6	0	-7.935678	1.812148	-1.910804
22	6	0	-7.997918	3.209822	-1.939671
23	6	0	-7.565820	3.858897	-3.085361
24	6	0	-7.117904	3.177568	-4.207319
25	6	0	-8.479609	3.969553	-0.719307
26	6	0	-9.533774	5.015608	-1.087686
27	1	0	-7.467403	0.031911	-2.992335
28	1	0	-7.539385	4.936364	-3.091104
29	1	0	-8.985948	3.248843	-0.066245
30	1	0	-9.175802	5.720348	-1.831670
31	1	0	-9.834849	5.568425	-0.200437
32	1	0	-10.406838	4.513789	-1.499106
33	8	0	-1.317183	5.641007	-4.032204
34	8	0	-4.160102	2.188675	-5.339812

35	6	0	-2.604020	5.304096	-4.351422
36	6	0	-2.818465	3.975160	-4.674119
37	6	0	-4.077042	3.513290	-5.025466
38	6	0	-5.159345	4.398820	-5.053361
39	6	0	-4.916030	5.722801	-4.719985
40	6	0	-3.661999	6.212549	-4.387081
41	6	0	-6.549111	3.901507	-5.413371
42	6	0	-7.491619	4.988675	-5.928734
43	1	0	-1.983410	3.293344	-4.652093
44	1	0	-5.740617	6.412929	-4.746133
45	1	0	-6.451192	3.172284	-6.225920
46	1	0	-7.757612	5.704682	-5.157188
47	1	0	-8.410399	4.524949	-6.281143
48	1	0	-7.030826	5.521124	-6.757949
49	8	0	-6.864051	2.423874	1.166854
50	8	0	-4.315286	6.187223	2.443861
51	6	0	-6.607781	3.747797	0.964976
52	6	0	-5.608006	4.296741	1.756377
53	6	0	-5.266982	5.630586	1.640086
54	6	0	-5.905494	6.434821	0.691289
55	6	0	-6.908481	5.867830	-0.075668
56	6	0	-7.306901	4.544364	0.055948
57	6	0	-5.450674	7.871655	0.544523
58	6	0	-6.533747	8.822263	0.032417
59	1	0	-5.101862	3.662349	2.467987
60	1	0	-7.422618	6.490352	-0.786974
61	1	0	-5.182918	8.228530	1.545291
62	1	0	-7.416076	8.750372	0.664588
63	1	0	-6.823319	8.609220	-0.991527
64	1	0	-6.161955	9.844054	0.067028
65	1	0	-3.379489	7.624287	1.999693
66	1	0	-0.046991	8.154053	-2.353200
67	1	0	-6.624140	0.138764	-5.058405
68	1	0	-7.855378	0.249240	-0.781481
69	1	0	-1.245495	6.569730	-3.722922
70	1	0	-5.088706	1.895532	-5.449967
71	1	0	-7.454157	2.049497	0.472121
72	1	0	-3.969670	5.518717	3.082444
73	8	0	2.206043	-7.045052	-0.312432
74	8	0	5.701816	-4.818944	-2.579541
75	6	0	3.551857	-6.832842	-0.412153
76	6	0	3.958488	-5.948945	-1.402020

77	6	0	5.298003	-5.652564	-1.579628
78	6	0	6.256255	-6.216266	-0.731016
79	6	0	5.827363	-7.109146	0.235148
80	6	0	4.496580	-7.463879	0.399849
81	6	0	7.707126	-5.816035	-0.898539
82	6	0	8.703702	-6.905079	-0.497768
83	1	0	3.215190	-5.490563	-2.035986
84	1	0	6.563341	-7.568698	0.870978
85	1	0	7.870008	-5.635602	-1.967066
86	1	0	8.683126	-7.117607	0.566127
87	1	0	9.711347	-6.584443	-0.754062
88	1	0	8.481340	-7.822403	-1.038020
89	8	0	6.921688	-1.054810	3.834113
90	8	0	3.536707	-3.561371	5.986559
91	6	0	6.494922	-2.290465	4.255720
92	6	0	5.252197	-2.328805	4.870600
93	6	0	4.738689	-3.519942	5.352764
94	6	0	5.473538	-4.703150	5.208140
95	6	0	6.704304	-4.637549	4.580193
96	6	0	7.253250	-3.452027	4.109944
97	6	0	4.879584	-5.994383	5.729219
98	6	0	5.921678	-7.036685	6.139576
99	1	0	4.686524	-1.415090	4.966749
100	1	0	7.271972	-5.544777	4.472199
101	1	0	4.325023	-5.745978	6.640860
102	1	0	5.421519	-7.873251	6.622774
103	1	0	6.626914	-6.598495	6.842676
104	1	0	6.474029	-7.427219	5.290931
105	8	0	1.979405	-5.778740	5.941657
106	8	0	1.316134	-8.275288	1.940814
107	6	0	2.524945	-6.462716	4.885273
108	6	0	1.653303	-7.050682	3.979510
109	6	0	2.141249	-7.721046	2.870167
110	6	0	3.522077	-7.793613	2.651217
111	6	0	4.367527	-7.195066	3.566758
112	6	0	3.906419	-6.558713	4.708887
113	6	0	4.055020	-8.496616	1.418629
114	6	0	5.137843	-9.518138	1.770108
115	1	0	0.588531	-6.972131	4.136862
116	1	0	5.428664	-7.217518	3.380109
117	1	0	3.229925	-9.070735	0.981075
118	1	0	5.959781	-9.076507	2.324856

119	1	0	5.531827	-9.969978	0.862349
120	1	0	4.702925	-10.300153	2.388533
121	8	0	7.791240	-3.182942	-2.158420
122	8	0	8.885122	-1.028951	1.933637
123	6	0	8.037330	-3.298971	-0.818258
124	6	0	8.360464	-2.139709	-0.126336
125	6	0	8.580692	-2.173956	1.239311
126	6	0	8.449276	-3.372240	1.944800
127	6	0	8.131682	-4.514206	1.228769
128	6	0	7.963771	-4.521684	-0.147396
129	6	0	8.621472	-3.395970	3.451790
130	6	0	9.567558	-4.510343	3.901432
131	1	0	8.438115	-1.209179	-0.669226
132	1	0	8.000402	-5.437251	1.767887
133	1	0	9.104973	-2.457208	3.747804
134	1	0	10.558136	-4.326880	3.490456
135	1	0	9.244677	-5.489615	3.563545
136	1	0	9.636842	-4.522006	4.986812
137	1	0	1.973518	-7.592699	0.468331
138	1	0	4.916958	-4.531746	-3.123499
139	1	0	7.721056	-1.134149	3.276213
140	1	0	3.049154	-2.697900	5.886541
141	1	0	2.567548	-5.023625	6.149145
142	1	0	0.356269	-8.161497	2.172900
143	1	0	7.135664	-3.867323	-2.417455
144	1	0	8.774476	-0.246951	1.356494
145	8	0	8.119321	-0.835222	-3.499359
146	8	0	4.736815	-2.578046	-6.321766
147	6	0	7.318210	-0.707707	-4.599909
148	6	0	6.413246	-1.694200	-4.947076
149	6	0	5.611907	-1.560575	-6.074301
150	6	0	5.734543	-0.432743	-6.890880
151	6	0	6.608932	0.564892	-6.485690
152	6	0	7.412683	0.458562	-5.364280
153	6	0	4.950406	-0.312342	-8.185958
154	6	0	5.779177	0.292321	-9.321320
155	1	0	6.326294	-2.586018	-4.346037
156	1	0	6.676534	1.459333	-7.079778
157	1	0	4.684646	-1.322189	-8.517994
158	1	0	6.073653	1.318235	-9.127760
159	1	0	5.197687	0.277232	-10.240467
160	1	0	6.681392	-0.297314	-9.468177

