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# Supporting Information

## The Hexameric Resorcinarene Capsule as a Hydrogen Bonding Catalyst in the Conjugate Addition of Pyrroles and Indoles to Nitroalkenes

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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 $^{1}H$ NMR and by TLC on Merck silica gel plates (0.25 mm) and visualized by UV light and spraying with H2SO4-Ce(SO4)2 or phosphomolybdic acid. Flash chromatography was performed on Merck silica gel (60, 40-63 μm). NMR spectra were recorded on Bruker Avance-600 spectrometer [600.13 MHz ($^{1}H$) and 150.03 MHz ($^{13}C$)], Bruker Avance-400 spectrometer [400 ($^{1}H$) and 100.57 MHz ($^{13}C$)], Bruker Avance-300 spectrometer [300 ($^{1}H$) and 75.48 MHz ($^{13}C$)], or Bruker Avance-250 spectrometer [250 ($^{1}H$) 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). DOSY experiments were performed on a Bruker Avance-600 spectrometer equipped with 5 mm PABBO BB|19F-1H\D Z-GRD Z114607/0109. The standard Bruker pulse program, ledbpgp2s, employing a double stimulated echo sequence and LED, bipolar gradient pulses for diffusion, and two spoil gradients were utilized. Diffusion times were 150 ms, eddy current delay was 5 ms, gradient recovery delays were 0.2 ms, and gradient pulse was 1400 ms. Individual rows of the quasi-2D diffusion databases were phased and baseline corrected. NOESY experiments were performed on Bruker Avance 400 and Bruker Avance 600 spectrometers with a D8 value range from 50 to 250 ms.

High-resolution mass spectra (HRMS) were acquired using a Bruker Solaris XR Fourier transform ion cyclotron resonance mass spectrometer equipped with a 7 T refrigerated actively-shielded superconducting magnet. The samples were ionized in positive ion mode using the ESI ion source (Bruker Daltonik GmbH, Bremen, Germany). The mass range was set to *m/z* 200-3000. The mass spectra were calibrated externally using a NaTFA solution in positive ion mode. Low resolution mass spectral analyses were carried out using an electrospray spectrometer Waters 4 micro

quadrupole. A linear calibration was applied. All final compounds purity was determined by elemental analysis on a Flash EA 1112 Series with Thermal Conductivity Detector, for C, H, N, and S. The final compounds were found to be >95% when analyzed. Resorcinarene was synthesized according to literature procedures.[1,2] Water saturated deuterated chloroform was prepared as reported in the literature.[3]

## 2. General Procedure

Resorcinarene **1** (281.6 mg, 254.7 μmol, 1.56 equiv.) was weighed in a 4 mL vial. Then, 1.1 mL of water-saturated chloroform was added, and the mixture was homogenized in an ultrasonic water bath at 40 °C for 10 min. To this clear yellow solution, the nucleophile (654.4 μmol, 4 equiv.) was added, and the solution was stirred at 50 °C for 10 minutes. Later, the electrophile (162.6 μmol, 1.0 equiv.) was added, and the reaction system was vigorously stirred (1400 rpm) at 50 °C for the appropriate time. The reaction was monitored by $^1$H NMR analysis taking aliquots of the reaction mixture (50 μL) at various time intervals and diluting with chloroform-d. The reaction was stopped pouring the solution in a 50 mL Eppendorf conical tube and diluting with 0.13% (v/v) DMSO in *n*-hexane (35 mL). The tube was placed in a freezer at −20 °C for at least 3 hrs and successively centrifugated at 1750 rpm for 10 minutes. The diluted reaction mixture was subjected three times to this process of centrifugation/dilution with *n*-hexane. Finally, the clear solution was removed and concentrated under reduced pressure. The oily residue thus obtained was purified by flash chromatography on silica gel to afford the desired title compounds. Regioisomeric ratios were determined by $^1$H NMR analysis via integration of proton signals of the title compounds in comparison with literature data.[4,5,6]

The compounds $\alpha$-**4a-e**[4], $\beta$-**4**[5], $\alpha$-**5a**[6], $\beta$-**7a**[6], $\beta$-**8a**[6] were previously described.

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[1] T.M. Bruer, Q. Zhang, K. Tiefenbacher, *Angew. Chem. Int. Ed.* **2016**, *55*, 7698-7701.
[2] Q. Zhang, K. Tiefenbacher, L. Catti, J. Pleiss, *J. Am. Chem. Soc.*, **2017**, *139*, 11482–11492
[3] G. La Sorella, L. Sperni, G. Strukul, A. Scarso, *Adv. Synth. Catal*. **2016**, *358*, 3443-3449.
[4] M. De Rosa, A, Soriente, *Tetrahedron,* **2010**, *66,* 2981-2986.
[5] N. Takenaka, R. S. Sarangthem, S. K. Seeria, *Org. Lett*, **2007**, *9*, 2819-2822.
[6] C. Lin, J. Hsu, M.N.V. Sastry, H. Fang, Z. Tu, J. T. Liu, Y. Ching-Fa, *Tetrahedron,* **2005**, *61,* 11751-11757.

## 3. Control experiments

### *3.1. Evidence of trace amounts of HCl/DCl in the $^1$H-NMR spectra of a solution of capsule C*

The capsule **C** was prepared in water saturated $CDCl_3$ (purchased from Sigma Aldrich) and freshly prepared HCl-saturated $CDCl_3$ (prepared according to the literature),[7] and $^1$H-NMR spectra were compared. The sharp signals in water saturated untreated $CDCl_3$ solution of **C** was a first evidence of the absence of trace amounts of HCl/DCl.

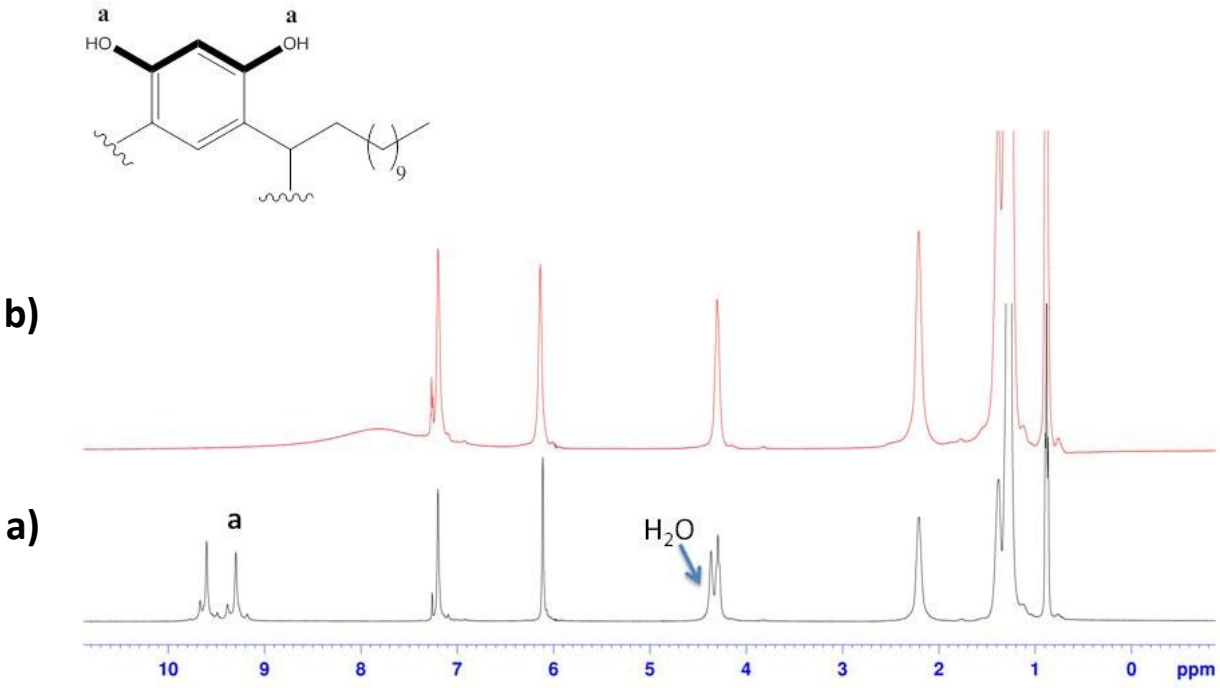



**Figure S1.** $^1$H-NMR spectra (400 MHz, $CDCl_3$, 298 K) of **C** in a) water saturated untreated $CDCl_3$ (5.0 mM), b) freshly prepared HCl-saturated $CDCl_3$ (5.0 mM).

[7] J. M. Köster, K. Tiefenbacher, *ChemCatChem* **2018**, *10*, 2941-2944.

### *3.2 Preparation of the capsule C in different batches of $CDCl_3$*

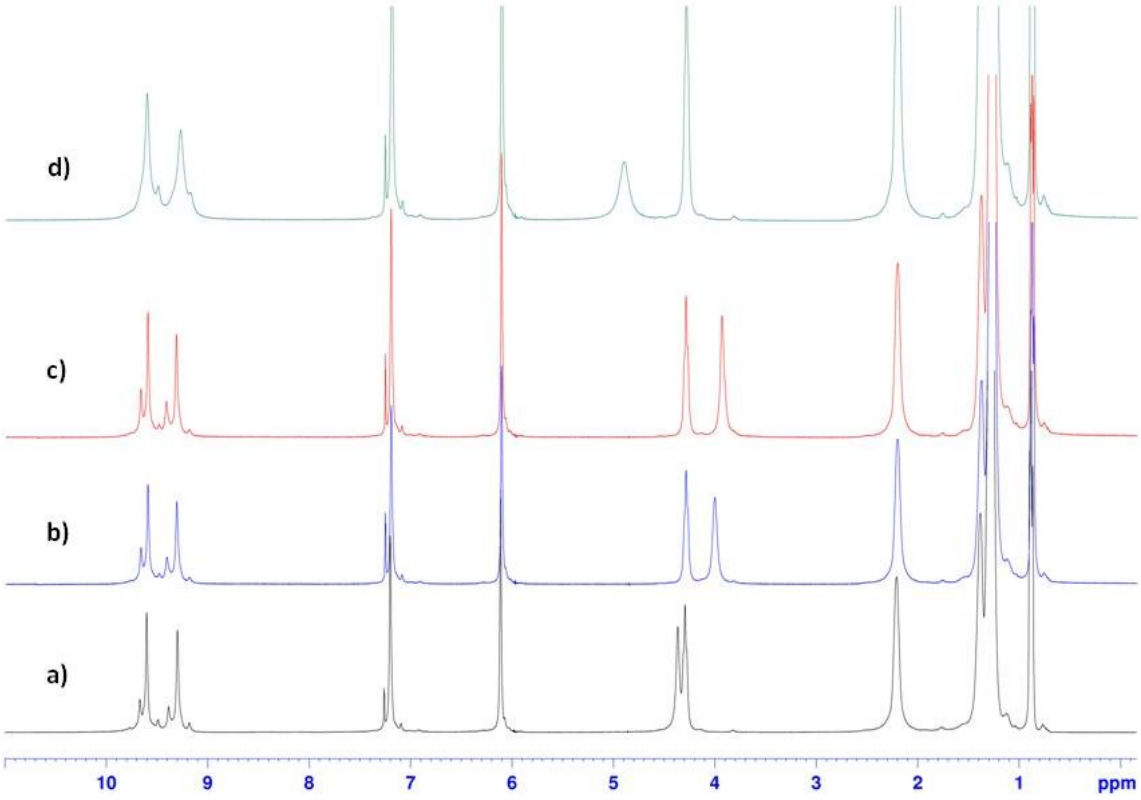



**Figure S2.** $^1$H-NMR spectra (400 MHz, $CDCl_3$, 298 K) of **C** (5mM) in: a) $CDCl_3$ from Sigma Aldrich just opened amber bottle without any treatment; b) $CDCl_3$ from Sigma Aldrich filtered through basic aluminium oxide layer ($Al_2O_3$); c) $CDCl_3$ from Sigma Aldrich stored in an amber bottle over 3 Å molecular sieves and freshly filtered through basic aluminium oxide layer ($Al_2O_3$); d) $CDCl_3$ from Euriso-top GmbH without any treatment.

### 3.3 *Influence of DCl-traces on the reaction outcome*

*3.3.1* In order to rule out a background reaction promoted by HCl from photodegradation of $CDCl_3$, the model reaction between *N*-methylpyrrole **2** and β-nitrostyrene **3a** was carried out in the absence of **C**. In the first experiment, **2** (654.4

µmol, 4 equiv.) and **3a** (162.6 µmol, 1.0 equiv) were dissolved in 1.1 mL of water saturated chloroform-d without any treatment. In the second experiment, the reaction was performed under identical conditions but using freshly prepared HCl-saturated $CDCl_3$ (1.1mL). The reactions was kept at 50 °C and observed by $^1$H-NMR spectra. In both cases, they did not show any conversion into products **4a**, even after prolonged reaction time.

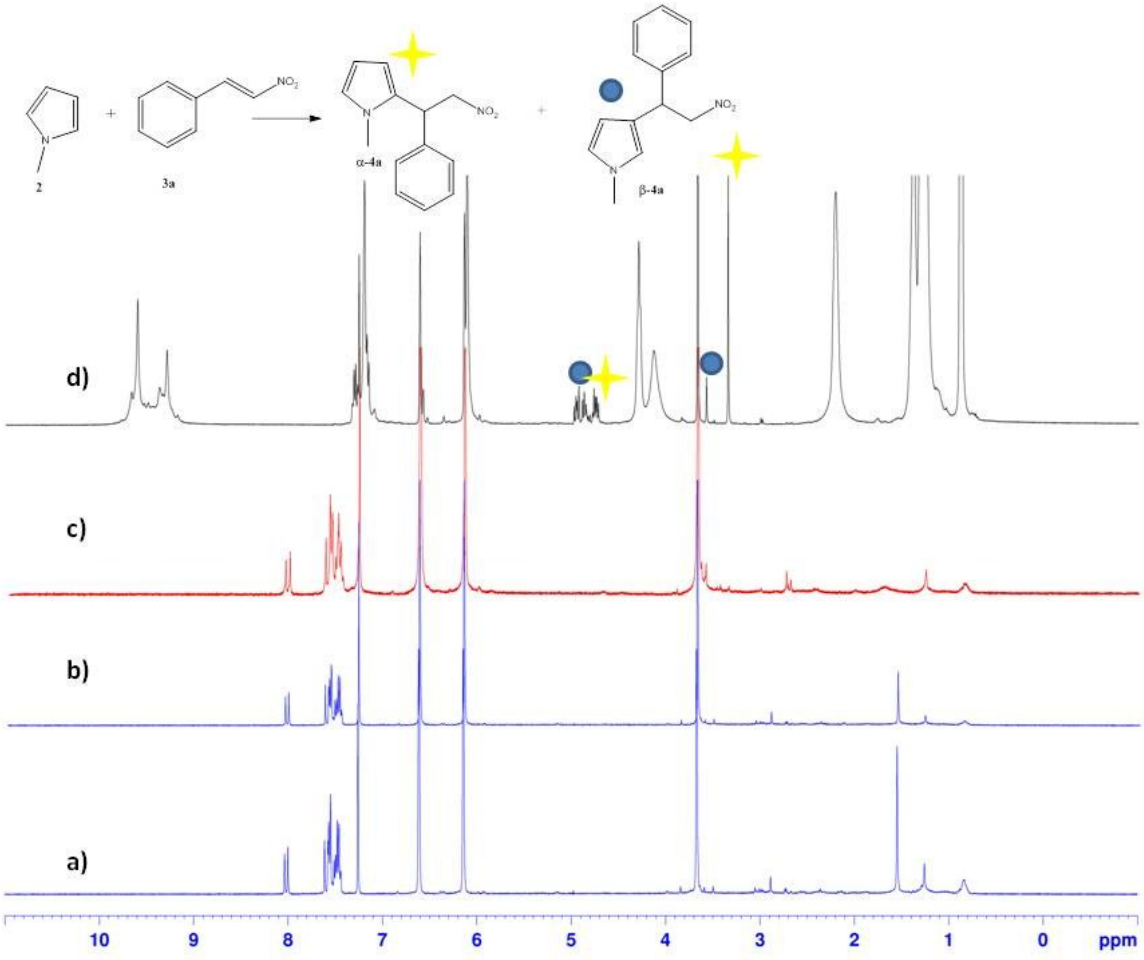
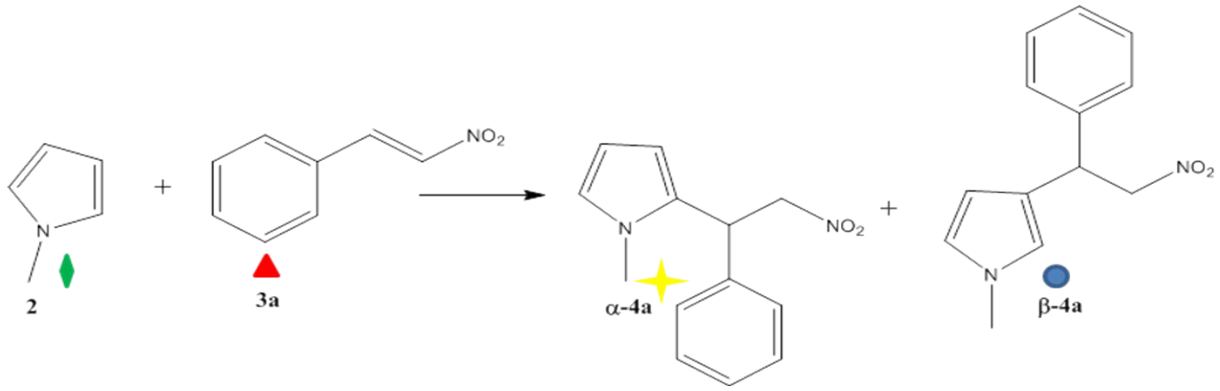



**Figure S3.** $^1$H-NMR spectra ( 400 MHz, $CDCl_3$, 298 K) of: **a)** reaction without **C** in $CDCl_3$ without any treatment after 4h; **b)** reaction without **C** in $CDCl_3$ without any treatment after 12h; **c)** reaction without **C** in freshly prepared HCl-saturated $CDCl_3$ after 4h; **d)** reaction in $CDCl_3$ without any treatment and in the presence of **C** after 2h.

*3.3.2 Influence of HCl on the reaction outcome*




The capsule **C** (0.039 M) was formed in freshly prepared HCl-saturated $CDCl_3$ (1.1 mL) and, subsequently, *N*-methylpyrrole **2** (0.59 M) and *β*-nitrostyrene **3a** (0.15 M) were added. The reaction was kept at 50 °C and monitored for 4 h by $^1$H-NMR spectra. Furthermore, the reaction outcome was compared with the reaction in $CDCl_3$ (from Sigma Aldrich) filtered through basic aluminium oxide. Both reactions afforded the adduct **4** in 94% of yield after 2h (80/20 *α*-**4a**/*β*-**4a** ratio), even if the control experiment with HCl-saturated $CDCl_3$ led to a retardation of the initial reaction progress.

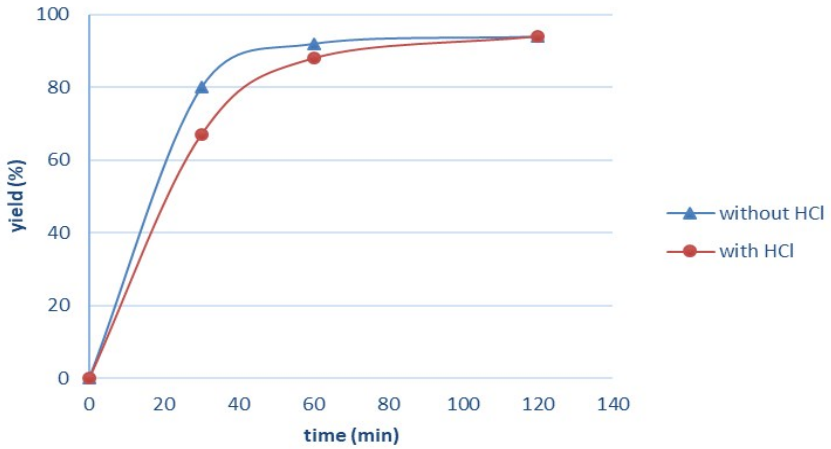



**Figure S4.** Reaction progress profile in different batches of $CDCl_3$: - - $CDCl_3$ filtered through basic $Al_2O_3$ (without HCl); - - freshly prepared HCl-saturated $CDCl_3$ (with HCl).

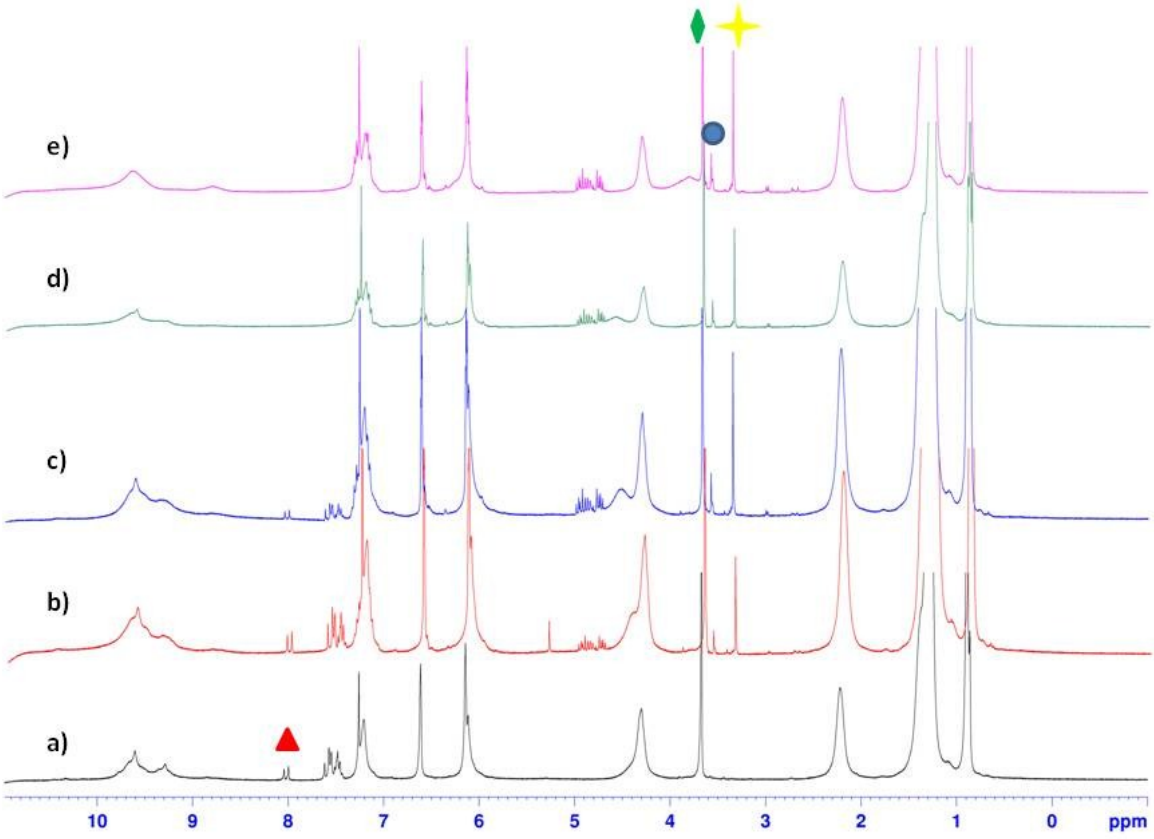



**Figure S5.** $^{1}$H-NMR spectra (400 MHz, $CDCl_3$, 298 K) of the reaction outcome in freshly prepared HCl-saturated $CDCl_3$: a) t = 0; b) t=30 min; c) t = 60 min; d) t = 120 min; e) t = 120 min after adding DMSO.

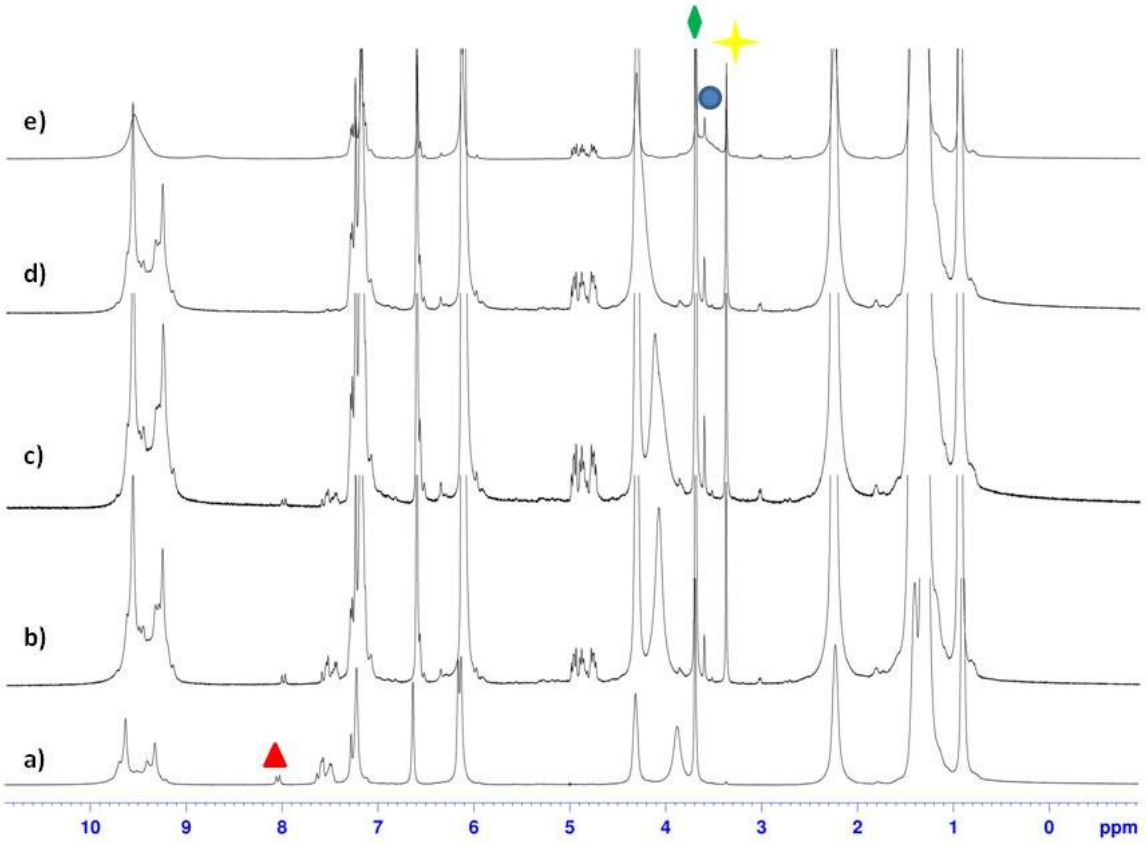



**Figure S6.** $^{1}$H-NMR spectra (400 MHz, $CDCl_3$, 298 K) of the reaction outcome in $CDCl_3$ (from Sigma Aldrich) filtered through basic aluminium oxide: **a)** t = 0; b) t = 30 min; c) t = 60 min; d) t = 120 min; e) t = 120 min after adding DMSO.

### *3.4 Reaction in presence of competitive guest*

In order to confirm that the reaction took place inside the capsule, a control experiment was performed in presence of a large amount of competitive guest for the capsule as hexamethonium bromide.[1]

To a solution of resorcinarene **1** (281.6 mg, 254.7 µmol, 1.56 equiv.) in water saturated chloroform-d (1.1 mL), hexamethonium bromide (763.8 µmol, 18 equiv. respect to resorcinarene capsule) was added. Subsequently, the nucleophile (654.4 µmol, 4 equiv.) was introduced followed by the electrophile (162.6 µmol, 1.0 equiv.). The

reaction system was kept under stirring (1400 rpm) at 50 °C for 16 h. No formation of product was observed.

### 3.5 *Reaction in presence of DMSO*

It is known that DMSO can disrupt the hexameric structure of the capsule thanks to its ability to make hydrogen bonds.[1,8] So, as a further evidence that the reaction took place inside the capsule, a reaction in presence of DMSO has been performed. To a resorcin[4]arene (281.6 mg, 254.7 μmol, 1.56 equiv.) solution in water saturated chloroform-d (1.1 mL), 90 μl of DMSO (1.27 mmol, ) were added. Next, **2** (654.4 μmol, 4 equiv.) and **3a** (162.6 μmol, 1.0 equiv.) were subsequently added. The reaction vial was maintained at 50°C using a thermostated oil bath under vigorous stirring. The reaction was monitored via $^1$H- NMR analysis by taking aliquots at different times and, in all cases, no formation of products was observed.

### 3.6 *Reaction without capsule in the presence of different Brønsted acids*

Since the capsule is a Brønsted acid[9] with p$K_a$ = 5.5–6.0, further investigation in the reaction mechanism was replacing it with a Brønsted acid, such as $CH_3COOH$ (p$K_a$ = 4.76), $CF_3COOH$ (p$K_a$ = −0.25) and $BrCH_2COOH$ (p$K_a$ = 2.86).

To a solution of **2** (654.4 μmol, 4 equiv.) and **3a** (162.6 μmol, 1.0 equiv) in 1.1 mL of water saturated chloroform-d, Brønsted acid additive (1 equiv) was added. The reaction system was kept under stirring (1400 rpm) at 50 °C for 2h.

**Table 1**:

| Entry | Additive | Yield (%)[a] | $\alpha$-**4a**/$\beta$-**4a** [b] |
|---|---|---|---|
| 1 | $CH_3COOH$ | NR | — |
| 2 | $CF_3COOH$ | 34% [c] | 78/22 |
| 3 | $BrCH_2COOH$ | 17% [c] | 59/41 |

[a]Yields of the isolated products after purification by column chromatography. [b] Determined by $^1$H NMR

[7]L. Avram, Y. Cohen, *Org. Lett*. **2003**, *5*, 3329-3332

[9] Q. Zhang, K. Tiefenbacher, *J. Am. Chem. Soc*. **2013**, *135*, 16213-16219.

spectroscopy of the crude reaction mixture after removing resorcinarene according to literature data. [c] Presence of several byproducts.

## 4. Incapsulation experiments

### 4.1 Encapsulation experiments of nitrostyrene **3a** inside the hexameric capsule **C**

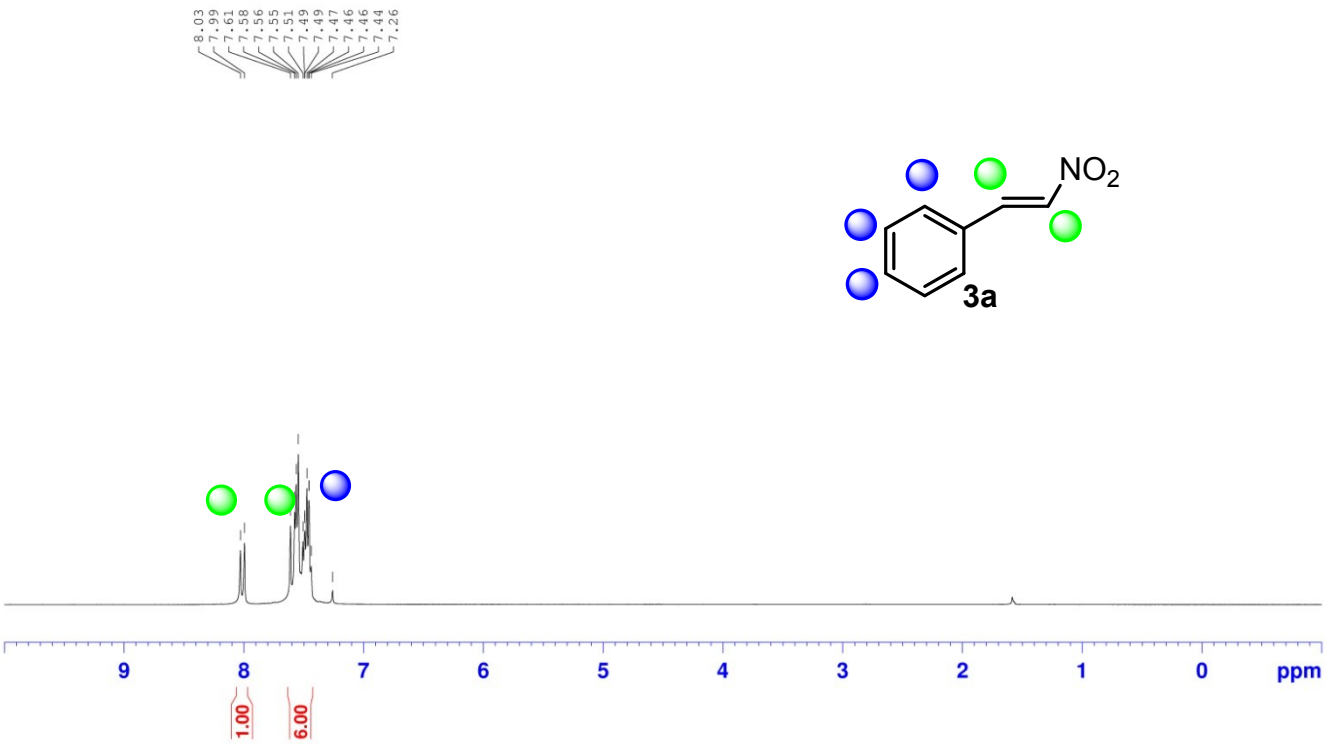
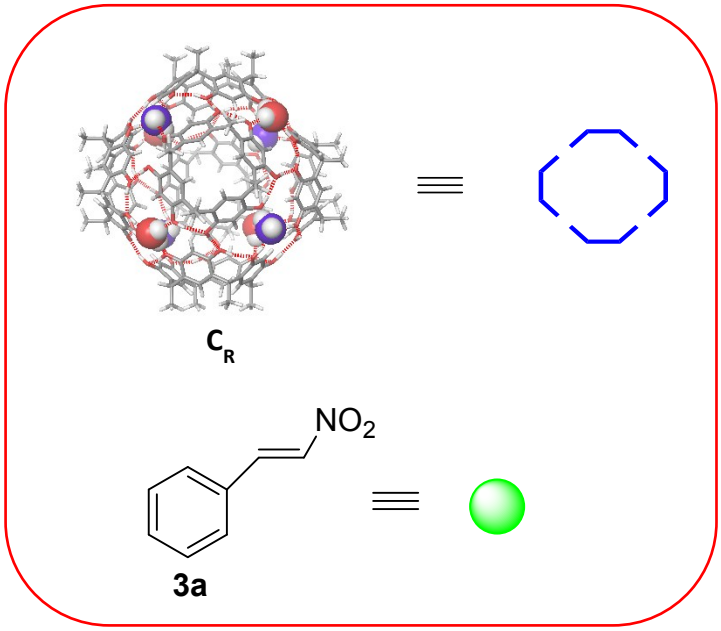



**Figure S7.** $^{1}$H NMR (400 MHz, $CDCl_3$, 298 K) of nitrostyrene **3a**.

2D EXSY experiments of a mixture of **C** and nitrostyrene **3a** revealed the presence of exchange cross-peaks between olefinic proton signals of **3a**, outside and inside the capsule respectively (Figure S8, S9).



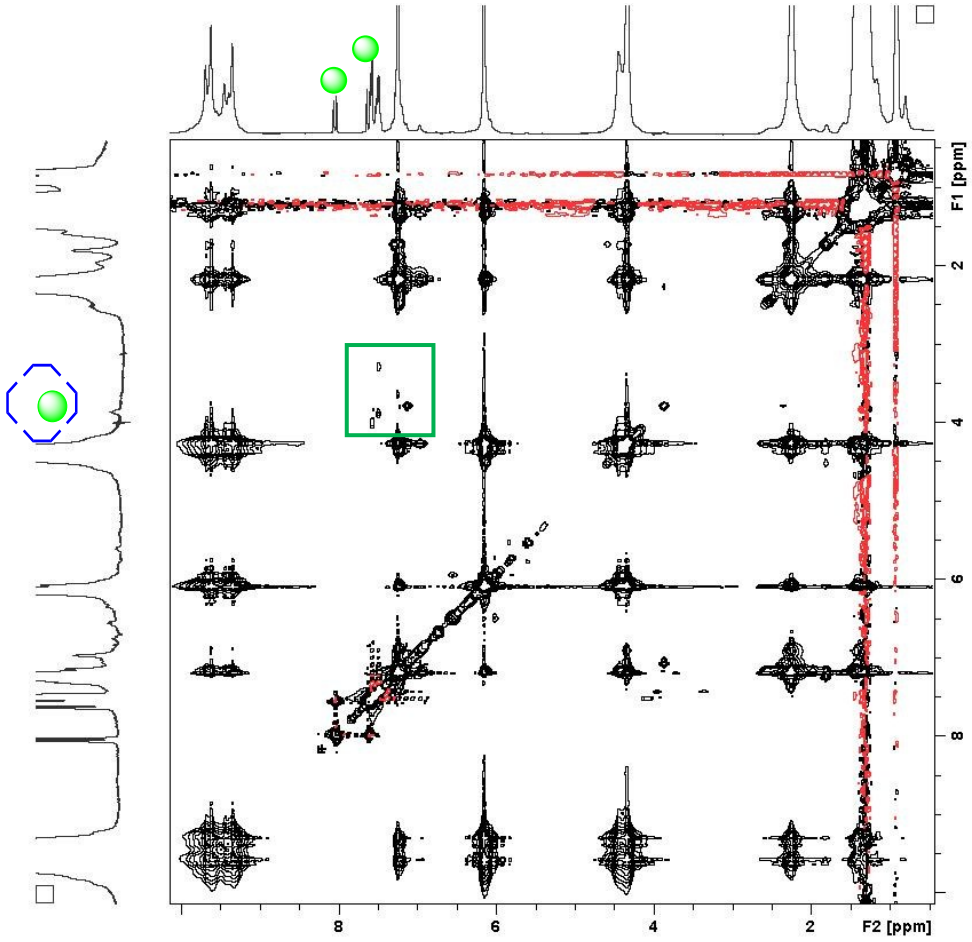
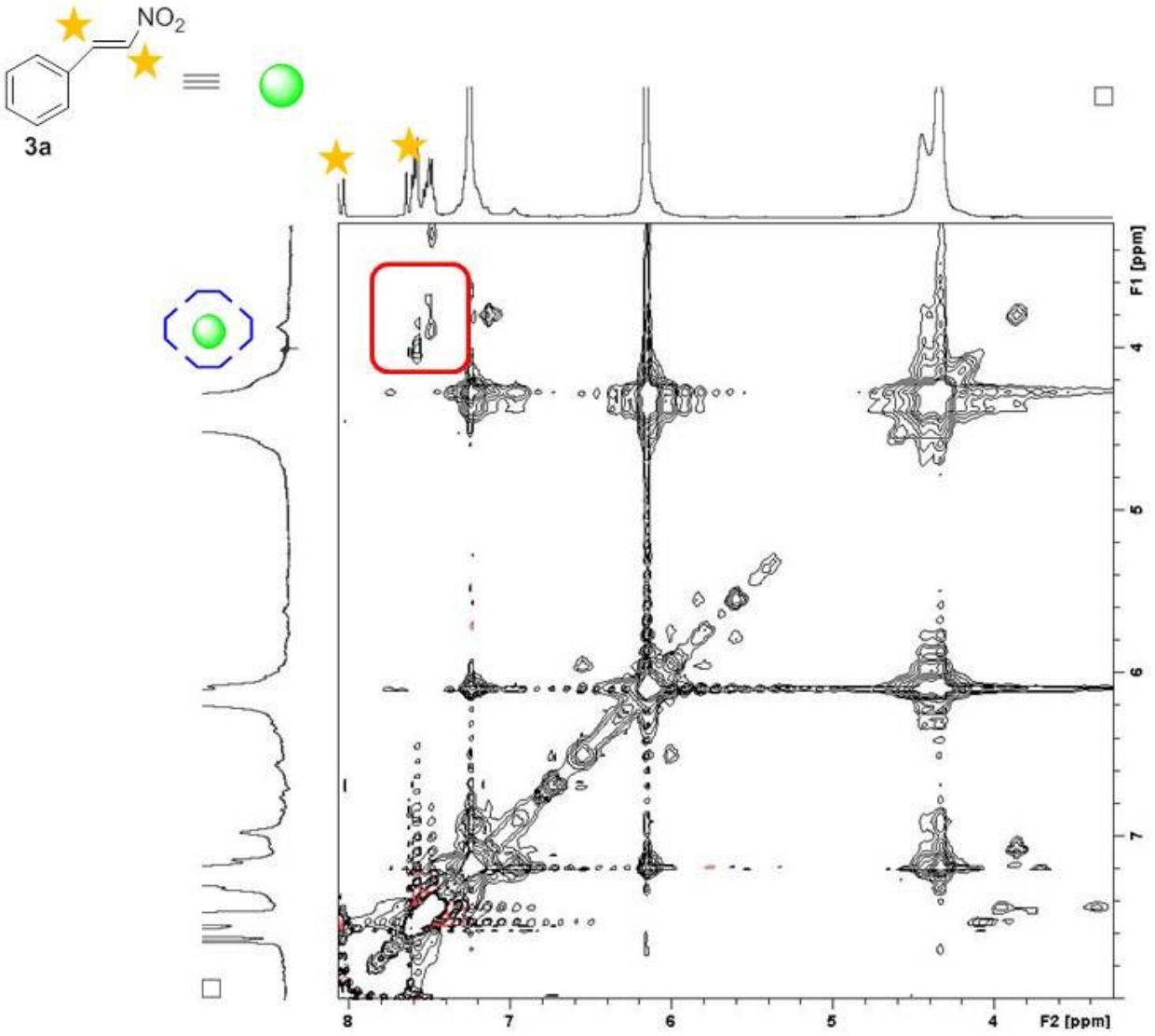




**Fig. S8.** 2D EXSY experiment (400 MHz, $CDCl_3$, 298 K, mixing time 250 ms) of the mixture of **C** (21 mM) and nitrostyrene **3a** (82 mM)**.**

**a)**



**b)**

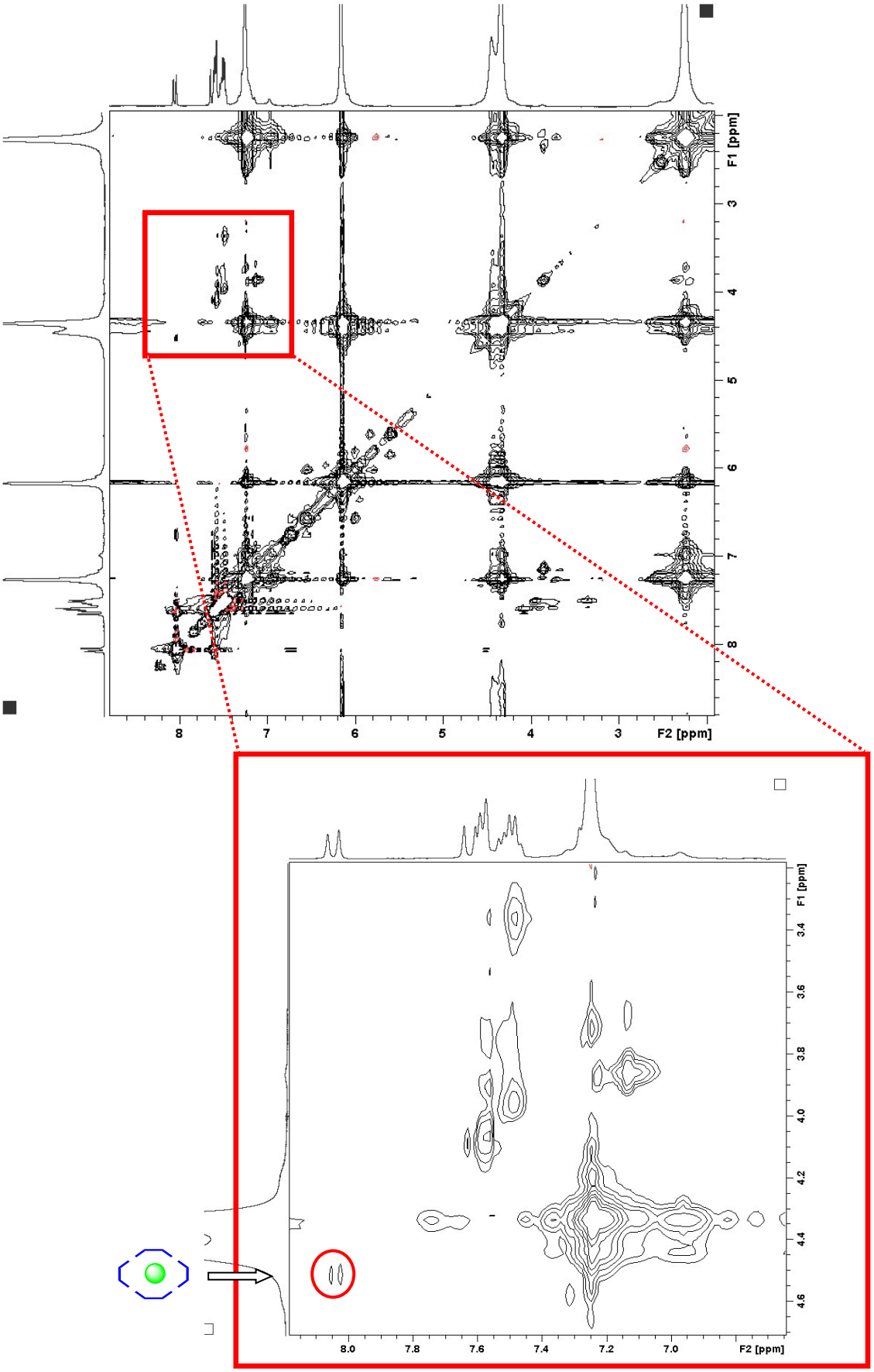



**Fig. S9.** Relevant regions of the 2D experiment in Figure S8. Exchange cross-peaks for free and encapsulated vinyl proton at 8.00 ppm of **3a**.

## 5. Reaction profile of nitrostyrene 3a with *N*-methylpyrrole 2 in the presence of C




The progress of the reaction was monitored by $^{1}$H-NMR spectra at different time intervals. As evidenced in Figure S10, the relative α/β ratio in the product profile was not affected substantially during the reaction.

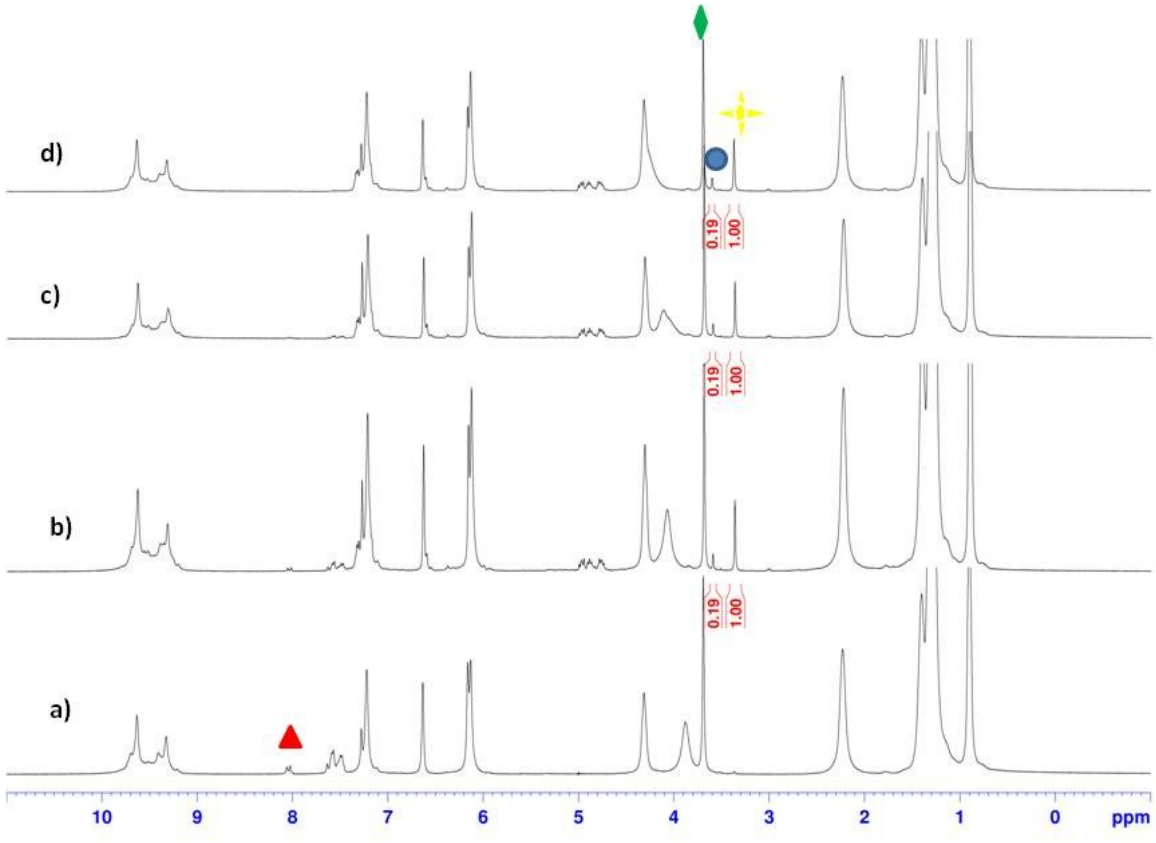



**Fig. S10.** $^{1}$H-NMR spectra (400 MHz, $CDCl_3$, 298 K) of the reaction course in $CDCl_3$ (from Sigma Aldrich) filtered through basic aluminium oxide: **a)** t = 0; b) t = 30 min; c) t = 60 min; d) t = 120 min.

