

Supporting Information

Supramolecular Catalysis in Confined Space: Making the Pyrogallol[4]arene Capsule Catalytically Active in Non-Competitive Solvent

Pellegrino La Manna,^[a] Carmen Talotta,^{*[a]} Carmine Gaeta,^[a] Yoram Cohen,^{*[b]} Sarit Slovak,^[b] Antonio Rescifina,^{*[c]} Paolo Della Sala,^[a] Margherita De Rosa,^[a] Annunziata Soriente,^[a] Placido Neri^{*[a]}

[a] Dr P. La Manna, Prof. C. Talotta, Prof. C. Gaeta, Dr P. Della Sala, Prof. M. De Rosa, Prof. A. Soriente and Prof. P. Neri
Laboratory of Supramolecular Chemistry,
Dipartimento di Chimica e Biologia "A. Zambelli",
Università di Salerno,
Via Giovanni Paolo II 132, I-84084 Fisciano (Salerno), Italy.
E-mail: ctalotta@unisa.it, neri@unisa.it

[b] Prof. Y. Cohen, Dr S. Slovak
School of Chemistry, The Sackler Faculty of Exact Sciences,
Tel Aviv University,
Ramat Aviv, 69978 Tel Aviv, Israel.
E-mail: ycohen@tauex.tau.ac.il

[c] Prof. A. Rescifina
Dipartimento di Scienze del Farmaco e della Salute
Università di Catania,
Viale Andrea Doria 6, I-95125 Catania, Italy.
E-mail: arescifina@unict.it

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1. General Remarks

All 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 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 (^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)], or Bruker Avance-250 spectrometer [250 (^1H) and 62.80 MHz (^{13}C)]; chemical shifts are reported relative to the residual solvent peak (CHCl_3 : δ 7.26, CDCl_3 : δ 77.23). For nitrone **3**, L-proline and iminium species, 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 was 0.2 ms, and gradient pulse was 1400 ms. Individual rows of the quasi2D diffusion databases were phased and baseline corrected. For crotonaldehyde **4**, a different approach was exploited (see section 4.3). EXSY 2D experiments were performed on Bruker Avance 400 and Bruker Avance 600 spectrometers with a D8 value range from 0.05 to 0.75 s. HPLC analysis was performed using a Jasco HPLC system equipped with PU-4180 HPLC pump, 20 μl loop injector (Rheodyne model 7725i) and MD-4015 Photodiode Array Detector at $\lambda = 210$ or 220 nm. As stationary phase, the following Chiralcel column was used: OD-H (250 x 4.6 mm) and OD guard (50 mm). C-undecylresorcin[4]rene **1**, pyrogallol[4]arene **2**, and nitrone **3** were synthesized according to literature procedures.^{1,2,3} Percentages of conversions, regioisomeric and diastereomeric ratios of isoxazolidines **5** and **6** were determined by ^1H NMR analysis in comparison with literature data.⁴

¹ Q. Zhang, K. Tiefenbacher, *Nature Chem.* **2015**, *7*, 197-202.

² Q. Zhang, L. Catti, V. R. I. Kaila, K. Tiefenbacher, *Chem. Sci.* **2017**, *8*, 1653-1657.

³ S. Pagoti, D. Dutta, J. Dash, *Adv. Synth. Catal.* **2013**, *355*, 3532-3538.

⁴ a) T. Otsuki, J. Kumagai, Y. Kohari, Y. Okuyama, E. Kwon, C. Seki, K. Uwai, Y. Mawatari, N. Kobayashi, T. Iwasa, M. Tokiwa, M. Takeshita, A. Maeda, A. Hashimoto, K. Turuga, H. Nakano, *Eur. J. Org. Chem.* **2015**, 7292-7300; b) X. Wang, C. Weigl, M. P. Doyle, *J. Am. Chem. Soc.* **2011**, *133*, 9572-9579; c) W. S. Jen, J. J. M. Wiener, D. W. C. MacMillan, *J. Am. Chem. Soc.* **2000**, *122*, 9874-9875; d) M. Lemay, J. Trant, W. W. Ogilvie, *Tetrahedron* **2007**, *63*, 11644-11655.

2. General Procedures

2.0 Monitoring of cycloaddition reaction

The progress of the cycloaddition reaction was controlled after 4 h and 16 h by following ^1H NMR signals associated with nitrones. The reaction was stopped after the consumption of nitron or when its conversion reached a plateau. The enantiomeric excess value was determined by HPLC analysis by converting the mixture of isoxazolidines to the corresponding alcohols. 50 μL of the reaction solution was poured in the vial, diluted with 350 μL of C_6D_6 , and the reaction progress was monitored by ^1H NMR. In Figure S1, the ^1H NMR spectrum of the reaction mixture for the experiment of Table 1, entry 7 (in the manuscript) can be seen.

2.1. General procedure for 1,3-dipolar cycloaddition reaction without capsule in the presence of L-proline, crotonaldehyde **4**, and nitron **3**

L-proline (16.3 μmol , 0.2 eq.) was weighed into a 4 mL vial and deuterated benzene (0.55 mL) was added. Next, crotonaldehyde **4** (325.2 μmol , 4.0 eq.) was added, followed by nitron **3** (81.3 μmol , 1.0 eq.). The vial was thermostatically controlled at 30 $^\circ\text{C}$ and maintained under vigorous stirring for an appropriate time. The progress of the reaction was monitored by ^1H NMR analysis by periodically sampling from the reaction mixture at different times.

2.2 General procedure for 1,3-dipolar cycloaddition reaction with capsule **CR**₆ in the presence of L-proline, crotonaldehyde **4**, and nitron **3**

C-undecylresorcin[4]arene **1** (140.8 mg, 127.4 μmol , 1.56 eq.) was weighed in a 4 mL vial. Then, 0.55 mL of water-saturated deuterated benzene was added and the mixture was stirred at 30 $^\circ\text{C}$ for 15 minutes until resorcinarene was completely dissolved. L-proline (16.3 μmol , 0.2 eq.) was added to the solution and the mixture was stirred for 30 minutes. Subsequently, crotonaldehyde **4** (325.2 μmol , 4.0 eq.) was added and the reaction mixture was stirred for further 5 minutes. Then nitron **3** (81.3 μmol , 1.0 eq.) was added and the reaction mixture was stirred at 30 $^\circ\text{C}$ and checked at the desired time (generally, 4 hrs). Quenching of the reaction was performed by adding the reaction mixture to a 50 mL conical eppendorf tube and diluting with 40 mL n-hexane. To this mixture, 40 μL of DMSO were added. The eppendorf tube was placed in a freezer at -20 $^\circ\text{C}$ for at least 2 h and successively centrifuged at 3000 rpm for 5 minutes. The diluted reaction mixture was subjected three times to this procedure. Finally, the clear solution was removed and concentrated under reduced pressure. The oily residue thus obtained was purified by flash chromatography on silica gel (hexane/ethyl acetate, from 100 to 80:20) to afford the desired compounds (isoxazolidines **5** and **6**).

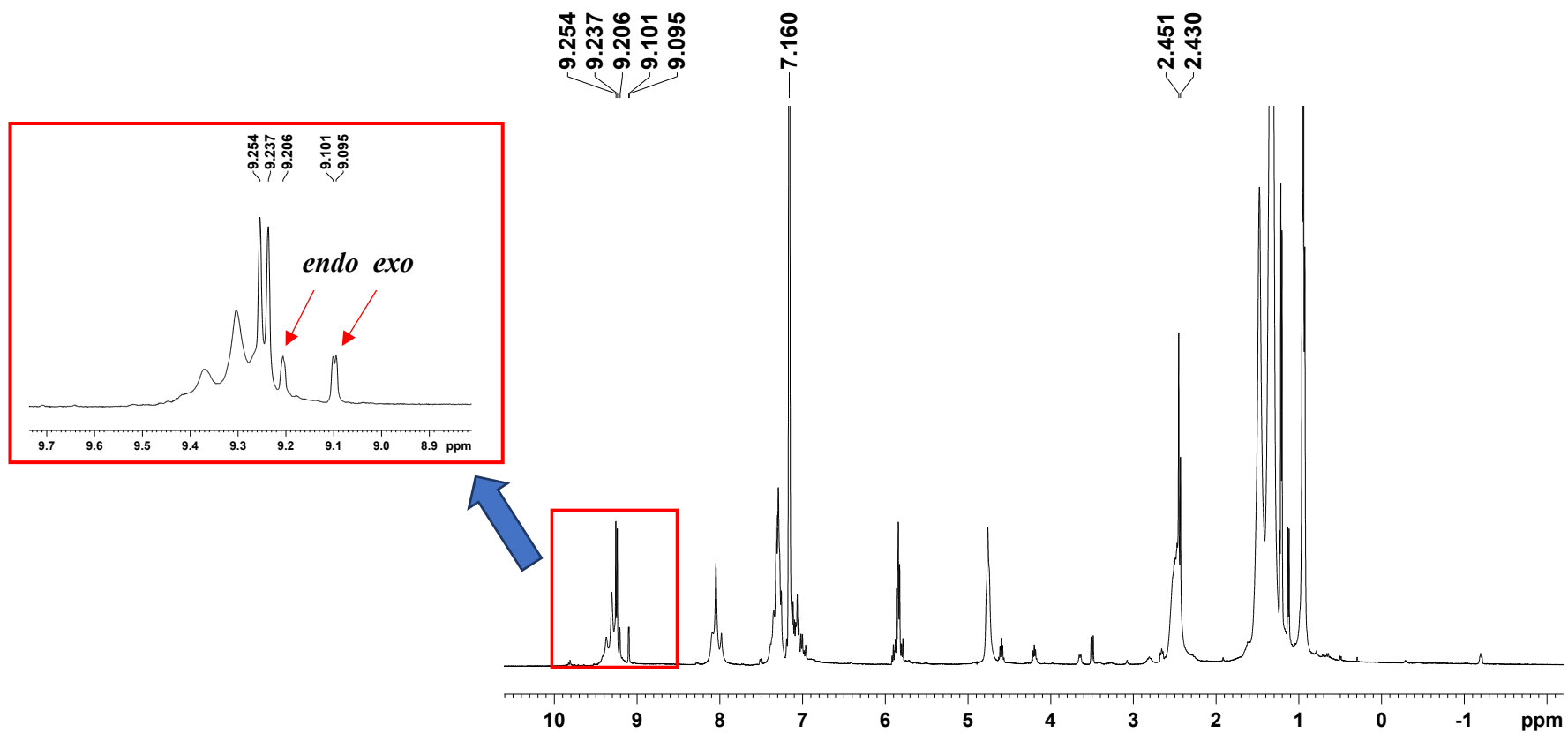


Figure S1. ¹H NMR (300 MHz, C₆D₆, 298 K) of the crude reaction mixture between **3** and **4** in the presence of CP₆ and L-proline as described in Table 1, entry 7 in the manuscript. Expansion of low field spectral zone, with crotonaldehyde **4** and *endo/exo*-**5** cycloadducts peaks (indicated by arrows), is visible.

2.3 General procedure for 1,3-dipolar cycloaddition reaction with capsule **CP₆** in the presence of L-proline, crotonaldehyde **4**, and nitrone **3**

C-undecylpyrogallol[4]arene **2** (127.4 μmol , 148 mg) was weighed in a 4 mL vial. Then, 0.55 mL of deuterated benzene was added and the mixture was stirred at 30 °C for 15 minutes until pyrogallolarene was completely dissolved. L-proline (1.9 mg, 16.3 μmol) was added to the solution and the mixture was stirred for 30 minutes. Subsequently, crotonaldehyde **4** (325.2 μmol , 26.9 μL) was added and the reaction mixture was stirred for further 5 minutes. Then, nitrone **3** (81.3 μmol , 11 mg) was added and the reaction mixture was stirred at 30 °C and checked at the desired time (generally, 4 hr). Quenching of the reaction was performed by adding the reaction mixture to a 50 mL conical eppendorf tube and diluting with 40 mL *n*-hexane. To this mixture, 70 μL of DMSO were added. The eppendorf tube was placed in a freezer at -20 °C for at least 2 h and successively centrifuged at 3000 rpm for 5 minutes. The diluted reaction mixture was subjected three times to this procedure. Finally, the clear solution was removed and concentrated under reduced pressure. The oily residue thus obtained was purified by flash chromatography on silica gel (hexane/ethyl acetate, from 100 to 80:20) to afford the desired compounds (isoxazolidines **5** and **6**). Figure S2 shows the mixture of isoxazolidines as isolated by FC means.

2.4 Procedure for the inhibition experiments

C-undecylpyrogallol[4]arene **2** (127.4 μmol , 148 mg) was weighed in a 4 mL vial. Then, 0.55 mL of deuterated benzene was added and the mixture was stirred at 30 °C for 15 minutes until pyrogallolarene was completely dissolved. L-proline (1.9 mg, 16.3 μmol), tetralkylammonium salt (concentration indicated in Table 1 in the main text) was added to the solution and the mixture was stirred for 30 minutes. Subsequently, crotonaldehyde **4** (325.2 μmol , 26.9 μL) was added and the reaction mixture was stirred for further 5 minutes. Then, nitrone **3** (81.3 μmol , 11 mg) was added and the reaction mixture was stirred at 30 °C and checked at the desired time (generally, 4 hr).

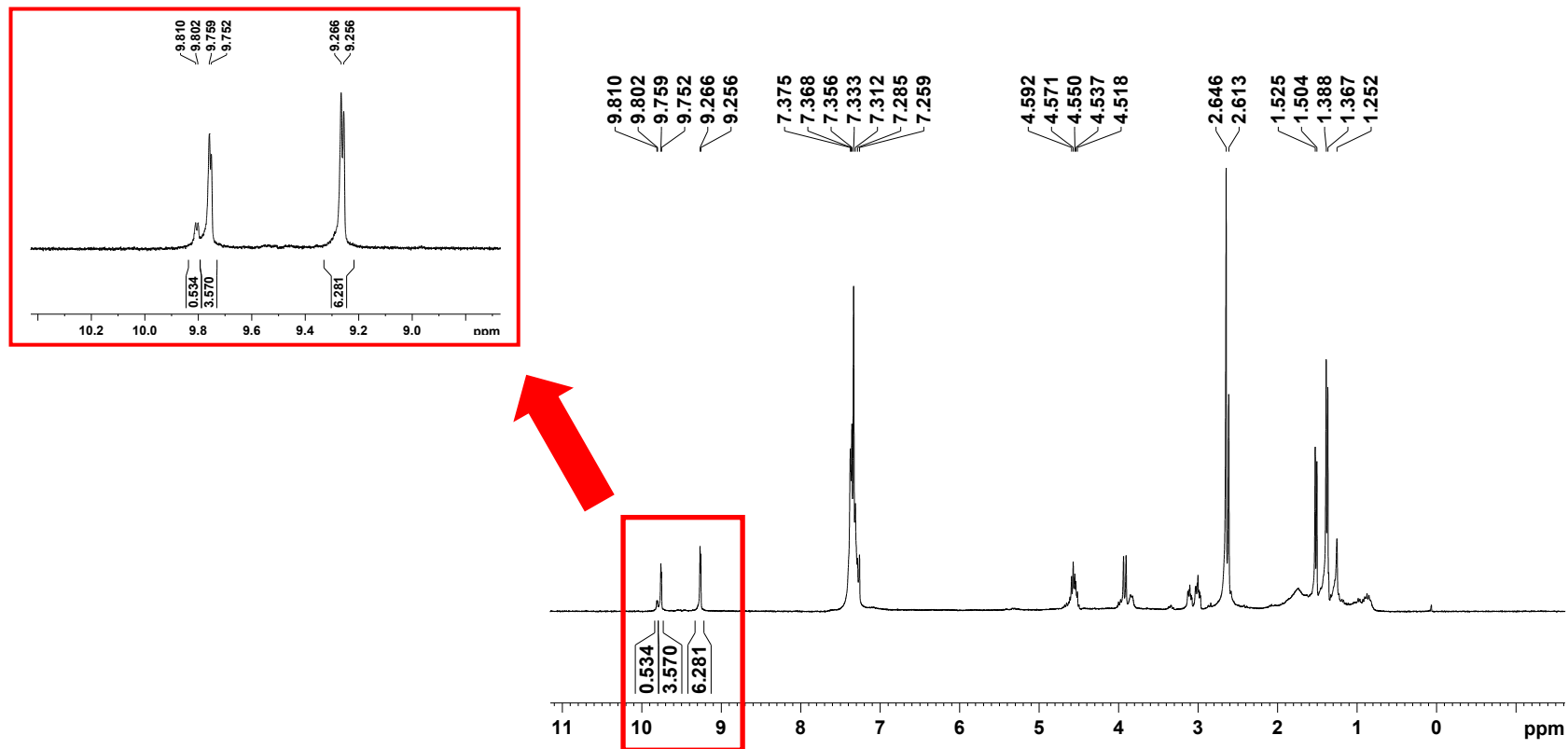


Figure S2. ^1H NMR (300 MHz, CDCl_3 , 298 K) of the crude reaction mixture between **3** and **4** in the presence of **CP**₆ and L-proline as described in **Table 1, entry 2** in the manuscript. Expansion of low field spectral zone, with aldehyde cycloadduct peaks (indicated by arrows), is visible.

2.5 General procedure for reduction of mixture of isoxazolidine adducts

To a solution of compounds **5** and **6** (0.15 mmol) in EtOH (2 mL), NaBH₄ (0.30 mmol, 2 eq.) was added and the resulting mixture was stirred at 30 °C for 75 min. The reaction was quenched by the addition of NH₄Cl saturated solution (5 mL), then EtOH was partially removed under reduced pressure and the residue was extracted with CH₂Cl₂ (3 × 10 mL). The combined organic phases were washed with deionized H₂O and dried over Na₂SO₄, filtered and concentrated under reduced pressure to give the corresponding purified mixture of alcohols as a yellowish oil, as confirmed by ¹H NMR analysis.

3. Inhibition Experiments

3.1. Inhibition experiments with DMSO

It has been widely reported that DMSO is able to break the hexameric assembly of the pyrogallolarene capsule **CP₆** by interfering with hydrogen bonding of hydroxyl groups. So, to highlight whether a capsule exerts a catalytically relevant role, a reaction in the presence of DMSO (151 μL, 3.86 M, 100 eq. in comparison to the capsule **CP₆**) and the capsule **CP₆** (38.6 mM) has been performed.

The ¹H NMR spectrum of the crude reaction mixture in Figure S3 shows very weak NMR signals at low field, indicative of the presence of a little amount of the aldehyde cycloadducts. After purification by FC, only scarce yields are obtained. This outcome can be attributed to the disassembling of the pyrogallolarene capsule in the presence of a hydrogen bonding competitor.

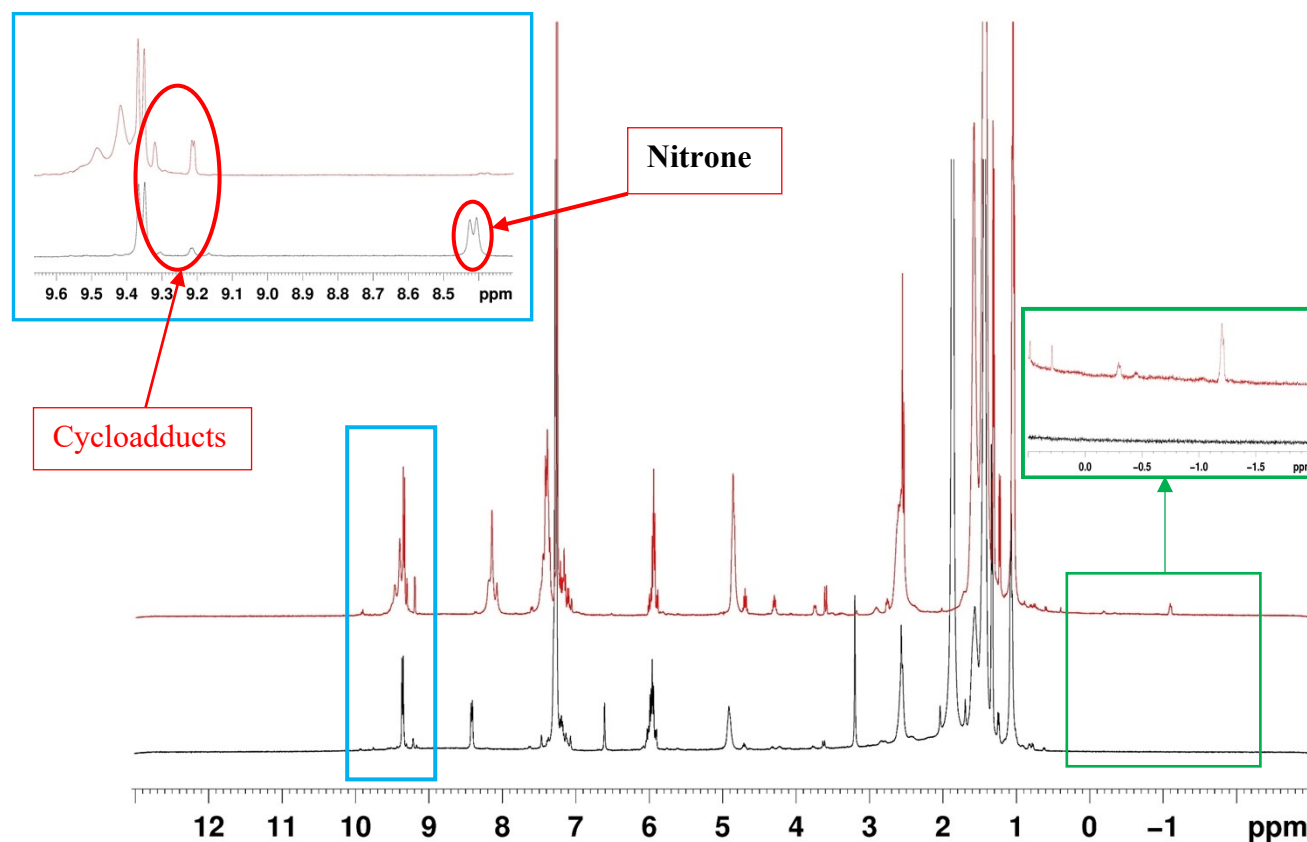
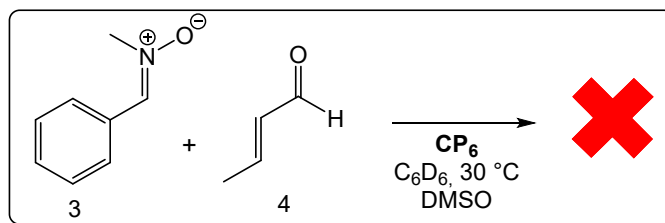


Figure S3. Stacked ^1H NMR spectra (400 MHz, C_6D_6 , 298 K) of: (bottom) reaction between **3** (148 mM, 1 equiv.) and **4** (591 mM, 4 equiv.) in the presence of L-proline (29.7 mM, 0.2 equiv.), capsule **CP₆** (38.6 mM, 0.26 equiv.) and DMSO (100 equiv. in comparison to **CP₆**) as inhibitor: the crude reaction mixture after 4 h at 30 °C; (top) similar reaction but without DMSO. It is clearly evident how the presence of inhibitor largely reduces the formation of products. It is also noteworthy to observe the absence of protonic signals associated to the encapsulated aldehyde at low field in the presence of DMSO.

3.2. Inhibition experiments with tetralkylammonium salts

An evidence that cycloaddition reaction occurred inside supramolecular host **CP**₆ has been furnished by control experiments performed in the presence of tetralkylammonium guests. Indeed, efficient competition of these salts for the inner space of capsule **CR**₆ has been reported by several authors. Moreover, encapsulation of ammonium salts by pyrogallolarene capsule **CP**₆ in benzene has been reported by Cohen et al⁵. Reaction performed in the presence of **NEt**₄**BF**₄ (3.5 eq. in comparison to the capsule **CP**₆) gave no trace of products after 4h. This result can be ascribed to an efficient blocking of the cavity by this ammonium salt.

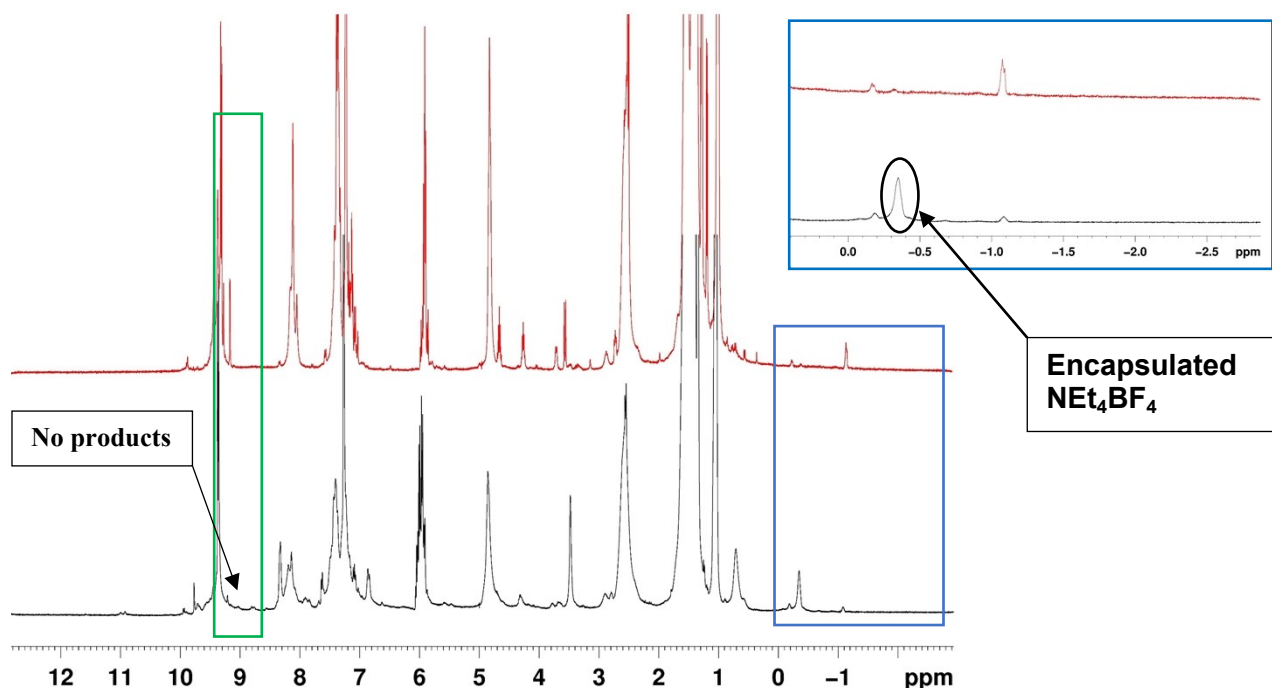
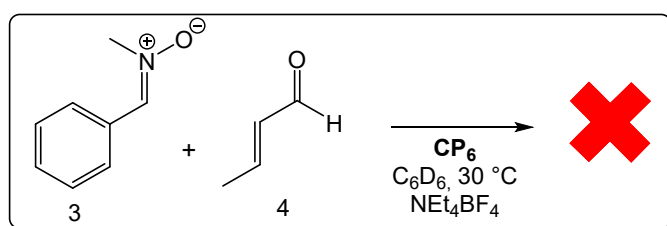


Figure S4. Stacked ¹H NMR spectra (400 MHz, C₆D₆, 298 K) of: (bottom) reaction between **3** (148 mM, 1 equiv.) and **4** (591 mM, 4 equiv.) in the presence of L-proline (29.7 mM, 0.2 equiv.), capsule **CP**₆ (38.6 mM, 0.26 equiv.), and **NEt**₄**BF**₄ (3.5 equiv. in comparison to **CP**₆) as inhibitor: the crude reaction mixture after 4 h at 30 °C; (top) similar reaction but without the ammonium salt. It is clearly evident how the presence of ammonium salt inhibits the reaction. Encapsulation of tetraethylammonium salt is also evident in the inset.

⁵ Cohen, Y.; Yariv-Shoushan, S.; Encapsulated or Not Encapsulated? Ammonium Salts Can Be Encapsulated in Hexameric Capsules of Pyrogallol[4]arene. *Org. Lett.* **2016**, *18*, 936–939. DOI: 10.1021/acs.orglett.5b03655.

4. Encapsulation Experiments

4.1 Encapsulation experiments of crotonaldehyde **4** inside capsule **CP₆**

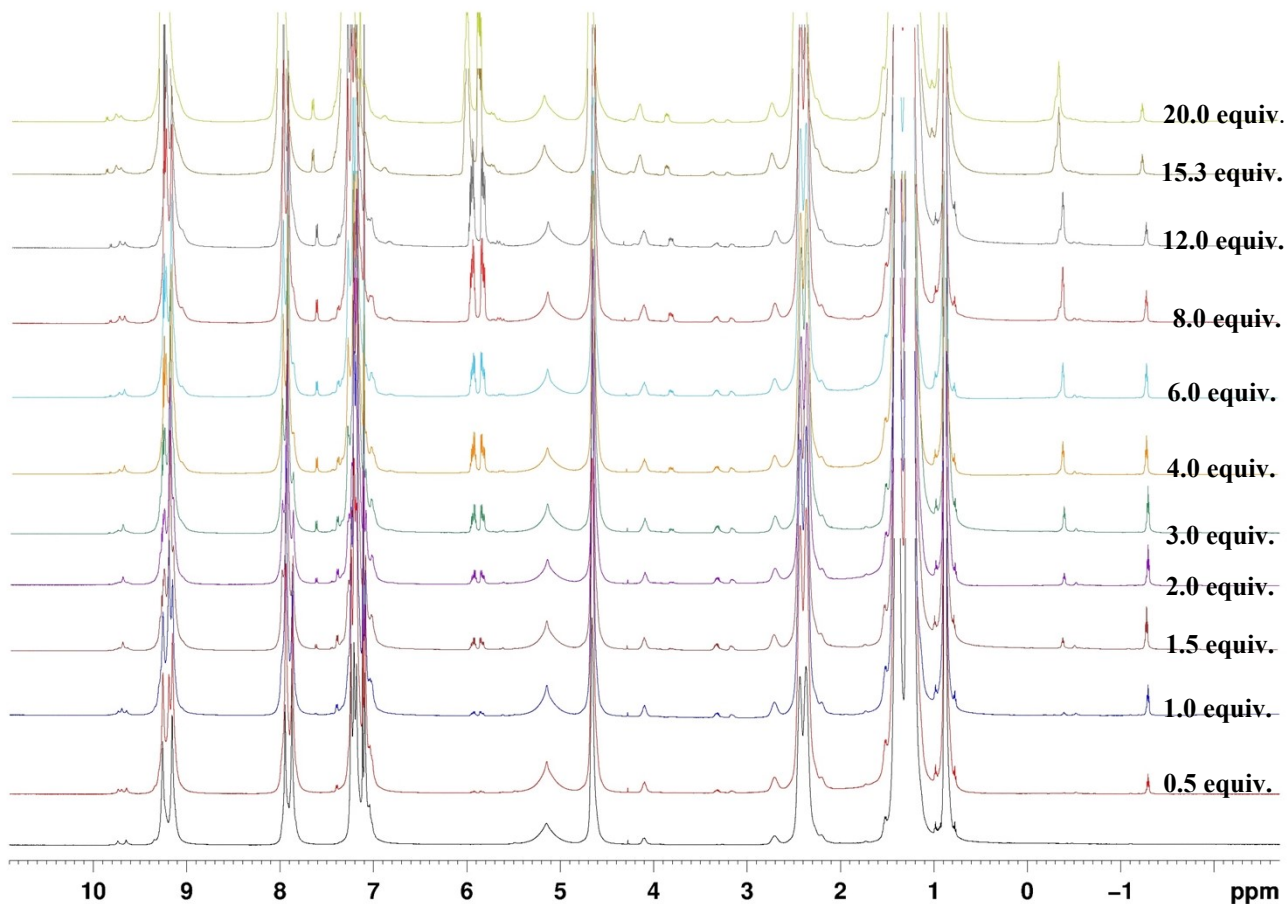


Figure S5. Stacked ¹H NMR spectra (600 MHz, CDCl₃, 298K) of crotonaldehyde **4** (from 0 to 20 equiv. in comparison to capsule **CP₆**, from bottom to top) and **CP₆** (21.2 μmol).

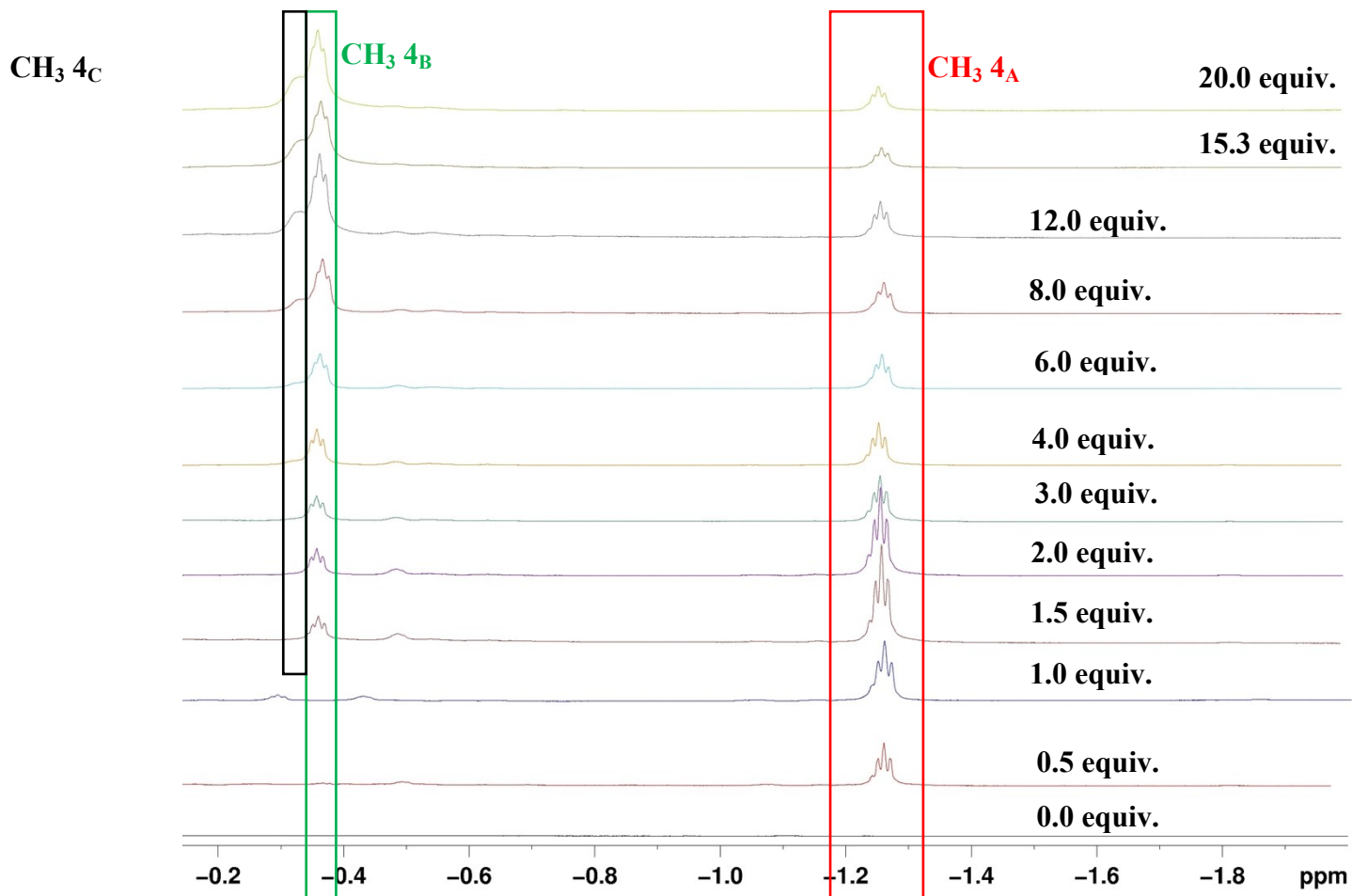


Figure S6. Significant portion of **Figure S5** between -0.2 and 2.0 ppm. Increasing concentration of guest **4** leads to an initial increase, followed by a later decrease, of the intensity of CH₃ **4**_A signal; instead, intensity of CH₃ **4**_B and CH₃ **4**_C shows a constant increasing pattern until the plateau (reached with 15.3 equiv. of crotonaldehyde **4**).

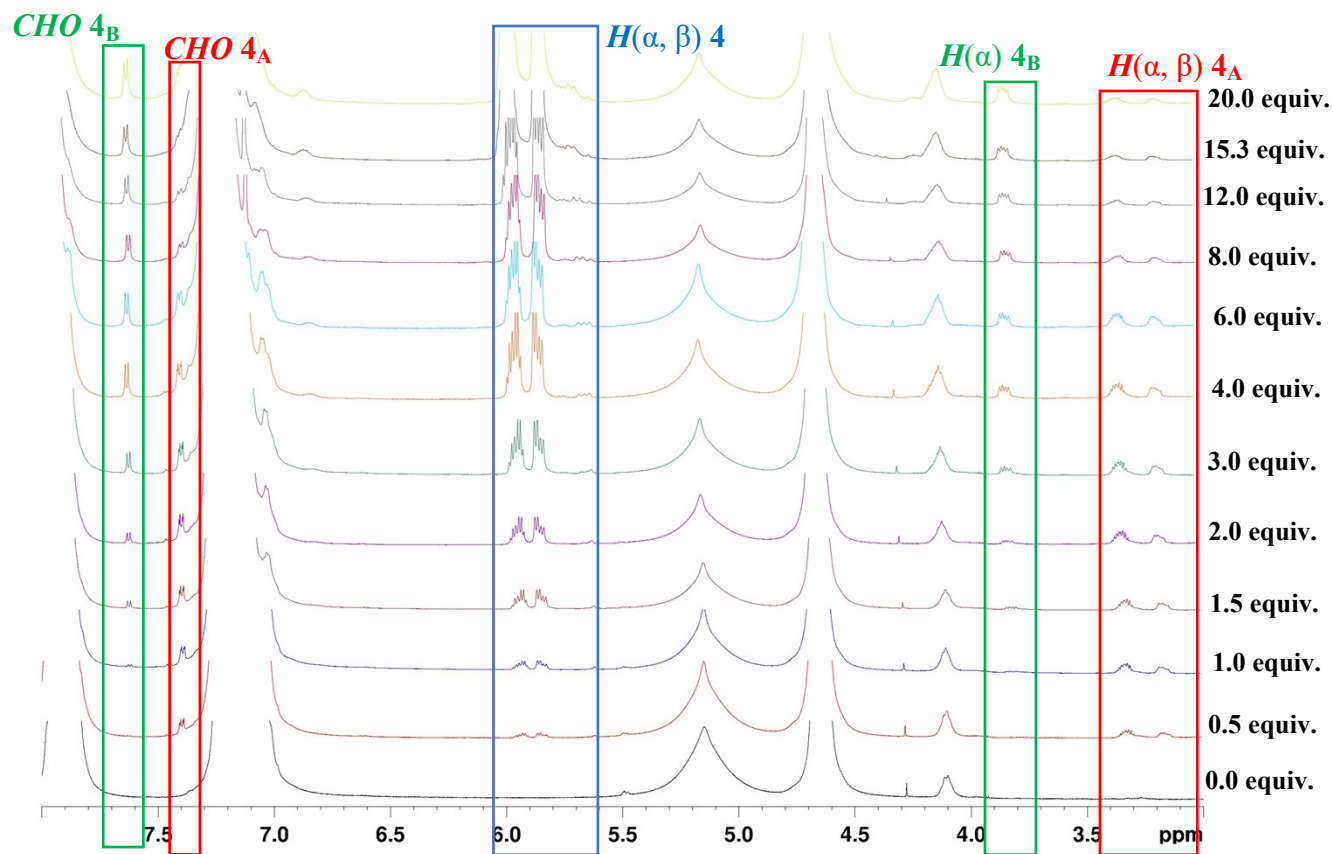


Figure S7. Significant portion of **Figure S5** between 8.0 and 3.0 ppm. The trend before observed for **CH₃ 4_A** and **CH₃ 4_B** is confirmed also for the **H(α,β) 4_A** and **4_B** signals.

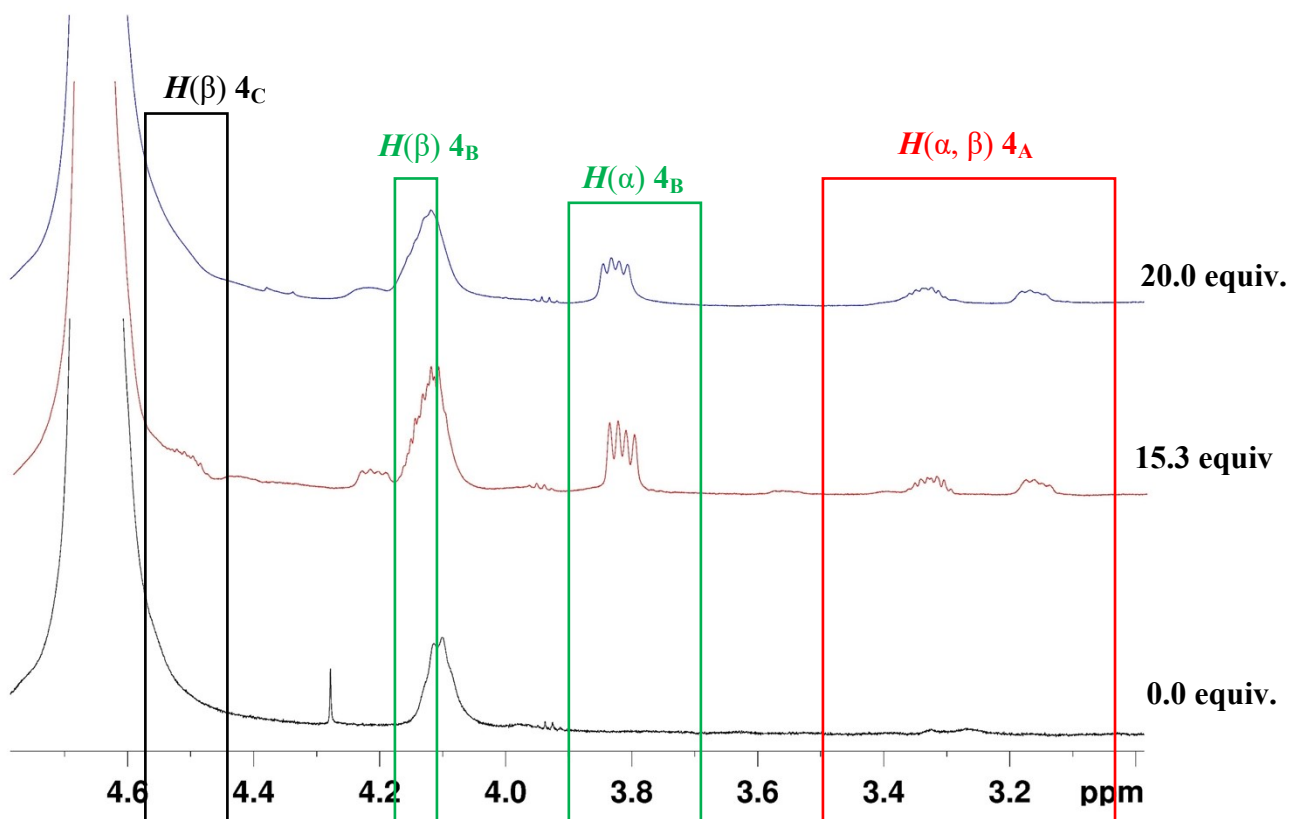


Figure S8. Significant portion of **Figure S5** between 4.8 and 3.3 ppm. A better scenario showing the signal $H(\beta) 4_c$ can be seen.

4.2 2D experiments for the encapsulation of crotonaldehyde **4** inside capsule **CP₆**

4.2.1 2D ROESY of the mixture of **CP₆** and crotonaldehyde **4**

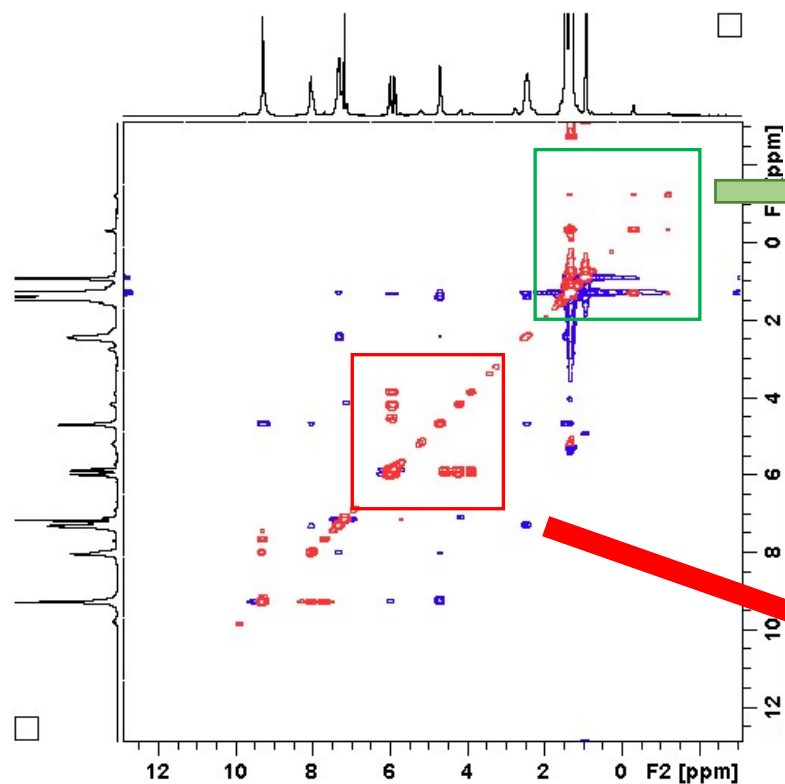


Figure S9. 2D ROESY spectrum (400 MHz, C₆D₆, 298 K, p15 = 0.50 s) of the mixture of **CP₆** (38.6 mM) and crotonaldehyde **4** (15.3 equiv).