161	8	0	0.352004	4.816502	-6.020358
162	8	0	3.472458	6.488650	-2.893393
163	6	0	1.650334	5.055500	-5.670567
164	6	0	1.961688	5.646572	-4.460190
165	6	0	3.280768	5.902468	-4.109449
166	6	0	4.316133	5.571068	-4.988368
167	6	0	3.976306	4.932949	-6.172924
168	6	0	2.669169	4.676714	-6.548620
169	6	0	5.762393	5.906284	-4.663733
170	6	0	6.529820	6.434273	-5.877077
171	1	0	1.176529	5.920400	-3.772602
172	1	0	4.766962	4.635442	-6.839551
173	1	0	5.767431	6.720027	-3.930102
174	1	0	6.609286	5.704162	-6.675387
175	1	0	7.536250	6.716023	-5.575242
176	1	0	6.024276	7.312575	-6.272278
177	8	0	2.543443	-1.661565	-7.699066
178	8	0	0.045452	2.295916	-7.037694
179	6	0	2.489801	-0.298142	-7.681093
180	6	0	1.310222	0.361871	-7.387163
181	6	0	1.248981	1.748737	-7.382753
182	6	0	2.378786	2.498404	-7.721402
183	6	0	3.562856	1.811378	-7.949815
184	6	0	3.653985	0.430430	-7.937575
185	6	0	2.304047	4.008572	-7.858053
186	6	0	3.123506	4.532188	-9.039566
187	1	0	0.419470	-0.201531	-7.160884
188	1	0	4.450519	2.380708	-8.162946
189	1	0	1.263870	4.276163	-8.076091
190	1	0	2.808544	4.031643	-9.952542
191	1	0	4.189216	4.372349	-8.915759
192	1	0	2.955149	5.601109	-9.150050
193	8	0	5.851242	5.614466	-1.881630
194	8	0	8.047057	1.428128	-2.027730
195	6	0	6.409424	4.609655	-2.615089
196	6	0	6.950430	3.497743	-1.994730
197	6	0	7.551795	2.491186	-2.736419
198	6	0	7.639625	2.599647	-4.125814
199	6	0	7.038685	3.698458	-4.724461
200	6	0	6.425980	4.712277	-4.008549
201	6	0	8.374745	1.551682	-4.942315
202	6	0	9.147317	2.150285	-6.119432

203	1	0	6.910549	3.415259	-0.919847
204	1	0	7.065057	3.773832	-5.797240
205	1	0	9.130146	1.088221	-4.297574
206	1	0	9.824223	2.921459	-5.758409
207	1	0	8.498066	2.591386	-6.868152
208	1	0	9.731341	1.369264	-6.601000
209	1	0	7.984503	-1.708141	-3.070611
210	1	0	4.042076	-2.289664	-6.946787
211	1	0	-0.241290	5.126607	-5.302366
212	1	0	4.385733	6.342414	-2.578422
213	1	0	1.638255	-2.025986	-7.601709
214	1	0	0.140082	3.247147	-6.828149
215	1	0	5.847566	5.363871	-0.934034
216	1	0	8.191533	0.655773	-2.615952
217	8	0	-6.949708	1.703437	3.801817
218	8	0	-7.523721	-2.588839	1.782072
219	6	0	-7.044108	0.340908	3.907225
220	6	0	-7.217106	-0.441805	2.779015
221	6	0	-7.333143	-1.817726	2.887382
222	6	0	-7.256406	-2.432589	4.141777
223	6	0	-7.042069	-1.629968	5.249349
224	6	0	-6.956315	-0.248997	5.170618
225	6	0	-7.378623	-3.940486	4.245644
226	6	0	-8.280726	-4.379943	5.400027
227	1	0	-7.261567	0.018577	1.803831
228	1	0	-6.943519	-2.099666	6.212892
229	1	0	-7.871577	-4.291319	3.331938
230	1	0	-9.285461	-3.995731	5.237722
231	1	0	-7.937166	-4.017058	6.363194
232	1	0	-8.323653	-5.466200	5.438408
233	8	0	-0.676253	-5.848010	6.500455
234	8	0	0.101011	-1.362117	7.819905
235	6	0	-1.145430	-4.664397	6.986040
236	6	0	-0.307320	-3.581696	7.182472
237	6	0	-0.794128	-2.392662	7.709379
238	6	0	-2.132739	-2.293799	8.095959
239	6	0	-2.967584	-3.364877	7.807209
240	6	0	-2.512835	-4.550446	7.259398
241	6	0	-2.646822	-1.076654	8.844786
242	6	0	-3.539355	-1.469323	10.025205
243	1	0	0.738275	-3.653710	6.927208
244	1	0	-4.017278	-3.271240	8.026724

245	1	0	-1.785299	-0.560324	9.283925
246	1	0	-2.986374	-2.122571	10.696402
247	1	0	-4.438659	-1.990311	9.714971
248	1	0	-3.835684	-0.575866	10.570687
249	8	0	-1.247597	1.083333	7.722128
250	8	0	-4.988136	2.729558	5.346657
251	6	0	-2.571418	0.969610	7.394012
252	6	0	-3.167514	1.888014	6.549849
253	6	0	-4.505500	1.775902	6.198999
254	6	0	-5.279166	0.734607	6.718013
255	6	0	-4.648858	-0.185765	7.543415
256	6	0	-3.315936	-0.094004	7.908262
257	6	0	-6.757430	0.629545	6.391036
258	6	0	-7.598570	0.181762	7.587752
259	1	0	-2.592675	2.714661	6.166386
260	1	0	-5.228307	-1.004319	7.932326
261	1	0	-7.119284	1.630860	6.130798
262	1	0	-7.363464	-0.826011	7.913120
263	1	0	-8.651858	0.209778	7.318105
264	1	0	-7.433140	0.857223	8.424496
265	8	0	-5.827538	-4.655320	1.871592
266	8	0	-2.213320	-6.300734	4.318810
267	6	0	-5.315540	-4.877298	3.117631
268	6	0	-4.063490	-5.466603	3.172374
269	6	0	-3.447589	-5.729312	4.386104
270	6	0	-4.099517	-5.412871	5.582545
271	6	0	-5.350021	-4.820548	5.496994
272	6	0	-5.992283	-4.556657	4.297219
273	6	0	-3.441248	-5.700784	6.921249
274	6	0	-4.435213	-6.009359	8.041490
275	1	0	-3.552326	-5.715269	2.255779
276	1	0	-5.859278	-4.571149	6.411115
277	1	0	-2.825547	-6.600591	6.811515
278	1	0	-5.095166	-6.817866	7.734949
279	1	0	-5.044167	-5.152164	8.310065
280	1	0	-3.889706	-6.321444	8.929334
281	1	0	-6.964853	1.956190	2.853612
282	1	0	-7.318373	-2.065115	0.962315
283	1	0	0.289975	-5.799857	6.330344
284	1	0	-0.368035	-0.516531	7.949375
285	1	0	-0.869908	1.852940	7.256158
286	1	0	-5.799041	2.415422	4.890987

287	1	0	-6.526054	-3.961083	1.890408
288	1	0	-1.748078	-6.256868	5.178629
289	8	0	-5.530593	-6.550519	-0.052422
290	8	0	-7.463531	-3.103892	-2.750525
291	6	0	-5.827683	-6.019345	-1.275408
292	6	0	-6.512179	-4.821005	-1.390432
293	6	0	-6.801270	-4.291582	-2.638048
294	6	0	-6.415279	-4.970953	-3.798731
295	6	0	-5.703524	-6.151145	-3.655565
296	6	0	-5.408406	-6.704367	-2.419866
297	6	0	-6.754099	-4.389251	-5.158496
298	6	0	-7.251405	-5.448927	-6.143267
299	1	0	-6.811979	-4.281667	-0.504441
300	1	0	-5.358801	-6.656814	-4.541548
301	1	0	-7.592041	-3.697503	-5.016173
302	1	0	-7.479678	-4.982521	-7.099347
303	1	0	-8.157234	-5.906858	-5.752134
304	1	0	-6.525988	-6.237787	-6.313122
305	8	0	-0.000682	-2.614027	-7.399366
306	8	0	1.934723	-6.020734	-4.840734
307	6	0	-0.158769	-3.865343	-6.870364
308	6	0	0.901579	-4.370317	-6.137522
309	6	0	0.835666	-5.622647	-5.547114
310	6	0	-0.317226	-6.400042	-5.695613
311	6	0	-1.372377	-5.858355	-6.414466
312	6	0	-1.321130	-4.620554	-7.036411
313	6	0	-0.413840	-7.790743	-5.092909
314	6	0	-1.037094	-8.804538	-6.053679
315	1	0	1.793310	-3.776075	-6.021469
316	1	0	-2.276459	-6.435747	-6.503656
317	1	0	0.602097	-8.149980	-4.895133
318	1	0	-1.050406	-9.786830	-5.586679
319	1	0	-0.441245	-8.857109	-6.962368
320	1	0	-2.053527	-8.549147	-6.333953
321	8	0	0.993206	-7.412146	-2.711883
322	8	0	-2.882334	-7.261229	-0.015496
323	6	0	-0.365143	-7.478603	-2.603773
324	6	0	-0.990195	-7.327445	-1.380193
325	6	0	-2.370052	-7.440292	-1.264725
326	6	0	-3.143028	-7.742982	-2.391139
327	6	0	-2.494449	-7.827323	-3.615581
328	6	0	-1.123542	-7.704539	-3.756957