## 6. $^{1}$H-NMR spectra of the reaction mixture with and without C

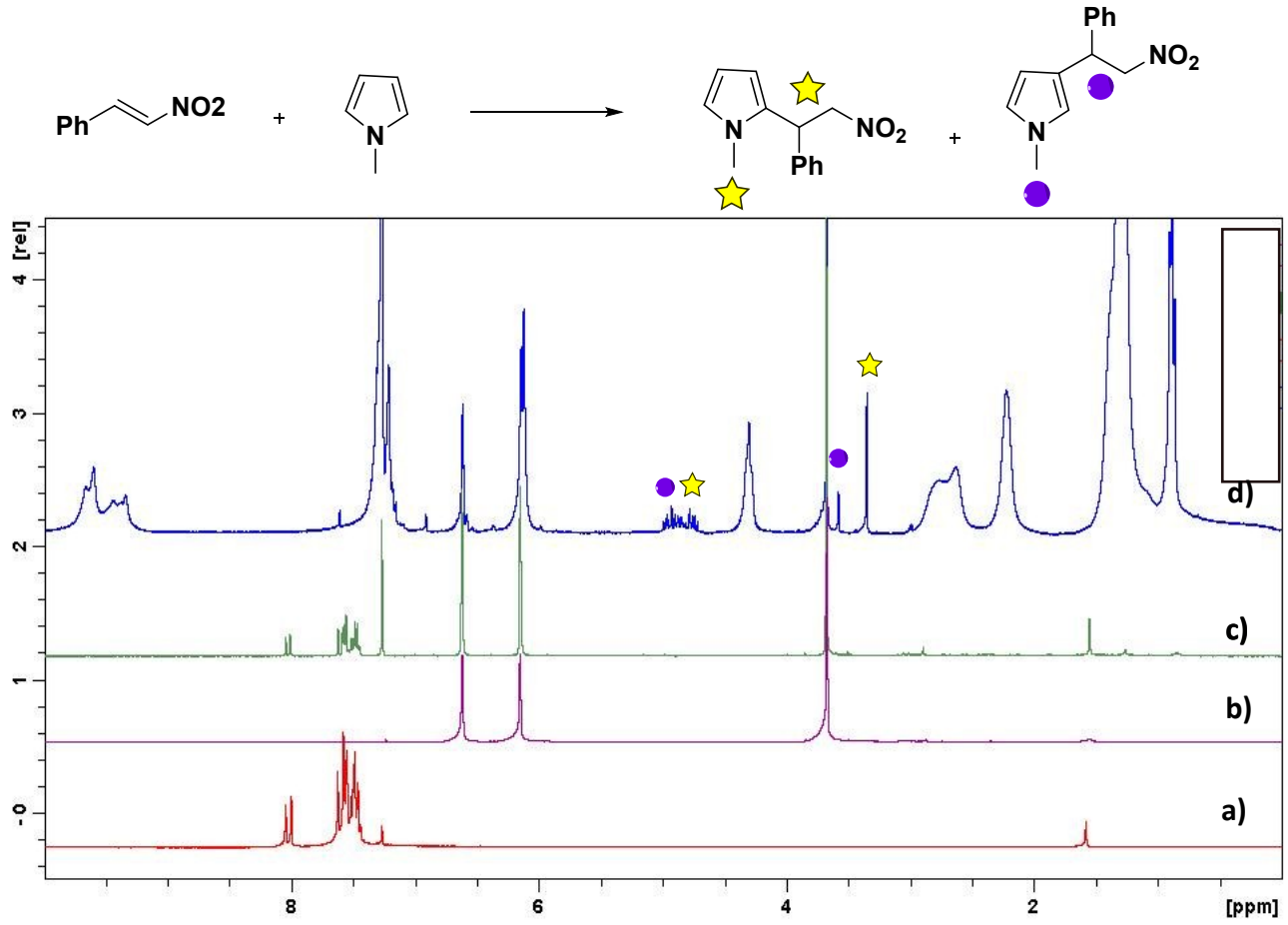
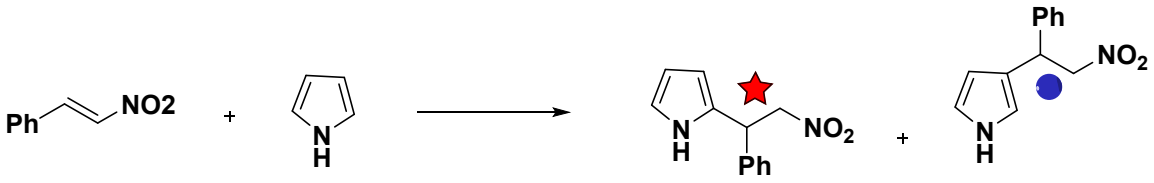



**Fig. S11.** $^{1}$H NMR (400 MHz, $CDCl_3$, 298 K) of: **a)** nitrostyrene **3a**; **b)** *N*-methylpyrrole **2**; **c)** reaction without capsule after t=2h and **d)** reaction in presence of **C** after t=2h.



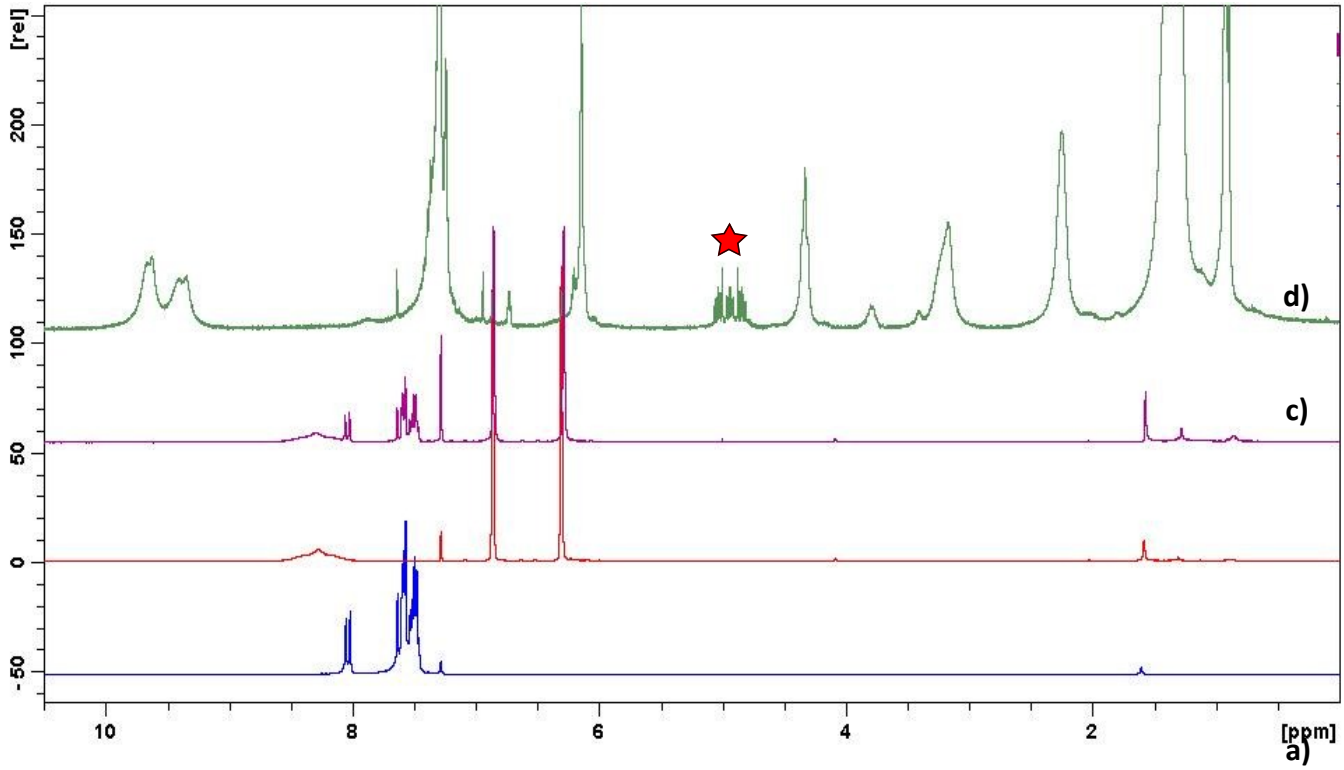




**Fig. S12.** $^{1}$H NMR (400 MHz, $CDCl_3$, 298 K) of: **a)** nitrostyrene **3a**; **b)** pyrrole; **c)** reaction without capsule after t= 2h and **d)** reaction in presence of **C** after t= 2h.

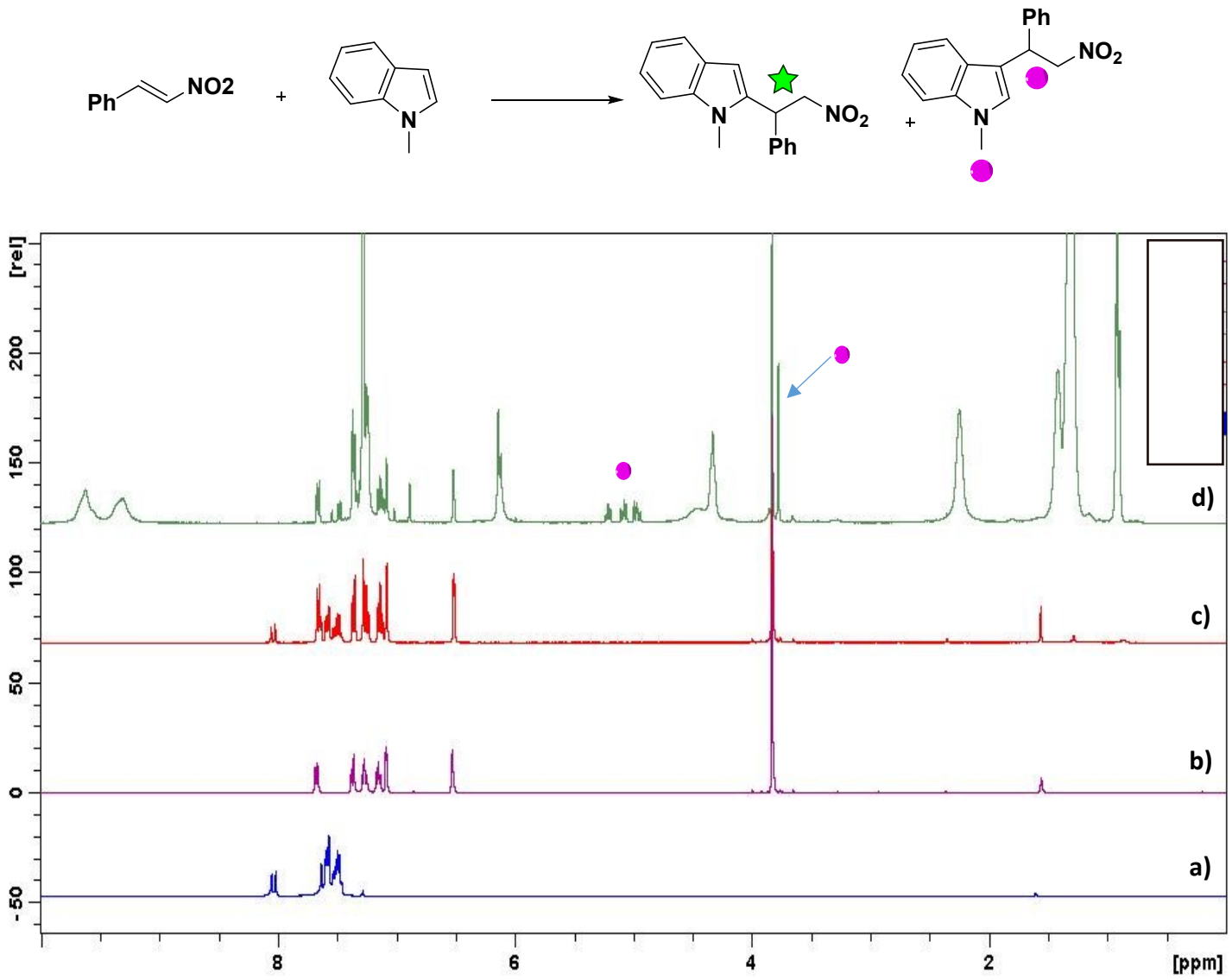



**Fig. S13.** $^{1}$H NMR (400 MHz, $CDCl_3$, 298 K) of: **a)** nitrostyrene **3a**; **b)** of *N*-Me indole; **c)** reaction without capsule after t= 2h and **d)** reaction in presence of **C** after t= 2h**.**

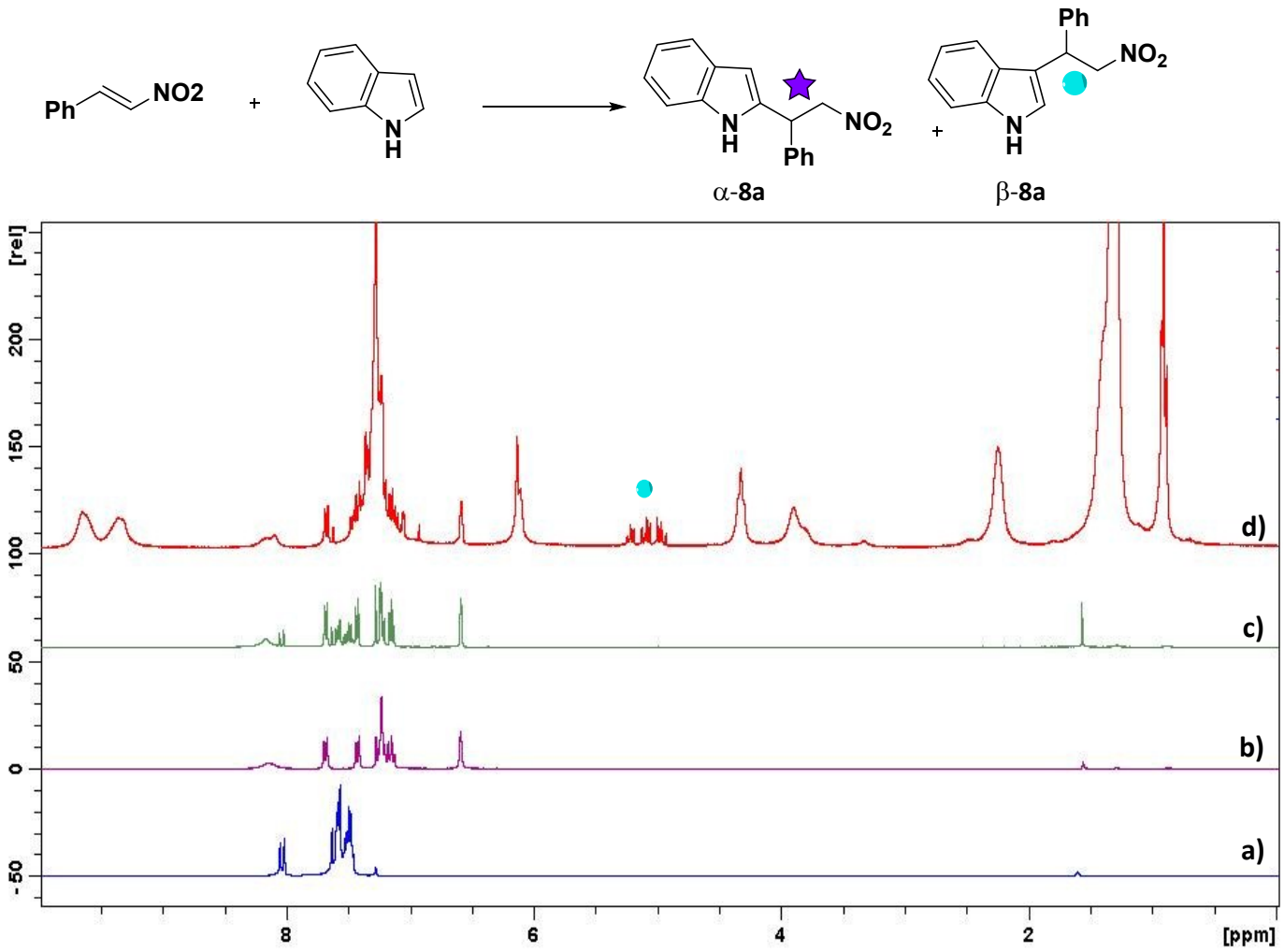



**Fig. S14.** $^{1}$H NMR (400 MHz, $CDCl_3$, 298 K) of: **a)** nitrostyrene **3a**; **b)** indole; **c)** reaction without capsule after t= 2h and **d)** reaction in presence of **C** after t= 2h**.**

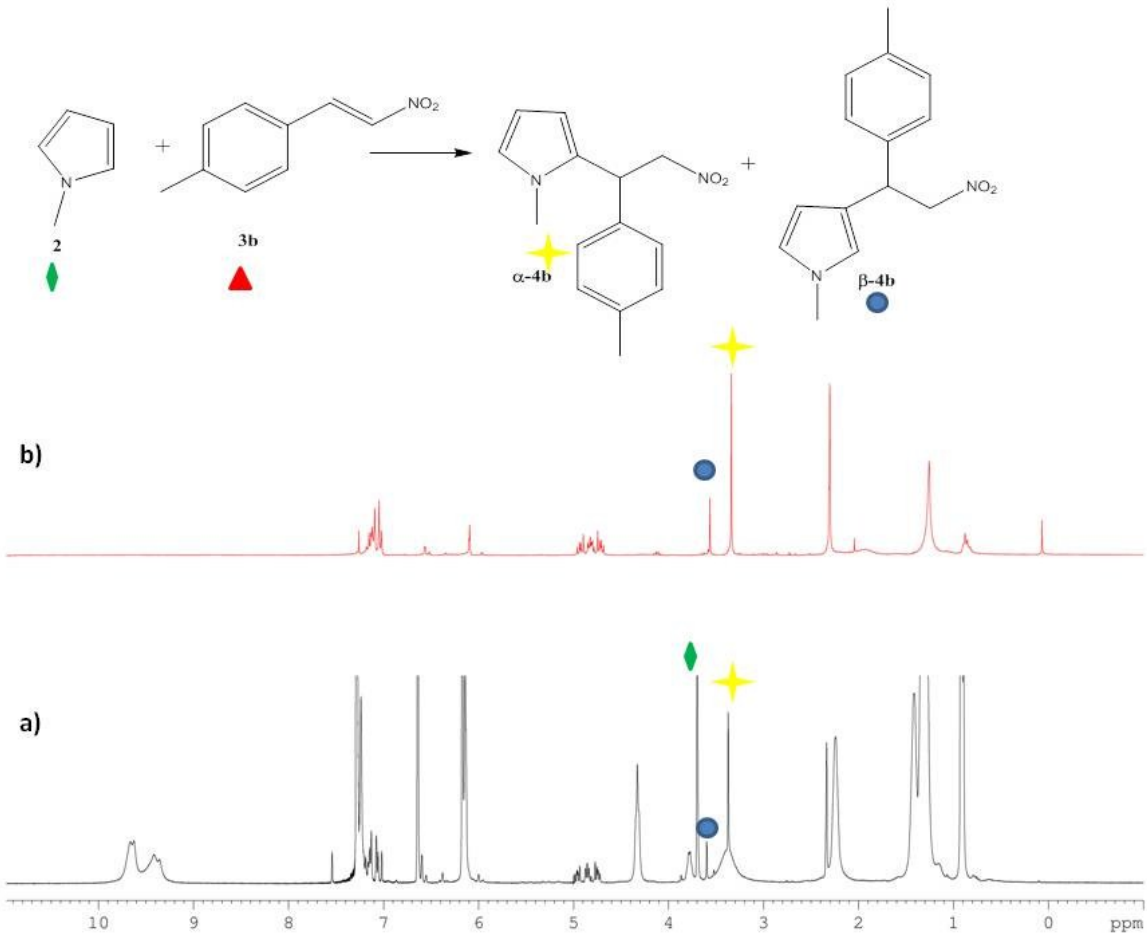



**Fig. S15.** $^{1}H$ NMR (300 MHz, $CDCl_3$, 298 K) of: a) control of the reaction with **C** at 2h; b) crude reaction mixture after work-up.

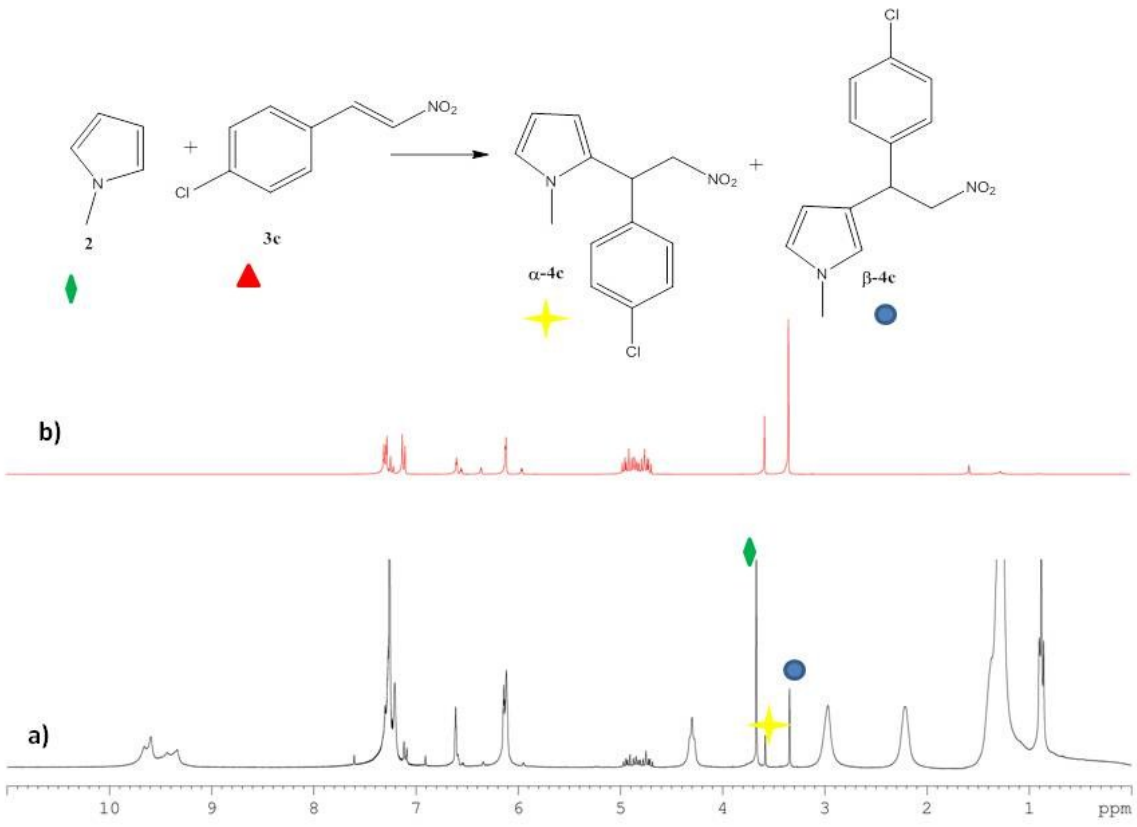



**Fig. S16.** $^{1}$H NMR (300 MHz, $CDCl_3$, 298 K) of: **a)** control of the reaction with **C** at 2h; **b)** crude reaction mixture after work-up.

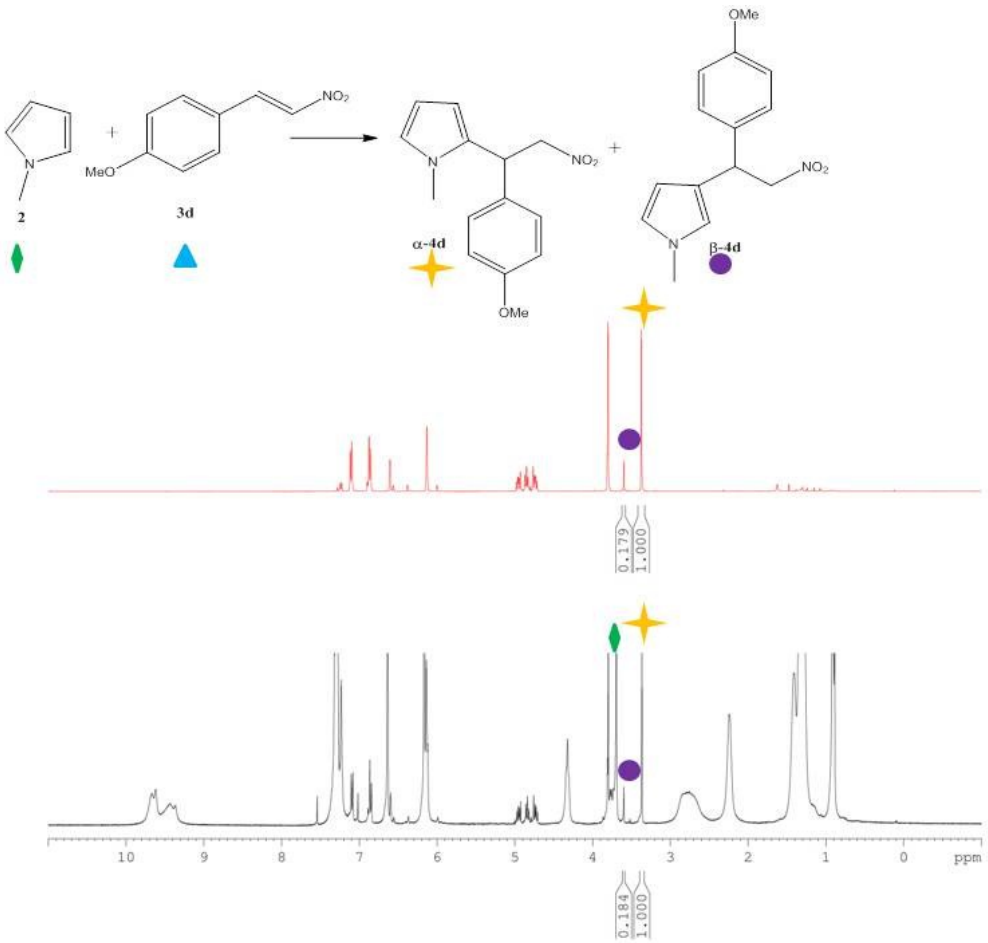



**Fig. S17.** $^{1}$H NMR (300 MHz, $CDCl_3$, 298 K) of: **a)** control of the reaction with **C** at 2h; **b)** crude reaction mixture after work-up.

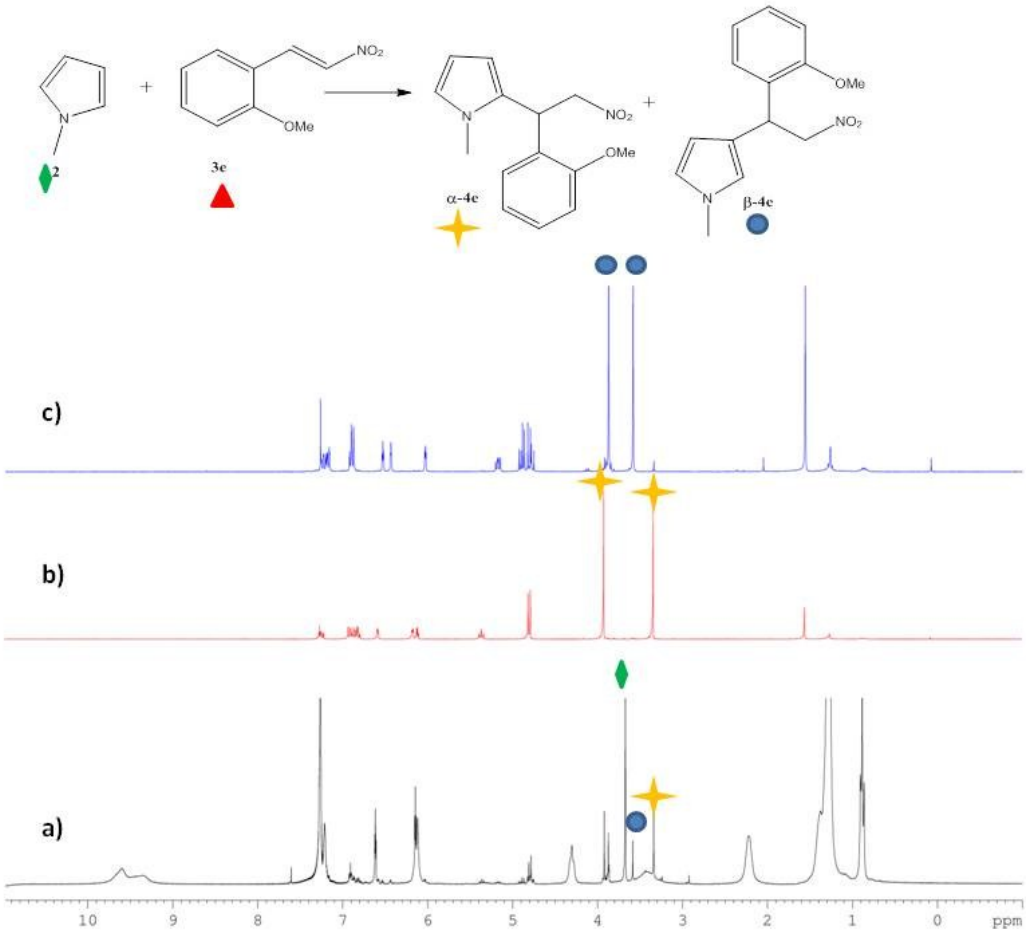



**Fig. S18.** $^{1}$H NMR (300 MHz, $CDCl_3$, 298 K) of: **a)** control of the reaction with **C** at 16h; **b)** α-**4e**; **c)** β-**4e**.

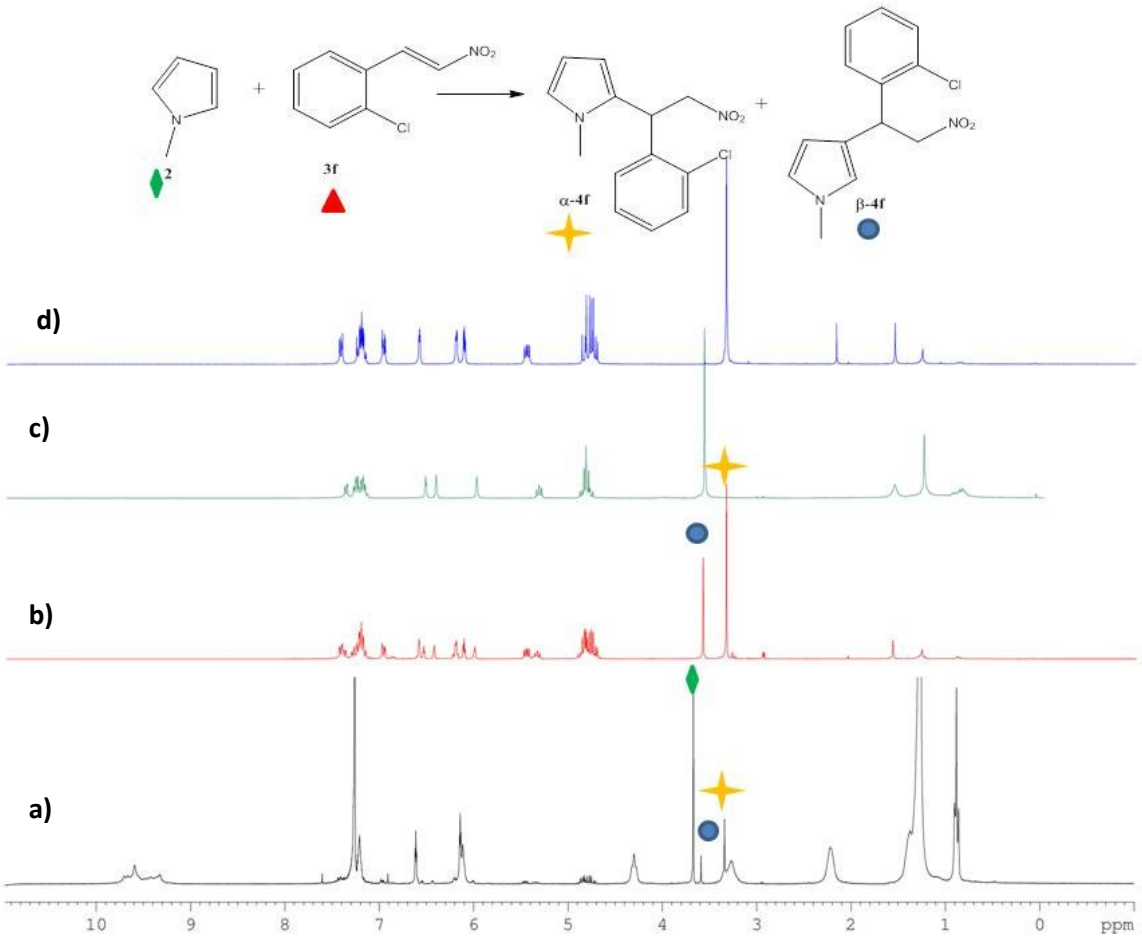



**Fig. S19.** $^{1}$H NMR (300 MHz, $CDCl_3$, 298 K) of: **a)** control of the reaction with **C** at 16h; **b)** crude reaction mixture after work-up; **c)** β-**4f** ; **d)** α-**4f**

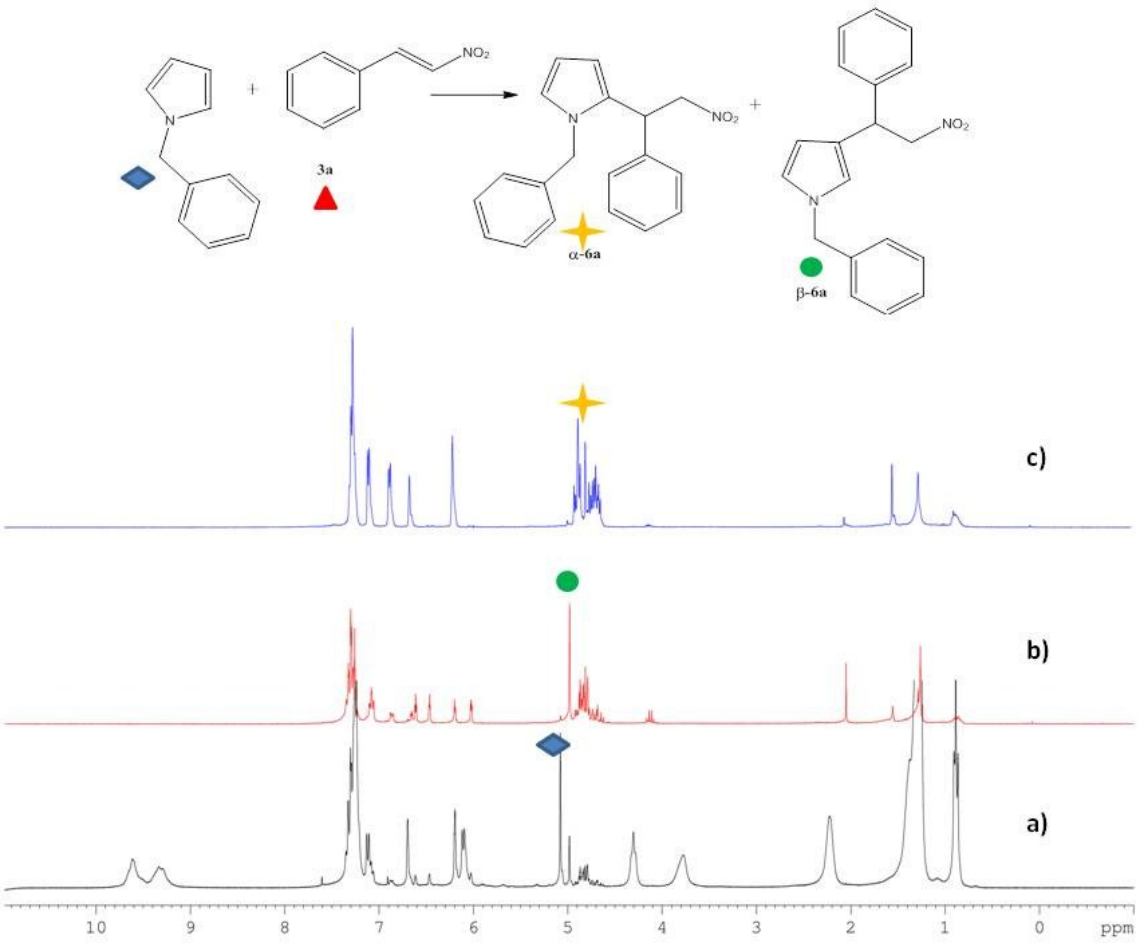



**Fig. S20.** $^{1}$H NMR (300 MHz, $CDCl_3$, 298 K) of: **a)** control of the reaction with **C** at 2h; **b)** β-**6a** ; **c)** α-**6a**

# 7. NMR spectra of novel compounds *β*-4b, *β*-4c, *β*-4d, *β*-4e, α-4f, *β*-4f, α-6a and *β*-6a

*1-methyl-3-(2-nitro-1-(p-tolyl)ethyl)-1H-pyrrole* (*β*-**4b**): isolated as a brown oil; $^{1}$H-NMR (300 MHz, $CDCl_3$, 298 K): $\delta$ 2.32 (s, 3H; $CH_3$), 3.58 (s, 3H; $CH_3$), 4.70-4.89 (m, 3H; $CH_2$ overlapped with CH), 5.97-5.98 (m, 1H, $=CH_{Py}$), 6.35-6.36 (m, 1H, $=CH_{Py}$), 6.52-6.54 (m, 1H, $=CH_{Py}$), 7.11-7.19 (m, 4H; ArH); $^{13}$C NMR (75 MHz, $CDCl_3$, 298 K): δ= 21.4 ($CH_3$), 36.5 ($CH_3$), 42.7 (*C*H), 80.9 ($CH_2$), 107.4 ($C_{Py}H$), 119.8 ($C_{Py}H$), 122.5 ($C_{Pyr}H$), 122.6 ($C_{Pyr}C$), 127.3 (2C, $C_{Ar}H$), 129.7 (2C, $C_{Ar}H$), 137.2 ($C_{Ar}C$), 137.5 ($C_{Ar}C$). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{14}H_{17}N_2O_2$: 245.12845, found 245.12795.

*3-(1-(4-chlorophenyl)-2-nitroethyl)-1-methyl-1H-pyrrole* (*β*-**4c**): isolated as a brown oil; $^{1}$H-NMR (300 MHz, $CDCl_3$, 298 K): $\delta$ 3.60 (s, 3H; $CH_3$), 4.73- 4.91 (m, 3H; $CH_2$ overlapped with CH), 5.96-5.98 (m, 1H, $=CH_{Py}$), 6.36-6.37 (m, 1H, $=CH_{Py}$), 6.55-6.57 (m, 1H, $=CH_{Py}$), 7.22-7.33 (m, 4H, ArH); $^{13}$C NMR (75 MHz, $CDCl_3$, 298 K): δ 36.4 ($CH_3$), 42.2 (*C*H), 80.4 ($CH_2$), 107.3 ($C_{Py}H$), 119.7($C_{Py}H$), 121.8 ($C_{Py}C$), 122.7 ($C_{Py}H$), 129.1 (2C, $C_{Ar}H$), 129.2 (2C, $C_{Ar}H$), 133.3 ($C_{Ar}C$), 139.0 ($C_{Ar}C$). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{13}H_{14}ClN_2O_2$: 265.07382, found 265.07440.

*3-(1-(4-methoxyphenyl)-2-nitroethyl)-1-methyl-1H-pyrrole* (*β*-**4d**): isolated as a brown oil; $^{1}$H-NMR (300 MHz, $CDCl_3$, 298 K): $\delta$ 3.59 (s, 3H; $CH_3$), 3.80 (s, 3H; $CH_3$), 4.71- 4.91 (m, 3H; $CH_2$ overlapped with CH), 5.98-5.99 (m, 1H, $=CH_{Py}$), 6.35-6.37 (m, 1H, $=CH_{Py}$), 6.55-6.57 (m, 1H, $=CH_{Py}$), 6.87 (d, *J*= 8.6 Hz, 2H, ArH), 7.22 (d, *J*= 8.6 Hz, 2H, ArH); $^{13}$C NMR (75 MHz, $CDCl_3$, 298 K): δ 36.4 ($CH_3$), 42.2 (*C*H), 55.4 ($CH_3$), 80.8 ($CH_2$), 107.3 ($C_{Py}H$), 114.3 (2C, $C_{Ar}H$), 119.7

($C_{Py}$H), 122.6 ($C_{Py}$H), 122.7 ($C_{Py}$C), 128.9 (2C, $C_{Ar}$H), 132.5 ($C_{Ar}$C), 158.9 ($C_{Ar}$C). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{14}H_{17}N_2O_3$: 261.12337, found 261.12287.

*3-(1-(2-methoxyphenyl)-2-nitroethyl)-1-methyl-1H-pyrrole* (*β*-**4e**): isolated as a yellow oil; $^1$H-NMR (300 MHz, $CDCl_3$, 298 K): δ= 3.60 (s, 3H; $CH_3$), 3.89 (s, 3H; $CH_3$), 4.81 (dd, $^2J$ = 12.3 Hz, $^3J$ = 9.2 Hz, 1H, CH), 4.90 (dd, $^2J$ = 12.3 Hz, $^3J$ = 6.7 Hz, 1H, CH), 5.19 (dd, $^3J$ = 9.2 Hz, $^3J$ = 6.7 Hz, 1H, CH), 6.04-6.05 (m, 1H, =$CH_{Py}$), 6.44-6.46 (m, 1H, =$CH_{Py}$), 6.55 (t, $^3J$ = 2.6 Hz, 1H, =$CH_{Py}$), 6.89-6.94 (m, 2H, ArH), 7.17-7.28 (m, 2H, ArH); $^{13}$C NMR (75 MHz, $CDCl_3$, 298 K): δ 36.0 ($CH_3$), 36.6 (*C*H), 55.3 ($OCH_3$), 79.1 ($CH_2$), 107.5 ($C_{Py}$H), 110.6 ($C_{Ar}$H), 119.7 ($C_{Py}$H), 120.5 ($C_{Ar}$H), 121.3 ($C_{Py}$C), 121.9 ($C_{Py}$H), 128.1 ($C_{Ar}$H), 128.4 ($C_{Ar}$C), 128.7 ($C_{Ar}$H), 156.6 ($C_{Ar}$OMe). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{14}H_{17}N_2O_3$: 261.12337, found 261.12475.

*2-(1-(2-chlorophenyl)-2-nitroethyl)-1-methyl-1H-pyrrole* (*α*-**4f**): isolated as a brown oil; $^1$H-NMR (300 MHz, $CDCl_3$, 298 K): δ= 3.36 (s, 3H; $CH_3$), 4.76 (dd, $^2J$ = 13.2 Hz, $^3J$ = 5.6 Hz, 1H, CH), 4.85 (dd, $^2J$ = 13.2 Hz, $^3J$ = 9.8 Hz, 1H, CH), 5.48 (dd, J=9.8, J=5.6 Hz, 1H, CH), 6.13-6.15 (m, 1H, =$CH_{Py}$), 6.21-6.23 (m, 1H, =$CH_{Py}$), 6.60-6.62 (m, 1H, =$CH_{Py}$), 6.97-7.00 (m, 1H, ArH), 7.18-7.28 (m, 2H, ArH), 7.43-7.46 (m, 1H, ArH); $^{13}$C NMR (75 MHz, $CDCl_3$, 298 K): δ= 33.8 ($CH_3$), 38.2 (*C*H), 77.1 ($CH_2$), 107.0 ($C_{Py}$H), 107.3 ($C_{Py}$H), 123.4 ($C_{Py}$H), 127.9 ($C_{Ar}$H), 128.7 ($C_{Py}$C), 129.4 ($C_{Ar}$H), 130. 0 ($C_{Ar}$H), 130.2 ($C_{Ar}$H), 133.5 ($C_{Ar}$C), 135.4 ($C_{Ar}$C). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{13}H_{14}N_2O_2$: 265.07385, found 265.07385.

*3-(1-(2-chlorophenyl)-2-nitroethyl)-1-methyl-1H-pyrrole* (*β*-**4f**)*:* yellow oil; $^1$H NMR (300 MHz, $CDCl_3$, 298 K): δ 3.60 (s, 3H; $CH_3$), 4.79-4.92 (m, 2H, $CH_2$), 5.33-5.39 (m, 1H, CH), 6.02 (m, 1H, =$CH_{Py}$), 6.45 (m, 1H, =$CH_{Py}$), 6.55-6.57

(m, 1H, =$CH_{Py}$), 7.18-7.42 (m, 4H, ArH); $^{13}$C NMR (75 MHz, $CDCl_3$, 298 K): δ 36.4 ($CH_3$), 39.2 (CH), 79.0 ($CH_2$), 107.6 ($C_{Py}H$), 120.2 ($C_{Py}H$), 120.7 ($C_{Py}C$), 122.7 ($C_{Py}H$), 127.4 ($C_{Ar}H$), 128.7 ($C_{Ar}H$), 128.8 ($C_{Ar}H$), 130.3 ($C_{Ar}H$), 133.9 ($C_{Ar}C$), 138.0 ($C_{Ar}C$). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{13}H_{14}N_2O_2$: 265.07385, found 265.07385.

*1-benzyl-2-(2-nitro-1-phenylethyl)-1H-pyrrole* (*α*-**6a**)*:* colourless oil; $^1$H NMR (600 MHz, $CDCl_3$, 298 K): δ 4.67-4.93 (m, 5H, $CH_2$, CH, $CH_2$Ph overlapped), 6.21-6.22 (m, 2H, =$CH_{Py}$), 6.67-6.68 (m, 1H, =$CH_{Py}$), 6.88-6.89 (m, 2H, ArH), 7.10-7.12 (m, 2H, ArH), 7.24-7.31 (m, 7H, ArH); $^{13}$C NMR (150 MHz, $CDCl_3$, 298 K): δ 41.8 (CH), 50.7 ($CH_2$Ph), 79.5 ($CH_2$), 107.0 ($C_{Py}H$), 107.7 ($C_{Py}H$), 123.2 ($C_{Py}H$), 126.6 (2C, $C_{Ar}H$), 127.8 ($C_{Ar}H$), 128.0 ($C_{Ar}H$), 128.1(2C, $C_{Ar}H$), 129.0 (2C, $C_{Ar}H$), 129.3 (2C, $C_{Ar}H$), 129.6 ($C_{Py}C$), 137.6 ($C_{Ar}C$), 138.4 ($C_{Ar}C$). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{19}H_{19}N_2O_2$: 307.14410 , found 307.14415.

*1-benzyl-3-(2-nitro-1-phenylethyl)-1H-pyrrole* (*β*-**6a**)*:* brown oil; $^1$H NMR (400 MHz, $CDCl_3$, 298 K): δ 4.78-4.93 (m, 3H, $CH_2$ and CH overlapped), 5.00 (s, 2H, $CH_2$Ph), 6.04-6.06 (m, 1H, =$CH_{Py}$), 6.48-6.50 (m, 1H, =$CH_{Py}$), 6.63-6.65 (m, 1H, =$CH_{Py}$ ), 7.08-7.11. (m, 2H, ArH), 7.27-7.37 (m, 8H, ArH); $^{13}$C NMR (150 MHz, $CDCl_3$, 298 K):δ 43.0 (CH), 53.6 ($CH_2$Ph), 80.8 ($CH_2$),107.9 ($C_{Py}H$), 119.3 ($C_{Py}H$), 122.1 ($C_{Py}H$), 122.6 ($C_{Py}C$), 127.2 (2C, $C_{Ar}H$), 127.5 ($C_{Ar}H$), 127.9 (2C, $C_{Ar}H$), 128.0 (2C, $C_{Ar}H$), 128.9 (2C, $C_{Ar}H$), 129.0 ($C_{Ar}H$), 137.9 ($C_{Ar}C$), 140.5 ($C_{Ar}C$). HRMS (MALDI-FT ICR): exact mass $[M+H]^+$ calculated for $C_{19}H_{19}N_2O_2$: 307.14410 , found 307.14413.