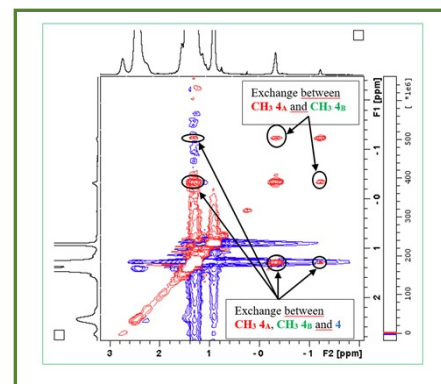


Figure S10. Relevant portion of 2D ROESY spectrum (400 MHz, C₆D₆, 298 K, p15 = 0.50 s) in **Figure S9**.

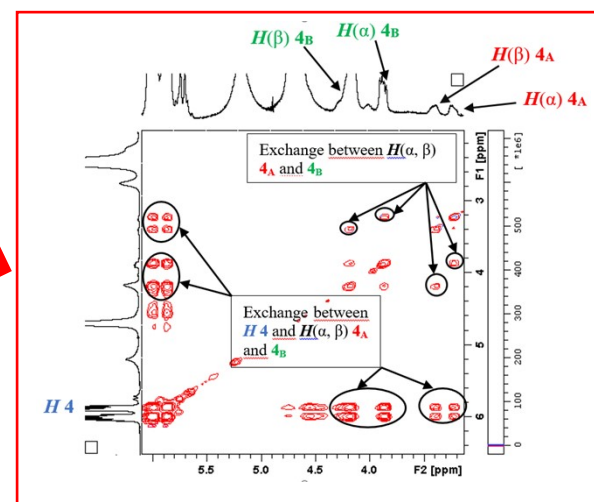


Figure S11. Relevant portion of 2D ROESY (400 MHz, C₆D₆, 298 K, p15 = 0.50 s) in **Figure S9**.

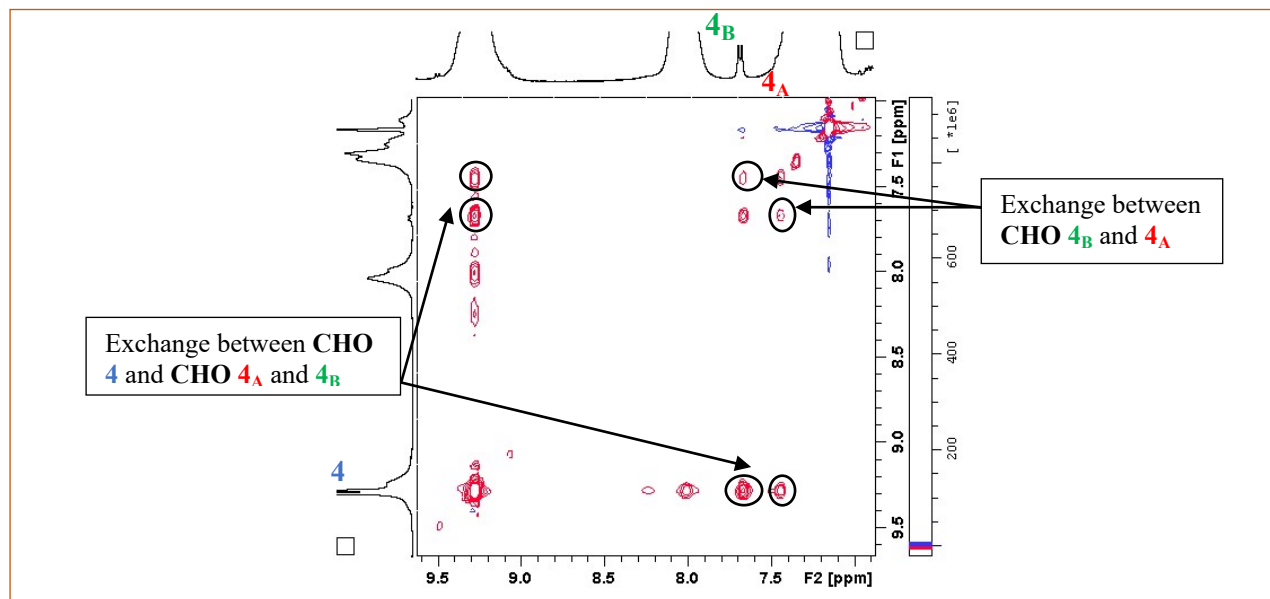


Figure S12. Relevant portion of 2D ROESY spectrum (400 MHz, C₆D₆, 298 K, p15 = 0.50 s) in **Figure S9**.

4.2.2 2D COSY of the mixture of CP₆ and crotonaldehyde 4

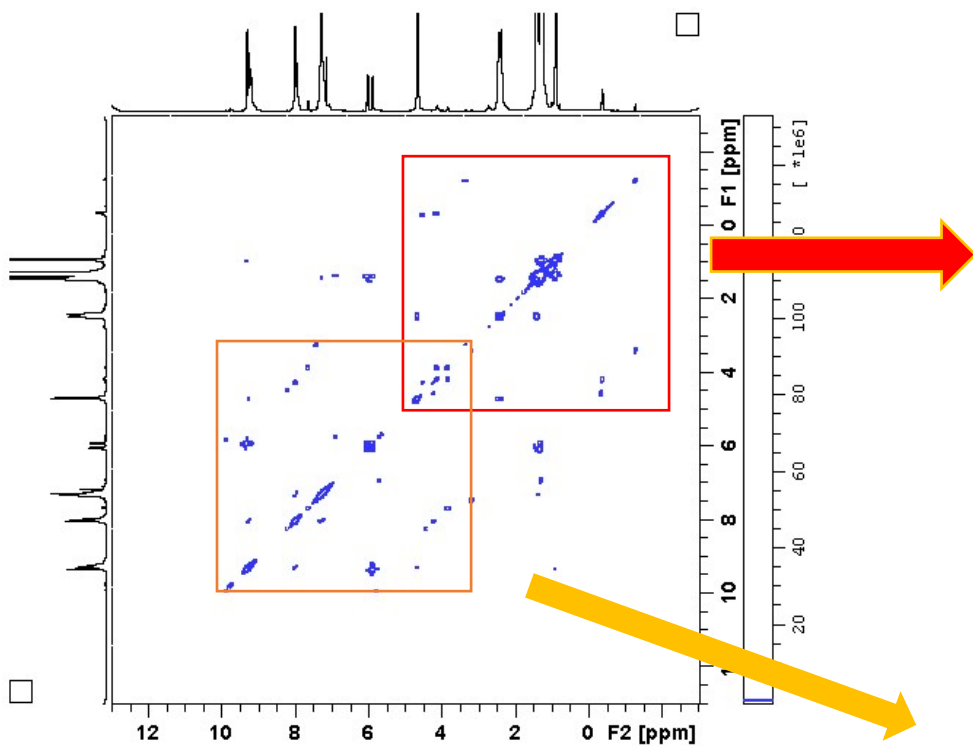


Figure S13. 2D COSY (600 MHz, C₆D₆, 298 K) of the mixture of CP₆ (38.6 mM) and crotonaldehyde 4 (15.3 equiv).

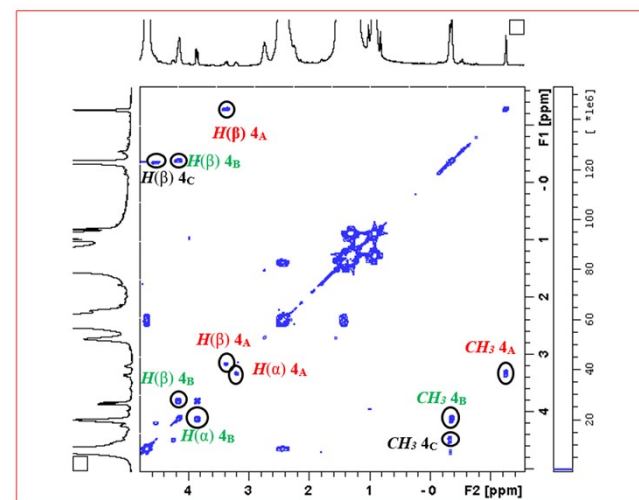


Figure S14. Relevant portion of 2D COSY (400 MHz, C₆D₆, 298 K) in Figure S13.

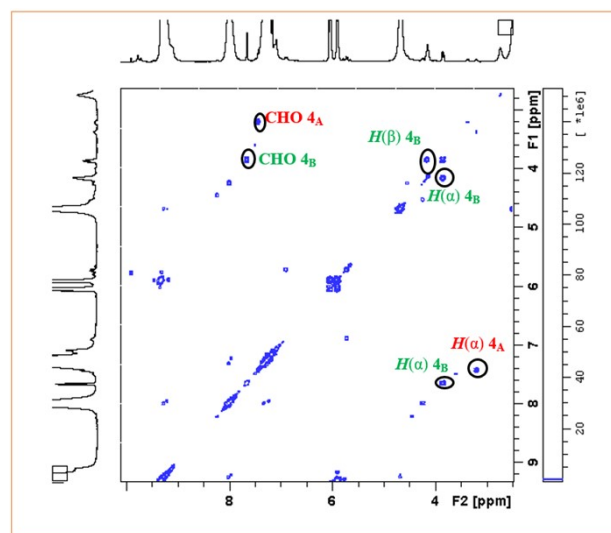


Figure S15. Relevant portion of 2D COSY spectrum (400 MHz, C₆D₆, 298 K) in Figure S13.

4.2.3 2D HSQC of the mixture of CP₆ and crotonaldehyde 4

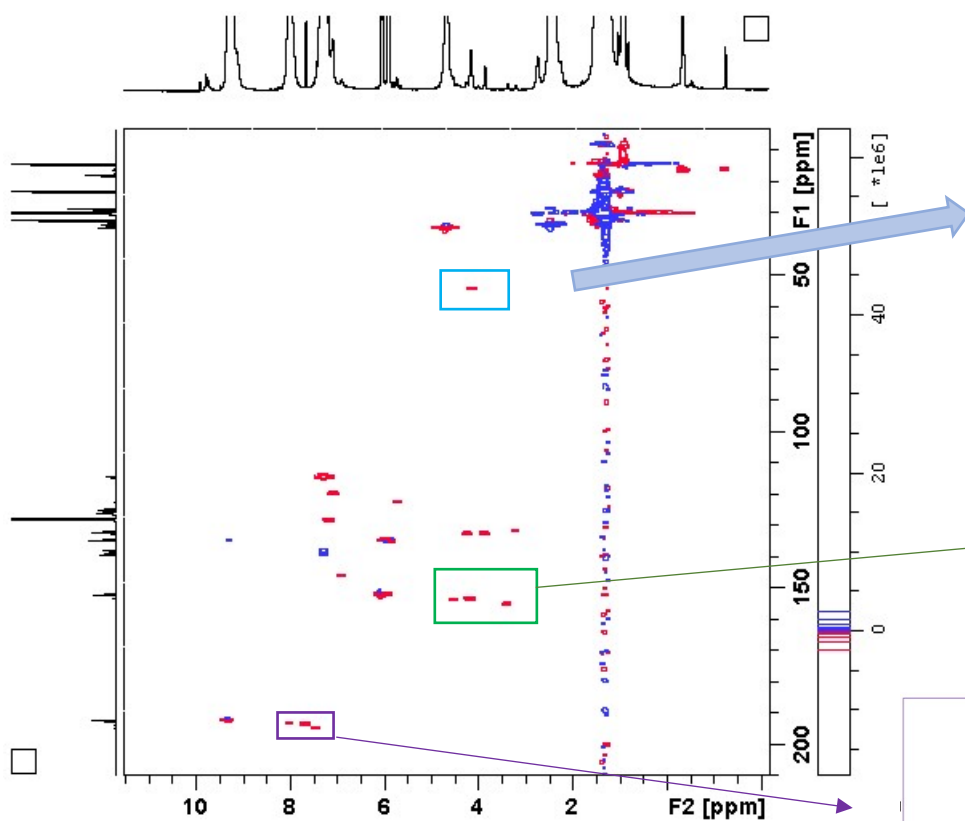


Figure S16. 2D HSQC (600 MHz, C₆D₆, 298 K) of the mixture of CP₆ (38.6 mM) and crotonaldehyde 4 (15.3 equiv).

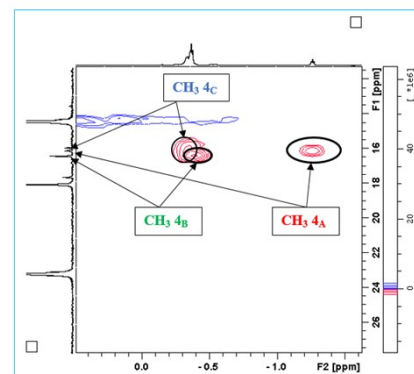


Figure S17. Relevant region of 2D HSQC (600 MHz, C₆D₆, 298 K) in Figure S16.

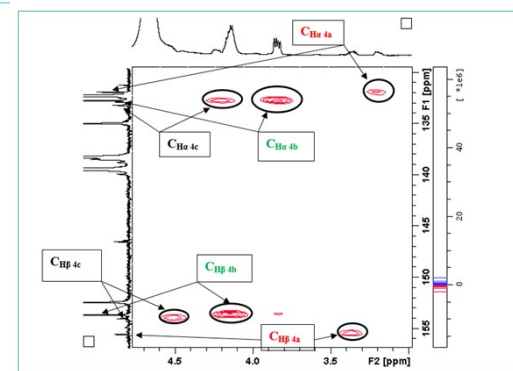


Figure S18. Relevant region of 2D HSQC (600 MHz, C₆D₆, 298 K) in Figure S16.

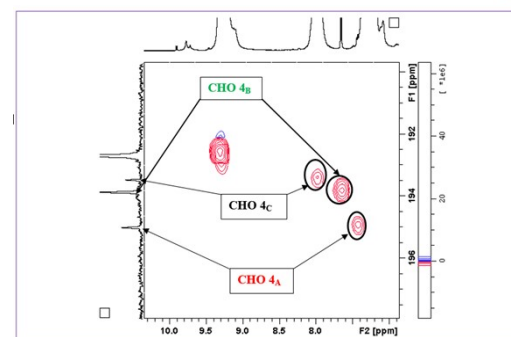


Figure S19. Relevant region of 2D HSQC (600 MHz, C₆D₆, 298 K) in Figure S16.

4.2.4 ^{13}C NMR of the mixture of CP_6 and crotonaldehyde **4**

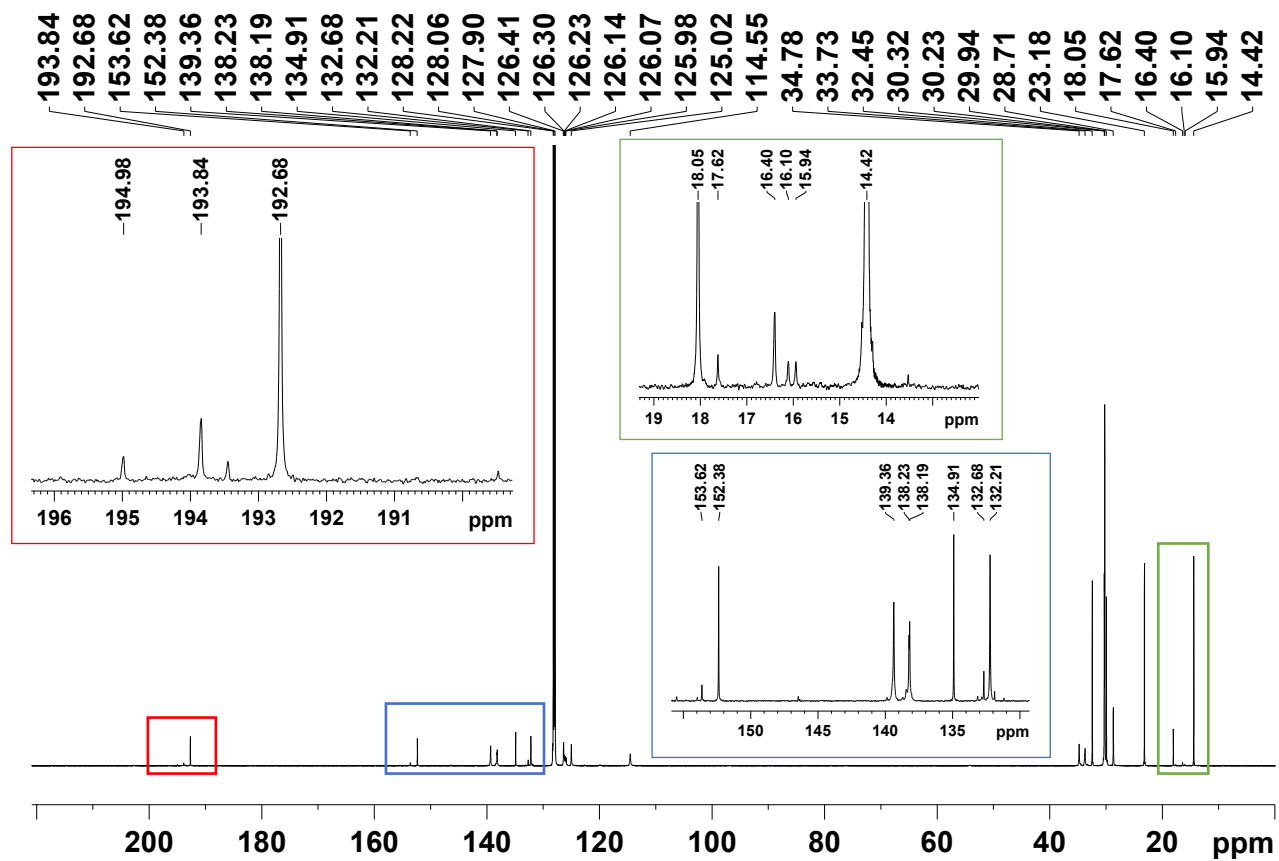


Figure S20. ^{13}C NMR (100 MHz, C_6D_6 , 298K) of the mixture of CP_6 (38.6 mM) and crotonaldehyde **4** (15.3 equiv).

4.2.4 ^{13}C NMR of the mixture of CP_6 and crotonaldehyde **4**

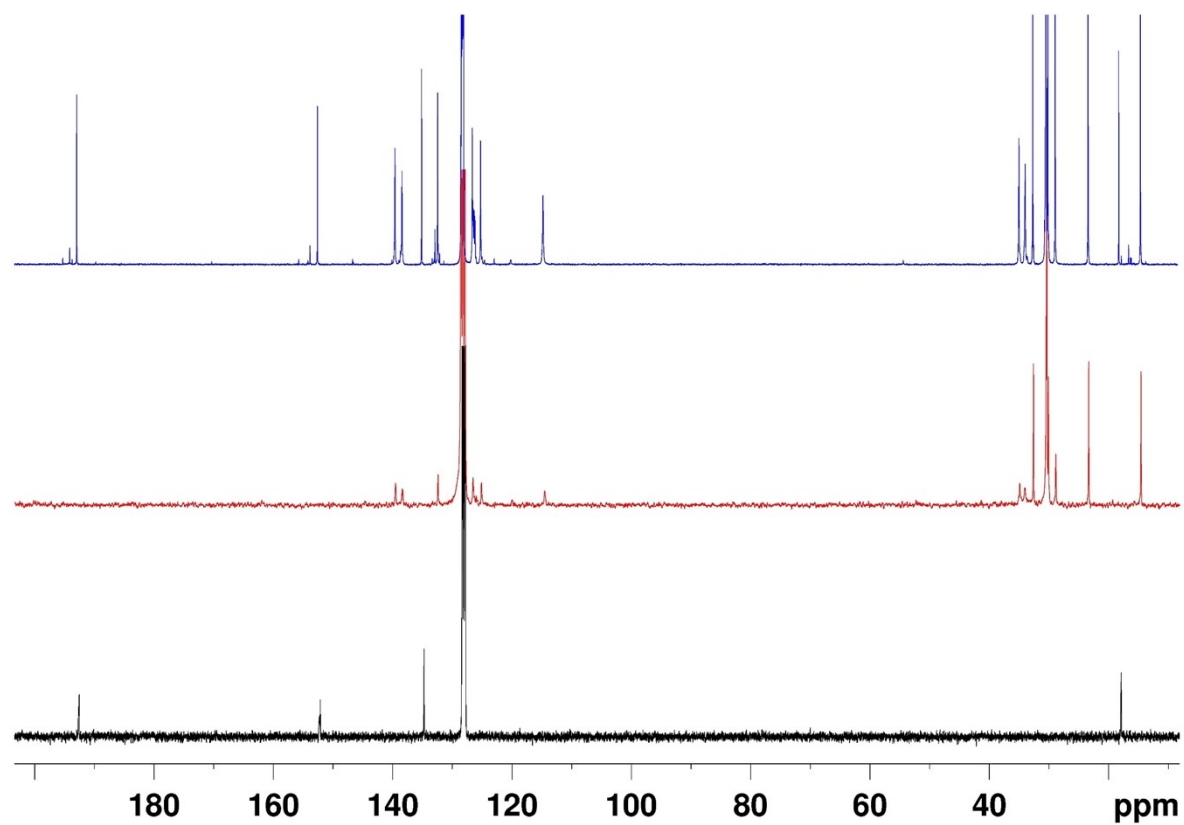


Figure S21. Stacked ^{13}C NMR (100 MHz, C_6D_6 , 298K) of (from bottom to top): crotonaldehyde **4**, CP_6 , and mixture of CP_6 (38.6 mM) and crotonaldehyde **4** (15.3 equiv).

4.3 Diffusion NMR experiments for the encapsulation of crotonaldehyde **4** inside capsule **CP₆**

Diffusion NMR and DOSY data were collected at 9.4 T, on Avance III Bruker NMR spectrometers, operating at 400.13 MHz for ¹H, equipped with a z-gradient system capable of producing maximal gradient pulses of about 50 G/cm. ¹H-diffusion NMR and DOSY experiments were performed using the eddy currents delays (LED) pulse sequence¹ using sine-shaped pulse gradients incremented from 0.7 to 32.2 G/cm (effective gradient strength: $G(2/\pi)$). The diffusion coefficients were extracted from: $\ln I/I_0 = -\gamma^2 \delta^2 G^2 (2/\pi)^2 (\Delta - \delta/4) D = -bD$, where I and I_0 are the echo intensity in the presence and absence of the gradient pulses, respectively, γ is the gyromagnetic ratio, G is the pulse gradient strength, $2/\pi$ is a geometrical correction factor due to the sine shape of the pulse gradients used, δ is the duration of the pulse gradient, Δ is the time interval between the leading edges of the pulse gradient used, and D is the diffusion coefficient. All diffusion NMR experiments were performed at 298 K in triplicates. The given values represent means \pm the standard error of the means (SEM). For routine diffusion NMR and DOSY measurements the sine-shaped pulse gradients were incremented from 0.7 to 32.2 G/cm in 10 steps and D was set to 50 ms, d to 6 ms and t_e to 5 ms unless specified differently. When the dependency of the diffusion time and t_e was explored the diffusion NMR and DOSY data included at least 28 and 32 gradient steps. Note that diffusion NMR and DOSY data were analyzed using the Bruker software.

Table S1: Diffusion coefficients, as deduced from diffusion NMR, of representative signals of **4**, **3**, **CP₆**, a mixture of **CP₆** and **4**, and the entire reaction mixture used for catalysis in C₆D₆ at 298K

Sample in C ₆ D ₆		^c Diffusion coefficients [x10 ⁻⁵ cm ² s ⁻¹]
Hexameric Capsule of CP₆ (38.6mM)	CP₆ (4.66ppm)	0.07 \pm 0.01 ^a
	C ₆ H ₆ (7.16ppm)	1.18 \pm 0.14 ^a
4 (590mM)	4 (5.65ppm)	2.60 \pm 0.01 ^b
	C ₆ H ₆ (7.16ppm)	2.29 \pm 0.02 ^b
3 (150mM)	3 (3.06ppm)	1.50 \pm 0.01 ^b
	C ₆ H ₆ (7.16ppm)	2.41 \pm 0.09 ^b
Hexameric Capsule of CP₆ (38.6mM) with 12 eq. of 4 (relative to hexamer)	Encapsulated 4 (-0.34ppm)	0.07 \pm 0.01 ^a
	CP₆ (4.66ppm)	0.07 \pm 0.01 ^a
	Free 4 (6.06ppm)	1.54 \pm 0.01 ^a
	C ₆ H ₆ (7.16ppm)	1.37 \pm 0.01 ^a

^a $\Delta/\delta/t_e = 50/6/5$ ms. ^b $\Delta/\delta/t_e = 30/2/5$ ms. ^cThe diffusion coefficients are means \pm standard error of the mean (SEM) of at least three independent measurements. In all measurements only 10 gradient values were collected and a single component fit function was used to analyze the diffusion data.

Table S2: Diffusion coefficients at different Δ and t_e -values, as deduced from diffusion NMR, of representative signals of the mixture of hexameric capsule of **CP₆** (38.6mM), **4** (590mM), **3** (150mM), L-proline (29.7mM) in C₆D₆ solution with 4 μ l of C₆H₆.

Diffusion time (Δ)	peak (ppm)	^a Diffusion coefficients [$\times 10^{-5}$ cm ² s ⁻¹]		
		$t_e=5\text{ms}$	$t_e=250\text{ms}$	$t_e=1\text{s}$
15ms	-1.2 (encapsulated 4)	0.07 \pm 0.01	0.08 \pm 0.01	0.17 \pm 0.01
	-0.34 (encapsulated 4)	0.07 \pm 0.01	0.18 \pm 0.01	0.56 \pm 0.02
	0.93 (CP₆)	0.06 \pm 0.01	0.07 \pm 0.01	0.07 \pm 0.01
	4.66 (CP₆)	0.07 \pm 0.01	0.07 \pm 0.01	0.09 \pm 0.01
	6.06 (4)	1.54 \pm 0.03	1.34 \pm 0.01	1.07 \pm 0.02
	7.16 (C ₆ H ₆)	1.19 \pm 0.03	1.18 \pm 0.01	1.25 \pm 0.04
50ms	-1.2 (encapsulated 4)	0.07 \pm 0.01	0.07 \pm 0.01	0.10 \pm 0.01
	-0.34 (encapsulated 4)	0.06 \pm 0.01	0.10 \pm 0.01	0.37 \pm 0.04
	0.93 (CP₆)	0.07 \pm 0.01	0.07 \pm 0.01	0.07 \pm 0.01
	4.66 (CP₆)	0.07 \pm 0.01	0.07 \pm 0.01	0.08 \pm 0.01
	6.06 (4)	1.52 \pm 0.01	1.39 \pm 0.01	1.16 \pm 0.03
	7.16 (C ₆ H ₆)	1.26 \pm 0.02	1.29 \pm 0.04	1.29 \pm 0.02
100ms	-1.2 (encapsulated 4)	0.06 \pm 0.01	0.07 \pm 0.01	0.09 \pm 0.01
	-0.34 (encapsulated 4)	0.06 \pm 0.01	0.09 \pm 0.02	0.50 \pm 0.02
	0.93 (CP₆)	0.07 \pm 0.01	0.07 \pm 0.01	0.07 \pm 0.01
	4.66 (CP₆)	0.07 \pm 0.01	0.07 \pm 0.01	0.07 \pm 0.01
	6.06 (4)	1.46 \pm 0.01	1.40 \pm 0.01	1.23 \pm 0.01
	7.16 (C ₆ H ₆)	1.26 \pm 0.01	1.30 \pm 0.02	1.33 \pm 0.05
200ms	-1.2 (encapsulated 4)	0.06 \pm 0.01	0.06 \pm 0.01	0.09 \pm 0.04
	-0.34 (encapsulated 4)	0.06 \pm 0.01	0.08 \pm 0.01	0.72 \pm 0.06
	0.93 (CP₆)	0.07 \pm 0.01	0.07 \pm 0.01	0.07 \pm 0.01
	4.66 (CP₆)	0.06 \pm 0.01	0.07 \pm 0.01	0.08 \pm 0.01
	6.06 (4)	1.44 \pm 0.01	1.38 \pm 0.01	1.28 \pm 0.03
	7.16 (C ₆ H ₆)	1.29 \pm 0.04	1.28 \pm 0.05	1.29 \pm 0.03

^aThe diffusion coefficients are mean \pm standard error of the mean (SEM) of at least three independent measurements. In all measurements only 10 gradient values were collected and a single component fit function was used to fit the data.

The data presented in Tables S1 and S2 clearly show that the diffusion coefficient of only one of the signals at high field (i.e., the signal at -0.34 ppm) is sensitive to the t_e -values and appear to increase with the increase in t_e . Some smaller changes, in the opposite direction, are observed for the signal at ~6.0 ppm attributed to unbound **4**. All these results are consistent with exchange of magnetization between two pools that differ considerably in their diffusion coefficients. Based on these results we decided to repeat the diffusion NMR and DOSY measurements with significantly more gradient values to allow for reliable fitting the diffusion data by two component fitting function.

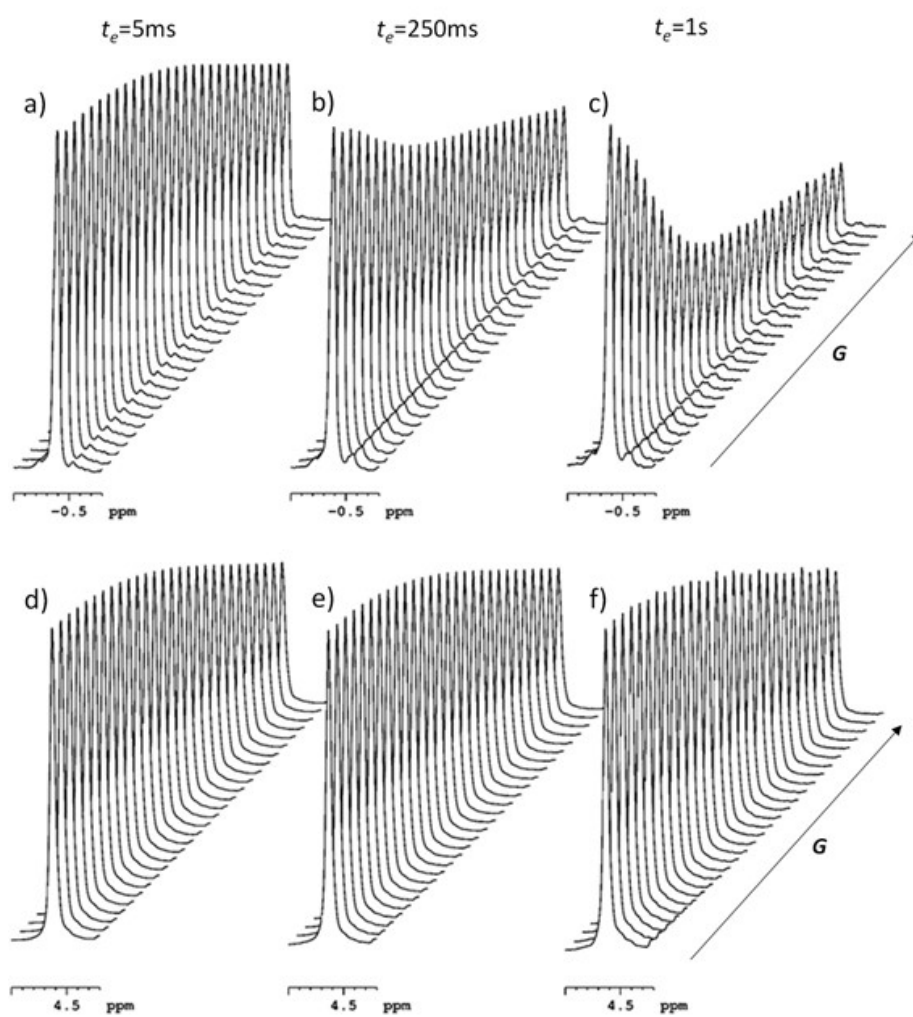


Figure S22. Signal decay of the peaks of a mixture of **4** and **CP₆** as a function of gradient strength (G) at three t_e values for one peak of **CP₆** (d-f) and one peak attributed to bound aldehydes (a-c) at different t_e values.

4.4 Encapsulation experiments of nitrone **3** inside capsule **CP**₆

4.4.1 ¹H NMR spectra of mixture of **CP**₆ and nitrone **3**

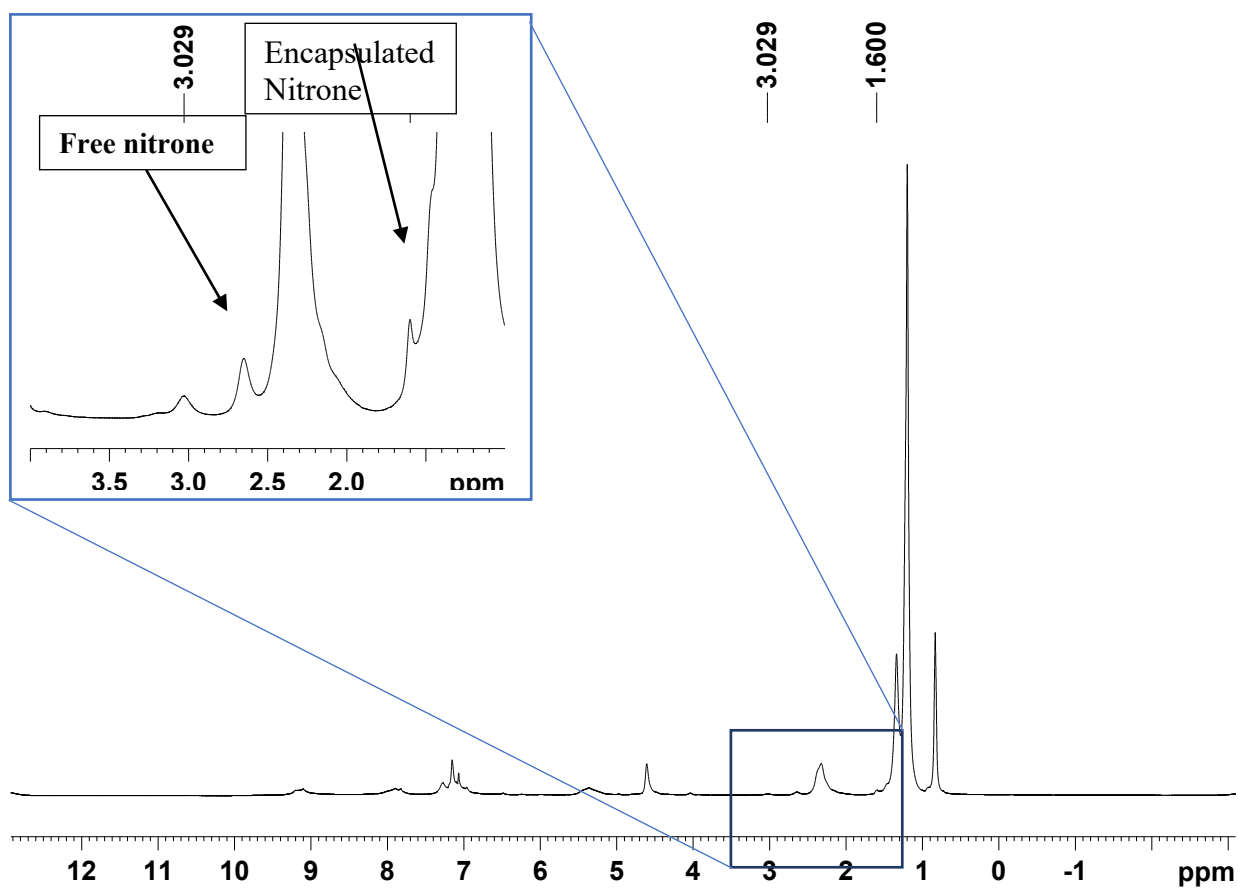


Figure S23. ¹H NMR spectrum (400 MHz, C_6D_6 , 298K) of mixture of **CP**₆ (38.6 mM) and nitrone **3** (148 mM, 3.8 equiv) in C_6D_6 (0.55 mL). A blue inset, showing free and encapsulated guest **3**, is present.

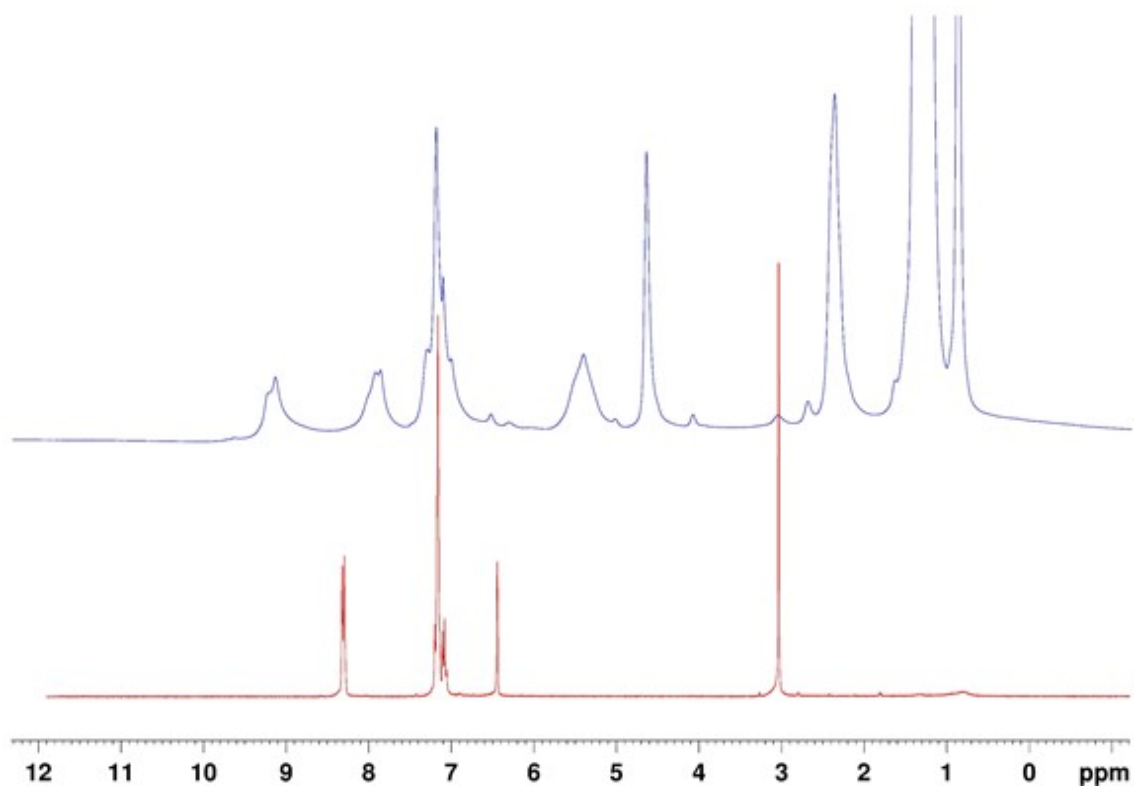


Figure S24. Stacked ¹H NMR spectra (400 MHz, C₆D₆, 298 K) of nitrone **3** (bottom) and mixture of CP₆ (38.6 mM) and nitrone **3** (148 mM, 3.8 equiv) in C₆D₆ (0.55 mL).

4.4.2 2D EXSY NMR of mixture of CP₆ and nitrone 3

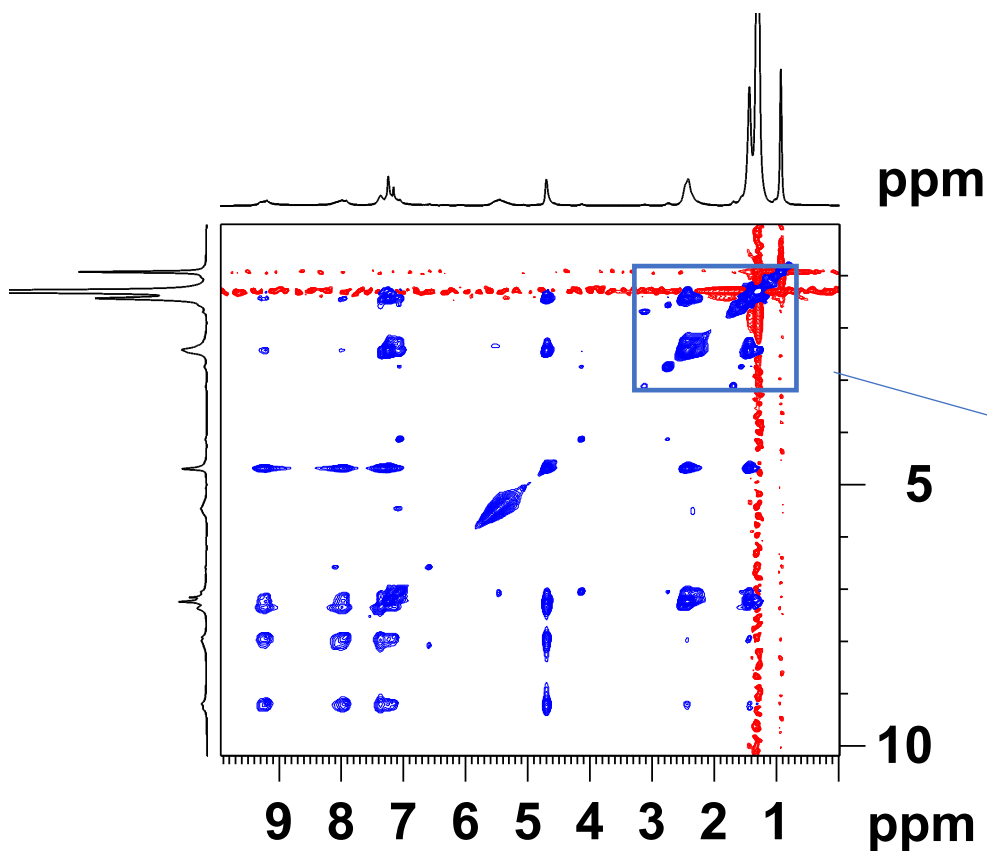


Figure S25. 2D EXSY NMR (600 MHz, 298 K, C₆D₆, d8 = 250 ms) of mixture of CP₆ (38.6 mM) and nitrone 3 (148 mM, 3.8 equiv) in C₆D₆ (0.55 mL).

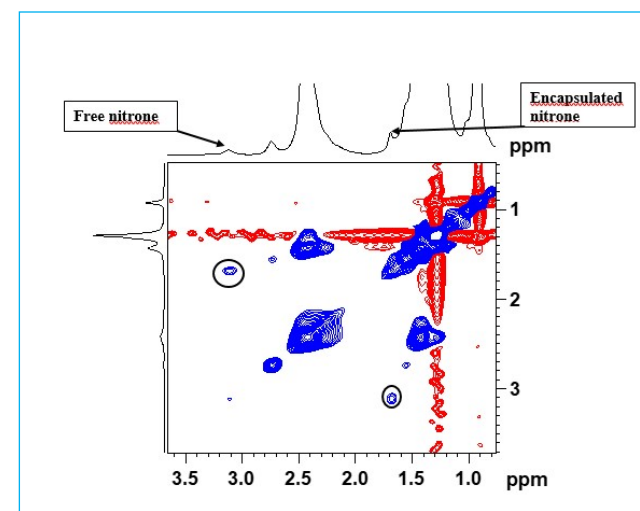


Figure S26. Relevant region of 2D EXSY NMR in **Figure S25**. Exchange cross peaks between free and encapsulated nitrone 3 are visible.

4.4.3 ^{13}C NMR spectrum of nitrone **3**

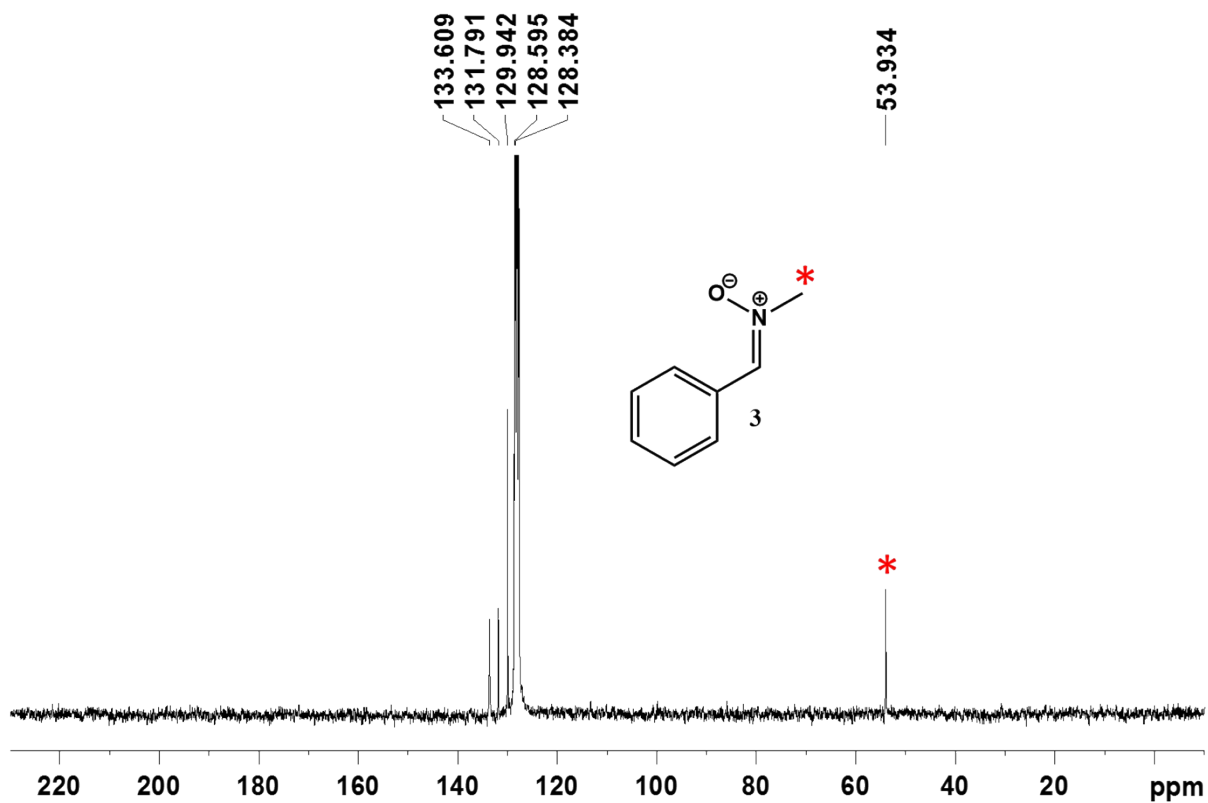


Figure S27. ^{13}C NMR (75 MHz, C_6D_6 , 298K) of nitrone **3**. ^{13}C NMR signal attributable to methyl carbon is evidenced with a red asterisk.