329	6	0	-4.635415	-7.999116	-2.267075
330	6	0	-5.133387	-9.091349	-3.216458
331	1	0	-0.406039	-7.124013	-0.495861
332	1	0	-3.083947	-8.022890	-4.494216
333	1	0	-4.828657	-8.374299	-1.255813
334	1	0	-5.077349	-8.798153	-4.259662
335	1	0	-6.172815	-9.318205	-2.989514
336	1	0	-4.540561	-9.993275	-3.081428
337	8	0	-6.341789	-1.546874	-4.619728
338	8	0	-2.361279	-1.375777	-7.152800
339	6	0	-5.446558	-2.234580	-5.382307
340	6	0	-4.374446	-1.506444	-5.879864
341	6	0	-3.415559	-2.105432	-6.677298
342	6	0	-3.521902	-3.462370	-6.998214
343	6	0	-4.591644	-4.170572	-6.475678
344	6	0	-5.573861	-3.592930	-5.684797
345	6	0	-2.470979	-4.102816	-7.882794
346	6	0	-3.035126	-5.179077	-8.812285
347	1	0	-4.289422	-0.461489	-5.625398
348	1	0	-4.672214	-5.217702	-6.708689
349	1	0	-2.083845	-3.315706	-8.539880
350	1	0	-3.842395	-4.759557	-9.408841
351	1	0	-3.420639	-6.038561	-8.274342
352	1	0	-2.250400	-5.527163	-9.480416
353	1	0	-5.746573	-5.905044	0.653936
354	1	0	-7.326958	-2.567459	-1.928713
355	1	0	-0.878896	-2.182472	-7.490487
356	1	0	1.672914	-6.662277	-4.148848
357	1	0	1.392544	-7.262925	-1.827231
358	1	0	-3.855578	-7.156002	-0.041589
359	1	0	-6.834209	-2.151189	-4.016500
360	1	0	-2.244025	-0.557387	-6.604208
361	8	0	5.788621	4.872321	0.745736
362	8	0	1.786508	7.265853	0.963526
363	6	0	5.046953	5.778097	1.457958
364	6	0	3.814400	6.113648	0.923828
365	6	0	2.982064	7.015958	1.566734
366	6	0	3.394887	7.617296	2.759570
367	6	0	4.632858	7.260357	3.271456
368	6	0	5.484440	6.359935	2.648335
369	6	0	2.482997	8.610058	3.456201
370	6	0	3.208208	9.576814	4.392973

371	1	0	3.490364	5.663700	-0.000750
372	1	0	4.958736	7.721450	4.186929
373	1	0	2.005921	9.231233	2.689398
374	1	0	2.505065	10.329536	4.742571
375	1	0	4.015194	10.075813	3.861192
376	1	0	3.619150	9.077121	5.264827
377	8	0	-0.226422	3.236739	6.240091
378	8	0	3.778999	0.844372	6.138626
379	6	0	1.129512	3.281249	6.475477
380	6	0	1.824900	2.115944	6.208049
381	6	0	3.194537	2.042249	6.411676
382	6	0	3.885061	3.160964	6.888474
383	6	0	3.158940	4.313648	7.144581
384	6	0	1.785825	4.406246	6.970313
385	6	0	5.386565	3.090401	7.090297
386	6	0	5.927666	4.090604	8.112620
387	1	0	1.293650	1.256712	5.830647
388	1	0	3.683517	5.173892	7.520391
389	1	0	5.632554	2.095808	7.479375
390	1	0	6.979493	3.881514	8.294061
391	1	0	5.386924	3.993211	9.051398
392	1	0	5.849172	5.117024	7.768107
393	8	0	-0.152462	8.470028	2.495979
394	8	0	-1.540454	5.576902	6.060679
395	6	0	0.097184	7.796824	3.654694
396	6	0	-0.882393	7.046618	4.285213
397	6	0	-0.591454	6.355276	5.450261
398	6	0	0.688159	6.407999	6.006650
399	6	0	1.660570	7.128646	5.333748
400	6	0	1.393972	7.839641	4.177196
401	6	0	1.000247	5.663547	7.291312
402	6	0	1.681371	6.573027	8.314884
403	1	0	-1.875037	6.990038	3.862611
404	1	0	2.668192	7.120221	5.715388
405	1	0	0.047617	5.362756	7.744145
406	1	0	2.589028	7.023711	7.926212
407	1	0	1.926445	6.007379	9.211131
408	1	0	1.001208	7.377384	8.585869
409	8	0	6.483605	0.904053	5.694351
410	8	0	7.879929	3.640960	2.019336
411	6	0	6.602881	2.125707	5.097559
412	6	0	7.213788	2.261964	3.861211

413	6	0	7.303316	3.504349	3.255289
414	6	0	6.768107	4.634844	3.877426
415	6	0	6.141370	4.467496	5.101382
416	6	0	6.066565	3.242922	5.742949
417	6	0	6.847013	5.994820	3.209859
418	6	0	7.432740	7.047278	4.152215
419	1	0	7.618520	1.391073	3.366135
420	1	0	5.677455	5.323221	5.563630
421	1	0	7.550550	5.917137	2.371923
422	1	0	6.871286	7.129822	5.077582
423	1	0	7.446867	8.018442	3.662718
424	1	0	8.453630	6.770942	4.406627
425	1	0	6.594838	4.611192	1.233246
426	1	0	1.204162	7.813254	1.525520
427	1	0	-0.635045	4.127966	6.340721
428	1	0	4.755931	0.897548	6.149314
429	1	0	-1.087848	8.366750	2.215402
430	1	0	-2.286371	5.409916	5.436004
431	1	0	6.735536	0.197224	5.062026
432	1	0	8.087105	2.758318	1.647421
433	8	0	-1.775377	0.727535	-5.583109
434	1	0	-2.577890	1.268727	-5.499177
435	1	0	-1.157913	1.247481	-6.125886
436	8	0	7.899390	1.222294	0.674704
437	1	0	8.054561	1.381805	-0.278499
438	1	0	6.970935	0.986644	0.754617
439	8	0	-1.296982	-7.980341	2.277801
440	1	0	-1.789568	-7.790983	1.467092
441	1	0	-1.667640	-7.403151	2.962322
442	8	0	2.063358	-1.363288	5.807024
443	1	0	2.615414	-0.581511	5.958380
444	1	0	1.423878	-1.397292	6.537873
445	8	0	3.733360	-4.001078	-4.133592
446	1	0	4.133926	-3.619645	-4.932164
447	1	0	3.140310	-4.713929	-4.428002
448	8	0	-1.312197	2.731788	3.677844
449	1	0	-0.759971	2.810528	4.472247
450	1	0	-1.627477	1.823491	3.648945
451	8	0	1.484272	8.115912	-1.683489
452	1	0	1.605187	7.789289	-0.778444
453	1	0	2.140538	7.645359	-2.216607
454	8	0	-3.238874	4.538830	4.259382