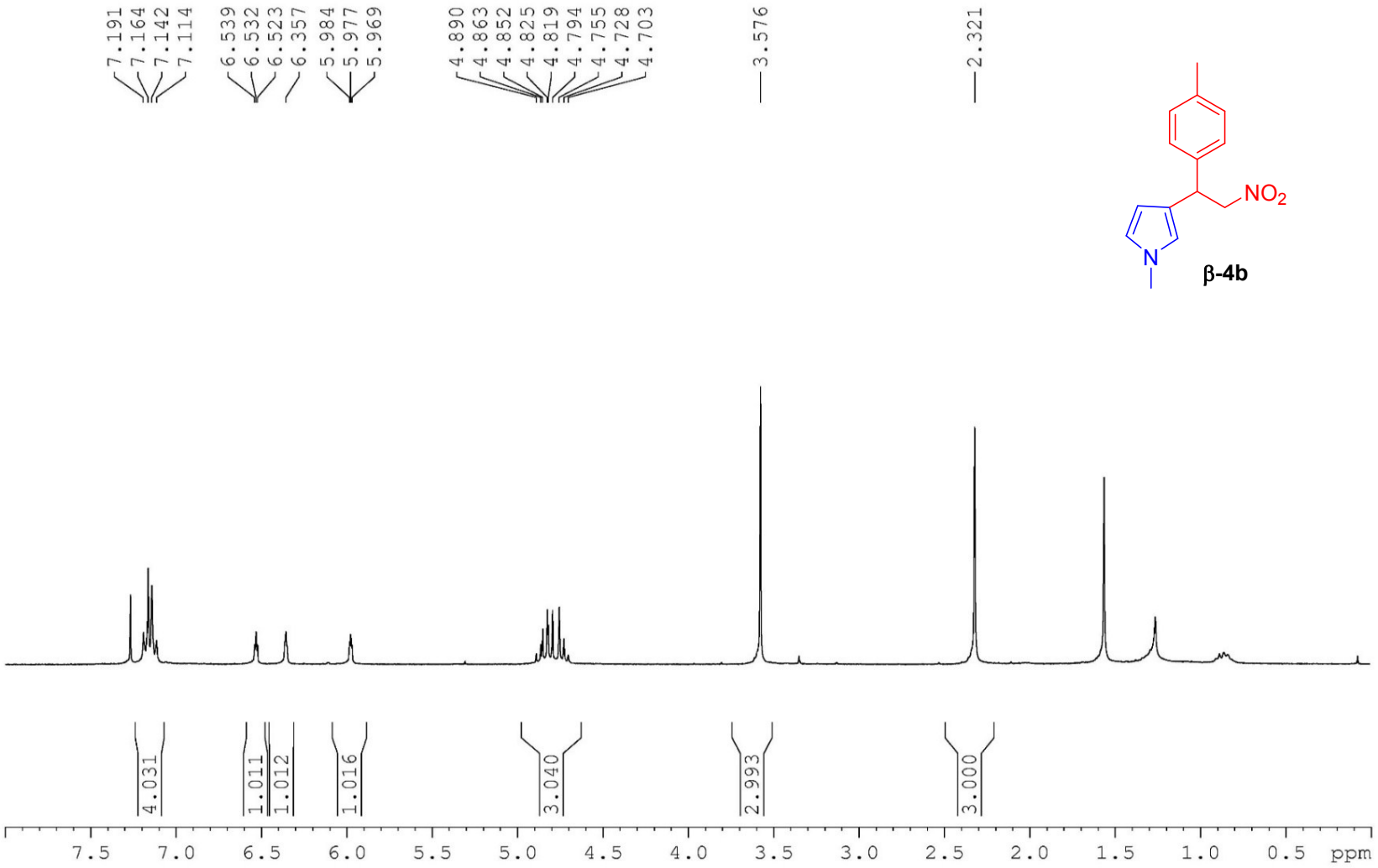



**Figure S17**.[1]H NMR spectrum of derivative ***β*-4b** (300 MHz, $CDCl_3$, 298 K).

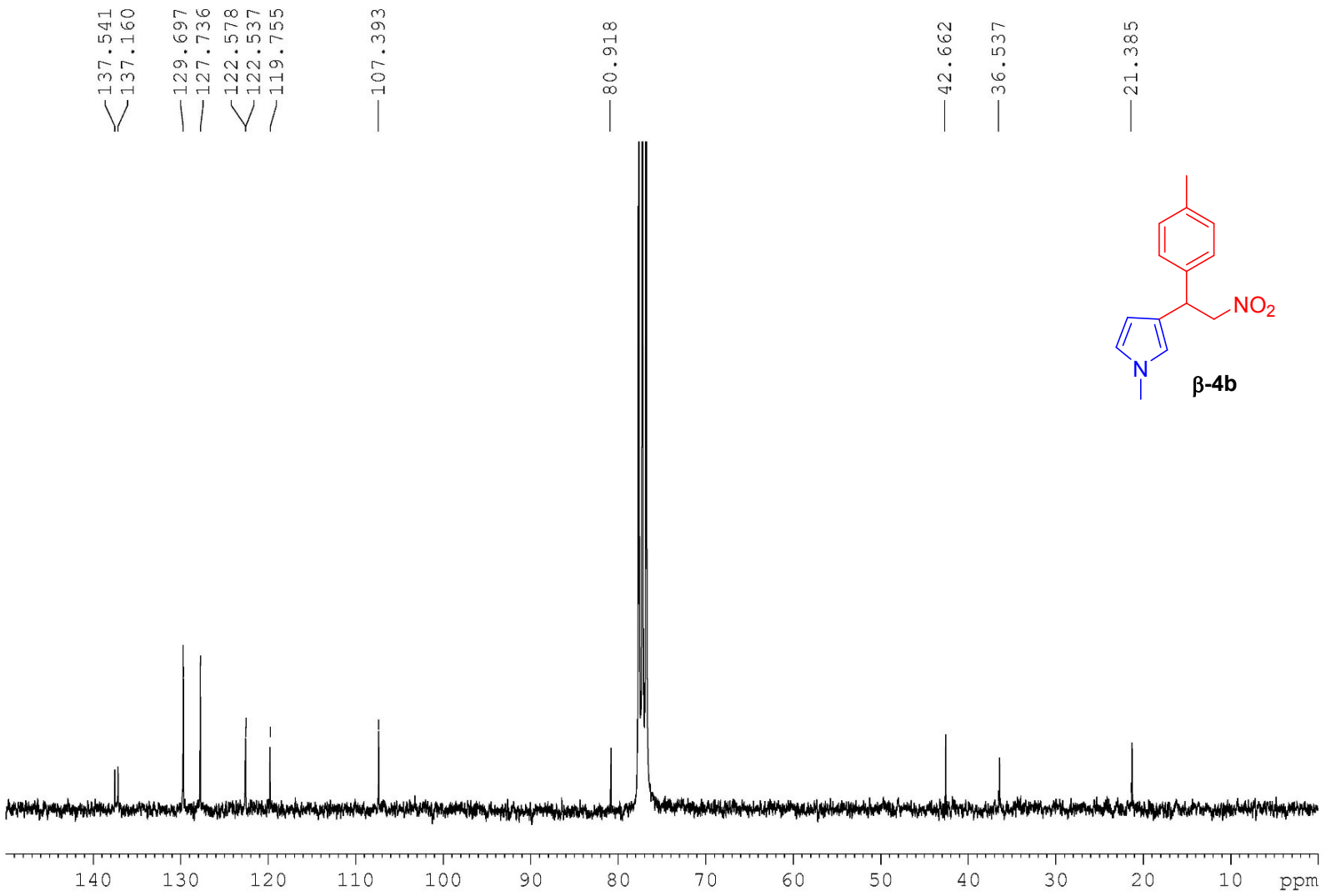



**Figure S18**.[13]C NMR spectrum of derivative ***β*-4b** (300 MHz, $CDCl_3$, 298 K).

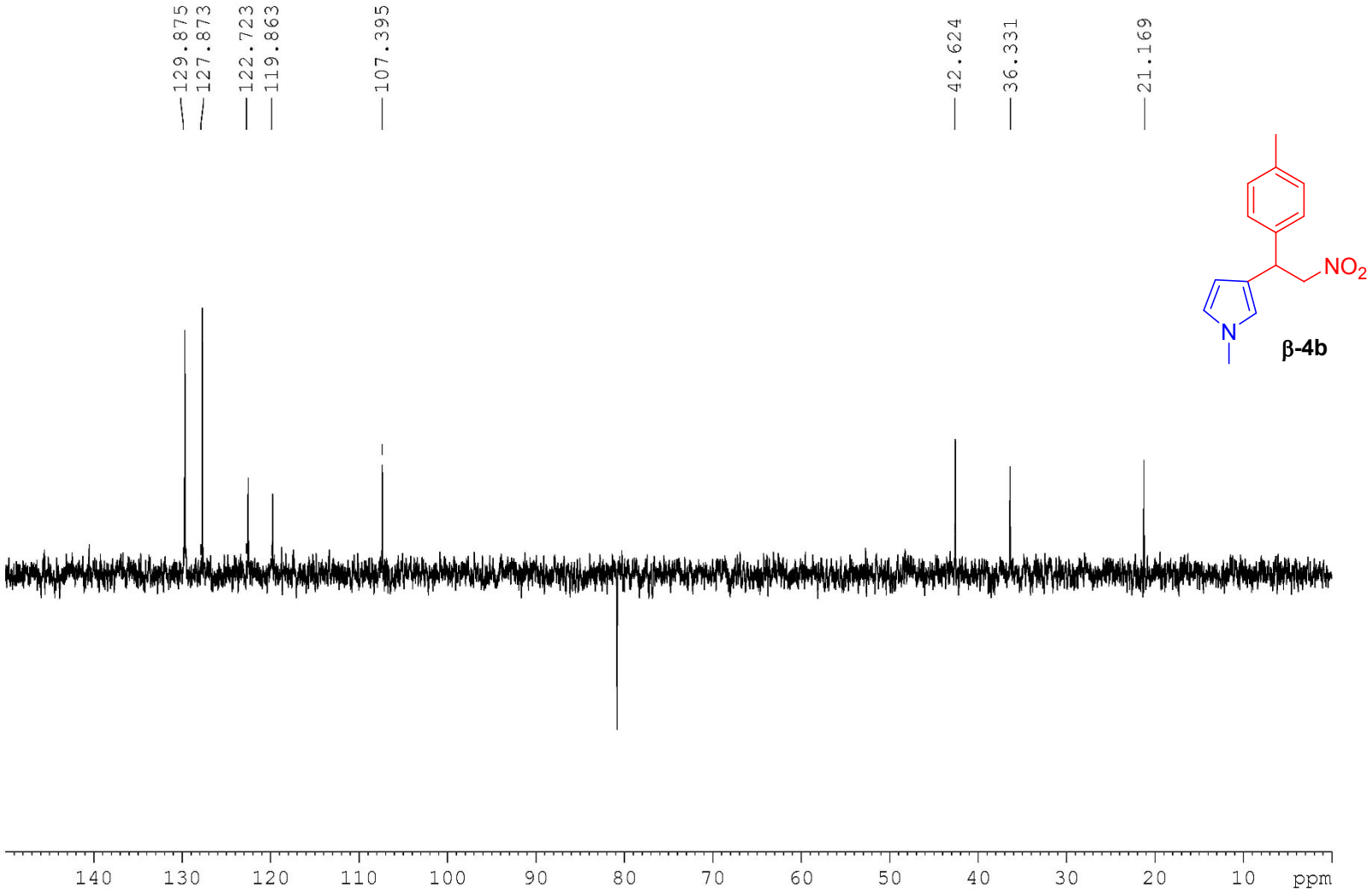



**Figure S19**.DEPT $^{13}$CNMR spectrum of derivative ***β*-4b** (300 MHz, $CDCl_3$, 298 K).

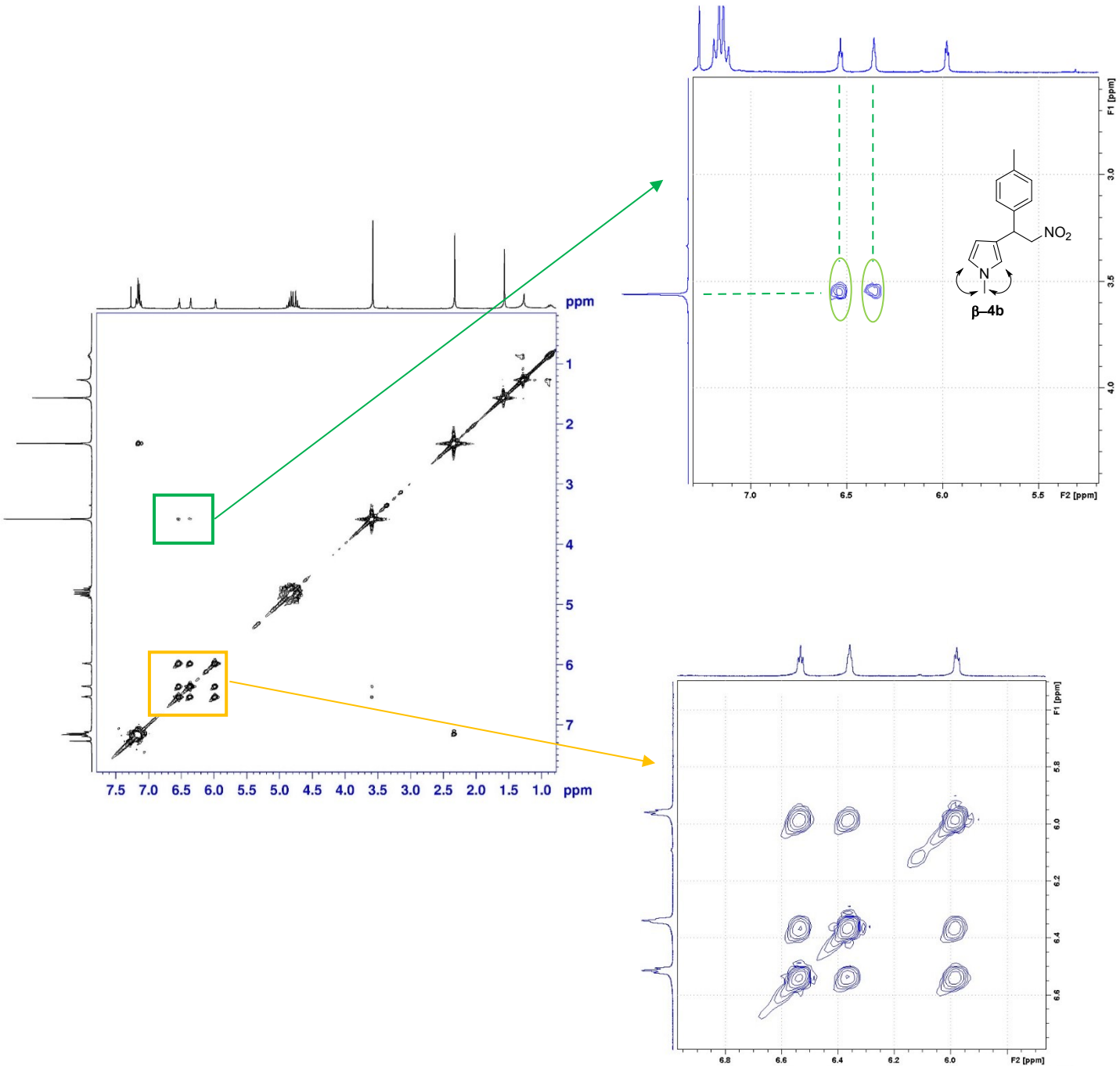



**Figure S20**. COSY NMR spectrum of derivative ***β*-4b** (300 MHz, $CDCl_3$, 298 K).

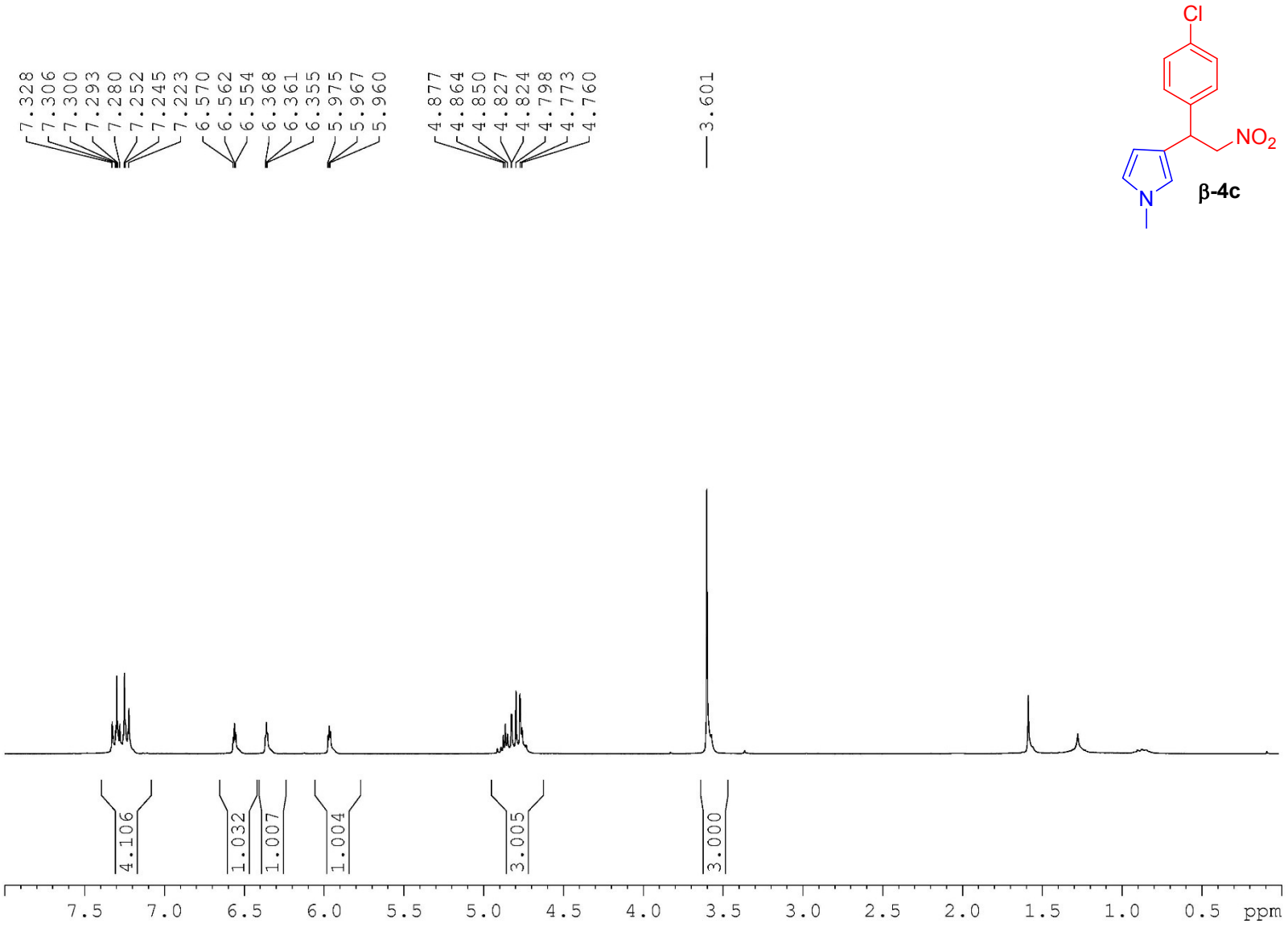



**Figure S21** $^{1}$H NMR spectrum of derivative ***β*-4c** (300 MHz, $CDCl_3$, 298 K).

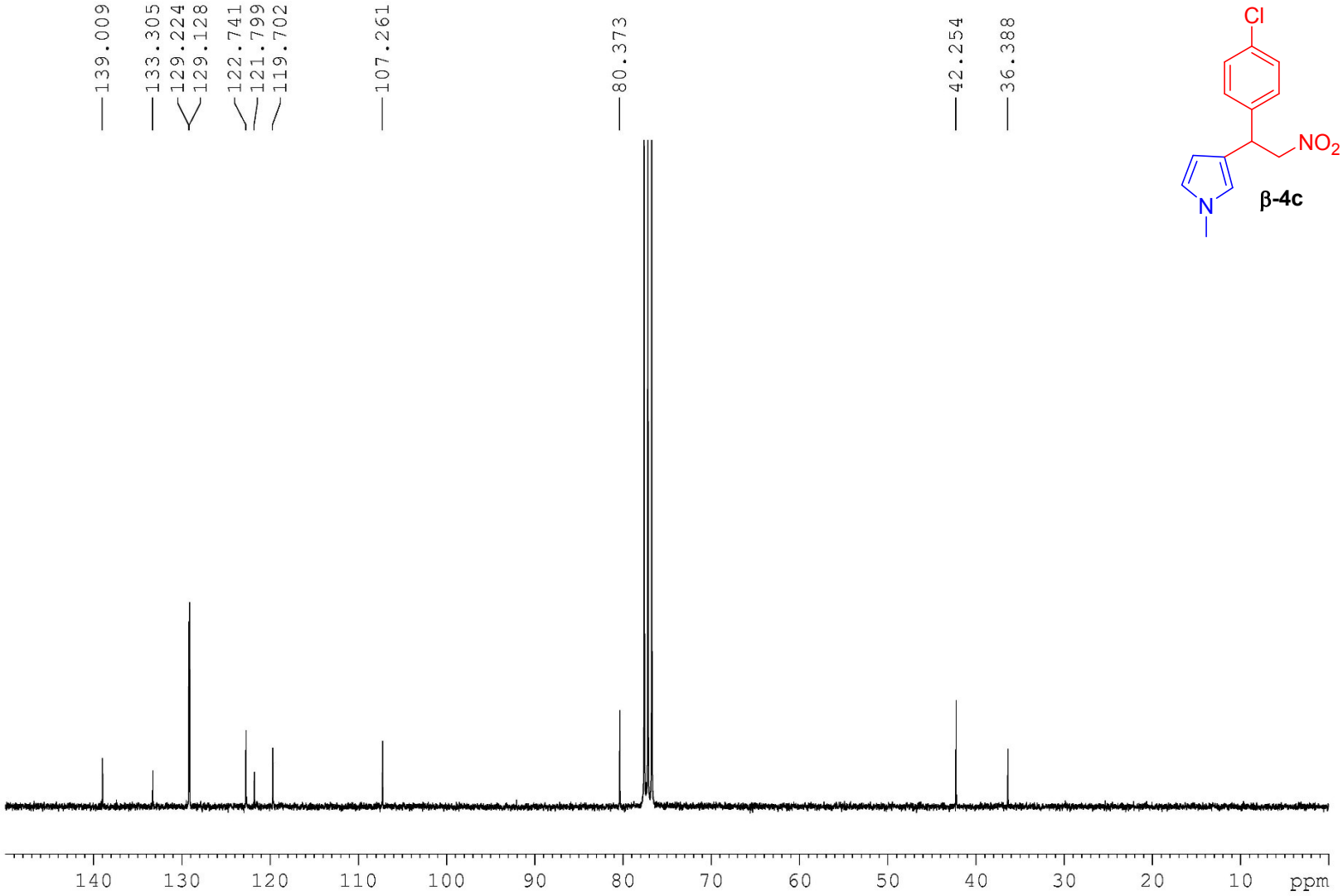



**Figure S22** $^{13}C$ NMR spectrum of derivative ***β*-4c** (300 MHz, $CDCl_3$, 298 K)

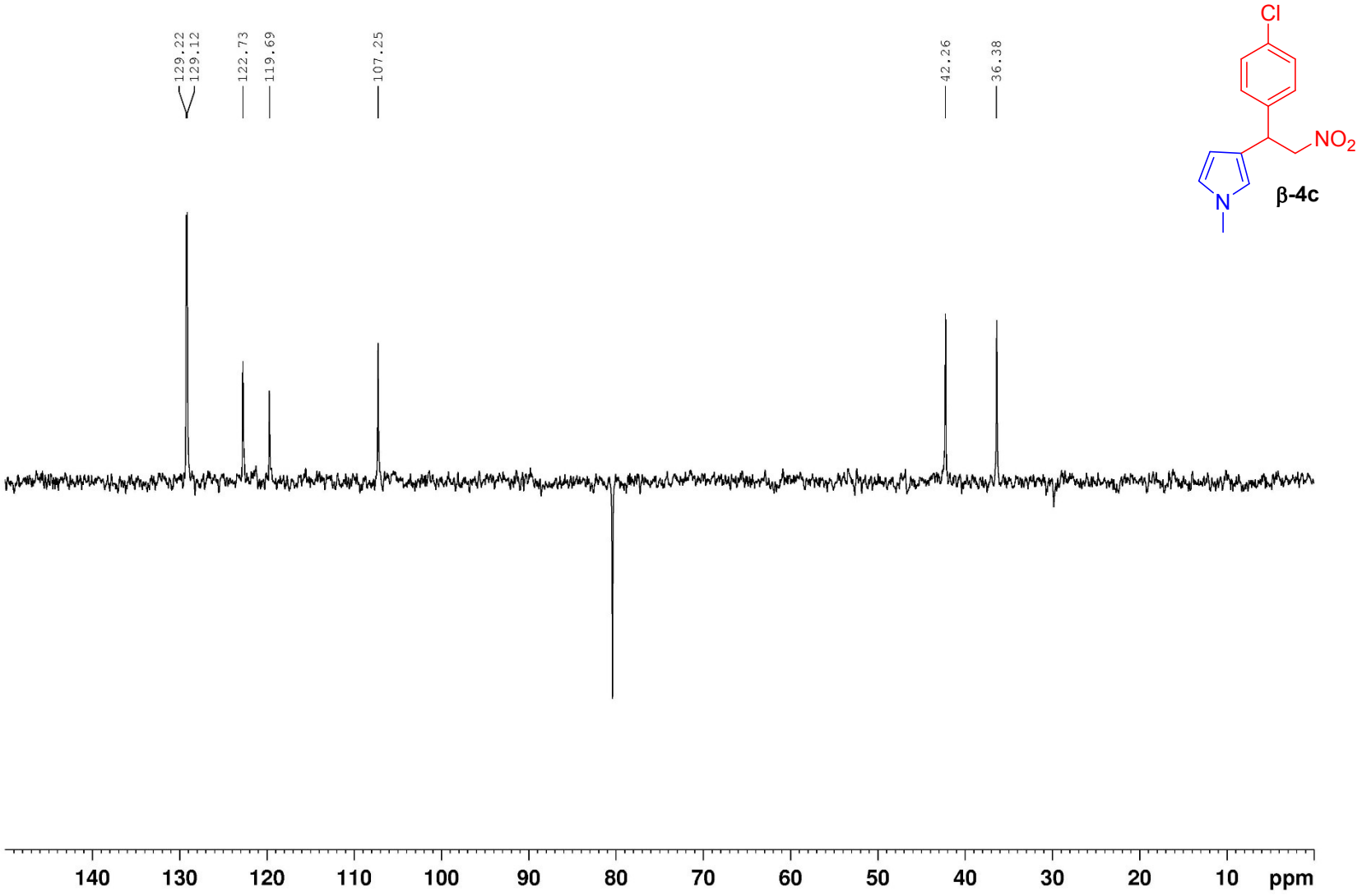



**Figure S23.** DEPT 135 NMR spectrum of derivative ***β*-4c** (300 MHz, $CDCl_3$, 298 K).

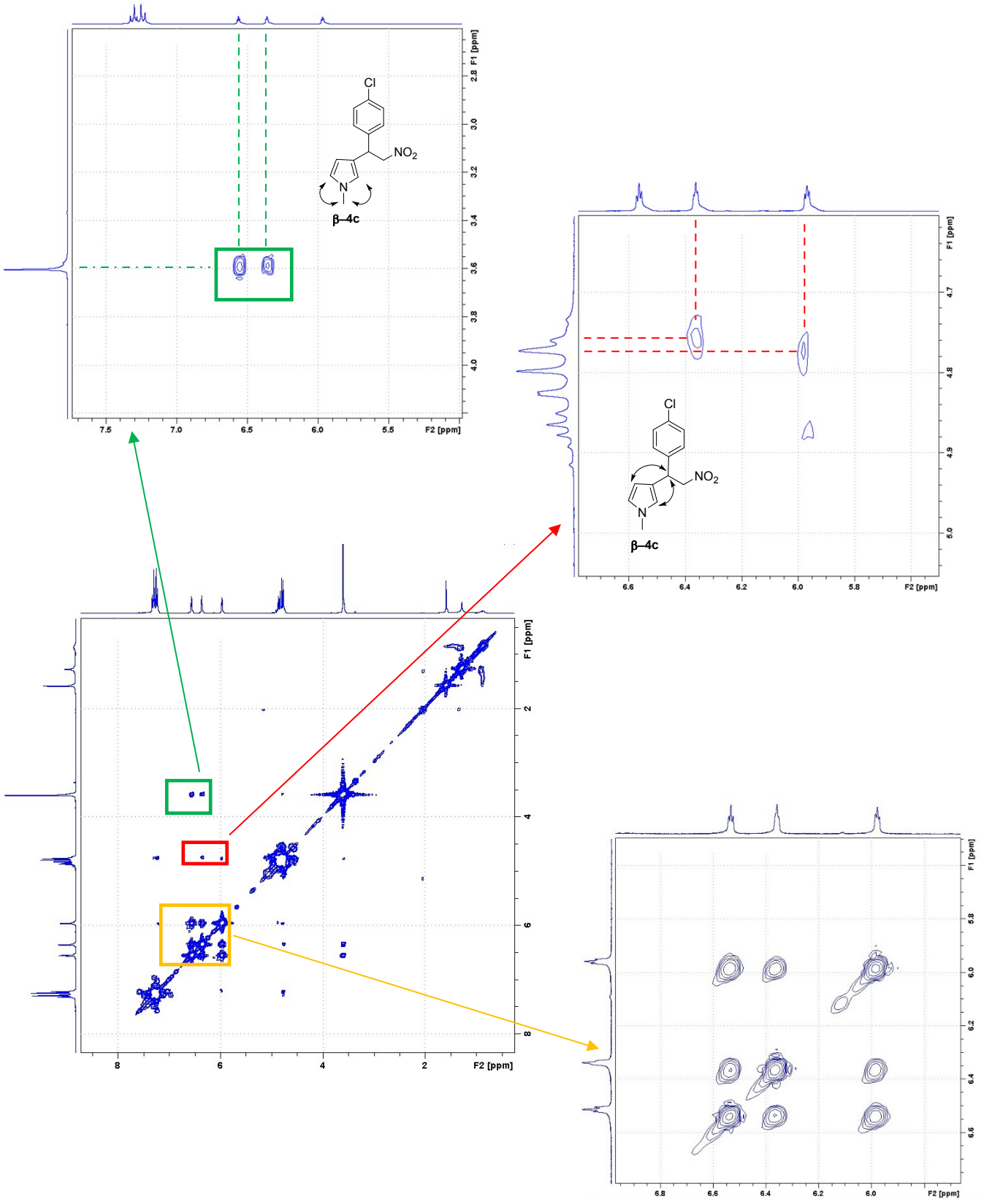



**Figure S24.** COSY NMR spectrum of derivative ***β*-4c** (300 MHz, $CDCl_3$, 298 K).

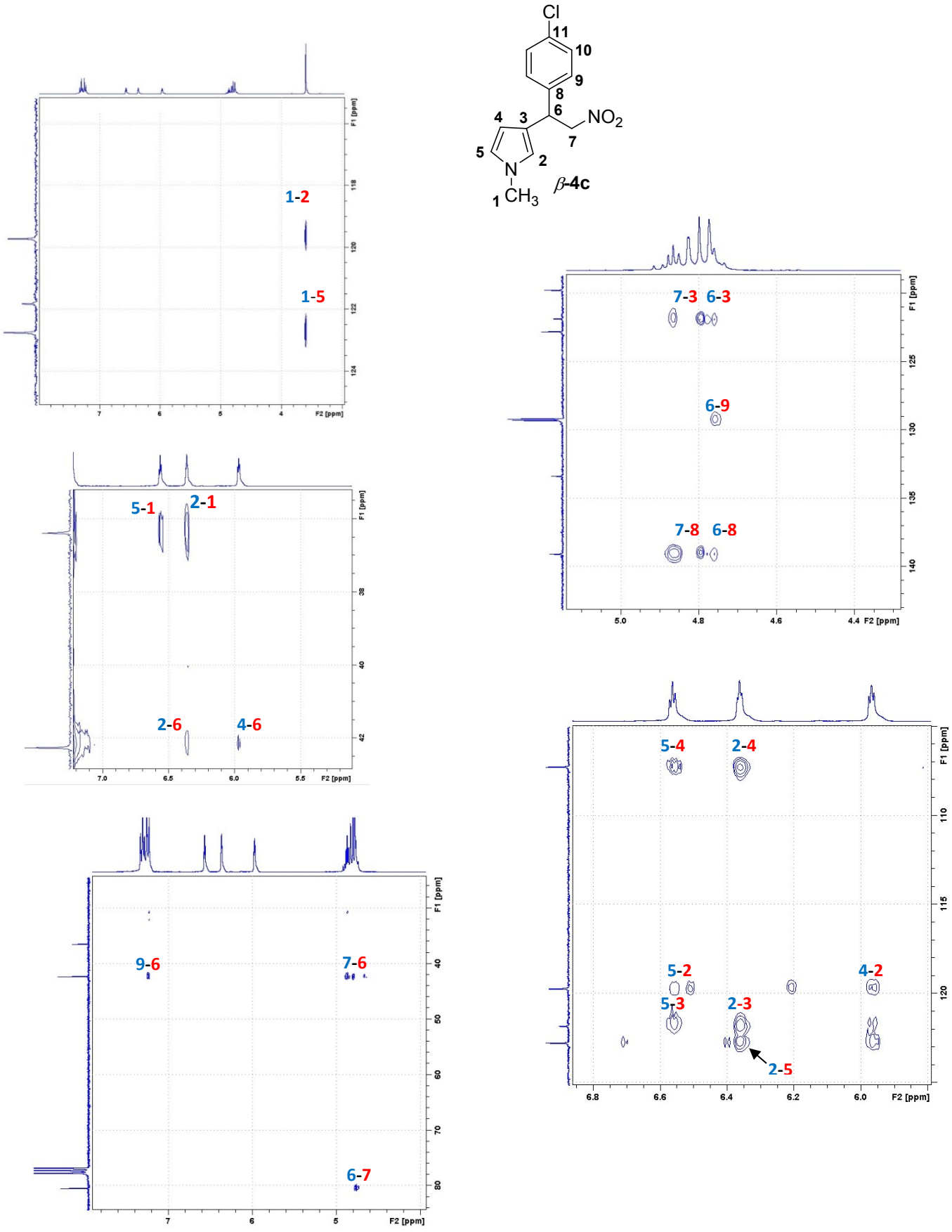



**Figure S25.** Relevant region of HMBC NMR spectrum of derivative ***β*-4c** (600 MHz, $CDCl_3$, 298 K). Protons are indicated with blue color and carbons with red color.