4.4.4 ^{13}C NMR spectrum of mixture of CP_6 and nitrone **3**

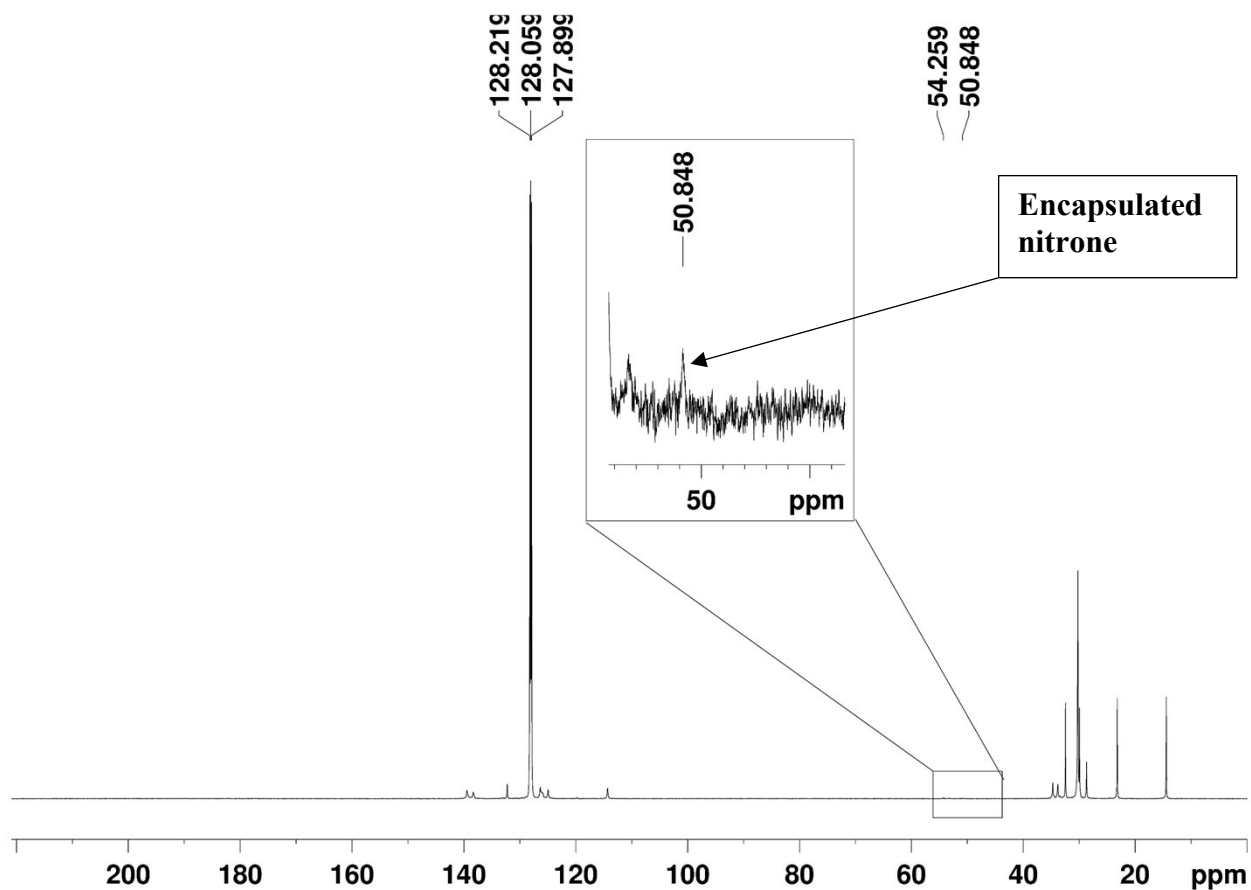


Figure S28. ^{13}C NMR (75 MHz, C_6D_6 , 298 K) of mixture of CP_6 (38.6 mM) and nitrone **3** (148 mM, 3.8 equiv) in C_6D_6 (0.55 mL). An inset showing methyl signal of encapsulated nitrone is present.

4.4.5 2D HSQC NMR of mixture of CP₆ and nitrone 3

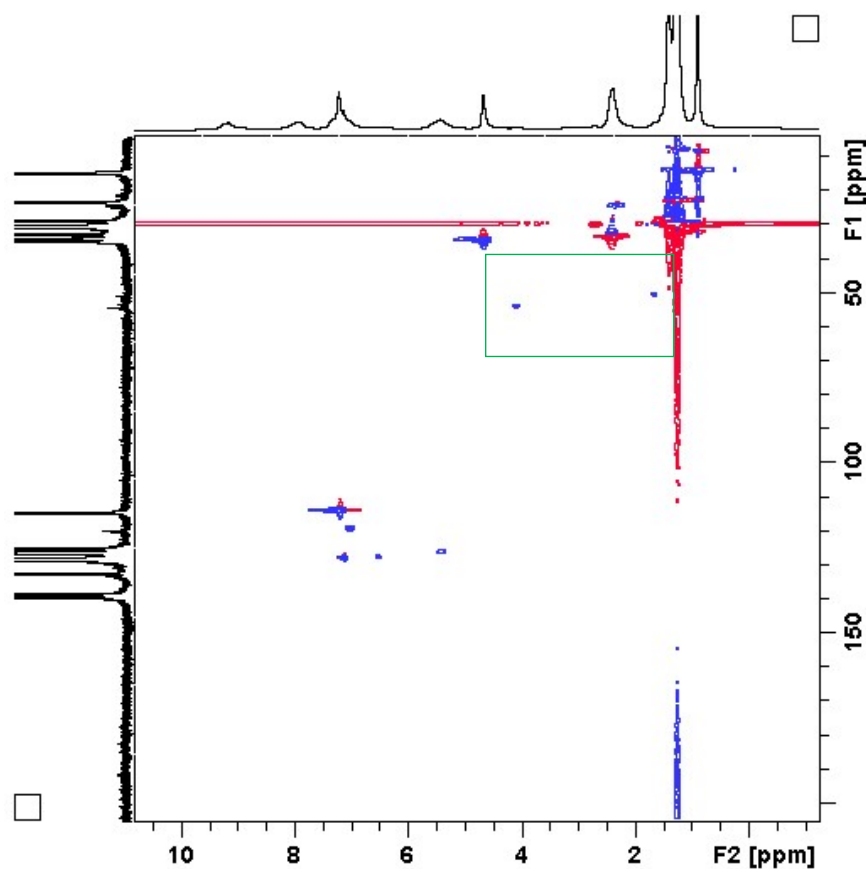


Figure S29. 2D HSQC NMR (600 MHz, C₆D₆, 298 K) of the mixture of CP₆ (38.6 mM) and nitrone 3 (148 mM, 3.8 equiv) in C₆D₆ (0.55 mL).

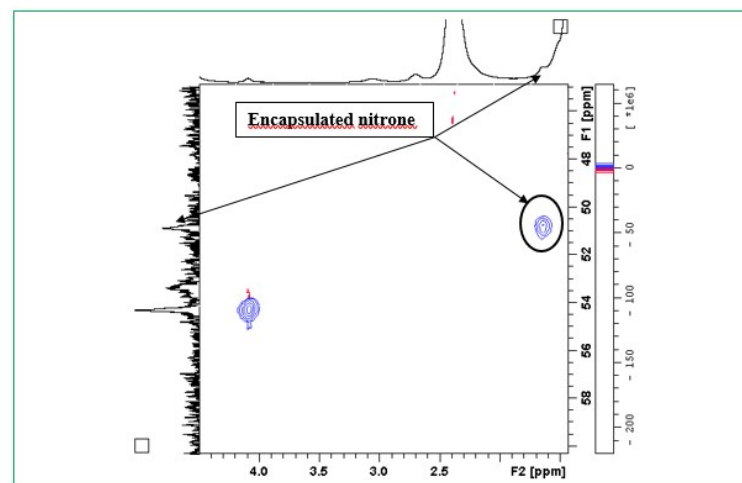


Figure S30. Relevant portion of 2D HSQC NMR (600 MHz, C₆D₆, 298 K) of the mixture of CP₆ (38.6 mM) and nitrone 3 (148 mM, 3.8 equiv) in C₆D₆ (0.55 mL).

4.4.6 2D DOSY NMR of mixture of CP₆ and nitrone 3

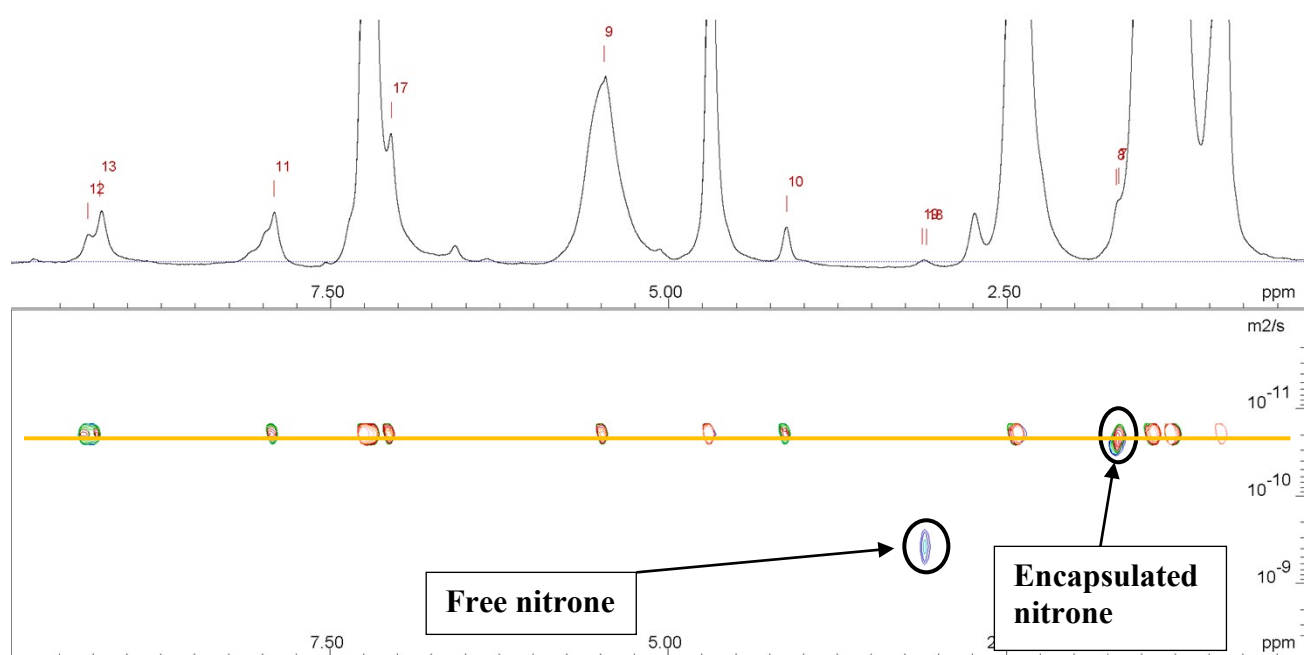


Figure S31. 2D DOSY NMR (600 MHz, C₆D₆, 298 K, p₃₀ = 1400 μs) of the mixture of CP₆ (38.6 mM) and nitrone **3** (148 mM, 3.8 equiv) in C₆D₆ (0.55 mL). Free and encapsulated guest are evidenced.

4.5 Encapsulation L-proline inside capsule CP_6

4.5.1 1H NMR spectrum of mixture of CP_6 and L-proline

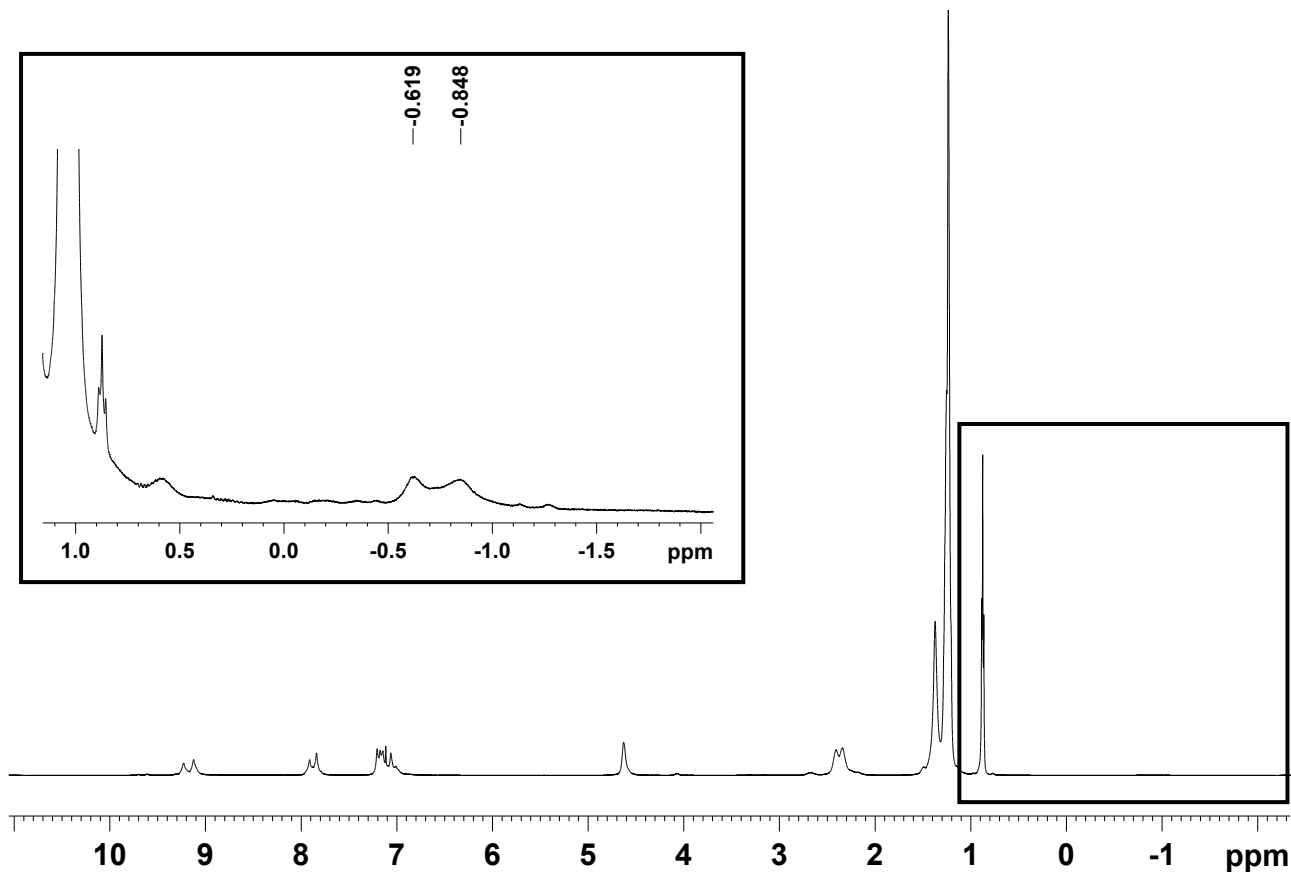


Figure S32. 1H NMR (600 MHz, C_6D_6 , 298 K) of the mixture of CP_6 (38.6 mM) and L-proline (50.2 mM, 1.3 equiv) in C_6D_6 (0.55 mL). Inset showing signals attributable to the encapsulated guest is present.

4.5.2 2D HSQC NMR of mixture of CP₆ and L-proline

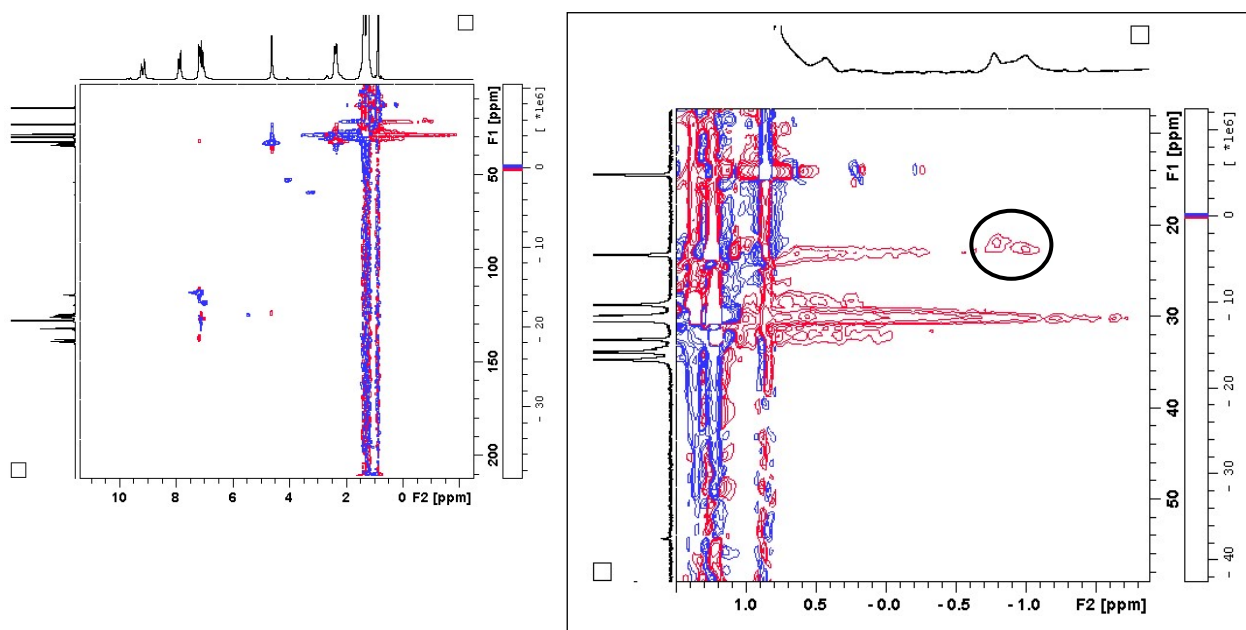


Figure S33. 2D HSQC NMR (600 MHz, C₆D₆, 298 K) of the mixture of CP₆ (38.6 mM) and L-proline (50.2 mM, 1.3 equiv) in C₆D₆ (0.55 mL). Inset showing cross-peak signal attributable to the encapsulated guest is present.

4.5.3 2D DOSY NMR of mixture of CP_6 and L-proline

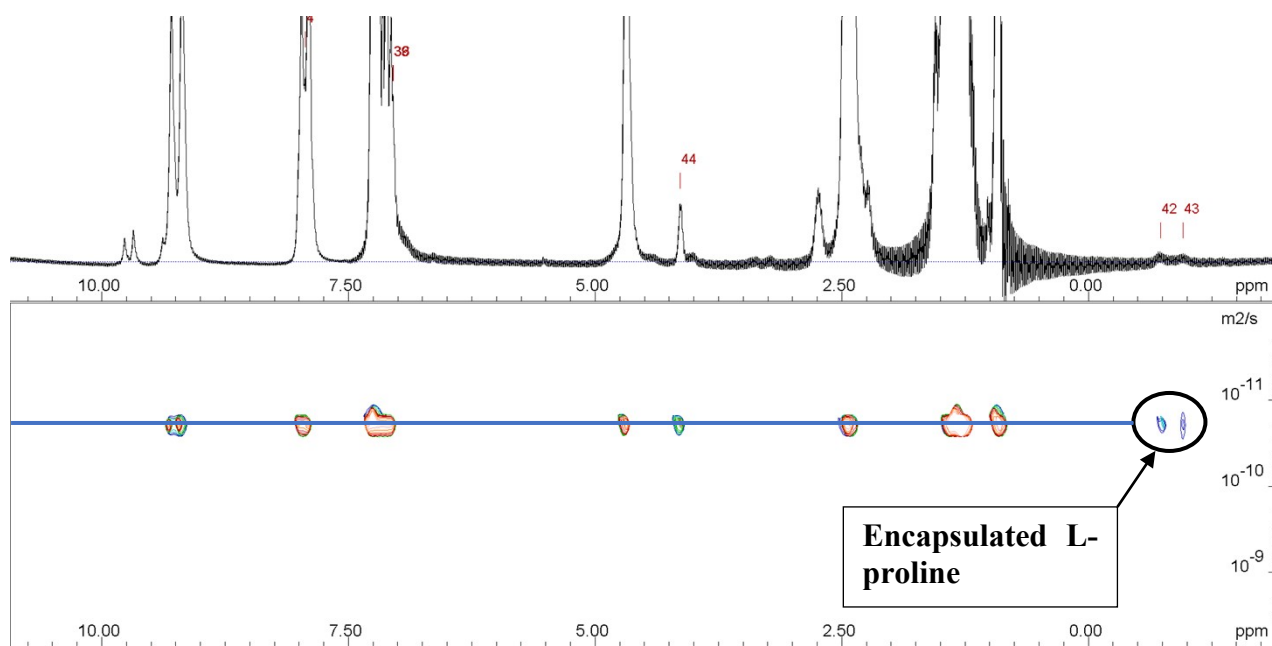


Figure S34. 2D DOSY NMR (600 MHz, C_6D_6 , 298 K, $p_{30} = 1400 \mu\text{s}$) of the mixture of CP_6 (38.6 mM) and L-proline (50.2 mM, 1.3 equiv.) in C_6D_6 (0.55 mL). Free and encapsulated guest are evidenced.

4.6 Encapsulation of iminium species inside capsule CP_6

4.6.1 1H NMR spectra of mixture of CP_6 , L-proline, and crotonaldehyde

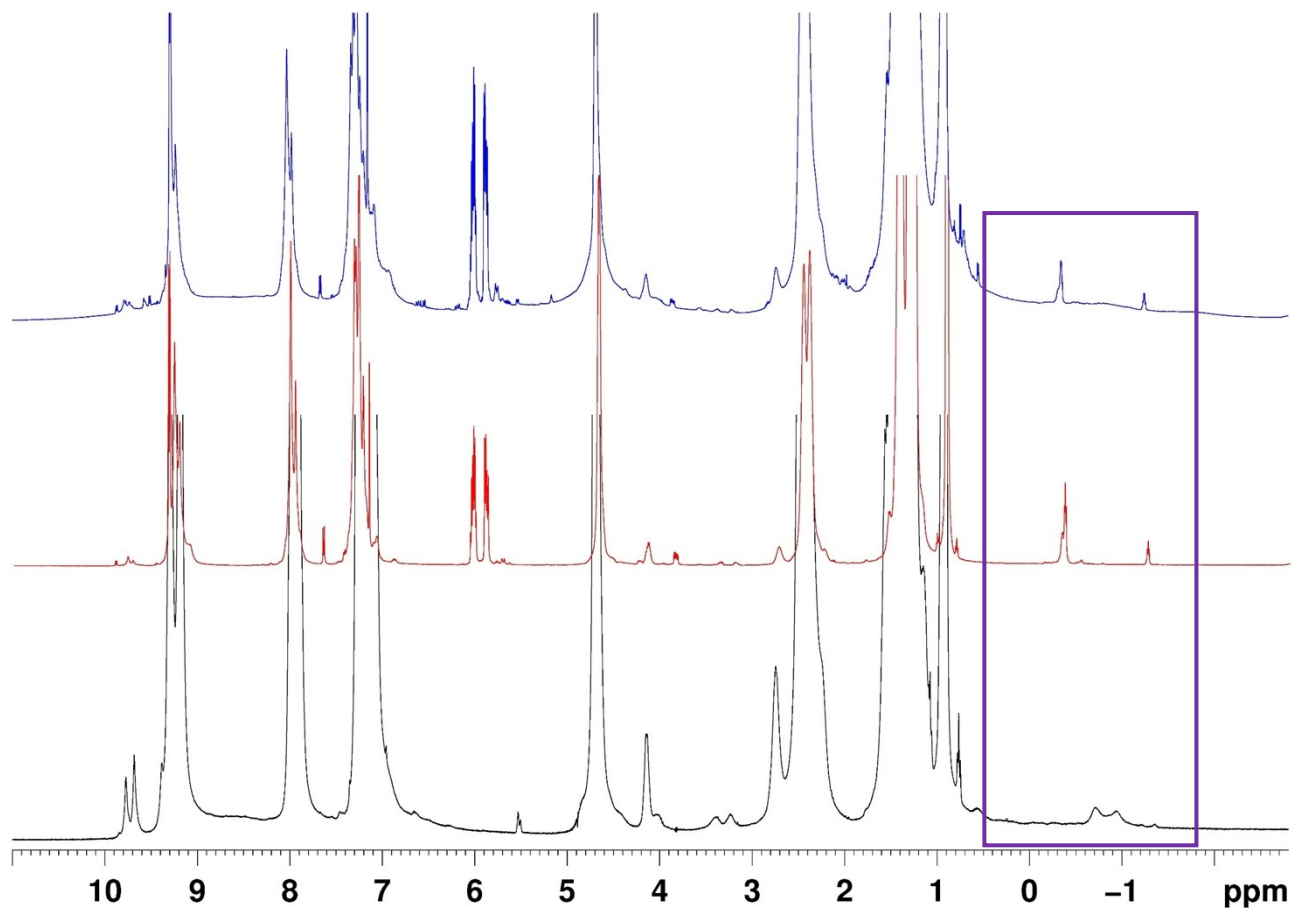


Figure S35. Stacked 1H NMR spectra (600 MHz, C_6D_6 , 298 K) of mixture of CP_6 (38.6 mM) and L-proline (50.2 mM, 1.3 equiv.) (bottom), mixture of CP_6 (38.6 mM) and crotonaldehyde **4** (591 mM, 15.3 equiv) (middle); mixture of CP_6 (38.6 mM), L-proline (50.2 mM, 1.3 equiv.), and crotonaldehyde **4** (591 mM, 15.3 equiv.) (top) in C_6D_6 (0.55 mL).

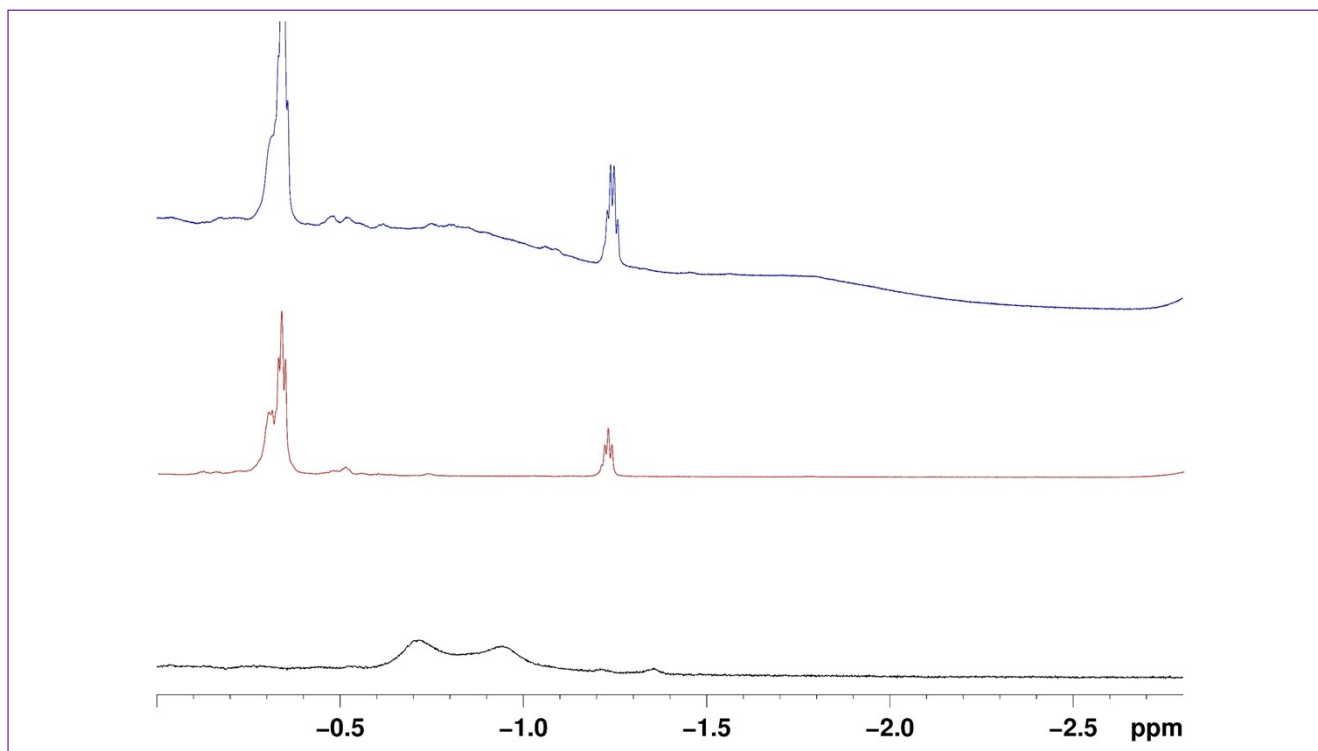


Figure S36. High field region of the spectrum in Figure S36. A new set of signals, arising from the presence of iminium species inside the nanocontainer CP_6 , is evidenced.

4.6.2 2D DOSY NMR of mixture of CP_6 , L-proline, and crotonaldehyde

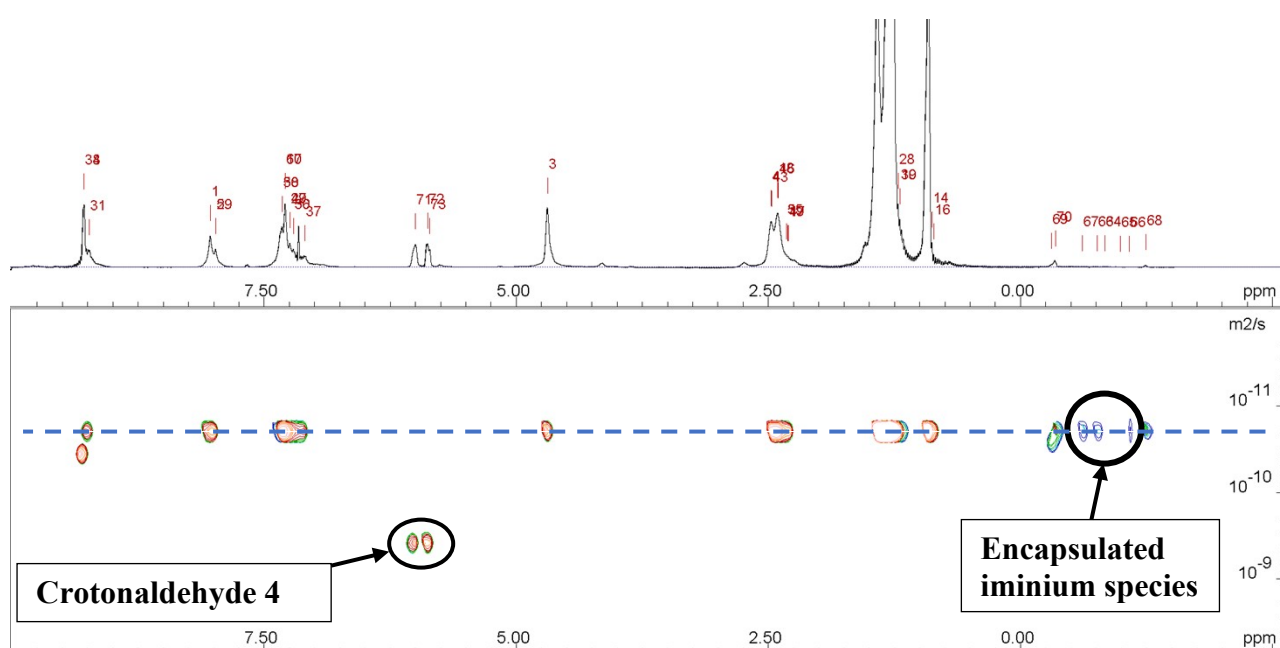


Figure S37. 2D DOSY NMR spectrum (600 MHz, C_6D_6 , 298 K, $p_{30} = 1400 \mu\text{s}$) for the mixture of CP_6 (38.6 mM), L-proline (50.2 mM, 1.3 equiv.), and crotonaldehyde **4** (591 mM, 15.3 equiv.) in C_6D_6 (0.55 mL).

5. ¹H NMR Spectra of the products arising from the 1,3-dipolar cycloaddition reactions and of reduced cycloadducts

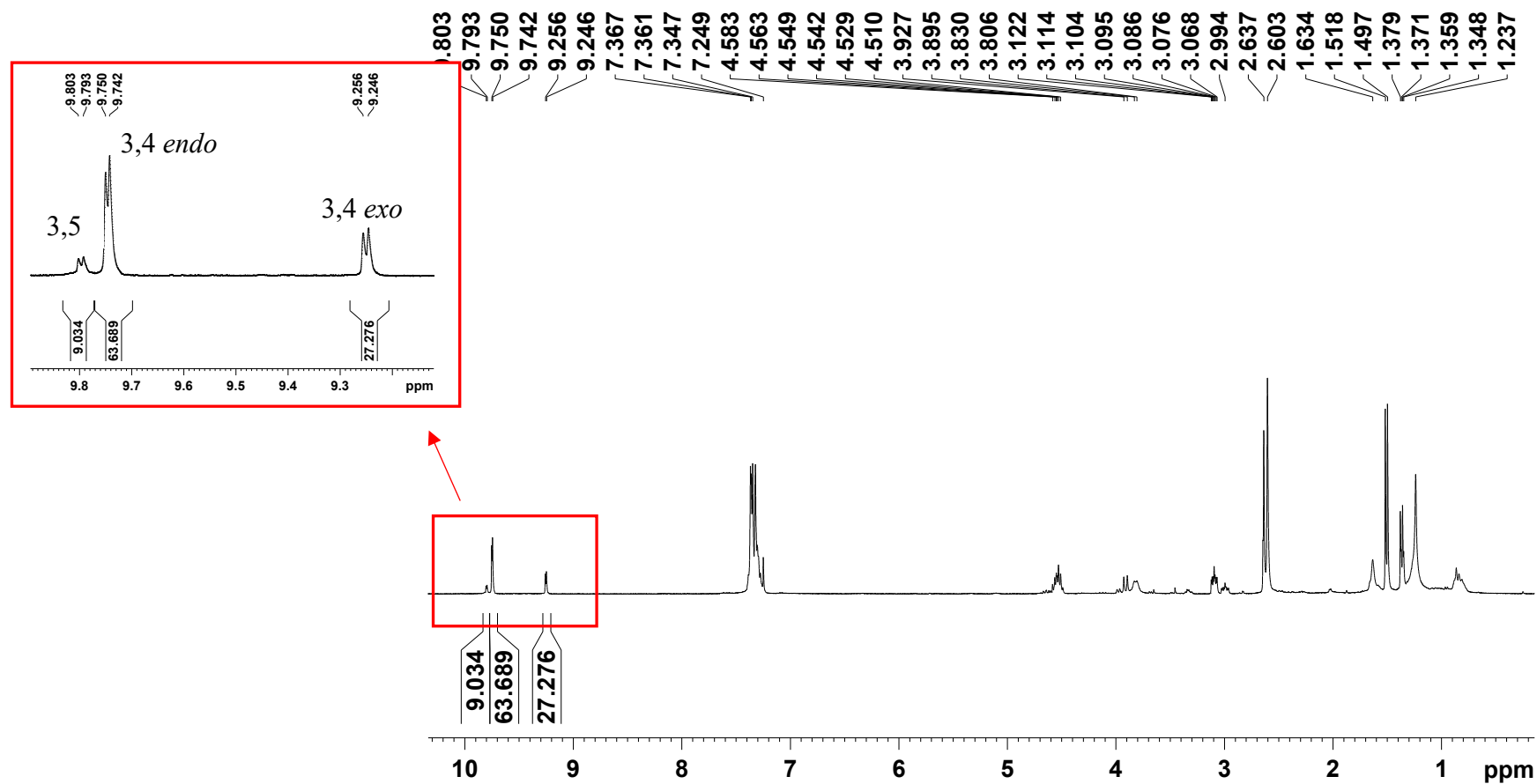


Figure S38. ¹H NMR spectrum (300 MHz, CDCl₃, 298 K) for entry 1, Table 1.

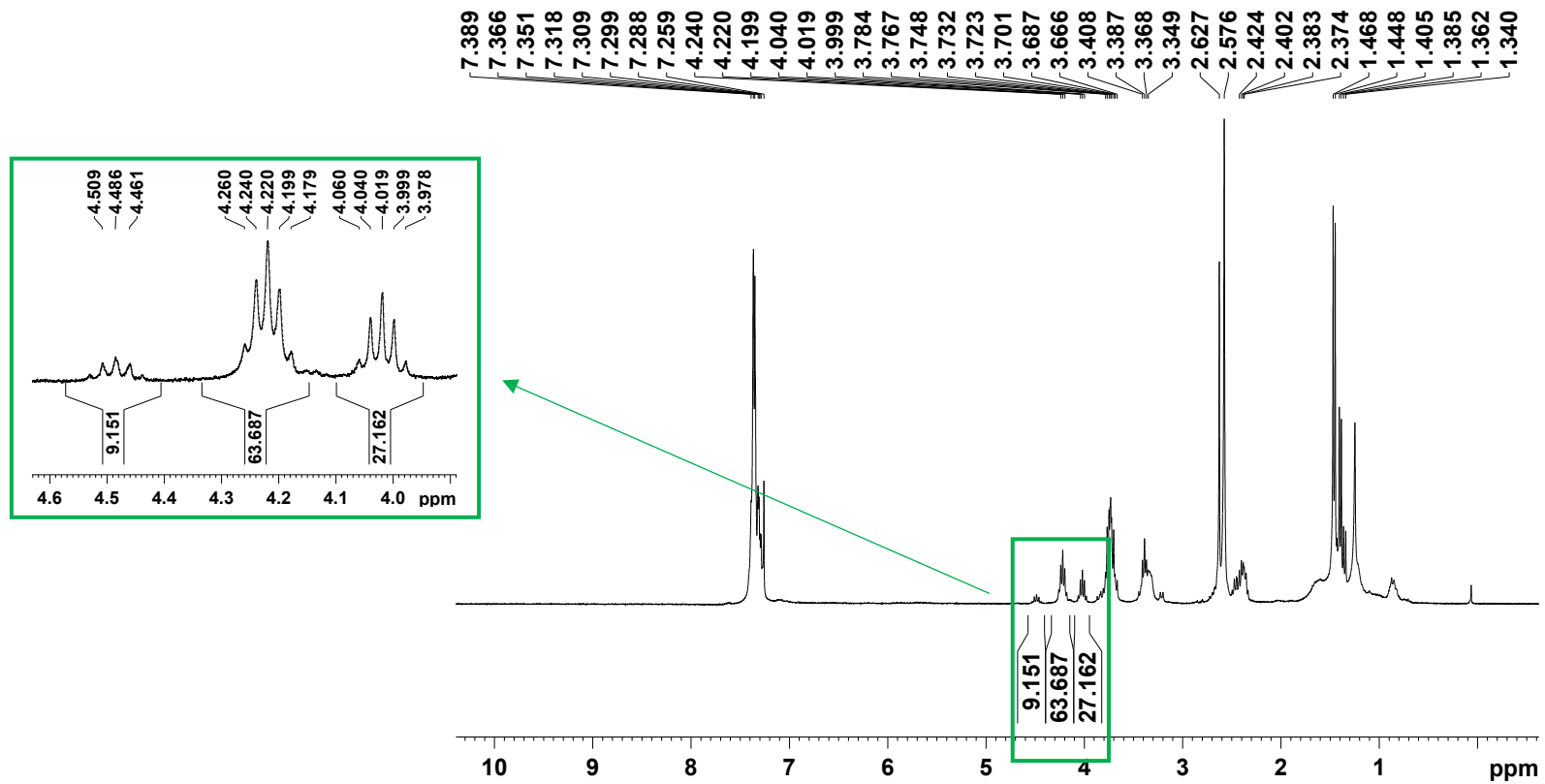


Figure S39. ¹H NMR spectrum (300 MHz, CDCl₃, 298 K) of the reduced mixture for entry 1, Table 1.

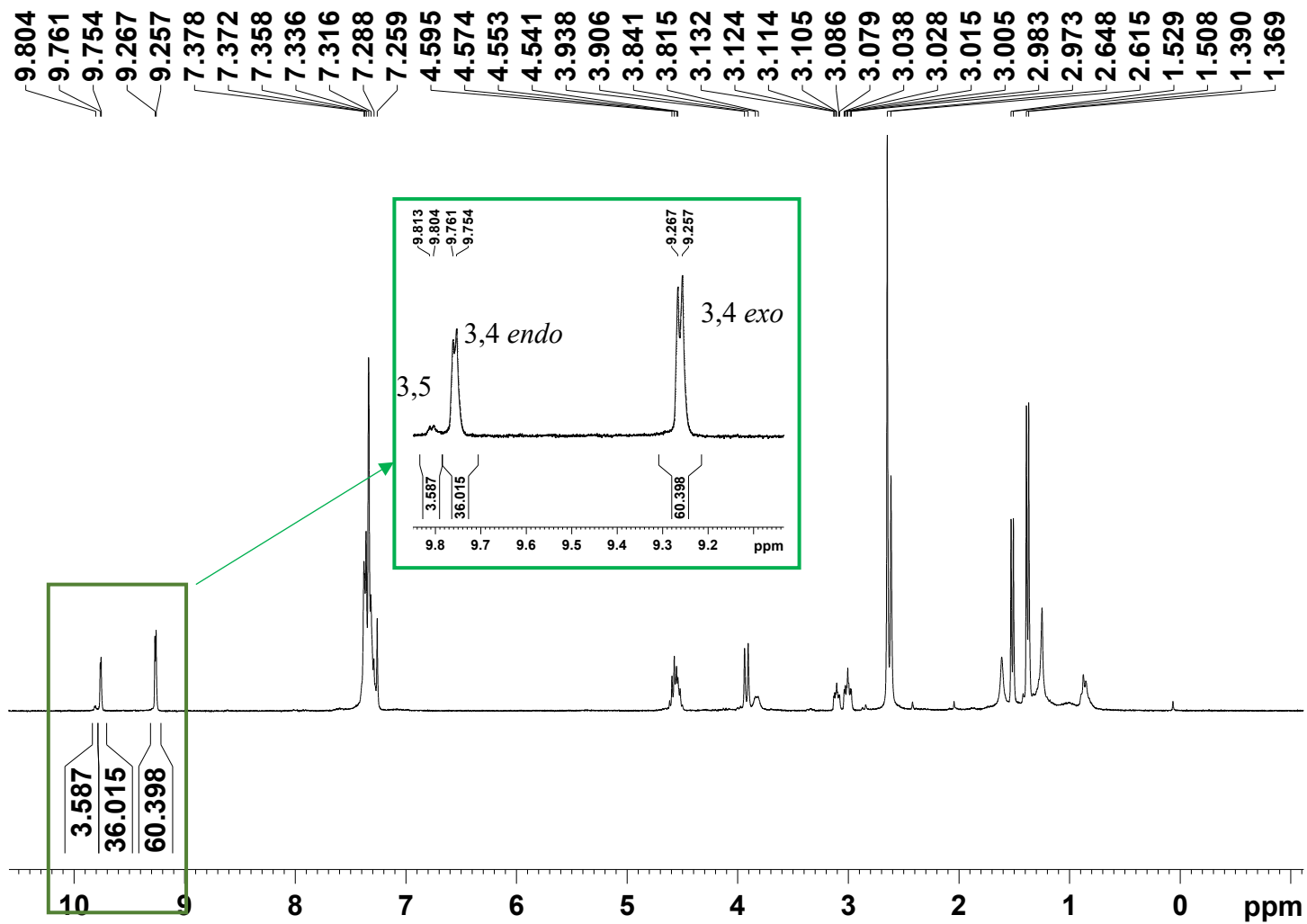


Figure S40. ¹H NMR spectrum (400 MHz, CDCl₃, 298 K) for entry 2, **Table 1** in the manuscript.