455	1	0	-2.561717	3.928359	3.896854
456	1	0	-3.900886	3.973098	4.698935
457	6	0	-2.159791	0.011409	1.292151
458	6	0	-1.034071	-0.483927	1.936067
459	6	0	-1.058996	-0.719099	3.302511
460	6	0	-2.216688	-0.486764	4.027825
461	6	0	-3.343971	0.006963	3.386031
462	6	0	-3.314809	0.268012	2.027369
463	6	0	-2.212760	0.184849	-0.213981
464	6	0	-2.756024	-1.084549	-0.874441
465	6	0	-2.908753	1.484472	-0.568140
466	6	0	-4.007753	1.562703	-1.409498
467	6	0	-4.530592	2.802394	-1.739402
468	6	0	-3.971884	3.963136	-1.236844
469	6	0	-2.893287	3.887198	-0.371695
470	6	0	-2.365310	2.655163	-0.036150
471	6	0	-2.696725	-1.216380	-2.256875
472	6	0	-3.068042	-2.400595	-2.867790
473	6	0	-3.511006	-3.467612	-2.105410
474	6	0	-3.603964	-3.329573	-0.732865
475	6	0	-3.223824	-2.150685	-0.116331
476	17	0	-6.505973	-1.251440	-0.643536
477	1	0	-0.142869	-0.707732	1.371294
478	1	0	-0.179876	-1.107458	3.793830
479	1	0	-2.253906	-0.703872	5.084289
480	1	0	-4.252691	0.164308	3.944624
481	1	0	-4.197113	0.637451	1.527586
482	1	0	-4.464279	0.665672	-1.797505
483	1	0	-5.378531	2.860203	-2.397763
484	1	0	-4.381323	4.922423	-1.509845
485	1	0	-2.462916	4.787214	0.039160
486	1	0	-1.526653	2.594512	0.643752
487	1	0	-2.349176	-0.399806	-2.875725
488	1	0	-3.004773	-2.492124	-3.940344
489	1	0	-3.781497	-4.395504	-2.584550
490	1	0	-3.968120	-4.139788	-0.122816
491	1	0	-3.306269	-2.073237	0.955556
492	6	0	0.602808	-1.801169	-2.503965
493	6	0	1.623983	-1.964035	-1.673040
494	6	0	2.654755	-0.878545	-1.738238
495	6	0	1.948615	0.449982	-1.392430
496	6	0	0.793444	0.683176	-2.388885

497	6	0	0.684940	-0.575385	-3.348134
498	6	0	2.001425	-0.613398	-4.138254
499	6	0	3.176687	-0.848529	-3.183320
500	6	0	-0.521212	0.845548	-1.775932
501	1	0	-1.259671	1.472612	-2.278112
502	8	0	-0.824758	0.241626	-0.709756
503	6	0	2.893352	1.648590	-1.377168
504	1	0	-0.227164	-2.480162	-2.599045
505	1	0	1.736511	-2.799494	-1.004387
506	1	0	3.474843	-1.053617	-1.040851
507	1	0	1.527668	0.338722	-0.388361
508	1	0	0.996453	1.541609	-3.032980
509	1	0	-0.161284	-0.453301	-4.023971
510	1	0	1.924020	-1.430254	-4.854295
511	1	0	2.124958	0.311322	-4.702453
512	1	0	3.937948	-0.078932	-3.300131
513	1	0	3.641741	-1.810392	-3.390120
514	1	0	3.722557	1.461016	-0.700124
515	1	0	3.297109	1.853382	-2.365098
516	1	0	2.370270	2.537137	-1.031133

6-*exo*@$\mathbf{C_M}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.073658	5.974065	3.465302
2	8	0	-1.351215	8.330003	0.373395
3	6	0	-3.994437	6.714277	2.307042
4	6	0	-2.702103	7.125294	1.960666
5	6	0	-2.559919	7.848380	0.771290
6	6	0	-3.658394	8.112445	-0.086237
7	6	0	-4.925458	7.698078	0.325307
8	6	0	-5.132422	7.031815	1.541915
9	6	0	-3.419203	8.812162	-1.406833
10	6	0	-4.467399	9.889029	-1.701275
11	1	0	-1.850048	6.881175	2.588340
12	1	0	-5.785582	7.906104	-0.314826
13	1	0	-2.423840	9.348063	-1.332767
14	1	0	-4.478249	10.645509	-0.906331
15	1	0	-5.481198	9.483578	-1.777947

16	1	0	-4.246473	10.401893	-2.645347
17	8	0	-4.942725	3.339515	-5.919473
18	8	0	-7.804527	1.405895	-2.556268
19	6	0	-5.803672	3.444158	-4.852083
20	6	0	-6.325632	2.303215	-4.239718
21	6	0	-7.232457	2.496682	-3.194500
22	6	0	-7.619106	3.776116	-2.743104
23	6	0	-7.027271	4.883533	-3.361674
24	6	0	-6.121421	4.751178	-4.421126
25	6	0	-8.645198	3.890991	-1.637175
26	6	0	-9.648898	5.022032	-1.885385
27	1	0	-6.039652	1.298589	-4.557218
28	1	0	-7.283866	5.884647	-3.010167
29	1	0	-9.244724	2.929492	-1.635739
30	1	0	-9.176104	6.008244	-1.918437
31	1	0	-10.409509	5.048572	-1.095518
32	1	0	-10.167221	4.875850	-2.841580
33	8	0	-0.889257	7.577077	-2.170470
34	8	0	-2.753217	5.000310	-5.575547
35	6	0	-2.042159	7.237413	-2.834802
36	6	0	-1.859623	6.307609	-3.864546
37	6	0	-2.996911	5.907344	-4.574214
38	6	0	-4.285759	6.409972	-4.289787
39	6	0	-4.406786	7.333781	-3.245916
40	6	0	-3.302002	7.784012	-2.512922
41	6	0	-5.476372	5.940169	-5.099529
42	6	0	-6.476769	7.062665	-5.391009
43	1	0	-0.877095	5.908352	-4.093025
44	1	0	-5.397248	7.723394	-2.999376
45	1	0	-5.088527	5.590095	-6.104761
46	1	0	-6.932689	7.469550	-4.483039
47	1	0	-7.292300	6.697286	-6.028200
48	1	0	-5.990360	7.893495	-5.916297
49	8	0	-8.119355	1.601460	0.103245
50	8	0	-6.264025	4.320602	3.512153
51	6	0	-7.773228	2.858030	0.512526
52	6	0	-7.210235	2.921011	1.794631
53	6	0	-6.820647	4.178012	2.264014
54	6	0	-6.967681	5.354131	1.497042
55	6	0	-7.537915	5.234107	0.224902
56	6	0	-7.969300	4.006345	-0.287298
57	6	0	-6.512179	6.682146	2.057094

58	6	0	-7.529137	7.801215	1.810125
59	1	0	-7.080944	2.020781	2.387315
60	1	0	-7.653792	6.131723	-0.387079
61	1	0	-6.434787	6.565474	3.181807
62	1	0	-8.500735	7.546674	2.251958
63	1	0	-7.696905	7.992692	0.745616
64	1	0	-7.192673	8.742079	2.262433
65	1	0	-5.024205	5.626709	3.638634
66	1	0	-0.580988	8.201422	1.096359
67	1	0	-4.808007	2.371178	-6.207213
68	1	0	-7.269048	0.571066	-2.739997
69	1	0	-1.060435	8.185724	-1.362347
70	1	0	-3.613350	4.599472	-5.954721
71	1	0	-8.315843	1.549052	-0.909321
72	1	0	-6.041607	3.411743	3.943793
73	8	0	3.399320	-6.381148	-2.606483
74	8	0	7.055153	-3.369944	-2.707966
75	6	0	4.659582	-6.072565	-2.148203
76	6	0	5.181101	-4.875686	-2.653977
77	6	0	6.451550	-4.489939	-2.212735
78	6	0	7.180350	-5.245469	-1.262873
79	6	0	6.614734	-6.437917	-0.804604
80	6	0	5.371454	-6.899885	-1.256375
81	6	0	8.515486	-4.730462	-0.775144
82	6	0	9.523013	-5.844978	-0.476851
83	1	0	4.605482	-4.270562	-3.349420
84	1	0	7.164328	-7.036575	-0.074623
85	1	0	8.960876	-4.112756	-1.613843
86	1	0	9.194538	-6.506388	0.331088
87	1	0	10.492022	-5.425103	-0.180530
88	1	0	9.687341	-6.467936	-1.364905
89	8	0	5.645777	-2.105596	4.969694
90	8	0	2.323147	-5.479828	4.982481
91	6	0	5.335873	-3.432933	4.742996
92	6	0	3.987133	-3.748322	4.940052
93	6	0	3.607005	-5.082596	4.759393
94	6	0	4.537472	-6.082193	4.376221
95	6	0	5.865197	-5.702481	4.179541
96	6	0	6.305523	-4.385135	4.380009
97	6	0	4.051617	-7.499651	4.168667
98	6	0	5.098648	-8.560169	4.522129
99	1	0	3.268961	-2.975910	5.203876