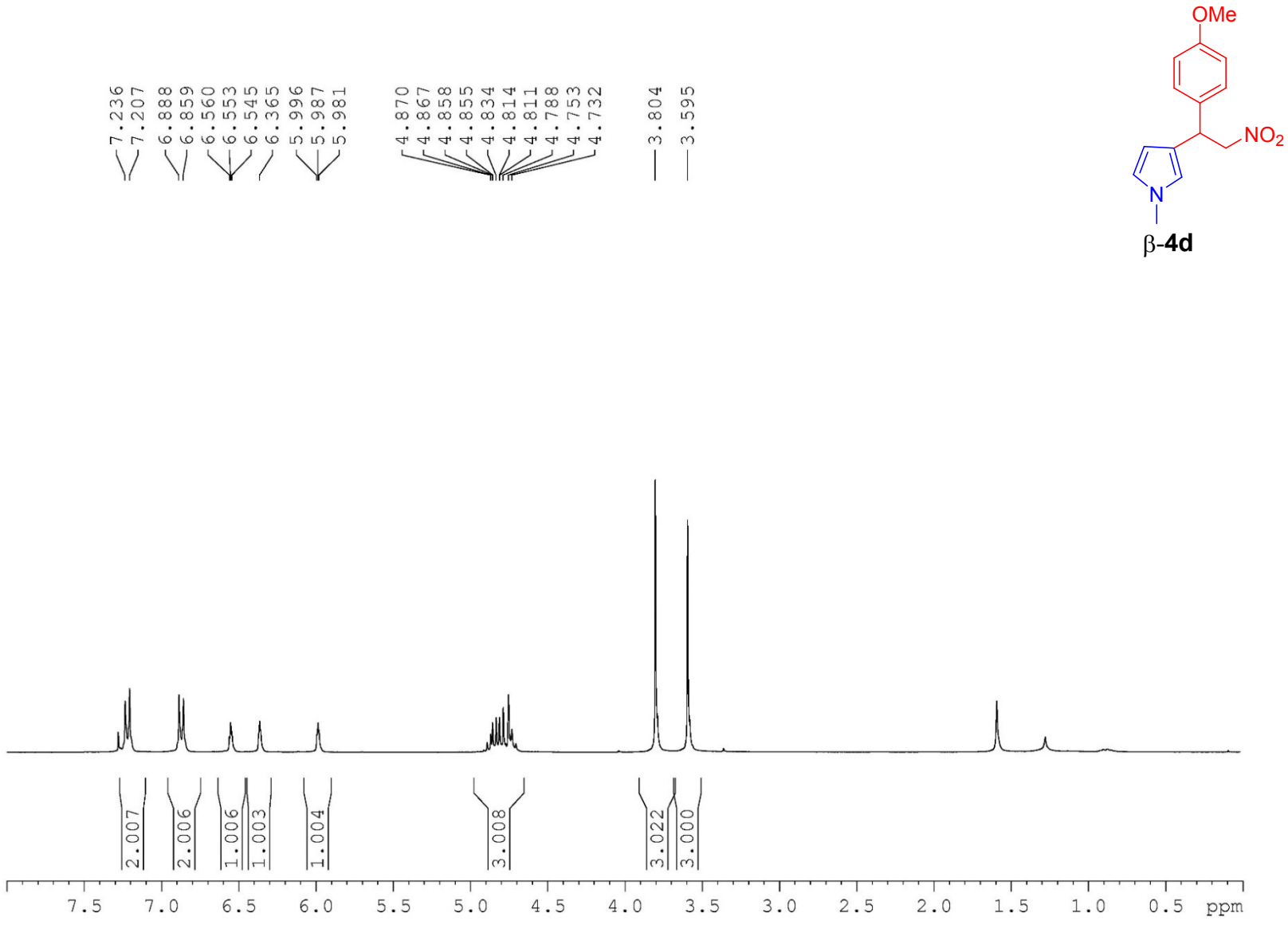



**Figure S26.** $^{1}$H NMR spectrum of derivative ***β*-4d** (300 MHz, $CDCl_3$, 298 K).

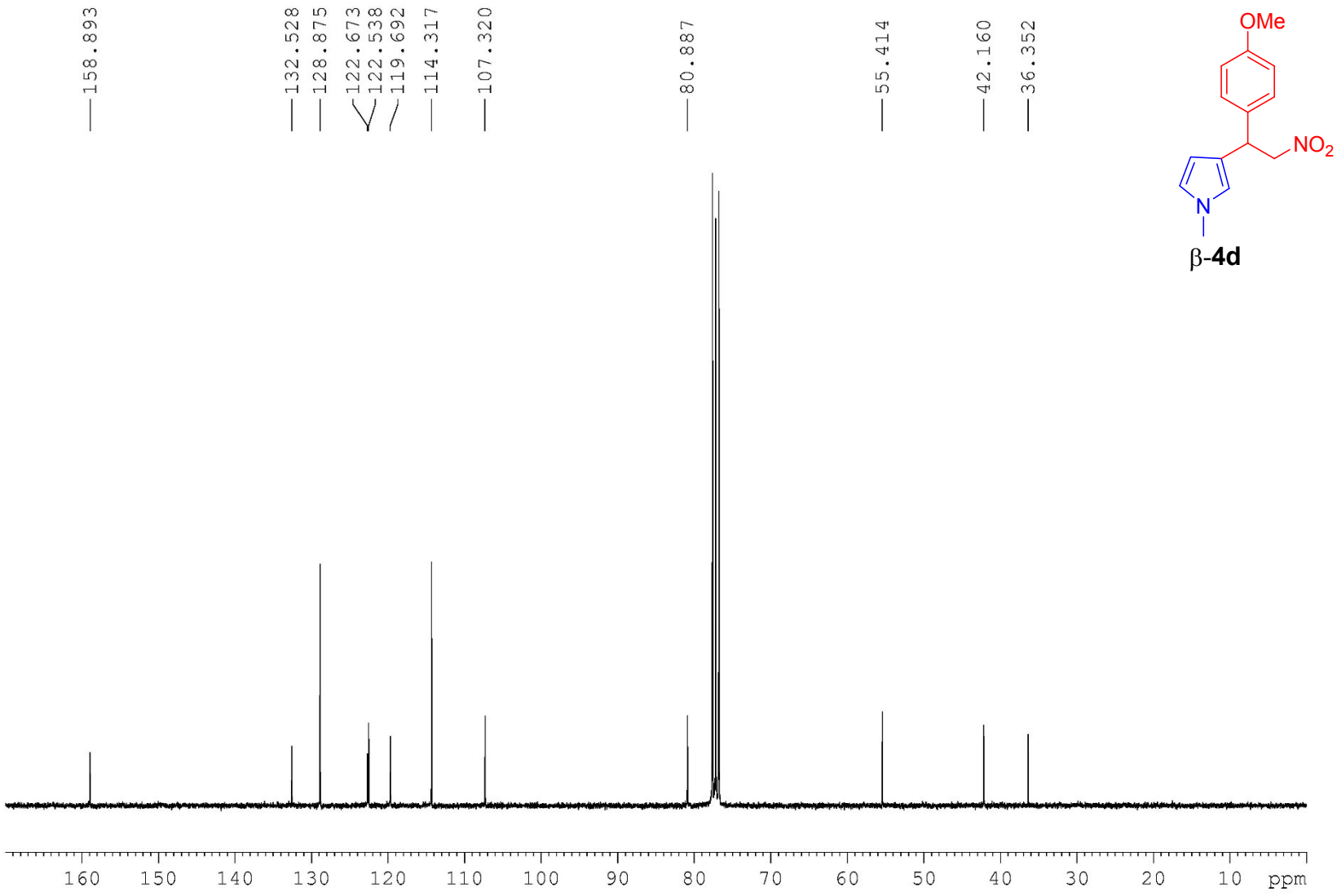



**Figure S27.** $^{13}C$ NMR spectrum of derivative ***β*-4d** (300 MHz, $CDCl_3$, 298 K).

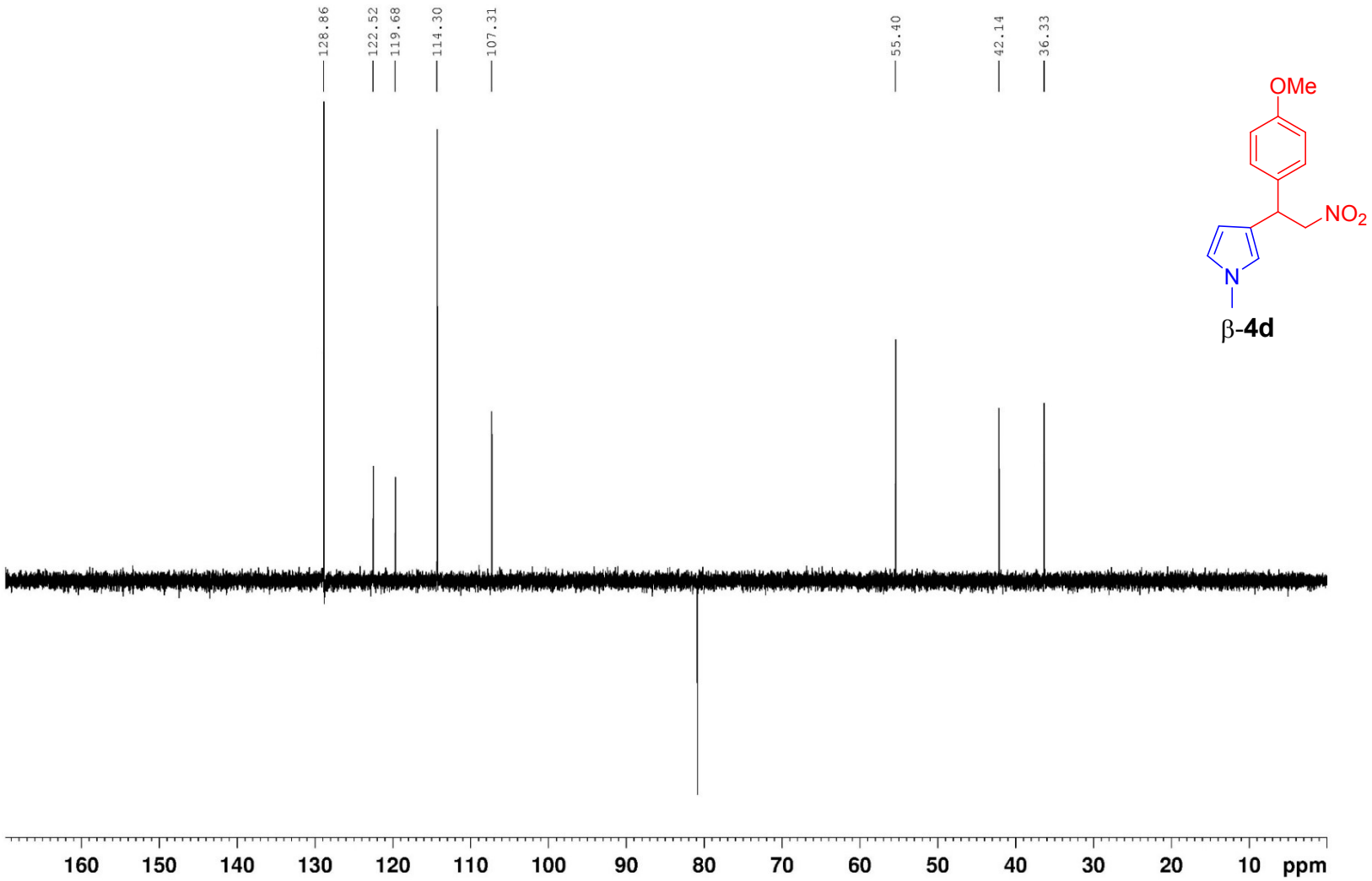



**Figure S28.** DEPT 135 NMR spectrum of derivative ***β*-4d** (300 MHz, $CDCl_3$, 298 K).

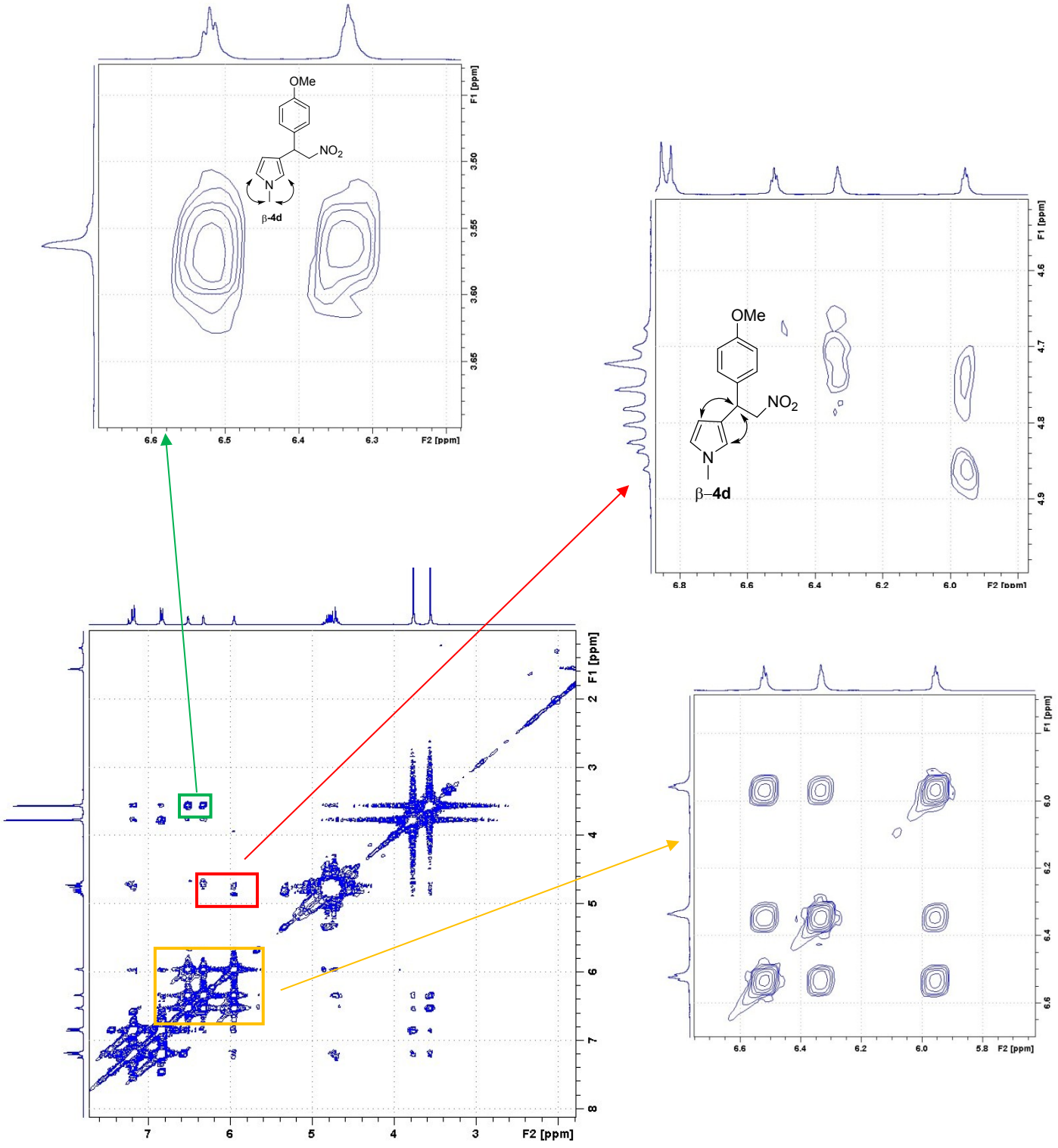



**Figure S29.** COSY NMR spectrum of derivative ***β*-4d** (300 MHz, $CDCl_3$, 298 K).

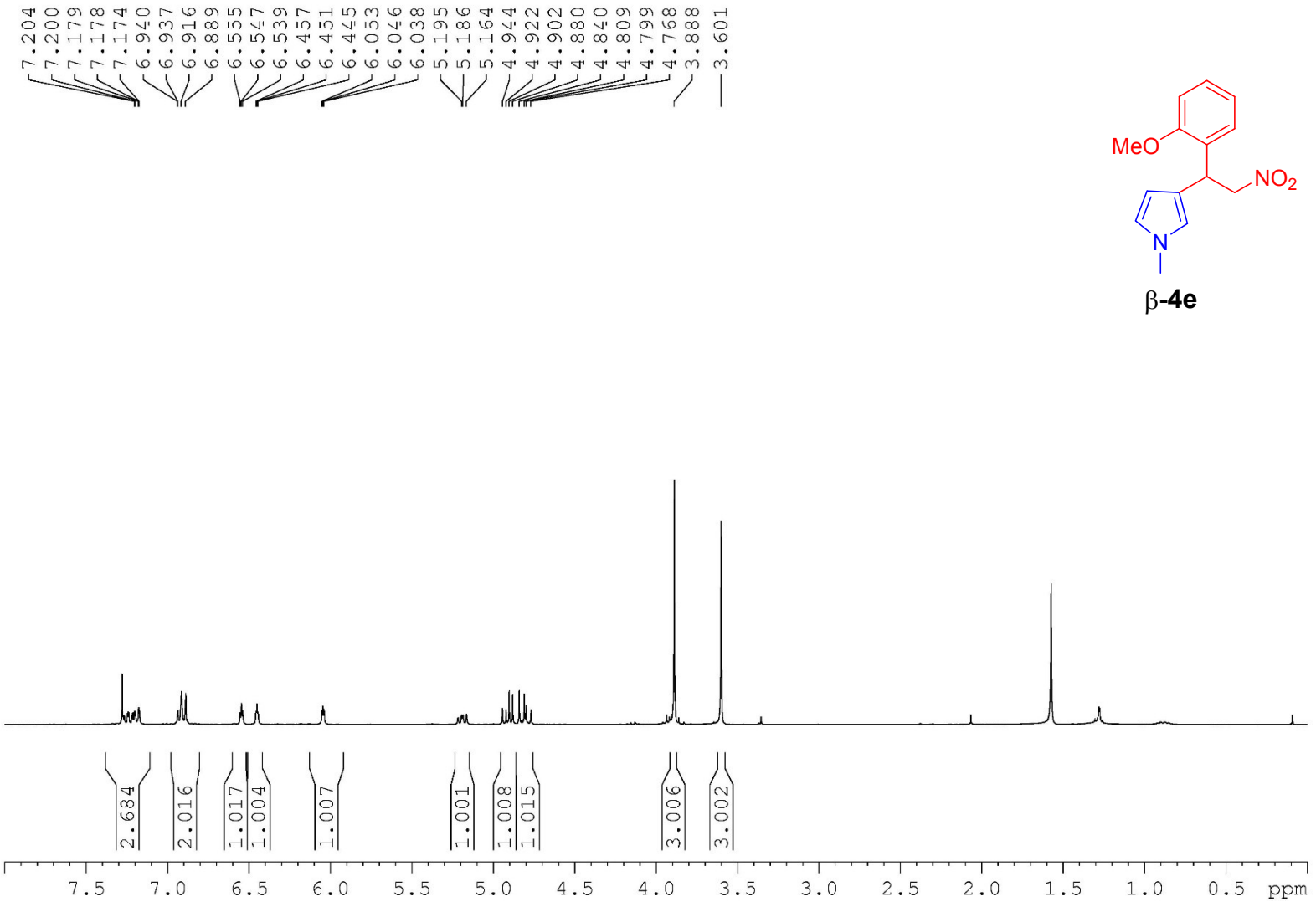



**Figure S30.** $^{1}$H NMR spectrum of derivative ***β*-4e** (300 MHz, $CDCl_3$, 298 K).

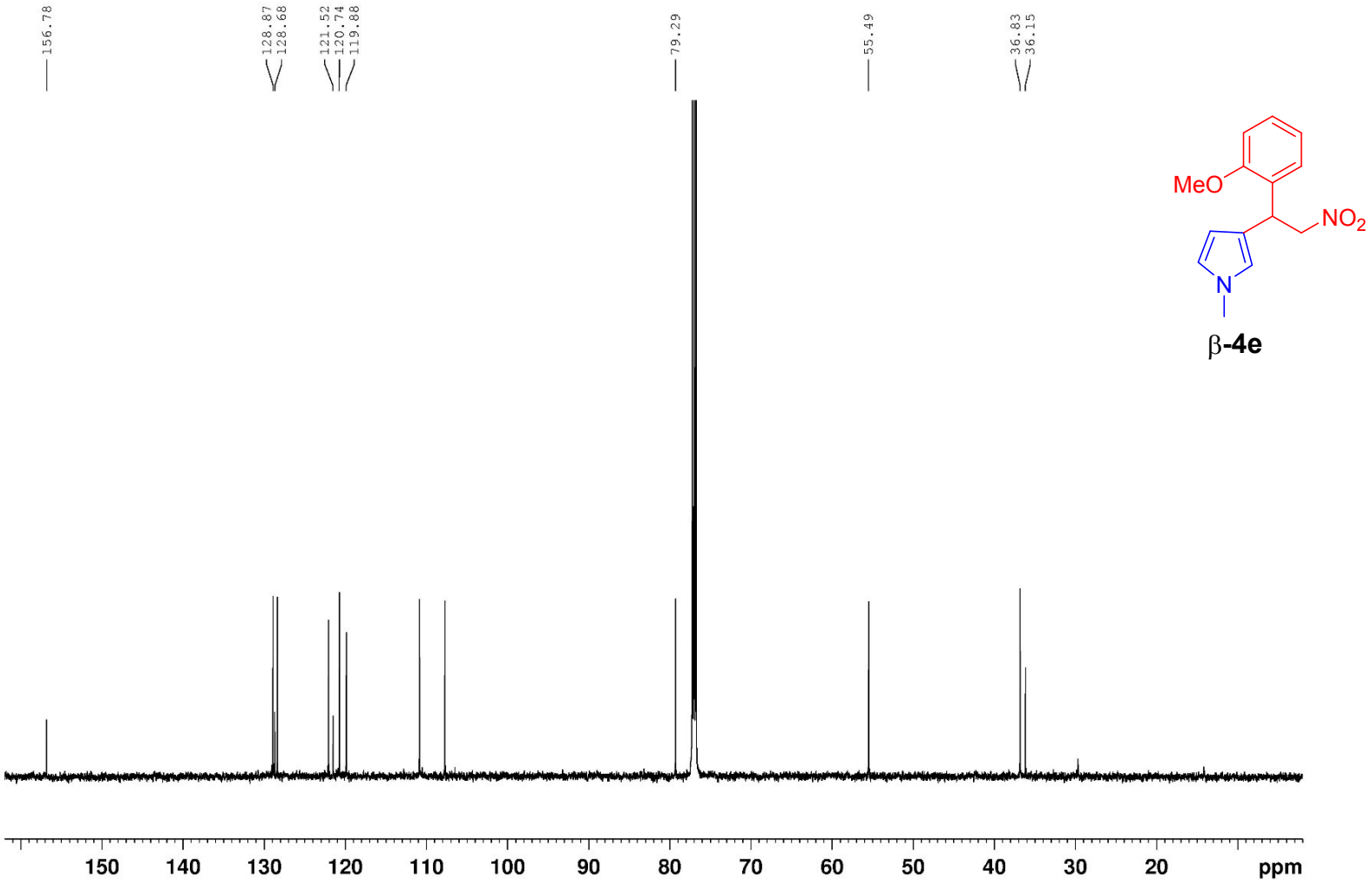



**Figure S31** $^{13}C$ NMR spectrum of derivative ***β*-4e** (300 MHz, $CDCl_3$, 298 K).

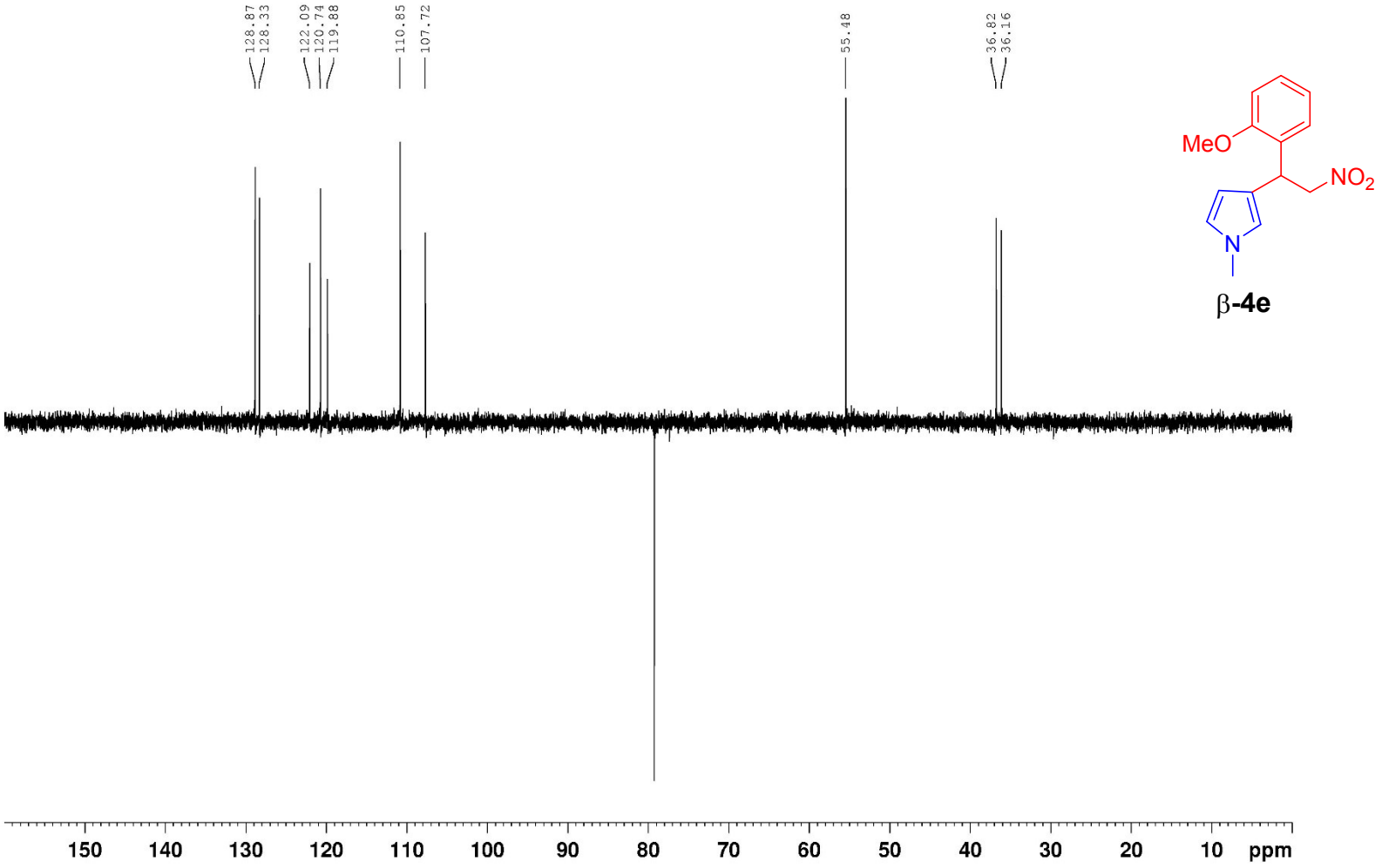



**Figure S32.** DEPT 135 NMR spectrum of derivative ***β*-4e** (600 MHz, $CDCl_3$, 298 K).

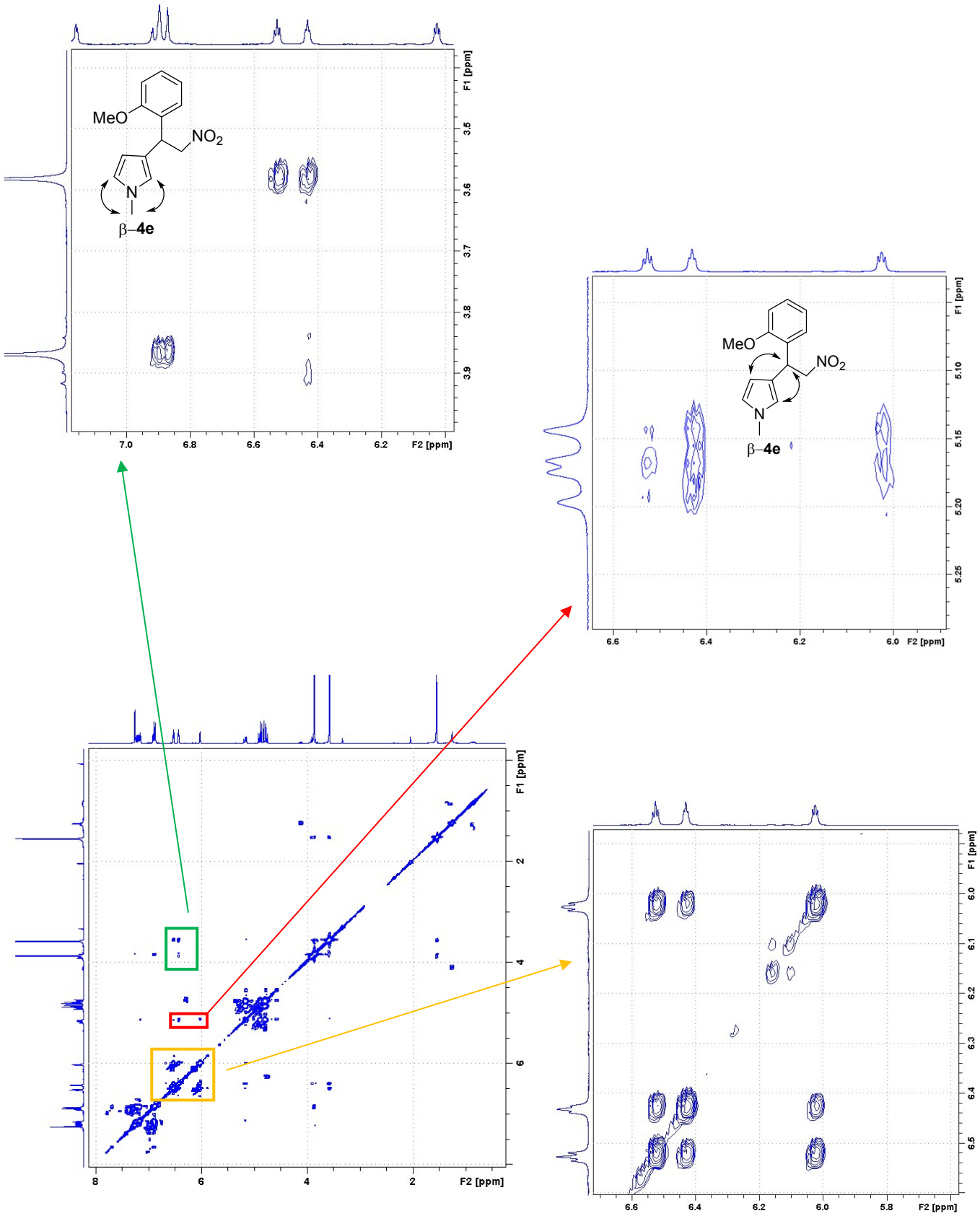
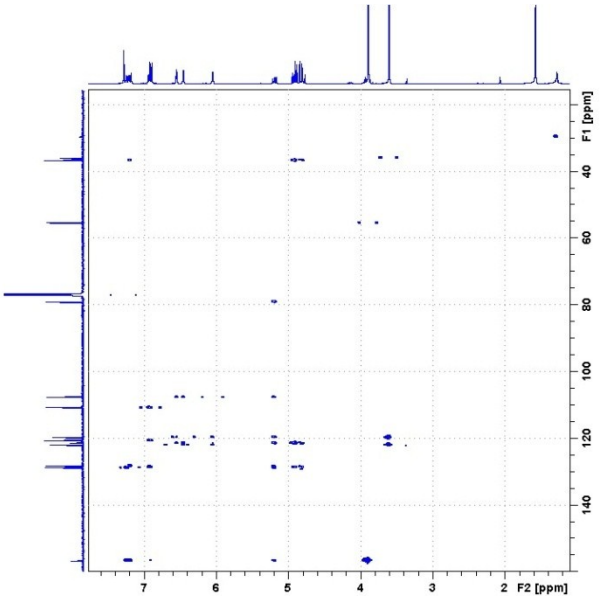
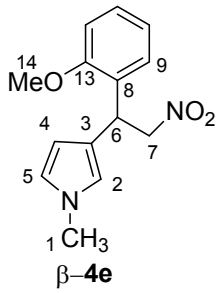



**Figure S33.** COSY NMR spectrum of derivative ***β*-4e** (300 MHz, $CDCl_3$, 298 K).

**a)**




β–**4e**

**b)**

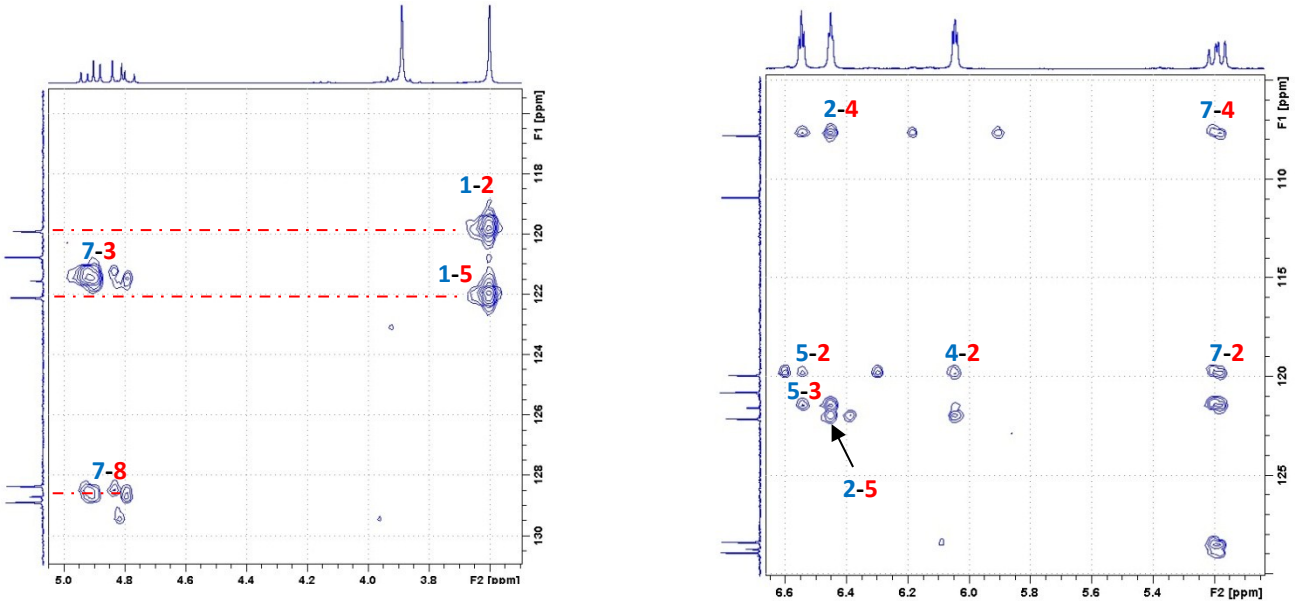



**Figure S34.** a) HMBC NMR spectrum of derivative ***β*-4e** (600 MHz, $CDCl_3$, 298 K). b) Relevant region of HMBC NMR spectrum of derivative ***β*-4e**. Protons are indicated with blue color and carbons with red color.

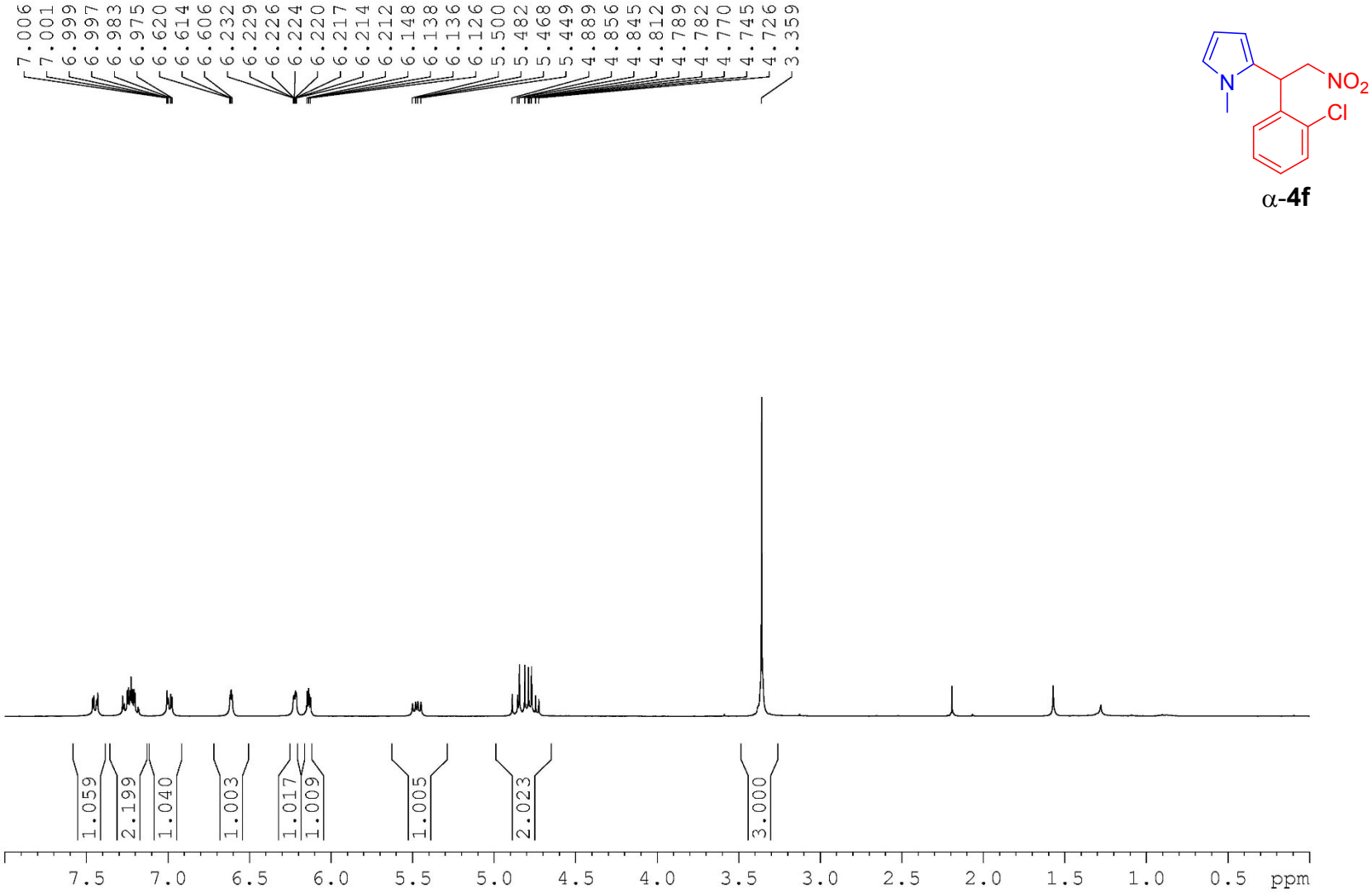



**Figure S35.** $^{1}$H NMR spectrum of derivative ***α*-4f** (300 MHz, $CDCl_3$, 298 K).

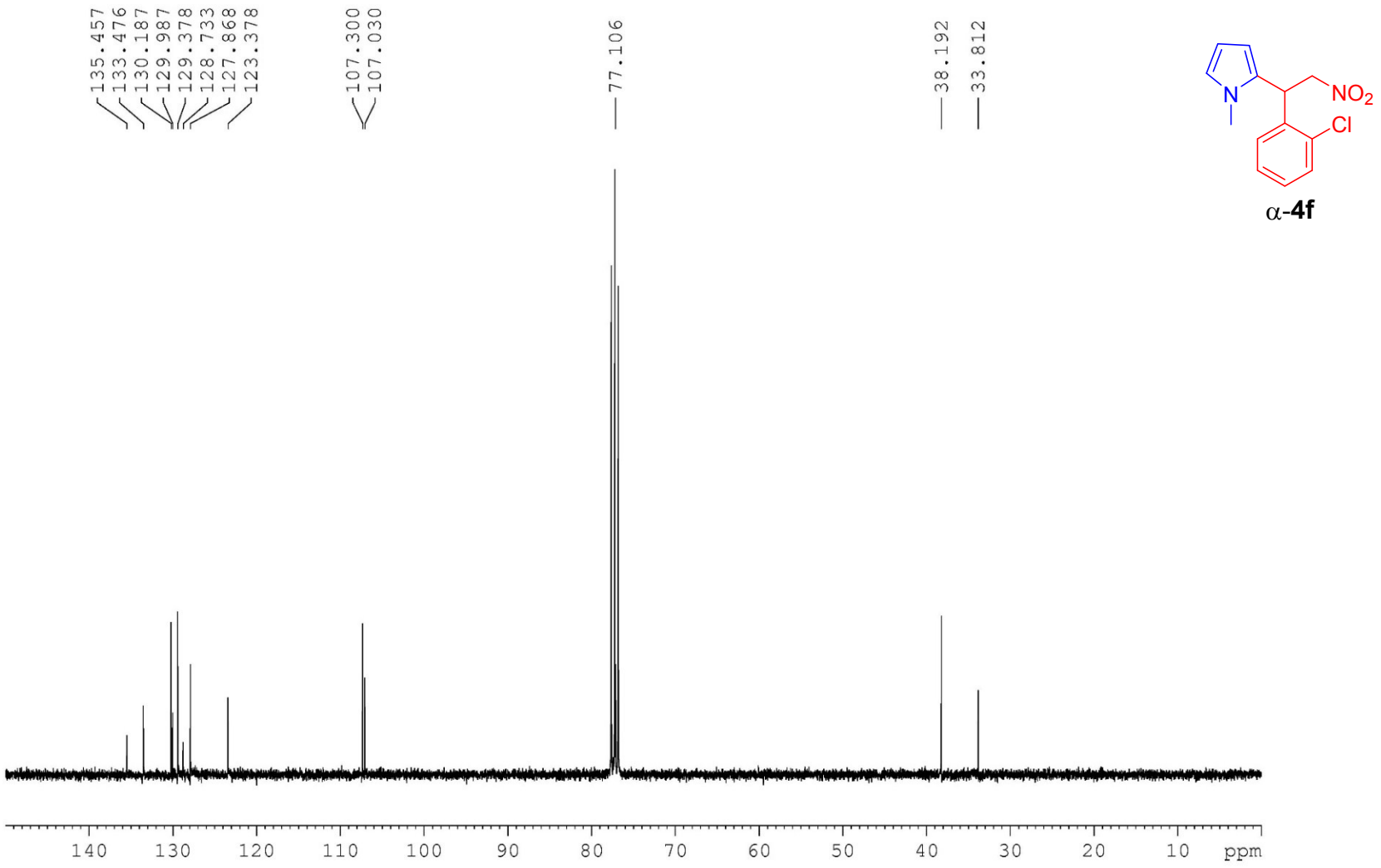



**Figure S36.** $^{13}C$ NMR spectrum of derivative ***α*-4f** (300 MHz, $CDCl_3$, 298 K).

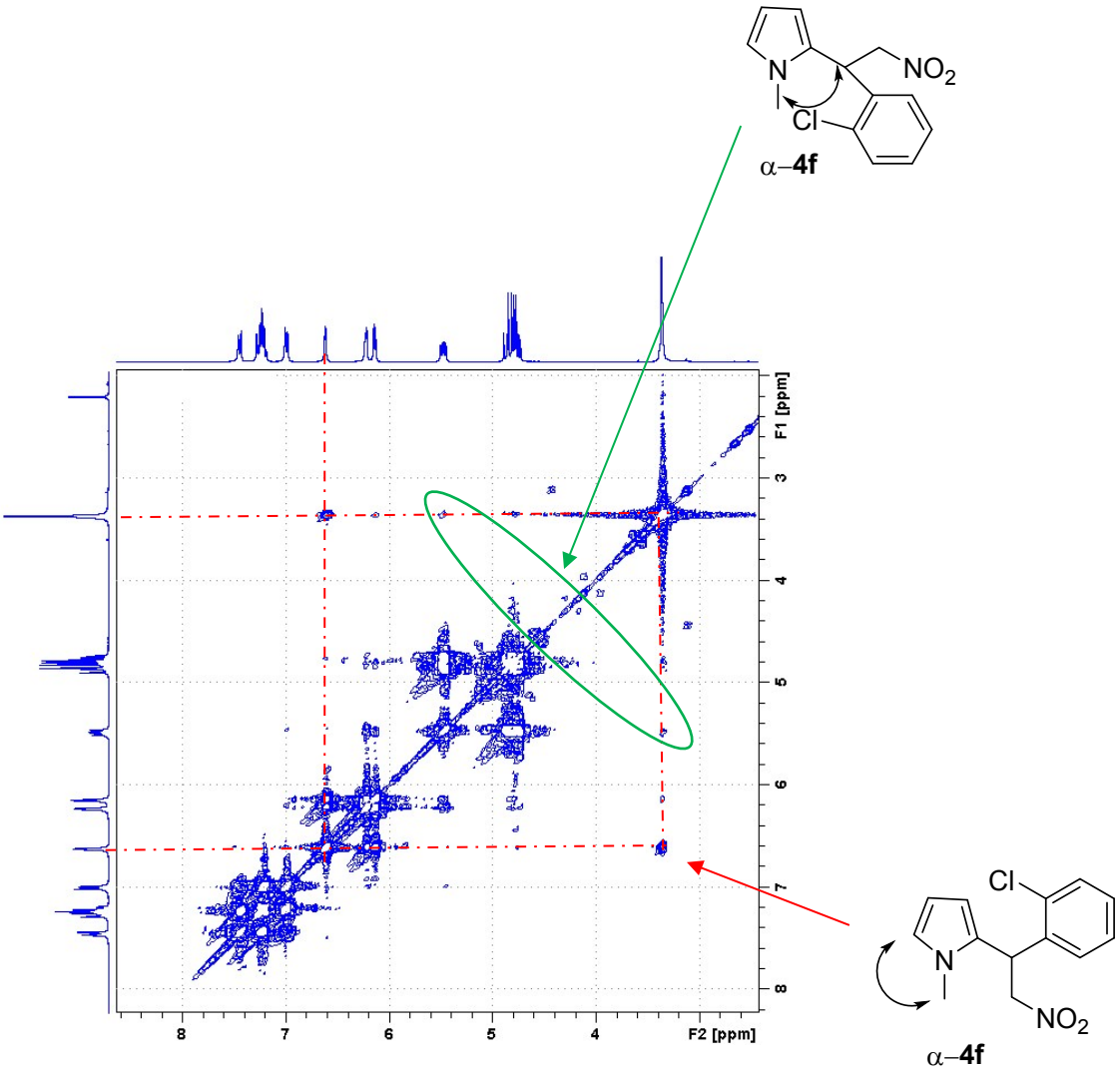



**Figure S37.** COSY NMR spectrum of derivative ***α*-4f** (300 MHz, $CDCl_3$, 298 K).

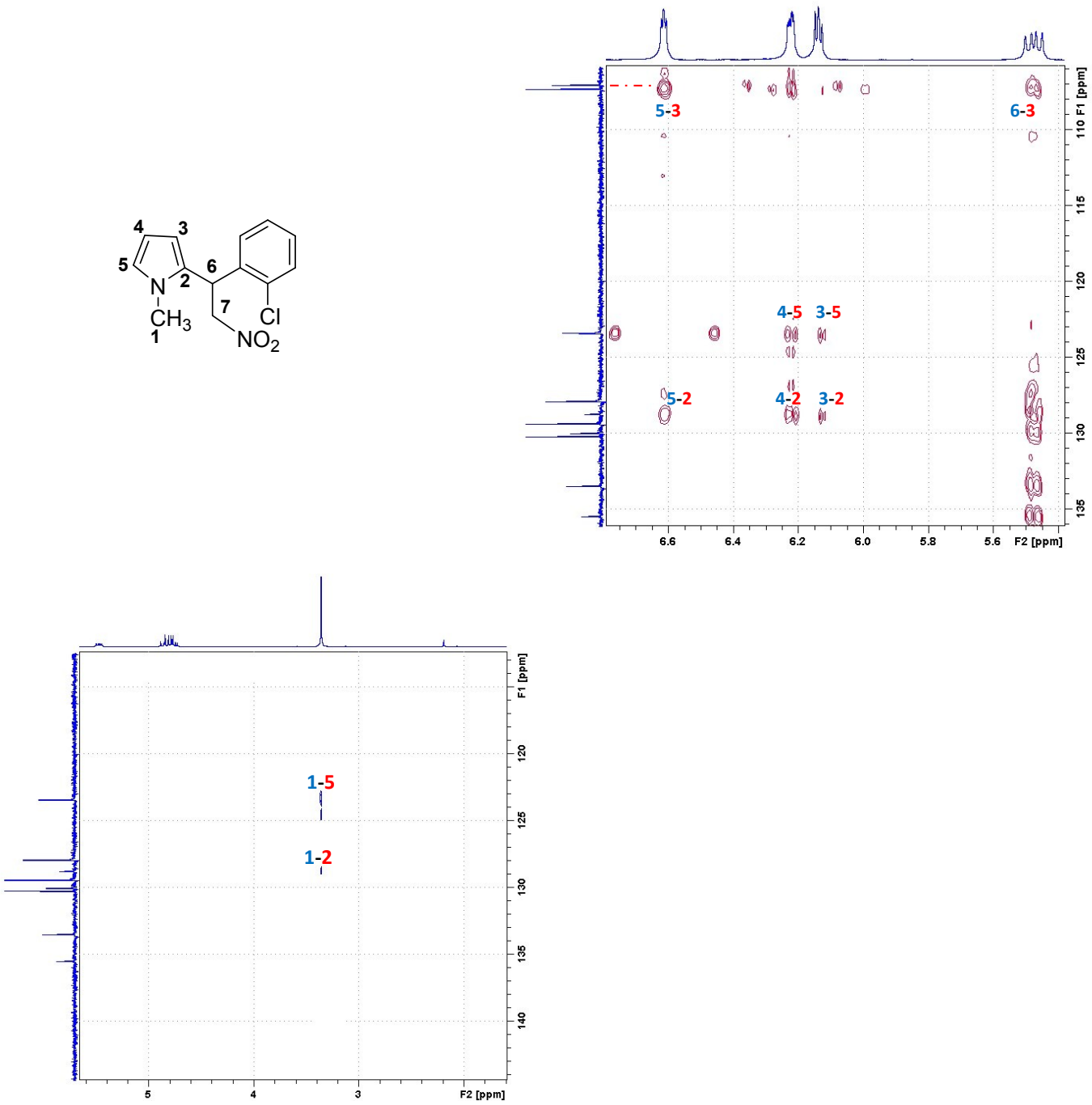



**Figure S38.** Relevant region of HMBC NMR spectrum of derivative ***a*-4f**. Protons are indicated with blue color and carbons with red color (600 MHz, $CDCl_3$, 298 K).