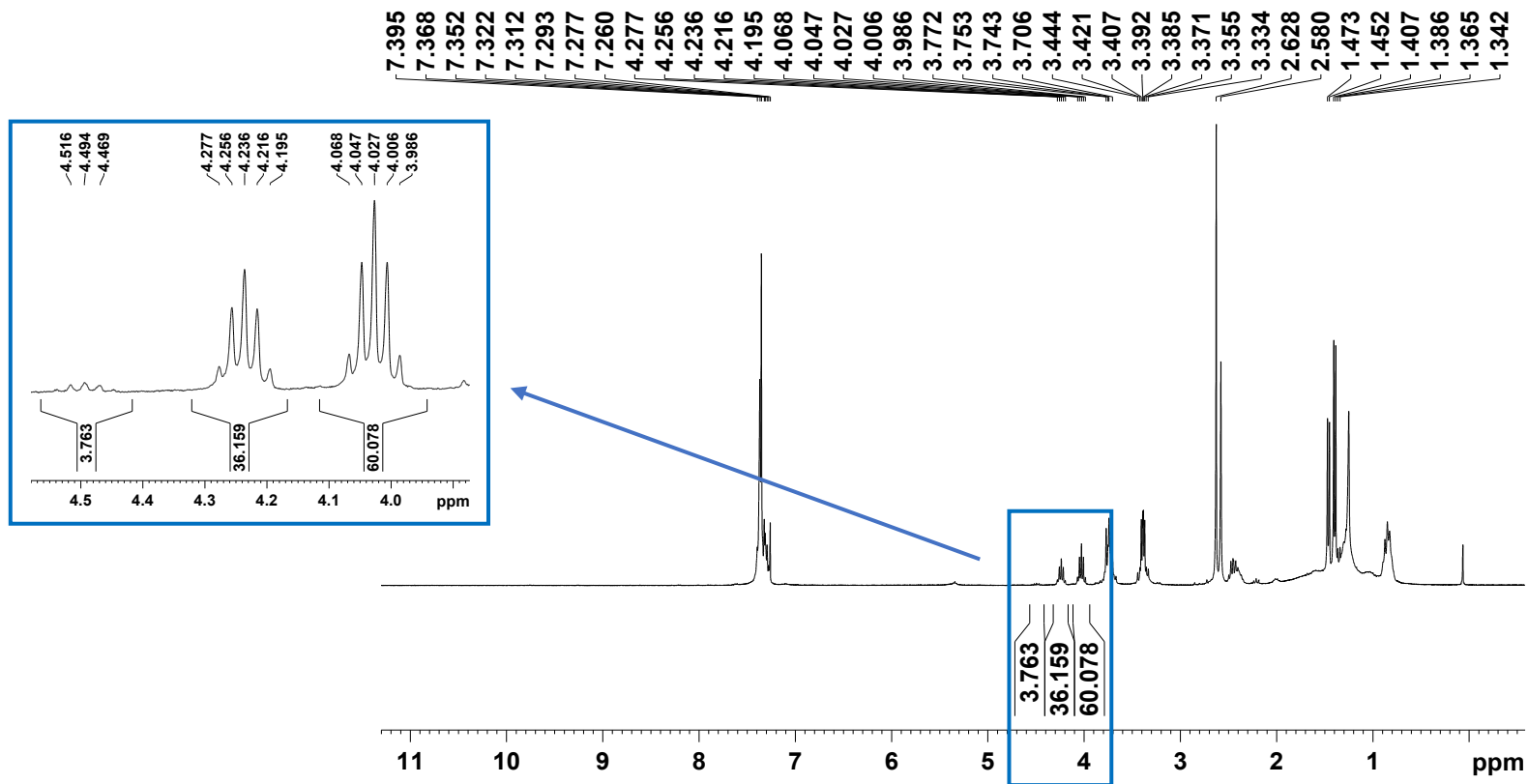


Figure S41. ^1H NMR spectrum (400 MHz, CDCl_3 , 298 K) of the reduced mixture for entry 2, **Table 1** in the manuscript.

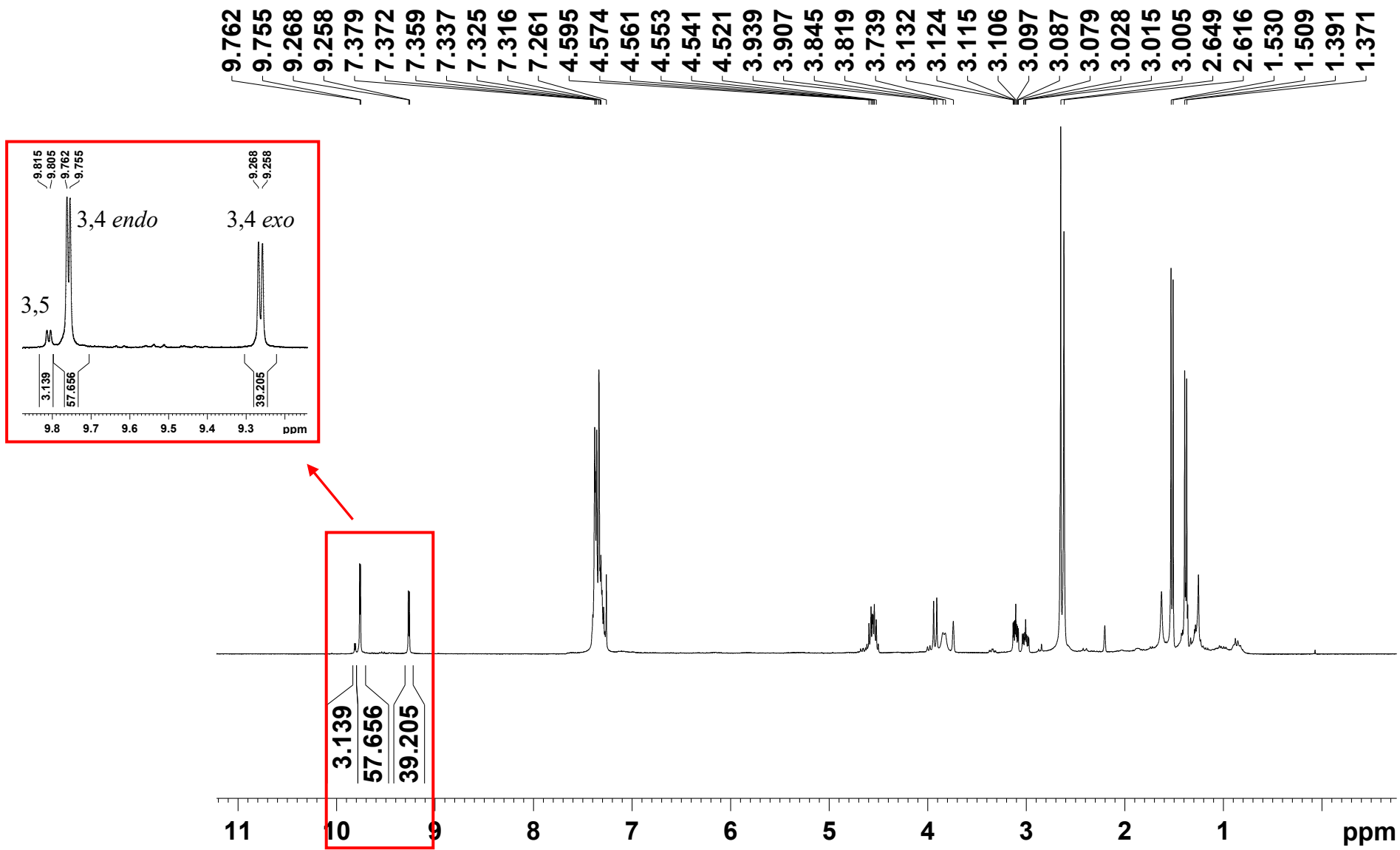


Figure S42. ¹H NMR spectrum (300 MHz, CDCl₃, 298 K) for entry 4, Table 1 in the manuscript.

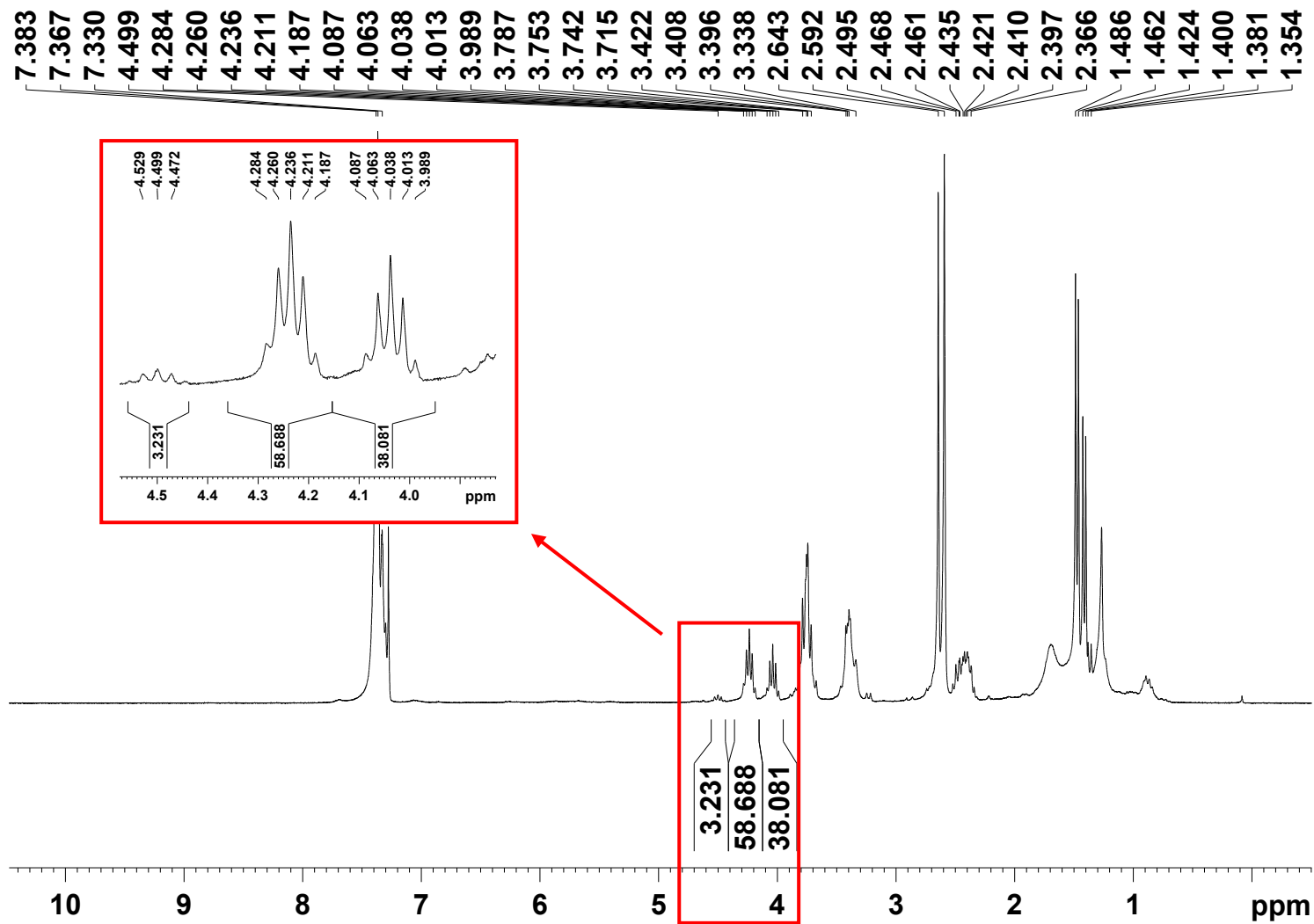


Figure S43. ^1H NMR spectrum (250 MHz, CDCl_3 , 298 K) of the reduced mixture for entry 4, **Table 1** in the manuscript.

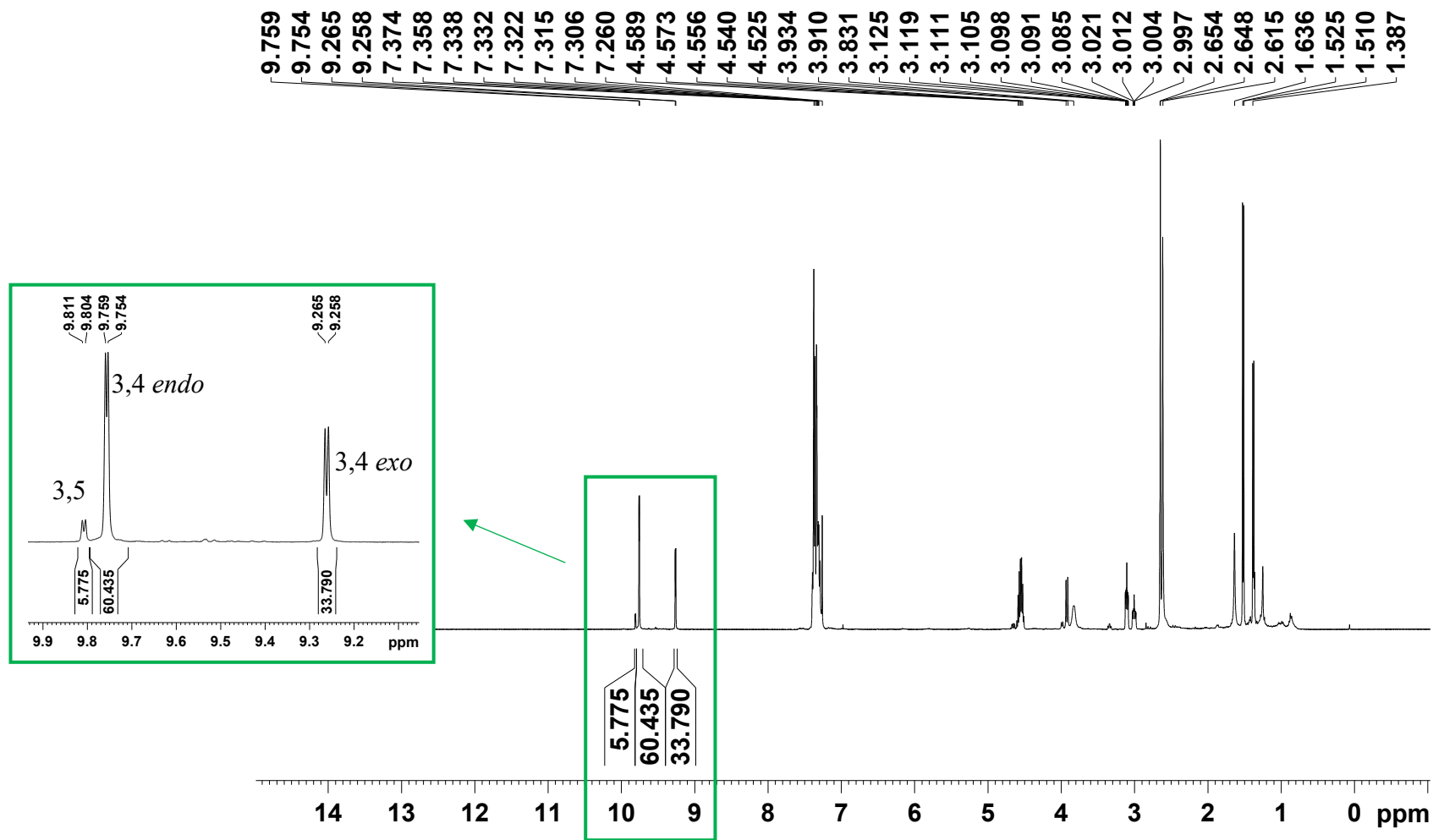


Figure S44. ¹H NMR spectrum (400 MHz, CDCl₃, 298 K) for entry 5, **Table 1** in the manuscript.

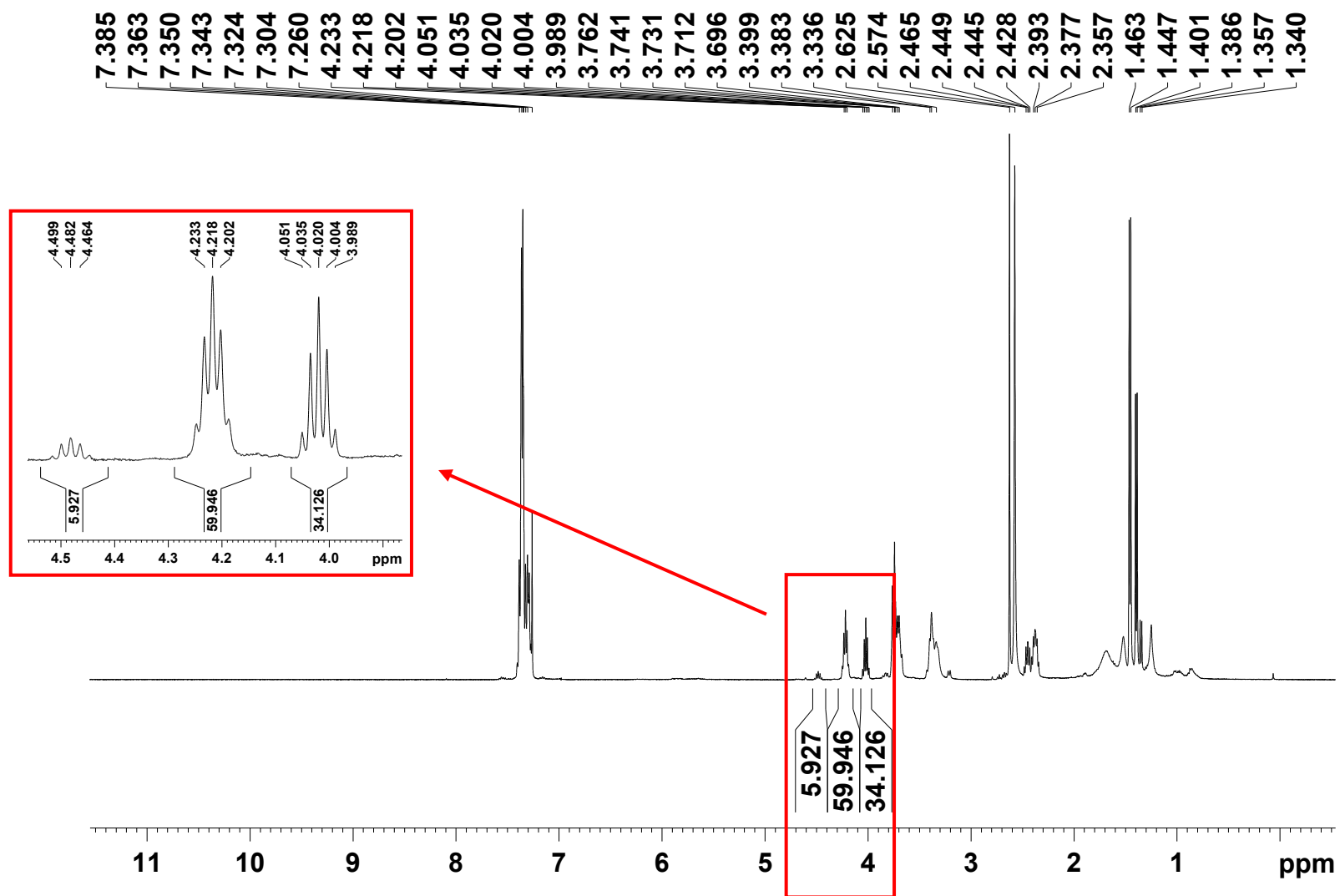


Figure S45. ^1H NMR spectrum (400 MHz, CDCl_3 , 298 K) of the reduced mixture for entry 5, **Table 1** in the manuscript.

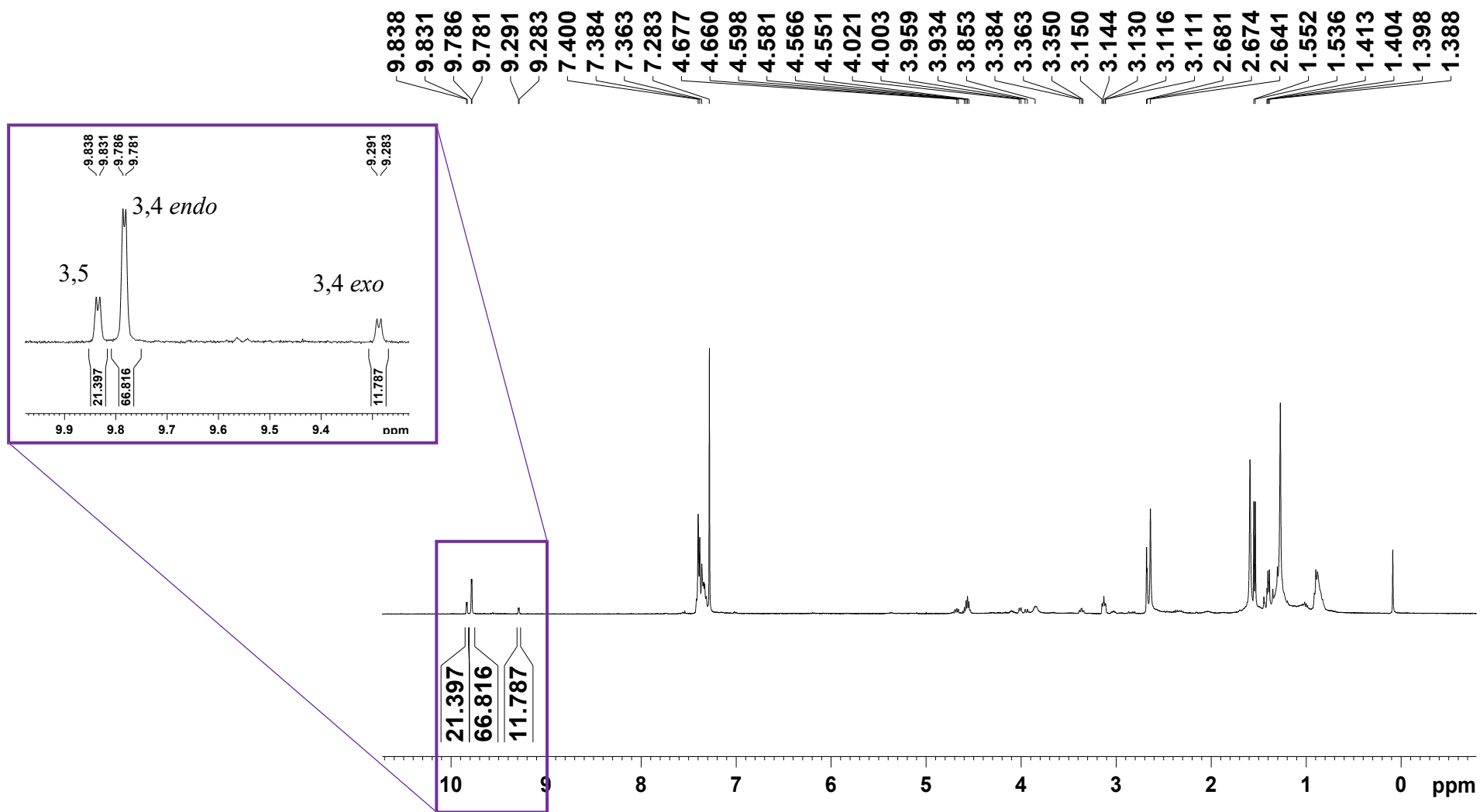


Figure S46. ¹H NMR spectrum (400 MHz, CDCl₃, 298 K) for entry 6, Table 1 in the manuscript.

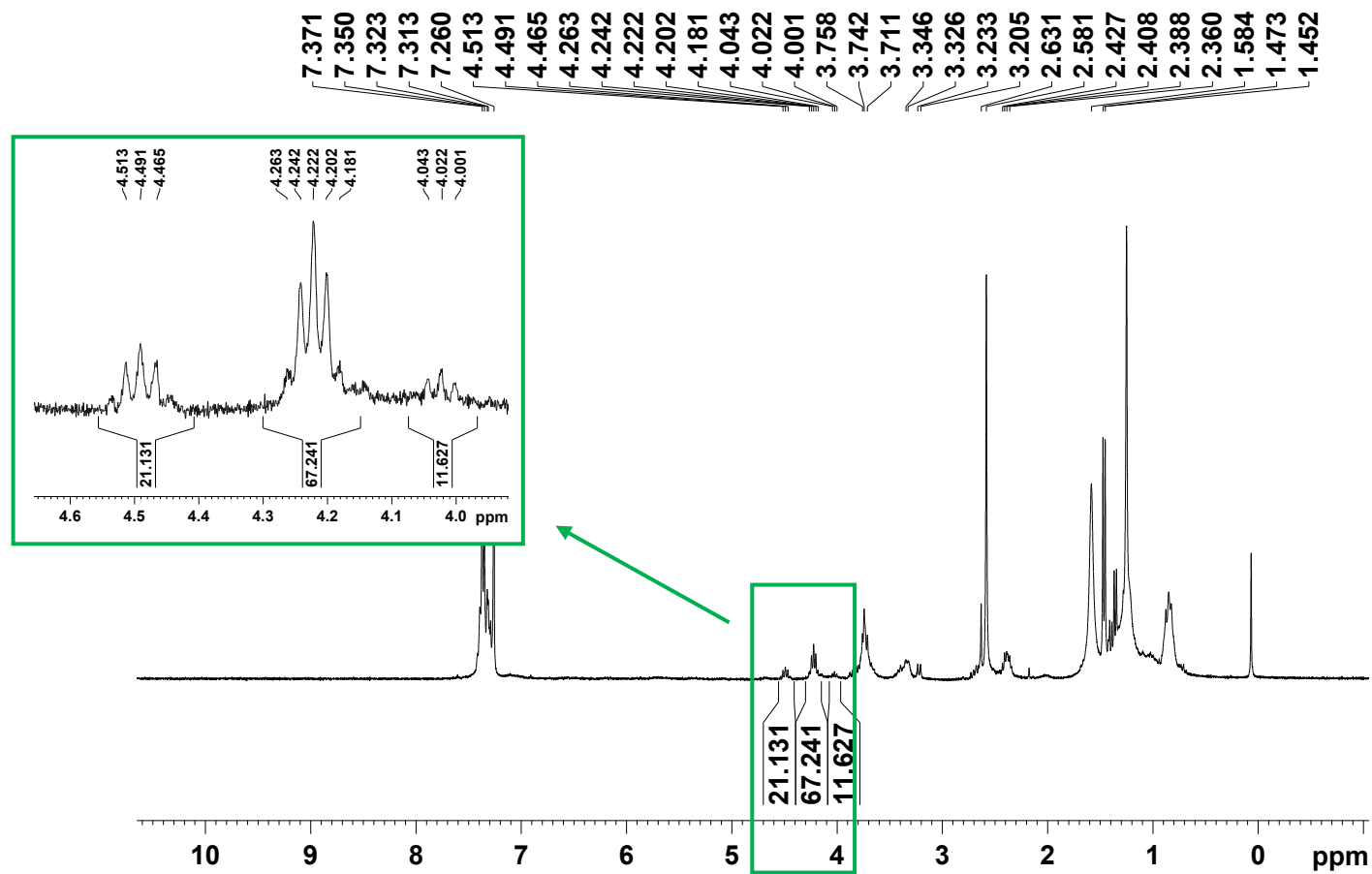


Figure S47. ^1H NMR spectrum (300 MHz, CDCl_3 , 298 K) of the reduced mixture for entry 6, **Table 1** in the manuscript.

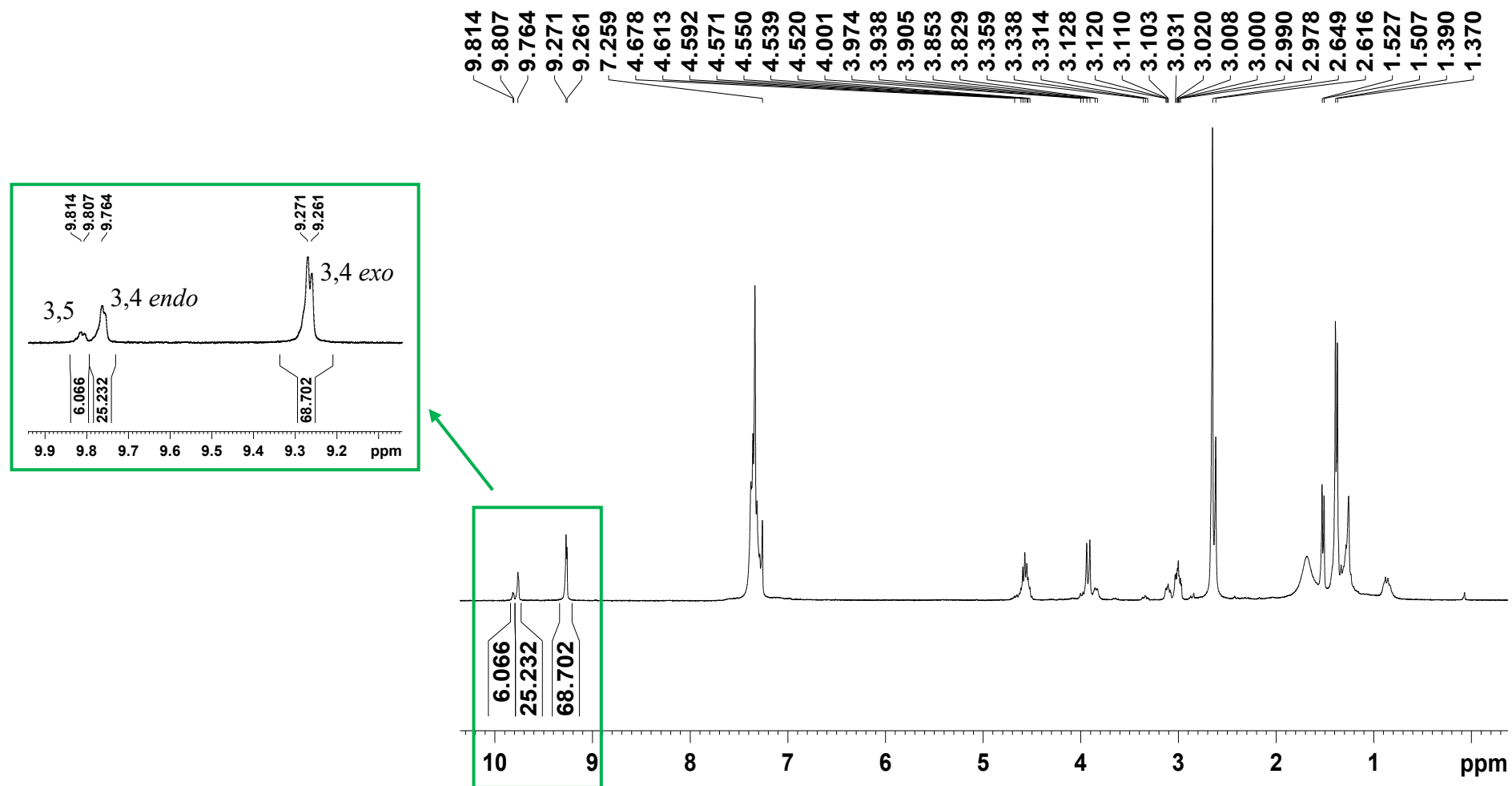


Figure S48. ^1H NMR spectrum (300 MHz, CDCl_3 , 298 K) for entry 7, **Table 1** in the manuscript.

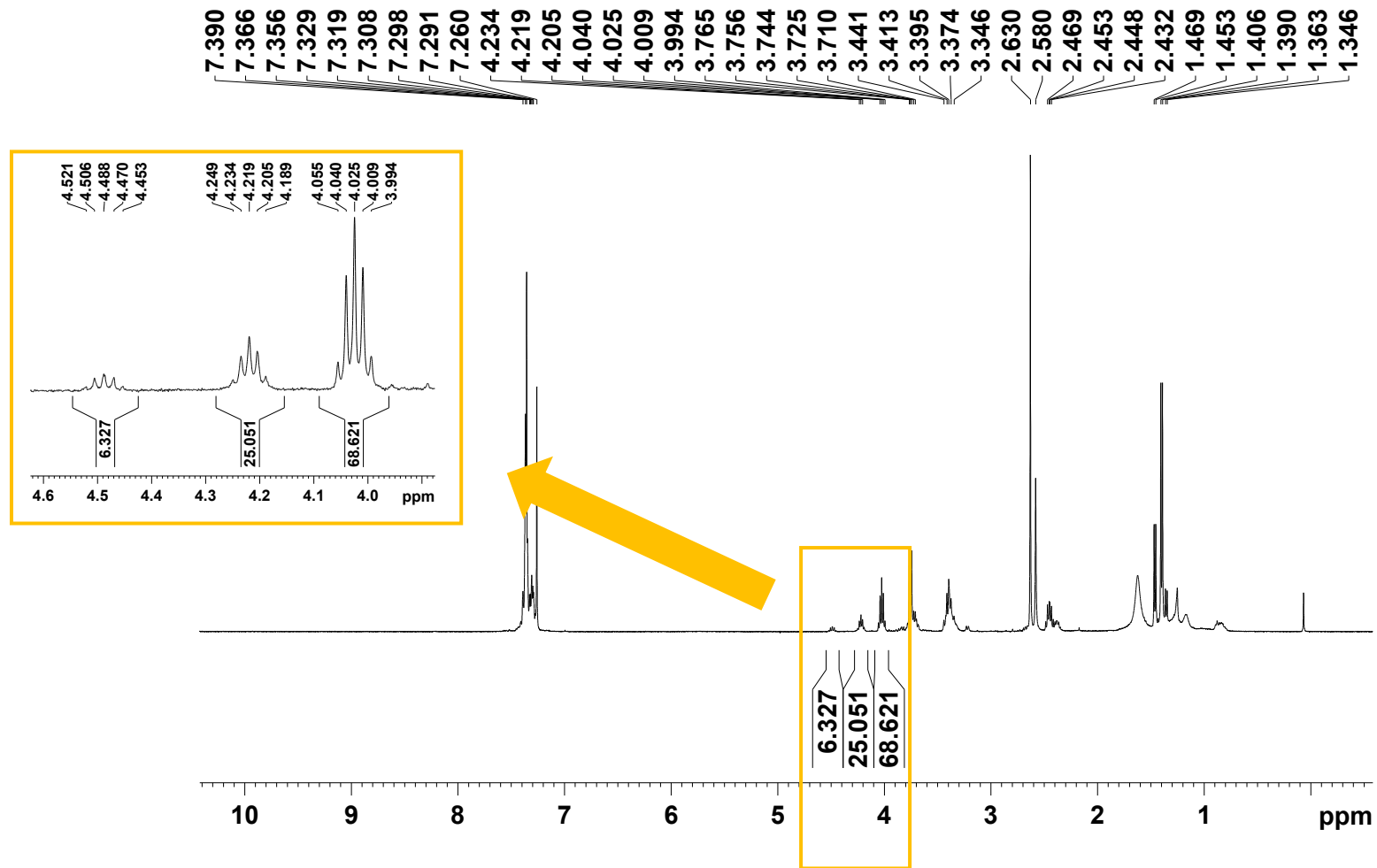


Figure S49. ^1H NMR spectrum (400 MHz, CDCl_3 , 298 K) for the reduced mixture of entry 7, **Table 1** in the manuscript.

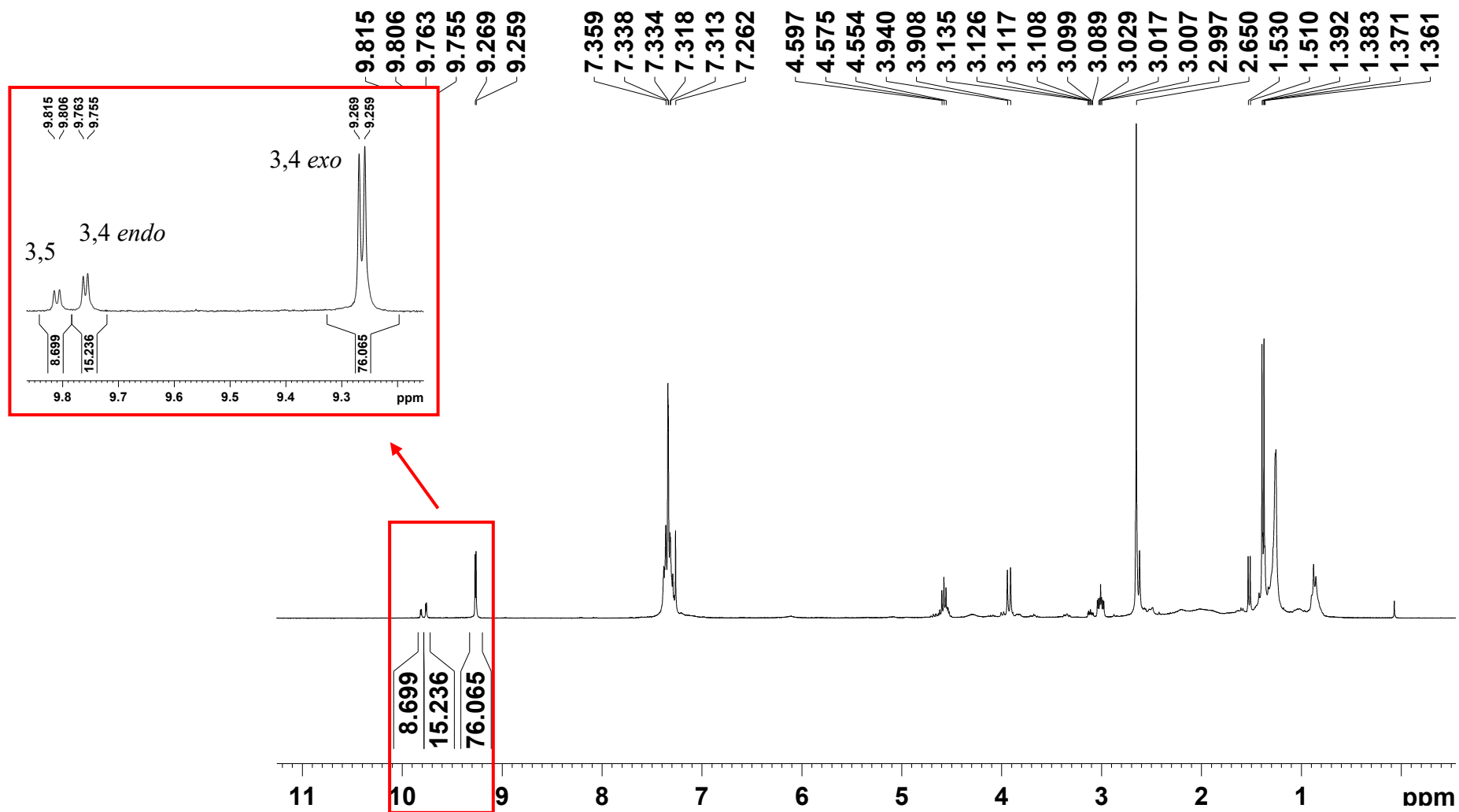


Figure S50. ^1H NMR spectrum (300 MHz, CDCl_3 , 298 K) for entry 8, **Table 1** in the manuscript.

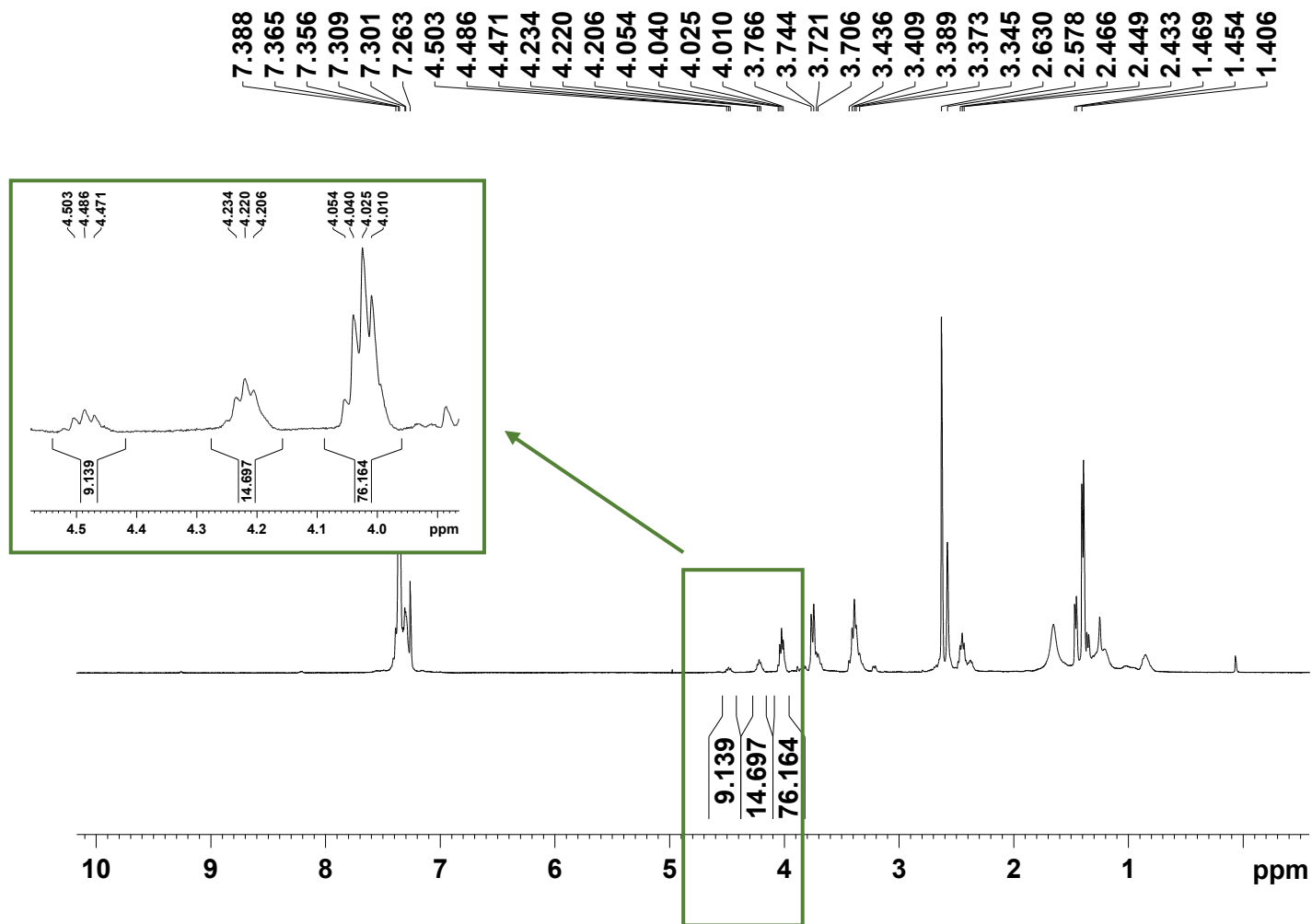


Figure S51. ^1H NMR spectrum (400 MHz, CDCl_3 , 298 K) of the reduced mixture for entry 8, **Table 1** in the manuscript.

6. HPLC chromatograms

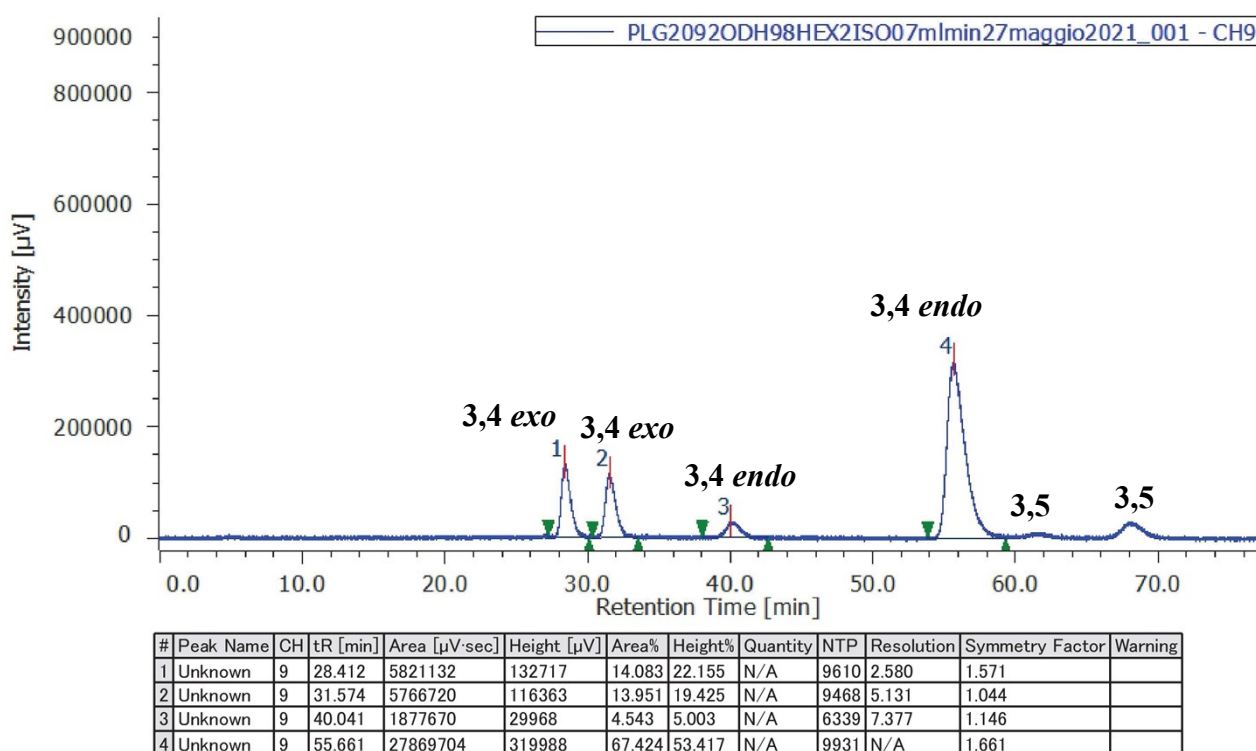


Figure S52. HPLC chromatogram for entry 1, Table 1 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4** and nitrene **3** in the presence of capsule **CR₆**. The analysis was performed with Chiralcel OD-H as column, 98:2 hexane/isopropanol as eluent phase, 0.7 mL min⁻¹ at $\lambda = 214$ nm.