100	1	0	6.590252	-6.456933	3.865647
101	1	0	3.182623	-7.657218	4.879672
102	1	0	4.680029	-9.568554	4.412220
103	1	0	5.434332	-8.449226	5.559964
104	1	0	5.983774	-8.508556	3.880170
105	8	0	1.238425	-7.405535	3.520769
106	8	0	2.035448	-8.239823	-1.090967
107	6	0	2.142690	-7.633662	2.511708
108	6	0	1.586367	-7.840652	1.244725
109	6	0	2.477370	-8.046211	0.186402
110	6	0	3.881974	-8.041224	0.366794
111	6	0	4.378195	-7.842418	1.657169
112	6	0	3.530251	-7.664456	2.757193
113	6	0	4.791938	-8.231151	-0.826780
114	6	0	5.861838	-9.297612	-0.568671
115	1	0	0.511503	-7.815193	1.093686
116	1	0	5.458367	-7.824637	1.813454
117	1	0	4.161350	-8.617349	-1.683778
118	1	0	6.516472	-9.045006	0.270965
119	1	0	6.494531	-9.440131	-1.452672
120	1	0	5.393166	-10.262248	-0.335270
121	8	0	8.473120	-1.840398	-0.998063
122	8	0	7.940270	-1.245715	3.688877
123	6	0	8.328237	-2.415574	0.238086
124	6	0	8.217762	-1.513880	1.304657
125	6	0	8.053144	-2.059049	2.580934
126	6	0	7.983626	-3.448053	2.815418
127	6	0	8.110336	-4.301220	1.711893
128	6	0	8.313981	-3.815125	0.416209
129	6	0	7.753057	-3.972665	4.217156
130	6	0	8.743280	-5.082065	4.584493
131	1	0	8.254693	-0.444381	1.133380
132	1	0	8.046686	-5.380396	1.869189
133	1	0	7.945714	-3.123197	4.939403
134	1	0	9.775909	-4.717456	4.516331
135	1	0	8.664157	-5.953396	3.926324
136	1	0	8.579235	-5.429305	5.611798
137	1	0	3.001000	-7.213699	-2.155565
138	1	0	6.395797	-2.773311	-3.291130
139	1	0	6.609593	-1.883640	4.712634
140	1	0	1.634391	-4.668549	4.998430
141	1	0	1.690833	-7.040331	4.365132

142	1	0	0.980322	-8.285892	-1.166575
143	1	0	8.249104	-2.497718	-1.760299
144	1	0	7.890140	-0.256044	3.442641
145	8	0	8.662358	0.943436	-1.049791
146	8	0	6.605078	0.423878	-5.298743
147	6	0	8.187628	1.472148	-2.228220
148	6	0	7.596465	0.655142	-3.194623
149	6	0	7.165564	1.271219	-4.376010
150	6	0	7.317910	2.655930	-4.607932
151	6	0	7.877327	3.430559	-3.585614
152	6	0	8.334237	2.866417	-2.389263
153	6	0	6.895821	3.254486	-5.933337
154	6	0	7.954234	4.205641	-6.501072
155	1	0	7.472697	-0.414634	-3.044518
156	1	0	7.969533	4.508962	-3.730139
157	1	0	6.798157	2.405015	-6.677610
158	1	0	8.134016	5.071607	-5.856589
159	1	0	7.648007	4.586000	-7.483522
160	1	0	8.913782	3.689245	-6.627991
161	8	0	1.424617	7.549146	-3.715477
162	8	0	3.180332	7.591367	0.695358
163	6	0	2.484976	7.504138	-2.844139
164	6	0	2.288915	7.562171	-1.462184
165	6	0	3.432087	7.559002	-0.653297
166	6	0	4.738727	7.534642	-1.186433
167	6	0	4.871491	7.414505	-2.576180
168	6	0	3.765998	7.398454	-3.431019
169	6	0	5.938385	7.659957	-0.271956
170	6	0	7.000071	8.612122	-0.832445
171	1	0	1.293502	7.594639	-1.027819
172	1	0	5.872220	7.339325	-3.006612
173	1	0	5.579657	8.120235	0.699411
174	1	0	7.426754	8.261399	-1.777322
175	1	0	7.828118	8.733426	-0.123426
176	1	0	6.572372	9.605434	-1.018165
177	8	0	4.590183	1.861416	-6.555224
178	8	0	1.669698	5.447619	-5.516969
179	6	0	4.379588	3.143126	-6.117537
180	6	0	3.087204	3.661764	-6.000565
181	6	0	2.963332	4.996672	-5.595114
182	6	0	4.081189	5.809928	-5.310234
183	6	0	5.349767	5.222323	-5.399196

184	6	0	5.533477	3.898815	-5.809417
185	6	0	3.890195	7.263931	-4.933327
186	6	0	4.976851	8.176488	-5.510947
187	1	0	2.207693	3.060595	-6.217527
188	1	0	6.227180	5.823382	-5.150430
189	1	0	2.912460	7.607039	-5.390454
190	1	0	5.023203	8.084752	-6.603123
191	1	0	5.973176	7.948527	-5.119940
192	1	0	4.765926	9.226850	-5.273900
193	8	0	5.265933	6.360869	2.070263
194	8	0	7.844056	2.483541	1.118459
195	6	0	6.103141	5.649856	1.250442
196	6	0	6.543906	4.368772	1.598133
197	6	0	7.444818	3.745670	0.726896
198	6	0	7.925142	4.363431	-0.443833
199	6	0	7.404936	5.624356	-0.770738
200	6	0	6.501225	6.294461	0.056778
201	6	0	8.978984	3.683439	-1.292185
202	6	0	10.018179	4.668320	-1.838990
203	1	0	6.191949	3.874161	2.497617
204	1	0	7.726598	6.102570	-1.698873
205	1	0	9.544663	2.967631	-0.621770
206	1	0	10.498779	5.223824	-1.024780
207	1	0	9.585526	5.402009	-2.526395
208	1	0	10.804514	4.134553	-2.387987
209	1	0	8.563248	-0.072973	-1.018284
210	1	0	6.115072	0.934468	-6.035265
211	1	0	0.530572	7.638899	-3.231884
212	1	0	4.025693	7.460197	1.249080
213	1	0	3.713997	1.363638	-6.739433
214	1	0	1.602119	6.376812	-5.101713
215	1	0	4.968791	5.821278	2.885867
216	1	0	8.332994	1.986488	0.365921
217	8	0	-8.030396	-0.430244	2.106826
218	8	0	-7.248057	-3.440163	-1.582495
219	6	0	-7.855034	-1.690063	1.581036
220	6	0	-7.595153	-1.868624	0.220720
221	6	0	-7.476718	-3.182998	-0.238343
222	6	0	-7.597117	-4.304409	0.609941
223	6	0	-7.808944	-4.064688	1.970662
224	6	0	-7.948146	-2.768758	2.485504
225	6	0	-7.485783	-5.694120	0.020646