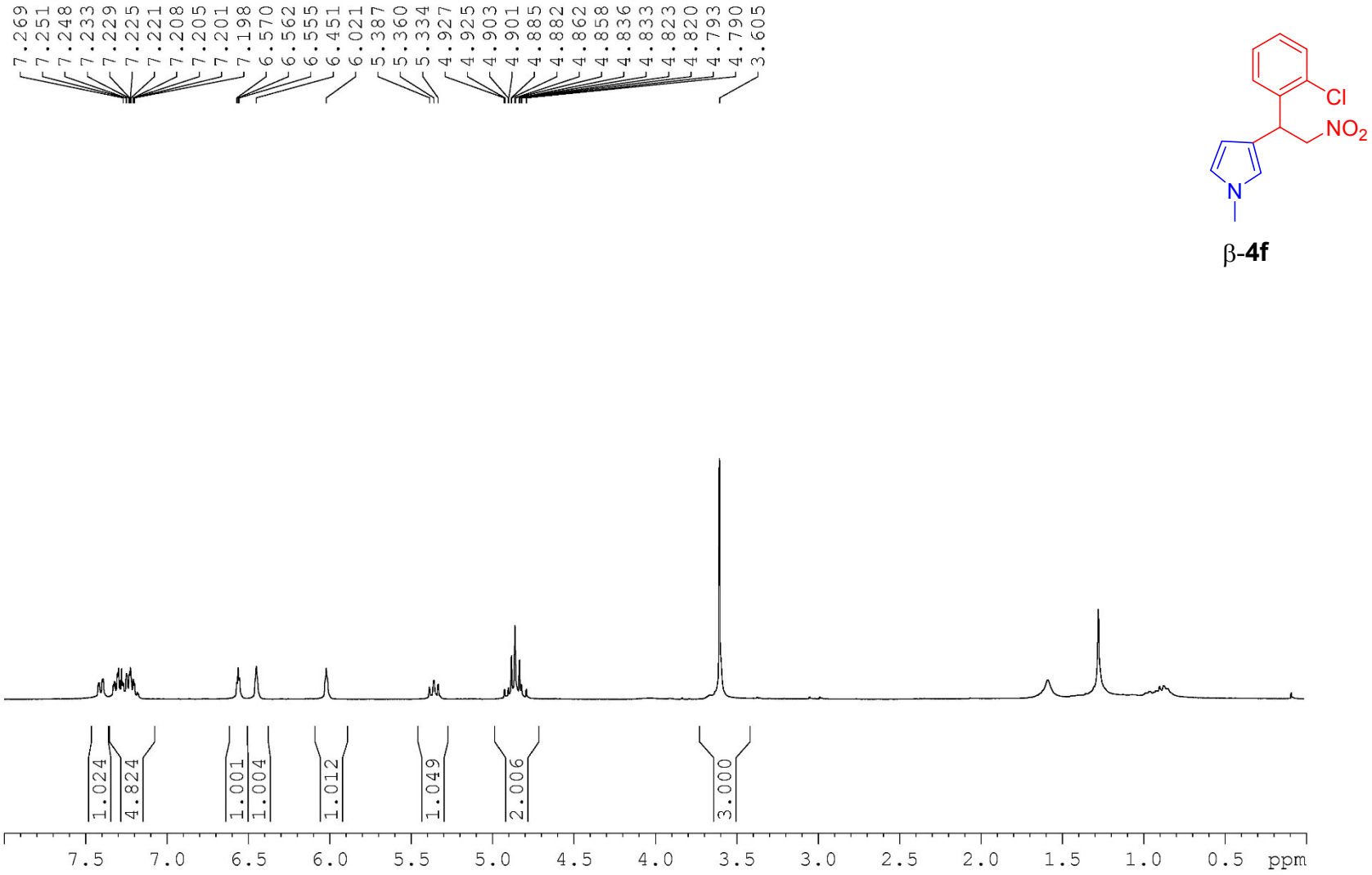



**Figure S39.** $^{1}$H NMR spectrum of derivative ***β*-4f** (300 MHz, $CDCl_3$, 298 K).

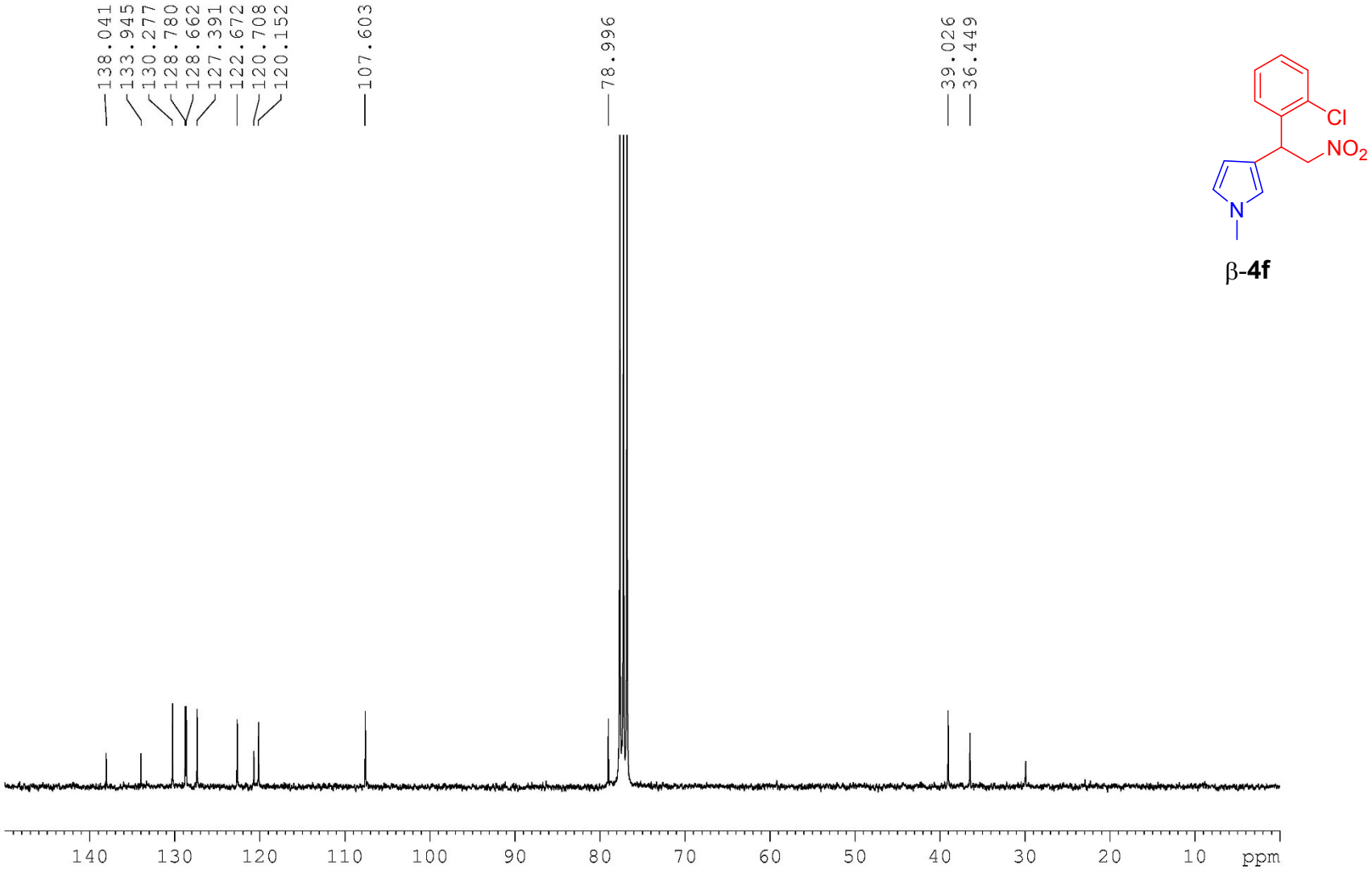



**Figure S40.** $^{13}C$ NMR spectrum of derivative ***β*-4f** (300 MHz, $CDCl_3$, 298 K).

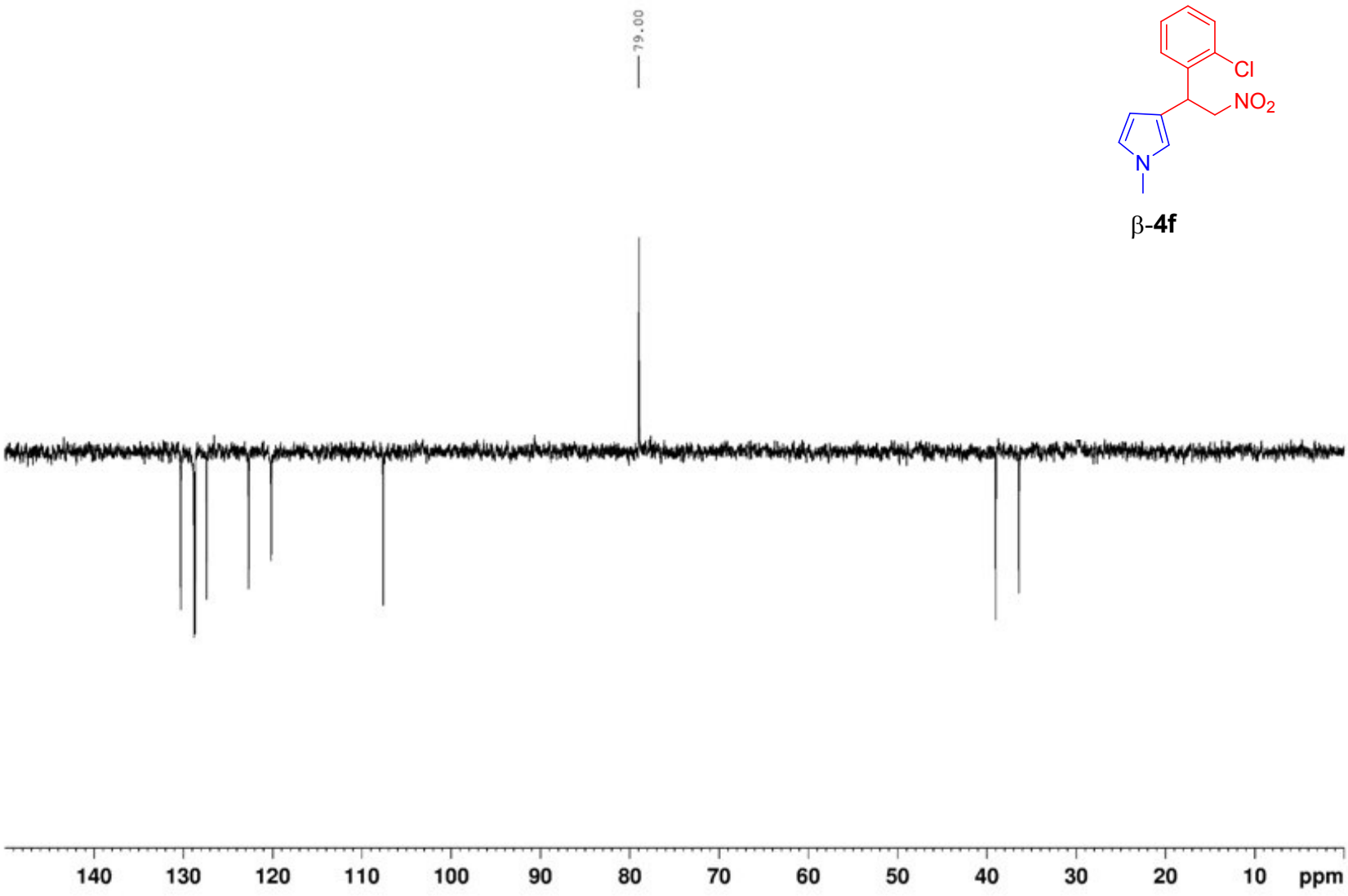



**Figure S41.** DEPT 135 NMR spectrum of derivative ***β*-4f** (300 MHz, $CDCl_3$, 298 K).

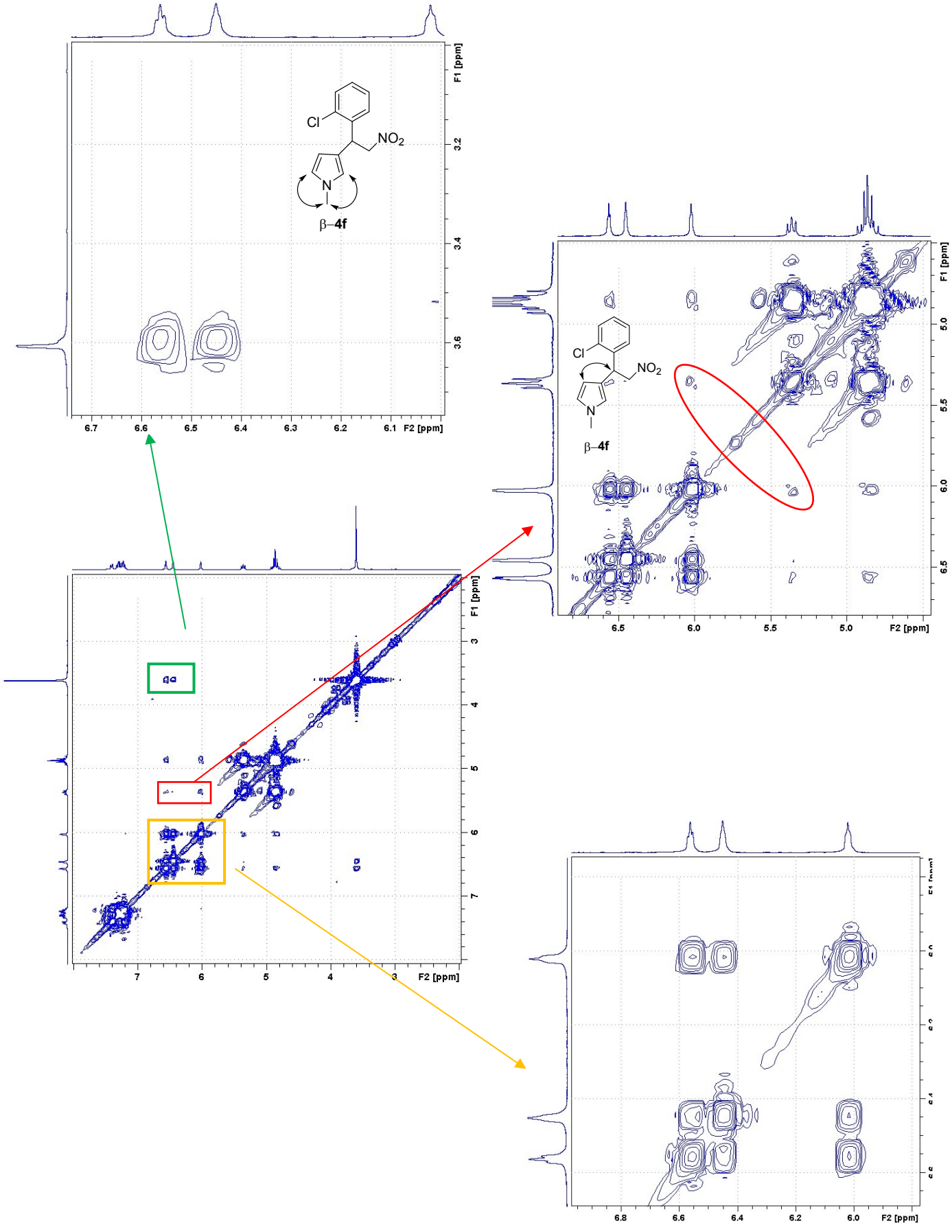



**Figure S42.** COSY NMR spectrum of derivative ***β*-4f** (300 MHz, $CDCl_3$, 298 K).

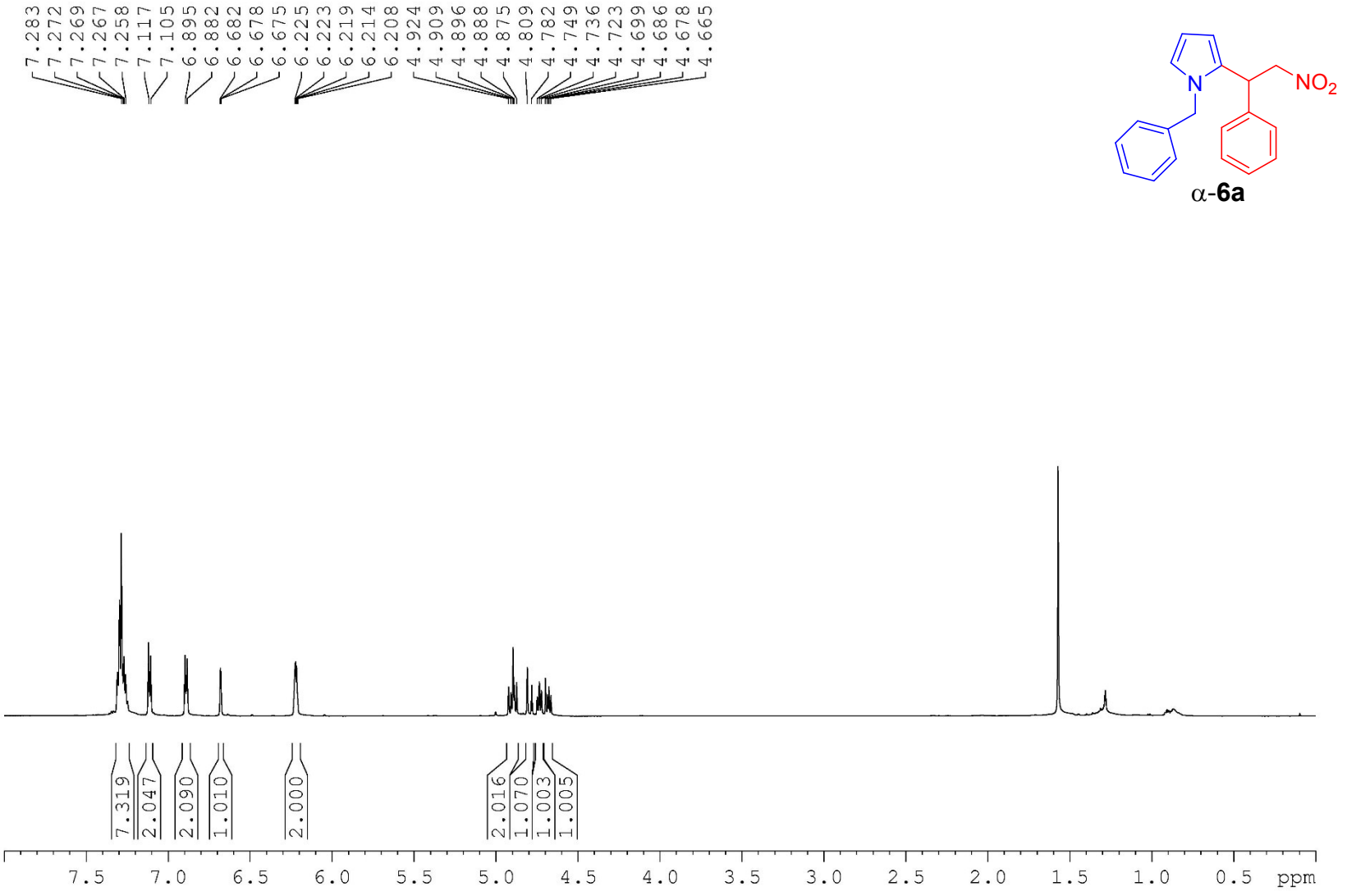



**Figure S43.** $^{1}$H NMR spectrum of derivative ***α*-6a** (600 MHz, $CDCl_3$, 298 K).

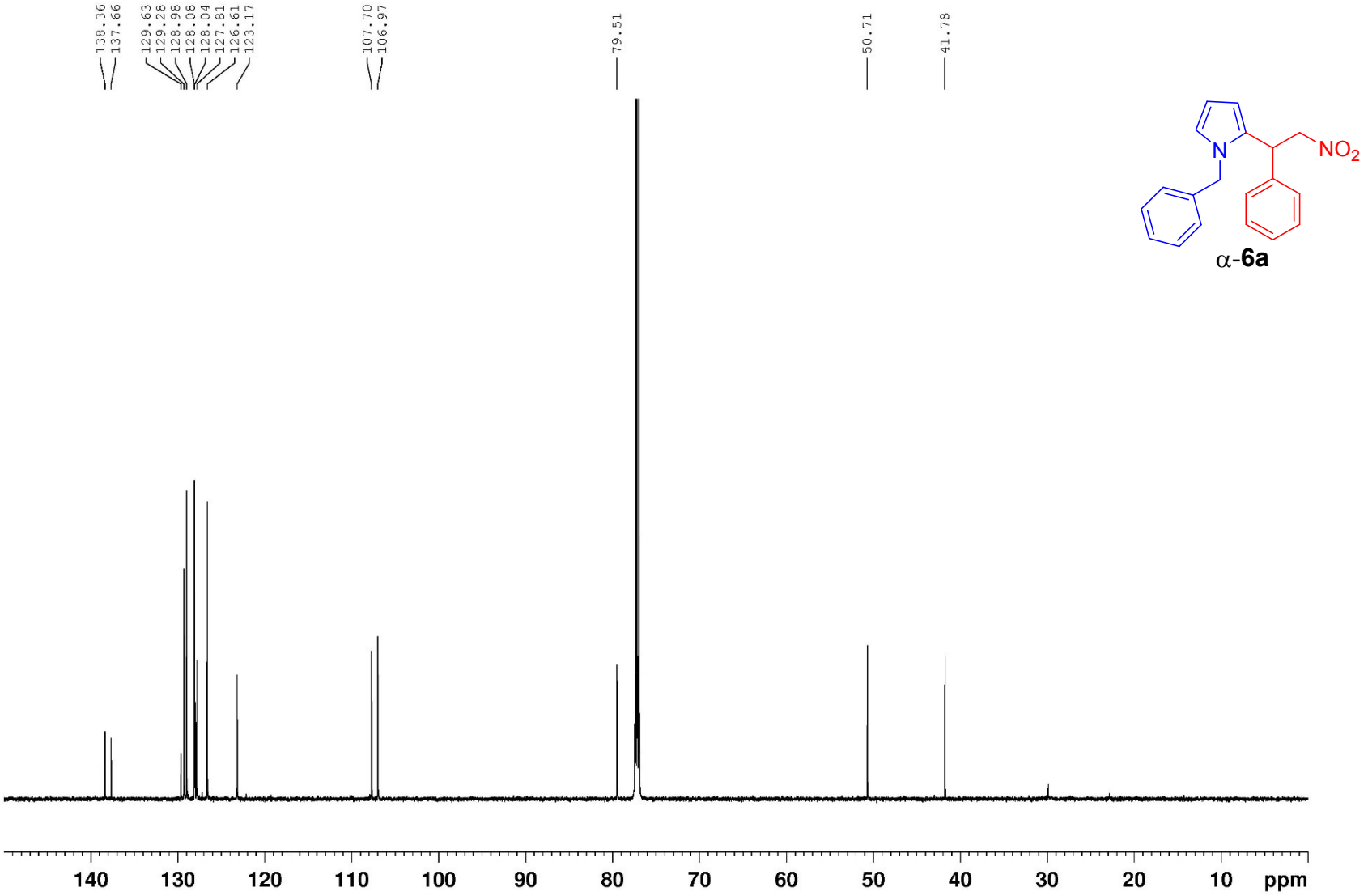



**Figure S44.** $^{13}C$ NMR spectrum of derivative ***α*-6a** (600 MHz, $CDCl_3$, 298 K).

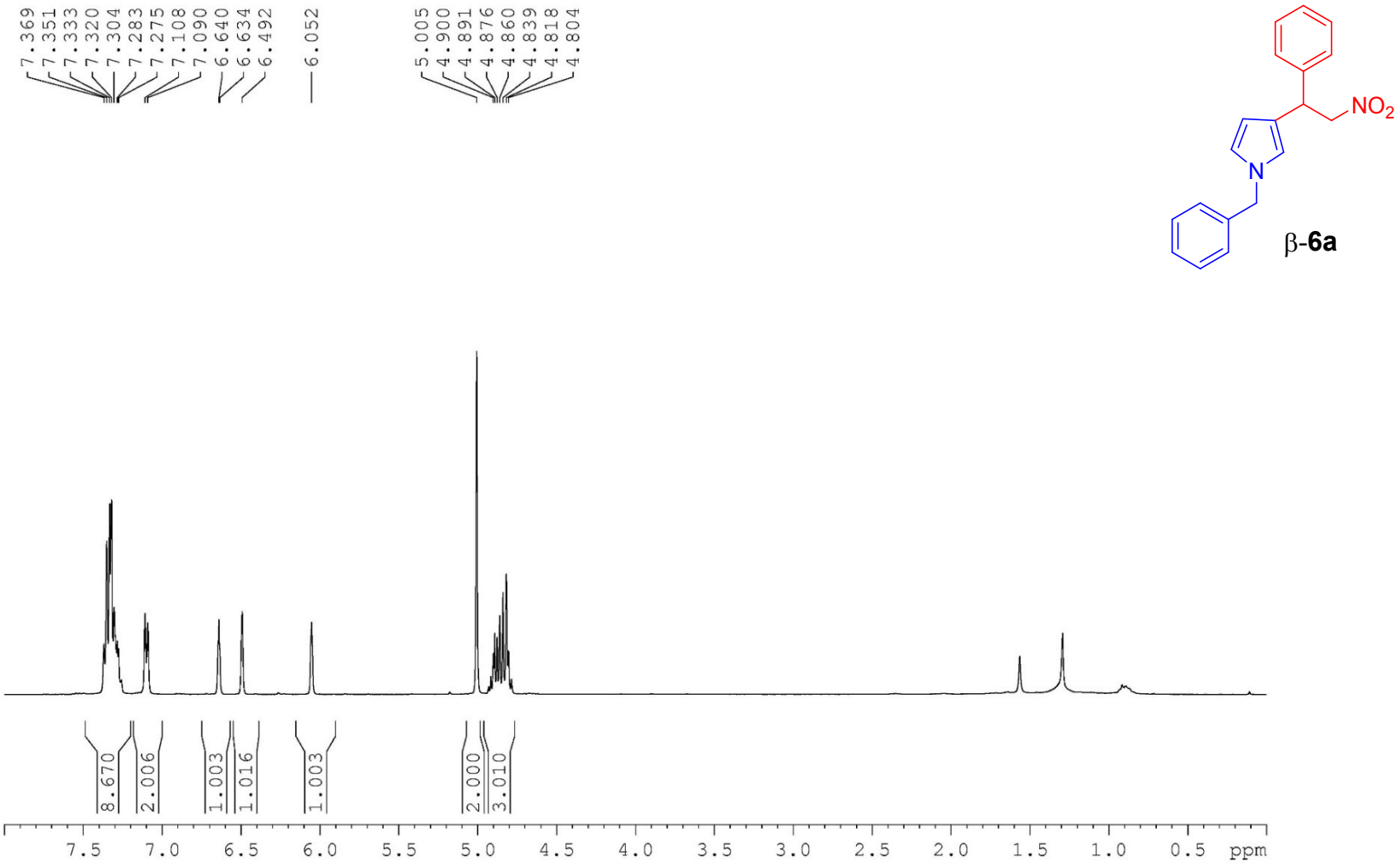



**Figure S45.** $^{1}$H NMR spectrum of derivative ***β*-6a** (400 MHz, $CDCl_3$, 298 K).

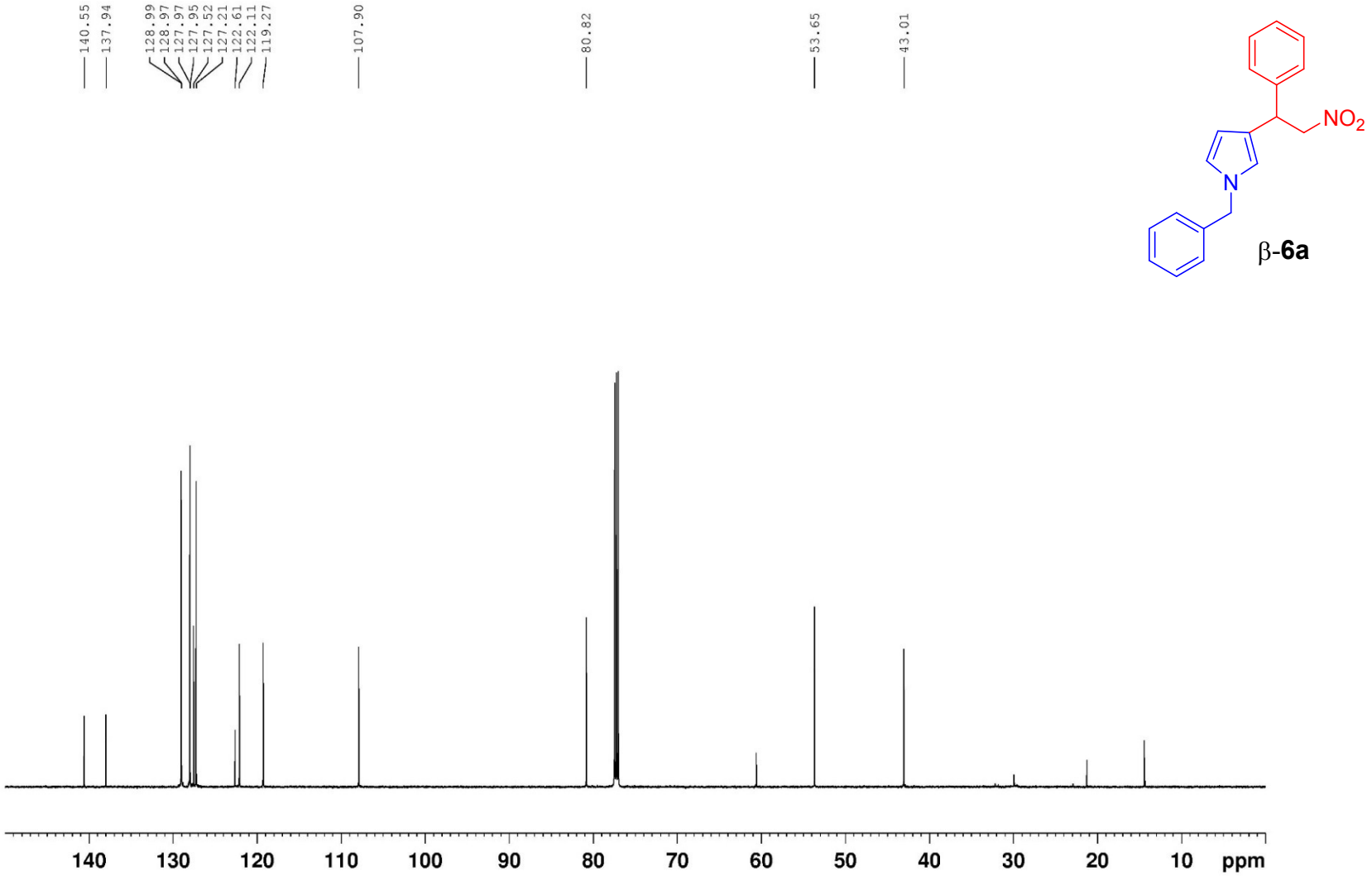



**Figure S46.** $^{13}$CNMR spectrum of derivative ***β*-6a** (400 MHz, $CDCl_3$, 298 K).

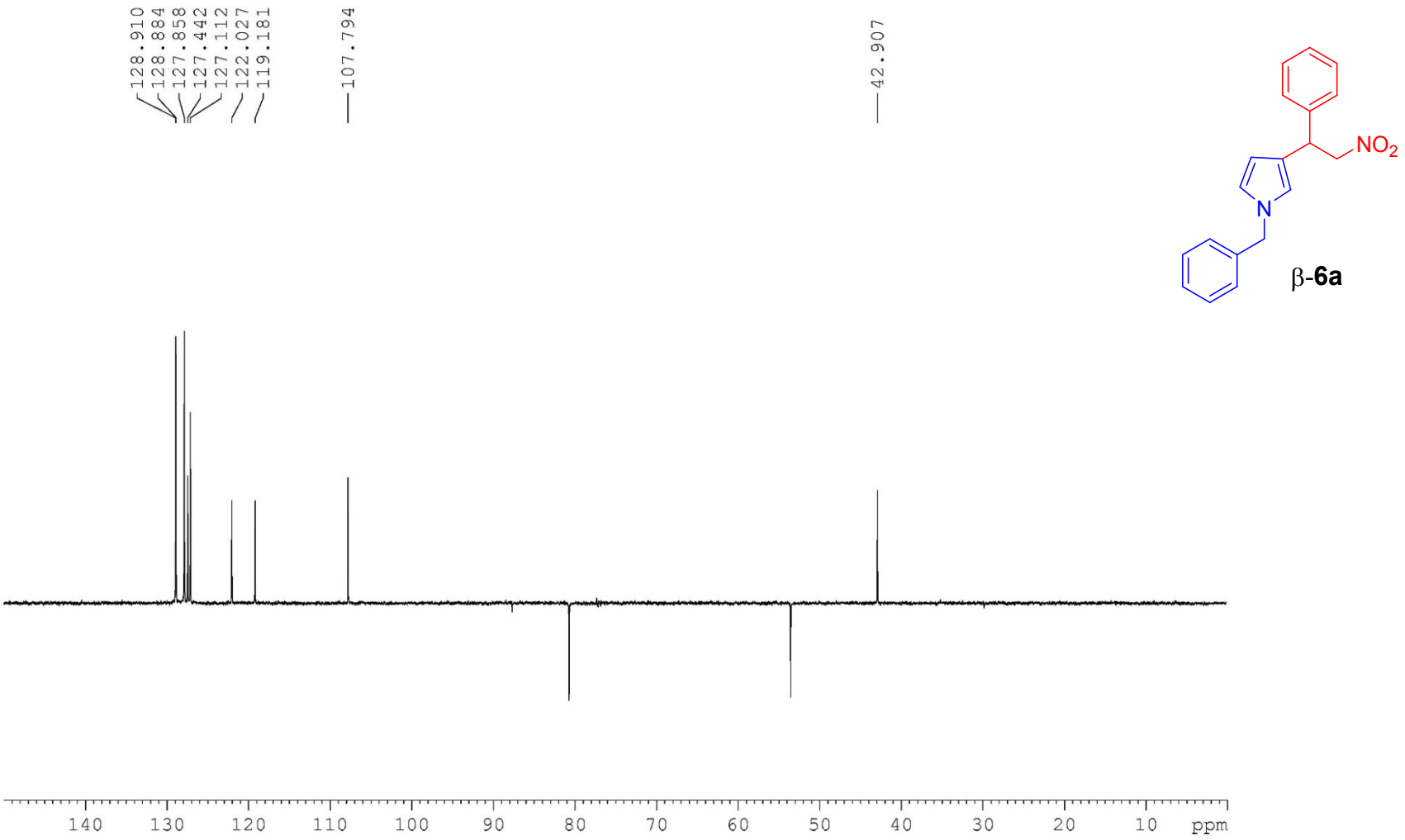



**Figure S47.** DEPT 135 NMR spectrum of derivative ***β*-6a** (400 MHz, $CDCl_3$, 298 K).

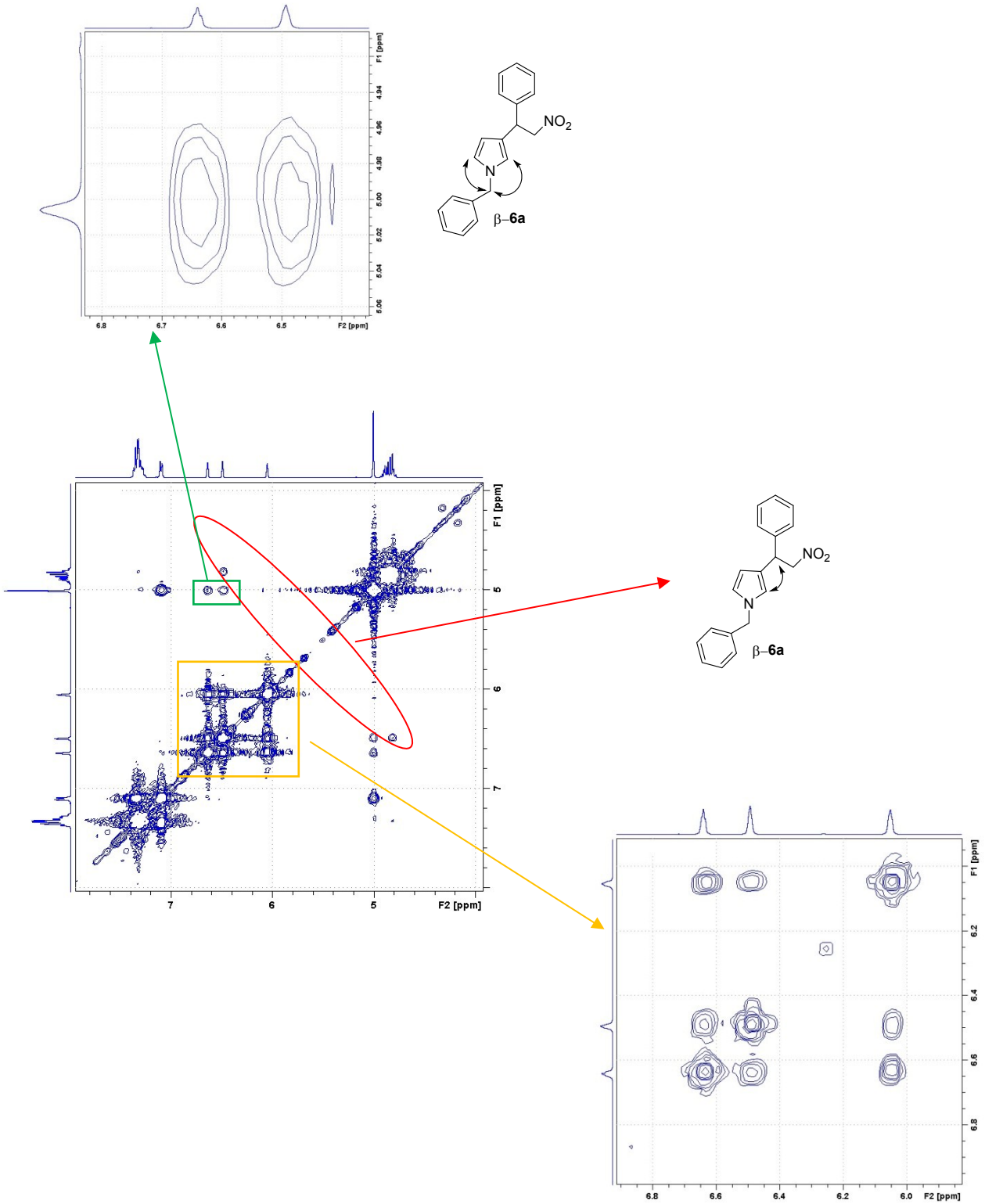



**Figure S48.** COSY NMR spectrum of derivative ***β*-6a** (400 MHz, $CDCl_3$, 298 K).

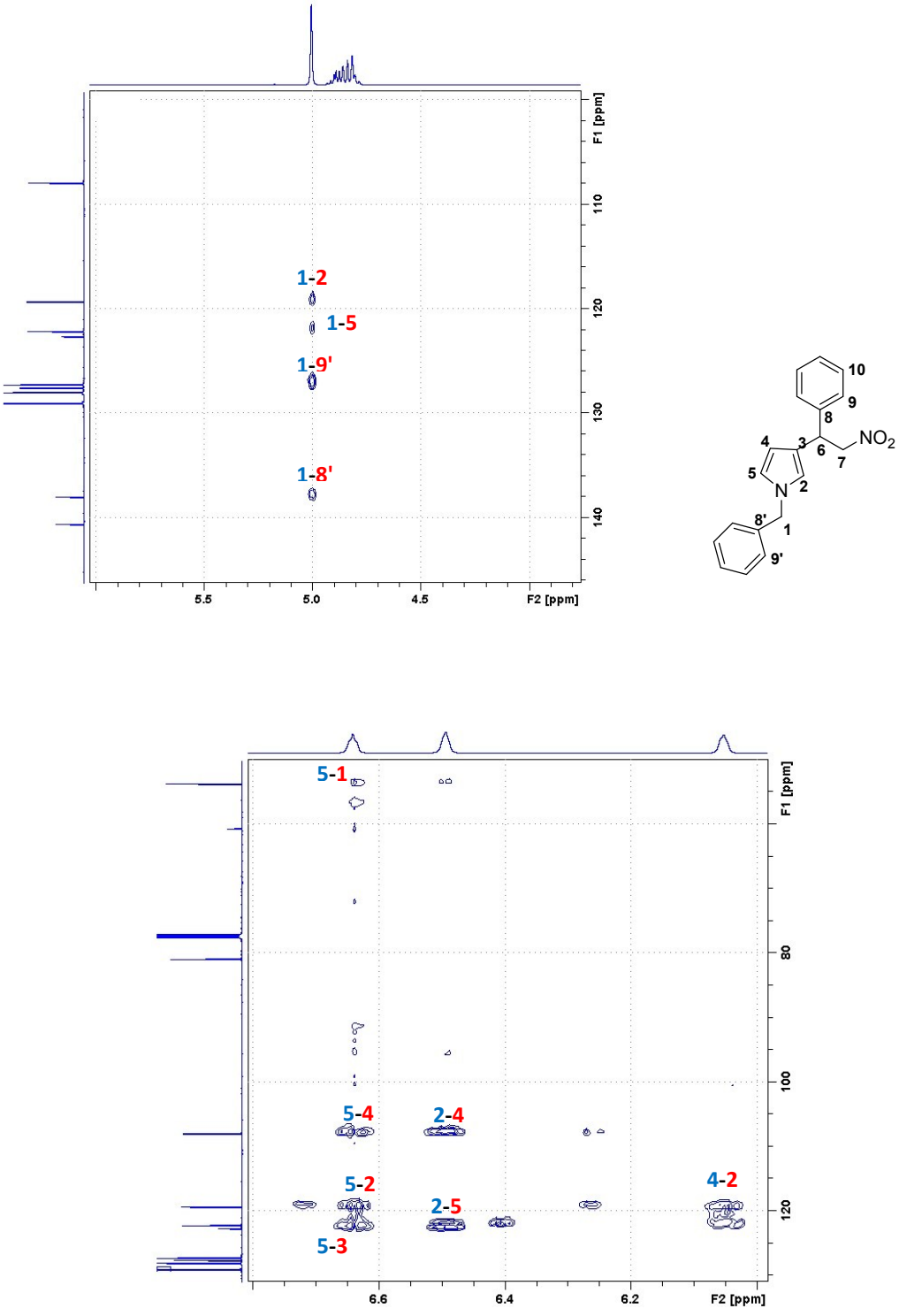



**Figure S49.** HMBC NMR spectrum of derivative ***β*-6a** (400 MHz, $CDCl_3$, 298 K).

## 8. Computational Studies

*Computational details*

Due to the high computational cost derived from the large number of atoms involved we choose to conduct an *in silico* investigation using the ONIOM method upon a reduced model of $(\mathbf{1})_6 \bullet 8H_2O$, namely $\mathbf{C_R}$ substituting the undecylic residues (the so-called "feet") present in the hexameric capsule with the methyl ones.

The calculations have been performed using the ONIOM method incorporated in the Gaussian16 package, for the reaction between the *N*-methylpyrrole **2** and the nitrostyrene **3a**. The reactive species (**2** and **3a**) together with one of the four acidic molecules of water directly involved in the supramolecular assembly and the corresponding three phenolic hydroxyl groups surrounding it were modeled using the M06-2X DFT functional, employing the cc-pVDZ basis set, while the semiempirical method PM6 was employed for all the other atoms.

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 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/cc-pVDZ:PM6] level (zero-point energy-corrected ONIOM values). The optimizations were carried out using the Berny analytical gradient optimization method. All calculations were carried out with the Gaussian 16 suite of programs.

*Cartesian coordinates, energies (Hartree), and frequencies for selected fully optimized compounds, intermediates, and transition states*

**2@$C_R$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 5.652737 | 0.943315 | -6.767020 |
| 2 | 8 | 0 | 2.791999 | -2.881348 | -7.486921 |
| 3 | 6 | 0 | 4.543894 | 0.330054 | -7.299826 |
| 4 | 6 | 0 | 4.273230 | -1.021162 | -7.061394 |
| 5 | 6 | 0 | 3.134423 | -1.559694 | -7.667465 |
| 6 | 6 | 0 | 2.279931 | -0.799034 | -8.493853 |
| 7 | 6 | 0 | 2.579791 | 0.557556 | -8.666996 |
| 8 | 6 | 0 | 3.708728 | 1.148491 | -8.090537 |
| 9 | 6 | 0 | 1.074333 | -1.444163 | -9.143273 |
| 10 | 6 | 0 | 1.008388 | -1.145453 | -10.644479 |
| 11 | 1 | 0 | 4.915140 | -1.617334 | -6.419680 |
| 12 | 1 | 0 | 1.906908 | 1.174601 | -9.266114 |
| 13 | 1 | 0 | 1.190842 | -2.566439 | -9.047924 |
| 14 | 1 | 0 | 0.924273 | -0.075519 | -10.858892 |
| 15 | 1 | 0 | 1.913127 | -1.506636 | -11.149779 |
| 16 | 1 | 0 | 0.147896 | -1.645148 | -11.105695 |
| 17 | 8 | 0 | -4.742000 | 2.321075 | -6.548172 |
| 18 | 8 | 0 | -1.903776 | 6.090196 | -5.515190 |
| 19 | 6 | 0 | -3.630972 | 3.105030 | -6.746551 |

| | | | | | |
|---|---|---|---|---|---|
| 20 | 6 | 0 | -3.378685 | 4.229064 | -5.953733 |
| 21 | 6 | 0 | -2.230204 | 4.970577 | -6.249245 |
| 22 | 6 | 0 | -1.348836 | 4.628574 | -7.295543 |
| 23 | 6 | 0 | -1.635046 | 3.473743 | -8.035383 |
| 24 | 6 | 0 | -2.773709 | 2.699582 | -7.792039 |
| 25 | 6 | 0 | -0.134994 | 5.487738 | -7.579887 |
| 26 | 6 | 0 | -0.045322 | 5.868407 | -9.061297 |
| 27 | 1 | 0 | -4.038495 | 4.502083 | -5.136855 |
| 28 | 1 | 0 | -0.943566 | 3.166084 | -8.822796 |
| 29 | 1 | 0 | -0.258604 | 6.457837 | -7.009643 |
| 30 | 1 | 0 | 0.044517 | 4.995823 | -9.716229 |
| 31 | 1 | 0 | 0.821152 | 6.513843 | -9.248911 |
| 32 | 1 | 0 | -0.943144 | 6.416029 | -9.374585 |
| 33 | 8 | 0 | 0.139472 | -2.864074 | -6.782036 |
| 34 | 8 | 0 | -3.693244 | -0.266661 | -6.270363 |
| 35 | 6 | 0 | -0.584068 | -1.801883 | -7.267186 |
| 36 | 6 | 0 | -1.760529 | -1.533784 | -6.559452 |
| 37 | 6 | 0 | -2.550354 | -0.469351 | -7.005645 |
| 38 | 6 | 0 | -2.199428 | 0.315194 | -8.127584 |
| 39 | 6 | 0 | -1.004894 | 0.006180 | -8.789205 |
| 40 | 6 | 0 | -0.187395 | -1.060008 | -8.400649 |
| 41 | 6 | 0 | -3.097344 | 1.446703 | -8.578869 |
| 42 | 6 | 0 | -3.052988 | 1.696910 | -10.089695 |
| 43 | 1 | 0 | -2.036688 | -2.128660 | -5.693467 |
| 44 | 1 | 0 | -0.706295 | 0.612163 | -9.647799 |
| 45 | 1 | 0 | -4.162201 | 1.148313 | -8.339078 |
| 46 | 1 | 0 | -2.068295 | 2.027556 | -10.434672 |
| 47 | 1 | 0 | -3.773660 | 2.474243 | -10.373151 |
| 48 | 1 | 0 | -3.310362 | 0.786530 | -10.644750 |
| 49 | 8 | 0 | 0.759323 | 5.740861 | -4.820135 |
| 50 | 8 | 0 | 4.581144 | 3.147027 | -5.433348 |
| 51 | 6 | 0 | 1.496290 | 4.989108 | -5.710440 |
| 52 | 6 | 0 | 2.658048 | 4.430943 | -5.169990 |
| 53 | 6 | 0 | 3.456416 | 3.660226 | -6.023483 |
| 54 | 6 | 0 | 3.126318 | 3.448132 | -7.382509 |
| 55 | 6 | 0 | 1.943605 | 4.021060 | -7.860716 |
| 56 | 6 | 0 | 1.117778 | 4.817944 | -7.057753 |
| 57 | 6 | 0 | 4.037124 | 2.616638 | -8.261377 |
| 58 | 6 | 0 | 4.015861 | 3.038596 | -9.733840 |
| 59 | 1 | 0 | 2.911568 | 4.554459 | -4.120438 |
| 60 | 1 | 0 | 1.658154 | 3.850527 | -8.901501 |
| 61 | 1 | 0 | 5.096878 | 2.781442 | -7.899959 |
| 62 | 1 | 0 | 4.742751 | 2.453392 | -10.311738 |
| 63 | 1 | 0 | 4.280377 | 4.097183 | -9.842577 |
| 64 | 1 | 0 | 3.037777 | 2.890268 | -10.202041 |
| 65 | 1 | 0 | -0.117266 | 6.075086 | -5.223731 |
| 66 | 1 | 0 | 6.182721 | 0.317835 | -6.160654 |
| 67 | 1 | 0 | 3.331967 | -3.328722 | -6.739966 |
| 68 | 1 | 0 | -5.285379 | 2.621371 | -5.739195 |
| 69 | 1 | 0 | -2.516022 | 6.212157 | -4.703102 |
| 70 | 1 | 0 | 1.023866 | -2.996762 | -7.280339 |
| 71 | 1 | 0 | -4.199976 | 0.569526 | -6.553754 |
| 72 | 1 | 0 | 5.099687 | 2.516449 | -6.046421 |
| 73 | 8 | 0 | -5.178831 | -0.039738 | 6.667545 |
| 74 | 8 | 0 | -4.242490 | -4.688687 | 5.715894 |
| 75 | 6 | 0 | -4.506415 | -1.217271 | 6.892477 |
| 76 | 6 | 0 | -4.753781 | -2.351107 | 6.111461 |
| 77 | 6 | 0 | -4.041640 | -3.509249 | 6.433324 |
| 78 | 6 | 0 | -3.100204 | -3.566814 | 7.478597 |
| 79 | 6 | 0 | -2.873213 | -2.393529 | 8.209797 |
| 80 | 6 | 0 | -3.571790 | -1.209313 | 7.950810 |
| 81 | 6 | 0 | -2.359685 | -4.857537 | 7.760149 |
| 82 | 6 | 0 | -2.394179 | -5.222371 | 9.247308 |
| 83 | 1 | 0 | -5.469020 | -2.330385 | 5.294234 |
| 84 | 1 | 0 | -2.123739 | -2.403761 | 9.004090 |
| 85 | 1 | 0 | -2.900254 | -5.690645 | 7.215862 |
| 86 | 1 | 0 | -1.879286 | -6.173760 | 9.428915 |
| 87 | 1 | 0 | -3.429349 | -5.333193 | 9.594398 |
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| 89 | 8 | 0 | 4.751262 | -3.129444 | 6.705273 |
| 90 | 8 | 0 | 3.751223 | 1.542819 | 7.408688 |
| 91 | 6 | 0 | 4.012978 | -2.107348 | 7.247819 |
| 92 | 6 | 0 | 4.314249 | -0.767264 | 6.984570 |

| | | | | | |
|---|---|---|---|---|---|
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| 94 | 6 | 0 | 2.462102 | -0.131234 | 8.481716 |
| 95 | 6 | 0 | 2.179016 | -1.489804 | 8.675167 |
| 96 | 6 | 0 | 2.941016 | -2.499233 | 8.080354 |
| 97 | 6 | 0 | 1.668130 | 0.961774 | 9.163485 |
| 98 | 6 | 0 | 1.534719 | 0.714515 | 10.669790 |
| 99 | 1 | 0 | 5.121312 | -0.496283 | 6.310249 |
| 100 | 1 | 0 | 1.334021 | -1.767945 | 9.308386 |
| 101 | 1 | 0 | 2.247892 | 1.927871 | 9.050618 |
| 102 | 1 | 0 | 2.524494 | 0.653722 | 11.140052 |
| 103 | 1 | 0 | 1.011596 | -0.219137 | 10.899593 |
| 104 | 1 | 0 | 0.985021 | 1.530141 | 11.154432 |
| 105 | 8 | 0 | 1.317581 | 2.717502 | 6.867534 |
| 106 | 8 | 0 | -3.270170 | 1.979483 | 6.540905 |
| 107 | 6 | 0 | 0.236725 | 2.032846 | 7.373663 |
| 108 | 6 | 0 | -0.971261 | 2.299928 | 6.722071 |
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| 110 | 6 | 0 | -2.074016 | 0.738518 | 8.279699 |
| 111 | 6 | 0 | -0.833732 | 0.502316 | 8.883303 |
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| 113 | 6 | 0 | -3.345279 | 0.060636 | 8.744437 |
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| 115 | 1 | 0 | -1.011138 | 2.960048 | 5.860507 |
| 116 | 1 | 0 | -0.777110 | -0.207208 | 9.712220 |
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| 118 | 1 | 0 | -3.241311 | 0.739892 | 10.812385 |
| 119 | 1 | 0 | -2.597852 | -0.890484 | 10.582390 |
| 120 | 1 | 0 | -4.341298 | -0.623909 | 10.553853 |
| 121 | 8 | 0 | -1.733197 | -5.508059 | 4.985427 |
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| 130 | 6 | 0 | 2.496421 | -4.333180 | 9.756045 |
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| 133 | 1 | 0 | 3.530205 | -4.560265 | 7.891296 |
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| 136 | 1 | 0 | 2.306789 | -5.406310 | 9.879950 |
| 137 | 1 | 0 | 4.423731 | 1.712207 | 6.654161 |
| 138 | 1 | 0 | 2.200283 | 2.432295 | 7.302638 |
| 139 | 1 | 0 | -4.055892 | 1.376152 | 6.784904 |
| 140 | 1 | 0 | -2.653891 | -5.496651 | 5.428577 |
| 141 | 1 | 0 | 3.585224 | -4.365653 | 6.036323 |
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| 148 | 8 | 0 | 6.329312 | 4.541534 | -3.690166 |
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| 154 | 8 | 0 | 3.826495 | -6.696906 | 3.652957 |
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| 156 | 1 | 0 | 3.210657 | -7.153077 | 3.046682 |
| 157 | 1 | 0 | -1.173576 | -6.822841 | 3.889011 |
| 158 | 8 | 0 | -1.010479 | -7.556807 | 3.202614 |
| 159 | 8 | 0 | -5.014263 | -5.848487 | 1.276339 |
| 160 | 6 | 0 | -1.963223 | -7.563110 | 2.214759 |
| 161 | 6 | 0 | -3.026131 | -6.654431 | 2.227608 |
| 162 | 6 | 0 | -3.978514 | -6.777663 | 1.211196 |
| 163 | 6 | 0 | -3.924394 | -7.778009 | 0.222560 |
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| 165 | 6 | 0 | -1.813803 | -8.542781 | 1.207681 |

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|---|---|---|---|---|---|
| 166 | 6 | 0 | -5.056139 | -7.941269 | -0.769702 |
| 167 | 6 | 0 | -5.325233 | -9.410242 | -1.119000 |
| 168 | 1 | 0 | -3.101025 | -5.880670 | 2.985092 |
| 169 | 1 | 0 | -2.708798 | -9.372937 | -0.561939 |
| 170 | 1 | 0 | -5.997818 | -7.560353 | -0.270895 |
| 171 | 1 | 0 | -4.485179 | -9.880970 | -1.639157 |
| 172 | 1 | 0 | -6.199641 | -9.493927 | -1.776814 |
| 173 | 1 | 0 | -5.528547 | -9.997526 | -0.216083 |
| 174 | 8 | 0 | -1.533391 | -5.071419 | -6.332041 |
| 175 | 8 | 0 | 2.589469 | -6.263113 | -4.320265 |
| 176 | 6 | 0 | -0.791647 | -5.897875 | -5.549571 |
| 177 | 6 | 0 | 0.558156 | -5.635659 | -5.283715 |
| 178 | 6 | 0 | 1.261690 | -6.585963 | -4.536852 |
| 179 | 6 | 0 | 0.677788 | -7.777029 | -4.072438 |
| 180 | 6 | 0 | -0.697924 | -7.956662 | -4.309418 |
| 181 | 6 | 0 | -1.455172 | -7.047642 | -5.045459 |
| 182 | 6 | 0 | 1.521626 | -8.824367 | -3.377959 |
| 183 | 6 | 0 | 1.121594 | -10.253174 | -3.764464 |
| 184 | 1 | 0 | 1.031701 | -4.725071 | -5.633299 |
| 185 | 1 | 0 | -1.182827 | -8.851087 | -3.913430 |
| 186 | 1 | 0 | 2.587784 | -8.688614 | -3.732405 |
| 187 | 1 | 0 | 1.173778 | -10.391393 | -4.851158 |
| 188 | 1 | 0 | 0.103035 | -10.504427 | -3.452310 |
| 189 | 1 | 0 | 1.795638 | -10.983363 | -3.300603 |
| 190 | 8 | 0 | -6.342231 | -5.506681 | -1.138467 |
| 191 | 8 | 0 | -4.370615 | -4.834450 | -5.474152 |
| 192 | 6 | 0 | -5.503812 | -5.884389 | -2.168346 |
| 193 | 6 | 0 | -5.365644 | -5.083124 | -3.303367 |
| 194 | 6 | 0 | -4.517438 | -5.544518 | -4.319944 |
| 195 | 6 | 0 | -3.800325 | -6.762659 | -4.211431 |
| 196 | 6 | 0 | -3.957330 | -7.502423 | -3.037869 |
| 197 | 6 | 0 | -4.821105 | -7.103581 | -2.005511 |
| 198 | 6 | 0 | -2.926071 | -7.231747 | -5.355670 |
| 199 | 6 | 0 | -3.254290 | -8.675578 | -5.758585 |
| 200 | 1 | 0 | -5.901891 | -4.145128 | -3.401042 |
| 201 | 1 | 0 | -3.394949 | -8.430669 | -2.919392 |
| 202 | 1 | 0 | -3.163882 | -6.577996 | -6.250699 |
| 203 | 1 | 0 | -4.308372 | -8.764296 | -6.047596 |
| 204 | 1 | 0 | -3.075076 | -9.391259 | -4.951723 |
| 205 | 1 | 0 | -2.647061 | -8.984753 | -6.617276 |
| 206 | 8 | 0 | 3.620312 | -7.557240 | -2.078055 |
| 207 | 8 | 0 | 1.609872 | -7.816918 | 2.217107 |
| 208 | 6 | 0 | 2.582609 | -7.938616 | -1.256996 |
| 209 | 6 | 0 | 2.615639 | -7.665336 | 0.112554 |
| 210 | 6 | 0 | 1.541908 | -8.128893 | 0.882110 |
| 211 | 6 | 0 | 0.479840 | -8.874982 | 0.327683 |
| 212 | 6 | 0 | 0.472594 | -9.067448 | -1.059575 |
| 213 | 6 | 0 | 1.511530 | -8.616056 | -1.879259 |
| 214 | 6 | 0 | -0.599460 | -9.444025 | 1.223270 |
| 215 | 6 | 0 | -0.936957 | -10.897574 | 0.875638 |
| 216 | 1 | 0 | 3.427104 | -7.100598 | 0.562805 |
| 217 | 1 | 0 | -0.368352 | -9.593847 | -1.515758 |
| 218 | 1 | 0 | -0.197853 | -9.453935 | 2.282528 |
| 219 | 1 | 0 | -0.042962 | -11.530115 | 0.939738 |
| 220 | 1 | 0 | -1.339509 | -11.007100 | -0.136357 |
| 221 | 1 | 0 | -1.682972 | -11.301034 | 1.570956 |
| 222 | 1 | 0 | -5.538542 | -5.827062 | 0.428732 |
| 223 | 1 | 0 | -1.016099 | -4.252711 | -6.627307 |
| 224 | 1 | 0 | 3.025161 | -6.875788 | -3.628895 |
| 225 | 1 | 0 | -6.787690 | -4.614081 | -1.321961 |
| 226 | 1 | 0 | -4.787812 | -3.917195 | -5.406250 |
| 227 | 1 | 0 | 4.350693 | -7.068995 | -1.563352 |
| 228 | 1 | 0 | 0.737796 | -8.017251 | 2.702418 |
| 229 | 1 | 0 | 1.796118 | 6.818158 | -3.897291 |
| 230 | 1 | 0 | -2.578781 | 8.082432 | -0.489841 |
| 231 | 1 | 0 | 0.869905 | 4.418952 | 6.545967 |
| 232 | 8 | 0 | 2.268715 | 7.436278 | -3.233083 |
| 233 | 8 | 0 | -2.071977 | 7.823340 | -1.341919 |
| 234 | 6 | 0 | 1.426547 | 7.887168 | -2.251245 |
| 235 | 6 | 0 | 0.058587 | 7.597012 | -2.278213 |
| 236 | 6 | 0 | -0.732393 | 8.147998 | -1.263545 |
| 237 | 6 | 0 | -0.209530 | 8.983233 | -0.257082 |
| 238 | 6 | 0 | 1.176869 | 9.197294 | -0.250468 |

| | | | | | |
|---|---|---|---|---|---|
| 239 | 6 | 0 | 2.017205 | 8.673234 | -1.234644 |
| 240 | 6 | 0 | -1.124376 | 9.628472 | 0.762623 |
| 241 | 6 | 0 | -0.702013 | 11.059351 | 1.113066 |
| 242 | 1 | 0 | -0.367913 | 6.956097 | -3.043399 |
| 243 | 1 | 0 | 1.611979 | 9.803885 | 0.547053 |
| 244 | 1 | 0 | -2.151712 | 9.708448 | 0.294284 |
| 245 | 1 | 0 | 0.278290 | 11.104335 | 1.597855 |
| 246 | 1 | 0 | -1.425055 | 11.518748 | 1.798827 |
| 247 | 1 | 0 | -0.652400 | 11.684348 | 0.213221 |
| 248 | 8 | 0 | 0.765817 | 5.388904 | 6.246772 |
| 249 | 8 | 0 | 5.010212 | 4.617517 | 4.263597 |
| 250 | 6 | 0 | 1.828533 | 5.812938 | 5.490166 |
| 251 | 6 | 0 | 2.913128 | 4.969234 | 5.231272 |
| 252 | 6 | 0 | 3.975296 | 5.500066 | 4.490229 |
| 253 | 6 | 0 | 3.994219 | 6.833476 | 4.034470 |
| 254 | 6 | 0 | 2.857729 | 7.616975 | 4.280418 |
| 255 | 6 | 0 | 1.765821 | 7.140949 | 5.010844 |
| 256 | 6 | 0 | 5.210433 | 7.386028 | 3.320435 |
| 257 | 6 | 0 | 5.511140 | 8.838586 | 3.705713 |
| 258 | 1 | 0 | 2.920937 | 3.938841 | 5.574289 |
| 259 | 1 | 0 | 2.830460 | 8.639504 | 3.896999 |
| 260 | 1 | 0 | 6.105456 | 6.779278 | 3.654656 |
| 261 | 1 | 0 | 4.715600 | 9.528716 | 3.407992 |
| 262 | 1 | 0 | 6.435702 | 9.181676 | 3.224175 |
| 263 | 1 | 0 | 5.643798 | 8.936903 | 4.789803 |
| 264 | 8 | 0 | 6.463691 | 5.304552 | 2.002006 |
| 265 | 8 | 0 | 4.695529 | 6.432264 | -2.256811 |
| 266 | 6 | 0 | 5.698149 | 6.112818 | 1.192658 |
| 267 | 6 | 0 | 5.569678 | 5.849436 | -0.172477 |
| 268 | 6 | 0 | 4.807478 | 6.749152 | -0.928198 |
| 269 | 6 | 0 | 4.217122 | 7.901916 | -0.363996 |
| 270 | 6 | 0 | 4.331807 | 8.081119 | 1.019825 |
| 271 | 6 | 0 | 5.068628 | 7.206664 | 1.825339 |
| 272 | 6 | 0 | 3.511846 | 8.905895 | -1.250631 |
| 273 | 6 | 0 | 3.884957 | 10.350593 | -0.900992 |
| 274 | 1 | 0 | 6.023484 | 4.974585 | -0.630978 |
| 275 | 1 | 0 | 3.838125 | 8.936897 | 1.484397 |
| 276 | 1 | 0 | 3.868742 | 8.733441 | -2.312260 |
| 277 | 1 | 0 | 3.580663 | 10.632953 | 0.111519 |
| 278 | 1 | 0 | 3.409490 | 11.054241 | -1.595175 |
| 279 | 1 | 0 | 4.970102 | 10.498635 | -0.967785 |
| 280 | 8 | 0 | -3.314291 | 7.981277 | 1.129975 |
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| 282 | 6 | 0 | -2.368750 | 7.904782 | 2.128415 |
| 283 | 6 | 0 | -2.533556 | 7.035502 | 3.208430 |
| 284 | 6 | 0 | -1.543034 | 7.051219 | 4.198268 |
| 285 | 6 | 0 | -0.434417 | 7.923600 | 4.147196 |
| 286 | 6 | 0 | -0.295255 | 8.733656 | 3.013117 |
| 287 | 6 | 0 | -1.248243 | 8.751710 | 1.989314 |
| 288 | 6 | 0 | 0.541824 | 7.979984 | 5.303044 |
| 289 | 6 | 0 | 0.895920 | 9.419808 | 5.690483 |
| 290 | 1 | 0 | -3.387317 | 6.366447 | 3.279332 |
| 291 | 1 | 0 | 0.581352 | 9.379215 | 2.929508 |
| 292 | 1 | 0 | 0.028872 | 7.524642 | 6.205230 |
| 293 | 1 | 0 | 1.405271 | 9.960903 | 4.887076 |
| 294 | 1 | 0 | 1.556241 | 9.435765 | 6.566286 |
| 295 | 1 | 0 | -0.007667 | 9.988070 | 5.943948 |
| 296 | 1 | 0 | 6.903886 | 4.546464 | 1.477634 |
| 297 | 1 | 0 | 4.010407 | 7.014216 | -2.737005 |
| 298 | 1 | 0 | -4.098395 | 7.354182 | 1.300979 |
| 299 | 1 | 0 | -0.925358 | 6.078139 | 5.824502 |
| 300 | 1 | 0 | 5.666634 | 4.965603 | 3.555813 |
| 301 | 1 | 0 | -5.647997 | 5.748791 | 2.609223 |
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| 303 | 1 | 0 | -8.084298 | -2.739206 | -2.547504 |
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| 305 | 8 | 0 | -5.360550 | 6.164005 | 1.711227 |
| 306 | 8 | 0 | -5.755227 | 5.594843 | -2.987671 |
| 307 | 6 | 0 | -6.086666 | 5.675910 | 0.657766 |
| 308 | 6 | 0 | -5.532231 | 5.908739 | -0.606893 |
| 309 | 6 | 0 | -6.232360 | 5.409655 | -1.708764 |
| 310 | 6 | 0 | -7.440761 | 4.691485 | -1.585379 |
| 311 | 6 | 0 | -7.954304 | 4.500449 | -0.296906 |