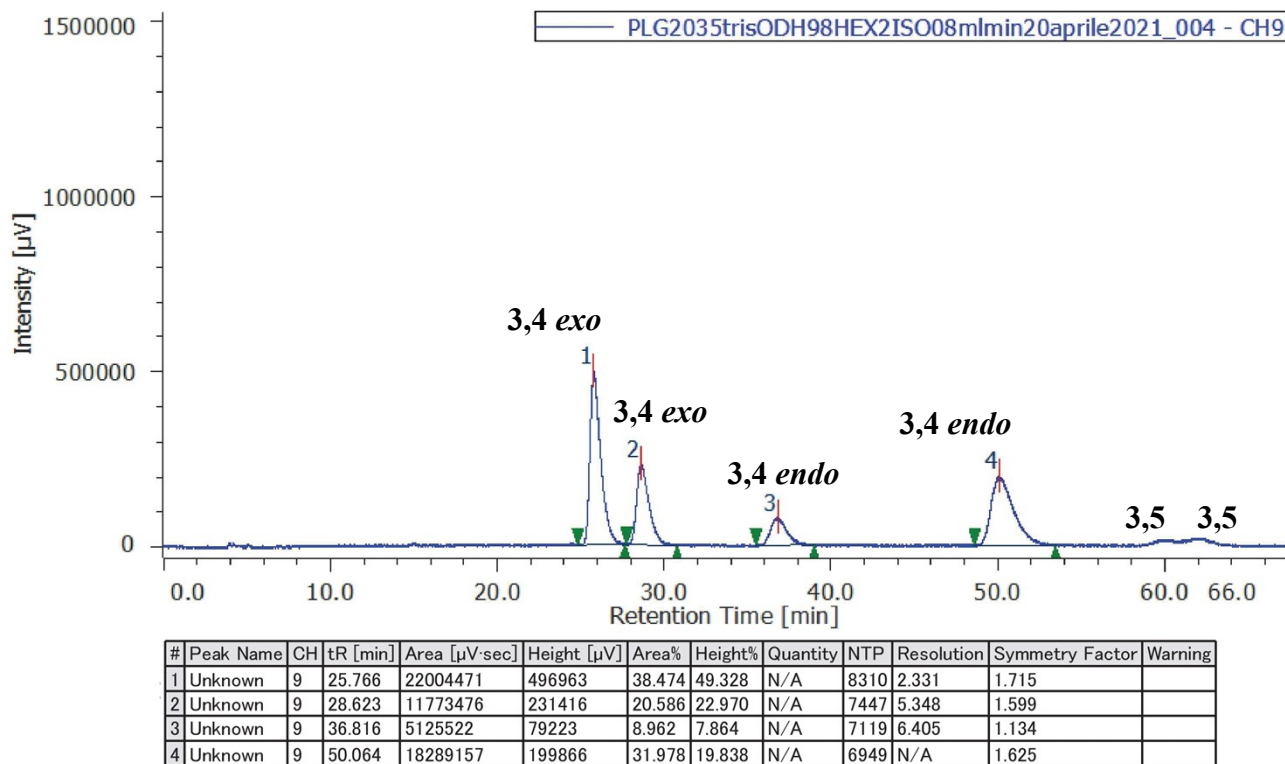


Figure S53. HPLC chromatogram for entry 2, Table 1 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4** and nitrene **3** in the presence of capsule **CP₆**. The analysis was performed with Chiralcel OD-H as column, 98:2 hexane/isopropanol as eluent phase, 0.7 mL min⁻¹ at $\lambda = 214$ nm.

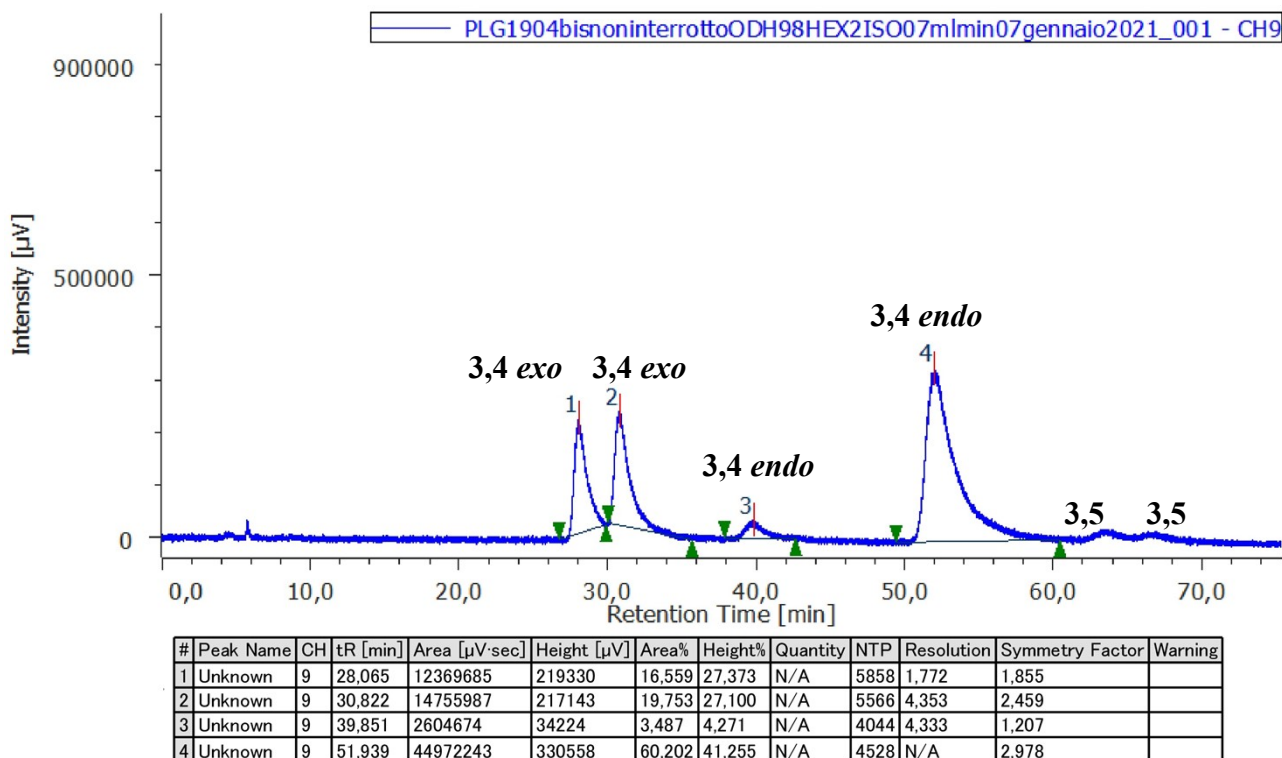


Figure S54. HPLC chromatogram for entry 4, Table 1 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4** and nitrene **3** in the presence of capsule **CP₆**. The analysis was performed with Chiralcel OD-H as column, 98:2 hexane/isopropanol as eluent phase, 0.7 mL min⁻¹ at λ = 214 nm.

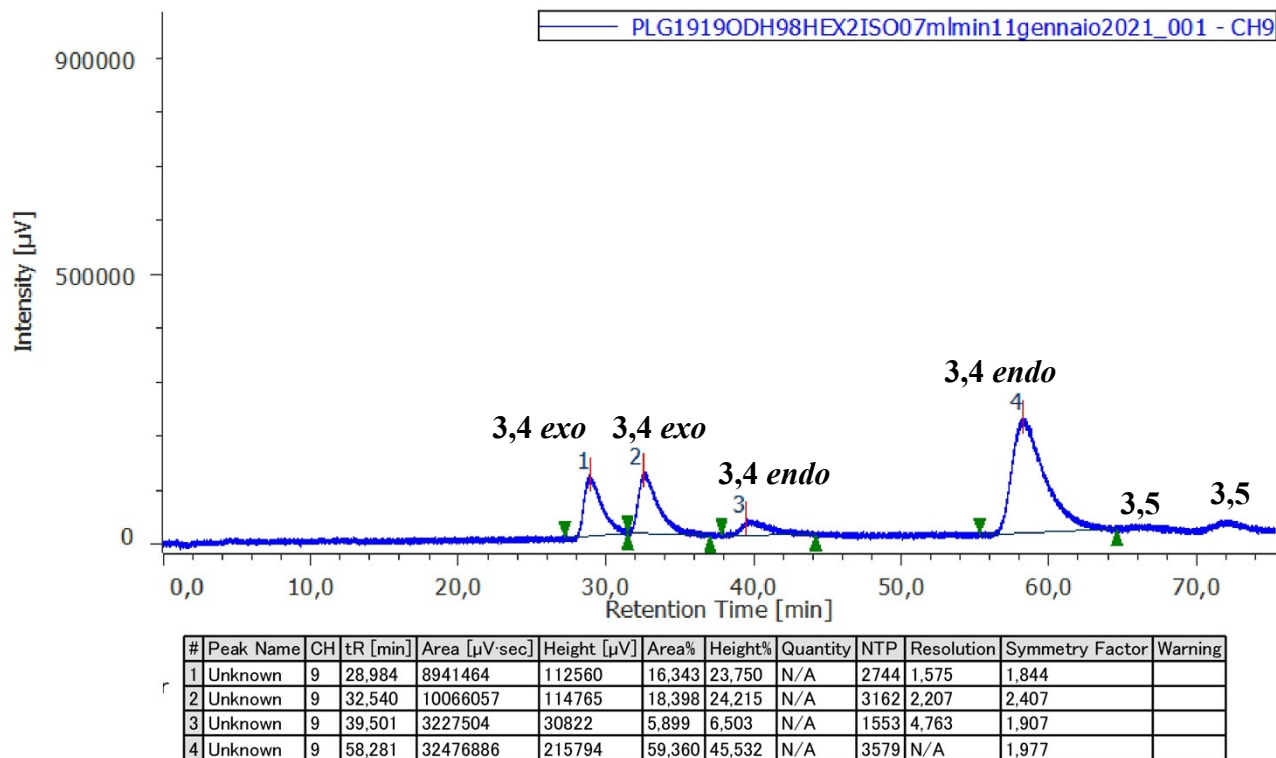


Figure S55. HPLC chromatogram for entry 5, Table 1 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4** and nitrene **3** in the presence of capsule **CP₆**. The analysis was performed with Chiralcel OD-H as column, 98:2 hexane/isopropanol as eluent phase, 0.7 mL min⁻¹ at λ = 214 nm.

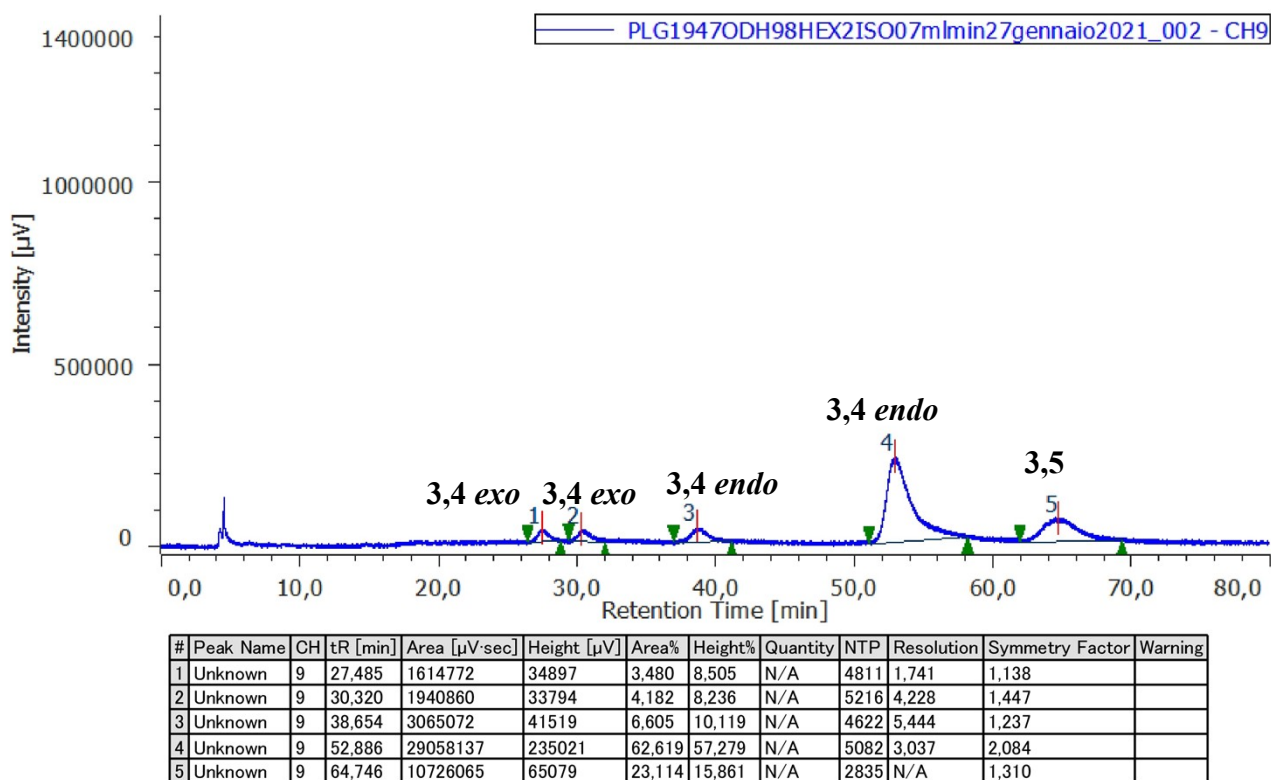


Figure S56. HPLC chromatogram for entry 6, Table 1 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4** and nitrene **3** in the presence of capsule **CP₆**. The analysis was performed with Chiralcel OD-H as column, 98:2 hexane/isopropanol as eluent phase, 0.7 mL min⁻¹ at λ = 214 nm.

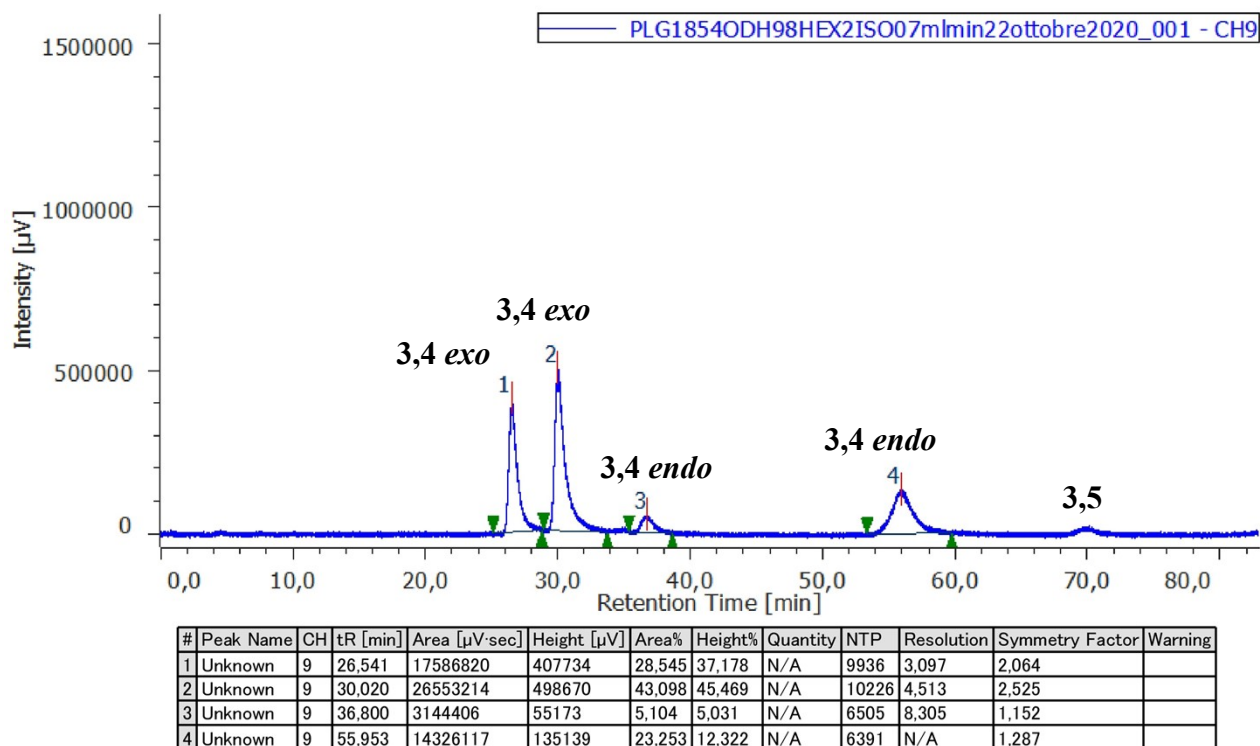


Figure S57. HPLC chromatogram for entry 7, Table 1 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4** and nitrene **3** in the presence of capsule **CP₆**. The analysis was performed with Chiralcel OD-H as column, 98:2 hexane/isopropanol as eluent phase, 0.7 mL min⁻¹ at λ = 214 nm.

7. Computational Studies

7.1. 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 on a reduced model of **CP₆**, namely **CP_{6R}** 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@**CP_{6R}** complexes, a preliminary molecular dynamics (MD) study (10 ns) in benzene, 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 benzene as implicit solvent, to locate the structure with the plausible lowest minima. The so located most stable complex has been submitted to a conformational search using CREST combined to the xTB at the GFN-FF level of theory. CREST employ an iterative conformational search workflow that generates conformer/rotamer ensembles by extensive metadynamic sampling, with an additional genetic z-matrix crossing step at the end. The final ensemble file, containing the most stable generated conformers, has been processed with the *screen* option to optimize each point on the ensemble file with GFN2-xTB (benzene as implicit solvent), and sort the resulting ensemble. The most stable structure has been utilized as starting point for the QM/SE calculations. The MD calculations have been performed with the YASARA Structure software, the semiempirical extended tight binding with the xTB program,⁶ the conformational search with the CREST program,⁷ and the DFT and ONIOM ones with the Gaussian 16 suite of programs.⁸ For the MD calculations, 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 benzene of 1.0 Å, and a density of 0.874 g mL⁻¹ with explicit solvent. The final system dimensions were approximately 43 × 43 × 43 Å³. 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 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

⁶ C. Bannwarth, E. Caldeweyher, S. Ehlert, A. Hansen, P. Pracht, J. Seibert, *et al.* *WIREs Computational Molecular Science* **n/a**, e01493.

⁷ P. Pracht, F. Bohle, S. Grimme, *Physical Chemistry Chemical Physics* **2020**, *22*, 7169–7192.

⁸ 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 C.01.

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 MD simulations without any restrictions were conducted, and the conformations of each system were recorded every 100 ps. For the QM/SE calculations, the reactive species together with the two resorcinol hydroxyl groups with which the carboxylate moiety of **1** establishes the hydrogen bonds were modeled using the M06-2X DFT functional, employing the Def2SVP basis set, while the semiempirical method PM6 was employed for all the other atoms. All pure DFT calculations were performed at M06-2X/Def2SVP 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/Def2SVP:PM6] level (zero-point energy-corrected ONIOM values). The optimizations were carried out using the Bery analytical gradient optimization method.

Table S3. Gibbs free energies (G , in Hartree), number of negative frequencies, relative Gibbs free energies (ΔG ,^a in kcal/mol), and activation free energies (ΔG^\ddagger ,^b in kcal/mol) of all investigated structures.

Structure	G	Neg. Freq.	ΔG	ΔG^\ddagger
3	-439.529503	0	—	—
I	-555.107284	0	—	—
CP_{6R}	-154.061100	0	—	—
I@CP_{6R-in}	-709.212695	0	-27.81	—
I@CP_{6R-out}	-709.195646	0	-17.11	—
MC1a@CP_{6R-in}	-1148.758868	0	-38.27	—
TS1a@CP_{6R-in}	-1148.750316	1	-32.90	5.37
IN1a@CP_{6R-in}	-1148.755829	0	-36.36	—
TS2a@CP_{6R-in}	-1148.742870	1	-28.23	10.04
P1a@CP_{6R-in}	-1148.765768	0	-42.60	—
MC1b@CP_{6R-in}	-1148.755900	0	-36.40	—
TS2b@CP_{6R-in}	-1148.738450	1	-25.45	10.95
MC1c@CP_{6R-in}	-1148.747903	0	-31.39	—
TS2c@CP_{6R-in}	-1148.727967	1	-18.88	12.51
MC1d@CP_{6R-in}	-1148.742797	0	-28.18	—
TS2d@CP_{6R-in}	-1148.725172	1	-17.12	11.06
MC1a@CP_{6R-out}	-1148.741158	0	-27.15	—
TS2a@CP_{6R-out}	-1148.724515	1	-16.71	10.44
MC1b@CP_{6R-out}	-1148.741218	0	-27.19	—
TS2b@CP_{6R-out}	-1148.724868	1	-16.93	10.26
MC1c@CP_{6R-out}	-1148.730451	0	-20.43	—
TS2c@CP_{6R-out}	-1148.710037	1	-7.62	12.81
MC1d@CP_{6R-out}	-1148.732184	0	-21.52	—
TS2d@CP_{6R-out}	-1148.715356	1	-10.96	10.56

MC2a@CP _{6R} -in	-1148.749130	0	-32.16	—
TS3a@CP _{6R} -in	-1148.720153	1	-13.97	18.18
MC2b@CP _{6R} -in	-1148.758240	0	-37.87	—
TS3b@CP _{6R} -in	-1148.738878	1	-25.72	12.15
MC2c@CP _{6R} -in	-1148.753040	0	-34.61	—
TS3c@CP _{6R} -in	-1148.721739	1	-14.97	19.64
MC2d@CP _{6R} -in	-1148.741520	0	-27.38	—
TS3d@CP _{6R} -in	-1148.715305	1	-10.93	16.45
MC2a@CP _{6R} -out	-1148.735132	0	-23.37	—
TS3a@CP _{6R} -out	-1148.705996	1	-5.09	18.28
MC2b@CP _{6R} -out	-1148.728524	0	-19.23	—
TS3b@CP _{6R} -out	-1148.710006	1	-7.61	11.62
MC2c@CP _{6R} -out	-1148.746056	0	-30.23	—
TS3c@CP _{6R} -out	-1148.709569	1	-7.33	22.90
MC2d@CP _{6R} -out	-1148.727034	0	-18.29	—
TS3d@CP _{6R} -out	-1148.700245	1	-1.48	16.81

^a Referred to those of the CP_{6R} host and the corresponding **3** and **I** non-encapsulated guests.

^b Relative to the corresponding MC@CP_{6R}.

7.2. Cartesian coordinates for selected fully optimized compounds and transition states

MC1a@CP_{6R}-in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.628624	8.290053	-2.557617
2	8	0	-2.677666	4.065512	-6.839283
3	8	0	-0.112082	2.701533	-7.577831
4	6	0	-0.048047	7.263018	-0.402543
5	8	0	-2.287580	7.273541	-1.040191
6	8	0	2.155403	7.243309	0.410983
7	8	0	4.493549	2.975914	-6.313794
8	6	0	3.152628	8.664044	-1.972894
9	8	0	-3.960672	7.108008	-3.289490
10	6	0	-1.677999	8.648118	-3.590702
11	8	0	2.340466	1.473877	-7.108316
12	6	0	-1.935749	7.446262	-4.476874
13	8	0	-0.382504	6.533926	0.717090
14	6	0	1.699387	8.284748	-1.776423
15	6	0	4.440944	5.726228	-5.951825
16	8	0	6.025913	4.195566	-4.045272
17	8	0	4.927815	7.188978	-0.469524
18	8	0	6.365521	5.042279	-1.402592
19	8	0	-4.468261	4.735916	-4.822283
20	6	0	1.302640	7.606569	-0.604673
21	6	0	-0.426118	5.589910	-7.487029
22	6	0	-1.001650	7.622251	-1.377894
23	6	0	3.191767	4.966004	-6.339460
24	6	0	2.145537	2.822408	-6.916425
25	6	0	0.846539	4.897295	-7.046815
26	6	0	3.274076	3.570197	-6.517040
27	6	0	3.758988	7.118597	-3.922021
28	6	0	-3.342714	5.511223	-5.014441
29	6	0	1.969253	5.599508	-6.594440
30	6	0	-1.311690	5.947786	-6.315343
31	6	0	-1.060434	7.056030	-5.496293
32	6	0	-3.096673	6.675455	-4.266846
33	6	0	0.727405	8.590507	-2.735649
34	6	0	4.477816	6.050871	-4.472791
35	6	0	-2.452094	5.163291	-6.048829
36	6	0	0.936929	3.496139	-7.167894
37	6	0	3.904155	7.498338	-2.582830
38	6	0	5.315609	5.296719	-3.625774
39	6	0	5.497597	5.658467	-2.277519
40	6	0	4.794563	6.768797	-1.771825
41	6	0	3.344999	9.946019	-2.788702
42	6	0	-0.137520	6.805373	-8.375158
43	6	0	4.641590	6.981121	-6.808869

44	6	0	-1.331092	9.895831	-4.407650
45	1	0	-3.538618	3.601680	-6.561807
46	1	0	-0.974583	3.242516	-7.645723
47	1	0	-2.909008	7.230734	-1.852763
48	1	0	3.129152	7.240366	0.112644
49	1	0	4.469428	1.994034	-6.582802
50	1	0	3.591450	8.873272	-0.951023
51	1	0	-4.766775	6.482165	-3.197185
52	1	0	-2.633866	8.889602	-3.036549
53	1	0	1.459472	0.984645	-7.228654
54	1	0	-1.390260	6.550547	0.867321
55	1	0	5.324646	5.046166	-6.171921
56	1	0	5.743661	3.917848	-4.987415
57	1	0	5.630933	6.650944	0.027500
58	1	0	6.731703	4.178161	-1.785866
59	1	0	-4.515060	4.433906	-3.838668
60	1	0	-1.004881	4.854967	-8.131897
61	1	0	3.070460	7.678356	-4.556770
62	1	0	1.898017	6.679820	-6.460932
63	1	0	-0.153721	7.640613	-5.663452
64	1	0	1.037085	9.091962	-3.655121
65	1	0	4.408114	10.217203	-2.833368
66	1	0	2.993925	9.848570	-3.821077
67	1	0	2.808104	10.786665	-2.332248
68	1	0	0.463456	6.518558	-9.247287
69	1	0	-1.071379	7.247266	-8.745319
70	1	0	0.408599	7.593722	-7.847710
71	1	0	3.841326	7.715847	-6.675845
72	1	0	5.586531	7.479095	-6.557346
73	1	0	4.675462	6.722959	-7.874975
74	1	0	-1.173886	10.762320	-3.753514
75	1	0	-0.427984	9.769238	-5.013334
76	1	0	-2.149884	10.144938	-5.095513
77	6	0	4.216933	0.558451	7.162970
78	8	0	-1.390747	3.779392	7.250778
79	8	0	-0.736863	5.987740	5.600877
80	6	0	4.993780	-0.787043	5.277727
81	8	0	3.299743	-1.625794	6.783268
82	8	0	6.661087	-0.066622	3.816168
83	8	0	2.830904	7.608650	2.745371
84	6	0	7.149124	2.371595	5.434484
85	8	0	0.760238	-0.386074	8.128710
86	6	0	3.302999	0.719242	8.359702
87	8	0	0.026170	7.175644	3.223695
88	6	0	2.101038	1.580798	8.030314
89	8	0	4.875612	-1.965612	4.568739
90	6	0	6.049326	1.370804	5.731615
91	6	0	4.799224	6.820490	4.537372
92	8	0	4.993508	6.087999	1.694976
93	8	0	7.628172	2.244355	2.688103
94	8	0	6.393644	3.858479	0.860311
95	8	0	-1.483868	0.997111	7.449251
96	6	0	5.921065	0.214352	4.942293
97	6	0	1.060304	5.271883	7.635675
98	6	0	4.161665	-0.631232	6.404403
99	6	0	3.333296	6.593305	4.831178
100	6	0	1.000247	6.769433	4.110391
101	6	0	1.534922	5.814552	6.305989
102	6	0	2.370426	6.992707	3.883729
103	6	0	5.938201	4.571659	4.938582
104	6	0	-0.311842	1.716006	7.606645
105	6	0	2.891746	6.000508	6.019280
106	6	0	1.030085	3.757970	7.649224
107	6	0	2.167148	2.972126	7.881110
108	6	0	0.839830	0.960399	7.914122
109	6	0	5.157460	1.531292	6.802444
110	6	0	5.430649	5.531859	4.053237
111	6	0	-0.209154	3.108633	7.479373
112	6	0	0.591091	6.183012	5.324795
113	6	0	6.628414	3.438194	4.495417
114	6	0	5.530166	5.284093	2.671369
115	6	0	6.230280	4.161677	2.189837
116	6	0	6.828033	3.281767	3.110109
117	6	0	7.771375	2.957659	6.704940
118	6	0	1.860487	5.834397	8.815578
119	6	0	5.545629	7.427611	5.729367
120	6	0	4.050803	1.247609	9.589676
121	1	0	-1.210584	4.746388	6.975376

122	1	0	-1.314731	6.208047	4.789249
123	1	0	3.495188	-2.484947	6.267302
124	1	0	7.159025	0.759598	3.466093
125	1	0	2.068905	7.849416	2.109744
126	1	0	7.980198	1.819537	4.900585
127	1	0	-0.169185	-0.721600	7.938317
128	1	0	2.919634	-0.314507	8.626073
129	1	0	0.252337	6.863778	2.265986
130	1	0	5.591083	-2.020365	3.841483
131	1	0	4.872695	7.577509	3.699323
132	1	0	4.269387	6.706398	2.067214
133	1	0	7.741417	2.256260	1.670094
134	1	0	5.939335	4.555250	0.266071
135	1	0	-2.284587	1.607417	7.563050
136	1	0	-0.006897	5.634710	7.774277
137	1	0	5.800353	4.717614	6.011256
138	1	0	3.633548	5.682453	6.754895
139	1	0	3.137301	3.463588	7.965645
140	1	0	5.212295	2.447447	7.393968
141	1	0	8.169403	2.161763	7.347136
142	1	0	8.602081	3.629984	6.455444
143	1	0	7.054818	3.530950	7.302264
144	1	0	2.912948	5.534215	8.792908
145	1	0	1.444518	5.484174	9.768874
146	1	0	1.830466	6.930964	8.821750
147	1	0	5.525068	6.785123	6.615422
148	1	0	5.101432	8.389959	6.014326
149	1	0	6.598681	7.608315	5.479767
150	1	0	4.899159	0.598619	9.838139
151	1	0	3.386506	1.272480	10.462608
152	1	0	4.439340	2.260074	9.447298
153	6	0	5.578905	-3.472044	-5.296509
154	8	0	5.001621	-7.398567	-0.160758
155	8	0	5.921670	-5.720805	1.755916
156	6	0	4.323592	-1.423304	-5.754536
157	8	0	3.316419	-3.613494	-6.032234
158	8	0	5.306390	0.687240	-5.584506
159	8	0	8.096853	-1.546172	2.461087
160	6	0	7.894621	-0.437092	-4.766414
161	8	0	3.055266	-5.943076	-4.257503
162	6	0	5.619841	-4.984709	-5.280221
163	8	0	6.338715	-3.519878	3.292501
164	6	0	5.445434	-5.529687	-3.877963
165	8	0	3.135437	-0.851136	-6.149191
166	6	0	6.672136	-1.287506	-5.056019
167	6	0	9.374977	-1.558047	-0.002824
168	8	0	7.595993	0.663564	0.814850
169	8	0	6.746910	1.904995	-3.684426
170	8	0	6.478422	2.370989	-1.043887
171	8	0	2.880868	-7.294771	-1.814109
172	6	0	5.470174	-0.667423	-5.445788
173	6	0	7.501716	-6.258851	-0.700763
174	6	0	4.388405	-2.828624	-5.695597
175	6	0	8.532144	-2.732720	0.445769
176	6	0	6.980268	-3.674382	2.082850
177	6	0	7.571106	-4.961875	0.081515
178	6	0	7.859367	-2.655467	1.682253
179	6	0	8.602071	-0.960775	-2.359838
180	6	0	4.029498	-6.687802	-2.249515
181	6	0	8.379548	-3.890804	-0.323413
182	6	0	6.378361	-6.195130	-1.711506
183	6	0	6.509044	-5.595409	-2.969681
184	6	0	4.184665	-6.034959	-3.490900
185	6	0	6.689243	-2.685528	-4.967920
186	6	0	8.585129	-0.710666	-0.980603
187	6	0	5.132641	-6.754118	-1.380385
188	6	0	6.829381	-4.817496	1.269185
189	6	0	7.949843	-0.135191	-3.283310
190	6	0	7.817627	0.372636	-0.510269
191	6	0	7.193519	1.254849	-1.411622
192	6	0	7.285163	1.003915	-2.792242
193	6	0	9.185919	-1.061792	-5.300219
194	6	0	8.840816	-6.637967	-1.339583
195	6	0	10.733468	-1.994059	-0.558620
196	6	0	6.880317	-5.535036	-5.956571
197	1	0	4.017968	-7.535381	0.036888
198	1	0	5.743964	-6.498533	1.093217
199	1	0	2.514424	-3.037699	-6.306980

200	1	0	5.966650	1.210226	-4.995702
201	1	0	7.602083	-1.596895	3.349201
202	1	0	7.767940	0.546562	-5.310281
203	1	0	3.199049	-5.313966	-5.043655
204	1	0	4.741909	-5.350956	-5.898833
205	1	0	5.576293	-4.199680	3.384225
206	1	0	3.224539	0.167206	-6.150537
207	1	0	9.595471	-0.920272	0.905512
208	1	0	7.886719	-0.096913	1.432338
209	1	0	6.099892	2.540165	-3.206700
210	1	0	6.094508	2.248935	-0.101837
211	1	0	2.068701	-6.694953	-2.040622
212	1	0	7.257080	-7.084545	0.034226
213	1	0	9.149228	-1.830211	-2.729237
214	1	0	8.917989	-3.966171	-1.270619
215	1	0	7.473018	-5.172848	-3.254351
216	1	0	7.607706	-3.182006	-4.651067
217	1	0	9.117012	-1.228836	-6.382962
218	1	0	10.042157	-0.399614	-5.120437
219	1	0	9.413369	-2.027206	-4.836664
220	1	0	9.169700	-5.916883	-2.094731
221	1	0	9.631272	-6.709231	-0.582392
222	1	0	8.766885	-7.615000	-1.835443
223	1	0	10.645607	-2.642254	-1.436603
224	1	0	11.332638	-1.123009	-0.853071
225	1	0	11.302509	-2.547502	0.199511
226	1	0	7.799962	-5.235567	-5.444543
227	1	0	6.861702	-6.632027	-5.979102
228	1	0	6.951549	-5.181101	-6.992597
229	6	0	-4.826158	-0.564332	-6.922347
230	8	0	0.908083	-3.028137	-5.505160
231	8	0	-0.062359	-4.930818	-3.713650
232	6	0	-5.916555	0.948042	-5.331535
233	8	0	-3.990828	1.695820	-6.426991
234	8	0	-7.878794	0.319356	-4.182842
235	8	0	-3.994676	-7.132681	-1.865393
236	6	0	-7.938754	-2.293000	-5.445798
237	8	0	-1.519039	0.728450	-7.174709
238	6	0	-3.738117	-0.796132	-7.951099
239	8	0	-1.462037	-6.422014	-1.498778
240	6	0	-2.528221	-1.433096	-7.299859
241	8	0	-6.009598	2.145964	-4.648022
242	6	0	-6.842283	-1.283946	-5.721547
243	6	0	-5.519862	-6.591980	-4.151023
244	8	0	-6.499236	-6.076796	-1.435205
245	8	0	-8.699277	-2.054031	-2.764635
246	8	0	-8.012624	-3.877196	-0.799490
247	8	0	0.718653	-0.304616	-5.994437
248	6	0	-6.890633	-0.033770	-5.072295
249	6	0	-1.190326	-4.884304	-6.253276
250	6	0	-4.885169	0.671543	-6.249753
251	6	0	-4.050639	-6.237229	-4.075973
252	6	0	-2.004155	-6.078297	-2.729848
253	6	0	-1.993377	-5.325742	-5.049522
254	6	0	-3.348697	-6.476022	-2.881677
255	6	0	-6.700462	-4.402241	-4.727203
256	6	0	-0.288884	-1.176266	-6.328400
257	6	0	-3.344476	-5.673940	-5.146012
258	6	0	-1.314766	-3.394328	-6.476070
259	6	0	-2.447258	-2.809133	-7.052649
260	6	0	-1.438326	-0.624105	-6.926540
261	6	0	-5.798943	-1.527243	-6.622514
262	6	0	-6.342669	-5.372809	-3.784561
263	6	0	-0.241351	-2.564079	-6.103604
264	6	0	-1.342810	-5.452157	-3.801224
265	6	0	-7.496575	-3.297414	-4.402719
266	6	0	-6.768942	-5.197853	-2.453339
267	6	0	-7.549154	-4.084799	-2.085654
268	6	0	-7.916093	-3.142194	-3.065074
269	6	0	-8.438321	-2.969932	-6.726190
270	6	0	-1.537434	-5.680006	-7.515620
271	6	0	-5.921724	-7.193787	-5.499453
272	6	0	-4.230293	-1.594310	-9.162033
273	1	0	0.756455	-3.949118	-5.082294
274	1	0	0.404091	-5.211550	-2.873759
275	1	0	-3.109023	1.359804	-6.837156
276	1	0	-8.308280	-0.507922	-3.763305
277	1	0	-3.381313	-7.253466	-1.045660

278	1	0	-8.824666	-1.729406	-5.019064
279	1	0	-0.735351	1.225047	-6.739087
280	1	0	-3.420780	0.216033	-8.347032
281	1	0	-0.514437	-6.088276	-1.400559
282	1	0	-5.482964	2.865009	-5.125974
283	1	0	-5.718060	-7.390440	-3.372404
284	1	0	-5.724120	-6.698564	-1.686982
285	1	0	-8.923007	-2.019449	-1.773414
286	1	0	-7.695670	-4.624512	-0.196861
287	1	0	1.405078	-0.775609	-5.392201
288	1	0	-0.102191	-5.111508	-6.021445
289	1	0	-6.354921	-4.515987	-5.756534
290	1	0	-3.863351	-5.517017	-6.093299
291	1	0	-3.292529	-3.444551	-7.320084
292	1	0	-5.749058	-2.498162	-7.119201
293	1	0	-7.661521	-3.556933	-7.226449
294	1	0	-8.800571	-2.224750	-7.445522
295	1	0	-9.270433	-3.650962	-6.505910
296	1	0	-1.409082	-6.756798	-7.346065
297	1	0	-0.881395	-5.394945	-8.347876
298	1	0	-2.568430	-5.520619	-7.846775
299	1	0	-5.340640	-8.101438	-5.707865
300	1	0	-5.762601	-6.505018	-6.335422
301	1	0	-6.983315	-7.471688	-5.501542
302	1	0	-3.435335	-1.686781	-9.913564
303	1	0	-5.081828	-1.094163	-9.640020
304	1	0	-4.548899	-2.608539	-8.900667
305	6	0	-5.937441	4.015657	5.321736
306	8	0	-4.242704	7.680781	0.282994
307	8	0	-4.883190	5.655825	-1.597424
308	6	0	-4.801906	1.909201	5.837628
309	8	0	-3.681661	4.032508	6.114234
310	8	0	-5.870025	-0.163743	5.608376
311	8	0	-7.136563	1.522859	-2.099558
312	6	0	-8.361651	1.079833	4.709621
313	8	0	-3.154902	6.435401	4.773055
314	6	0	-5.884635	5.527246	5.289576
315	8	0	-5.011284	3.237354	-2.652916
316	6	0	-5.421553	6.014643	3.932004
317	8	0	-3.647565	1.326612	6.297385
318	6	0	-7.117190	1.880379	5.038376
319	6	0	-9.175919	2.157844	-0.210449
320	8	0	-8.265837	-0.569118	-0.747838
321	8	0	-7.688755	-1.503889	3.910582
322	8	0	-7.582334	-2.312349	1.242907
323	8	0	-2.391758	7.464101	2.282495
324	6	0	-5.960803	1.201608	5.471283
325	6	0	-6.813648	6.647969	0.398278
326	6	0	-4.794651	3.315176	5.751702
327	6	0	-8.056215	3.125385	-0.528168
328	6	0	-6.009808	3.605646	-1.786858
329	6	0	-6.900745	5.270954	-0.231612
330	6	0	-7.094422	2.760885	-1.484761
331	6	0	-8.711119	1.578817	2.232404
332	6	0	-3.666559	7.010205	2.545496
333	6	0	-7.926179	4.372897	0.094427
334	6	0	-5.893387	6.595947	1.600252
335	6	0	-6.283630	6.053309	2.829551
336	6	0	-4.094374	6.461229	3.767990
337	6	0	-7.071502	3.278014	4.957588
338	6	0	-8.730576	1.207513	0.881698
339	6	0	-4.586283	7.105703	1.483651
340	6	0	-5.931907	4.872752	-1.174009
341	6	0	-8.360590	0.681489	3.247406
342	6	0	-8.325820	-0.095637	0.543207
343	6	0	-7.963404	-1.026624	1.537182
344	6	0	-8.000529	-0.633748	2.887824
345	6	0	-9.654681	1.798549	5.105774
346	6	0	-8.180689	7.240501	0.751972
347	6	0	-10.494902	2.852996	0.137565
348	6	0	-7.205394	6.179460	5.708519
349	1	0	-3.279552	8.026126	0.301518
350	1	0	-4.607906	6.343979	-0.894295
351	1	0	-2.883643	3.411267	6.269682
352	1	0	-6.640936	-0.646628	5.141316
353	1	0	-7.312689	1.620668	-3.108101
354	1	0	-8.325883	0.129755	5.325919
355	1	0	-3.438555	5.785912	5.512851

356	1	0	-5.111708	5.849078	6.054582
357	1	0	-5.191712	2.294733	-3.022657
358	1	0	-3.642409	0.316297	6.126114
359	1	0	-9.368800	1.549477	-1.144280
360	1	0	-7.953038	0.173390	-1.388373
361	1	0	-7.426730	-2.412214	3.551321
362	1	0	-7.542673	-2.441610	0.224094
363	1	0	-1.853778	7.545208	3.136671
364	1	0	-6.356281	7.344956	-0.366415
365	1	0	-8.979240	2.601271	2.502419
366	1	0	-8.658157	4.661224	0.850761
367	1	0	-7.292988	5.651229	2.932869
368	1	0	-7.955666	3.814228	4.608831
369	1	0	-9.650465	2.050311	6.173690
370	1	0	-9.810573	2.727702	4.548283
371	1	0	-10.526146	1.157515	4.919378
372	1	0	-8.827610	7.291156	-0.132560
373	1	0	-8.709380	6.661226	1.516031
374	1	0	-8.068762	8.261712	1.139423
375	1	0	-10.818788	3.510877	-0.678261
376	1	0	-11.289705	2.114036	0.303414
377	1	0	-10.426370	3.461521	1.045269
378	1	0	-8.028453	5.944352	5.025989
379	1	0	-7.503942	5.846440	6.710626
380	1	0	-7.108795	7.272265	5.736468
381	6	0	0.049367	-8.546671	2.780689
382	8	0	2.614549	-3.043362	4.751458
383	8	0	0.290168	-1.379471	5.933276
384	6	0	-0.849820	-8.605287	0.495079
385	8	0	1.527068	-8.633470	0.890656
386	8	0	-3.173507	-8.631557	0.082690
387	8	0	-4.379167	-2.085862	5.684152
388	6	0	-3.795563	-8.743000	2.921288
389	8	0	3.187164	-6.975448	2.118449
390	6	0	1.252941	-8.485206	3.698793
391	8	0	-2.223280	-0.451614	5.403351
392	6	0	1.607668	-7.041170	3.997130
393	8	0	-0.517463	-8.649082	-0.831479
394	6	0	-2.374637	-8.633562	2.407089
395	6	0	-4.237590	-4.827970	6.151237
396	8	0	-5.956680	-3.602699	4.080753
397	8	0	-5.480308	-7.341009	1.174202
398	8	0	-6.507232	-4.850883	1.712743
399	8	0	3.839614	-4.369187	2.643959
400	6	0	-2.156446	-8.616546	1.014520
401	6	0	0.832853	-4.224864	6.511807
402	6	0	0.242484	-8.585264	1.388233
403	6	0	-2.981532	-3.987094	6.055043
404	6	0	-1.988810	-1.770740	5.724878
405	6	0	-0.548967	-3.686279	6.212209
406	6	0	-3.112533	-2.607362	5.802898
407	6	0	-4.017247	-6.732151	4.472781
408	6	0	2.928382	-5.054747	3.427157
409	6	0	-1.691537	-4.499753	6.231912
410	6	0	1.393741	-4.994661	5.334746
411	6	0	1.038819	-6.319721	5.054288
412	6	0	2.558735	-6.392671	3.184297
413	6	0	-1.267685	-8.568805	3.260463
414	6	0	-4.537425	-5.478595	4.816834
415	6	0	2.333066	-4.359709	4.495269
416	6	0	-0.705275	-2.312183	5.944227
417	6	0	-4.331659	-7.371785	3.268284
418	6	0	-5.375793	-4.829997	3.888958
419	6	0	-5.693364	-5.433526	2.656283
420	6	0	-5.175248	-6.707038	2.357582
421	6	0	-3.923777	-9.732592	4.082263
422	6	0	0.857857	-5.050457	7.802056
423	6	0	-4.174654	-5.837216	7.301662
424	6	0	1.076547	-9.321477	4.968054
425	1	0	3.323414	-2.671090	4.112196
426	1	0	1.212930	-1.771239	6.138873
427	1	0	1.526640	-8.492726	-0.115918
428	1	0	-4.084696	-8.563669	0.540687
429	1	0	-4.356685	-1.106349	5.382939
430	1	0	-4.434904	-9.154196	2.078049
431	1	0	2.774994	-7.892132	1.904836
432	1	0	2.125343	-8.940397	3.134466
433	1	0	-1.490755	0.151296	5.800241