226	6	0	-8.575999	-6.633047	0.548293
227	1	0	-7.491451	-1.024863	-0.462245
228	1	0	-7.872614	-4.913935	2.653509
229	1	0	-7.657004	-5.607043	-1.095060
230	1	0	-9.572307	-6.234014	0.319600
231	1	0	-8.523815	-6.776128	1.631826
232	1	0	-8.498329	-7.622065	0.080561
233	8	0	-1.389465	-8.176241	3.190043
234	8	0	-1.714493	-4.816706	6.536378
235	6	0	-2.129421	-7.333457	3.979899
236	6	0	-1.522478	-6.456109	4.881406
237	6	0	-2.367052	-5.677922	5.682062
238	6	0	-3.771807	-5.772694	5.623855
239	6	0	-4.326031	-6.626555	4.658249
240	6	0	-3.533018	-7.418302	3.825289
241	6	0	-4.624082	-5.004527	6.610794
242	6	0	-5.719988	-5.881841	7.226047
243	1	0	-0.441522	-6.375793	4.960809
244	1	0	-5.412197	-6.677537	4.559759
245	1	0	-3.950345	-4.689497	7.467216
246	1	0	-5.284526	-6.760629	7.717872
247	1	0	-6.434539	-6.248556	6.482462
248	1	0	-6.288575	-5.324412	7.980365
249	8	0	-3.365412	-2.556959	6.956246
250	8	0	-6.551387	-0.122958	4.426711
251	6	0	-4.508397	-2.513245	6.195671
252	6	0	-4.966557	-1.306841	5.659511
253	6	0	-6.153754	-1.339491	4.917998
254	6	0	-6.881649	-2.530912	4.710065
255	6	0	-6.354492	-3.715827	5.237292
256	6	0	-5.177295	-3.739893	5.993112
257	6	0	-8.192212	-2.495566	3.952490
258	6	0	-9.248988	-3.427227	4.553976
259	1	0	-4.436661	-0.369931	5.809350
260	1	0	-6.887266	-4.653750	5.062596
261	1	0	-8.607985	-1.445440	4.039819
262	1	0	-8.960456	-4.481886	4.505675
263	1	0	-10.201426	-3.327109	4.017669
264	1	0	-9.432309	-3.183335	5.607291
265	8	0	-5.300244	-5.288602	-1.885659
266	8	0	-2.221259	-7.761744	0.586231
267	6	0	-5.086594	-6.019761	-0.748300

268	6	0	-3.794777	-6.544575	-0.625825
269	6	0	-3.505834	-7.286110	0.525392
270	6	0	-4.464192	-7.522540	1.536551
271	6	0	-5.738407	-6.972152	1.361443
272	6	0	-6.088583	-6.237647	0.224285
273	6	0	-4.104308	-8.333809	2.762440
274	6	0	-5.266598	-9.180213	3.290728
275	1	0	-3.039137	-6.358233	-1.382004
276	1	0	-6.491083	-7.129601	2.137683
277	1	0	-3.292672	-9.063201	2.460975
278	1	0	-5.643342	-9.854447	2.511687
279	1	0	-6.109491	-8.573350	3.635646
280	1	0	-4.941394	-9.798106	4.136988
281	1	0	-8.020980	0.288805	1.386213
282	1	0	-6.907846	-2.609822	-2.043591
283	1	0	-0.385540	-8.040374	3.311643
284	1	0	-2.363210	-4.183000	7.000335
285	1	0	-2.933767	-1.640973	7.046765
286	1	0	-7.331268	-0.203379	3.770900
287	1	0	-6.179383	-4.745751	-1.855322
288	1	0	-2.009494	-8.203993	1.479892
289	8	0	-4.022485	-5.978960	-4.305668
290	8	0	-5.662748	-1.702909	-5.825455
291	6	0	-4.088660	-4.958989	-5.224019
292	6	0	-4.862720	-3.820571	-4.988016
293	6	0	-4.889788	-2.844319	-5.988602
294	6	0	-4.168040	-2.963398	-7.194760
295	6	0	-3.387285	-4.112204	-7.366802
296	6	0	-3.333456	-5.129210	-6.406139
297	6	0	-4.262765	-1.860541	-8.227071
298	6	0	-4.312839	-2.399221	-9.660624
299	1	0	-5.410518	-3.678667	-4.056308
300	1	0	-2.801716	-4.220497	-8.281813
301	1	0	-5.245285	-1.324198	-8.054172
302	1	0	-4.431685	-1.580143	-10.380345
303	1	0	-5.162872	-3.081163	-9.788269
304	1	0	-3.408309	-2.949443	-9.937363
305	8	0	2.083839	0.746546	-6.790150
306	8	0	3.792713	-3.425091	-5.646704
307	6	0	2.084275	-0.597531	-7.079682
308	6	0	2.898536	-1.366201	-6.243050
309	6	0	2.945385	-2.744935	-6.480365

310	6	0	2.192171	-3.364355	-7.502979
311	6	0	1.392156	-2.543196	-8.305360
312	6	0	1.338275	-1.154184	-8.139142
313	6	0	2.242016	-4.868058	-7.683906
314	6	0	2.077607	-5.310229	-9.140567
315	1	0	3.444644	-0.911221	-5.419105
316	1	0	0.792534	-3.001231	-9.095888
317	1	0	3.268128	-5.217112	-7.359795
318	1	0	2.174528	-6.400175	-9.225388
319	1	0	2.847408	-4.857223	-9.776760
320	1	0	1.102659	-5.038600	-9.557758
321	8	0	2.987963	-5.974142	-5.266871
322	8	0	-1.455565	-6.987732	-3.931093
323	6	0	1.634560	-5.999198	-5.506611
324	6	0	0.737895	-6.489752	-4.555025
325	6	0	-0.614721	-6.539320	-4.916951
326	6	0	-1.070053	-6.160957	-6.198980
327	6	0	-0.135383	-5.608923	-7.084272
328	6	0	1.222050	-5.507578	-6.764993
329	6	0	-2.515247	-6.387514	-6.589348
330	6	0	-2.647608	-6.968275	-8.001778
331	1	0	1.065380	-6.808695	-3.569965
332	1	0	-0.477210	-5.250717	-8.057535
333	1	0	-2.937419	-7.168427	-5.884451
334	1	0	-2.276433	-6.288264	-8.774624
335	1	0	-3.697735	-7.184753	-8.234501
336	1	0	-2.085199	-7.905476	-8.092622
337	8	0	-4.566716	0.583447	-6.645039
338	8	0	-0.147554	2.011785	-7.552668
339	6	0	-3.378858	0.317169	-7.267763
340	6	0	-2.396610	1.300226	-7.084115
341	6	0	-1.151633	1.088094	-7.682479
342	6	0	-0.865632	-0.069885	-8.440415
343	6	0	-1.879504	-1.021712	-8.585824
344	6	0	-3.152171	-0.850352	-8.027949
345	6	0	0.512557	-0.256048	-9.036406
346	6	0	0.460065	-0.742383	-10.487851
347	1	0	-2.602491	2.187154	-6.493199
348	1	0	-1.670842	-1.930782	-9.154470
349	1	0	1.015921	0.757446	-9.058826
350	1	0	-0.095269	-0.031226	-11.112659
351	1	0	-0.031574	-1.715001	-10.590477

352	1	0	1.469139	-0.836646	-10.906410
353	1	0	-4.540684	-5.769490	-3.452766
354	1	0	-5.831861	-1.530058	-4.847774
355	1	0	1.367421	1.266896	-7.329915
356	1	0	3.702638	-4.443318	-5.725389
357	1	0	3.220195	-6.259596	-4.309736
358	1	0	-2.439042	-6.914798	-4.198128
359	1	0	-5.182846	-0.246598	-6.590555
360	1	0	-0.345715	2.707896	-6.773217
361	8	0	4.548776	4.628417	4.095310
362	8	0	0.302373	6.542915	4.091812
363	6	0	3.493503	5.060293	4.870130
364	6	0	2.421042	5.583743	4.142212
365	6	0	1.313255	6.037469	4.868238
366	6	0	1.258473	5.981479	6.280072
367	6	0	2.360079	5.440308	6.951228
368	6	0	3.504220	4.993843	6.278237
369	6	0	0.031548	6.484809	7.012341
370	6	0	0.330433	7.013829	8.418045
371	1	0	2.432823	5.609579	3.056343
372	1	0	2.332069	5.371980	8.041591
373	1	0	-0.376130	7.361476	6.424029
374	1	0	-0.579139	7.425335	8.874867
375	1	0	1.076775	7.816675	8.385742
376	1	0	0.705650	6.237303	9.091920
377	8	0	-2.372206	0.074058	6.723011
378	8	0	1.882235	-1.783446	6.981636
379	6	0	-1.128925	0.158818	7.316917
380	6	0	-0.216740	-0.799893	6.869000
381	6	0	1.062842	-0.788671	7.439797
382	6	0	1.446306	0.158035	8.417094
383	6	0	0.492032	1.098684	8.817091
384	6	0	-0.813488	1.107721	8.309249
385	6	0	2.851131	0.140363	8.982046
386	6	0	2.943589	0.673816	10.414590
387	1	0	-0.480348	-1.511891	6.090910
388	1	0	0.769981	1.848675	9.562120
389	1	0	3.185070	-0.939797	9.024293
390	1	0	3.968824	0.577855	10.795118
391	1	0	2.286889	0.109041	11.087369
392	1	0	2.669132	1.730546	10.491918
393	8	0	-2.173111	6.601951	5.353382