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| 312 | 6 | 0 | -7.314041 | 5.003632 | 0.839938 |
| 313 | 6 | 0 | -8.129854 | 4.140028 | -2.815192 |
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| 315 | 1 | 0 | -4.592218 | 6.438897 | -0.713040 |
| 316 | 1 | 0 | -8.884100 | 3.940080 | -0.177379 |
| 317 | 1 | 0 | -7.672257 | 4.642999 | -3.720243 |
| 318 | 1 | 0 | -9.766188 | 5.574449 | -2.819111 |
| 319 | 1 | 0 | -10.166990 | 4.072084 | -1.986621 |
| 320 | 1 | 0 | -10.097308 | 4.106144 | -3.752523 |
| 321 | 8 | 0 | -7.996952 | -3.236447 | -1.659146 |
| 322 | 8 | 0 | -7.547504 | -2.415246 | 3.009488 |
| 323 | 6 | 0 | -8.278956 | -2.424480 | -0.592236 |
| 324 | 6 | 0 | -7.824086 | -2.893417 | 0.647491 |
| 325 | 6 | 0 | -8.057304 | -2.079503 | 1.755540 |
| 326 | 6 | 0 | -8.779371 | -0.871123 | 1.686958 |
| 327 | 6 | 0 | -9.220289 | -0.454275 | 0.424740 |
| 328 | 6 | 0 | -8.982428 | -1.207096 | -0.729636 |
| 329 | 6 | 0 | -9.049623 | -0.078895 | 2.948307 |
| 330 | 6 | 0 | -10.520962 | 0.333971 | 3.056504 |
| 331 | 1 | 0 | -7.317700 | -3.852035 | 0.724482 |
| 332 | 1 | 0 | -9.758606 | 0.492119 | 0.339538 |
| 333 | 1 | 0 | -8.846773 | -0.762760 | 3.829149 |
| 334 | 1 | 0 | -11.172794 | -0.549021 | 3.046330 |
| 335 | 1 | 0 | -10.840480 | 0.980986 | 2.233573 |
| 336 | 1 | 0 | -10.708170 | 0.874430 | 3.992505 |
| 337 | 8 | 0 | -6.420014 | -0.289508 | 4.180687 |
| 338 | 8 | 0 | -5.544773 | 4.334715 | 3.653777 |
| 339 | 6 | 0 | -6.848749 | 0.926875 | 3.694830 |
| 340 | 6 | 0 | -5.949736 | 1.980262 | 3.891687 |
| 341 | 6 | 0 | -6.330800 | 3.247663 | 3.435324 |
| 342 | 6 | 0 | -7.558087 | 3.460220 | 2.756116 |
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| 347 | 1 | 0 | -4.989393 | 1.811255 | 4.372351 |
| 348 | 1 | 0 | -9.354361 | 2.514897 | 2.051504 |
| 349 | 1 | 0 | -7.359824 | 5.585334 | 2.911105 |
| 350 | 1 | 0 | -9.754156 | 5.093500 | 3.318871 |
| 351 | 1 | 0 | -9.554917 | 6.207803 | 1.956692 |
| 352 | 1 | 0 | -9.982770 | 4.521875 | 1.662538 |
| 353 | 8 | 0 | -5.750425 | 3.065481 | -4.103375 |
| 354 | 8 | 0 | -7.172332 | -1.417193 | -3.534951 |
| 355 | 6 | 0 | -6.698929 | 2.205655 | -3.599068 |
| 356 | 6 | 0 | -6.419046 | 0.850744 | -3.812592 |
| 357 | 6 | 0 | -7.345417 | -0.080375 | -3.331617 |
| 358 | 6 | 0 | -8.510094 | 0.312243 | -2.625960 |
| 359 | 6 | 0 | -8.734331 | 1.678279 | -2.442309 |
| 360 | 6 | 0 | -7.861678 | 2.655021 | -2.942664 |
| 361 | 6 | 0 | -9.444321 | -0.754938 | -2.099779 |
| 362 | 6 | 0 | -10.915571 | -0.331670 | -2.100116 |
| 363 | 1 | 0 | -5.510076 | 0.548263 | -4.324397 |
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| 365 | 1 | 0 | -9.364327 | -1.640983 | -2.803054 |
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| 368 | 1 | 0 | -11.112666 | 0.515620 | -1.435944 |
| 369 | 1 | 0 | -7.103416 | -1.036758 | 4.004538 |
| 370 | 1 | 0 | -4.556973 | 4.074924 | 3.998561 |
| 371 | 1 | 0 | -5.941429 | 4.043372 | -3.874548 |
| 372 | 1 | 0 | -6.264886 | -1.642878 | -4.002472 |
| 373 | 1 | 0 | 5.707580 | -6.207234 | 0.460102 |
| 374 | 1 | 0 | 5.232535 | -3.900408 | -4.715931 |
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| 376 | 1 | 0 | 6.699343 | -1.879300 | -4.947408 |
| 377 | 8 | 0 | 5.400371 | -6.054368 | -0.507447 |
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| 380 | 6 | 0 | 5.752369 | -4.827498 | -2.459356 |
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| 384 | 6 | 0 | 7.503641 | -4.832964 | -0.720615 |

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| 385 | 6 | 0 | 8.608933 | -2.538951 | -3.604485 |
| 386 | 6 | 0 | 10.104708 | -2.872108 | -3.616873 |
| 387 | 1 | 0 | 4.777574 | -5.156280 | -2.804237 |
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| 389 | 1 | 0 | 8.248388 | -2.653120 | -4.672560 |
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| 393 | 8 | 0 | 7.465666 | 3.220279 | 0.446632 |
| 394 | 8 | 0 | 7.197087 | 0.659189 | 4.428372 |
| 395 | 6 | 0 | 7.900498 | 2.124874 | 1.147104 |
| 396 | 6 | 0 | 7.306397 | 1.968097 | 2.406900 |
| 397 | 6 | 0 | 7.696198 | 0.858640 | 3.162100 |
| 398 | 6 | 0 | 8.622804 | -0.096182 | 2.689680 |
| 399 | 6 | 0 | 9.193147 | 0.120760 | 1.430770 |
| 400 | 6 | 0 | 8.883007 | 1.242402 | 0.652426 |
| 401 | 6 | 0 | 8.948770 | -1.310165 | 3.531243 |
| 402 | 6 | 0 | 10.442166 | -1.652561 | 3.519060 |
| 403 | 1 | 0 | 6.561700 | 2.672782 | 2.759251 |
| 404 | 1 | 0 | 9.911848 | -0.606399 | 1.045872 |
| 405 | 1 | 0 | 8.688593 | -1.055860 | 4.604335 |
| 406 | 1 | 0 | 11.039291 | -0.805231 | 3.876954 |
| 407 | 1 | 0 | 10.807067 | -1.911171 | 2.519933 |
| 408 | 1 | 0 | 10.650101 | -2.508900 | 4.172397 |
| 409 | 8 | 0 | 6.621464 | -0.862839 | -4.891040 |
| 410 | 8 | 0 | 7.767899 | 2.913729 | -2.251658 |
| 411 | 6 | 0 | 7.387358 | -0.337694 | -3.875757 |
| 412 | 6 | 0 | 7.158498 | 1.016300 | -3.605612 |
| 413 | 6 | 0 | 7.901419 | 1.594672 | -2.571045 |
| 414 | 6 | 0 | 8.829158 | 0.851000 | -1.800750 |
| 415 | 6 | 0 | 9.021374 | -0.493957 | -2.124156 |
| 416 | 6 | 0 | 8.341925 | -1.109372 | -3.183951 |
| 417 | 6 | 0 | 9.566539 | 1.529518 | -0.668144 |
| 418 | 6 | 0 | 11.057835 | 1.176800 | -0.647332 |
| 419 | 1 | 0 | 6.416057 | 1.579810 | -4.162765 |
| 420 | 1 | 0 | 9.730243 | -1.083276 | -1.539230 |
| 421 | 1 | 0 | 9.507468 | 2.646654 | -0.845278 |
| 422 | 1 | 0 | 11.575064 | 1.711250 | 0.158301 |
| 423 | 1 | 0 | 11.533701 | 1.459598 | -1.594822 |
| 424 | 1 | 0 | 11.237175 | 0.107210 | -0.500633 |
| 425 | 8 | 0 | 6.443873 | -1.961186 | 4.841678 |
| 426 | 8 | 0 | 5.810717 | -5.852395 | 2.197595 |
| 427 | 6 | 0 | 6.897280 | -2.765851 | 3.820593 |
| 428 | 6 | 0 | 6.099733 | -3.884264 | 3.554556 |
| 429 | 6 | 0 | 6.506244 | -4.724972 | 2.512389 |
| 430 | 6 | 0 | 7.658596 | -4.455155 | 1.731834 |
| 431 | 6 | 0 | 8.418972 | -3.329266 | 2.051949 |
| 432 | 6 | 0 | 8.084852 | -2.482621 | 3.118392 |
| 433 | 6 | 0 | 8.016497 | -5.384133 | 0.593242 |
| 434 | 6 | 0 | 9.514297 | -5.706215 | 0.549555 |
| 435 | 1 | 0 | 5.193288 | -4.073291 | 4.121391 |
| 436 | 1 | 0 | 9.307931 | -3.104321 | 1.459419 |
| 437 | 1 | 0 | 7.485881 | -6.367663 | 0.779293 |
| 438 | 1 | 0 | 10.133069 | -4.817950 | 0.389648 |
| 439 | 1 | 0 | 9.738175 | -6.412851 | -0.258571 |
| 440 | 1 | 0 | 9.837971 | -6.164223 | 1.492586 |
| 441 | 1 | 0 | 7.107578 | 3.439441 | -2.895157 |
| 442 | 1 | 0 | 6.975284 | -1.094308 | 4.915736 |
| 443 | 1 | 0 | 4.990695 | -6.039520 | 2.847746 |
| 444 | 1 | 0 | 7.805285 | 3.238316 | -0.523580 |
| 445 | 8 | 0 | -5.250057 | -3.948009 | 3.175746 |
| 446 | 1 | 0 | -4.514054 | -3.347313 | 2.973777 |
| 447 | 1 | 0 | -5.137590 | -4.677926 | 2.520933 |
| 448 | 8 | 0 | 3.686949 | -4.345057 | -5.350944 |
| 449 | 1 | 0 | 3.671616 | -5.291351 | -5.619649 |
| 450 | 1 | 0 | 3.000305 | -4.295363 | -4.647747 |
| 451 | 8 | 0 | -3.164415 | 6.587816 | -3.127755 |
| 452 | 1 | 0 | -2.594414 | 6.209175 | -2.421172 |
| 453 | 1 | 0 | -3.074618 | 7.558153 | -3.005316 |
| 454 | 8 | 0 | 5.230955 | 2.416322 | 5.278503 |
| 455 | 1 | 0 | 5.615060 | 3.277735 | 5.551258 |
| 456 | 1 | 0 | 4.602753 | 2.654280 | 4.561645 |
| 457 | 6 | 0 | -3.768316 | -3.240466 | -0.723873 |

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| 458 | 6 | 0 | -4.638412 | -2.628165 | 0.154351 |
| 459 | 7 | 0 | -4.613577 | -1.278608 | -0.080467 |
| 460 | 6 | 0 | -3.744486 | -1.018053 | -1.099684 |
| 461 | 6 | 0 | -3.199856 | -2.214607 | -1.528091 |
| 462 | 6 | 0 | -5.406822 | -0.296035 | 0.631684 |
| 463 | 1 | 0 | -3.555595 | -4.307459 | -0.764701 |
| 464 | 1 | 0 | -5.284223 | -3.026682 | 0.930299 |
| 465 | 1 | 0 | -3.562446 | 0.004463 | -1.420922 |
| 466 | 1 | 0 | -2.424773 | -2.330304 | -2.280187 |
| 467 | 1 | 0 | -5.893669 | -0.783164 | 1.486338 |
| 468 | 1 | 0 | -4.767647 | 0.516323 | 1.004187 |
| 469 | 1 | 0 | -6.184297 | 0.131275 | -0.020036 |

Sum of electronic and thermal Free Energies = -555.408608
ONIOM Total Energy = -558.567381
0 imaginary frequency

**3a@$C_R$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 5.782549 | -0.447003 | 6.744339 |
| 2 | 8 | 0 | 2.508755 | 2.965050 | 7.722668 |
| 3 | 6 | 0 | 4.630636 | 0.005261 | 7.341395 |
| 4 | 6 | 0 | 4.179749 | 1.316301 | 7.159438 |
| 5 | 6 | 0 | 3.018395 | 1.692411 | 7.841808 |
| 6 | 6 | 0 | 2.315562 | 0.810064 | 8.690223 |
| 7 | 6 | 0 | 2.787879 | -0.503768 | 8.798415 |
| 8 | 6 | 0 | 3.945680 | -0.933775 | 8.142911 |
| 9 | 6 | 0 | 1.092012 | 1.287987 | 9.441232 |
| 10 | 6 | 0 | 1.155062 | 0.921499 | 10.927702 |
| 11 | 1 | 0 | 4.705067 | 2.005515 | 6.505079 |
| 12 | 1 | 0 | 2.232021 | -1.215590 | 9.412118 |
| 13 | 1 | 0 | 1.082221 | 2.419854 | 9.393696 |
| 14 | 1 | 0 | 1.197355 | -0.159200 | 11.095122 |
| 15 | 1 | 0 | 2.047632 | 1.356581 | 11.395116 |
| 16 | 1 | 0 | 0.278459 | 1.305573 | 11.463308 |
| 17 | 8 | 0 | -4.349816 | -2.997438 | 6.911615 |
| 18 | 8 | 0 | -1.140809 | -6.324680 | 5.515355 |
| 19 | 6 | 0 | -3.142959 | -3.648930 | 7.013630 |
| 20 | 6 | 0 | -2.796855 | -4.678571 | 6.132826 |
| 21 | 6 | 0 | -1.560242 | -5.299454 | 6.333799 |
| 22 | 6 | 0 | -0.680498 | -4.927140 | 7.371941 |
| 23 | 6 | 0 | -1.063204 | -3.863571 | 8.198792 |
| 24 | 6 | 0 | -2.293078 | -3.213135 | 8.052494 |
| 25 | 6 | 0 | 0.629595 | -5.663049 | 7.557013 |
| 26 | 6 | 0 | 0.828695 | -6.111660 | 9.008436 |
| 27 | 1 | 0 | -3.457618 | -4.969367 | 5.321690 |
| 28 | 1 | 0 | -0.378143 | -3.530696 | 8.981543 |
| 29 | 1 | 0 | 0.583101 | -6.608700 | 6.936076 |
| 30 | 1 | 0 | 0.857479 | -5.271622 | 9.709739 |
| 31 | 1 | 0 | 1.766554 | -6.668772 | 9.121566 |
| 32 | 1 | 0 | 0.009802 | -6.769573 | 9.325763 |
| 33 | 8 | 0 | -0.201268 | 2.745165 | 7.286450 |
| 34 | 8 | 0 | -3.753908 | -0.252896 | 6.885846 |
| 35 | 6 | 0 | -0.757188 | 1.576608 | 7.740506 |
| 36 | 6 | 0 | -1.960732 | 1.223455 | 7.119560 |
| 37 | 6 | 0 | -2.566543 | 0.032355 | 7.529147 |
| 38 | 6 | 0 | -2.018230 | -0.795953 | 8.531394 |
| 39 | 6 | 0 | -0.811770 | -0.391185 | 9.118096 |
| 40 | 6 | 0 | -0.171589 | 0.800301 | 8.765208 |
| 41 | 6 | 0 | -2.725817 | -2.068754 | 8.944820 |
| 42 | 6 | 0 | -2.548724 | -2.403974 | 10.429374 |
| 43 | 1 | 0 | -2.390933 | 1.852761 | 6.343715 |
| 44 | 1 | 0 | -0.362238 | -1.023048 | 9.887586 |
| 45 | 1 | 0 | -3.834427 | -1.906396 | 8.787969 |
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| 50 | 8 | 0 | 4.978729 | -2.721327 | 5.377469 |

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| 51 | 6 | 0 | 2.129565 | -4.908879 | 5.663012 |
| 52 | 6 | 0 | 3.203806 | -4.203038 | 5.114448 |
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| 54 | 6 | 0 | 3.627720 | -3.255800 | 7.351420 |
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| 60 | 1 | 0 | 2.265114 | -3.881860 | 8.892981 |
| 61 | 1 | 0 | 5.518790 | -2.369576 | 7.837970 |
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| 63 | 1 | 0 | 4.945086 | -3.857160 | 9.741376 |
| 64 | 1 | 0 | 3.573627 | -2.835796 | 10.193910 |
| 65 | 1 | 0 | 0.624497 | -6.139951 | 5.176751 |
| 66 | 1 | 0 | 6.198320 | 0.252790 | 6.128001 |
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| 361 | 6 | 0 | -9.325022 | -0.284572 | 2.431219 |
| 362 | 6 | 0 | -10.768670 | -0.797108 | 2.475515 |
| 363 | 1 | 0 | -5.494346 | -1.374191 | 4.940470 |
| 364 | 1 | 0 | -9.215058 | -3.013986 | 2.042132 |
| 365 | 1 | 0 | -9.288933 | 0.623268 | 3.109199 |
| 366 | 1 | 0 | -11.465601 | -0.026434 | 2.122933 |
| 367 | 1 | 0 | -11.056412 | -1.062976 | 3.499955 |
| 368 | 1 | 0 | -10.922089 | -1.682792 | 1.851293 |
| 369 | 1 | 0 | -7.517690 | 0.350239 | -3.855372 |
| 370 | 1 | 0 | -4.380341 | -4.400417 | -4.085742 |
| 371 | 1 | 0 | -5.542120 | -4.854227 | 4.206655 |
| 372 | 1 | 0 | -6.441498 | 0.742112 | 4.698574 |
| 373 | 1 | 0 | 4.880164 | 6.836954 | -0.232898 |
| 374 | 1 | 0 | 4.750849 | 4.333396 | 4.874431 |
| 375 | 1 | 0 | 6.540015 | -0.490637 | -4.763208 |
| 376 | 1 | 0 | 6.395655 | 2.468446 | 4.961259 |
| 377 | 8 | 0 | 4.607389 | 6.615285 | 0.731926 |
| 378 | 8 | 0 | 5.717245 | 4.118416 | 4.606220 |
| 379 | 6 | 0 | 5.543821 | 5.864367 | 1.391336 |
| 380 | 6 | 0 | 5.125410 | 5.377966 | 2.637687 |
| 381 | 6 | 0 | 6.034330 | 4.597483 | 3.356358 |
| 382 | 6 | 0 | 7.315876 | 4.272537 | 2.860293 |
| 383 | 6 | 0 | 7.682162 | 4.793564 | 1.614358 |
| 384 | 6 | 0 | 6.833608 | 5.623293 | 0.872816 |
| 385 | 6 | 0 | 8.231987 | 3.377400 | 3.664195 |
| 386 | 6 | 0 | 9.679792 | 3.879176 | 3.678502 |
| 387 | 1 | 0 | 4.127533 | 5.590485 | 3.007336 |
| 388 | 1 | 0 | 8.668072 | 4.551375 | 1.211554 |
| 389 | 1 | 0 | 7.874684 | 3.405955 | 4.738816 |
| 390 | 1 | 0 | 10.309872 | 3.233718 | 4.302486 |
| 391 | 1 | 0 | 9.734414 | 4.895919 | 4.086528 |
| 392 | 1 | 0 | 10.127380 | 3.904279 | 2.679979 |
| 393 | 8 | 0 | 7.777889 | -2.366006 | -0.595345 |
| 394 | 8 | 0 | 7.154723 | 0.275833 | -4.485859 |
| 395 | 6 | 0 | 8.059143 | -1.199314 | -1.257786 |
| 396 | 6 | 0 | 7.447175 | -1.081102 | -2.513435 |
| 397 | 6 | 0 | 7.680880 | 0.097686 | -3.227034 |
| 398 | 6 | 0 | 8.468623 | 1.152712 | -2.718044 |
| 399 | 6 | 0 | 9.066147 | 0.971056 | -1.466023 |
| 400 | 6 | 0 | 8.913291 | -0.209502 | -0.729208 |
| 401 | 6 | 0 | 8.624719 | 2.428942 | -3.515324 |
| 402 | 6 | 0 | 10.064163 | 2.953810 | -3.507684 |
| 403 | 1 | 0 | 6.809278 | -1.869848 | -2.894766 |
| 404 | 1 | 0 | 9.679547 | 1.775407 | -1.053368 |
| 405 | 1 | 0 | 8.380151 | 2.184938 | -4.594463 |
| 406 | 1 | 0 | 10.755168 | 2.202735 | -3.909015 |
| 407 | 1 | 0 | 10.412451 | 3.214790 | -2.503249 |
| 408 | 1 | 0 | 10.152871 | 3.855303 | -4.126522 |
| 409 | 8 | 0 | 6.416904 | 1.452430 | 4.855239 |
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| 411 | 6 | 0 | 7.249700 | 1.050307 | 3.836107 |
| 412 | 6 | 0 | 7.173501 | -0.310015 | 3.516840 |
| 413 | 6 | 0 | 7.983199 | -0.765893 | 2.471134 |
| 414 | 6 | 0 | 8.825379 | 0.103172 | 1.734461 |
| 415 | 6 | 0 | 8.869650 | 1.447589 | 2.110043 |

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| 416 | 6 | 0 | 8.121996 | 1.945309 | 3.185636 |
| 417 | 6 | 0 | 9.633640 | -0.448430 | 0.581650 |
| 418 | 6 | 0 | 11.071017 | 0.082711 | 0.565300 |
| 419 | 1 | 0 | 6.492512 | -0.970525 | 4.045784 |
| 420 | 1 | 0 | 9.514536 | 2.131724 | 1.554951 |
| 421 | 1 | 0 | 9.711083 | -1.569078 | 0.727829 |
| 422 | 1 | 0 | 11.644171 | -0.364654 | -0.255482 |
| 423 | 1 | 0 | 11.583819 | -0.164039 | 1.503579 |
| 424 | 1 | 0 | 11.118914 | 1.169471 | 0.445160 |
| 425 | 8 | 0 | 6.019062 | 2.783868 | -4.744282 |
| 426 | 8 | 0 | 4.977086 | 6.498468 | -1.976777 |
| 427 | 6 | 0 | 6.396072 | 3.616084 | -3.711990 |
| 428 | 6 | 0 | 5.471070 | 4.616774 | -3.395531 |
| 429 | 6 | 0 | 5.795681 | 5.475528 | -2.338907 |
| 430 | 6 | 0 | 6.992285 | 5.329886 | -1.590719 |
| 431 | 6 | 0 | 7.879669 | 4.319337 | -1.961516 |
| 432 | 6 | 0 | 7.627954 | 3.467034 | -3.046581 |
| 433 | 6 | 0 | 7.258108 | 6.264498 | -0.431682 |
| 434 | 6 | 0 | 8.708413 | 6.758535 | -0.396554 |
| 435 | 1 | 0 | 4.532798 | 4.703332 | -3.936045 |
| 436 | 1 | 0 | 8.805112 | 4.192724 | -1.396248 |
| 437 | 1 | 0 | 6.613166 | 7.183690 | -0.584398 |
| 438 | 1 | 0 | 9.429056 | 5.945499 | -0.266162 |
| 439 | 1 | 0 | 8.859436 | 7.466778 | 0.427033 |
| 440 | 1 | 0 | 8.963070 | 7.274522 | -1.330793 |
| 441 | 1 | 0 | 7.419562 | -2.700937 | 2.745290 |
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| 443 | 1 | 0 | 4.131812 | 6.620246 | -2.617198 |
| 444 | 1 | 0 | 8.112345 | -2.366940 | 0.377107 |
| 445 | 8 | 0 | -6.158339 | 3.538674 | -2.969924 |
| 446 | 1 | 0 | -5.473002 | 2.881919 | -2.729143 |
| 447 | 1 | 0 | -6.053493 | 4.255240 | -2.307394 |
| 448 | 8 | 0 | 3.188820 | 4.578534 | 5.610048 |
| 449 | 1 | 0 | 3.093917 | 5.504693 | 5.927998 |
| 450 | 1 | 0 | 2.474439 | 4.495555 | 4.936642 |
| 451 | 8 | 0 | -2.367328 | -6.833208 | 3.124975 |
| 452 | 1 | 0 | -1.850231 | -6.377657 | 2.424289 |
| 453 | 1 | 0 | -2.203971 | -7.786658 | 2.955890 |
| 454 | 8 | 0 | 5.411336 | -1.674603 | -5.402013 |
| 455 | 1 | 0 | 5.883465 | -2.476797 | -5.712414 |
| 456 | 1 | 0 | 4.829645 | -2.006372 | -4.684419 |
| 457 | 6 | 0 | -1.858924 | 0.210327 | -2.991349 |
| 458 | 6 | 0 | -0.675934 | -0.640984 | -3.086220 |
| 459 | 6 | 0 | -1.888734 | 1.541951 | -3.134694 |
| 460 | 7 | 0 | -3.136623 | 2.247541 | -2.977321 |
| 461 | 6 | 0 | 0.624161 | -0.122024 | -3.209591 |
| 462 | 6 | 0 | 1.717345 | -0.975472 | -3.270204 |
| 463 | 6 | 0 | 1.531922 | -2.359746 | -3.212307 |
| 464 | 6 | 0 | 0.247323 | -2.886152 | -3.098624 |
| 465 | 6 | 0 | -0.849755 | -2.031769 | -3.030517 |
| 466 | 8 | 0 | -3.115387 | 3.449742 | -3.150780 |
| 467 | 8 | 0 | -4.149510 | 1.620842 | -2.685137 |
| 468 | 1 | 0 | -2.813548 | -0.279074 | -2.779155 |
| 469 | 1 | 0 | -1.070643 | 2.219459 | -3.367030 |
| 470 | 1 | 0 | 0.783317 | 0.957013 | -3.243060 |
| 471 | 1 | 0 | 2.720025 | -0.557753 | -3.350594 |
| 472 | 1 | 0 | 2.391605 | -3.030229 | -3.248562 |
| 473 | 1 | 0 | 0.098344 | -3.965237 | -3.048763 |
| 474 | 1 | 0 | -1.858668 | -2.447270 | -2.937545 |

Sum of electronic and thermal Free Energies = -819.991546
ONIOM Total Energy = -823.174616
0 imaginary frequency

**[2+3a]@$C_R$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 5.422662 | -1.490077 | 6.946139 |
| 2 | 8 | 0 | 3.412857 | 2.881782 | 7.370506 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 6 | 0 | 4.467373 | -0.624804 | 7.424070 |
| 4 | 6 | 0 | 4.479006 | 0.732979 | 7.089876 |
| 5 | 6 | 0 | 3.479231 | 1.535524 | 7.647969 |
| 6 | 6 | 0 | 2.493503 | 1.026355 | 8.520829 |
| 7 | 6 | 0 | 2.507873 | -0.347551 | 8.788836 |
| 8 | 6 | 0 | 3.485602 | -1.197204 | 8.261093 |
| 9 | 6 | 0 | 1.455841 | 1.950793 | 9.120903 |
| 10 | 6 | 0 | 1.352213 | 1.779119 | 10.639864 |
| 11 | 1 | 0 | 5.225540 | 1.138797 | 6.413762 |
| 12 | 1 | 0 | 1.727077 | -0.769523 | 9.424992 |
| 13 | 1 | 0 | 1.800312 | 3.015167 | 8.944781 |
| 14 | 1 | 0 | 1.053047 | 0.767549 | 10.931248 |
| 15 | 1 | 0 | 2.319142 | 1.981151 | 11.117933 |
| 16 | 1 | 0 | 0.619661 | 2.476876 | 11.063512 |
| 17 | 8 | 0 | -5.065495 | -0.693648 | 6.806129 |
| 18 | 8 | 0 | -3.051676 | -5.001776 | 5.959185 |
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| 20 | 6 | 0 | -4.120787 | -2.863427 | 6.307014 |
| 21 | 6 | 0 | -3.139035 | -3.803310 | 6.635606 |
| 22 | 6 | 0 | -2.191108 | -3.592602 | 7.657431 |
| 23 | 6 | 0 | -2.223698 | -2.364407 | 8.331194 |
| 24 | 6 | 0 | -3.185439 | -1.389532 | 8.050155 |
| 25 | 6 | 0 | -1.176321 | -4.666519 | 7.986940 |
| 26 | 6 | 0 | -1.152134 | -4.980301 | 9.486393 |
| 27 | 1 | 0 | -4.837089 | -3.039549 | 5.510923 |
| 28 | 1 | 0 | -1.470332 | -2.161011 | 9.095384 |
| 29 | 1 | 0 | -1.501369 | -5.618964 | 7.468673 |
| 30 | 1 | 0 | -0.880790 | -4.111619 | 10.094911 |
| 31 | 1 | 0 | -0.433934 | -5.778421 | 9.709393 |
| 32 | 1 | 0 | -2.139907 | -5.316172 | 9.826741 |
| 33 | 8 | 0 | 0.793070 | 3.376080 | 6.674434 |
| 34 | 8 | 0 | -3.501687 | 1.595768 | 6.353910 |
| 35 | 6 | 0 | -0.126278 | 2.521676 | 7.231798 |
| 36 | 6 | 0 | -1.345924 | 2.458315 | 6.549607 |
| 37 | 6 | 0 | -2.328006 | 1.608522 | 7.068190 |
| 38 | 6 | 0 | -2.124939 | 0.838955 | 8.236128 |
| 39 | 6 | 0 | -0.880936 | 0.937177 | 8.870885 |
| 40 | 6 | 0 | 0.130237 | 1.785844 | 8.409271 |
| 41 | 6 | 0 | -3.228575 | -0.053247 | 8.761856 |
| 42 | 6 | 0 | -3.208361 | -0.218928 | 10.284617 |
| 43 | 1 | 0 | -1.514010 | 3.048809 | 5.652282 |
| 44 | 1 | 0 | -0.697380 | 0.338599 | 9.766103 |
| 45 | 1 | 0 | -4.213253 | 0.445008 | 8.510893 |
| 46 | 1 | 0 | -2.306688 | -0.725309 | 10.643003 |
| 47 | 1 | 0 | -4.068554 | -0.811984 | 10.619756 |
| 48 | 1 | 0 | -3.261938 | 0.755969 | 10.784703 |
| 49 | 8 | 0 | -0.388005 | -5.215296 | 5.235505 |
| 50 | 8 | 0 | 3.907558 | -3.481336 | 5.734636 |
| 51 | 6 | 0 | 0.502704 | -4.603069 | 6.094026 |
| 52 | 6 | 0 | 1.752275 | -4.332558 | 5.529843 |
| 53 | 6 | 0 | 2.703500 | -3.708840 | 6.346475 |
| 54 | 6 | 0 | 2.434810 | -3.361731 | 7.691306 |
| 55 | 6 | 0 | 1.163131 | -3.651054 | 8.195311 |
| 56 | 6 | 0 | 0.181627 | -4.295628 | 7.431241 |
| 57 | 6 | 0 | 3.502416 | -2.687509 | 8.527808 |
| 58 | 6 | 0 | 3.397570 | -3.002094 | 10.023149 |
| 59 | 1 | 0 | 1.967530 | -4.561155 | 4.489760 |
| 60 | 1 | 0 | 0.928363 | -3.374095 | 9.226015 |
| 61 | 1 | 0 | 4.503134 | -3.092454 | 8.188474 |
| 62 | 1 | 0 | 4.231940 | -2.544968 | 10.570859 |
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| 66 | 1 | 0 | 6.066863 | -1.033177 | 6.299566 |
| 67 | 1 | 0 | 4.034153 | 3.156267 | 6.601630 |
| 68 | 1 | 0 | -5.695055 | -0.936636 | 6.042126 |
| 69 | 1 | 0 | -3.681106 | -5.036685 | 5.153542 |
| 70 | 1 | 0 | 1.694140 | 3.352362 | 7.158171 |
| 71 | 1 | 0 | -4.168249 | 0.912763 | 6.704510 |
| 72 | 1 | 0 | 4.553952 | -2.941842 | 6.314953 |
| 73 | 8 | 0 | -4.881272 | 0.515257 | -6.813944 |
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| 75 | 6 | 0 | -3.960775 | 1.516712 | -7.024586 |

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| 76 | 6 | 0 | -3.954306 | 2.669839 | -6.234727 |
| 77 | 6 | 0 | -3.021038 | 3.655490 | -6.562053 |
| 78 | 6 | 0 | -2.105219 | 3.519137 | -7.625455 |
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| 86 | 1 | 0 | -0.435348 | 5.806202 | -9.643345 |
| 87 | 1 | 0 | -2.117529 | 5.268581 | -9.780343 |
| 88 | 1 | 0 | -0.800806 | 4.126911 | -10.055993 |
| 89 | 8 | 0 | 5.476508 | 1.579637 | -6.819453 |
| 90 | 8 | 0 | 3.528899 | -2.819800 | -7.236781 |
| 91 | 6 | 0 | 4.538160 | 0.701758 | -7.301342 |
| 92 | 6 | 0 | 4.553140 | -0.651236 | -6.947040 |
| 93 | 6 | 0 | 3.583724 | -1.473360 | -7.529685 |
| 94 | 6 | 0 | 2.626096 | -0.991418 | -8.445004 |
| 95 | 6 | 0 | 2.626578 | 0.382141 | -8.724070 |
| 96 | 6 | 0 | 3.572557 | 1.251385 | -8.174470 |
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| 100 | 1 | 0 | 1.861295 | 0.785247 | -9.390636 |
| 101 | 1 | 0 | 2.014328 | -2.996929 | -8.903730 |
| 102 | 1 | 0 | 2.571523 | -1.930356 | -11.052993 |
| 103 | 1 | 0 | 1.259882 | -0.761958 | -10.902146 |
| 104 | 1 | 0 | 0.888155 | -2.482851 | -11.060112 |
| 105 | 8 | 0 | 0.896070 | -3.475668 | -6.725312 |
| 106 | 8 | 0 | -3.460654 | -1.827474 | -6.582214 |
| 107 | 6 | 0 | -0.015405 | -2.616858 | -7.296116 |
| 108 | 6 | 0 | -1.269534 | -2.611544 | -6.676713 |
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| 110 | 6 | 0 | -1.992016 | -0.921289 | -8.320444 |
| 111 | 6 | 0 | -0.716788 | -0.968338 | -8.894031 |
| 112 | 6 | 0 | 0.283686 | -1.828548 | -8.425769 |
| 113 | 6 | 0 | -3.077751 | -0.003195 | -8.842299 |
| 114 | 6 | 0 | -3.012309 | 0.213121 | -10.357132 |
| 115 | 1 | 0 | -1.467650 | -3.223518 | -5.802897 |
| 116 | 1 | 0 | -0.496512 | -0.319401 | -9.745202 |
| 117 | 1 | 0 | -4.072509 | -0.501871 | -8.635913 |
| 118 | 1 | 0 | -3.066889 | -0.742235 | -10.892596 |
| 119 | 1 | 0 | -2.093738 | 0.717820 | -10.673014 |
| 120 | 1 | 0 | -3.853567 | 0.832308 | -10.694259 |
| 121 | 8 | 0 | -0.333075 | 5.310020 | -5.227825 |
| 122 | 8 | 0 | 3.984016 | 3.626578 | -5.692071 |
| 123 | 6 | 0 | 0.557382 | 4.680223 | -6.063476 |
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| 148 | 8 | 0 | 5.295230 | -5.393684 | 4.163943 |

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| 149 | 1 | 0 | 4.762389 | -5.989484 | 3.605344 |
| 150 | 1 | 0 | 4.655789 | -4.817197 | 4.628529 |
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| 171 | 1 | 0 | -2.220733 | 10.814233 | 0.819132 |
| 172 | 1 | 0 | -3.975915 | 10.811375 | 0.993162 |
| 173 | 1 | 0 | -3.242602 | 11.085141 | -0.597082 |
| 174 | 8 | 0 | -0.370026 | 5.847201 | 5.999113 |
| 175 | 8 | 0 | 3.928214 | 5.985000 | 3.998774 |
| 176 | 6 | 0 | 0.524871 | 6.416085 | 5.149583 |
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| 472 | 1 | 0 | -0.941935 | -4.828708 | 1.143475 |
| 473 | 1 | 0 | -2.355956 | -5.082670 | -0.887896 |
| 474 | 1 | 0 | -3.092316 | -3.071144 | -2.151008 |
| 475 | 6 | 0 | -2.902961 | 2.766684 | 1.000620 |
| 476 | 6 | 0 | -3.922151 | 2.611974 | 0.082441 |
| 477 | 7 | 0 | -4.505565 | 1.390238 | 0.284321 |
| 478 | 6 | 0 | -3.881916 | 0.760220 | 1.322866 |
| 479 | 6 | 0 | -2.879081 | 1.585363 | 1.797023 |
| 480 | 6 | 0 | -5.607472 | 0.852999 | -0.490960 |
| 481 | 1 | 0 | -2.235568 | 3.623176 | 1.065663 |
| 482 | 1 | 0 | -4.264031 | 3.250890 | -0.730699 |
| 483 | 1 | 0 | -4.194345 | -0.234063 | 1.634985 |
| 484 | 1 | 0 | -2.180884 | 1.339476 | 2.593297 |
| 485 | 1 | 0 | -5.700230 | 1.423362 | -1.423324 |
| 486 | 1 | 0 | -5.411591 | -0.200893 | -0.735234 |
| 487 | 1 | 0 | -6.552281 | 0.915732 | 0.072471 |

Sum of electronic and thermal Free Energies = -1069.303228
ONIOM Total Energy = -1072.589912
0 imaginary frequency

MC

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | -0.000001326 | 0.000000966 | 0.000000024 |
| 2 | 1 | -0.000000368 | 0.000003700 | -0.000000603 |
| 3 | 1 | -0.000001853 | -0.000000273 | 0.000002036 |
| 4 | 1 | -0.000002550 | -0.000001187 | 0.000001677 |
| 5 | 1 | -0.000001000 | -0.000000066 | 0.000001281 |
| 6 | 1 | -0.000001486 | 0.000000693 | -0.000000190 |
| 7 | 1 | 0.000001234 | 0.000001655 | -0.000001681 |
| 8 | 6 | -0.000001027 | -0.000001512 | 0.000000840 |
| 9 | 8 | -0.000003812 | 0.000003981 | 0.000001276 |
| 10 | 8 | 0.000002138 | 0.000000703 | -0.000002248 |
| 11 | 6 | -0.000004839 | 0.000001206 | -0.000002003 |
| 12 | 6 | -0.000000329 | -0.000000343 | 0.000001124 |
| 13 | 6 | 0.000003413 | 0.000004720 | 0.000000651 |
| 14 | 6 | 0.000000141 | -0.000000022 | -0.000001767 |

| | | | | |
|---|---|---|---|---|
| 15 | 6 | -0.000005056 | -0.000007530 | -0.000001261 |
| 16 | 7 | 0.000002005 | -0.000000200 | 0.000001082 |
| 17 | 6 | 0.000000259 | 0.000001479 | 0.000003095 |
| 18 | 6 | -0.000004759 | 0.000000752 | 0.000000270 |
| 19 | 7 | 0.000003082 | -0.000000327 | 0.000000554 |
| 20 | 6 | 0.000000211 | 0.000001162 | -0.000003323 |
| 21 | 6 | 0.000003506 | 0.000002407 | 0.000005869 |
| 22 | 6 | -0.000000315 | -0.000002461 | -0.000000052 |
| 23 | 6 | 0.000000241 | -0.000002824 | 0.000001193 |
| 24 | 1 | 0.000000747 | -0.000002067 | -0.000000849 |
| 25 | 1 | 0.000000275 | -0.000000140 | 0.000000323 |
| 26 | 1 | 0.000002483 | -0.000000217 | -0.000000215 |
| 27 | 1 | 0.000002055 | -0.000000425 | -0.000002298 |
| 28 | 6 | 0.000001201 | -0.000013176 | 0.000004621 |
| 29 | 1 | 0.000002185 | 0.000006980 | -0.000005221 |
| 30 | 1 | 0.000001629 | 0.000002719 | -0.000000484 |
| 31 | 1 | 0.000001913 | -0.000000353 | -0.000003719 |

Sum of electronic and thermal Free Energies = -763.190439
0 imaginary frequency

*α*-TS1

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | -0.000001008 | 0.000002619 | 0.000000659 |
| 2 | 1 | 0.000002387 | -0.000003083 | 0.000001039 |
| 3 | 1 | -0.000002301 | 0.000003038 | 0.000002330 |
| 4 | 1 | -0.000002032 | 0.000003986 | 0.000005019 |
| 5 | 1 | 0.000000500 | 0.000002117 | 0.000006097 |
| 6 | 1 | 0.000002697 | -0.000000587 | 0.000004575 |
| 7 | 1 | 0.000002644 | -0.000001499 | 0.000001943 |
| 8 | 6 | -0.000000844 | 0.000001517 | 0.000002793 |
| 9 | 8 | 0.000000385 | 0.000000164 | -0.000003013 |
| 10 | 8 | 0.000002734 | -0.000001190 | 0.000000648 |
| 11 | 6 | 0.000001524 | 0.000000441 | 0.000002653 |
| 12 | 6 | 0.000001780 | 0.000000296 | 0.000004154 |
| 13 | 6 | 0.000001372 | 0.000004756 | 0.000005193 |
| 14 | 6 | -0.000000775 | -0.000000052 | 0.000001368 |
| 15 | 6 | 0.000001895 | -0.000003154 | -0.000009068 |
| 16 | 7 | -0.000001862 | -0.000006400 | 0.000003581 |
| 17 | 6 | -0.000001382 | 0.000002839 | 0.000004476 |
| 18 | 6 | 0.000000329 | 0.000001808 | 0.000004625 |
| 19 | 7 | -0.000003713 | 0.000009361 | 0.000005984 |
| 20 | 6 | 0.000003366 | -0.000014317 | -0.000005146 |
| 21 | 6 | -0.000002131 | -0.000003256 | -0.000001508 |
| 22 | 6 | -0.000001445 | -0.000002221 | -0.000005679 |
| 23 | 6 | 0.000004384 | 0.000004209 | -0.000005361 |
| 24 | 1 | -0.000002567 | 0.000000250 | -0.000001802 |
| 25 | 1 | 0.000000186 | -0.000000684 | -0.000001809 |
| 26 | 1 | 0.000000181 | -0.000000282 | -0.000004884 |
| 27 | 1 | 0.000002768 | -0.000003161 | -0.000002848 |
| 28 | 6 | -0.000001360 | 0.000000660 | -0.000004220 |
| 29 | 1 | -0.000002883 | 0.000001133 | -0.000002548 |
| 30 | 1 | -0.000001966 | 0.000000025 | -0.000004470 |
| 31 | 1 | -0.000002863 | 0.000000667 | -0.000004781 |

Sum of electronic and thermal Free Energies = -763.138036
1 imaginary frequency = -471.47

*β*-TS1

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 0.000001234 | -0.000000375 | -0.000000783 |
| 2 | 1 | -0.000000938 | 0.000000314 | 0.000000897 |
| 3 | 1 | -0.000000230 | -0.000000076 | -0.000000326 |
| 4 | 1 | -0.000000526 | -0.000000090 | -0.000000090 |
| 5 | 1 | -0.000000245 | 0.000000181 | -0.000000570 |
| 6 | 1 | 0.000000077 | 0.000000317 | -0.000000785 |

| | | | | |
|---|---|---|---|---|
| 7 | 1 | 0.000000057 | 0.000000170 | -0.000001311 |
| 8 | 6 | -0.000000705 | -0.000000981 | 0.000000426 |
| 9 | 8 | 0.000014249 | 0.000002629 | -0.000011221 |
| 10 | 8 | 0.000001694 | -0.000000173 | 0.000003924 |
| 11 | 6 | 0.000000253 | -0.000000230 | -0.000000556 |
| 12 | 6 | -0.000000376 | 0.000000361 | -0.000000721 |
| 13 | 6 | -0.000003331 | -0.000005059 | 0.000018373 |
| 14 | 6 | 0.000003030 | 0.000000319 | -0.000003523 |
| 15 | 6 | 0.000000527 | -0.000005103 | -0.000010546 |
| 16 | 7 | -0.000014516 | 0.000004766 | -0.000003132 |
| 17 | 6 | -0.000000536 | 0.000000024 | 0.000000105 |
| 18 | 6 | -0.000000088 | 0.000000080 | -0.000000415 |
| 19 | 7 | 0.000011481 | -0.000001864 | 0.000001347 |
| 20 | 6 | -0.000002603 | 0.000005271 | 0.000006031 |
| 21 | 6 | -0.000002373 | 0.000001325 | 0.000013745 |
| 22 | 6 | 0.000001240 | 0.000003381 | -0.000014214 |
| 23 | 6 | -0.000002708 | -0.000007706 | 0.000003594 |
| 24 | 1 | -0.000001367 | 0.000001792 | 0.000004018 |
| 25 | 1 | -0.000001491 | -0.000002041 | -0.000000363 |
| 26 | 1 | 0.000000071 | -0.000000206 | -0.000001008 |
| 27 | 1 | -0.000000216 | 0.000000254 | -0.000001237 |
| 28 | 6 | 0.000000612 | 0.000001704 | -0.000004677 |
| 29 | 1 | -0.000000111 | 0.000002567 | 0.000002066 |
| 30 | 1 | 0.000001309 | 0.000000897 | 0.000000163 |
| 31 | 1 | -0.000003476 | -0.000002448 | 0.000000787 |

Sum of electronic and thermal Free Energies = -763.128624
1 imaginary frequency = -448.85

MC-TFA

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 0.000002127 | -0.000000429 | 0.000001860 |
| 2 | 1 | -0.000000491 | 0.000002012 | -0.000000292 |
| 3 | 1 | -0.000000828 | -0.000000454 | 0.000000999 |
| 4 | 1 | -0.000000677 | -0.000000831 | 0.000000972 |
| 5 | 1 | 0.000000382 | 0.000000174 | -0.000000704 |
| 6 | 1 | -0.000000313 | 0.000001021 | -0.000001203 |
| 7 | 1 | 0.000000907 | -0.000003652 | -0.000002023 |
| 8 | 6 | -0.000000597 | 0.000000839 | 0.000000347 |
| 9 | 8 | -0.000023689 | 0.000001789 | 0.000000181 |
| 10 | 8 | -0.000001810 | 0.000000020 | 0.000006787 |
| 11 | 6 | 0.000002391 | 0.000003397 | 0.000003550 |
| 12 | 6 | 0.000000124 | -0.000002267 | -0.000000959 |
| 13 | 6 | 0.000002278 | 0.000001707 | 0.000006421 |
| 14 | 6 | -0.000003633 | -0.000005072 | -0.000005459 |
| 15 | 6 | 0.000001232 | -0.000000706 | 0.000002725 |
| 16 | 7 | 0.000009091 | -0.000000439 | -0.000012896 |
| 17 | 6 | -0.000000439 | -0.000000967 | 0.000001055 |
| 18 | 6 | -0.000001750 | -0.000000059 | -0.000000465 |
| 19 | 1 | -0.000001043 | -0.000001232 | 0.000001301 |
| 20 | 8 | 0.000008678 | 0.000014067 | 0.000010429 |
| 21 | 6 | -0.000009600 | -0.000018980 | -0.000017072 |
| 22 | 8 | 0.000013820 | 0.000008893 | 0.000003769 |
| 23 | 6 | 0.000004785 | -0.000001114 | -0.000004265 |
| 24 | 9 | -0.000007567 | 0.000004264 | 0.000013552 |
| 25 | 9 | -0.000001510 | -0.000007389 | -0.000003617 |
| 26 | 9 | 0.000010871 | 0.000003711 | 0.000006675 |
| 27 | 7 | 0.000000999 | 0.000000591 | 0.000002568 |
| 28 | 6 | -0.000000880 | 0.000002897 | -0.000009722 |
| 29 | 6 | -0.000002736 | -0.000002435 | 0.000008848 |
| 30 | 6 | 0.000002416 | -0.000000363 | -0.000009823 |
| 31 | 6 | 0.000000481 | -0.000003636 | 0.000003399 |
| 32 | 1 | 0.000000422 | 0.000000598 | -0.000002569 |
| 33 | 1 | 0.000001542 | 0.000000965 | 0.000000237 |
| 34 | 1 | 0.000001224 | 0.000001330 | 0.000000053 |
| 35 | 1 | -0.000000947 | 0.000001061 | -0.000002273 |
| 36 | 6 | -0.000007154 | 0.000016667 | 0.000001625 |
| 37 | 1 | -0.000005924 | -0.000008649 | 0.000009670 |
| 38 | 1 | 0.000007321 | -0.000007088 | -0.000008258 |

| | | | | |
|---|---|---|---|---|
| 39 | 1 | 0.000000500 | -0.000000241 | -0.000005423 |