434	1	0	-1.269230	-8.270040	-1.402496
435	1	0	-5.096759	-4.129928	6.390747
436	1	0	-5.496229	-3.081614	4.834029
437	1	0	-6.058801	-6.749118	0.594729
438	1	0	-6.668637	-3.879219	1.952110
439	1	0	4.255105	-5.014563	1.949200
440	1	0	1.512424	-3.329518	6.689102
441	1	0	-3.348104	-7.235355	5.173209
442	1	0	-1.571391	-5.569829	6.409149
443	1	0	0.295501	-6.810074	5.686229
444	1	0	-1.434503	-8.543720	4.338311
445	1	0	-4.971768	-9.835522	4.391802
446	1	0	-3.563773	-10.727097	3.789462
447	1	0	-3.352861	-9.425934	4.964645
448	1	0	0.521228	-4.449102	8.656436
449	1	0	0.212409	-5.932913	7.752630
450	1	0	1.874063	-5.399151	8.024886
451	1	0	-4.020323	-5.323890	8.259441
452	1	0	-5.112556	-6.402122	7.376209
453	1	0	-3.363339	-6.562824	7.185582
454	1	0	1.985072	-9.295388	5.583040
455	1	0	0.248158	-8.972498	5.593305
456	1	0	0.876381	-10.371427	4.717173
457	1	0	-1.347114	0.803421	-2.815523
458	1	0	-1.202954	-1.632043	-3.377262
459	1	0	0.908055	-2.842953	-3.087685
460	1	0	6.216424	-2.306990	-2.208923
461	1	0	5.023650	-3.569726	-1.664903
462	1	0	5.793321	-2.445708	-0.484165
463	1	0	3.127427	-3.005125	-2.398703
464	1	0	4.615730	1.259049	2.323728
465	1	0	5.162677	1.163096	0.633092
466	1	0	3.491681	1.729465	1.012036
467	1	0	4.602247	-1.146638	1.408168
468	1	0	1.766365	-0.073796	0.840152
469	1	0	3.077778	-2.913062	1.248356
470	1	0	-1.008598	-4.160702	1.740306
471	1	0	-0.996051	-5.228020	0.308111
472	1	0	1.353121	-4.635825	1.611392
473	1	0	-0.521411	-1.521049	1.300876
474	6	0	-1.022019	-3.081882	-0.144844
475	6	0	-0.106442	-1.981936	0.387853
476	7	0	1.119572	-2.718841	0.766343
477	8	0	4.647001	-0.386587	-1.316445
478	6	0	3.198621	-1.946057	-2.168680
479	6	0	-0.405249	0.263825	-2.697524
480	6	0	1.647644	-4.738187	-0.515592
481	8	0	2.824262	-4.411175	-0.626753
482	6	0	2.018175	-1.117328	-2.364067
483	8	0	0.993801	-5.505534	-1.296182
484	6	0	2.277709	-2.196552	1.019511
485	6	0	2.564290	-0.795616	1.028376
486	6	0	3.836413	-0.381707	1.231420
487	7	0	4.345521	-1.562245	-1.676022
488	6	0	5.409194	-2.558018	-1.506358
489	6	0	0.732557	0.934139	-2.239389
490	1	0	-0.797538	-3.308299	-1.197910
491	6	0	0.890075	-4.180862	0.721163
492	6	0	-0.629212	-4.283889	0.711437
493	6	0	-0.327144	-1.093572	-3.009893
494	6	0	0.873023	-1.779525	-2.845238
495	6	0	1.941180	0.260548	-2.076762
496	1	0	0.136321	-1.191282	-0.334100
497	1	0	-2.080877	-2.804669	-0.063833
498	6	0	4.290381	1.030732	1.292505
499	1	0	0.676929	2.000388	-2.007049
500	1	0	2.832508	0.772090	-1.719892

TS1a@CP6R-in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.690506	8.115310	-2.988753
2	8	0	-2.305004	4.160035	-6.955828
3	8	0	-0.051351	2.298045	-7.547436

4	6	0	1.192740	7.067204	-0.823450
5	8	0	-1.040886	7.433696	-1.367808
6	8	0	3.398259	6.701646	-0.101240
7	8	0	4.595643	1.822651	-6.528838
8	6	0	4.503992	7.869172	-2.572810
9	8	0	-2.845399	7.548878	-3.530608
10	6	0	-0.332258	8.615555	-3.988967
11	8	0	2.155196	0.683391	-7.048948
12	6	0	-0.847669	7.445738	-4.802667
13	8	0	0.795067	6.437980	0.334578
14	6	0	3.019041	7.742687	-2.304358
15	6	0	5.062683	4.559980	-6.429686
16	8	0	6.567417	2.933974	-4.546174
17	8	0	6.126766	6.216201	-1.082425
18	8	0	7.192191	3.844040	-1.979071
19	8	0	-3.855951	5.250449	-4.929127
20	6	0	2.570748	7.174326	-1.093533
21	6	0	0.171454	5.191865	-7.746201
22	6	0	0.267588	7.553048	-1.771427
23	6	0	3.677115	4.011788	-6.690321
24	6	0	2.224547	2.057776	-6.996593
25	6	0	1.320611	4.316976	-7.291144
26	6	0	3.493802	2.614596	-6.729559
27	6	0	4.737247	6.148759	-4.453768
28	6	0	-2.614329	5.790972	-5.194147
29	6	0	2.577148	4.835559	-6.959181
30	6	0	-0.589498	5.771890	-6.575785
31	6	0	-0.102426	6.850294	-5.825934
32	6	0	-2.123347	6.919353	-4.515792
33	6	0	2.067728	8.179279	-3.233180
34	6	0	5.256411	4.960503	-4.981268
35	6	0	-1.845955	5.232916	-6.234505
36	6	0	1.145875	2.918694	-7.267820
37	6	0	5.030144	6.571534	-3.151841
38	6	0	6.041534	4.142081	-4.144321
39	6	0	6.363998	4.538024	-2.832860
40	6	0	5.857778	5.760868	-2.351551
41	6	0	4.867713	9.063950	-3.459638
42	6	0	0.626989	6.280971	-8.723509
43	6	0	5.422666	5.707942	-7.379216
44	6	0	0.185390	9.745724	-4.882985
45	1	0	-3.226862	3.883975	-6.627517
46	1	0	-0.802471	2.980054	-7.653909
47	1	0	-1.700679	7.492597	-2.147679
48	1	0	4.344227	6.540364	-0.435192
49	1	0	4.372580	0.841665	-6.696447
50	1	0	5.015173	8.048476	-1.579242
51	1	0	-3.751460	7.094419	-3.380993
52	1	0	-1.197811	9.048049	-3.403357
53	1	0	1.193229	0.363248	-7.087873
54	1	0	-0.184520	6.637983	0.533339
55	1	0	5.796013	3.720229	-6.652279
56	1	0	6.162477	2.643172	-5.438885
57	1	0	6.794125	5.619204	-0.606926
58	1	0	7.412382	2.922601	-2.339306
59	1	0	-3.917462	5.001195	-3.931089
60	1	0	-0.549222	4.529039	-8.321749
61	1	0	4.090365	6.768528	-5.076485
62	1	0	2.711802	5.918000	-6.935762
63	1	0	0.891032	7.243067	-6.050615
64	1	0	2.413139	8.595670	-4.181910
65	1	0	5.958010	9.156024	-3.552244
66	1	0	4.464868	8.977296	-4.473929
67	1	0	4.492235	10.001041	-3.030420
68	1	0	1.141896	5.841629	-9.587046
69	1	0	-0.233424	6.847525	-9.102150
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73	1	0	5.327843	5.392562	-8.426019
74	1	0	0.530849	10.595718	-4.281732
75	1	0	1.015437	9.433128	-5.524651
76	1	0	-0.613412	10.110328	-5.542380
77	6	0	4.610116	0.191342	6.936910
78	8	0	-0.347774	4.337051	7.160216
79	8	0	0.604137	6.211952	5.258622
80	6	0	5.038368	-1.297147	5.047313
81	8	0	3.285578	-1.788197	6.634543

82	8	0	6.767942	-0.935450	3.525775
83	8	0	4.256759	7.061482	2.186389
84	6	0	7.756684	1.397725	5.058632
85	8	0	1.088667	-0.098740	8.174069
86	6	0	3.794893	0.535377	8.165701
87	8	0	1.441576	7.096069	2.776747
88	6	0	2.744493	1.584169	7.862053
89	8	0	4.653030	-2.426667	4.354656
90	6	0	6.503216	0.626349	5.422496
91	6	0	6.157355	6.129276	3.985973
92	8	0	6.294952	5.304426	1.177029
93	8	0	8.235692	1.096251	2.327953
94	8	0	7.394617	2.886270	0.417954
95	8	0	-0.921373	1.635593	7.553097
96	6	0	6.130365	-0.498643	4.666334
97	6	0	2.350574	5.376081	7.289147
98	6	0	4.298794	-0.974274	6.203317
99	6	0	4.685526	6.135524	4.330632
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101	6	0	2.849564	5.742812	5.909374
102	6	0	3.757001	6.604314	3.380596
103	6	0	6.911087	3.738711	4.472491
104	6	0	0.369527	2.134230	7.589151
105	6	0	4.206459	5.701355	5.571779
106	6	0	2.052859	3.896220	7.407645
107	6	0	3.046241	2.930133	7.618271
108	6	0	1.387835	1.198152	7.869077
109	6	0	5.700532	0.965997	6.521415
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112	6	0	1.933556	6.179624	4.929425
113	6	0	7.421762	2.498369	4.074067
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116	6	0	7.622825	2.272782	2.697867
117	6	0	8.505224	1.924753	6.286471
118	6	0	3.291304	5.852972	8.401174
119	6	0	7.028638	6.671850	5.123353
120	6	0	4.676831	0.957520	9.346961
121	1	0	-0.018096	5.230811	6.792783
122	1	0	0.033242	6.465673	4.453105
123	1	0	3.293714	-2.671293	6.117927
124	1	0	7.411081	-0.233304	3.149502
125	1	0	3.514209	7.383095	1.563556
126	1	0	8.462002	0.677758	4.543946
127	1	0	0.107756	-0.279095	8.039172
128	1	0	3.254096	-0.411010	8.479481
129	1	0	1.573028	6.681409	1.841820
130	1	0	5.322952	-2.639753	3.617624
131	1	0	6.308687	6.829231	3.109067
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133	1	0	8.369470	1.052777	1.317458
134	1	0	6.978404	3.592266	-0.191326
135	1	0	-1.586871	2.386681	7.683201
136	1	0	1.372720	5.934083	7.439404
137	1	0	6.772088	3.933129	5.537418
138	1	0	4.920996	5.330500	6.309751
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140	1	0	5.949127	1.862998	7.092171
141	1	0	8.766850	1.103836	6.966096
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143	1	0	7.919653	2.650279	6.860580
144	1	0	4.268318	5.360466	8.366896
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148	1	0	6.734049	7.696991	5.381773
149	1	0	8.085446	6.693577	4.829106
150	1	0	5.420683	0.184611	9.574249
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152	1	0	5.214577	1.891758	9.161641
153	6	0	4.575234	-4.610925	-5.178635
154	8	0	3.854297	-8.290791	0.112271
155	8	0	5.014163	-6.550903	1.823924
156	6	0	3.623218	-2.390625	-5.555513
157	8	0	2.247352	-4.387702	-5.631668
158	8	0	4.929870	-0.465493	-5.538058
159	8	0	7.815205	-2.720808	2.209302

160	6	0	7.395868	-1.989257	-4.986669
161	8	0	1.805041	-6.846047	-3.944268
162	6	0	4.374385	-6.110206	-5.126022
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166	6	0	6.027278	-2.630302	-5.119527
167	6	0	9.017080	-3.086647	-0.264457
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170	8	0	6.913513	1.291923	-1.421165
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172	6	0	4.904194	-1.827708	-5.393436
173	6	0	6.406842	-7.460087	-0.633632
174	6	0	3.463599	-3.786519	-5.458709
175	6	0	8.005548	-4.078920	0.266979
176	6	0	6.359796	-4.655582	1.981279
177	6	0	6.698735	-6.146505	0.064557
178	6	0	7.381220	-3.816914	1.503248
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190	6	0	7.853541	-0.907173	-0.813834
191	6	0	7.349675	0.028535	-1.736904
192	6	0	7.268372	-0.329071	-3.095115
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245	8	0	-9.009761	-0.649375	-2.293126
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275	1	0	-3.226354	1.597462	-6.810640
276	1	0	-8.489456	0.788540	-3.417226
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285	1	0	-9.165675	-0.545293	-1.294641
286	1	0	-8.249971	-3.235890	0.336185
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309	8	0	-2.661622	4.929074	6.145909
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324	6	0	-5.410013	2.503527	5.716352
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326	6	0	-3.887701	4.392139	5.835630
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328	6	0	-5.408593	4.519044	-1.780845
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335	6	0	-4.993803	7.177829	2.728966
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347	6	0	-9.828438	4.649378	0.414040
348	6	0	-5.742471	7.619655	5.615029
349	1	0	-1.805536	8.411145	-0.029990
350	1	0	-3.485058	6.981640	-1.087975
351	1	0	-1.983525	4.190354	6.347198
352	1	0	-6.406491	0.787457	5.506568
353	1	0	-7.130537	2.748427	-2.927116
354	1	0	-7.905674	1.830454	5.630420
355	1	0	-2.110952	6.482566	5.297035
356	1	0	-3.723885	6.951100	5.910296
357	1	0	-4.919482	3.043232	-3.004771
358	1	0	-3.261004	1.280390	6.434884
359	1	0	-9.022855	3.109858	-0.847292
360	1	0	-7.873976	1.498168	-1.086642
361	1	0	-7.505173	-0.909730	3.955643
362	1	0	-7.847855	-1.068868	0.647142
363	1	0	-0.348810	7.788271	2.755259
364	1	0	-4.991478	8.308184	-0.526718
365	1	0	-8.254397	4.244900	2.711523
366	1	0	-7.661289	6.132320	0.940925
367	1	0	-6.055057	6.988541	2.899489
368	1	0	-6.921579	5.351029	4.641560
369	1	0	-8.854115	3.983016	6.420643
370	1	0	-8.954692	4.609414	4.770736
371	1	0	-9.914189	3.202499	5.235453
372	1	0	-7.417050	8.715723	-0.190261
373	1	0	-7.334419	8.144547	1.481434
374	1	0	-6.435122	9.584617	1.000087
375	1	0	-10.084286	5.313304	-0.420794
376	1	0	-10.726320	4.069154	0.663952
377	1	0	-9.601023	5.279958	1.279797
378	1	0	-6.628152	7.482720	4.986363
379	1	0	-6.040919	7.414991	6.651110
380	1	0	-5.459749	8.678150	5.553416
381	6	0	-1.363831	-8.278763	3.155228
382	8	0	2.282749	-3.184908	4.684464
383	8	0	0.326285	-1.039870	6.040684
384	6	0	-2.403028	-8.525648	0.940198
385	8	0	-0.037593	-8.892893	1.251594
386	8	0	-4.723077	-8.182234	0.624854
387	8	0	-4.403115	-0.962883	6.040942
388	6	0	-5.163918	-7.745428	3.461297
389	8	0	1.874767	-7.203252	2.166087
390	6	0	-0.116871	-8.326091	4.013965
391	8	0	-2.029692	0.292609	5.636029
392	6	0	0.483238	-6.943737	4.179520
393	8	0	-2.168261	-8.844841	-0.368544

394	6	0	-3.782829	-7.980104	2.883982
395	6	0	-4.697492	-3.686195	6.502412
396	8	0	-6.096651	-2.200485	4.339468
397	8	0	-6.435410	-6.077787	1.612075
398	8	0	-6.843384	-3.381003	2.012995
399	8	0	3.132628	-4.848682	2.598823
400	6	0	-3.655584	-8.215169	1.500358
401	6	0	0.419647	-3.938153	6.592781
402	6	0	-1.269908	-8.553967	1.779909
403	6	0	-3.322119	-3.070072	6.343918
404	6	0	-1.993763	-1.046947	5.952296
405	6	0	-0.868932	-3.177875	6.367470
406	6	0	-3.233187	-1.686906	6.095888
407	6	0	-4.927434	-5.667274	4.919365
408	6	0	2.123601	-5.272770	3.447263
409	6	0	-2.128019	-3.791540	6.452211
410	6	0	0.749029	-4.841244	5.422939
411	6	0	0.138253	-6.086156	5.233587
412	6	0	1.464461	-6.506691	3.269860
413	6	0	-2.631353	-7.990019	3.679021
414	6	0	-5.141741	-4.311197	5.196464
415	6	0	1.739714	-4.430045	4.504192
416	6	0	-0.808358	-1.795261	6.105200
417	6	0	-5.366919	-6.273162	3.737630
418	6	0	-5.798941	-3.533651	4.223165
419	6	0	-6.222362	-4.103396	3.005315
420	6	0	-6.013515	-5.474982	2.773590
421	6	0	-5.432489	-8.624839	4.685204
422	6	0	0.399981	-4.704267	7.919833
423	6	0	-4.758405	-4.655207	7.687109
424	6	0	-0.364541	-9.021396	5.356261
425	1	0	2.945068	-2.944639	3.946708
426	1	0	1.181652	-1.583978	6.173787
427	1	0	-0.065850	-8.845425	0.236086
428	1	0	-5.556778	-7.827720	1.098869
429	1	0	-4.232507	0.000914	5.729256
430	1	0	-5.926101	-8.047689	2.675072
431	1	0	1.216123	-7.964722	1.934822
432	1	0	0.644837	-8.960832	3.466213
433	1	0	-1.171337	0.762933	5.949247
434	1	0	-2.889044	-8.452953	-0.972280
435	1	0	-5.423261	-2.851111	6.742365
436	1	0	-5.562201	-1.750672	5.091792
437	1	0	-6.851025	-5.396162	0.989970
438	1	0	-6.793414	-2.388211	2.230511
439	1	0	3.459128	-5.650026	2.037534
440	1	0	1.255010	-3.169998	6.676487
441	1	0	-4.405591	-6.279591	5.657441
442	1	0	-2.178213	-4.867993	6.623159
443	1	0	-0.632278	-6.404897	5.938904
444	1	0	-2.723832	-7.771621	4.743641
445	1	0	-6.449505	-8.465114	5.065148
446	1	0	-5.334531	-9.687937	4.430679
447	1	0	-4.740094	-8.424609	5.509397
448	1	0	0.248263	-4.018907	8.763650
449	1	0	-0.397280	-5.452782	7.963696
450	1	0	1.350560	-5.226198	8.085991
451	1	0	-4.491744	-4.141798	8.619966
452	1	0	-5.771289	-5.058935	7.809765
453	1	0	-4.076073	-5.503994	7.576247
454	1	0	0.563173	-9.090479	5.937977
455	1	0	-1.102426	-8.499504	5.974050
456	1	0	-0.734491	-10.043270	5.200268
457	1	0	-1.163640	1.319887	-2.236150
458	1	0	-1.589260	-1.033369	-2.932881
459	1	0	0.262846	-2.693924	-2.896378
460	1	0	5.704813	-3.181587	-2.282927
461	1	0	4.279697	-4.299359	-2.274700
462	1	0	5.054744	-3.785079	-0.735311
463	1	0	2.472622	-3.256986	-2.701825
464	1	0	4.649430	-0.282840	2.441757
465	1	0	5.554128	-0.228899	0.906474
466	1	0	3.971566	0.608815	1.055203
467	1	0	4.428579	-2.454974	1.025622
468	1	0	1.850110	-0.752930	1.002318
469	1	0	2.503720	-3.800948	0.769560
470	1	0	-1.772574	-4.310217	1.755494
471	1	0	-2.076851	-5.011290	0.142089

472	1	0	0.408922	-5.172448	1.322873
473	1	0	-0.635050	-1.743892	1.746363
474	6	0	-1.675524	-2.844519	0.162555
475	6	0	-0.460667	-2.107226	0.717527
476	7	0	0.576366	-3.145228	0.741214
477	8	0	4.401124	-1.327317	-0.979036
478	6	0	2.736300	-2.327258	-2.206064
479	6	0	-0.350199	0.591661	-2.233546
480	6	0	0.449441	-5.080691	-0.810033
481	8	0	1.366286	-4.555143	-1.433026
482	6	0	1.735522	-1.267822	-2.201858
483	8	0	-0.185319	-6.132927	-1.168291
484	6	0	1.867722	-2.908003	0.812098
485	6	0	2.464845	-1.654155	0.951531
486	6	0	3.851123	-1.528716	0.922148
487	7	0	3.917750	-2.310514	-1.668180
488	6	0	4.787923	-3.480175	-1.755898
489	6	0	0.935122	0.985141	-1.847443
490	1	0	-1.641098	-2.843776	-0.937366
491	6	0	0.017345	-4.491652	0.547328
492	6	0	-1.492475	-4.268249	0.690323
493	6	0	-0.589504	-0.725964	-2.622422
494	6	0	0.447826	-1.655829	-2.610367
495	6	0	1.978537	0.066323	-1.827234
496	1	0	-0.135369	-1.257711	0.099092
497	1	0	-2.619974	-2.380336	0.475735
498	6	0	4.548467	-0.279745	1.342748
499	1	0	1.121911	2.020945	-1.555832
500	1	0	2.980135	0.357606	-1.515591

IN1a@CP_{6R}-in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.872752	8.156681	-2.825487
2	8	0	-2.234584	4.377560	-6.872314
3	8	0	-0.032192	2.471601	-7.461271
4	6	0	1.355286	7.033494	-0.693194
5	8	0	-0.870243	7.462453	-1.222444
6	8	0	3.553258	6.600618	0.013899
7	8	0	4.604125	1.858640	-6.470462
8	6	0	4.680500	7.816097	-2.424081
9	8	0	-2.682306	7.702127	-3.371753
10	6	0	-0.141048	8.709073	-3.807275
11	8	0	2.126966	0.792237	-6.983463
12	6	0	-0.689612	7.574280	-4.648559
13	8	0	0.946243	6.378382	0.445885
14	6	0	3.193540	7.713715	-2.157304
15	6	0	5.148715	4.582542	-6.356695
16	8	0	6.655963	2.899477	-4.530171
17	8	0	6.283950	6.101466	-0.982809
18	8	0	7.308937	3.735533	-1.944105
19	8	0	-3.755646	5.462451	-4.827218
20	6	0	2.734913	7.119799	-0.962724
21	6	0	0.269998	5.360102	-7.641547
22	6	0	0.439581	7.567007	-1.624769
23	6	0	3.747330	4.074507	-6.614223
24	6	0	2.238276	2.164575	-6.923376
25	6	0	1.397142	4.449741	-7.200967
26	6	0	3.524042	2.683324	-6.660502
27	6	0	4.868457	6.133915	-4.343801
28	6	0	-2.500667	5.977841	-5.076787
29	6	0	2.669689	4.930386	-6.872891
30	6	0	-0.476527	5.935380	-6.459615
31	6	0	0.039118	6.983513	-5.685969
32	6	0	-1.979555	7.076436	-4.372689
33	6	0	2.250636	8.198418	-3.070742
34	6	0	5.364830	4.950284	-4.902635
35	6	0	-1.746583	5.423202	-6.129517
36	6	0	1.182723	3.056904	-7.184920
37	6	0	5.179944	6.522634	-3.035544
38	6	0	6.147420	4.103692	-4.092154
39	6	0	6.485487	4.462684	-2.774484
40	6	0	6.000870	5.681203	-2.260257
41	6	0	5.069309	9.023885	-3.282104

42	6	0	0.751005	6.456404	-8.598092
43	6	0	5.530651	5.739417	-7.286369
44	6	0	0.400898	9.848641	-4.674438
45	1	0	-3.162771	4.119495	-6.546729
46	1	0	-0.763928	3.175150	-7.568075
47	1	0	-1.530926	7.575509	-1.995328
48	1	0	4.496996	6.437982	-0.323092
49	1	0	4.350407	0.885470	-6.637395
50	1	0	5.195555	7.960597	-1.426769
51	1	0	-3.600273	7.269099	-3.229607
52	1	0	-0.992649	9.147991	-3.206079
53	1	0	1.154453	0.503343	-7.018585
54	1	0	-0.025966	6.600984	0.658873
55	1	0	5.857832	3.728440	-6.602303
56	1	0	6.230924	2.633356	-5.421156
57	1	0	6.947277	5.485098	-0.526618
58	1	0	7.508516	2.818645	-2.325043
59	1	0	-3.827419	5.192176	-3.835023
60	1	0	-0.465613	4.725131	-8.229261
61	1	0	4.224775	6.777079	-4.945913
62	1	0	2.835027	6.008660	-6.844488
63	1	0	1.042546	7.354884	-5.902448
64	1	0	2.603572	8.636077	-4.007009
65	1	0	6.161332	9.096201	-3.372055
66	1	0	4.665525	8.969918	-4.298254
67	1	0	4.712793	9.958015	-2.830581
68	1	0	1.257644	6.022253	-9.469053
69	1	0	-0.096526	7.048239	-8.967452
70	1	0	1.450382	7.153098	-8.125324
71	1	0	4.918029	6.631878	-7.123273
72	1	0	6.577358	6.032878	-7.135397
73	1	0	5.415396	5.449608	-8.338491
74	1	0	0.770588	10.673790	-4.053227
75	1	0	1.219520	9.532137	-5.328666
76	1	0	-0.391634	10.250570	-5.319639
77	6	0	4.631246	-0.069406	6.890385
78	8	0	-0.226224	4.182951	7.248472
79	8	0	0.770147	6.057162	5.364186
80	6	0	5.009701	-1.506077	4.948804
81	8	0	3.248412	-1.997423	6.524169
82	8	0	6.754009	-1.147305	3.440110
83	8	0	4.437163	6.889146	2.305481
84	6	0	7.810277	1.101486	5.045864
85	8	0	1.107475	-0.308839	8.151362
86	6	0	3.828202	0.257305	8.131736
87	8	0	1.625930	6.967682	2.895983
88	6	0	2.801772	1.338899	7.862791
89	8	0	4.579173	-2.596991	4.224411
90	6	0	6.534050	0.357833	5.386951
91	6	0	6.321298	5.894027	4.091340
92	8	0	6.488212	5.153521	1.263291
93	8	0	8.327194	0.871471	2.315585
94	8	0	7.567278	2.745625	0.444536
95	8	0	-0.864117	1.488326	7.581122
96	6	0	6.126103	-0.730378	4.594868
97	6	0	2.498550	5.150886	7.378543
98	6	0	4.282712	-1.198536	6.118420
99	6	0	4.849449	5.918342	4.434125
100	6	0	2.551760	6.445080	3.774623
101	6	0	3.005684	5.532774	6.005815
102	6	0	3.930281	6.420323	3.492398
103	6	0	7.017700	3.474048	4.516854
104	6	0	0.438984	1.953301	7.621006
105	6	0	4.361375	5.471307	5.667508
106	6	0	2.164378	3.676878	7.466776
107	6	0	3.135186	2.681971	7.647499
108	6	0	1.435801	0.986167	7.871836
109	6	0	5.744312	0.685468	6.498264
110	6	0	6.725998	4.512043	3.622436
111	6	0	0.810323	3.290299	7.421032
112	6	0	2.098170	6.004094	5.033578
113	6	0	7.512493	2.237091	4.088978
114	6	0	6.841838	4.257163	2.243379
115	6	0	7.359690	3.034171	1.777475
116	6	0	7.734002	2.050275	2.709856
117	6	0	8.570508	1.576919	6.287680
118	6	0	3.451377	5.580833	8.499406
119	6	0	7.201112	6.390783	5.243096

120	6	0	4.722241	0.624132	9.322397
121	1	0	0.122766	5.074157	6.895006
122	1	0	0.203826	6.335387	4.563853
123	1	0	3.223496	-2.858438	5.966035
124	1	0	7.415875	-0.453827	3.090200
125	1	0	3.699884	7.242980	1.694353
126	1	0	8.495880	0.373908	4.515616
127	1	0	0.124080	-0.466934	8.004463
128	1	0	3.266323	-0.685346	8.418915
129	1	0	1.742413	6.556943	1.958090
130	1	0	5.209601	-2.785453	3.448582
131	1	0	6.485755	6.613973	3.233067
132	1	0	5.843792	5.861359	1.620690
133	1	0	8.485457	0.857644	1.310403
134	1	0	7.153059	3.468759	-0.144523
135	1	0	-1.508950	2.250510	7.742567
136	1	0	1.535105	5.730083	7.540915
137	1	0	6.861840	3.637493	5.584822
138	1	0	5.068435	5.074140	6.399077
139	1	0	4.188118	2.966019	7.633075
140	1	0	6.020766	1.554415	7.098334
141	1	0	8.804492	0.732370	6.948322
142	1	0	9.519082	2.050350	6.004744
143	1	0	8.004689	2.305517	6.877477
144	1	0	4.414674	5.062708	8.455440
145	1	0	3.014354	5.365389	9.482958
146	1	0	3.651933	6.658077	8.452656
147	1	0	7.120347	5.766407	6.138644
148	1	0	6.922221	7.412412	5.531081
149	1	0	8.258075	6.404694	4.949082
150	1	0	5.450040	-0.171133	9.522882
151	1	0	4.118776	0.756766	10.229176
152	1	0	5.278992	1.552054	9.163751
153	6	0	4.427345	-4.564870	-5.268896
154	8	0	3.690508	-8.371361	-0.078202
155	8	0	4.904278	-6.699646	1.653918
156	6	0	3.525659	-2.306689	-5.522410
157	8	0	2.094621	-4.260467	-5.637210
158	8	0	4.877992	-0.417374	-5.460481
159	8	0	7.766318	-2.922936	2.093652
160	6	0	7.322891	-2.028268	-5.056441
161	8	0	1.619918	-6.804059	-4.074806
162	6	0	4.185622	-6.059192	-5.261610
163	8	0	5.688761	-4.474734	3.030281
164	6	0	4.055177	-6.588463	-3.848631
165	8	0	2.421597	-1.511071	-5.719270
166	6	0	5.933984	-2.626374	-5.176652
167	6	0	8.967694	-3.276785	-0.380914
168	8	0	7.881241	-0.664099	0.448405
169	8	0	6.888945	0.550013	-4.043916
170	8	0	6.980888	1.186653	-1.418518
171	8	0	1.455486	-7.963987	-1.555101
172	6	0	4.825843	-1.783559	-5.380827
173	6	0	6.249236	-7.574074	-0.836677
174	6	0	3.330702	-3.700922	-5.483922
175	6	0	7.930449	-4.252620	0.129479
176	6	0	6.270969	-4.821936	1.834706
177	6	0	6.578434	-6.285017	-0.110443
178	6	0	7.310003	-3.997000	1.368564
179	6	0	8.123834	-2.612147	-2.692493
180	6	0	2.637181	-7.549584	-2.094149
181	6	0	7.549919	-5.393670	-0.583602
182	6	0	5.064503	-7.359479	-1.753612
183	6	0	5.170461	-6.776869	-3.020448
184	6	0	2.781363	-6.955689	-3.369193
185	6	0	5.700227	-4.006917	-5.109403
186	6	0	8.309597	-2.303282	-1.338722
187	6	0	3.788258	-7.756643	-1.315084
188	6	0	5.916720	-5.968416	1.092181
189	6	0	7.595592	-1.691027	-3.604327
190	6	0	7.874999	-1.047592	-0.870331
191	6	0	7.386855	-0.077706	-1.766769
192	6	0	7.282966	-0.402997	-3.131736
193	6	0	8.409909	-2.910337	-5.673828
194	6	0	7.449117	-8.175149	-1.573473
195	6	0	10.183707	-3.972861	-0.997318
196	6	0	5.247031	-6.825937	-6.057540
197	1	0	2.719856	-8.438862	0.193547

198	1	0	4.644829	-7.520904	1.082358
199	1	0	1.382929	-3.547494	-5.844293
200	1	0	5.783839	-0.042054	-5.146192
201	1	0	7.279591	-2.835385	2.988239
202	1	0	7.330272	-1.059123	-5.640513
203	1	0	1.719414	-6.096413	-4.791806
204	1	0	3.198103	-6.240175	-5.789630
205	1	0	4.811592	-4.993311	3.175405
206	1	0	2.706429	-0.539459	-5.870553
207	1	0	9.354721	-2.687467	0.504575
208	1	0	7.973919	-1.469499	1.079565
209	1	0	6.510599	1.379927	-3.573113
210	1	0	6.955412	1.295688	-0.399174
211	1	0	0.676066	-7.355868	-1.901143
212	1	0	5.947566	-8.334248	-0.052871
213	1	0	8.408184	-3.603581	-3.050542
214	1	0	8.040562	-5.605276	-1.535936
215	1	0	6.153080	-6.472481	-3.380585
216	1	0	6.547216	-4.676226	-4.943752
217	1	0	8.199561	-3.104575	-6.733610
218	1	0	9.389406	-2.417987	-5.616028
219	1	0	8.503070	-3.881527	-5.176646
220	1	0	7.814120	-7.535656	-2.383313
221	1	0	8.285046	-8.351891	-0.885413
222	1	0	7.179187	-9.141113	-2.021474
223	1	0	9.927490	-4.591038	-1.863785
224	1	0	10.928726	-3.238167	-1.328445
225	1	0	10.668687	-4.628078	-0.261728
226	1	0	6.247783	-6.738551	-5.623665
227	1	0	5.003564	-7.896075	-6.094200
228	1	0	5.300452	-6.461826	-7.090811
229	6	0	-5.265821	0.248696	-6.699329
230	8	0	-0.195838	-3.204747	-5.081310
231	8	0	-1.247559	-5.389286	-3.710122
232	6	0	-5.990219	2.005501	-5.149782
233	8	0	-4.038714	2.356399	-6.392203
234	8	0	-7.957087	1.776864	-3.865255
235	8	0	-5.500019	-6.514943	-1.603650
236	6	0	-8.553588	-0.824924	-5.000963
237	8	0	-1.815004	0.866791	-6.960856
238	6	0	-4.277054	-0.232032	-7.743090
239	8	0	-2.861975	-6.544159	-1.416384
240	6	0	-3.205064	-1.075545	-7.084442
241	8	0	-5.831187	3.228882	-4.524890
242	6	0	-7.310482	-0.042965	-5.374834
243	6	0	-6.974012	-5.512006	-3.762692
244	8	0	-7.564834	-4.754450	-0.994800
245	8	0	-9.026958	-0.394061	-2.281605
246	8	0	-8.555481	-2.279170	-0.316858
247	8	0	0.134847	-0.510449	-5.664313
248	6	0	-7.102016	1.222131	-4.788641
249	6	0	-2.492724	-4.718825	-6.074147
250	6	0	-5.079595	1.510506	-6.102694
251	6	0	-5.460907	-5.515532	-3.769584
252	6	0	-3.359920	-5.990806	-2.587170
253	6	0	-3.305674	-5.074621	-4.848589
254	6	0	-4.769816	-6.001450	-2.647088
255	6	0	-7.709662	-3.130574	-4.314245
256	6	0	-0.998028	-1.205717	-6.023819
257	6	0	-4.703377	-5.058777	-4.855803
258	6	0	-2.369001	-3.219573	-6.233963
259	6	0	-3.360808	-2.447606	-6.850779
260	6	0	-2.001391	-0.468119	-6.680887
261	6	0	-6.374711	-0.511375	-6.304345
262	6	0	-7.477685	-4.137667	-3.371174
263	6	0	-1.202511	-2.575778	-5.778682
264	6	0	-2.628497	-5.492155	-3.679816
265	6	0	-8.234715	-1.880864	-3.964648
266	6	0	-7.739339	-3.855480	-2.015362
267	6	0	-8.246021	-2.600668	-1.624467
268	6	0	-8.499979	-1.621321	-2.604347
269	6	0	-9.256754	-1.408394	-6.230775
270	6	0	-3.038128	-5.390672	-7.339401
271	6	0	-7.567545	-6.009827	-5.083331
272	6	0	-4.957884	-0.950337	-8.910942
273	1	0	-0.523584	-4.093370	-4.664870
274	1	0	-0.816970	-5.759915	-2.874047
275	1	0	-3.259628	1.849317	-6.828731

276	1	0	-8.491529	1.051454	-3.380705
277	1	0	-4.884736	-6.816876	-0.830905
278	1	0	-9.287558	-0.100915	-4.529681
279	1	0	-0.972146	1.220781	-6.503908
280	1	0	-3.769555	0.679974	-8.182329
281	1	0	-1.860578	-6.408413	-1.333254
282	1	0	-5.212040	3.819589	-5.061806
283	1	0	-7.314634	-6.241711	-2.965800
284	1	0	-6.977763	-5.542248	-1.292166
285	1	0	-9.171487	-0.303209	-1.279837
286	1	0	-8.311385	-3.047047	0.295386
287	1	0	0.701712	-1.076164	-5.033520
288	1	0	-1.449777	-5.135937	-5.920757
289	1	0	-7.487175	-3.331106	-5.363961
290	1	0	-5.223486	-4.691245	-5.741456
291	1	0	-4.285911	-2.933574	-7.166209
292	1	0	-6.519678	-1.499923	-6.744361
293	1	0	-8.636612	-2.130840	-6.770862
294	1	0	-9.527429	-0.614974	-6.938585
295	1	0	-10.181026	-1.924593	-5.940749
296	1	0	-3.054925	-6.482057	-7.219808
297	1	0	-2.407614	-5.161703	-8.207164
298	1	0	-4.057894	-5.075818	-7.581604
299	1	0	-7.226211	-7.030569	-5.299587
300	1	0	-7.285464	-5.385158	-5.936743
301	1	0	-8.663481	-6.029202	-5.036367
302	1	0	-4.222115	-1.236394	-9.673633
303	1	0	-5.697964	-0.298363	-9.392066
304	1	0	-5.478434	-1.862858	-8.602105
305	6	0	-4.751838	5.235245	5.467005
306	8	0	-2.616703	8.299871	0.182625
307	8	0	-3.788567	6.466300	-1.624488
308	6	0	-4.063399	2.979058	6.124447
309	8	0	-2.532467	4.844876	6.266754
310	8	0	-5.535602	1.155441	6.009316
311	8	0	-6.853911	2.866768	-1.879249
312	6	0	-7.727873	2.819931	5.042701
313	8	0	-1.563849	6.927456	4.641176
314	6	0	-4.396126	6.700478	5.344646
315	8	0	-4.479513	4.114773	-2.619456
316	6	0	-3.916120	7.020195	3.944089
317	8	0	-3.054756	2.210096	6.645093
318	6	0	-6.342204	3.371419	5.313321
319	6	0	-8.583418	3.915450	0.134987
320	8	0	-8.232627	1.052039	-0.353731
321	8	0	-7.572774	0.136822	4.295313
322	8	0	-7.787983	-0.739903	1.654315
323	8	0	-0.745156	7.715500	2.082678
324	6	0	-5.343765	2.500372	5.792654
325	6	0	-5.340541	7.850467	0.463756
326	6	0	-3.772066	4.345806	5.945860
327	6	0	-7.321825	4.637422	-0.286871
328	6	0	-5.317600	4.685265	-1.694637
329	6	0	-5.743841	6.510887	-0.122816
330	6	0	-6.524371	4.078406	-1.298802
331	6	0	-8.093954	3.317082	2.568861
332	6	0	-2.070432	7.560037	2.429868
333	6	0	-6.901977	5.840703	0.293840
334	6	0	-4.385860	7.629267	1.618485
335	6	0	-4.812064	7.220647	2.887058
336	6	0	-2.534413	7.147209	3.692364
337	6	0	-6.015594	4.722716	5.144683
338	6	0	-8.257898	2.925353	1.233895
339	6	0	-3.008196	7.835314	1.416487
340	6	0	-4.942855	5.915086	-1.117179
341	6	0	-7.863170	2.393977	3.595056
342	6	0	-8.124670	1.561463	0.920521
343	6	0	-7.888088	0.602697	1.925536
344	6	0	-7.772605	1.025662	3.263244
345	6	0	-8.838832	3.787558	5.462080
346	6	0	-6.536728	8.717151	0.867544
347	6	0	-9.716105	4.865231	0.534045
348	6	0	-5.537441	7.623497	5.782785
349	1	0	-1.601661	8.426965	0.143485
350	1	0	-3.322203	7.071203	-0.944924
351	1	0	-1.874828	4.084628	6.457718
352	1	0	-6.385924	0.816171	5.553524
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355	1	0	-1.937745	6.375859	5.420990
356	1	0	-3.536126	6.897108	6.056822
357	1	0	-4.885262	3.236550	-2.970872
358	1	0	-3.224674	1.210333	6.492372
359	1	0	-8.953026	3.331710	-0.760432
360	1	0	-7.825084	1.701852	-1.038005
361	1	0	-7.506814	-0.815272	3.954581
362	1	0	-7.830521	-0.896353	0.640243
363	1	0	-0.150541	7.693720	2.902134
364	1	0	-4.792001	8.425322	-0.341341
365	1	0	-8.152895	4.377520	2.818104
366	1	0	-7.505836	6.277954	1.090822
367	1	0	-5.877670	7.059239	3.059256
368	1	0	-6.775550	5.404297	4.759757
369	1	0	-8.745305	4.052986	6.522632
370	1	0	-8.827946	4.719161	4.887476
371	1	0	-9.825875	3.328701	5.320366
372	1	0	-7.205316	8.885874	0.014346
373	1	0	-7.132217	8.270793	1.670753
374	1	0	-6.198041	9.699296	1.222659
375	1	0	-9.961616	5.550035	-0.286824
376	1	0	-10.625496	4.300979	0.779055
377	1	0	-9.469368	5.474365	1.409836
378	1	0	-6.429636	7.519966	5.157007
379	1	0	-5.835808	7.408363	6.816832
380	1	0	-5.227767	8.675199	5.738077
381	6	0	-1.524511	-8.326308	3.010317
382	8	0	2.214189	-3.325995	4.545777
383	8	0	0.305554	-1.154842	5.989104
384	6	0	-2.568284	-8.483868	0.788988
385	8	0	-0.216008	-8.927271	1.089127
386	8	0	-4.877954	-8.069835	0.481593
387	8	0	-4.423133	-1.005417	6.036353
388	6	0	-5.313533	-7.725314	3.332454
389	8	0	1.779900	-7.369145	2.062786
390	6	0	-0.278920	-8.422647	3.867528
391	8	0	-2.032989	0.224585	5.643925
392	6	0	0.361767	-7.060582	4.049112
393	8	0	-2.339706	-8.772784	-0.528083
394	6	0	-3.936586	-7.965023	2.747490
395	6	0	-4.751276	-3.735446	6.448685
396	8	0	-6.174721	-2.191716	4.348132
397	8	0	-6.621440	-6.010866	1.551677
398	8	0	-6.999183	-3.319336	2.020365
399	8	0	3.075245	-5.027406	2.496012
400	6	0	-3.813089	-8.158012	1.356920
401	6	0	0.360778	-4.063228	6.471395
402	6	0	-1.436788	-8.566208	1.627957
403	6	0	-3.370078	-3.135419	6.281802
404	6	0	-2.015740	-1.124253	5.922295
405	6	0	-0.919013	-3.281437	6.273018
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407	6	0	-5.027331	-5.680574	4.828006
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410	6	0	0.664822	-4.964634	5.293777
411	6	0	0.029061	-6.196479	5.101817
412	6	0	1.366319	-6.649531	3.153376
413	6	0	-2.785897	-8.024007	3.541600
414	6	0	-5.224748	-4.329299	5.138643
415	6	0	1.660273	-4.567782	4.373276
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418	6	0	-5.895355	-3.525375	4.196460
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420	6	0	-6.163536	-5.434919	2.714007
421	6	0	-5.592069	-8.627875	4.537426
422	6	0	0.347349	-4.838193	7.793924
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424	6	0	-0.544642	-9.126236	5.201991
425	1	0	2.822332	-3.065373	3.768450
426	1	0	1.153789	-1.720553	6.074382
427	1	0	-0.241548	-8.846663	0.076323
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435	1	0	-5.461461	-2.895304	6.715981
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437	1	0	-7.046719	-5.313700	0.955952
438	1	0	-6.919349	-2.332303	2.248343
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441	1	0	-4.492612	-6.312158	5.540112
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443	1	0	-0.752116	-6.498504	5.802143
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445	1	0	-6.608109	-8.466505	4.919079
446	1	0	-5.503231	-9.686152	4.260822
447	1	0	-4.899363	-8.450713	5.366626
448	1	0	0.219493	-4.156379	8.644309
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450	1	0	1.291456	-5.376941	7.942182
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452	1	0	-5.824578	-5.119724	7.744321
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454	1	0	0.382510	-9.230892	5.779300
455	1	0	-1.262570	-8.587287	5.828669
456	1	0	-0.947630	-10.133597	5.035632
457	1	0	-1.336401	1.331980	-2.060345
458	1	0	-1.783201	-0.992779	-2.830036
459	1	0	0.068040	-2.655056	-2.898039
460	1	0	5.519318	-3.146806	-2.363897
461	1	0	4.113470	-4.284648	-2.440553
462	1	0	4.885930	-3.902785	-0.869817
463	1	0	2.301466	-3.178926	-2.855990
464	1	0	4.601259	-0.634938	2.345713
465	1	0	5.663315	-0.432870	0.921454
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475	6	0	-0.472198	-2.193969	0.825183
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479	6	0	-0.524287	0.603231	-2.099062
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487	7	0	3.705464	-2.379725	-1.677620
488	6	0	4.612140	-3.504823	-1.855142
489	6	0	0.767304	0.984678	-1.723019
490	1	0	-1.760122	-2.805498	-0.803361
491	6	0	-0.030076	-4.557605	0.479106
492	6	0	-1.532898	-4.343998	0.704588
493	6	0	-0.776797	-0.699088	-2.530051
494	6	0	0.257985	-1.628586	-2.577145
495	6	0	1.806412	0.063088	-1.749663
496	1	0	-0.161564	-1.328982	0.214132
497	1	0	-2.651713	-2.438275	0.691568
498	6	0	4.617793	-0.506247	1.254259
499	1	0	0.961378	2.009302	-1.399893
500	1	0	2.811349	0.352409	-1.447674

TS2a@CP_{6R}-in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.808310	8.122700	-2.782183