394	8	0	-3.863292	2.344730	6.875357
395	6	0	-2.121080	5.477956	6.142557
396	6	0	-3.093592	4.477759	6.051757
397	6	0	-2.966486	3.383971	6.913788
398	6	0	-1.920388	3.277402	7.855303
399	6	0	-0.951623	4.287542	7.873287
400	6	0	-1.025095	5.400308	7.028925
401	6	0	-1.865567	2.085679	8.786025
402	6	0	-1.684029	2.511009	10.246270
403	1	0	-3.910291	4.545501	5.338294
404	1	0	-0.108783	4.199953	8.561944
405	1	0	-2.865414	1.557495	8.732174
406	1	0	-0.756287	3.067344	10.413004
407	1	0	-1.673918	1.639587	10.911848
408	1	0	-2.510359	3.160847	10.562954
409	8	0	4.570613	-1.214917	7.301480
410	8	0	6.272700	2.848988	5.330934
411	6	0	4.626967	0.151833	7.181144
412	6	0	5.475879	0.767657	6.256317
413	6	0	5.474446	2.165155	6.221779
414	6	0	4.666500	2.948127	7.072098
415	6	0	3.814025	2.277194	7.958622
416	6	0	3.778541	0.881962	8.041920
417	6	0	4.723747	4.458957	6.998280
418	6	0	4.936231	5.086599	8.379399
419	1	0	6.096919	0.182535	5.584587
420	1	0	3.151326	2.863385	8.598883
421	1	0	5.628745	4.740136	6.379058
422	1	0	4.129183	4.849573	9.079966
423	1	0	5.004164	6.178881	8.308833
424	1	0	5.869615	4.723743	8.828737
425	1	0	5.294554	4.203198	4.651472
426	1	0	-0.517833	6.816357	4.636648
427	1	0	-3.001311	0.838746	7.023434
428	1	0	2.845222	-1.705919	7.317070
429	1	0	-2.966072	6.583747	4.710723
430	1	0	-4.496901	2.400736	6.042853
431	1	0	5.115831	-1.687910	6.572074
432	1	0	6.756260	2.216704	4.682489
433	8	0	-0.385163	3.442448	-5.388683
434	1	0	-1.212364	3.975822	-5.366810
435	1	0	0.346107	4.099837	-5.396823

436	8	0	7.429866	1.448125	3.270084
437	1	0	8.199235	1.991954	2.991286
438	1	0	6.802146	1.531173	2.517476
439	8	0	-0.519541	-8.494709	-1.619455
440	1	0	-0.720741	-8.046459	-2.461108
441	1	0	-1.172254	-8.165713	-0.972859
442	8	0	0.501023	-3.611642	5.195219
443	1	0	0.891507	-2.992355	5.849002
444	1	0	-0.218735	-4.084608	5.677063
445	8	0	5.423766	-1.766736	-3.956866
446	1	0	5.895611	-1.172884	-4.579089
447	1	0	4.785658	-2.276516	-4.500323
448	8	0	-3.229409	0.585150	3.896865
449	1	0	-2.623161	0.279773	4.588813
450	1	0	-3.293867	-0.152725	3.274056
451	8	0	0.715964	8.341568	1.942404
452	1	0	0.776518	7.648344	2.629495
453	1	0	1.504747	8.230722	1.376739
454	8	0	-4.937295	2.225125	4.480424
455	1	0	-4.100565	2.245097	3.953264
456	1	0	-5.245466	1.280343	4.394723
457	6	0	-2.427319	-1.218962	0.873907
458	6	0	-1.414523	-1.623742	1.742502
459	6	0	-1.714709	-2.455119	2.827470
460	6	0	-3.022222	-2.881483	3.042953
461	6	0	-4.038093	-2.469926	2.173344
462	6	0	-3.745133	-1.642181	1.094584
463	6	0	-2.197907	-0.331904	-0.337175
464	6	0	-2.396991	-1.039424	-1.667353
465	6	0	-2.881974	1.013287	-0.138941
466	6	0	-4.056568	1.336932	-0.821649
467	6	0	-4.664678	2.571838	-0.592445
468	6	0	-4.111314	3.477974	0.309788
469	6	0	-2.966272	3.133163	1.028929
470	6	0	-2.359619	1.899931	0.813716
471	6	0	-2.477018	-0.306277	-2.858715
472	6	0	-2.398765	-0.951323	-4.087353
473	6	0	-2.232767	-2.334659	-4.141672
474	6	0	-2.189982	-3.074103	-2.962916
475	6	0	-2.268231	-2.429529	-1.728929
476	17	0	-6.035742	-1.017695	-2.898226
477	1	0	-0.384637	-1.313997	1.580922

478	1	0	-0.911303	-2.779593	3.494309
479	1	0	-3.255511	-3.539511	3.880136
480	1	0	-5.061751	-2.805106	2.333017
481	1	0	-4.534015	-1.342768	0.406896
482	1	0	-4.509804	0.636869	-1.521308
483	1	0	-5.573785	2.822289	-1.133845
484	1	0	-4.579013	4.451493	0.463756
485	1	0	-2.544723	3.827187	1.755042
486	1	0	-1.482631	1.624030	1.401938
487	1	0	-2.609482	0.773376	-2.843574
488	1	0	-2.462664	-0.370942	-5.004531
489	1	0	-2.142157	-2.834745	-5.106026
490	1	0	-2.071903	-4.155565	-2.998942
491	1	0	-2.204208	-3.015675	-0.814401
492	6	0	3.075921	-0.719665	-1.382112
493	6	0	2.197867	0.188935	-0.485487
494	6	0	1.207701	0.950755	-1.390974
495	6	0	1.340966	0.437767	-2.904856
496	6	0	2.774031	0.720135	-3.273576
497	6	0	3.672636	0.110657	-2.492048
498	6	0	-0.211942	0.828901	-1.086838
499	1	0	-0.926310	1.505428	-1.570041
500	8	0	-0.665491	-0.075530	-0.348652
501	6	0	3.015344	1.164381	0.356045
502	1	0	3.845026	-1.198966	-0.767410
503	1	0	1.631736	-0.471710	0.183341
504	1	0	1.427679	2.026571	-1.436816
505	1	0	0.628127	0.964066	-3.549509
506	1	0	3.017619	1.354810	-4.124093
507	1	0	4.749019	0.174866	-2.651305
508	1	0	3.699397	0.619023	1.015064
509	1	0	3.606597	1.823755	-0.292979
510	1	0	2.364337	1.790438	0.979021
511	6	0	1.116352	-1.088411	-2.935295
512	1	0	0.091629	-1.339716	-2.645676
513	1	0	1.235327	-1.412457	-3.974969
514	6	0	2.152007	-1.782818	-2.019774
515	1	0	2.757079	-2.495550	-2.589333
516	1	0	1.647499	-2.344015	-1.222715

TS-*endo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.650040	-1.776700	1.333520
2	6	0	-1.366609	-2.956227	0.584193
3	6	0	-2.226579	-3.388788	-0.400513
4	6	0	-1.408921	-2.210487	-2.089724
5	6	0	-1.599472	-0.874032	-1.731809
6	6	0	-2.753432	-1.031727	1.039736
7	6	0	-3.882948	-1.534544	0.195609
8	6	0	-3.676134	-2.964187	-0.344745
9	6	0	-0.676113	-0.165298	-0.982391
10	1	0	-0.850544	0.884556	-0.734280
11	8	0	0.458853	-0.735309	-0.651342
12	6	0	-2.239040	-2.814568	-3.186685
13	1	0	-0.915077	-1.409178	2.043221
14	1	0	-0.398224	-3.440617	0.715197
15	1	0	-1.998423	-4.323693	-0.911205
16	1	0	-0.411908	-2.627383	-1.956956
17	1	0	-2.502838	-0.335120	-1.999550
18	1	0	-2.867397	-0.032160	1.465515
19	1	0	-4.783046	-1.505135	0.825540
20	1	0	-4.073488	-0.795667	-0.589566
21	1	0	-4.153598	-3.085354	-1.323301
22	1	0	-4.175035	-3.681575	0.323002
23	1	0	-2.326383	-3.902757	-3.106410
24	1	0	-3.236900	-2.366036	-3.222510
25	1	0	-1.740148	-2.593290	-4.140652
26	6	0	0.059967	0.196970	4.118143
27	6	0	-0.467518	1.057462	3.154498
28	6	0	0.041742	1.052336	1.857776
29	6	0	1.072378	0.171883	1.502323
30	6	0	1.603275	-0.681983	2.474895
31	6	0	1.100621	-0.666343	3.776998
32	6	0	1.499853	0.059499	0.038138
33	6	0	2.770984	-0.773077	-0.124936
34	6	0	1.665443	1.393661	-0.688632
35	6	0	4.008037	-0.172274	0.128790
36	6	0	5.183165	-0.914519	0.055657
37	6	0	5.140170	-2.268249	-0.281201
38	6	0	3.911760	-2.869871	-0.540696
39	6	0	2.731666	-2.128106	-0.459159