Sum of electronic and thermal Free Energies = -1289.848656
0 imaginary frequency

$\alpha$-TS1-TFA

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | -0.000003672 | -0.000004269 | -0.000001024 |
| 2 | 1 | 0.000000210 | 0.000003324 | 0.000000441 |
| 3 | 1 | -0.000005317 | -0.000004982 | -0.000003536 |
| 4 | 1 | -0.000000991 | -0.000000646 | -0.000000558 |
| 5 | 1 | 0.000000037 | -0.000000185 | 0.000000209 |
| 6 | 1 | -0.000000149 | 0.000001135 | -0.000001277 |
| 7 | 1 | -0.000000032 | 0.000003797 | -0.000001623 |
| 8 | 6 | -0.000006728 | 0.000001271 | 0.000004057 |
| 9 | 8 | -0.000007835 | -0.000004530 | -0.000008854 |
| 10 | 8 | -0.000008214 | 0.000002855 | 0.000004921 |
| 11 | 6 | -0.000000120 | -0.000004222 | 0.000002847 |
| 12 | 6 | -0.000001278 | 0.000001400 | 0.000000780 |
| 13 | 6 | 0.000013240 | -0.000002790 | -0.000000088 |
| 14 | 6 | -0.000000592 | 0.000001636 | -0.000004353 |
| 15 | 6 | -0.000015456 | -0.000014026 | -0.000000678 |
| 16 | 7 | 0.000011907 | 0.000013150 | -0.000003482 |
| 17 | 6 | -0.000001109 | -0.000002015 | 0.000000205 |
| 18 | 6 | 0.000001385 | 0.000001081 | -0.000001348 |
| 19 | 1 | 0.000006940 | 0.000001606 | 0.000006575 |
| 20 | 8 | -0.000000622 | -0.000002853 | 0.000007080 |
| 21 | 6 | 0.000031578 | 0.000015946 | 0.000139285 |
| 22 | 8 | -0.000028750 | -0.000009959 | -0.000137487 |
| 23 | 6 | 0.000025265 | 0.000012938 | 0.000118022 |
| 24 | 9 | -0.000001449 | 0.000001843 | -0.000001777 |
| 25 | 9 | -0.000000764 | 0.000003705 | 0.000001116 |
| 26 | 9 | -0.000024709 | -0.000018105 | -0.000125313 |
| 27 | 7 | 0.000000129 | -0.000014048 | -0.000000621 |
| 28 | 6 | -0.000001907 | 0.000002870 | 0.000002082 |
| 29 | 6 | 0.000006789 | 0.000007821 | -0.000003412 |
| 30 | 6 | -0.000002456 | -0.000000152 | 0.000002917 |
| 31 | 6 | 0.000002958 | 0.000003605 | 0.000002750 |
| 32 | 1 | 0.000006871 | 0.000002023 | -0.000002200 |
| 33 | 1 | 0.000000053 | -0.000001215 | -0.000001398 |
| 34 | 1 | 0.000000858 | -0.000000087 | 0.000002008 |
| 35 | 1 | -0.000000352 | 0.000001701 | 0.000001674 |
| 36 | 6 | 0.000001699 | 0.000004909 | -0.000000471 |
| 37 | 1 | -0.000001325 | -0.000000278 | 0.000001393 |
| 38 | 1 | 0.000002456 | -0.000003479 | 0.000001161 |
| 39 | 1 | 0.000001453 | -0.000000775 | -0.000000022 |

Sum of electronic and thermal Free Energies = -1289.810668
1 imaginary frequency = -353.21

$\beta$-TS1-TFA

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 0.000000977 | 0.000001115 | 0.000001036 |
| 2 | 1 | 0.000001120 | -0.000001589 | 0.000002841 |
| 3 | 1 | 0.000002614 | 0.000000394 | -0.000000995 |
| 4 | 1 | 0.000003161 | 0.000000242 | -0.000000557 |
| 5 | 1 | 0.000001955 | -0.000000837 | 0.000001666 |
| 6 | 1 | 0.000000246 | -0.000001619 | 0.000003437 |
| 7 | 1 | -0.000000257 | -0.000001440 | 0.000002875 |
| 8 | 6 | 0.000002019 | -0.000000033 | 0.000000122 |
| 9 | 8 | 0.000000708 | -0.000001991 | -0.000002385 |
| 10 | 8 | 0.000001625 | -0.000000983 | 0.000002563 |
| 11 | 6 | 0.000000251 | -0.000000936 | 0.000002378 |
| 12 | 6 | 0.000000765 | -0.000000939 | 0.000002438 |
| 13 | 6 | -0.000001543 | 0.000000517 | 0.000003638 |

| | | | | |
|---|---|---|---|---|
| 14 | 6 | 0.000002283 | 0.000000375 | -0.000000552 |
| 15 | 6 | 0.000001668 | 0.000002833 | 0.000002527 |
| 16 | 7 | 0.000002154 | -0.000003357 | 0.000000514 |
| 17 | 6 | 0.000002480 | -0.000000089 | 0.000000288 |
| 18 | 6 | 0.000001857 | -0.000000836 | 0.000001452 |
| 19 | 1 | 0.000003948 | -0.000000983 | 0.000002977 |
| 20 | 8 | -0.000001153 | 0.000000874 | -0.000003674 |
| 21 | 6 | -0.000005249 | 0.000000540 | 0.000004002 |
| 22 | 8 | -0.000004375 | -0.000006734 | -0.000007168 |
| 23 | 6 | 0.000000937 | 0.000002629 | -0.000001035 |
| 24 | 9 | 0.000001312 | 0.000004415 | -0.000002433 |
| 25 | 9 | -0.000000398 | -0.000004953 | 0.000003723 |
| 26 | 9 | -0.000000757 | 0.000003834 | 0.000002376 |
| 27 | 7 | -0.000005479 | 0.000000630 | -0.000001794 |
| 28 | 6 | -0.000002158 | 0.000000857 | -0.000002108 |
| 29 | 6 | 0.000002265 | -0.000000438 | 0.000001102 |
| 30 | 6 | 0.000000778 | -0.000001052 | -0.000000108 |
| 31 | 6 | -0.000000034 | 0.000002279 | -0.000003580 |
| 32 | 1 | -0.000001841 | 0.000000658 | 0.000000141 |
| 33 | 1 | -0.000001860 | -0.000001374 | 0.000001187 |
| 34 | 1 | -0.000001162 | 0.000001698 | -0.000003581 |
| 35 | 1 | -0.000001001 | 0.000000725 | -0.000001677 |
| 36 | 6 | -0.000005415 | -0.000000304 | -0.000002601 |
| 37 | 1 | -0.000001261 | 0.000003458 | -0.000001603 |
| 38 | 1 | -0.000002052 | 0.000001654 | -0.000005232 |
| 39 | 1 | 0.000000872 | 0.000000761 | -0.000002201 |

Sum of electronic and thermal Free Energies = -1289.808280
1 imaginary frequency = -384.47

**$\alpha$-TS1@$C_R$**

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | 0.000000010 | 0.000000067 | -0.000000037 |
| 2 | 8 | 0.000000037 | 0.000000051 | -0.000000086 |
| 3 | 6 | -0.000000020 | -0.000000008 | 0.000000032 |
| 4 | 6 | -0.000000029 | -0.000000020 | 0.000000077 |
| 5 | 6 | -0.000000013 | -0.000000012 | 0.000000047 |
| 6 | 6 | 0.000000009 | 0.000000057 | 0.000000031 |
| 7 | 6 | 0.000000029 | 0.000000067 | 0.000000034 |
| 8 | 6 | -0.000000038 | 0.000000020 | 0.000000033 |
| 9 | 6 | -0.000000026 | 0.000000034 | 0.000000018 |
| 10 | 6 | -0.000000009 | 0.000000016 | 0.000000039 |
| 11 | 1 | -0.000000017 | 0.000000006 | 0.000000047 |
| 12 | 1 | 0.000000002 | 0.000000029 | 0.000000026 |
| 13 | 1 | -0.000000010 | 0.000000028 | 0.000000023 |
| 14 | 1 | -0.000000015 | 0.000000010 | 0.000000038 |
| 15 | 1 | -0.000000005 | 0.000000019 | 0.000000046 |
| 16 | 1 | -0.000000001 | 0.000000023 | 0.000000029 |
| 17 | 8 | -0.000000017 | -0.000000062 | -0.000000085 |
| 18 | 8 | -0.000000030 | -0.000000031 | 0.000000038 |
| 19 | 6 | -0.000000052 | 0.000000028 | 0.000000041 |
| 20 | 6 | -0.000000020 | -0.000000062 | -0.000000040 |
| 21 | 6 | 0.000000029 | -0.000000001 | 0.000000009 |
| 22 | 6 | -0.000000033 | -0.000000058 | 0.000000042 |
| 23 | 6 | -0.000000073 | 0.000000008 | -0.000000005 |
| 24 | 6 | 0.000000013 | 0.000000034 | 0.000000035 |
| 25 | 6 | -0.000000031 | -0.000000018 | 0.000000026 |
| 26 | 6 | -0.000000048 | -0.000000007 | 0.000000028 |
| 27 | 1 | -0.000000023 | -0.000000020 | 0.000000000 |
| 28 | 1 | -0.000000031 | 0.000000001 | 0.000000033 |
| 29 | 1 | -0.000000040 | -0.000000016 | 0.000000023 |
| 30 | 1 | -0.000000030 | 0.000000002 | 0.000000035 |
| 31 | 1 | -0.000000037 | -0.000000020 | 0.000000043 |
| 32 | 1 | -0.000000038 | -0.000000010 | 0.000000036 |
| 33 | 8 | -0.000000041 | 0.000000051 | 0.000000066 |
| 34 | 8 | -0.000000002 | 0.000000028 | 0.000000049 |
| 35 | 6 | 0.000000012 | -0.000000026 | 0.000000011 |
| 36 | 6 | -0.000000008 | 0.000000040 | 0.000000014 |

| | | | | |
|---|---|---|---|---|
| 37 | 6 | 0.000000018 | 0.000000027 | -0.000000034 |
| 38 | 6 | -0.000000035 | -0.000000016 | 0.000000033 |
| 39 | 6 | 0.000000008 | 0.000000000 | 0.000000038 |
| 40 | 6 | -0.000000008 | 0.000000004 | 0.000000018 |
| 41 | 6 | -0.000000017 | -0.000000020 | 0.000000016 |
| 42 | 6 | -0.000000025 | -0.000000001 | 0.000000025 |
| 43 | 1 | 0.000000001 | 0.000000009 | -0.000000006 |
| 44 | 1 | -0.000000007 | 0.000000005 | 0.000000040 |
| 45 | 1 | -0.000000012 | -0.000000003 | 0.000000014 |
| 46 | 1 | -0.000000017 | -0.000000008 | 0.000000026 |
| 47 | 1 | -0.000000017 | -0.000000004 | 0.000000026 |
| 48 | 1 | -0.000000018 | 0.000000008 | 0.000000024 |
| 49 | 8 | -0.000000043 | -0.000000016 | -0.000000014 |
| 50 | 8 | -0.000000021 | 0.000000000 | 0.000000028 |
| 51 | 6 | -0.000000051 | 0.000000000 | 0.000000021 |
| 52 | 6 | -0.000000025 | -0.000000014 | -0.000000012 |
| 53 | 6 | -0.000000024 | -0.000000020 | 0.000000072 |
| 54 | 6 | -0.000000036 | 0.000000024 | 0.000000018 |
| 55 | 6 | 0.000000000 | 0.000000015 | 0.000000030 |
| 56 | 6 | -0.000000027 | -0.000000012 | 0.000000078 |
| 57 | 6 | -0.000000015 | 0.000000010 | 0.000000052 |
| 58 | 6 | -0.000000022 | 0.000000013 | 0.000000045 |
| 59 | 1 | -0.000000028 | -0.000000004 | 0.000000015 |
| 60 | 1 | -0.000000027 | 0.000000007 | 0.000000040 |
| 61 | 1 | -0.000000022 | 0.000000013 | 0.000000046 |
| 62 | 1 | -0.000000026 | 0.000000017 | 0.000000051 |
| 63 | 1 | -0.000000028 | 0.000000004 | 0.000000053 |
| 64 | 1 | -0.000000030 | 0.000000011 | 0.000000049 |
| 65 | 1 | -0.000000032 | -0.000000007 | 0.000000035 |
| 66 | 1 | -0.000000016 | -0.000000055 | 0.000000189 |
| 67 | 1 | -0.000000035 | -0.000000047 | 0.000000170 |
| 68 | 1 | -0.000000040 | 0.000000068 | 0.000000098 |
| 69 | 1 | -0.000000012 | -0.000000007 | -0.000000011 |
| 70 | 1 | 0.000000000 | 0.000000024 | 0.000000021 |
| 71 | 1 | -0.000000009 | -0.000000002 | -0.000000001 |
| 72 | 1 | -0.000000017 | 0.000000014 | 0.000000038 |
| 73 | 8 | 0.000000018 | 0.000000032 | -0.000000004 |
| 74 | 8 | -0.000000124 | -0.000000141 | 0.000000028 |
| 75 | 6 | 0.000000035 | -0.000000054 | 0.000000032 |
| 76 | 6 | -0.000000016 | 0.000000050 | -0.000000109 |
| 77 | 6 | 0.000000135 | 0.000000136 | -0.000000033 |
| 78 | 6 | 0.000000048 | -0.000000027 | 0.000000022 |
| 79 | 6 | 0.000000005 | 0.000000041 | -0.000000107 |
| 80 | 6 | -0.000000008 | -0.000000016 | -0.000000051 |
| 81 | 6 | 0.000000025 | 0.000000031 | 0.000000012 |
| 82 | 6 | 0.000000022 | 0.000000030 | -0.000000009 |
| 83 | 1 | 0.000000034 | -0.000000033 | -0.000000040 |
| 84 | 1 | 0.000000022 | -0.000000003 | -0.000000041 |
| 85 | 1 | 0.000000047 | 0.000000009 | -0.000000035 |
| 86 | 1 | 0.000000042 | 0.000000013 | -0.000000042 |
| 87 | 1 | 0.000000038 | 0.000000002 | -0.000000052 |
| 88 | 1 | 0.000000027 | -0.000000010 | -0.000000046 |
| 89 | 8 | 0.000000110 | 0.000000039 | 0.000000015 |
| 90 | 8 | 0.000000050 | 0.000000056 | 0.000000013 |
| 91 | 6 | 0.000000053 | -0.000000021 | 0.000000074 |
| 92 | 6 | 0.000000069 | 0.000000017 | -0.000000044 |
| 93 | 6 | -0.000000039 | -0.000000023 | -0.000000020 |
| 94 | 6 | 0.000000057 | 0.000000019 | -0.000000002 |
| 95 | 6 | 0.000000005 | 0.000000019 | -0.000000066 |
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| 97 | 6 | -0.000000028 | -0.000000023 | 0.000000005 |
| 98 | 6 | 0.000000009 | -0.000000003 | -0.000000035 |
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| 104 | 1 | 0.000000003 | -0.000000019 | -0.000000033 |
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| 107 | 6 | -0.000000009 | 0.000000030 | 0.000000007 |
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| 110 | 6 | -0.000000020 | 0.000000078 | -0.000000016 |
| 111 | 6 | 0.000000057 | 0.000000008 | -0.000000030 |
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| 116 | 1 | 0.000000020 | -0.000000003 | -0.000000045 |
| 117 | 1 | 0.000000014 | -0.000000023 | -0.000000039 |
| 118 | 1 | 0.000000012 | -0.000000034 | -0.000000049 |
| 119 | 1 | 0.000000017 | -0.000000006 | -0.000000048 |
| 120 | 1 | 0.000000021 | -0.000000017 | -0.000000055 |
| 121 | 8 | 0.000000031 | 0.000000028 | -0.000000041 |
| 122 | 8 | 0.000000013 | 0.000000176 | 0.000000093 |
| 123 | 6 | 0.000000050 | 0.000000077 | -0.000000029 |
| 124 | 6 | 0.000000005 | 0.000000044 | -0.000000020 |
| 125 | 6 | -0.000000002 | 0.000000057 | 0.000000016 |
| 126 | 6 | 0.000000048 | -0.000000021 | -0.000000021 |
| 127 | 6 | 0.000000008 | -0.000000025 | -0.000000067 |
| 128 | 6 | 0.000000052 | -0.000000070 | -0.000000001 |
| 129 | 6 | -0.000000012 | -0.000000022 | -0.000000045 |
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| 141 | 1 | 0.000000137 | 0.000000021 | -0.000000054 |
| 142 | 1 | -0.000000016 | -0.000000123 | -0.000000127 |
| 143 | 1 | 0.000000085 | 0.000000073 | -0.000000063 |
| 144 | 1 | 0.000000015 | 0.000000064 | -0.000000020 |
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| 152 | 1 | -0.000000019 | -0.000000042 | 0.000000029 |
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| 155 | 1 | -0.000000080 | -0.000000395 | -0.000000335 |
| 156 | 1 | 0.000000094 | 0.000000263 | 0.000000238 |
| 157 | 1 | 0.000000021 | 0.000000046 | 0.000000011 |
| 158 | 8 | 0.000000113 | -0.000000064 | 0.000000040 |
| 159 | 8 | -0.000000146 | 0.000000123 | 0.000000329 |
| 160 | 6 | 0.000000013 | 0.000000057 | 0.000000000 |
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| 162 | 6 | -0.000000008 | 0.000000050 | -0.000000163 |
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| 164 | 6 | 0.000000018 | -0.000000010 | -0.000000074 |
| 165 | 6 | 0.000000037 | 0.000000051 | -0.000000090 |
| 166 | 6 | -0.000000002 | -0.000000004 | -0.000000017 |
| 167 | 6 | 0.000000047 | 0.000000013 | -0.000000031 |
| 168 | 1 | 0.000000030 | 0.000000023 | -0.000000008 |
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| 172 | 1 | 0.000000036 | 0.000000015 | -0.000000018 |
| 173 | 1 | 0.000000043 | 0.000000017 | -0.000000024 |
| 174 | 8 | 0.000000068 | 0.000000013 | 0.000000006 |
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| 180 | 6 | 0.000000033 | 0.000000054 | 0.000000021 |
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| 182 | 6 | 0.000000017 | 0.000000062 | 0.000000087 |

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| 183 | 6 | 0.000000042 | 0.000000032 | 0.000000010 |
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| 191 | 8 | 0.000000002 | 0.000000008 | -0.000000008 |
| 192 | 6 | -0.000000031 | 0.000000055 | 0.000000055 |
| 193 | 6 | 0.000000000 | -0.000000036 | -0.000000041 |
| 194 | 6 | 0.000000056 | -0.000000006 | -0.000000067 |
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| 196 | 6 | 0.000000022 | -0.000000067 | -0.000000007 |
| 197 | 6 | 0.000000097 | 0.000000026 | -0.000000078 |
| 198 | 6 | 0.000000044 | 0.000000026 | -0.000000004 |
| 199 | 6 | 0.000000031 | 0.000000035 | -0.000000010 |
| 200 | 1 | 0.000000016 | 0.000000007 | -0.000000014 |
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| 203 | 1 | 0.000000034 | 0.000000025 | -0.000000005 |
| 204 | 1 | 0.000000027 | 0.000000023 | 0.000000002 |
| 205 | 1 | 0.000000033 | 0.000000018 | -0.000000004 |
| 206 | 8 | -0.000000116 | 0.000000032 | -0.000000033 |
| 207 | 8 | 0.000000031 | 0.000000031 | -0.000000150 |
| 208 | 6 | 0.000000011 | 0.000000135 | -0.000000069 |
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| 210 | 6 | 0.000000091 | 0.000000049 | 0.000000030 |
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| 222 | 1 | 0.000000121 | -0.000000073 | -0.000000109 |
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| 224 | 1 | 0.000000020 | 0.000000025 | 0.000000020 |
| 225 | 1 | 0.000000015 | 0.000000075 | -0.000000044 |
| 226 | 1 | 0.000000016 | 0.000000006 | -0.000000003 |
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| 230 | 1 | -0.000000034 | -0.000000034 | -0.000000009 |
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| 232 | 8 | -0.000000073 | -0.000000030 | 0.000000027 |
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| 236 | 6 | -0.000000018 | -0.000000073 | 0.000000080 |
| 237 | 6 | -0.000000129 | -0.000000024 | -0.000000068 |
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| 242 | 1 | -0.000000031 | -0.000000019 | 0.000000017 |
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| 251 | 6 | -0.000000081 | 0.000000006 | 0.000000004 |
| 252 | 6 | -0.000000019 | 0.000000028 | 0.000000049 |
| 253 | 6 | -0.000000004 | -0.000000010 | -0.000000047 |
| 254 | 6 | -0.000000079 | -0.000000062 | 0.000000013 |
| 255 | 6 | 0.000000010 | 0.000000022 | 0.000000060 |

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| 256 | 6 | -0.000000034 | -0.000000014 | -0.000000015 |
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| 266 | 6 | -0.000000033 | -0.000000025 | 0.000000025 |
| 267 | 6 | -0.000000004 | -0.000000003 | 0.000000037 |
| 268 | 6 | -0.000000022 | 0.000000005 | 0.000000042 |
| 269 | 6 | -0.000000055 | -0.000000022 | 0.000000002 |
| 270 | 6 | -0.000000037 | -0.000000036 | -0.000000004 |
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| 273 | 6 | -0.000000045 | -0.000000027 | 0.000000023 |
| 274 | 1 | -0.000000016 | -0.000000001 | 0.000000033 |
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| 276 | 1 | -0.000000043 | -0.000000017 | 0.000000025 |
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| 297 | 1 | -0.000000036 | -0.000000008 | 0.000000023 |
| 298 | 1 | -0.000000022 | -0.000000032 | -0.000000029 |
| 299 | 1 | 0.000000005 | -0.000000020 | -0.000000009 |
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| 301 | 1 | -0.000000040 | 0.000000003 | -0.000000043 |
| 302 | 1 | -0.000000063 | -0.000000042 | 0.000000016 |
| 303 | 1 | 0.000000011 | -0.000000026 | -0.000000038 |
| 304 | 1 | 0.000000301 | -0.000000029 | -0.000000116 |
| 305 | 8 | -0.000000005 | -0.000000075 | 0.000000025 |
| 306 | 8 | 0.000000018 | 0.000000001 | -0.000000042 |
| 307 | 6 | -0.000000004 | 0.000000000 | -0.000000028 |
| 308 | 6 | -0.000000015 | -0.000000065 | -0.000000048 |
| 309 | 6 | 0.000000019 | -0.000000086 | -0.000000099 |
| 310 | 6 | -0.000000001 | -0.000000048 | -0.000000021 |
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| 312 | 6 | -0.000000068 | 0.000000000 | -0.000000020 |
| 313 | 6 | -0.000000028 | -0.000000011 | -0.000000022 |
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| 315 | 1 | -0.000000033 | -0.000000025 | -0.000000007 |
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| 319 | 1 | -0.000000027 | -0.000000028 | -0.000000033 |
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| 321 | 8 | 0.000000050 | -0.000000032 | -0.000000021 |
| 322 | 8 | -0.000000320 | -0.000000066 | 0.000000231 |
| 323 | 6 | 0.000000029 | 0.000000019 | -0.000000012 |
| 324 | 6 | 0.000000031 | -0.000000054 | 0.000000032 |
| 325 | 6 | 0.000000201 | 0.000000082 | -0.000000214 |
| 326 | 6 | -0.000000019 | 0.000000027 | -0.000000044 |
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| 329 | 6 | 0.000000006 | -0.000000061 | -0.000000025 |
| 330 | 6 | 0.000000001 | -0.000000030 | -0.000000052 |
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| 333 | 1 | 0.000000003 | -0.000000004 | -0.000000038 |
| 334 | 1 | 0.000000006 | -0.000000016 | -0.000000046 |
| 335 | 1 | 0.000000009 | -0.000000034 | -0.000000037 |
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| 339 | 6 | 0.000000051 | -0.000000094 | -0.000000108 |
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| 343 | 6 | 0.000000022 | -0.000000071 | -0.000000135 |
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| 346 | 6 | -0.000000017 | -0.000000040 | -0.000000035 |
| 347 | 1 | -0.000000012 | -0.000000021 | -0.000000038 |
| 348 | 1 | 0.000000005 | -0.000000010 | -0.000000054 |
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| 352 | 1 | -0.000000015 | -0.000000039 | -0.000000040 |
| 353 | 8 | 0.000000062 | -0.000000065 | 0.000000032 |
| 354 | 8 | -0.000000022 | -0.000000007 | -0.000000027 |
| 355 | 6 | -0.000000064 | -0.000000073 | -0.000000082 |
| 356 | 6 | -0.000000025 | 0.000000044 | 0.000000014 |
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| 358 | 6 | -0.000000052 | 0.000000009 | -0.000000027 |
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| 360 | 6 | 0.000000057 | -0.000000032 | 0.000000006 |
| 361 | 6 | -0.000000007 | -0.000000015 | -0.000000024 |
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| 363 | 1 | -0.000000011 | -0.000000022 | -0.000000016 |
| 364 | 1 | -0.000000002 | -0.000000025 | -0.000000025 |
| 365 | 1 | 0.000000001 | -0.000000016 | -0.000000036 |
| 366 | 1 | 0.000000004 | -0.000000030 | -0.000000027 |
| 367 | 1 | 0.000000001 | -0.000000021 | -0.000000038 |
| 368 | 1 | 0.000000014 | -0.000000015 | -0.000000026 |
| 369 | 1 | -0.000000036 | 0.000000053 | -0.000000085 |
| 370 | 1 | -0.000000024 | -0.000000050 | -0.000000033 |
| 371 | 1 | -0.000000036 | 0.000000010 | -0.000000016 |
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| 373 | 1 | 0.000000002 | 0.000000026 | 0.000000019 |
| 374 | 1 | 0.000000001 | 0.000000045 | 0.000000010 |
| 375 | 1 | -0.000000014 | 0.000000006 | 0.000000013 |
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| 377 | 8 | 0.000000088 | -0.000000074 | 0.000000072 |
| 378 | 8 | 0.000000006 | 0.000000059 | 0.000000036 |
| 379 | 6 | 0.000000044 | 0.000000106 | 0.000000037 |
| 380 | 6 | 0.000000028 | 0.000000009 | 0.000000000 |
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| 385 | 6 | -0.000000004 | 0.000000015 | 0.000000047 |
| 386 | 6 | 0.000000004 | 0.000000042 | 0.000000051 |
| 387 | 1 | 0.000000015 | 0.000000032 | 0.000000003 |
| 388 | 1 | 0.000000004 | 0.000000037 | 0.000000048 |
| 389 | 1 | 0.000000001 | 0.000000030 | 0.000000046 |
| 390 | 1 | -0.000000004 | 0.000000039 | 0.000000058 |
| 391 | 1 | 0.000000006 | 0.000000050 | 0.000000046 |
| 392 | 1 | 0.000000012 | 0.000000035 | 0.000000041 |
| 393 | 8 | 0.000000004 | 0.000000030 | 0.000000034 |
| 394 | 8 | 0.000000018 | 0.000000002 | 0.000000043 |
| 395 | 6 | 0.000000011 | 0.000000021 | 0.000000024 |
| 396 | 6 | 0.000000006 | 0.000000018 | 0.000000069 |
| 397 | 6 | 0.000000016 | -0.000000005 | 0.000000008 |
| 398 | 6 | -0.000000014 | -0.000000011 | 0.000000054 |
| 399 | 6 | -0.000000009 | 0.000000054 | 0.000000014 |
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| 401 | 6 | 0.000000028 | 0.000000014 | -0.000000014 |

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| 402 | 6 | 0.000000009 | 0.000000030 | 0.000000037 |
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| 411 | 6 | 0.000000007 | 0.000000017 | 0.000000030 |
| 412 | 6 | -0.000000046 | -0.000000022 | 0.000000039 |
| 413 | 6 | -0.000000016 | 0.000000052 | 0.000000049 |
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| 418 | 6 | -0.000000010 | 0.000000020 | 0.000000051 |
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| 421 | 1 | -0.000000016 | 0.000000023 | 0.000000038 |
| 422 | 1 | 0.000000002 | 0.000000037 | 0.000000048 |
| 423 | 1 | -0.000000020 | 0.000000030 | 0.000000033 |
| 424 | 1 | -0.000000011 | 0.000000017 | 0.000000047 |
| 425 | 8 | -0.000000051 | -0.000000021 | 0.000000011 |
| 426 | 8 | 0.000000095 | 0.000000065 | 0.000000067 |
| 427 | 6 | -0.000000013 | 0.000000017 | 0.000000127 |
| 428 | 6 | -0.000000035 | 0.000000058 | -0.000000032 |
| 429 | 6 | 0.000000060 | -0.000000020 | 0.000000059 |
| 430 | 6 | 0.000000086 | 0.000000009 | 0.000000086 |
| 431 | 6 | 0.000000000 | 0.000000016 | -0.000000052 |
| 432 | 6 | 0.000000025 | 0.000000030 | 0.000000023 |
| 433 | 6 | 0.000000015 | 0.000000014 | 0.000000028 |
| 434 | 6 | 0.000000018 | 0.000000044 | 0.000000038 |
| 435 | 1 | 0.000000021 | 0.000000028 | 0.000000017 |
| 436 | 1 | 0.000000022 | 0.000000015 | 0.000000021 |
| 437 | 1 | 0.000000024 | 0.000000033 | 0.000000024 |
| 438 | 1 | 0.000000019 | 0.000000055 | 0.000000027 |
| 439 | 1 | 0.000000021 | 0.000000034 | 0.000000024 |
| 440 | 1 | 0.000000028 | 0.000000040 | 0.000000043 |
| 441 | 1 | -0.000000011 | 0.000000001 | 0.000000026 |
| 442 | 1 | 0.000000023 | 0.000000016 | -0.000000004 |
| 443 | 1 | -0.000000059 | 0.000000011 | -0.000000138 |
| 444 | 1 | -0.000000027 | 0.000000003 | 0.000000019 |
| 445 | 8 | -0.000000140 | 0.000000191 | 0.000000124 |
| 446 | 1 | 0.000000018 | -0.000000115 | 0.000000037 |
| 447 | 1 | 0.000000251 | -0.000000152 | -0.000000341 |
| 448 | 8 | 0.000000023 | 0.000000060 | -0.000000057 |
| 449 | 1 | -0.000000003 | -0.000000001 | 0.000000041 |
| 450 | 1 | 0.000000016 | -0.000000001 | 0.000000030 |
| 451 | 8 | -0.000000029 | -0.000000014 | -0.000000019 |
| 452 | 1 | -0.000000027 | -0.000000017 | 0.000000009 |
| 453 | 1 | -0.000000039 | -0.000000038 | 0.000000006 |
| 454 | 8 | -0.000000040 | -0.000000070 | 0.000000015 |
| 455 | 1 | -0.000000005 | 0.000000022 | 0.000000016 |
| 456 | 1 | -0.000000002 | -0.000000007 | 0.000000014 |
| 457 | 6 | 0.000000005 | -0.000000375 | -0.000000599 |
| 458 | 6 | 0.000000255 | 0.000000349 | 0.000000042 |
| 459 | 6 | -0.000000096 | -0.000000087 | 0.000000603 |
| 460 | 7 | 0.000000011 | -0.000000248 | -0.000000424 |
| 461 | 6 | 0.000000054 | 0.000000227 | 0.000000481 |
| 462 | 6 | -0.000000145 | 0.000000052 | -0.000000528 |
| 463 | 6 | -0.000000166 | -0.000000381 | 0.000000618 |
| 464 | 6 | 0.000000360 | 0.000000064 | -0.000000221 |
| 465 | 6 | 0.000000073 | -0.000000331 | -0.000000185 |
| 466 | 8 | -0.000000097 | 0.000000347 | 0.000000328 |
| 467 | 8 | 0.000000126 | 0.000000159 | 0.000000099 |
| 468 | 1 | -0.000000079 | -0.000000066 | -0.000000147 |
| 469 | 1 | 0.000000156 | 0.000000082 | -0.000000154 |
| 470 | 1 | -0.000000069 | 0.000000004 | -0.000000153 |
| 471 | 1 | -0.000000112 | -0.000000051 | -0.000000015 |
| 472 | 1 | 0.000000014 | 0.000000087 | -0.000000087 |
| 473 | 1 | -0.000000037 | 0.000000071 | 0.000000193 |
| 474 | 1 | -0.000000031 | -0.000000138 | 0.000000095 |

| | | | | |
|---|---|---|---|---|
| 475 | 6 | -0.000000009 | -0.000000246 | 0.000000372 |
| 476 | 6 | 0.000000523 | 0.000000026 | -0.000000606 |
| 477 | 7 | -0.000000559 | -0.000000285 | 0.000000073 |
| 478 | 6 | 0.000000189 | 0.000000747 | 0.000000296 |
| 479 | 6 | -0.000000008 | -0.000000125 | -0.000000231 |
| 480 | 6 | 0.000000273 | -0.000000083 | -0.000000088 |
| 481 | 1 | -0.000000093 | -0.000000033 | 0.000000069 |
| 482 | 1 | 0.000000056 | 0.000000110 | -0.000000157 |
| 483 | 1 | -0.000000057 | -0.000000120 | -0.000000135 |
| 484 | 1 | -0.000000218 | -0.000000163 | 0.000000245 |
| 485 | 1 | -0.000000129 | 0.000000021 | -0.000000080 |
| 486 | 1 | -0.000000343 | -0.000000106 | -0.000000308 |
| 487 | 1 | -0.000000024 | 0.000000092 | 0.000000122 |

Sum of electronic and thermal Free Energies = -1069.255528
ONIOM Total Energy = -1072.545357
1 imaginary frequency = -392.89

**$\alpha$-I1@$C_R$**

| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | -0.000001882 | 0.000003215 | 0.000002424 |
| 2 | 8 | -0.000002174 | 0.000002069 | 0.000005515 |
| 3 | 6 | -0.000001571 | -0.000001679 | -0.000004265 |
| 4 | 6 | -0.000000143 | -0.000000055 | 0.000000108 |
| 5 | 6 | 0.000003572 | -0.000004779 | -0.000003959 |
| 6 | 6 | -0.000001111 | 0.000001104 | 0.000001225 |
| 7 | 6 | -0.000000720 | -0.000000427 | -0.000001025 |
| 8 | 6 | 0.000001667 | 0.000001798 | 0.000001135 |
| 9 | 6 | -0.000000182 | -0.000000256 | -0.000000302 |
| 10 | 6 | -0.000000016 | 0.000000531 | -0.000000336 |
| 11 | 1 | -0.000001664 | 0.000001048 | 0.000000412 |
| 12 | 1 | -0.000000183 | 0.000000411 | -0.000000364 |
| 13 | 1 | -0.000000139 | 0.000000213 | 0.000000341 |
| 14 | 1 | -0.000000003 | 0.000000254 | 0.000000187 |
| 15 | 1 | -0.000000009 | 0.000000097 | -0.000000131 |
| 16 | 1 | -0.000000202 | 0.000000016 | 0.000000157 |
| 17 | 8 | -0.000009662 | 0.000002750 | 0.000004322 |
| 18 | 8 | -0.000005775 | -0.000007186 | 0.000004218 |
| 19 | 6 | -0.000002167 | -0.000000214 | -0.000002564 |
| 20 | 6 | 0.000002731 | 0.000001475 | 0.000003298 |
| 21 | 6 | -0.000001331 | -0.000000498 | -0.000003508 |
| 22 | 6 | 0.000001343 | 0.000000993 | -0.000002252 |
| 23 | 6 | 0.000000482 | 0.000000641 | 0.000003334 |
| 24 | 6 | -0.000000261 | -0.000001081 | -0.000001150 |
| 25 | 6 | 0.000001408 | -0.000001782 | 0.000003762 |
| 26 | 6 | -0.000000358 | -0.000000013 | 0.000000107 |
| 27 | 1 | -0.000000533 | -0.000001704 | -0.000000141 |
| 28 | 1 | 0.000000304 | 0.000000769 | -0.000000809 |
| 29 | 1 | 0.000000398 | 0.000000257 | -0.000002394 |
| 30 | 1 | -0.000000098 | 0.000000464 | -0.000000410 |
| 31 | 1 | 0.000000020 | 0.000000211 | 0.000000005 |
| 32 | 1 | -0.000000176 | 0.000000333 | -0.000000100 |
| 33 | 8 | 0.000017111 | 0.000000878 | -0.000009232 |
| 34 | 8 | 0.000001039 | -0.000001790 | -0.000001112 |
| 35 | 6 | -0.000004074 | 0.000002200 | 0.000000161 |
| 36 | 6 | -0.000001616 | -0.000002726 | -0.000002019 |
| 37 | 6 | 0.000000763 | 0.000003234 | 0.000000243 |
| 38 | 6 | 0.000001639 | -0.000000768 | 0.000001029 |
| 39 | 6 | -0.000000628 | -0.000001252 | -0.000000066 |
| 40 | 6 | -0.000000345 | -0.000000461 | 0.000001993 |
| 41 | 6 | -0.000005867 | -0.000000767 | -0.000000537 |
| 42 | 6 | 0.000000226 | 0.000002244 | -0.000001054 |
| 43 | 1 | 0.000000204 | -0.000000557 | -0.000000690 |
| 44 | 1 | 0.000001141 | 0.000000772 | -0.000000599 |
| 45 | 1 | 0.000003055 | 0.000001929 | -0.000000496 |
| 46 | 1 | 0.000000051 | -0.000000313 | 0.000000112 |
| 47 | 1 | -0.000000193 | -0.000000259 | 0.000000139 |
| 48 | 1 | 0.000000038 | -0.000000507 | 0.000001081 |
| 49 | 8 | 0.000003850 | 0.000001521 | 0.000001126 |

| | | | | |
|---|---|---|---|---|
| 50 | 8 | 0.000000172 | 0.000001486 | 0.000002340 |
| 51 | 6 | -0.000000717 | -0.000001158 | -0.000001229 |
| 52 | 6 | -0.000001713 | 0.000000199 | -0.000000057 |
| 53 | 6 | 0.000000466 | -0.000001712 | 0.000001181 |
| 54 | 6 | 0.000000377 | 0.000001019 | 0.000000774 |
| 55 | 6 | -0.000001534 | -0.000000612 | 0.000001035 |
| 56 | 6 | 0.000000090 | -0.000000753 | -0.000001098 |
| 57 | 6 | 0.000001084 | -0.000002651 | -0.000000529 |
| 58 | 6 | -0.000000763 | 0.000000365 | -0.000000878 |
| 59 | 1 | -0.000000165 | 0.000001186 | 0.000000090 |
| 60 | 1 | -0.000000363 | 0.000000755 | -0.000000201 |
| 61 | 1 | -0.000001001 | 0.000000317 | 0.000000011 |
| 62 | 1 | -0.000000047 | 0.000000083 | 0.000000224 |
| 63 | 1 | 0.000000137 | 0.000000287 | 0.000000578 |
| 64 | 1 | 0.000000048 | 0.000000017 | 0.000000029 |
| 65 | 1 | 0.000001979 | -0.000000936 | 0.000001037 |
| 66 | 1 | 0.000003208 | -0.000002971 | -0.000001220 |
| 67 | 1 | -0.000003792 | 0.000008729 | -0.000001850 |
| 68 | 1 | 0.000015436 | -0.000002531 | 0.000012258 |
| 69 | 1 | 0.000007653 | 0.000015510 | -0.000002499 |
| 70 | 1 | -0.000004291 | 0.000000525 | 0.000007083 |
| 71 | 1 | -0.000000602 | -0.000002113 | -0.000003534 |
| 72 | 1 | 0.000000479 | -0.000000292 | -0.000000173 |
| 73 | 8 | -0.000007253 | 0.000000781 | -0.000000306 |
| 74 | 8 | -0.000004991 | 0.000003869 | -0.000005862 |
| 75 | 6 | 0.000002057 | 0.000001276 | 0.000003129 |
| 76 | 6 | -0.000008186 | -0.000002316 | -0.000003793 |
| 77 | 6 | -0.000003248 | 0.000006996 | 0.000005881 |
| 78 | 6 | 0.000002981 | -0.000003086 | 0.000001194 |
| 79 | 6 | 0.000003623 | -0.000004014 | -0.000001886 |
| 80 | 6 | 0.000000046 | 0.000001011 | 0.000000493 |
| 81 | 6 | 0.000001908 | 0.000003429 | 0.000002008 |
| 82 | 6 | -0.000001883 | -0.000000033 | 0.000000098 |
| 83 | 1 | 0.000005938 | -0.000001225 | 0.000000916 |
| 84 | 1 | -0.000002090 | 0.000001781 | -0.000000845 |
| 85 | 1 | -0.000000157 | 0.000000337 | -0.000000130 |
| 86 | 1 | 0.000000284 | -0.000000865 | -0.000000506 |
| 87 | 1 | 0.000000964 | 0.000000161 | -0.000000090 |
| 88 | 1 | -0.000000105 | -0.000000098 | 0.000000637 |
| 89 | 8 | 0.000002312 | 0.000005316 | -0.000001885 |
| 90 | 8 | -0.000004166 | 0.000003199 | 0.000003420 |
| 91 | 6 | -0.000000276 | -0.000000282 | 0.000001426 |
| 92 | 6 | -0.000000369 | 0.000000581 | 0.000001820 |
| 93 | 6 | -0.000000474 | 0.000001476 | -0.000001518 |
| 94 | 6 | -0.000000128 | -0.000000130 | 0.000002918 |
| 95 | 6 | -0.000001178 | -0.000000250 | 0.000001297 |
| 96 | 6 | 0.000001767 | -0.000001067 | -0.000001863 |
| 97 | 6 | -0.000001897 | 0.000004432 | -0.000001598 |
| 98 | 6 | -0.000000087 | -0.000000752 | 0.000000486 |
| 99 | 1 | 0.000000244 | -0.000000777 | 0.000000020 |
| 100 | 1 | 0.000000171 | 0.000000337 | -0.000000516 |
| 101 | 1 | -0.000000492 | -0.000000371 | -0.000001829 |
| 102 | 1 | -0.000000225 | -0.000000094 | 0.000000136 |
| 103 | 1 | -0.000000021 | -0.000000183 | -0.000000222 |
| 104 | 1 | 0.000000276 | -0.000000048 | -0.000000072 |
| 105 | 8 | 0.000003920 | -0.000002173 | 0.000002090 |
| 106 | 8 | 0.000010170 | -0.000007930 | 0.000007036 |
| 107 | 6 | 0.000006432 | -0.000003916 | -0.000000058 |
| 108 | 6 | -0.000003666 | -0.000001469 | 0.000001285 |
| 109 | 6 | -0.000005648 | -0.000005886 | -0.000001562 |
| 110 | 6 | 0.000002648 | 0.000000995 | -0.000000217 |
| 111 | 6 | -0.000005274 | 0.000000266 | -0.000002401 |
| 112 | 6 | 0.000002979 | 0.000003649 | 0.000002676 |
| 113 | 6 | 0.000000692 | -0.000001237 | 0.000000913 |
| 114 | 6 | 0.000000776 | 0.000003184 | -0.000000164 |
| 115 | 1 | 0.000001495 | 0.000000293 | 0.000000214 |
| 116 | 1 | 0.000000933 | -0.000000637 | -0.000000617 |
| 117 | 1 | 0.000000004 | 0.000001336 | -0.000001874 |
| 118 | 1 | 0.000000349 | -0.000000516 | 0.000000242 |
| 119 | 1 | -0.000000194 | -0.000000566 | 0.000000068 |
| 120 | 1 | -0.000000037 | -0.000000698 | -0.000000425 |
| 121 | 8 | -0.000006461 | 0.000004062 | 0.000001730 |
| 122 | 8 | -0.000010220 | 0.000001156 | 0.000000980 |

| | | | | |
|---|---|---|---|---|
| 123 | 6 | -0.000005306 | -0.000005535 | 0.000002497 |
| 124 | 6 | 0.000003792 | 0.000001062 | -0.000001888 |
| 125 | 6 | 0.000003329 | -0.000001762 | 0.000001901 |
| 126 | 6 | 0.000001534 | 0.000001707 | -0.000001235 |
| 127 | 6 | 0.000000719 | 0.000001440 | -0.000000483 |
| 128 | 6 | -0.000002249 | 0.000003104 | -0.000002504 |
| 129 | 6 | 0.000000485 | 0.000000189 | 0.000000662 |
| 130 | 6 | 0.000000079 | 0.000000817 | 0.000000569 |
| 131 | 1 | -0.000000868 | -0.000000671 | 0.000001162 |
| 132 | 1 | -0.000000650 | -0.000000897 | 0.000000760 |
| 133 | 1 | -0.000001331 | 0.000000199 | 0.000000048 |
| 134 | 1 | 0.000000051 | -0.000000066 | -0.000000004 |
| 135 | 1 | -0.000000065 | -0.000000192 | -0.000000089 |
| 136 | 1 | -0.000000068 | -0.000000323 | -0.000000129 |
| 137 | 1 | 0.000003464 | -0.000002330 | -0.000002752 |
| 138 | 1 | -0.000002044 | -0.000001221 | -0.000003706 |
| 139 | 1 | 0.000001443 | 0.000003394 | 0.000001318 |
| 140 | 1 | 0.000002206 | -0.000005704 | 0.000001857 |
| 141 | 1 | 0.000002884 | 0.000001448 | -0.000003909 |
| 142 | 1 | 0.000013365 | -0.000000584 | -0.000005023 |
| 143 | 1 | 0.000006173 | -0.000007786 | 0.000002963 |
| 144 | 1 | -0.000004091 | -0.000005335 | -0.000000621 |
| 145 | 8 | 0.000022472 | -0.000019696 | -0.000002884 |
| 146 | 1 | -0.000002948 | -0.000002122 | 0.000004793 |
| 147 | 1 | -0.000020255 | 0.000024041 | -0.000015935 |
| 148 | 8 | 0.000003130 | 0.000000185 | 0.000005541 |
| 149 | 1 | -0.000001439 | -0.000000326 | -0.000001526 |
| 150 | 1 | -0.000003967 | -0.000002743 | -0.000002841 |
| 151 | 8 | -0.000008970 | 0.000008575 | -0.000001809 |
| 152 | 1 | 0.000007536 | 0.000000709 | 0.000002774 |
| 153 | 1 | 0.000003405 | -0.000007330 | -0.000002045 |
| 154 | 8 | -0.000002121 | 0.000001033 | -0.000000640 |
| 155 | 1 | 0.000007767 | -0.000004710 | 0.000004536 |
| 156 | 1 | -0.000000374 | -0.000000996 | 0.000002147 |
| 157 | 1 | 0.000004600 | -0.000001573 | -0.000006328 |
| 158 | 8 | 0.000002211 | -0.000000463 | 0.000006483 |
| 159 | 8 | 0.000001307 | 0.000007510 | 0.000003110 |
| 160 | 6 | -0.000006665 | 0.000002501 | -0.000000346 |
| 161 | 6 | -0.000004778 | 0.000004239 | 0.000003461 |
| 162 | 6 | 0.000005785 | -0.000007123 | 0.000002647 |
| 163 | 6 | 0.000000885 | -0.000001843 | 0.000003862 |
| 164 | 6 | -0.000000016 | -0.000000114 | -0.000007654 |
| 165 | 6 | 0.000003222 | -0.000001571 | -0.000002018 |
| 166 | 6 | -0.000002715 | -0.000001665 | -0.000006134 |
| 167 | 6 | -0.000000317 | -0.000001171 | 0.000003020 |
| 168 | 1 | 0.000001684 | -0.000001887 | 0.000003044 |
| 169 | 1 | 0.000000261 | 0.000001716 | 0.000003719 |
| 170 | 1 | -0.000002429 | -0.000001466 | 0.000001889 |
| 171 | 1 | 0.000000371 | -0.000000114 | -0.000000250 |
| 172 | 1 | 0.000000315 | 0.000000890 | -0.000000357 |
| 173 | 1 | 0.000000836 | 0.000000332 | 0.000000392 |
| 174 | 8 | 0.000002851 | 0.000004012 | 0.000004629 |
| 175 | 8 | 0.000001274 | -0.000002009 | -0.000001266 |
| 176 | 6 | -0.000003195 | -0.000001571 | -0.000003104 |
| 177 | 6 | 0.000001645 | 0.000003502 | 0.000002821 |
| 178 | 6 | 0.000001053 | -0.000009953 | -0.000006801 |
| 179 | 6 | 0.000001294 | 0.000000559 | -0.000001020 |
| 180 | 6 | -0.000001885 | 0.000001520 | 0.000000457 |
| 181 | 6 | 0.000003183 | -0.000001193 | -0.000000528 |
| 182 | 6 | -0.000001113 | 0.000000147 | 0.000001708 |
| 183 | 6 | -0.000001039 | -0.000000368 | 0.000001319 |
| 184 | 1 | 0.000000105 | 0.000000257 | 0.000000180 |
| 185 | 1 | 0.000001886 | 0.000001078 | 0.000001703 |
| 186 | 1 | -0.000000212 | 0.000001099 | 0.000002688 |
| 187 | 1 | -0.000000393 | 0.000000049 | -0.000000514 |
| 188 | 1 | 0.000000447 | 0.000000109 | -0.000000326 |
| 189 | 1 | 0.000000227 | -0.000000551 | -0.000000096 |
| 190 | 8 | 0.000011562 | 0.000000315 | -0.000004936 |
| 191 | 8 | -0.000000046 | 0.000003637 | -0.000005982 |
| 192 | 6 | -0.000011384 | -0.000009518 | 0.000004180 |
| 193 | 6 | 0.000003593 | 0.000005847 | -0.000004286 |
| 194 | 6 | -0.000003243 | -0.000008286 | 0.000002547 |
| 195 | 6 | 0.000002452 | 0.000004497 | -0.000001958 |