2	8	0	-2.885461	4.618154	-6.576052
3	8	0	-0.857791	2.605519	-7.272871
4	6	0	1.426994	6.945224	-0.717432
5	8	0	-0.811923	7.511201	-1.023576
6	8	0	3.646082	6.380130	-0.223964
7	8	0	3.811049	1.710060	-6.818359
8	6	0	4.608338	7.543845	-2.768225
9	8	0	-2.804932	7.879666	-2.990520
10	6	0	-0.260660	8.752952	-3.651991
11	8	0	1.223827	0.803555	-6.987167
12	6	0	-0.951771	7.669615	-4.454999
13	8	0	1.110356	6.307427	0.456049
14	6	0	3.152290	7.529670	-2.352237
15	6	0	4.535611	4.394931	-6.805466
16	8	0	6.036035	2.545367	-5.112131
17	8	0	6.063366	5.594775	-1.443831
18	8	0	6.810051	3.205694	-2.529029
19	8	0	-4.140121	5.740896	-4.380835
20	6	0	2.777241	6.954483	-1.121101
21	6	0	-0.402795	5.469191	-7.559881
22	6	0	0.458208	7.543793	-1.549027
23	6	0	3.085455	3.974375	-6.914398
24	6	0	1.432912	2.164177	-7.000341
25	6	0	0.711122	4.494962	-7.237591
26	6	0	2.771736	2.599638	-6.903682
27	6	0	4.558659	5.924123	-4.755589
28	6	0	-2.885790	6.190272	-4.737526
29	6	0	2.041886	4.894866	-7.070966
30	6	0	-1.004244	6.060728	-6.304839
31	6	0	-0.358450	7.060709	-5.565542
32	6	0	-2.237122	7.239954	-4.065676
33	6	0	2.154392	8.082205	-3.164190
34	6	0	4.906188	4.714433	-5.371176
35	6	0	-2.266751	5.617297	-5.865728
36	6	0	0.413359	3.119924	-7.162016
37	6	0	4.956716	6.236263	-3.450204
38	6	0	5.653242	3.776626	-4.632154
39	6	0	6.080611	4.061415	-3.321982
40	6	0	5.713569	5.287121	-2.738012
41	6	0	4.985692	8.748172	-3.636006
42	6	0	0.040375	6.557845	-8.542818
43	6	0	4.888962	5.546218	-7.751723
44	6	0	0.262059	9.878841	-4.548449
45	1	0	-3.790513	4.405655	-6.163514
46	1	0	-1.555894	3.347508	-7.329662
47	1	0	-1.534360	7.656259	-1.731118
48	1	0	4.525541	6.104011	-0.659168
49	1	0	3.480585	0.749726	-6.906665
50	1	0	5.230354	7.627802	-1.827024
51	1	0	-3.727189	7.494894	-2.768738
52	1	0	-1.024015	9.225941	-2.964422
53	1	0	0.236950	0.581094	-6.934812
54	1	0	0.172005	6.560306	0.767088
55	1	0	5.163250	3.507243	-7.132980
56	1	0	5.516747	2.304876	-5.957770
57	1	0	6.530631	4.803067	-0.994395
58	1	0	7.101762	2.379324	-3.043418
59	1	0	-4.138294	5.464140	-3.387956
60	1	0	-1.220996	4.881718	-8.083345
61	1	0	3.956387	6.646438	-5.309039
62	1	0	2.278336	5.960252	-7.087900
63	1	0	0.641197	7.377951	-5.868641
64	1	0	2.439197	8.508071	-4.128389
65	1	0	6.063443	8.750191	-3.845317
66	1	0	4.469121	8.754342	-4.601283
67	1	0	4.746250	9.689465	-3.125629
68	1	0	0.444478	6.115676	-9.462018
69	1	0	-0.808712	7.193700	-8.825534
70	1	0	0.811195	7.214570	-8.127270
71	1	0	4.347490	6.468297	-7.517133
72	1	0	5.960691	5.777579	-7.701545
73	1	0	4.654840	5.283065	-8.791160
74	1	0	0.738759	10.666451	-3.951821
75	1	0	0.993860	9.530605	-5.284305
76	1	0	-0.563343	10.340687	-5.106225
77	6	0	5.373442	-0.403152	6.386957
78	8	0	0.758079	4.003620	7.300912
79	8	0	1.620523	5.816007	5.284465

80	6	0	5.451329	-1.784701	4.371395
81	8	0	3.870576	-2.255053	6.137111
82	8	0	7.017815	-1.444687	2.669083
83	8	0	4.971790	6.548644	1.859585
84	6	0	8.377325	0.676050	4.229372
85	8	0	2.018886	-0.532383	8.090202
86	6	0	4.731476	-0.076730	7.718778
87	8	0	2.230629	6.705348	2.749756
88	6	0	3.723651	1.046008	7.580537
89	8	0	4.887208	-2.833798	3.676303
90	6	0	7.104931	-0.010007	4.681280
91	6	0	7.006589	5.534800	3.453118
92	8	0	7.262235	4.957786	0.622005
93	8	0	8.734121	0.479047	1.483846
94	8	0	8.127374	2.447141	-0.308218
95	8	0	0.059167	1.342980	7.747413
96	6	0	6.552755	-1.045719	3.906061
97	6	0	3.518345	4.864498	7.110036
98	6	0	4.885412	-1.489498	5.629697
99	6	0	5.575239	5.568161	3.936614
100	6	0	3.235397	6.152495	3.515428
101	6	0	3.893756	5.224523	5.689905
102	6	0	4.577300	6.094516	3.091334
103	6	0	7.617335	3.078404	3.789725
104	6	0	1.375708	1.752664	7.621620
105	6	0	5.205214	5.128590	5.213044
106	6	0	3.136777	3.405818	7.245784
107	6	0	4.082313	2.373792	7.317921
108	6	0	2.356419	0.747119	7.759826
109	6	0	6.468272	0.313161	5.888143
110	6	0	7.371906	4.159072	2.934749
111	6	0	1.772886	3.072520	7.363869
112	6	0	2.904774	5.722453	4.815718
113	6	0	8.064440	1.840511	3.312892
114	6	0	7.504607	3.963138	1.546081
115	6	0	7.942355	2.731453	1.029615
116	6	0	8.248659	1.688271	1.925286
117	6	0	9.272634	1.103390	5.397405
118	6	0	4.599165	5.257965	8.123313
119	6	0	7.999359	6.016978	4.515644
120	6	0	5.766377	0.235823	8.805844
121	1	0	1.095562	4.874123	6.890232
122	1	0	0.985631	6.127404	4.554157
123	1	0	3.729179	-3.089819	5.563706
124	1	0	7.642453	-0.754657	2.251228
125	1	0	4.200690	7.005451	1.367496
126	1	0	8.975593	-0.080727	3.637229
127	1	0	1.021305	-0.668262	8.030933
128	1	0	4.170853	-1.004515	8.052588
129	1	0	2.233311	6.308303	1.799887
130	1	0	5.413501	-3.022611	2.821098
131	1	0	7.084643	6.264549	2.586569
132	1	0	6.719118	5.714873	1.044355
133	1	0	8.876120	0.481709	0.476020
134	1	0	7.913721	3.249115	-0.881661
135	1	0	-0.532003	2.136550	7.952260
136	1	0	2.601024	5.482638	7.368094
137	1	0	7.465408	3.206068	4.863130
138	1	0	5.973654	4.715333	5.869727
139	1	0	5.136238	2.615576	7.175674
140	1	0	6.856694	1.145555	6.478447
141	1	0	9.518947	0.244660	6.034823
142	1	0	10.216772	1.523857	5.028396
143	1	0	8.805540	1.861351	6.034504
144	1	0	5.530508	4.700009	7.983946
145	1	0	4.257836	5.063861	9.148327
146	1	0	4.837516	6.325846	8.048378
147	1	0	8.021139	5.369664	5.398290
148	1	0	7.742947	7.027772	4.857723
149	1	0	9.019165	6.050615	4.112305
150	1	0	6.486521	-0.584675	8.907207
151	1	0	5.273689	0.365448	9.777928
152	1	0	6.329949	1.151089	8.603493
153	6	0	3.472553	-4.768939	-5.415327
154	8	0	3.333805	-8.368440	-0.018715
155	8	0	4.864707	-6.697637	1.419782
156	6	0	2.644493	-2.489000	-5.714406
157	8	0	1.129078	-4.381892	-5.603792

158	8	0	4.085686	-0.661212	-5.882751
159	8	0	8.127628	-3.251360	1.335787
160	6	0	6.474409	-2.362873	-5.647353
161	8	0	0.784294	-6.790884	-3.742993
162	6	0	3.180748	-6.251022	-5.313584
163	8	0	6.160479	-4.651449	2.647037
164	6	0	3.232153	-6.727741	-3.877233
165	8	0	1.563960	-1.647264	-5.881683
166	6	0	5.058510	-2.899355	-5.572895
167	6	0	8.843505	-3.708259	-1.324003
168	8	0	8.146883	-1.019569	-0.358237
169	8	0	6.260375	0.212863	-4.555115
170	8	0	6.877240	0.839020	-2.000395
171	8	0	0.890048	-7.736715	-1.163359
172	6	0	3.970989	-2.018778	-5.714440
173	6	0	5.778985	-7.797824	-1.195558
174	6	0	2.396545	-3.868585	-5.577788
175	6	0	7.857348	-4.607701	-0.610507
176	6	0	6.489721	-5.041210	1.363332
177	6	0	6.322115	-6.527213	-0.573087
178	6	0	7.485655	-4.294906	0.712672
179	6	0	7.625388	-2.994931	-3.447621
180	6	0	2.029481	-7.502260	-1.880809
181	6	0	7.277802	-5.728093	-1.216261
182	6	0	4.482919	-7.510049	-1.922479
183	6	0	4.441157	-6.971983	-3.212864
184	6	0	2.025740	-6.981394	-3.195966
185	6	0	4.776587	-4.261211	-5.399562
186	6	0	8.080046	-2.696401	-2.156664
187	6	0	3.264275	-7.790410	-1.274692
188	6	0	5.883366	-6.129498	0.704735
189	6	0	6.982640	-2.048786	-4.255306
190	6	0	7.812941	-1.416817	-1.630237
191	6	0	7.184686	-0.435897	-2.418805
192	6	0	6.798664	-0.755361	-3.733615
193	6	0	7.412643	-3.292257	-6.422630
194	6	0	6.797133	-8.508997	-2.091811
195	6	0	9.871053	-4.489691	-2.146860
196	6	0	4.095976	-7.082008	-6.220473
197	1	0	2.418741	-8.356381	0.428902
198	1	0	4.438426	-7.511370	0.931505
199	1	0	0.434125	-3.638846	-5.725713
200	1	0	4.967520	-0.305264	-5.492940
201	1	0	7.741187	-3.080126	2.268670
202	1	0	6.443038	-1.390694	-6.225240
203	1	0	0.797504	-6.031653	-4.413511
204	1	0	2.125111	-6.414297	-5.692248
205	1	0	5.475738	-5.275899	3.036740
206	1	0	1.893954	-0.695416	-6.044391
207	1	0	9.428931	-3.142857	-0.538410
208	1	0	8.219467	-1.821754	0.277106
209	1	0	5.961833	1.030898	-4.021891
210	1	0	7.192096	1.005609	-1.047718
211	1	0	0.119788	-7.100680	-1.530283
212	1	0	5.549946	-8.515018	-0.349936
213	1	0	7.782429	-4.001032	-3.841360
214	1	0	7.586063	-5.992003	-2.230548
215	1	0	5.378635	-6.748239	-3.722012
216	1	0	5.607239	-4.956437	-5.264257
217	1	0	7.035910	-3.464048	-7.439204
218	1	0	8.413594	-2.851478	-6.509650
219	1	0	7.525404	-4.272638	-5.948239
220	1	0	7.076824	-7.916508	-2.968821
221	1	0	7.715330	-8.740045	-1.538441
222	1	0	6.384826	-9.457458	-2.461745
223	1	0	9.413260	-5.089551	-2.940265
224	1	0	10.587655	-3.809240	-2.624078
225	1	0	10.440454	-5.175295	-1.506163
226	1	0	5.150994	-7.006931	-5.940542
227	1	0	3.822150	-8.144041	-6.176161
228	1	0	4.007208	-6.758702	-7.264785
229	6	0	-6.024436	0.594770	-6.097697
230	8	0	-1.039035	-3.052126	-4.846882
231	8	0	-1.997561	-5.357393	-3.656303
232	6	0	-6.537853	2.356867	-4.471463
233	8	0	-4.732663	2.677635	-5.927521
234	8	0	-8.351094	2.154432	-2.973386
235	8	0	-6.081420	-6.376702	-1.211087

236	6	0	-9.143579	-0.410132	-4.073332
237	8	0	-2.615568	1.090156	-6.577933
238	6	0	-5.151530	0.093287	-7.231445
239	8	0	-3.434010	-6.454675	-1.247124
240	6	0	-4.066857	-0.804742	-6.673320
241	8	0	-6.280748	3.569745	-3.859006
242	6	0	-7.922652	0.340525	-4.565436
243	6	0	-7.703372	-5.222186	-3.187539
244	8	0	-7.936501	-4.546099	-0.345954
245	8	0	-9.233094	-0.052811	-1.308229
246	8	0	-8.630412	-2.029192	0.525876
247	8	0	-0.636906	-0.395904	-5.404420
248	6	0	-7.619747	1.593638	-3.994613
249	6	0	-3.405330	-4.503467	-5.861389
250	6	0	-5.750438	1.850411	-5.522600
251	6	0	-6.200073	-5.304158	-3.342507
252	6	0	-4.025231	-5.885909	-2.365802
253	6	0	-4.131804	-4.902288	-4.595926
254	6	0	-5.434478	-5.854594	-2.300526
255	6	0	-8.358508	-2.784172	-3.570864
256	6	0	-1.816488	-1.030357	-5.730378
257	6	0	-5.523452	-4.836974	-4.477328
258	6	0	-3.249146	-3.000935	-5.944133
259	6	0	-4.246712	-2.179680	-6.486135
260	6	0	-2.824359	-0.244252	-6.317276
261	6	0	-7.102394	-0.143127	-5.591360
262	6	0	-8.078915	-3.838823	-2.695021
263	6	0	-2.055770	-2.399557	-5.503963
264	6	0	-3.376430	-5.392424	-3.508152
265	6	0	-8.755687	-1.519883	-3.120394
266	6	0	-8.158296	-3.594704	-1.309059
267	6	0	-8.516672	-2.323754	-0.818805
268	6	0	-8.827895	-1.295081	-1.729960
269	6	0	-10.008808	-0.912080	-5.234083
270	6	0	-4.070910	-5.088886	-7.111982
271	6	0	-8.449989	-5.630601	-4.459302
272	6	0	-5.962810	-0.571585	-8.345812
273	1	0	-1.363052	-3.934440	-4.419633
274	1	0	-1.526701	-5.728376	-2.850289
275	1	0	-4.017675	2.153041	-6.443044
276	1	0	-8.846536	1.433276	-2.444125
277	1	0	-5.401732	-6.734730	-0.511963
278	1	0	-9.786295	0.320736	-3.491396
279	1	0	-1.736468	1.411024	-6.176893
280	1	0	-4.641442	0.990045	-7.698687
281	1	0	-2.453487	-6.218360	-1.186734
282	1	0	-5.707862	4.149185	-4.455885
283	1	0	-8.005967	-5.964507	-2.386249
284	1	0	-7.544705	-5.401497	-0.753809
285	1	0	-9.249030	0.010171	-0.293989
286	1	0	-8.316100	-2.814629	1.082829
287	1	0	0.013386	-1.072570	-4.982707
288	1	0	-2.367550	-4.955520	-5.818878
289	1	0	-8.280109	-2.957511	-4.645802
290	1	0	-6.104414	-4.414939	-5.298820
291	1	0	-5.196483	-2.631114	-6.779476
292	1	0	-7.315143	-1.125531	-6.016966
293	1	0	-9.484037	-1.627057	-5.875597
294	1	0	-10.330397	-0.077587	-5.869845
295	1	0	-10.911565	-1.410788	-4.858663
296	1	0	-4.102427	-6.184980	-7.054074
297	1	0	-3.508994	-4.821606	-8.015508
298	1	0	-5.099643	-4.741819	-7.249044
299	1	0	-8.192217	-6.658591	-4.745906
300	1	0	-8.215500	-4.987031	-5.313286
301	1	0	-9.535625	-5.591369	-4.305279
302	1	0	-5.309460	-0.881584	-9.171575
303	1	0	-6.706671	0.124081	-8.754699
304	1	0	-6.502337	-1.461256	-8.004504
305	6	0	-3.924288	5.202696	6.027212
306	8	0	-2.345718	8.385732	0.593430
307	8	0	-3.805337	6.692068	-1.141590
308	6	0	-3.260565	2.931151	6.659106
309	8	0	-1.659897	4.747665	6.637227
310	8	0	-4.806185	1.159996	6.686797
311	8	0	-6.958607	3.157062	-1.119437
312	6	0	-7.001775	2.884055	5.873949
313	8	0	-0.804648	6.753355	4.815843

314	6	0	-3.535570	6.657091	5.878191
315	8	0	-4.677669	4.388504	-2.122773
316	6	0	-3.220186	6.993473	4.436103
317	8	0	-2.243984	2.135474	7.120539
318	6	0	-5.581996	3.393609	6.021923
319	6	0	-8.388724	4.161617	1.136866
320	8	0	-8.160929	1.310095	0.519480
321	8	0	-6.976353	0.222628	5.022393
322	8	0	-7.535779	-0.559185	2.407288
323	8	0	-0.279645	7.656016	2.217602
324	6	0	-4.578721	2.494839	6.434539
325	6	0	-5.028901	8.010478	1.190882
326	6	0	-2.938453	4.284208	6.433389
327	6	0	-7.174214	4.874047	0.581966
328	6	0	-5.371416	4.940662	-1.075918
329	6	0	-5.542319	6.707764	0.606805
330	6	0	-6.529229	4.340834	-0.545648
331	6	0	-7.625794	3.471401	3.473903
332	6	0	-1.556595	7.522807	2.722242
333	6	0	-6.652172	6.044247	1.147111
334	6	0	-3.949050	7.713142	2.210436
335	6	0	-4.230839	7.271919	3.508022
336	6	0	-1.876031	7.068898	4.014977
337	6	0	-5.226260	4.731367	5.811192
338	6	0	-7.953722	3.129244	2.155957
339	6	0	-2.599631	7.877992	1.845353
340	6	0	-4.894533	6.139627	-0.508433
341	6	0	-7.299313	2.509586	4.436950
342	6	0	-7.889850	1.774121	1.786730
343	6	0	-7.561550	0.777599	2.726318
344	6	0	-7.277530	1.151638	4.054223
345	6	0	-8.033821	3.865269	6.438723
346	6	0	-6.140046	8.890522	1.770250
347	6	0	-9.440635	5.120009	1.702386
348	6	0	-4.585210	7.603491	6.470539
349	1	0	-1.338425	8.470276	0.426660
350	1	0	-3.240585	7.259286	-0.504946
351	1	0	-1.013584	3.971385	6.786678
352	1	0	-5.699886	0.853567	6.295402
353	1	0	-7.344121	3.321483	-2.056432
354	1	0	-7.089795	1.938613	6.494831
355	1	0	-1.105271	6.198315	5.623717
356	1	0	-2.589005	6.816021	6.481743
357	1	0	-5.138248	3.523138	-2.435735
358	1	0	-2.469771	1.141500	7.022770
359	1	0	-8.880487	3.614849	0.277607
360	1	0	-7.823934	1.973985	-0.189357
361	1	0	-6.992990	-0.720063	4.644965
362	1	0	-7.741352	-0.684470	1.409910
363	1	0	0.416207	7.508185	2.935630
364	1	0	-4.563144	8.604124	0.348150
365	1	0	-7.632573	4.523590	3.762112
366	1	0	-7.134853	6.460361	2.032958
367	1	0	-5.272898	7.148612	3.808241
368	1	0	-5.991257	5.434679	5.479580
369	1	0	-7.825391	4.086731	7.493023
370	1	0	-8.050211	4.818201	5.900387
371	1	0	-9.044408	3.440800	6.381720
372	1	0	-6.900087	9.113515	1.011258
373	1	0	-6.649372	8.425869	2.620906
374	1	0	-5.730422	9.847053	2.120440
375	1	0	-9.770842	5.834834	0.938786
376	1	0	-10.324981	4.566141	2.043548
377	1	0	-9.072133	5.696908	2.556955
378	1	0	-5.553025	7.532882	5.964100
379	1	0	-4.754322	7.379992	7.531686
380	1	0	-4.254189	8.647158	6.399267
381	6	0	-1.457553	-8.264234	2.692354
382	8	0	2.475395	-3.350129	4.267049
383	8	0	0.881008	-1.360075	6.102392
384	6	0	-2.785420	-8.463916	0.634988
385	8	0	-0.378223	-8.800688	0.641769
386	8	0	-5.127622	-8.091707	0.651685
387	8	0	-3.829510	-1.056159	6.472692
388	6	0	-5.161477	-7.633655	3.513050
389	8	0	1.533809	-6.955098	1.316704
390	6	0	-0.102727	-8.360287	3.359507
391	8	0	-1.421084	0.119530	6.023694

392	6	0	0.501936	-6.986877	3.562907
393	8	0	-2.745713	-8.769419	-0.699285
394	6	0	-3.879647	-7.913050	2.755091
395	6	0	-4.231282	-3.793326	6.730889
396	8	0	-5.636160	-2.094851	4.735798
397	8	0	-6.407752	-5.779281	1.834363
398	8	0	-6.595623	-3.083890	2.401857
399	8	0	2.855886	-4.657986	1.858312
400	6	0	-3.944754	-8.146044	1.367115
401	6	0	0.849233	-4.304786	6.317087
402	6	0	-1.549074	-8.510548	1.310258
403	6	0	-2.841380	-3.229298	6.514569
404	6	0	-1.436788	-1.243968	6.205079
405	6	0	-0.405987	-3.459047	6.311453
406	6	0	-2.695825	-1.834806	6.385945
407	6	0	-4.692098	-5.662342	5.062497
408	6	0	2.004189	-5.218502	2.794853
409	6	0	-1.686345	-4.016362	6.449779
410	6	0	0.993033	-5.060566	5.013560
411	6	0	0.341803	-6.272827	4.760222
412	6	0	1.302190	-6.418110	2.554050
413	6	0	-2.632554	-7.958143	3.389131
414	6	0	-4.791668	-4.312480	5.423471
415	6	0	1.840927	-4.540282	4.014060
416	6	0	-0.289022	-2.062094	6.184866
417	6	0	-5.240197	-6.168850	3.879522
418	6	0	-5.443944	-3.437467	4.533558
419	6	0	-5.976411	-3.906753	3.315638
420	6	0	-5.880390	-5.274075	2.998610
421	6	0	-5.326438	-8.566608	4.715515
422	6	0	0.909000	-5.226872	7.538594
423	6	0	-4.253906	-4.831998	7.856647
424	6	0	-0.165796	-9.178738	4.654233
425	1	0	3.088347	-3.080819	3.490920
426	1	0	1.702373	-1.957946	6.005961
427	1	0	-0.545210	-8.912235	-0.355941
428	1	0	-5.876945	-7.737736	1.249958
429	1	0	-3.625293	-0.077054	6.235988
430	1	0	-6.034609	-7.847833	2.817246
431	1	0	0.705331	-7.440226	0.915956
432	1	0	0.585024	-8.927958	2.662268
433	1	0	-0.488040	0.505592	6.214129
434	1	0	-3.516159	-8.321945	-1.187773
435	1	0	-4.899759	-2.946154	7.072215
436	1	0	-5.018952	-1.720005	5.465716
437	1	0	-6.810925	-5.035446	1.276286
438	1	0	-6.468118	-2.112357	2.678677
439	1	0	3.340373	-5.411145	1.367589
440	1	0	1.736208	-3.598689	6.400447
441	1	0	-4.174617	-6.349948	5.734570
442	1	0	-1.784388	-5.100773	6.518004
443	1	0	-0.308514	-6.687818	5.533649
444	1	0	-2.574233	-7.749040	4.457616
445	1	0	-6.268838	-8.367365	5.240467
446	1	0	-5.337360	-9.616290	4.395114
447	1	0	-4.515287	-8.461867	5.443728
448	1	0	0.884998	-4.643905	8.468308
449	1	0	0.071439	-5.930696	7.577296
450	1	0	1.834395	-5.815791	7.541377
451	1	0	-3.902040	-4.388847	8.797241
452	1	0	-5.272435	-5.202787	8.026127
453	1	0	-3.617110	-5.697530	7.647322
454	1	0	0.828711	-9.274569	5.106344
455	1	0	-0.830110	-8.736866	5.403500
456	1	0	-0.535858	-10.192006	4.449946
457	1	0	2.583459	3.017809	-3.826685
458	1	0	0.783426	1.380741	-4.385620
459	1	0	0.889915	-0.927368	-3.501768
460	1	0	4.782724	-4.438158	-1.289186
461	1	0	3.134265	-4.540789	-2.021665
462	1	0	3.312216	-4.341640	-0.256749
463	1	0	1.946824	-2.664985	-2.362413
464	1	0	3.508172	-0.333849	2.369812
465	1	0	5.083867	-0.667632	1.601202
466	1	0	3.902280	0.409262	0.797646
467	1	0	3.471388	-2.592794	1.335572
468	1	0	1.673507	-0.500200	-0.003394
469	1	0	1.488525	-3.507731	0.754457

470	1	0	-2.857280	-2.998582	0.452656
471	1	0	-2.880379	-4.174764	-0.883646
472	1	0	-0.886212	-4.346085	0.933216
473	1	0	-1.203764	-0.716541	0.040079
474	6	0	-2.004409	-2.191433	-1.378455
475	6	0	-0.845727	-1.477833	-0.674258
476	7	0	-0.165374	-2.551828	0.056043
477	8	0	4.387248	-1.962711	-0.439046
478	6	0	2.698094	-2.001107	-1.921481
479	6	0	2.626605	1.998803	-3.436943
480	6	0	-0.281834	-4.709314	-1.116223
481	8	0	0.677096	-4.305462	-1.768048
482	6	0	2.729923	-0.608702	-2.406783
483	8	0	-0.881513	-5.831830	-1.270454
484	6	0	1.118525	-2.550365	0.353838
485	6	0	2.033872	-1.514677	0.178939
486	6	0	3.415346	-1.690269	0.700771
487	7	0	3.747132	-2.643441	-1.412744
488	6	0	3.745614	-4.081460	-1.239389
489	6	0	3.698165	1.597343	-2.637787
490	1	0	-1.683696	-2.579695	-2.355807
491	6	0	-0.907750	-3.813062	-0.029991
492	6	0	-2.311130	-3.356770	-0.435208
493	6	0	1.616449	1.087714	-3.743247
494	6	0	1.671733	-0.207368	-3.235798
495	6	0	3.756727	0.306419	-2.123507
496	1	0	-0.139856	-0.991132	-1.362327
497	1	0	-2.859937	-1.521106	-1.536045
498	6	0	4.014632	-0.496985	1.408695
499	1	0	4.497676	2.300128	-2.392023
500	1	0	4.600822	0.006127	-1.502873

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.302865	7.979844	-3.239271
2	8	0	-2.887642	3.896190	-6.919547
3	8	0	-0.640659	2.017075	-7.514659
4	6	0	0.908874	7.025289	-1.058648
5	8	0	-1.350494	7.372703	-1.510093
6	8	0	3.139870	6.683852	-0.425932
7	8	0	4.071838	1.615634	-6.813664
8	6	0	4.131410	7.733354	-3.007236
9	8	0	-3.256258	7.400581	-3.589773
10	6	0	-0.766686	8.445274	-4.206682
11	8	0	1.601479	0.438652	-7.098216
12	6	0	-1.321630	7.248955	-4.953087
13	8	0	0.583744	6.459302	0.149237
14	6	0	2.662090	7.626962	-2.655919
15	6	0	4.517095	4.358207	-6.840563
16	8	0	6.035884	2.724828	-4.946720
17	8	0	5.644371	5.977075	-1.487379
18	8	0	6.615742	3.593794	-2.382597
19	8	0	-4.336053	5.060693	-4.859628
20	6	0	2.272880	7.116080	-1.400972
21	6	0	-0.454765	4.900485	-7.871578
22	6	0	-0.061222	7.471959	-1.979327
23	6	0	3.124349	3.786536	-7.003002
24	6	0	1.670651	1.814220	-7.126666
25	6	0	0.729873	4.053531	-7.457026
26	6	0	2.952306	2.386434	-6.972529
27	6	0	4.310595	6.002048	-4.890403
28	6	0	-3.107690	5.587930	-5.202620
29	6	0	2.002642	4.591528	-7.234795
30	6	0	-1.153222	5.516185	-6.680346
31	6	0	-0.628207	6.617188	-5.990800
32	6	0	-2.582781	6.736573	-4.586854
33	6	0	1.665955	8.026997	-3.554621
34	6	0	4.775223	4.786688	-5.410195
35	6	0	-2.391706	4.992768	-6.259617
36	6	0	0.569351	2.657437	-7.358322
37	6	0	4.610043	6.418264	-3.587492
38	6	0	5.541065	3.950633	-4.574492
39	6	0	5.870725	4.342103	-3.262579

40	6	0	5.387769	5.570215	-2.777594
41	6	0	4.454442	8.910268	-3.932637
42	6	0	-0.072135	5.959143	-8.911638
43	6	0	4.804662	5.488932	-7.833439
44	6	0	-0.291929	9.541884	-5.164258
45	1	0	-3.796712	3.642636	-6.541658
46	1	0	-1.400702	2.688803	-7.621650
47	1	0	-2.043108	7.384050	-2.260876
48	1	0	4.053112	6.430761	-0.805877
49	1	0	3.852503	0.619118	-6.870962
50	1	0	4.699219	7.923117	-2.047530
51	1	0	-4.152268	6.953012	-3.380260
52	1	0	-1.602923	8.900334	-3.596131
53	1	0	0.642887	0.118421	-7.094620
54	1	0	-0.387464	6.653661	0.392254
55	1	0	5.248560	3.525274	-7.085070
56	1	0	5.590157	2.386025	-5.800329
57	1	0	6.136539	5.245077	-0.969586
58	1	0	6.946173	2.731894	-2.810179
59	1	0	-4.353415	4.858849	-3.849424
60	1	0	-1.199773	4.209875	-8.379478
61	1	0	3.694420	6.646099	-5.519484
62	1	0	2.130484	5.674828	-7.267694
63	1	0	0.353863	6.998947	-6.276647
64	1	0	1.965268	8.399822	-4.536284
65	1	0	5.537453	8.985459	-4.096445
66	1	0	3.984772	8.817130	-4.917226
67	1	0	4.119236	9.857986	-3.493384
68	1	0	0.400203	5.495816	-9.786903
69	1	0	-0.961227	6.499899	-9.260598
70	1	0	0.626503	6.704393	-8.518450
71	1	0	4.155941	6.357942	-7.684864
72	1	0	5.841357	5.836469	-7.738532
73	1	0	4.663081	5.145883	-8.866224
74	1	0	0.083064	10.411349	-4.610256
75	1	0	0.506630	9.204835	-5.832932
76	1	0	-1.120917	9.885301	-5.796987
77	6	0	4.994806	0.389092	6.651734
78	8	0	0.053211	4.535812	7.087851
79	8	0	0.893296	6.288048	5.018297
80	6	0	5.344310	-1.129208	4.767761
81	8	0	3.656296	-1.588032	6.436867
82	8	0	6.998042	-0.778256	3.156574
83	8	0	4.350244	7.049626	1.705205
84	6	0	8.042496	1.580620	4.617515
85	8	0	1.543778	0.131211	8.163167
86	6	0	4.243530	0.744212	7.917255
87	8	0	1.561867	7.071213	2.465915
88	6	0	3.177699	1.789242	7.659488
89	8	0	4.942685	-2.284445	4.126998
90	6	0	6.808363	0.811068	5.040772
91	6	0	6.367536	6.263464	3.444867
92	8	0	6.784126	5.514337	0.675902
93	8	0	8.539842	1.230352	1.910386
94	8	0	7.863807	3.013434	-0.036963
95	8	0	-0.500426	1.859088	7.640010
96	6	0	6.410541	-0.329166	4.319502
97	6	0	2.761031	5.559301	6.974529
98	6	0	4.653546	-0.785750	5.948082
99	6	0	4.914838	6.228189	3.859918
100	6	0	2.564979	6.631696	3.303459
101	6	0	3.177739	5.868649	5.554281
102	6	0	3.926436	6.639948	2.942194
103	6	0	7.133926	3.886620	3.980506
104	6	0	0.792206	2.348123	7.555095
105	6	0	4.513955	5.834367	5.141411
106	6	0	2.464374	4.087729	7.171767
107	6	0	3.466316	3.122639	7.341793
108	6	0	1.824276	1.415135	7.789416
109	6	0	6.059323	1.162453	6.172823
110	6	0	6.850105	4.885368	3.042021
111	6	0	1.118739	3.676110	7.245889
112	6	0	2.202072	6.253110	4.611299
113	6	0	7.687549	2.654965	3.610904
114	6	0	7.056075	4.605584	1.676554
115	6	0	7.602524	3.377320	1.267024
116	6	0	7.943510	2.422572	2.245967
117	6	0	8.823282	2.152481	5.805628

118	6	0	3.767433	6.072238	8.010552
119	6	0	7.270080	6.886212	4.514827
120	6	0	5.184618	1.181728	9.046326
121	1	0	0.358693	5.409065	6.656110
122	1	0	0.276396	6.525251	4.246912
123	1	0	3.611660	-2.465499	5.912824
124	1	0	7.596996	-0.068602	2.726902
125	1	0	3.577656	7.426742	1.152075
126	1	0	8.739191	0.847197	4.108925
127	1	0	0.553994	-0.042335	8.122292
128	1	0	3.722715	-0.199720	8.269073
129	1	0	1.643378	6.635954	1.536520
130	1	0	5.539637	-2.473593	3.319342
131	1	0	6.439764	6.936838	2.533197
132	1	0	6.181185	6.262826	1.024354
133	1	0	8.711588	1.168011	0.905963
134	1	0	7.621901	3.754526	-0.677452
135	1	0	-1.148392	2.620024	7.796884
136	1	0	1.796224	6.129810	7.159359
137	1	0	6.928385	4.076622	5.035321
138	1	0	5.275504	5.508789	5.853129
139	1	0	4.509359	3.423687	7.235305
140	1	0	6.331737	2.067376	6.719957
141	1	0	9.104376	1.356995	6.507323
142	1	0	9.747957	2.635508	5.464641
143	1	0	8.253656	2.899676	6.367432
144	1	0	4.737407	5.569737	7.940580
145	1	0	3.392560	5.909249	9.029138
146	1	0	3.942243	7.148177	7.888377
147	1	0	7.290485	6.303946	5.441606
148	1	0	6.929660	7.897540	4.770970
149	1	0	8.304551	6.963619	4.157201
150	1	0	5.947118	0.417276	9.237504
151	1	0	4.623930	1.329942	9.977912
152	1	0	5.702179	2.119899	8.826426
153	6	0	4.196781	-4.768441	-5.147033
154	8	0	3.960509	-8.190510	0.342918
155	8	0	5.211013	-6.294246	1.854718
156	6	0	3.156333	-2.600101	-5.565016
157	8	0	1.843682	-4.645726	-5.522959
158	8	0	4.400559	-0.627929	-5.655663
159	8	0	8.191351	-2.588870	1.896852
160	6	0	6.932974	-2.054791	-5.206745
161	8	0	1.613942	-7.057353	-3.663427
162	6	0	4.061891	-6.270901	-5.027109
163	8	0	6.248741	-4.108961	3.110477
164	6	0	4.040944	-6.708457	-3.577510
165	8	0	2.022442	-1.869037	-5.856784
166	6	0	5.582399	-2.741660	-5.224184
167	6	0	9.124296	-3.049078	-0.695506
168	8	0	8.154187	-0.404907	0.123741
169	8	0	6.346940	0.495874	-4.194514
170	8	0	6.800794	1.272029	-1.654399
171	8	0	1.618230	-8.038593	-1.075679
172	6	0	4.420284	-1.988652	-5.465193
173	6	0	6.434280	-7.391089	-0.635537
174	6	0	3.046430	-3.994298	-5.412158
175	6	0	8.172888	-4.012311	-0.018229
176	6	0	6.695267	-4.501722	1.862070
177	6	0	6.802344	-6.053474	-0.026259
178	6	0	7.678013	-3.696431	1.263417
179	6	0	7.986717	-2.517674	-2.916178
180	6	0	2.765093	-7.607219	-1.686262
181	6	0	7.736127	-5.195069	-0.624637
182	6	0	5.190044	-7.271781	-1.488333
183	6	0	5.203138	-6.778792	-2.797787
184	6	0	2.814935	-7.101955	-3.004894
185	6	0	5.434823	-4.123113	-5.042540
186	6	0	8.329498	-2.138388	-1.611416
187	6	0	3.958083	-7.686432	-0.950058
188	6	0	6.230605	-5.653647	1.196618
189	6	0	7.303828	-1.663786	-3.791437
190	6	0	7.914241	-0.874479	-1.148630
191	6	0	7.237187	0.013545	-2.002255
192	6	0	6.949500	-0.387779	-3.319121
193	6	0	8.020937	-2.889929	-5.889625
194	6	0	7.592482	-8.033675	-1.406067
195	6	0	10.270168	-3.759029	-1.421418

196	6	0	5.136205	-7.015358	-5.828211
197	1	0	3.011667	-8.266649	0.678245
198	1	0	4.880099	-7.134444	1.344683
199	1	0	1.088725	-3.983572	-5.694542
200	1	0	5.079940	-0.157139	-5.038817
201	1	0	7.760282	-2.446811	2.808780
202	1	0	6.839256	-1.102182	-5.809747
203	1	0	1.641180	-6.370888	-4.409584
204	1	0	3.065802	-6.556437	-5.487387
205	1	0	5.573094	-4.762553	3.461019
206	1	0	2.275273	-0.877058	-5.939779
207	1	0	9.602226	-2.409773	0.105261
208	1	0	8.160167	-1.168880	0.801925
209	1	0	5.944347	1.289007	-3.696436
210	1	0	7.008041	1.478948	-0.682243
211	1	0	0.814044	-7.489412	-1.443794
212	1	0	6.199697	-8.093900	0.220747
213	1	0	8.264854	-3.513147	-3.265479
214	1	0	8.141562	-5.460711	-1.603859
215	1	0	6.148382	-6.446438	-3.227205
216	1	0	6.321190	-4.721985	-4.826638
217	1	0	7.741841	-3.117274	-6.926239
218	1	0	8.972139	-2.343950	-5.913665
219	1	0	8.202092	-3.843854	-5.383886
220	1	0	7.889776	-7.452512	-2.284998
221	1	0	8.476173	-8.147639	-0.766874
222	1	0	7.308157	-9.033033	-1.761682
223	1	0	9.921239	-4.419882	-2.221688
224	1	0	10.953091	-3.029852	-1.875664
225	1	0	10.853840	-4.370389	-0.721830
226	1	0	6.148107	-6.820249	-5.459999
227	1	0	4.974802	-8.099595	-5.777800
228	1	0	5.107581	-6.722027	-6.884697
229	6	0	-5.724934	-0.291577	-6.328829
230	8	0	-0.504585	-3.545770	-4.832144
231	8	0	-1.395418	-5.785244	-3.428258
232	6	0	-6.419725	1.515465	-4.823993
233	8	0	-4.560551	1.869056	-6.199793
234	8	0	-8.292373	1.282044	-3.406357
235	8	0	-5.473221	-6.926595	-1.019077
236	6	0	-8.858696	-1.392609	-4.377175
237	8	0	-2.321177	0.397242	-6.787325
238	6	0	-4.782710	-0.789452	-7.406931
239	8	0	-2.817113	-6.884699	-1.005611
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241	8	0	-6.270829	2.774644	-4.273607
242	6	0	-7.671141	-0.587736	-4.865089
243	6	0	-7.105336	-6.007216	-3.099213
244	8	0	-7.499919	-5.163020	-0.324690
245	8	0	-9.122684	-0.868709	-1.649291
246	8	0	-8.455543	-2.660746	0.340565
247	8	0	-0.276113	-0.889809	-5.511111
248	6	0	-7.475867	0.712196	-4.355637
249	6	0	-2.794043	-5.175542	-5.715789
250	6	0	-5.550275	1.004126	-5.806355
251	6	0	-5.596119	-5.992156	-3.210912
252	6	0	-3.415101	-6.393267	-2.158513
253	6	0	-3.526387	-5.533986	-4.441174
254	6	0	-4.825038	-6.436039	-2.122752
255	6	0	-7.918773	-3.657736	-3.677389
256	6	0	-1.404393	-1.617098	-5.809576
257	6	0	-4.921772	-5.548589	-4.356318
258	6	0	-2.722457	-3.676250	-5.902807
259	6	0	-3.762913	-2.949807	-6.495872
260	6	0	-2.453477	-0.929398	-6.447844
261	6	0	-6.777703	-1.069330	-5.828970
262	6	0	-7.598926	-4.625770	-2.719162
263	6	0	-1.561845	-2.983745	-5.510450
264	6	0	-2.770340	-5.914107	-3.310292
265	6	0	-8.436124	-2.403665	-3.333016
266	6	0	-7.759872	-4.297367	-1.357948
267	6	0	-8.246792	-3.033278	-0.972610
268	6	0	-8.596275	-2.096616	-1.965980
269	6	0	-9.628623	-2.035526	-5.535232
270	6	0	-3.391423	-5.884191	-6.936487
271	6	0	-7.780717	-6.558896	-4.356964
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274	1	0	-0.916081	-6.112585	-2.611991
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276	1	0	-8.769898	0.563228	-2.859221
277	1	0	-4.800304	-7.197722	-0.280405
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279	1	0	-1.450746	0.785850	-6.423803
280	1	0	-4.320913	0.115282	-7.907378
281	1	0	-1.840392	-6.642057	-0.962870
282	1	0	-5.702077	3.355654	-4.874969
283	1	0	-7.379058	-6.712043	-2.254552
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285	1	0	-9.201537	-0.743831	-0.644348
286	1	0	-8.103092	-3.373023	0.967303
287	1	0	0.427060	-1.498987	-5.062092
288	1	0	-1.732065	-5.560144	-5.618035
289	1	0	-7.775922	-3.894432	-4.733519
290	1	0	-5.506943	-5.212210	-5.213820
291	1	0	-4.685111	-3.471079	-6.758867
292	1	0	-6.911699	-2.082865	-6.211418
293	1	0	-9.024409	-2.752423	-6.100161
294	1	0	-9.976449	-1.272477	-6.243065
295	1	0	-10.511654	-2.571993	-5.164994
296	1	0	-3.363473	-6.973687	-6.803147
297	1	0	-2.820971	-5.647628	-7.843517
298	1	0	-4.433381	-5.606200	-7.122433
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305	6	0	-4.636316	5.325163	5.514814
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311	8	0	-7.117151	2.524499	-1.551154
312	6	0	-7.520487	2.765833	5.399682
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328	6	0	-5.670136	4.425866	-1.564849
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331	6	0	-8.069738	3.125530	2.937957
332	6	0	-2.289723	7.612706	2.174310
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334	6	0	-4.659402	7.556091	1.539606
335	6	0	-4.971154	7.185008	2.852088
336	6	0	-2.637588	7.225457	3.481339
337	6	0	-5.890763	4.742598	5.288621
338	6	0	-8.307933	2.664588	1.637049
339	6	0	-3.311009	7.811539	1.225503
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345	6	0	-8.648376	3.701949	5.844751
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350	1	0	-3.773686	6.963271	-1.085389
351	1	0	-1.667755	4.364153	6.430864

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355	1	0	-1.883387	6.547347	5.185908
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357	1	0	-5.232460	2.925267	-2.777436
358	1	0	-2.894363	1.442411	6.724137
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362	1	0	-7.788347	-1.166649	1.194614
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378	1	0	-6.429793	7.516950	5.221446
379	1	0	-5.706137	7.521675	6.832690
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381	6	0	-1.029930	-8.163118	3.319199
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446	1	0	-4.914525	-9.615888	4.912431
447	1	0	-4.219767	-8.338217	5.909411
448	1	0	0.892663	-3.805090	8.764792
449	1	0	0.197104	-5.239345	8.009593
450	1	0	1.947050	-4.995158	7.987984
451	1	0	-3.915430	-3.990917	8.937901
452	1	0	-5.204830	-4.956441	8.203697
453	1	0	-3.509708	-5.355636	7.894221
454	1	0	1.156665	-8.776385	5.951531
455	1	0	-0.539290	-8.296419	6.100391
456	1	0	-0.124069	-9.830944	5.333950
457	1	0	2.238062	2.992873	-4.065025
458	1	0	0.748804	1.058366	-4.582804
459	1	0	1.115973	-1.123217	-3.476049
460	1	0	5.540156	-3.824390	-1.110562
461	1	0	4.163187	-4.097435	-2.221995
462	1	0	3.871906	-4.051090	-0.470425
463	1	0	2.371539	-2.541049	-2.066318
464	1	0	3.268029	-0.408841	2.480400
465	1	0	4.993616	-0.365654	2.032204
466	1	0	3.801474	0.555614	1.074820
467	1	0	3.885052	-2.508741	1.315608
468	1	0	1.895335	-0.657503	0.062130
469	1	0	2.042016	-3.611238	0.852226
470	1	0	-2.333109	-3.420537	0.661647
471	1	0	-2.311572	-4.707823	-0.567434
472	1	0	-0.230085	-4.563744	1.187345
473	1	0	-0.883798	-1.131311	0.046202
474	6	0	-1.596715	-2.731078	-1.268187
475	6	0	-0.484992	-1.867911	-0.671052
476	7	0	0.334010	-2.837954	0.086612
477	8	0	4.790726	-1.527838	-0.277500
478	6	0	2.939493	-1.750315	-1.556929
479	6	0	2.397567	2.028886	-3.577401
480	6	0	0.358000	-5.089374	-0.842016
481	8	0	1.403015	-4.722374	-1.362961
482	6	0	2.791543	-0.436072	-2.293493
483	8	0	-0.262206	-6.185536	-1.035674
484	6	0	1.589403	-2.746363	0.333587
485	6	0	2.446396	-1.603603	-0.046003
486	6	0	3.779573	-1.573251	0.730222
487	7	0	4.319945	-2.179050	-1.429123
488	6	0	4.477986	-3.616495	-1.288036
489	6	0	3.444781	1.865067	-2.669050
490	1	0	-1.277268	-3.187730	-2.216254
491	6	0	-0.347082	-4.143945	0.175593
492	6	0	-1.787555	-3.818697	-0.209570
493	6	0	1.562123	0.952161	-3.860920
494	6	0	1.763240	-0.274724	-3.224753
495	6	0	3.646135	0.643370	-2.033465
496	1	0	0.137016	-1.339787	-1.403697
497	1	0	-2.503115	-2.140775	-1.456144
498	6	0	3.969234	-0.375588	1.633733
499	1	0	4.105719	2.703087	-2.437922
500	1	0	4.477210	0.516057	-1.335655