40	6	0	1.639042	1.402695	-2.088408
41	6	0	1.829686	2.587459	-2.790219
42	6	0	2.072012	3.776924	-2.101555
43	6	0	2.128421	3.767832	-0.711594
44	6	0	1.924866	2.581267	-0.006019
45	1	0	-0.336461	0.200161	5.132123
46	1	0	-1.288149	1.732666	3.387898
47	1	0	-0.393216	1.739744	1.134875
48	1	0	2.407358	-1.369999	2.224089
49	1	0	1.523458	-1.336179	4.523738
50	1	0	4.052741	0.885531	0.382155
51	1	0	6.138061	-0.431680	0.256310
52	1	0	6.059781	-2.847523	-0.344400
53	1	0	3.866576	-3.924842	-0.806930
54	1	0	1.778449	-2.611448	-0.654180
55	1	0	1.464672	0.475880	-2.633765
56	1	0	1.789827	2.584061	-3.877895
57	1	0	2.211902	4.707154	-2.649234
58	1	0	2.314837	4.690550	-0.165894
59	1	0	1.960621	2.592299	1.080454
60	5	0	-2.786243	2.490027	0.011521
61	9	0	-3.609486	3.575074	-0.212797
62	9	0	-3.242950	1.347931	-0.714536
63	9	0	-1.454048	2.758555	-0.415891
64	9	0	-2.746265	2.142588	1.385868

Only one negative frequency: -252.38

TS-*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.364868	-3.379751	-0.574307
2	6	0	-1.569626	-2.158459	-2.185319
3	6	0	-1.628280	-0.825472	-1.746444
4	6	0	-2.837812	-1.111346	1.020229
5	6	0	-0.660821	-0.168035	-1.017262
6	1	0	-0.828002	0.877947	-0.742699
7	8	0	0.489077	-0.730147	-0.719268
8	6	0	-2.377162	-2.579820	-3.380073
9	1	0	-2.255617	-4.306781	-1.137494
10	1	0	-0.631640	-2.694138	-2.027611

11	1	0	-2.511155	-0.222424	-1.945691
12	1	0	-2.895842	-0.104691	1.441013
13	1	0	-2.555462	-3.660165	-3.402387
14	1	0	-3.333775	-2.048545	-3.412966
15	1	0	-1.815372	-2.314733	-4.286750
16	6	0	0.044292	-0.026089	4.090152
17	6	0	-0.494675	0.869758	3.166282
18	6	0	0.013705	0.929515	1.869996
19	6	0	1.058126	0.081690	1.476698
20	6	0	1.595005	-0.814120	2.408089
21	6	0	1.091653	-0.864245	3.708811
22	6	0	1.504257	0.056579	0.012500
23	6	0	2.802658	-0.726404	-0.177946
24	6	0	1.641781	1.429875	-0.643993
25	6	0	4.009934	-0.114597	0.176247
26	6	0	5.211500	-0.808509	0.074832
27	6	0	5.226154	-2.124244	-0.391802
28	6	0	4.028632	-2.735370	-0.751478
29	6	0	2.820696	-2.042552	-0.641535
30	6	0	1.618730	1.508804	-2.041576
31	6	0	1.783709	2.731532	-2.682138
32	6	0	1.996767	3.889920	-1.933557
33	6	0	2.049713	3.812052	-0.545612
34	6	0	1.871791	2.587220	0.098573
35	1	0	-0.348717	-0.070463	5.104645
36	1	0	-1.321569	1.525946	3.430270
37	1	0	-0.427074	1.646763	1.180283
38	1	0	2.406517	-1.480734	2.125292
39	1	0	1.520827	-1.564275	4.423620
40	1	0	4.009191	0.914433	0.531688
41	1	0	6.141989	-0.317761	0.355196
42	1	0	6.166735	-2.665772	-0.477443
43	1	0	4.028124	-3.760299	-1.119330
44	1	0	1.893272	-2.535536	-0.918200
45	1	0	1.467089	0.606862	-2.633437
46	1	0	1.746260	2.782025	-3.768728
47	1	0	2.116099	4.849580	-2.433174
48	1	0	2.212733	4.710255	0.046523
49	1	0	1.903248	2.545048	1.184448
50	5	0	-2.808279	2.473980	0.098375
51	9	0	-3.586070	3.607595	-0.035916
52	9	0	-3.328190	1.400915	-0.677798

53	9	0	-1.473065	2.717259	-0.341432
54	9	0	-2.749687	2.046898	1.452251
55	6	0	-1.362213	-3.135661	0.534171
56	1	0	-0.384084	-2.879389	0.110741
57	1	0	-1.218069	-4.087433	1.059426
58	6	0	-1.802762	-2.060708	1.545848
59	1	0	-0.936455	-1.511674	1.921001
60	1	0	-2.256238	-2.537053	2.428732
61	6	0	-3.589736	-2.743236	-0.581610
62	6	0	-3.777720	-1.519684	0.125156
63	1	0	-4.595412	-0.854529	-0.144302
64	1	0	-4.356282	-3.077039	-1.281944

Only one negative frequency: -227.89

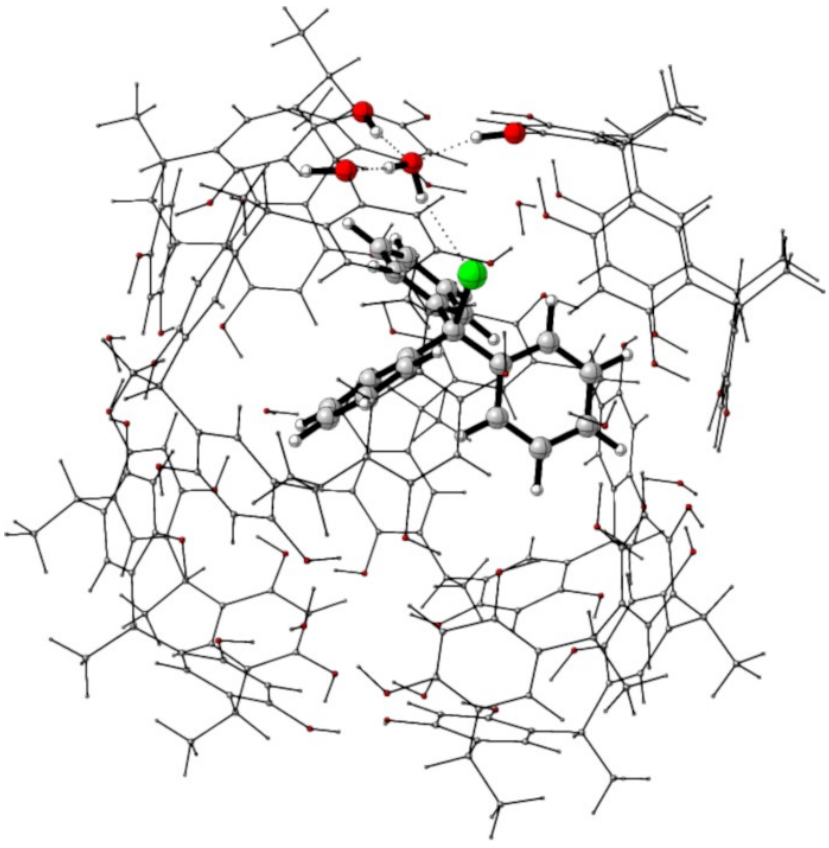


Figure S78. The most stable structure of **2a** inside $\mathbf{C_M}$