MC1a@CP_{6R-out}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	7.099046	2.294175	-5.279960
2	8	0	8.663098	3.573213	0.832920
3	8	0	6.299607	5.117809	1.161666
4	6	0	5.038731	1.112462	-5.890472
5	8	0	6.737621	-0.103345	-4.829698
6	8	0	3.315714	2.198520	-7.063264
7	8	0	2.922678	7.590446	-1.100643
8	6	0	4.734195	4.734324	-7.092098
9	8	0	8.680894	0.320327	-2.759521
10	6	0	8.500080	2.260283	-4.707713
11	8	0	3.734375	6.090753	1.036612
12	6	0	8.487907	2.627791	-3.238726
13	8	0	4.237031	-0.005358	-5.936714
14	6	0	5.293470	3.493266	-6.427094
15	6	0	4.515829	8.159532	-3.314996
16	8	0	1.629330	7.938668	-3.536281
17	8	0	1.940304	4.699439	-7.048336
18	8	0	0.405646	6.182219	-5.327907
19	8	0	8.722870	0.937738	0.084376
20	6	0	4.539249	2.302955	-6.458191
21	6	0	8.307293	5.705710	-0.927555
22	6	0	6.323710	1.119347	-5.311241
23	6	0	5.057904	7.372905	-2.141751
24	6	0	4.650452	6.332511	0.036628
25	6	0	6.864536	6.162998	-1.000843
26	6	0	4.198966	7.093032	-1.059589
27	6	0	4.571744	6.399097	-5.164898
28	6	0	8.678391	1.898871	-0.912953
29	6	0	6.370849	6.893224	-2.089838
30	6	0	8.426333	4.281245	-1.426734
31	6	0	8.370176	3.945543	-2.787091
32	6	0	8.609075	1.592871	-2.282642
33	6	0	6.550775	3.467001	-5.815276
34	6	0	3.844166	7.215760	-4.292615
35	6	0	8.597388	3.240345	-0.496250
36	6	0	5.978788	5.865054	0.052910
37	6	0	3.946760	5.564192	-6.099577
38	6	0	2.437591	7.152688	-4.330472
39	6	0	1.774582	6.305677	-5.235340
40	6	0	2.538438	5.520483	-6.123464
41	6	0	5.810825	5.563151	-7.800395
42	6	0	9.278162	6.642090	-1.653844
43	6	0	5.563927	9.040417	-3.998612
44	6	0	9.483924	3.128560	-5.500182
45	1	0	8.749345	2.732556	1.419761
46	1	0	7.188160	4.627607	1.059069
47	1	0	7.459214	-0.004049	-4.110307
48	1	0	2.862130	3.103943	-7.176060
49	1	0	2.375713	7.271728	-0.298925
50	1	0	4.016587	4.392129	-7.899572
51	1	0	8.637256	-0.396736	-2.005708
52	1	0	8.877789	1.196698	-4.795379
53	1	0	4.086361	5.373314	1.669904
54	1	0	4.787456	-0.847274	-5.753615
55	1	0	3.722875	8.860114	-2.904334
56	1	0	2.161319	8.303370	-2.742898
57	1	0	0.925629	4.689142	-6.934468
58	1	0	-0.049338	6.905475	-4.780804
59	1	0	9.547478	0.374513	0.009147
60	1	0	8.610619	5.721150	0.162420
61	1	0	5.661724	6.416351	-5.119322
62	1	0	7.037724	7.102215	-2.928719
63	1	0	8.226287	4.744006	-3.518372
64	1	0	7.134222	4.388113	-5.771954
65	1	0	5.359359	6.411278	-8.330725
66	1	0	6.554425	5.970820	-7.108368
67	1	0	6.346401	4.955296	-8.540237
68	1	0	9.199082	7.665616	-1.267113
69	1	0	10.314476	6.311413	-1.507389
70	1	0	9.100890	6.681056	-2.733436
71	1	0	5.106993	9.638301	-4.797718
72	1	0	6.019974	9.735033	-3.282374
73	1	0	6.371466	8.458069	-4.454536
74	1	0	9.235038	4.193694	-5.462058
75	1	0	10.502043	3.016940	-5.106701
76	1	0	9.501571	2.832421	-6.556466
77	6	0	-5.692184	-2.105652	-4.716428

78	8	0	-0.811286	-6.078670	-5.890575
79	8	0	0.917351	-4.028366	-6.397207
80	6	0	-5.596103	-0.746298	-2.684051
81	8	0	-5.771628	-3.067482	-2.443838
82	8	0	-5.384916	1.649899	-2.882564
83	8	0	1.483847	0.724976	-7.077182
84	6	0	-5.361019	1.623490	-5.672593
85	8	0	-4.985483	-5.476554	-3.625356
86	6	0	-5.857365	-3.468941	-5.355782
87	8	0	2.449363	-1.780237	-6.015602
88	6	0	-4.505498	-4.131308	-5.528870
89	8	0	-5.630410	-0.574929	-1.318051
90	6	0	-5.468562	0.339312	-4.874950
91	6	0	-1.000386	1.012722	-8.258284
92	8	0	0.099545	3.079599	-6.471615
93	8	0	-4.078105	3.668095	-4.256310
94	8	0	-1.424333	4.300224	-4.536058
95	8	0	-2.519616	-6.704698	-3.795782
96	6	0	-5.479643	0.423374	-3.465844
97	6	0	-1.461852	-4.066678	-7.879250
98	6	0	-5.681967	-1.998462	-3.314020
99	6	0	-0.498955	-0.343776	-7.810740
100	6	0	1.235504	-1.647515	-6.672562
101	6	0	-0.734073	-2.775349	-7.583501
102	6	0	0.762931	-0.425752	-7.180359
103	6	0	-3.135471	1.322234	-6.893830
104	6	0	-2.839516	-5.751125	-4.737561
105	6	0	-1.219179	-1.526291	-7.995762
106	6	0	-2.395982	-4.409144	-6.738260
107	6	0	-3.630748	-3.775834	-6.562385
108	6	0	-4.099054	-5.132390	-4.624780
109	6	0	-5.563899	-0.926654	-5.465412
110	6	0	-1.801292	1.666111	-7.150378
111	6	0	-2.005069	-5.394490	-5.812365
112	6	0	0.480654	-2.820662	-6.871505
113	6	0	-3.909444	1.975200	-5.926948
114	6	0	-1.210293	2.663048	-6.351648
115	6	0	-1.952667	3.334717	-5.367423
116	6	0	-3.310663	3.003002	-5.167927
117	6	0	-6.171068	1.585124	-6.973484
118	6	0	-2.182177	-4.061613	-9.229762
119	6	0	-1.786074	0.953928	-9.572647
120	6	0	-6.637503	-3.422104	-6.674168
121	1	0	-0.223785	-5.687241	-6.633425
122	1	0	1.827950	-3.921925	-5.915953
123	1	0	-5.396316	-3.925424	-2.849866
124	1	0	-5.292143	1.567530	-1.861501
125	1	0	2.470393	0.570474	-6.833760
126	1	0	-5.800880	2.447692	-5.032939
127	1	0	-4.602346	-6.202112	-3.026818
128	1	0	-6.467788	-4.105476	-4.648780
129	1	0	2.590197	-1.006921	-5.386878
130	1	0	-5.544330	-1.468091	-0.861569
131	1	0	-0.091883	1.657051	-8.458142
132	1	0	0.703246	2.309803	-6.754432
133	1	0	-3.520093	4.327965	-3.718320
134	1	0	-0.455727	4.494717	-4.776117
135	1	0	-1.509648	-6.883144	-3.798514
136	1	0	-0.671501	-4.881567	-7.938242
137	1	0	-3.590326	0.516591	-7.471364
138	1	0	-2.189984	-1.478552	-8.493723
139	1	0	-3.921380	-2.980293	-7.250642
140	1	0	-5.541655	-0.996916	-6.554033
141	1	0	-7.223842	1.359275	-6.773290
142	1	0	-6.127242	2.557456	-7.480330
143	1	0	-5.798193	0.836540	-7.679461
144	1	0	-1.483275	-3.836674	-10.045287
145	1	0	-2.986982	-3.320147	-9.274683
146	1	0	-2.632576	-5.040564	-9.435958
147	1	0	-2.702699	0.361564	-9.490828
148	1	0	-1.176498	0.516137	-10.372183
149	1	0	-2.079717	1.962120	-9.891580
150	1	0	-7.624137	-2.967304	-6.528592
151	1	0	-6.789027	-4.434073	-7.070185
152	1	0	-6.121130	-2.844853	-7.448575
153	6	0	-1.268601	7.617932	3.787943
154	8	0	-5.272171	2.548338	4.508152
155	8	0	-6.396327	2.351121	1.935756

156	6	0	0.953302	7.654708	2.749359
157	8	0	0.600777	6.837181	5.017435
158	8	0	1.267028	8.475027	0.561941
159	8	0	-6.244749	4.531806	-2.281993
160	6	0	-1.511583	9.327989	0.355006
161	8	0	-1.108265	4.583626	5.655913
162	6	0	-2.120530	7.269834	4.989555
163	8	0	-6.510593	2.239411	-0.764928
164	6	0	-2.902854	5.996660	4.744774
165	8	0	2.297218	7.402476	2.918776
166	6	0	-0.979521	8.558392	1.546023
167	6	0	-5.831588	7.071079	-1.185957
168	8	0	-4.217066	6.015511	-3.405082
169	8	0	-0.258498	8.131382	-1.828379
170	8	0	-1.561242	6.598257	-3.691437
171	8	0	-2.715746	2.333803	5.474650
172	6	0	0.390318	8.231238	1.595867
173	6	0	-6.339459	4.889957	3.418342
174	6	0	0.116367	7.366858	3.845118
175	6	0	-6.028131	5.857628	-0.301691
176	6	0	-6.321386	3.439800	-0.117458
177	6	0	-6.217340	4.808582	1.910591
178	6	0	-6.182825	4.591942	-0.905398
179	6	0	-3.638421	8.142118	-0.426903
180	6	0	-3.142764	3.577959	5.063044
181	6	0	-6.050993	5.936668	1.095576
182	6	0	-4.964216	4.864182	4.049309
183	6	0	-4.175746	6.013812	4.161300
184	6	0	-2.372579	4.754512	5.143714
185	6	0	-1.791349	8.205027	2.630260
186	6	0	-4.350252	7.351953	-1.338122
187	6	0	-4.449786	3.647739	4.542257
188	6	0	-6.297394	3.547789	1.290258
189	6	0	-2.277161	8.426328	-0.586242
190	6	0	-3.654269	6.807708	-2.434189
191	6	0	-2.284097	7.071621	-2.625114
192	6	0	-1.598448	7.865473	-1.686158
193	6	0	-2.324273	10.551726	0.790911
194	6	0	-7.173798	6.089238	3.877718
195	6	0	-6.617686	8.291926	-0.699768
196	6	0	-3.017082	8.440701	5.407812
197	1	0	-4.801159	1.717487	4.851239
198	1	0	-6.265491	2.445083	2.941636
199	1	0	1.612691	6.747743	4.998746
200	1	0	0.753959	8.724838	-0.289696
201	1	0	-6.051400	3.589389	-2.619806
202	1	0	-0.618499	9.726535	-0.221982
203	1	0	-0.515432	5.397600	5.493876
204	1	0	-1.426357	7.078115	5.863686
205	1	0	-6.659291	1.481507	-0.065353
206	1	0	2.800836	7.472330	2.037664
207	1	0	-6.238016	6.816264	-2.211779
208	1	0	-5.150098	5.684105	-3.131364
209	1	0	0.140340	7.566380	-2.582945
210	1	0	-2.107753	5.916575	-4.228965
211	1	0	-1.821910	2.393117	5.949009
212	1	0	-6.893734	3.964301	3.766617
213	1	0	-4.164727	8.555928	0.434327
214	1	0	-5.937892	6.913660	1.568090
215	1	0	-4.573649	6.960244	3.790513
216	1	0	-2.862734	8.403486	2.575547
217	1	0	-1.718104	11.220352	1.414861
218	1	0	-2.663082	11.124726	-0.081262
219	1	0	-3.212443	10.282531	1.371505
220	1	0	-8.181055	6.049671	3.444702
221	1	0	-7.282321	6.089767	4.969769
222	1	0	-6.730030	7.048088	3.592132
223	1	0	-6.309061	8.621287	0.298059
224	1	0	-6.478541	9.140581	-1.381216
225	1	0	-7.690737	8.071378	-0.654222
226	1	0	-2.410657	9.320444	5.658380
227	1	0	-3.715447	8.741209	4.620336
228	1	0	-3.610000	8.181907	6.293759
229	6	0	7.563563	1.788887	5.133449
230	8	0	2.219093	5.092093	5.551420
231	8	0	0.484616	3.572424	7.212090
232	6	0	7.544471	0.178883	3.280394
233	8	0	7.554361	2.447791	2.751476

234	8	0	7.613628	-2.133936	3.642181
235	8	0	0.388166	-1.194168	8.102640
236	6	0	7.523457	-1.788155	6.563360
237	8	0	6.573406	4.890862	3.623866
238	6	0	7.601426	3.227592	5.610756
239	8	0	-0.919825	1.182936	7.113119
240	6	0	6.186730	3.765366	5.690383
241	8	0	7.519895	-0.124950	1.939557
242	6	0	7.547475	-0.626497	5.589040
243	6	0	3.041847	-1.201455	8.974845
244	8	0	2.060846	-3.272561	7.159702
245	8	0	6.394944	-4.000287	5.308414
246	8	0	3.719479	-4.685725	5.512038
247	8	0	3.935828	5.664354	3.493108
248	6	0	7.562397	-0.886490	4.202629
249	6	0	3.131759	3.799930	8.030093
250	6	0	7.554031	1.505425	3.755632
251	6	0	2.382386	0.051796	8.442081
252	6	0	0.398799	1.166308	7.525573
253	6	0	2.429799	2.460688	7.994769
254	6	0	1.040478	0.010299	8.010150
255	6	0	5.256050	-1.495184	7.714311
256	6	0	4.349452	4.958219	4.595814
257	6	0	3.057475	1.276583	8.395146
258	6	0	4.014343	3.969961	6.811582
259	6	0	5.333601	3.497699	6.766831
260	6	0	5.694106	4.550369	4.629103
261	6	0	7.534773	0.705527	6.021246
262	6	0	3.914948	-1.847661	7.919513
263	6	0	3.514469	4.651881	5.687748
264	6	0	1.090890	2.391836	7.561638
265	6	0	6.082990	-2.185450	6.820101
266	6	0	3.376917	-2.880130	7.130983
267	6	0	4.184952	-3.616815	6.244818
268	6	0	5.544043	-3.281071	6.113899
269	6	0	8.291388	-1.509892	7.857743
270	6	0	3.899583	4.015094	9.338899
271	6	0	3.805715	-0.941259	10.277969
272	6	0	8.363715	3.406730	6.926612
273	1	0	1.577847	4.587054	6.164036
274	1	0	-0.481632	3.421969	6.927689
275	1	0	7.210617	3.358160	3.069523
276	1	0	7.396110	-2.868398	4.315504
277	1	0	-0.575066	-1.132579	7.762580
278	1	0	8.042493	-2.663030	6.066837
279	1	0	6.118897	5.491328	2.930525
280	1	0	8.161736	3.830951	4.835594
281	1	0	-1.110434	0.406120	6.467299
282	1	0	7.384285	0.727727	1.404801
283	1	0	2.219059	-1.935579	9.233057
284	1	0	1.456788	-2.559441	7.571491
285	1	0	5.897553	-4.728027	4.797315
286	1	0	2.708790	-4.795640	5.646828
287	1	0	2.931430	5.870115	3.550499
288	1	0	2.337636	4.605906	7.994442
289	1	0	5.673167	-0.656743	8.274134
290	1	0	4.105749	1.312424	8.699110
291	1	0	5.711775	2.906568	7.602159
292	1	0	7.508110	0.907372	7.093670
293	1	0	9.336012	-1.251484	7.644004
294	1	0	8.293606	-2.396814	8.504258
295	1	0	7.860687	-0.686405	8.436726
296	1	0	3.222672	3.949896	10.200184
297	1	0	4.366865	5.007698	9.357581
298	1	0	4.693459	3.277125	9.491254
299	1	0	4.233903	-1.872026	10.670702
300	1	0	3.135875	-0.533313	11.045478
301	1	0	4.628716	-0.230661	10.152053
302	1	0	7.894605	2.878595	7.763132
303	1	0	8.417137	4.468327	7.200211
304	1	0	9.391844	3.034843	6.836153
305	6	0	3.228260	-7.254566	-3.973031
306	8	0	7.385908	-2.571673	-5.391349
307	8	0	8.543485	-2.039026	-2.964196
308	6	0	1.177823	-6.762421	-2.736760
309	8	0	1.501202	-5.965866	-5.001930
310	8	0	0.869770	-7.427735	-0.530413
311	8	0	7.942271	-3.364953	1.577672

312	6	0	3.527781	-8.734692	-0.430062
313	8	0	3.294216	-4.709666	-6.634458
314	6	0	4.011890	-7.167520	-5.264399
315	8	0	8.449534	-1.345566	-0.427967
316	6	0	4.900198	-5.940816	-5.249542
317	8	0	-0.077978	-6.190277	-2.745343
318	6	0	2.987389	-8.014083	-1.649688
319	6	0	7.651235	-6.045803	0.967332
320	8	0	5.872737	-4.769289	2.937689
321	8	0	2.236475	-7.617593	1.779977
322	8	0	3.269909	-5.623705	3.308134
323	8	0	4.919033	-2.455671	-6.595480
324	6	0	1.708145	-7.427027	-1.613436
325	6	0	8.321440	-4.774982	-3.939960
326	6	0	1.953233	-6.654836	-3.906261
327	6	0	7.856749	-5.014593	-0.120348
328	6	0	8.221179	-2.677721	-0.740902
329	6	0	8.170162	-4.409865	-2.477997
330	6	0	8.009997	-3.657754	0.243966
331	6	0	5.560289	-7.338599	0.281605
332	6	0	5.271127	-3.622700	-5.954307
333	6	0	7.924208	-5.356044	-1.475712
334	6	0	6.968007	-4.788998	-4.620424
335	6	0	6.129884	-5.909794	-4.583758
336	6	0	4.476888	-4.783898	-5.931012
337	6	0	3.723046	-7.904548	-2.837037
338	6	0	6.182695	-6.390898	1.106435
339	6	0	6.529225	-3.645698	-5.318788
340	6	0	8.299727	-3.060091	-2.095240
341	6	0	4.232041	-7.738784	0.470150
342	6	0	5.415287	-5.766636	2.108172
343	6	0	4.083354	-6.160300	2.340867
344	6	0	3.516894	-7.163522	1.536047
345	6	0	4.416541	-9.930652	-0.782236
346	6	0	9.092027	-6.082813	-4.143062
347	6	0	8.518334	-7.292277	0.757301
348	6	0	4.792840	-8.445243	-5.580693
349	1	0	6.924736	-1.747160	-5.768493
350	1	0	8.377847	-2.306689	-3.939184
351	1	0	0.558028	-5.581585	-4.828426
352	1	0	1.370379	-7.583585	0.355977
353	1	0	8.039406	-2.366540	1.778689
354	1	0	2.645230	-9.153114	0.139772
355	1	0	2.746275	-5.565992	-6.506895
356	1	0	3.255409	-7.036660	-6.102372
357	1	0	7.641723	-0.950935	0.026357
358	1	0	-0.452031	-6.165963	-1.795865
359	1	0	7.991443	-5.586403	1.944242
360	1	0	6.615068	-4.219476	2.496279
361	1	0	1.771620	-7.038168	2.486726
362	1	0	3.719153	-4.801838	3.733142
363	1	0	3.947652	-2.498919	-6.911102
364	1	0	8.939232	-3.962493	-4.432393
365	1	0	6.131823	-7.783362	-0.534308
366	1	0	7.791882	-6.402054	-1.760631
367	1	0	6.449727	-6.790128	-4.024027
368	1	0	4.721036	-8.345238	-2.879452
369	1	0	3.872666	-10.650725	-1.406251
370	1	0	5.321128	-9.640330	-1.326560
371	1	0	4.737235	-10.455010	0.127145
372	1	0	9.235003	-6.287635	-5.211665
373	1	0	10.085089	-6.025057	-3.679865
374	1	0	8.579208	-6.947911	-3.710675
375	1	0	8.282353	-7.822440	-0.170582
376	1	0	9.581183	-7.021929	0.719094
377	1	0	8.385615	-8.002574	1.582935
378	1	0	5.297079	-8.364385	-6.551911
379	1	0	5.563393	-8.663952	-4.833851
380	1	0	4.122448	-9.312863	-5.623351
381	6	0	-5.130710	-2.442184	5.158675
382	8	0	-7.073783	-4.243114	-0.653421
383	8	0	-4.805812	-5.884788	-1.170321
384	6	0	-3.009339	-1.227892	5.346541
385	8	0	-4.814516	-0.153323	4.301455
386	8	0	-1.137530	-2.164812	6.415335
387	8	0	-1.099437	-8.066003	0.889936
388	6	0	-2.591855	-4.668260	6.997067
389	8	0	-7.290931	-0.743150	2.739690

390	6	0	-6.584277	-2.472609	4.737326
391	8	0	-2.220248	-6.821840	-1.287043
392	6	0	-6.701551	-2.962521	3.308083
393	8	0	-2.196519	-0.141688	5.128187
394	6	0	-3.201885	-3.501097	6.247940
395	6	0	-2.341344	-8.278514	3.376205
396	8	0	0.535146	-7.898197	3.485643
397	8	0	0.158090	-4.739348	7.065826
398	8	0	1.734936	-6.283293	5.415575
399	8	0	-7.521661	-1.685552	-0.135684
400	6	0	-2.445061	-2.335603	6.013388
401	6	0	-6.471983	-6.205517	1.240525
402	6	0	-4.355899	-1.289958	4.926327
403	6	0	-3.035865	-7.624358	2.204666
404	6	0	-2.967308	-6.904160	-0.135144
405	6	0	-5.010117	-6.591509	1.180756
406	6	0	-2.356187	-7.526138	0.973781
407	6	0	-2.433462	-6.411817	5.124077
408	6	0	-7.177324	-2.458040	0.969153
409	6	0	-4.346543	-7.142059	2.283520
410	6	0	-6.629117	-4.753854	1.636355
411	6	0	-6.483294	-4.297043	2.953912
412	6	0	-7.055770	-2.031693	2.304094
413	6	0	-4.525293	-3.532823	5.793666
414	6	0	-1.693395	-7.251061	4.281756
415	6	0	-6.948775	-3.810982	0.646450
416	6	0	-4.292704	-6.442623	-0.022609
417	6	0	-1.816603	-5.561903	6.049558
418	6	0	-0.287671	-7.171190	4.319099
419	6	0	0.368553	-6.341515	5.246067
420	6	0	-0.409310	-5.556356	6.118821
421	6	0	-3.614935	-5.473954	7.805078
422	6	0	-7.296722	-7.128268	2.144943
423	6	0	-3.264278	-9.210364	4.168587
424	6	0	-7.470054	-3.287463	5.685804
425	1	0	-7.086701	-3.440885	-1.303027
426	1	0	-5.658155	-5.349921	-0.988114
427	1	0	-5.675945	-0.322574	3.782354
428	1	0	-0.668055	-3.052119	6.568247
429	1	0	-0.766412	-8.047607	-0.078282
430	1	0	-1.865118	-4.239941	7.751863
431	1	0	-7.610800	-0.112113	1.993035
432	1	0	-6.971740	-1.408720	4.779719
433	1	0	-2.761050	-6.391562	-2.039172
434	1	0	-2.703675	0.598566	4.651164
435	1	0	-1.516098	-8.932008	2.946712
436	1	0	-0.008544	-8.337971	2.739217
437	1	0	1.164435	-4.879772	7.120049
438	1	0	2.223800	-6.678501	4.619120
439	1	0	-7.488374	-0.716777	0.098100
440	1	0	-6.893912	-6.328038	0.197056
441	1	0	-3.522494	-6.424144	5.061830
442	1	0	-4.877653	-7.220286	3.233653
443	1	0	-6.188821	-5.008616	3.727731
444	1	0	-5.113759	-4.438365	5.953777
445	1	0	-4.352900	-5.976866	7.172082
446	1	0	-3.111762	-6.250891	8.395593
447	1	0	-4.159599	-4.827962	8.504565
448	1	0	-7.184935	-8.176121	1.838640
449	1	0	-7.003484	-7.060851	3.197537
450	1	0	-8.362947	-6.877894	2.086616
451	1	0	-4.082975	-8.674093	4.659078
452	1	0	-3.711646	-9.967569	3.512734
453	1	0	-2.706668	-9.736821	4.953572
454	1	0	-7.370158	-2.927593	6.717947
455	1	0	-8.526069	-3.194060	5.405475
456	1	0	-7.224669	-4.354244	5.683174
457	1	0	-15.606148	2.182689	-0.695401
458	1	0	-13.955064	3.181251	0.887137
459	1	0	-12.116248	1.777866	1.809827
460	1	0	-10.591917	-3.212420	2.738226
461	1	0	-9.533210	-1.797808	2.316066
462	1	0	-9.670186	-3.211059	1.210580
463	1	0	-10.935571	-0.172656	2.021249
464	1	0	-11.681633	-4.199162	-1.559848
465	1	0	-12.234706	-3.220506	-2.955913
466	1	0	-10.695589	-4.138472	-3.035024
467	1	0	-9.714766	-2.627132	-1.212944

468	1	0	-11.812355	-0.793479	-2.533791
469	1	0	-9.291417	-0.497587	-0.681833
470	1	0	-9.797008	4.275106	-0.376084
471	1	0	-11.060796	3.267743	0.372181
472	1	0	-8.576980	2.309500	-1.127693
473	1	0	-11.386159	1.509371	-3.083742
474	6	0	-11.159251	3.304026	-1.813097
475	6	0	-11.420270	1.812399	-2.027713
476	7	0	-10.326064	1.148803	-1.293383
477	8	0	-11.998183	-2.814242	0.509572
478	6	0	-11.614861	-0.729153	1.376113
479	6	0	-14.803230	1.570964	-0.280511
480	6	0	-9.095830	1.525815	0.831185
481	8	0	-9.790342	1.756200	1.809041
482	6	0	-12.741345	-0.014673	0.786945
483	8	0	-8.068179	0.765586	0.769770
484	6	0	-10.131475	-0.131308	-1.278364
485	6	0	-10.935285	-1.098289	-1.959072
486	6	0	-10.614341	-2.403414	-1.800986
487	7	0	-11.347625	-2.000981	1.219892
488	6	0	-10.200694	-2.577784	1.934272
489	6	0	-14.702070	0.220999	-0.621296
490	1	0	-12.095377	3.875863	-1.792540
491	6	0	-9.497412	2.128202	-0.536746
492	6	0	-10.389291	3.358226	-0.491397
493	6	0	-13.878769	2.129352	0.605219
494	6	0	-12.856992	1.346490	1.133767
495	6	0	-13.685875	-0.576049	-0.095045
496	1	0	-12.378229	1.485137	-1.595487
497	1	0	-10.537859	3.698302	-2.631546
498	6	0	-11.357430	-3.546694	-2.383627
499	1	0	-15.431095	-0.222876	-1.301714
500	1	0	-13.607120	-1.630256	-0.349301

TS2a@CP_{6R}-out

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.374832	2.174321	-5.043137
2	8	0	8.842664	3.134381	1.151047
3	8	0	6.545717	4.776220	1.481552
4	6	0	5.272750	1.124770	-5.745785
5	8	0	6.881635	-0.216827	-4.696039
6	8	0	3.635928	2.342270	-6.911899
7	8	0	3.354735	7.502748	-0.758576
8	6	0	5.183275	4.800284	-6.812740
9	8	0	8.794245	0.026084	-2.567189
10	6	0	8.757313	2.046573	-4.439964
11	8	0	4.034965	5.879018	1.333457
12	6	0	8.725898	2.357114	-2.958127
13	8	0	4.416183	0.052845	-5.853643
14	6	0	5.661609	3.507811	-6.183490
15	6	0	5.032083	8.081518	-2.906861
16	8	0	2.145066	8.015714	-3.209710
17	8	0	2.391751	4.906580	-6.842620
18	8	0	0.885634	6.396274	-5.103046
19	8	0	8.793774	0.530583	0.299920
20	6	0	4.848326	2.360435	-6.277377
21	6	0	8.635088	5.348325	-0.530758
22	6	0	6.541831	1.043138	-5.138162
23	6	0	5.503987	7.222169	-1.754479
24	6	0	4.988234	6.115504	0.367529
25	6	0	7.218637	5.878968	-0.620720
26	6	0	4.603638	6.941389	-0.706702
27	6	0	5.051194	6.395123	-4.825020
28	6	0	8.821315	1.530107	-0.659487
29	6	0	6.790237	6.676315	-1.690145
30	6	0	8.698131	3.940144	-1.083532
31	6	0	8.660539	3.660596	-2.457173
32	6	0	8.772123	1.281224	-2.041553
33	6	0	6.900461	3.393290	-5.544754
34	6	0	4.341332	7.212567	-3.938982
35	6	0	8.794894	2.856816	-0.191612
36	6	0	6.291485	5.582745	0.397280
37	6	0	4.411318	5.630346	-5.808301

38	6	0	2.934918	7.222355	-4.015001
39	6	0	2.255639	6.446452	-4.970235
40	6	0	3.003731	5.659117	-5.869873
41	6	0	6.318603	5.600128	-7.460150
42	6	0	9.669078	6.262860	-1.195187
43	6	0	6.139592	8.935956	-3.527553
44	6	0	9.803616	2.893497	-5.173378
45	1	0	8.873735	2.268501	1.705626
46	1	0	7.412705	4.248479	1.381725
47	1	0	7.589293	-0.182270	-3.957246
48	1	0	3.232691	3.273858	-7.003138
49	1	0	2.771265	7.178983	0.015020
50	1	0	4.471877	4.526059	-7.651059
51	1	0	8.693188	-0.716381	-1.844311
52	1	0	9.083205	0.969258	-4.561220
53	1	0	4.333258	5.118348	1.943043
54	1	0	4.918054	-0.822953	-5.692115
55	1	0	4.263652	8.803550	-2.486862
56	1	0	2.672394	8.321039	-2.388853
57	1	0	1.374753	4.938720	-6.752842
58	1	0	0.450737	7.113228	-4.531533
59	1	0	9.587835	-0.073989	0.217662
60	1	0	8.910006	5.306480	0.566024
61	1	0	6.138968	6.355133	-4.751014
62	1	0	7.488606	6.885760	-2.502863
63	1	0	8.573832	4.492873	-3.159179
64	1	0	7.528759	4.280640	-5.452324
65	1	0	5.924160	6.489563	-7.967786
66	1	0	7.062087	5.943065	-6.733764
67	1	0	6.843465	4.994700	-8.209545
68	1	0	9.629595	7.273296	-0.769940
69	1	0	10.683854	5.875738	-1.036919
70	1	0	9.522216	6.352248	-2.276358
71	1	0	5.733406	9.587632	-4.311867
72	1	0	6.610112	9.577345	-2.772174
73	1	0	6.929212	8.332829	-3.987820
74	1	0	9.607645	3.967676	-5.098171
75	1	0	10.804386	2.714488	-4.760847
76	1	0	9.833179	2.638348	-6.240032
77	6	0	-5.634519	-1.576670	-4.943909
78	8	0	-0.935714	-5.753447	-6.151774
79	8	0	0.905884	-3.776217	-6.539433
80	6	0	-5.503513	-0.287870	-2.867706
81	8	0	-5.824688	-2.603075	-2.706863
82	8	0	-5.142030	2.097401	-2.990111
83	8	0	1.741753	0.958652	-7.053019
84	6	0	-5.086321	2.156244	-5.775588
85	8	0	-5.129133	-5.024905	-3.960379
86	6	0	-5.855515	-2.909541	-5.628727
87	8	0	2.544217	-1.626218	-6.046877
88	6	0	-4.534845	-3.633673	-5.796908
89	8	0	-5.548030	-0.152666	-1.499579
90	6	0	-5.273559	0.854985	-5.021679
91	6	0	-0.695654	1.418142	-8.274000
92	8	0	0.460834	3.356414	-6.380545
93	8	0	-3.742186	4.079504	-4.252442
94	8	0	-1.051333	4.581840	-4.438140
95	8	0	-2.724639	-6.371471	-4.123269
96	6	0	-5.304014	0.896204	-3.611401
97	6	0	-1.436017	-3.638731	-8.075598
98	6	0	-5.650028	-1.512896	-3.538456
99	6	0	-0.277830	0.022520	-7.862017
100	6	0	1.355777	-1.408251	-6.727671
101	6	0	-0.648468	-2.398715	-7.719472
102	6	0	0.962332	-0.147546	-7.206710
103	6	0	-2.848314	1.790073	-6.954760
104	6	0	-2.972813	-5.366021	-5.032832
105	6	0	-1.056020	-1.112630	-8.100992
106	6	0	-2.412626	-3.973041	-6.968281
107	6	0	-3.617702	-3.284040	-6.795092
108	6	0	-4.202292	-4.688396	-4.923887
109	6	0	-5.427093	-0.385168	-5.653574
110	6	0	-1.491486	2.072981	-7.163430
111	6	0	-2.095198	-5.011654	-6.073104
112	6	0	0.544547	-2.532003	-6.982269
113	6	0	-3.613557	2.444890	-5.982706
114	6	0	-0.872351	3.006107	-6.311128
115	6	0	-1.605962	3.678182	-5.320559

116	6	0	-2.984141	3.410799	-5.168741
117	6	0	-5.864191	2.197455	-7.095811
118	6	0	-2.124618	-3.548629	-9.439761
119	6	0	-1.447522	1.445216	-9.609039
120	6	0	-6.604784	-2.783397	-6.959756
121	1	0	-0.311845	-5.364476	-6.865411
122	1	0	1.807023	-3.733251	-6.032429
123	1	0	-5.498232	-3.466315	-3.137836
124	1	0	-5.081285	1.980325	-1.970001
125	1	0	2.709259	0.743640	-6.781909
126	1	0	-5.503079	2.980167	-5.120032
127	1	0	-4.799941	-5.793948	-3.385054
128	1	0	-6.511925	-3.535255	-4.953745
129	1	0	2.704567	-0.886603	-5.383535
130	1	0	-5.615044	-1.061916	-1.066832
131	1	0	0.249630	2.020597	-8.427749
132	1	0	1.030995	2.565854	-6.674841
133	1	0	-3.166740	4.682562	-3.669095
134	1	0	-0.068300	4.734151	-4.645851
135	1	0	-1.726243	-6.603014	-4.113049
136	1	0	-0.687562	-4.491294	-8.147844
137	1	0	-3.328079	1.031642	-7.574562
138	1	0	-2.011212	-0.996306	-8.617600
139	1	0	-3.850667	-2.448226	-7.457085
140	1	0	-5.388317	-0.423296	-6.743068
141	1	0	-6.931277	2.016801	-6.926656
142	1	0	-5.761811	3.181616	-7.569941
143	1	0	-5.510613	1.453126	-7.815937
144	1	0	-1.397224	-3.331594	-10.232030
145	1	0	-2.889383	-2.765294	-9.473706
146	1	0	-2.620062	-4.494892	-9.690285
147	1	0	-2.395098	0.898795	-9.571170
148	1	0	-0.839829	1.003955	-10.407968
149	1	0	-1.680918	2.477632	-9.898850
150	1	0	-7.570032	-2.283307	-6.817569
151	1	0	-6.799598	-3.773713	-7.389603
152	1	0	-6.044530	-2.209474	-7.705405
153	6	0	-0.955388	7.557766	4.026091
154	8	0	-5.239855	2.687212	4.465649
155	8	0	-6.290977	2.647178	1.840445
156	6	0	1.290886	7.515503	3.041950
157	8	0	0.838352	6.629263	5.265983
158	8	0	1.703184	8.403176	0.897551
159	8	0	-5.919002	4.980460	-2.283160
160	6	0	-1.020155	9.412081	0.660481
161	8	0	-1.008059	4.454034	5.798319
162	6	0	-1.854429	7.210236	5.192896
163	8	0	-6.294419	2.643415	-0.869489
164	6	0	-2.695233	5.989980	4.881531
165	8	0	2.614993	7.185266	3.232565
166	6	0	-0.560070	8.568661	1.831451
167	6	0	-5.409266	7.450521	-1.076290
168	8	0	-3.789672	6.390736	-3.292800
169	8	0	0.227472	8.237162	-1.538343
170	8	0	-1.101885	6.843814	-3.489765
171	8	0	-2.729841	2.301027	5.494376
172	6	0	0.788835	8.166324	1.899932
173	6	0	-6.146294	5.119328	3.422636
174	6	0	0.412295	7.230005	4.105236
175	6	0	-5.691234	6.216203	-0.245765
176	6	0	-6.095297	3.807516	-0.168022
177	6	0	-5.988684	5.090877	1.916187
178	6	0	-5.889696	4.984027	-0.903631
179	6	0	-3.184248	8.373104	-0.222042
180	6	0	-3.074922	3.579680	5.112345
181	6	0	-5.746769	6.241318	1.152233
182	6	0	-4.792962	4.995777	4.089402
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184	6	0	-2.244967	4.708762	5.254451
185	6	0	-1.416731	8.217078	2.881161
186	6	0	-3.911422	7.656845	-1.181004
187	6	0	-4.359961	3.738497	4.557407
188	6	0	-6.112136	3.860880	1.243676
189	6	0	-1.806059	8.590107	-0.335292
190	6	0	-3.214926	7.116381	-2.278817
191	6	0	-1.828033	7.315179	-2.424637
192	6	0	-1.128109	8.036440	-1.439154
193	6	0	-1.779771	10.658604	1.126657

194	6	0	-6.928080	6.343306	3.909681
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196	6	0	-2.700539	8.409804	5.634596
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202	1	0	-0.092800	9.785650	0.122284
203	1	0	-0.365762	5.235896	5.670862
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205	1	0	-6.471565	1.856300	-0.205192
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207	1	0	-5.801610	7.257377	-2.120734
208	1	0	-4.743191	6.089179	-3.052626
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220	1	0	-7.920691	6.379567	3.444073
221	1	0	-7.070876	6.304711	4.996771
222	1	0	-6.422771	7.286464	3.678724
223	1	0	-5.843441	8.965597	0.456264
224	1	0	-5.942106	9.557460	-1.204967
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227	1	0	-3.362990	8.774363	4.843102
228	1	0	-3.327714	8.149538	6.496099
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236	6	0	7.290314	-2.379177	6.637848
237	8	0	6.740598	4.441952	3.938485
238	6	0	7.637885	2.658806	5.884349
239	8	0	-1.013162	0.989911	7.127584
240	6	0	6.249029	3.261633	5.951435
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242	6	0	7.397020	-1.184225	5.710518
243	6	0	2.785832	-1.661557	8.969071
244	8	0	1.748043	-3.610667	7.051842
245	8	0	6.085263	-4.481062	5.270242
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256	6	0	4.498391	4.580636	4.859444
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259	6	0	5.357521	2.997164	6.997120
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275	1	0	7.320546	2.903892	3.340321
276	1	0	7.167624	-3.365428	4.345953
277	1	0	-0.794794	-1.369230	7.690709
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284	1	0	1.169310	-2.883416	7.475207
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293	1	0	9.099399	-1.976052	7.780510
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295	1	0	7.634466	-1.367197	8.559927
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312	6	0	3.142215	-8.843618	-0.716093
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318	6	0	2.665608	-8.048887	-1.916128
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326	6	0	1.751068	-6.549276	-4.135323
327	6	0	7.637499	-5.357691	-0.160966
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330	6	0	7.847162	-4.025046	0.260073
331	6	0	5.222332	-7.578896	0.096717
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337	6	0	3.432860	-7.927823	-3.082115
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353	1	0	7.901853	-2.796642	1.844837
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356	1	0	3.082237	-6.906491	-6.317588
357	1	0	7.612895	-1.295829	0.137063
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359	1	0	7.694289	-6.014320	1.881887
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366	1	0	7.544684	-6.676176	-1.855873
367	1	0	6.235174	-6.906051	-4.162224
368	1	0	4.408975	-8.415141	-3.121902
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370	1	0	4.910366	-9.798801	-1.610960
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374	1	0	8.345941	-7.185164	-3.809248
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377	1	0	7.979644	-8.431364	1.434093
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381	6	0	-5.355783	-2.384691	4.968662
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408	6	0	-7.246666	-2.094070	0.732586
409	6	0	-4.715699	-6.969746	1.883368
410	6	0	-6.861922	-4.450173	1.296027
411	6	0	-6.742541	-4.072255	2.640453
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414	6	0	-2.121072	-7.295060	3.938163
415	6	0	-7.091954	-3.440806	0.346292
416	6	0	-4.565172	-6.176446	-0.387632
417	6	0	-2.202038	-5.683491	5.779332
418	6	0	-0.714039	-7.281265	4.003426
419	6	0	-0.039143	-6.524236	4.978045
420	6	0	-0.797487	-5.743790	5.871919
421	6	0	-4.027811	-5.592715	7.506449
422	6	0	-7.658998	-6.811874	1.660910
423	6	0	-3.786002	-9.164700	3.705805
424	6	0	-7.738324	-3.164871	5.397385
425	1	0	-7.178983	-2.967001	-1.585328
426	1	0	-5.830634	-4.954166	-1.334612
427	1	0	-5.764938	-0.182855	3.665050

428	1	0	-0.955845	-3.254242	6.438627
429	1	0	-1.123509	-7.955302	-0.427277
430	1	0	-2.224047	-4.437950	7.538871
431	1	0	-7.536672	0.221005	1.870218
432	1	0	-7.146554	-1.262641	4.603896
433	1	0	-2.981006	-6.112997	-2.360444
434	1	0	-2.793574	0.564593	4.642863
435	1	0	-1.995690	-8.926438	2.537874
436	1	0	-0.456627	-8.384527	2.374808
437	1	0	0.786460	-5.177872	6.925054
438	1	0	1.811388	-6.920373	4.371293
439	1	0	-7.463933	-0.281638	-0.033069
440	1	0	-7.161250	-5.933079	-0.230511
441	1	0	-3.925708	-6.421340	4.723940
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443	1	0	-6.519781	-4.838878	3.384827
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446	1	0	-3.571018	-6.416861	8.069936
447	1	0	-4.556836	-4.954146	8.224397
448	1	0	-7.595647	-7.845037	1.297051
449	1	0	-7.387925	-6.819780	2.721516
450	1	0	-8.708253	-6.499182	1.594803
451	1	0	-4.590119	-8.607722	4.197296
452	1	0	-4.252464	-9.871401	3.008240
453	1	0	-3.276039	-9.749414	4.481802
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456	1	0	-7.524964	-4.237787	5.352127
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462	1	0	-9.504277	-1.193334	1.108727
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465	1	0	-13.119136	-2.875719	-1.741091
466	1	0	-11.629349	-3.169241	-2.681033
467	1	0	-10.237496	-2.367120	-0.774480
468	1	0	-12.403189	-0.420301	-1.750879
469	1	0	-9.460405	-0.287288	-0.768793
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471	1	0	-10.408109	3.841694	-0.153258
472	1	0	-8.319245	2.171974	-1.608969
473	1	0	-11.770090	1.700108	-3.033523
474	6	0	-10.825905	3.552785	-2.267468
475	6	0	-11.422677	2.157923	-2.095395
476	7	0	-10.311919	1.392727	-1.537519
477	8	0	-11.833481	-2.379479	0.578264
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484	6	0	-10.387899	0.127008	-1.180838
485	6	0	-11.508447	-0.704083	-1.192111
486	6	0	-11.314203	-2.135642	-0.818542
487	7	0	-11.601062	-1.279801	1.333815
488	6	0	-10.267037	-1.202984	1.904223
489	6	0	-15.851723	-0.984349	0.188448
490	1	0	-11.592089	4.338130	-2.273408
491	6	0	-9.234865	2.261328	-0.996925
492	6	0	-9.857466	3.654109	-1.086234
493	6	0	-15.526576	1.407101	0.230767
494	6	0	-14.170095	1.211273	0.473791
495	6	0	-14.494358	-1.186672	0.421314
496	1	0	-12.264084	2.156428	-1.381494
497	1	0	-10.275923	3.606845	-3.219628
498	6	0	-12.055123	-3.142726	-1.669579
499	1	0	-16.513306	-1.846301	0.090514
500	1	0	-14.093230	-2.195021	0.509136