| | | | | |
|---|---|---|---|---|
| 196 | 6 | -0.000001200 | -0.000004719 | 0.000001044 |
| 197 | 6 | 0.000010286 | 0.000009445 | -0.000006628 |
| 198 | 6 | 0.000000092 | -0.000000767 | 0.000001566 |
| 199 | 6 | 0.000001120 | 0.000000858 | -0.000000629 |
| 200 | 1 | -0.000000060 | -0.000000402 | 0.000003222 |
| 201 | 1 | -0.000001084 | 0.000000105 | -0.000000252 |
| 202 | 1 | -0.000000996 | 0.000000358 | -0.000000375 |
| 203 | 1 | -0.000000540 | 0.000000059 | 0.000000112 |
| 204 | 1 | -0.000000125 | 0.000000044 | 0.000000390 |
| 205 | 1 | -0.000000708 | -0.000000468 | 0.000000711 |
| 206 | 8 | -0.000006207 | -0.000000145 | 0.000004617 |
| 207 | 8 | -0.000001946 | 0.000002013 | -0.000001113 |
| 208 | 6 | 0.000007755 | 0.000005029 | 0.000000289 |
| 209 | 6 | 0.000001253 | 0.000002181 | -0.000000431 |
| 210 | 6 | -0.000001736 | -0.000001133 | -0.000001818 |
| 211 | 6 | -0.000000916 | -0.000003127 | 0.000002614 |
| 212 | 6 | -0.000000836 | 0.000003715 | -0.000002094 |
| 213 | 6 | 0.000001443 | 0.000000123 | -0.000002111 |
| 214 | 6 | 0.000000645 | 0.000004039 | 0.000000043 |
| 215 | 6 | -0.000000437 | -0.000001045 | -0.000002124 |
| 216 | 1 | 0.000000902 | -0.000000331 | 0.000001018 |
| 217 | 1 | 0.000000560 | 0.000000327 | 0.000001518 |
| 218 | 1 | 0.000000927 | -0.000002063 | 0.000000580 |
| 219 | 1 | -0.000000458 | 0.000000443 | 0.000000571 |
| 220 | 1 | 0.000000483 | 0.000000080 | 0.000000690 |
| 221 | 1 | 0.000000474 | 0.000000192 | 0.000000397 |
| 222 | 1 | -0.000000948 | -0.000002575 | 0.000000147 |
| 223 | 1 | -0.000009188 | -0.000006273 | -0.000001190 |
| 224 | 1 | -0.000001395 | -0.000003349 | -0.000000427 |
| 225 | 1 | -0.000012551 | 0.000008770 | 0.000008345 |
| 226 | 1 | -0.000000595 | 0.000002959 | 0.000004400 |
| 227 | 1 | -0.000000052 | 0.000000164 | -0.000001117 |
| 228 | 1 | 0.000000838 | -0.000000479 | -0.000001239 |
| 229 | 1 | -0.000003331 | -0.000001891 | 0.000000481 |
| 230 | 1 | 0.000000634 | 0.000000388 | -0.000000626 |
| 231 | 1 | -0.000000884 | 0.000000619 | -0.000000559 |
| 232 | 8 | -0.000000286 | -0.000000743 | 0.000000808 |
| 233 | 8 | 0.000000698 | 0.000001419 | -0.000002272 |
| 234 | 6 | -0.000000379 | 0.000001362 | -0.000000637 |
| 235 | 6 | 0.000000651 | -0.000000028 | -0.000000507 |
| 236 | 6 | -0.000005766 | -0.000001050 | -0.000000845 |
| 237 | 6 | 0.000002943 | 0.000002407 | 0.000001725 |
| 238 | 6 | -0.000001378 | -0.000001717 | 0.000001185 |
| 239 | 6 | 0.000003277 | 0.000002415 | -0.000002507 |
| 240 | 6 | -0.000000915 | -0.000001660 | 0.000000591 |
| 241 | 6 | -0.000000017 | 0.000000512 | -0.000000475 |
| 242 | 1 | -0.000000312 | -0.000000016 | 0.000000095 |
| 243 | 1 | -0.000000748 | -0.000000490 | -0.000000313 |
| 244 | 1 | -0.000000164 | -0.000000534 | -0.000001300 |
| 245 | 1 | 0.000000550 | 0.000000066 | 0.000000084 |
| 246 | 1 | 0.000000052 | -0.000000004 | 0.000000046 |
| 247 | 1 | 0.000000257 | 0.000000158 | 0.000000210 |
| 248 | 8 | -0.000000885 | -0.000000245 | -0.000000666 |
| 249 | 8 | 0.000000500 | -0.000001717 | -0.000002376 |
| 250 | 6 | -0.000001222 | 0.000002438 | 0.000002704 |
| 251 | 6 | 0.000002129 | -0.000001570 | -0.000001869 |
| 252 | 6 | 0.000001909 | 0.000002236 | -0.000001221 |
| 253 | 6 | -0.000002774 | -0.000002516 | 0.000000379 |
| 254 | 6 | 0.000001361 | -0.000000366 | -0.000000912 |
| 255 | 6 | -0.000002279 | -0.000001844 | 0.000000525 |
| 256 | 6 | 0.000000960 | 0.000000878 | -0.000001261 |
| 257 | 6 | 0.000000142 | -0.000000628 | 0.000001213 |
| 258 | 1 | -0.000000335 | 0.000001409 | 0.000001397 |
| 259 | 1 | 0.000000702 | 0.000000303 | -0.000000370 |
| 260 | 1 | -0.000001088 | 0.000000460 | -0.000000027 |
| 261 | 1 | -0.000000439 | 0.000000129 | 0.000000114 |
| 262 | 1 | 0.000000279 | 0.000000285 | 0.000000009 |
| 263 | 1 | -0.000000036 | 0.000000109 | -0.000000116 |
| 264 | 8 | -0.000000859 | 0.000000636 | 0.000000175 |
| 265 | 8 | 0.000001763 | 0.000000717 | -0.000003202 |
| 266 | 6 | 0.000001969 | -0.000002612 | -0.000000155 |
| 267 | 6 | 0.000001572 | -0.000001490 | 0.000001180 |
| 268 | 6 | -0.000000430 | 0.000003055 | 0.000000121 |

| | | | | |
|---|---|---|---|---|
| 269 | 6 | -0.000001590 | 0.000002841 | -0.000001748 |
| 270 | 6 | 0.000000481 | -0.000001758 | 0.000000113 |
| 271 | 6 | -0.000000749 | 0.000000340 | 0.000000352 |
| 272 | 6 | 0.000000344 | 0.000000239 | 0.000000341 |
| 273 | 6 | -0.000000354 | 0.000000696 | 0.000000302 |
| 274 | 1 | -0.000000050 | 0.000000078 | -0.000001099 |
| 275 | 1 | 0.000000801 | -0.000000661 | 0.000000617 |
| 276 | 1 | -0.000000144 | -0.000001686 | 0.000000982 |
| 277 | 1 | -0.000000180 | 0.000000062 | -0.000000152 |
| 278 | 1 | 0.000000200 | -0.000000406 | -0.000000282 |
| 279 | 1 | -0.000000344 | -0.000000128 | -0.000000276 |
| 280 | 8 | 0.000004603 | -0.000003844 | 0.000002492 |
| 281 | 8 | 0.000001317 | -0.000000795 | -0.000001375 |
| 282 | 6 | -0.000003722 | 0.000009867 | -0.000001173 |
| 283 | 6 | -0.000000889 | -0.000004469 | -0.000000114 |
| 284 | 6 | 0.000002441 | 0.000003238 | 0.000003828 |
| 285 | 6 | 0.000000018 | -0.000005071 | -0.000001085 |
| 286 | 6 | -0.000000178 | 0.000001719 | 0.000000104 |
| 287 | 6 | 0.000001564 | -0.000002539 | -0.000000020 |
| 288 | 6 | -0.000001342 | 0.000000065 | -0.000000255 |
| 289 | 6 | -0.000000546 | 0.000000399 | -0.000000541 |
| 290 | 1 | -0.000000841 | 0.000000977 | -0.000000377 |
| 291 | 1 | -0.000000533 | 0.000000154 | -0.000000216 |
| 292 | 1 | 0.000000487 | 0.000000907 | -0.000000943 |
| 293 | 1 | -0.000000015 | -0.000000387 | 0.000000019 |
| 294 | 1 | 0.000000254 | -0.000000073 | -0.000000001 |
| 295 | 1 | 0.000000197 | 0.000000181 | -0.000000139 |
| 296 | 1 | 0.000000228 | 0.000001745 | -0.000000770 |
| 297 | 1 | -0.000000218 | -0.000000227 | 0.000001041 |
| 298 | 1 | -0.000003227 | -0.000006891 | -0.000003963 |
| 299 | 1 | -0.000000310 | 0.000000721 | 0.000000122 |
| 300 | 1 | 0.000000221 | 0.000000707 | 0.000000131 |
| 301 | 1 | -0.000001540 | -0.000005538 | 0.000003291 |
| 302 | 1 | -0.000002694 | 0.000001197 | -0.000002354 |
| 303 | 1 | -0.000000910 | 0.000006535 | 0.000001906 |
| 304 | 1 | -0.000034251 | 0.000014065 | 0.000023551 |
| 305 | 8 | 0.000009368 | 0.000013058 | 0.000003184 |
| 306 | 8 | 0.000003704 | 0.000001440 | 0.000000826 |
| 307 | 6 | -0.000005441 | 0.000002579 | -0.000004411 |
| 308 | 6 | 0.000000070 | 0.000000605 | -0.000002081 |
| 309 | 6 | 0.000003982 | 0.000000776 | 0.000002315 |
| 310 | 6 | -0.000004079 | -0.000005451 | 0.000001219 |
| 311 | 6 | 0.000001628 | 0.000006139 | -0.000000997 |
| 312 | 6 | -0.000002192 | -0.000001540 | 0.000001312 |
| 313 | 6 | 0.000004649 | 0.000007197 | -0.000001596 |
| 314 | 6 | -0.000000763 | 0.000000039 | 0.000000704 |
| 315 | 1 | -0.000001055 | -0.000001774 | 0.000000562 |
| 316 | 1 | -0.000000705 | -0.000002220 | -0.000000865 |
| 317 | 1 | -0.000000772 | -0.000004688 | 0.000000118 |
| 318 | 1 | 0.000000295 | 0.000000060 | -0.000000343 |
| 319 | 1 | -0.000000409 | -0.000000722 | -0.000000493 |
| 320 | 1 | -0.000000159 | -0.000000379 | -0.000000165 |
| 321 | 8 | 0.000003442 | -0.000007754 | -0.000007925 |
| 322 | 8 | 0.000020812 | -0.000017839 | -0.000016261 |
| 323 | 6 | -0.000001043 | 0.000000821 | 0.000000398 |
| 324 | 6 | -0.000003276 | -0.000002992 | 0.000003984 |
| 325 | 6 | -0.000003960 | 0.000011292 | -0.000006156 |
| 326 | 6 | 0.000002397 | -0.000004231 | 0.000001492 |
| 327 | 6 | -0.000002415 | 0.000001946 | -0.000001451 |
| 328 | 6 | 0.000003172 | -0.000000063 | -0.000001847 |
| 329 | 6 | 0.000000892 | 0.000001930 | 0.000000851 |
| 330 | 6 | -0.000001020 | -0.000000287 | -0.000001345 |
| 331 | 1 | 0.000002154 | 0.000001560 | 0.000000491 |
| 332 | 1 | -0.000000123 | -0.000000433 | 0.000002440 |
| 333 | 1 | -0.000000741 | -0.000000107 | 0.000000868 |
| 334 | 1 | 0.000000568 | 0.000000060 | 0.000000813 |
| 335 | 1 | -0.000000547 | 0.000001168 | -0.000000000 |
| 336 | 1 | 0.000000250 | -0.000000673 | 0.000000167 |
| 337 | 8 | 0.000002657 | 0.000002887 | 0.000010378 |
| 338 | 8 | 0.000003065 | -0.000006171 | 0.000004730 |
| 339 | 6 | 0.000000286 | 0.000000733 | 0.000004175 |
| 340 | 6 | -0.000007927 | -0.000001840 | -0.000007882 |
| 341 | 6 | 0.000005302 | 0.000002879 | 0.000002571 |

| | | | | |
|---|---|---|---|---|
| 342 | 6 | 0.000002007 | -0.000003139 | -0.000004095 |
| 343 | 6 | 0.000000817 | 0.000000610 | 0.000000787 |
| 344 | 6 | 0.000000210 | 0.000000751 | -0.000004577 |
| 345 | 6 | -0.000000220 | -0.000000017 | -0.000003285 |
| 346 | 6 | 0.000000976 | 0.000000190 | 0.000002415 |
| 347 | 1 | -0.000000417 | -0.000001114 | 0.000001481 |
| 348 | 1 | -0.000002462 | 0.000001121 | -0.000000483 |
| 349 | 1 | 0.000000659 | 0.000000507 | 0.000003053 |
| 350 | 1 | 0.000000064 | 0.000000253 | -0.000000115 |
| 351 | 1 | -0.000000008 | -0.000000685 | -0.000000337 |
| 352 | 1 | -0.000000040 | 0.000000140 | -0.000000892 |
| 353 | 8 | -0.000008205 | -0.000006061 | -0.000014597 |
| 354 | 8 | -0.000008305 | -0.000015050 | 0.000002614 |
| 355 | 6 | -0.000000055 | 0.000001592 | 0.000004507 |
| 356 | 6 | -0.000000845 | 0.000000135 | 0.000000917 |
| 357 | 6 | 0.000000068 | -0.000000044 | -0.000001895 |
| 358 | 6 | 0.000002258 | 0.000002563 | -0.000000958 |
| 359 | 6 | 0.000001776 | -0.000000235 | -0.000003509 |
| 360 | 6 | -0.000000488 | -0.000003400 | 0.000003103 |
| 361 | 6 | -0.000000639 | 0.000000821 | 0.000002609 |
| 362 | 6 | -0.000000196 | -0.000000955 | -0.000000538 |
| 363 | 1 | 0.000000358 | -0.000001963 | 0.000000614 |
| 364 | 1 | -0.000002607 | -0.000001238 | 0.000001040 |
| 365 | 1 | 0.000000738 | -0.000000365 | 0.000000234 |
| 366 | 1 | 0.000000246 | -0.000000377 | -0.000000025 |
| 367 | 1 | -0.000000178 | 0.000000576 | 0.000000418 |
| 368 | 1 | -0.000000402 | 0.000000337 | -0.000000117 |
| 369 | 1 | 0.000000774 | -0.000002944 | -0.000001079 |
| 370 | 1 | -0.000012820 | 0.000008744 | 0.000001281 |
| 371 | 1 | 0.000001815 | 0.000007737 | -0.000001497 |
| 372 | 1 | 0.000004509 | 0.000008508 | -0.000001341 |
| 373 | 1 | 0.000000998 | 0.000001748 | -0.000000163 |
| 374 | 1 | -0.000005276 | -0.000001673 | -0.000003280 |
| 375 | 1 | -0.000000706 | -0.000000325 | -0.000002156 |
| 376 | 1 | 0.000000888 | -0.000003511 | -0.000001342 |
| 377 | 8 | -0.000003866 | -0.000004133 | -0.000002550 |
| 378 | 8 | 0.000008819 | -0.000001315 | 0.000005577 |
| 379 | 6 | -0.000004188 | 0.000004093 | -0.000003151 |
| 380 | 6 | 0.000003366 | -0.000001466 | -0.000000151 |
| 381 | 6 | -0.000007853 | 0.000004673 | -0.000002814 |
| 382 | 6 | 0.000004033 | 0.000001087 | 0.000001740 |
| 383 | 6 | 0.000001552 | -0.000001998 | 0.000000367 |
| 384 | 6 | 0.000003691 | 0.000001903 | 0.000002318 |
| 385 | 6 | -0.000003406 | -0.000000008 | -0.000001201 |
| 386 | 6 | -0.000000663 | 0.000000259 | -0.000000844 |
| 387 | 1 | -0.000000860 | -0.000000274 | 0.000000928 |
| 388 | 1 | -0.000000966 | 0.000000666 | -0.000000422 |
| 389 | 1 | 0.000000843 | -0.000002620 | 0.000002190 |
| 390 | 1 | 0.000000325 | 0.000000143 | -0.000000147 |
| 391 | 1 | 0.000000418 | -0.000000066 | 0.000000536 |
| 392 | 1 | 0.000000731 | -0.000000634 | 0.000000012 |
| 393 | 8 | -0.000004233 | -0.000003637 | -0.000001422 |
| 394 | 8 | -0.000001039 | -0.000000351 | -0.000000757 |
| 395 | 6 | 0.000003009 | -0.000000493 | -0.000001375 |
| 396 | 6 | -0.000000220 | 0.000000263 | 0.000000191 |
| 397 | 6 | 0.000001074 | -0.000003048 | -0.000001736 |
| 398 | 6 | 0.000000729 | 0.000001026 | 0.000000305 |
| 399 | 6 | -0.000000174 | -0.000001136 | -0.000000265 |
| 400 | 6 | -0.000000778 | 0.000001512 | 0.000001146 |
| 401 | 6 | -0.000002283 | 0.000001334 | -0.000000677 |
| 402 | 6 | 0.000000702 | -0.000000314 | -0.000000209 |
| 403 | 1 | -0.000000236 | -0.000000353 | 0.000000792 |
| 404 | 1 | -0.000000387 | -0.000000595 | 0.000000222 |
| 405 | 1 | -0.000000865 | -0.000000169 | 0.000000124 |
| 406 | 1 | 0.000000147 | 0.000000064 | 0.000000114 |
| 407 | 1 | 0.000000133 | 0.000000213 | -0.000000199 |
| 408 | 1 | 0.000000131 | 0.000000118 | -0.000000015 |
| 409 | 8 | 0.000000129 | 0.000003772 | -0.000000280 |
| 410 | 8 | 0.000000862 | -0.000003953 | 0.000001953 |
| 411 | 6 | 0.000000210 | -0.000002745 | -0.000001658 |
| 412 | 6 | 0.000001516 | 0.000000293 | -0.000001373 |
| 413 | 6 | 0.000002337 | 0.000000671 | -0.000000738 |
| 414 | 6 | -0.000000027 | 0.000000097 | 0.000002200 |

| | | | | |
|---|---|---|---|---|
| 415 | 6 | -0.000000698 | -0.000000447 | -0.000001700 |
| 416 | 6 | -0.000003192 | 0.000003150 | -0.000000009 |
| 417 | 6 | 0.000000732 | -0.000001019 | -0.000000378 |
| 418 | 6 | -0.000000048 | 0.000000051 | 0.000000984 |
| 419 | 1 | -0.000000600 | -0.000000229 | -0.000000049 |
| 420 | 1 | 0.000000453 | -0.000000046 | -0.000000187 |
| 421 | 1 | 0.000000393 | 0.000000374 | 0.000000019 |
| 422 | 1 | -0.000000326 | 0.000000143 | -0.000000211 |
| 423 | 1 | -0.000000127 | -0.000000101 | 0.000000046 |
| 424 | 1 | -0.000000117 | 0.000000060 | 0.000000012 |
| 425 | 8 | 0.000002769 | -0.000002334 | 0.000007630 |
| 426 | 8 | 0.000002936 | 0.000003360 | 0.000002624 |
| 427 | 6 | -0.000000310 | 0.000002813 | -0.000004993 |
| 428 | 6 | 0.000001483 | 0.000000432 | 0.000001527 |
| 429 | 6 | 0.000000293 | 0.000000399 | -0.000000046 |
| 430 | 6 | -0.000002181 | -0.000003285 | -0.000001223 |
| 431 | 6 | 0.000000186 | 0.000000748 | -0.000000813 |
| 432 | 6 | 0.000000131 | -0.000001806 | 0.000002239 |
| 433 | 6 | 0.000000546 | 0.000000317 | -0.000000240 |
| 434 | 6 | 0.000001064 | 0.000000290 | -0.000000062 |
| 435 | 1 | 0.000000226 | -0.000000392 | 0.000000476 |
| 436 | 1 | 0.000000149 | 0.000000827 | 0.000001115 |
| 437 | 1 | -0.000001089 | -0.000000453 | 0.000000363 |
| 438 | 1 | -0.000000661 | -0.000000134 | -0.000000314 |
| 439 | 1 | -0.000000216 | 0.000000049 | 0.000000451 |
| 440 | 1 | -0.000000309 | -0.000000052 | 0.000000150 |
| 441 | 1 | -0.000003534 | 0.000003645 | 0.000001338 |
| 442 | 1 | -0.000001249 | 0.000002174 | -0.000002941 |
| 443 | 1 | -0.000001062 | -0.000000194 | -0.000003556 |
| 444 | 1 | 0.000000660 | 0.000002894 | 0.000002435 |
| 445 | 8 | 0.000028636 | -0.000000497 | 0.000006505 |
| 446 | 1 | -0.000000307 | 0.000003502 | -0.000009771 |
| 447 | 1 | -0.000008941 | -0.000001698 | -0.000007712 |
| 448 | 8 | 0.000009561 | -0.000004584 | -0.000003208 |
| 449 | 1 | -0.000001075 | 0.000000610 | 0.000007184 |
| 450 | 1 | -0.000002618 | -0.000001196 | 0.000000376 |
| 451 | 8 | -0.000004428 | -0.000016323 | 0.000007446 |
| 452 | 1 | 0.000000111 | 0.000003746 | 0.000001898 |
| 453 | 1 | 0.000002323 | 0.000000716 | -0.000003677 |
| 454 | 8 | 0.000004143 | -0.000000983 | 0.000002702 |
| 455 | 1 | -0.000004921 | 0.000000342 | -0.000000313 |
| 456 | 1 | -0.000000968 | 0.000002653 | 0.000001609 |
| 457 | 6 | -0.000045025 | 0.000005362 | 0.000000188 |
| 458 | 6 | 0.000002630 | 0.000010219 | 0.000024750 |
| 459 | 6 | 0.000029300 | -0.000015303 | -0.000013489 |
| 460 | 7 | 0.000024549 | 0.000004020 | -0.000010182 |
| 461 | 6 | 0.000006358 | 0.000000400 | 0.000000957 |
| 462 | 6 | -0.000002927 | 0.000001766 | -0.000005998 |
| 463 | 6 | 0.000000977 | 0.000000351 | 0.000001701 |
| 464 | 6 | 0.000001210 | -0.000004423 | -0.000000871 |
| 465 | 6 | -0.000003345 | 0.000005500 | -0.000005533 |
| 466 | 8 | -0.000002437 | -0.000007334 | -0.000008974 |
| 467 | 8 | -0.000031493 | -0.000006482 | 0.000013969 |
| 468 | 1 | 0.000006992 | 0.000003755 | -0.000003419 |
| 469 | 1 | -0.000005183 | 0.000001507 | -0.000004614 |
| 470 | 1 | -0.000001083 | -0.000000446 | -0.000002447 |
| 471 | 1 | 0.000003574 | 0.000000015 | 0.000000177 |
| 472 | 1 | 0.000000200 | 0.000001234 | -0.000001213 |
| 473 | 1 | -0.000002169 | 0.000002093 | 0.000000005 |
| 474 | 1 | 0.000003745 | -0.000002892 | 0.000000707 |
| 475 | 6 | 0.000010461 | -0.000008652 | 0.000008462 |
| 476 | 6 | 0.000003723 | -0.000004613 | -0.000011310 |
| 477 | 7 | -0.000006528 | -0.000013679 | 0.000012316 |
| 478 | 6 | 0.000013372 | 0.000007449 | -0.000000383 |
| 479 | 6 | -0.000018662 | 0.000010834 | 0.000008567 |
| 480 | 6 | -0.000004135 | 0.000013060 | -0.000010033 |
| 481 | 1 | -0.000002107 | 0.000001861 | -0.000001940 |
| 482 | 1 | 0.000002311 | -0.000000097 | -0.000000993 |
| 483 | 1 | -0.000005035 | -0.000003990 | 0.000003458 |
| 484 | 1 | 0.000010109 | -0.000003781 | -0.000004860 |
| 485 | 1 | 0.000002230 | -0.000000851 | 0.000005464 |
| 486 | 1 | 0.000000632 | -0.000002139 | 0.000000553 |
| 487 | 1 | -0.000000345 | 0.000001090 | -0.000000531 |

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Sum of electronic and thermal Free Energies = -1069.257423
ONIOM Total Energy = -1072.550715
0 imaginary frequency

**$\alpha$-TS2@$C_R$**

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| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | 0.000000476 | -0.000001127 | 0.000002914 |
| 2 | 8 | 0.000000221 | 0.000000738 | -0.000001770 |
| 3 | 6 | 0.000000251 | 0.000000332 | -0.000000136 |
| 4 | 6 | 0.000000190 | 0.000000002 | 0.000000231 |
| 5 | 6 | -0.000000211 | 0.000000544 | -0.000000049 |
| 6 | 6 | 0.000000225 | -0.000000295 | -0.000000142 |
| 7 | 6 | 0.000000126 | -0.000000123 | 0.000000204 |
| 8 | 6 | 0.000000151 | -0.000000159 | -0.000000100 |
| 9 | 6 | -0.000000002 | 0.000000001 | 0.000000095 |
| 10 | 6 | 0.000000034 | -0.000000035 | 0.000000027 |
| 11 | 1 | 0.000000022 | -0.000000030 | 0.000000044 |
| 12 | 1 | 0.000000020 | 0.000000002 | 0.000000046 |
| 13 | 1 | 0.000000054 | -0.000000059 | 0.000000069 |
| 14 | 1 | 0.000000046 | 0.000000009 | 0.000000037 |
| 15 | 1 | 0.000000032 | 0.000000013 | 0.000000032 |
| 16 | 1 | 0.000000029 | 0.000000021 | 0.000000046 |
| 17 | 8 | 0.000000084 | -0.000002242 | -0.000002438 |
| 18 | 8 | -0.000000999 | 0.000000381 | -0.000001124 |
| 19 | 6 | -0.000000341 | 0.000000336 | -0.000000042 |
| 20 | 6 | -0.000000178 | -0.000000282 | -0.000000142 |
| 21 | 6 | 0.000000189 | 0.000000658 | -0.000000399 |
| 22 | 6 | -0.000000337 | -0.000000022 | 0.000000076 |
| 23 | 6 | -0.000000139 | -0.000000200 | -0.000000158 |
| 24 | 6 | 0.000000111 | 0.000000109 | 0.000000165 |
| 25 | 6 | -0.000000134 | 0.000000191 | -0.000000054 |
| 26 | 6 | -0.000000040 | -0.000000063 | -0.000000000 |
| 27 | 1 | -0.000000078 | 0.000000009 | 0.000000036 |
| 28 | 1 | 0.000000001 | -0.000000011 | 0.000000024 |
| 29 | 1 | 0.000000004 | -0.000000071 | 0.000000057 |
| 30 | 1 | 0.000000038 | -0.000000012 | 0.000000040 |
| 31 | 1 | -0.000000016 | -0.000000016 | 0.000000057 |
| 32 | 1 | -0.000000014 | 0.000000000 | -0.000000002 |
| 33 | 8 | 0.000000114 | 0.000000202 | -0.000000022 |
| 34 | 8 | 0.000000100 | -0.000000132 | -0.000000019 |
| 35 | 6 | 0.000000134 | 0.000000013 | 0.000000028 |
| 36 | 6 | -0.000000072 | -0.000000015 | 0.000000077 |
| 37 | 6 | -0.000000050 | -0.000000092 | -0.000000061 |
| 38 | 6 | 0.000000223 | 0.000000214 | -0.000000005 |
| 39 | 6 | -0.000000125 | -0.000000160 | -0.000000012 |
| 40 | 6 | -0.000000071 | 0.000000192 | 0.000000156 |
| 41 | 6 | 0.000000231 | -0.000000040 | -0.000000126 |
| 42 | 6 | 0.000000084 | -0.000000076 | 0.000000037 |
| 43 | 1 | 0.000000000 | 0.000000018 | -0.000000037 |
| 44 | 1 | -0.000000002 | -0.000000026 | 0.000000013 |
| 45 | 1 | 0.000000022 | -0.000000019 | -0.000000024 |
| 46 | 1 | 0.000000014 | 0.000000000 | 0.000000017 |
| 47 | 1 | 0.000000010 | 0.000000009 | 0.000000008 |
| 48 | 1 | 0.000000030 | 0.000000003 | 0.000000009 |
| 49 | 8 | 0.000000449 | -0.000000232 | -0.000000227 |
| 50 | 8 | -0.000000339 | -0.000000710 | 0.000000425 |
| 51 | 6 | -0.000000102 | -0.000000131 | 0.000000145 |
| 52 | 6 | 0.000000078 | -0.000000029 | -0.000000071 |
| 53 | 6 | -0.000000314 | -0.000000662 | 0.000000288 |
| 54 | 6 | -0.000000335 | 0.000000524 | -0.000000138 |
| 55 | 6 | 0.000000219 | 0.000000079 | 0.000000016 |
| 56 | 6 | 0.000000095 | 0.000000102 | 0.000000117 |
| 57 | 6 | -0.000000179 | 0.000000109 | 0.000000113 |
| 58 | 6 | -0.000000041 | -0.000000050 | -0.000000038 |
| 59 | 1 | -0.000000000 | 0.000000033 | 0.000000032 |
| 60 | 1 | 0.000000017 | -0.000000008 | 0.000000071 |
| 61 | 1 | 0.000000047 | 0.000000025 | 0.000000100 |
| 62 | 1 | 0.000000069 | 0.000000008 | 0.000000106 |

| | | | | |
|---|---|---|---|---|
| 63 | 1 | -0.000000055 | -0.000000013 | 0.000000077 |
| 64 | 1 | 0.000000041 | -0.000000003 | -0.000000028 |
| 65 | 1 | -0.000000105 | -0.000000050 | 0.000000177 |
| 66 | 1 | -0.000001226 | 0.000001916 | -0.000004445 |
| 67 | 1 | -0.000000784 | -0.000001259 | 0.000003068 |
| 68 | 1 | 0.000000308 | 0.000003242 | 0.000003422 |
| 69 | 1 | 0.000001766 | -0.000000838 | 0.000002201 |
| 70 | 1 | 0.000000038 | -0.000000034 | 0.000000038 |
| 71 | 1 | -0.000000076 | 0.000000018 | -0.000000067 |
| 72 | 1 | 0.000000561 | 0.000000095 | 0.000000261 |
| 73 | 8 | -0.000000330 | -0.000000340 | -0.000000252 |
| 74 | 8 | 0.000000087 | 0.000000095 | -0.000000416 |
| 75 | 6 | 0.000000127 | 0.000000003 | -0.000000115 |
| 76 | 6 | 0.000000095 | -0.000000082 | 0.000000074 |
| 77 | 6 | -0.000000051 | -0.000000044 | 0.000000172 |
| 78 | 6 | 0.000000017 | -0.000000140 | 0.000000161 |
| 79 | 6 | -0.000000076 | 0.000000129 | -0.000000074 |
| 80 | 6 | -0.000000238 | 0.000000231 | -0.000000156 |
| 81 | 6 | 0.000000109 | 0.000000022 | 0.000000109 |
| 82 | 6 | -0.000000019 | 0.000000122 | 0.000000064 |
| 83 | 1 | -0.000000013 | 0.000000058 | -0.000000041 |
| 84 | 1 | -0.000000036 | 0.000000045 | -0.000000041 |
| 85 | 1 | -0.000000077 | 0.000000073 | 0.000000034 |
| 86 | 1 | 0.000000173 | 0.000000041 | 0.000000049 |
| 87 | 1 | 0.000000007 | -0.000000003 | -0.000000238 |
| 88 | 1 | -0.000000175 | 0.000000022 | 0.000000055 |
| 89 | 8 | 0.000000173 | -0.000000106 | -0.000000109 |
| 90 | 8 | 0.000000524 | 0.000000381 | 0.000000206 |
| 91 | 6 | -0.000000065 | 0.000000072 | -0.000000247 |
| 92 | 6 | 0.000000178 | 0.000000032 | 0.000000048 |
| 93 | 6 | -0.000000126 | -0.000000161 | -0.000000202 |
| 94 | 6 | 0.000000059 | -0.000000186 | -0.000000160 |
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| 96 | 6 | -0.000000154 | -0.000000090 | 0.000000135 |
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| 99 | 1 | -0.000000021 | -0.000000006 | 0.000000019 |
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| 104 | 1 | -0.000000087 | -0.000000010 | -0.000000062 |
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| 107 | 6 | -0.000000154 | 0.000000192 | -0.000000047 |
| 108 | 6 | 0.000000266 | 0.000000030 | -0.000000066 |
| 109 | 6 | -0.000000233 | -0.000000262 | 0.000000034 |
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| 111 | 6 | 0.000000160 | -0.000000175 | 0.000000105 |
| 112 | 6 | -0.000000148 | -0.000000104 | 0.000000100 |
| 113 | 6 | 0.000000204 | -0.000000145 | -0.000000093 |
| 114 | 6 | -0.000000036 | -0.000000000 | -0.000000211 |
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| 120 | 1 | -0.000000058 | 0.000000012 | 0.000000050 |
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| 124 | 6 | -0.000000122 | 0.000000507 | -0.000000097 |
| 125 | 6 | 0.000000320 | -0.000000322 | -0.000000058 |
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| 130 | 6 | -0.000000080 | 0.000000076 | 0.000000156 |
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| 155 | 1 | -0.000005487 | 0.000000839 | -0.000001710 |
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| 157 | 1 | -0.000000494 | 0.000000882 | -0.000000374 |
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| 187 | 1 | -0.000000025 | 0.000000050 | 0.000000030 |
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| 216 | 1 | 0.000000075 | -0.000000072 | -0.000000029 |
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| 224 | 1 | -0.000000034 | 0.000000058 | 0.000000010 |
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| 249 | 8 | -0.000000203 | 0.000000578 | 0.000000576 |
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| 263 | 1 | -0.000000033 | -0.000000033 | 0.000000023 |
| 264 | 8 | 0.000000264 | -0.000000154 | -0.000000049 |
| 265 | 8 | 0.000000259 | 0.000000042 | -0.000000014 |
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| 283 | 6 | -0.000000358 | -0.000000017 | 0.000000190 |
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| 285 | 6 | -0.000000073 | 0.000000021 | 0.000000113 |
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| 320 | 1 | -0.000000034 | -0.000000055 | -0.000000100 |
| 321 | 8 | -0.000000977 | 0.000000659 | -0.000000171 |
| 322 | 8 | 0.000000223 | 0.000000804 | 0.000000071 |
| 323 | 6 | 0.000000139 | -0.000000298 | 0.000000224 |
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| 332 | 1 | 0.000000044 | -0.000000003 | -0.000000032 |
| 333 | 1 | 0.000000021 | -0.000000115 | -0.000000009 |
| 334 | 1 | -0.000000011 | -0.000000016 | -0.000000051 |
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| 388 | 1 | -0.000000007 | 0.000000013 | -0.000000019 |
| 389 | 1 | 0.000000051 | -0.000000012 | 0.000000122 |
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| 391 | 1 | 0.000000027 | -0.000000132 | 0.000000051 |
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| 393 | 8 | -0.000001035 | 0.000000105 | 0.000000079 |
| 394 | 8 | -0.000000090 | -0.000000057 | -0.000000073 |
| 395 | 6 | -0.000000013 | 0.000000082 | 0.000000043 |
| 396 | 6 | -0.000000346 | 0.000000051 | 0.000000143 |
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| 400 | 6 | 0.000000299 | -0.000000166 | 0.000000316 |
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| 412 | 6 | -0.000000065 | -0.000000194 | -0.000000201 |
| 413 | 6 | 0.000000513 | 0.000000564 | -0.000000125 |
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| 415 | 6 | -0.000000154 | -0.000000054 | -0.000000206 |
| 416 | 6 | -0.000000224 | 0.000000100 | 0.000000097 |
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| 422 | 1 | -0.000000034 | -0.000000126 | -0.000000008 |
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| 428 | 6 | 0.000000106 | -0.000000046 | -0.000000031 |
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| 430 | 6 | 0.000000204 | 0.000000000 | -0.000000111 |
| 431 | 6 | -0.000000068 | 0.000000153 | 0.000000092 |
| 432 | 6 | -0.000000078 | 0.000000144 | 0.000000059 |
| 433 | 6 | -0.000000162 | 0.000000203 | 0.000000390 |
| 434 | 6 | -0.000000114 | 0.000000155 | 0.000000238 |
| 435 | 1 | -0.000000029 | 0.000000091 | 0.000000071 |
| 436 | 1 | 0.000000000 | 0.000000031 | 0.000000051 |
| 437 | 1 | 0.000000038 | -0.000000046 | 0.000000096 |
| 438 | 1 | 0.000000028 | -0.000000144 | 0.000000117 |
| 439 | 1 | 0.000000036 | 0.000000150 | 0.000000138 |
| 440 | 1 | -0.000000025 | 0.000000017 | -0.000000106 |
| 441 | 1 | -0.000000466 | 0.000000062 | 0.000000551 |
| 442 | 1 | 0.000000008 | 0.000000120 | 0.000000047 |
| 443 | 1 | -0.000000134 | 0.000000291 | 0.000000250 |
| 444 | 1 | 0.000000398 | -0.000000090 | 0.000000193 |
| 445 | 8 | -0.000000497 | -0.000000207 | -0.000000650 |
| 446 | 1 | 0.000000539 | 0.000000604 | 0.000000155 |
| 447 | 1 | 0.000000249 | 0.000000038 | 0.000000203 |
| 448 | 8 | 0.000000311 | 0.000000529 | -0.000001092 |
| 449 | 1 | -0.000000062 | 0.000000008 | -0.000000013 |
| 450 | 1 | 0.000000129 | -0.000000004 | 0.000000144 |
| 451 | 8 | -0.000000724 | -0.000000109 | -0.000000453 |
| 452 | 1 | -0.000000014 | 0.000000027 | -0.000000003 |
| 453 | 1 | -0.000000096 | 0.000000048 | 0.000000062 |
| 454 | 8 | 0.000000283 | -0.000000747 | -0.000000308 |
| 455 | 1 | 0.000000198 | -0.000000021 | -0.000000002 |
| 456 | 1 | -0.000000201 | -0.000000350 | -0.000000328 |
| 457 | 6 | 0.000000408 | -0.000001285 | 0.000000615 |
| 458 | 6 | 0.000000260 | -0.000000539 | -0.000000216 |
| 459 | 6 | 0.000000095 | 0.000000226 | -0.000000836 |
| 460 | 7 | -0.000003521 | 0.000000937 | 0.000000802 |
| 461 | 6 | 0.000000240 | 0.000000478 | -0.000000274 |
| 462 | 6 | 0.000000025 | -0.000000192 | -0.000000040 |
| 463 | 6 | 0.000000146 | 0.000000160 | -0.000000135 |
| 464 | 6 | -0.000000200 | -0.000000232 | 0.000000100 |
| 465 | 6 | -0.000000525 | -0.000000191 | 0.000000273 |
| 466 | 8 | 0.000001340 | -0.000000571 | -0.000000341 |
| 467 | 8 | 0.000000906 | 0.000001817 | 0.000000635 |
| 468 | 1 | 0.000000137 | 0.000000507 | 0.000000334 |
| 469 | 1 | -0.000000028 | 0.000000355 | 0.000000263 |
| 470 | 1 | 0.000000172 | -0.000000104 | 0.000000157 |
| 471 | 1 | 0.000000086 | 0.000000060 | -0.000000005 |
| 472 | 1 | 0.000000024 | 0.000000085 | 0.000000076 |
| 473 | 1 | 0.000000077 | 0.000000152 | -0.000000211 |
| 474 | 1 | -0.000000050 | -0.000000044 | 0.000000028 |
| 475 | 6 | -0.000000832 | 0.000001390 | -0.000001777 |
| 476 | 6 | -0.000002954 | -0.000007072 | -0.000001977 |
| 477 | 7 | -0.000001838 | 0.000000758 | 0.000000540 |
| 478 | 6 | 0.000000215 | -0.000000753 | 0.000001160 |
| 479 | 6 | 0.000001547 | -0.000000911 | -0.000000411 |
| 480 | 6 | 0.000000269 | -0.000000001 | 0.000000038 |
| 481 | 1 | -0.000000203 | 0.000000040 | 0.000000133 |
| 482 | 1 | 0.000003728 | 0.000003539 | 0.000000375 |
| 483 | 1 | -0.000000130 | 0.000000072 | 0.000000051 |
| 484 | 1 | -0.000000062 | 0.000000262 | -0.000000213 |
| 485 | 1 | 0.000000323 | 0.000000027 | 0.000000030 |
| 486 | 1 | 0.000000002 | 0.000000183 | -0.000000047 |
| 487 | 1 | -0.000000204 | -0.000000102 | -0.000000308 |

Sum of electronic and thermal Free Energies = -1069.257506
ONIOM Total Energy = -1072.547535
1 imaginary frequency = -455.50

**$\alpha$-I2@$C_R$**

| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | -0.000005739 | -0.000007600 | 0.000000416 |
| 2 | 8 | -0.000001928 | -0.000004263 | 0.000000711 |

| | | | | |
|---|---|---|---|---|
| 3 | 6 | -0.000000953 | 0.000002555 | -0.000000372 |
| 4 | 6 | 0.000001648 | -0.000000552 | 0.000001756 |
| 5 | 6 | -0.000004465 | 0.000000729 | -0.000000166 |
| 6 | 6 | -0.000000489 | 0.000001524 | 0.000002221 |
| 7 | 6 | -0.000000678 | 0.000000693 | -0.000000488 |
| 8 | 6 | 0.000002032 | -0.000001005 | -0.000001573 |
| 9 | 6 | -0.000001346 | -0.000002989 | 0.000003105 |
| 10 | 6 | -0.000000289 | -0.000001848 | -0.000000703 |
| 11 | 1 | 0.000000574 | -0.000000041 | -0.000000179 |
| 12 | 1 | -0.000000104 | -0.000000962 | 0.000000315 |
| 13 | 1 | 0.000000352 | -0.000001432 | -0.000000444 |
| 14 | 1 | -0.000000110 | 0.000000129 | 0.000000184 |
| 15 | 1 | -0.000000007 | -0.000000002 | 0.000000140 |
| 16 | 1 | -0.000000047 | 0.000000129 | 0.000000208 |
| 17 | 8 | -0.000004544 | -0.000005592 | 0.000001147 |
| 18 | 8 | 0.000002172 | -0.000008790 | 0.000008428 |
| 19 | 6 | -0.000000477 | -0.000003004 | 0.000003103 |
| 20 | 6 | -0.000001395 | -0.000000695 | 0.000000549 |
| 21 | 6 | -0.000005766 | -0.000004822 | -0.000001706 |
| 22 | 6 | 0.000004916 | 0.000002448 | -0.000000227 |
| 23 | 6 | 0.000000036 | 0.000001191 | -0.000002065 |
| 24 | 6 | 0.000002219 | 0.000002580 | -0.000001451 |
| 25 | 6 | 0.000001170 | 0.000002495 | 0.000000718 |
| 26 | 6 | 0.000000192 | 0.000000705 | -0.000000592 |
| 27 | 1 | 0.000001059 | 0.000001212 | -0.000000562 |
| 28 | 1 | -0.000000464 | -0.000000068 | 0.000000250 |
| 29 | 1 | 0.000000149 | -0.000000562 | 0.000000551 |
| 30 | 1 | -0.000000319 | -0.000000424 | 0.000000637 |
| 31 | 1 | -0.000000015 | -0.000000040 | 0.000000159 |
| 32 | 1 | -0.000000059 | -0.000000131 | 0.000000239 |
| 33 | 8 | 0.000008316 | 0.000002543 | -0.000006983 |
| 34 | 8 | -0.000003775 | -0.000002473 | 0.000006689 |
| 35 | 6 | -0.000000649 | 0.000006004 | 0.000005904 |
| 36 | 6 | 0.000001729 | 0.000001222 | -0.000002414 |
| 37 | 6 | -0.000005981 | 0.000003602 | 0.000003254 |
| 38 | 6 | 0.000000370 | -0.000005282 | -0.000003026 |
| 39 | 6 | -0.000004204 | -0.000003035 | 0.000001606 |
| 40 | 6 | 0.000002642 | -0.000001133 | -0.000002672 |
| 41 | 6 | -0.000000160 | -0.000003097 | -0.000002368 |
| 42 | 6 | 0.000000072 | 0.000001076 | 0.000000142 |
| 43 | 1 | -0.000002057 | -0.000000055 | -0.000000725 |
| 44 | 1 | 0.000000914 | -0.000000001 | 0.000000465 |
| 45 | 1 | 0.000001250 | 0.000000864 | -0.000000143 |
| 46 | 1 | -0.000000134 | -0.000000171 | -0.000000215 |
| 47 | 1 | 0.000000065 | -0.000000383 | 0.000000087 |
| 48 | 1 | -0.000000028 | -0.000000216 | 0.000000185 |
| 49 | 8 | -0.000004152 | 0.000004314 | -0.000003308 |
| 50 | 8 | -0.000001126 | 0.000001873 | 0.000005187 |
| 51 | 6 | -0.000000349 | -0.000003400 | 0.000001837 |
| 52 | 6 | 0.000001303 | 0.000002269 | -0.000001066 |
| 53 | 6 | -0.000002607 | -0.000006269 | 0.000002648 |
| 54 | 6 | -0.000000669 | 0.000003448 | -0.000000762 |
| 55 | 6 | -0.000001227 | 0.000001362 | -0.000001191 |
| 56 | 6 | -0.000001740 | -0.000001088 | 0.000000801 |
| 57 | 6 | -0.000000308 | 0.000000773 | -0.000000992 |
| 58 | 6 | 0.000000196 | 0.000001199 | -0.000000032 |
| 59 | 1 | 0.000000379 | 0.000000537 | 0.000000543 |
| 60 | 1 | 0.000000445 | 0.000000154 | -0.000000371 |
| 61 | 1 | 0.000001181 | -0.000000186 | -0.000000048 |
| 62 | 1 | 0.000000052 | -0.000000150 | 0.000000157 |
| 63 | 1 | 0.000000007 | -0.000000168 | -0.000000162 |
| 64 | 1 | 0.000000064 | -0.000000302 | -0.000000010 |
| 65 | 1 | 0.000002915 | 0.000001335 | -0.000003282 |
| 66 | 1 | 0.000008858 | 0.000012326 | 0.000002656 |
| 67 | 1 | -0.000002633 | 0.000012798 | -0.000008560 |
| 68 | 1 | 0.000005978 | 0.000009477 | -0.000010444 |
| 69 | 1 | -0.000004997 | 0.000014971 | -0.000010264 |
| 70 | 1 | -0.000001252 | 0.000000525 | 0.000004193 |
| 71 | 1 | 0.000006327 | -0.000001050 | -0.000008754 |
| 72 | 1 | 0.000001594 | 0.000000146 | -0.000000075 |
| 73 | 8 | 0.000009974 | -0.000020130 | -0.000003510 |
| 74 | 8 | 0.000018528 | 0.000012649 | -0.000025340 |
| 75 | 6 | 0.000008388 | -0.000011826 | 0.000013205 |

| | | | | |
|---|---|---|---|---|
| 76 | 6 | 0.000001042 | 0.000001418 | -0.000011379 |
| 77 | 6 | -0.000008938 | 0.000002510 | 0.000007348 |
| 78 | 6 | 0.000004737 | -0.000003115 | -0.000007511 |
| 79 | 6 | 0.000003423 | -0.000000328 | -0.000006547 |
| 80 | 6 | -0.000013119 | 0.000007989 | 0.000000847 |
| 81 | 6 | -0.000002565 | 0.000001782 | 0.000003639 |
| 82 | 6 | -0.000001047 | -0.000002376 | 0.000000643 |
| 83 | 1 | -0.000000391 | 0.000001182 | 0.000000597 |
| 84 | 1 | 0.000000664 | -0.000001316 | 0.000000650 |
| 85 | 1 | 0.000000866 | 0.000000140 | 0.000000479 |
| 86 | 1 | 0.000000080 | 0.000000714 | -0.000000156 |
| 87 | 1 | 0.000000539 | 0.000000872 | -0.000000109 |
| 88 | 1 | -0.000000155 | 0.000001044 | -0.000000204 |
| 89 | 8 | 0.000001773 | 0.000001243 | 0.000005673 |
| 90 | 8 | -0.000013486 | -0.000007316 | -0.000001789 |
| 91 | 6 | -0.000000704 | 0.000000047 | 0.000001187 |
| 92 | 6 | -0.000003602 | 0.000000455 | 0.000004504 |
| 93 | 6 | 0.000005120 | 0.000000555 | -0.000002751 |
| 94 | 6 | 0.000001227 | -0.000002594 | 0.000002804 |
| 95 | 6 | -0.000003526 | -0.000000092 | 0.000002240 |
| 96 | 6 | 0.000006090 | 0.000001858 | 0.000002241 |
| 97 | 6 | -0.000001406 | 0.000003893 | -0.000002165 |
| 98 | 6 | -0.000000876 | -0.000001600 | -0.000000112 |
| 99 | 1 | 0.000001137 | -0.000002088 | -0.000000246 |
| 100 | 1 | -0.000000703 | 0.000000895 | -0.000000103 |
| 101 | 1 | -0.000000419 | 0.000001617 | 0.000000208 |
| 102 | 1 | -0.000000185 | 0.000000796 | 0.000000232 |
| 103 | 1 | 0.000000517 | 0.000001378 | 0.000000009 |
| 104 | 1 | 0.000000452 | 0.000000785 | -0.000000959 |
| 105 | 8 | 0.000006892 | 0.000007167 | -0.000011792 |
| 106 | 8 | 0.000007803 | 0.000032713 | -0.000071384 |
| 107 | 6 | -0.000009465 | 0.000001686 | 0.000003890 |
| 108 | 6 | 0.000011150 | 0.000003823 | 0.000004898 |
| 109 | 6 | -0.000017363 | 0.000014234 | 0.000002689 |
| 110 | 6 | 0.000010173 | -0.000011667 | 0.000000175 |
| 111 | 6 | 0.000004278 | 0.000002679 | 0.000001825 |
| 112 | 6 | -0.000002993 | -0.000009383 | -0.000003936 |
| 113 | 6 | 0.000001054 | -0.000001534 | -0.000001235 |
| 114 | 6 | 0.000000130 | 0.000001254 | 0.000000048 |
| 115 | 1 | -0.000001157 | -0.000000788 | 0.000000309 |
| 116 | 1 | -0.000000631 | 0.000001935 | 0.000000950 |
| 117 | 1 | -0.000002311 | 0.000000416 | 0.000002004 |
| 118 | 1 | 0.000000069 | 0.000000355 | -0.000000392 |
| 119 | 1 | 0.000000506 | 0.000000515 | 0.000000339 |
| 120 | 1 | 0.000000517 | 0.000000138 | -0.000000068 |
| 121 | 8 | 0.000013780 | -0.000028302 | 0.000008577 |
| 122 | 8 | 0.000020052 | 0.000006722 | 0.000005373 |
| 123 | 6 | -0.000015178 | 0.000021284 | -0.000008544 |
| 124 | 6 | 0.000014772 | -0.000009419 | 0.000008930 |
| 125 | 6 | -0.000011807 | 0.000014270 | -0.000013355 |
| 126 | 6 | 0.000000116 | -0.000014210 | 0.000004241 |
| 127 | 6 | 0.000000034 | -0.000000516 | -0.000001544 |
| 128 | 6 | 0.000007744 | -0.000005723 | 0.000006988 |
| 129 | 6 | -0.000004708 | -0.000002534 | -0.000000197 |
| 130 | 6 | 0.000001628 | 0.000000556 | 0.000002028 |
| 131 | 1 | -0.000003964 | 0.000001132 | -0.000001268 |
| 132 | 1 | -0.000000741 | -0.000000008 | -0.000001942 |
| 133 | 1 | 0.000001556 | 0.000000080 | -0.000002710 |
| 134 | 1 | -0.000000276 | 0.000000155 | 0.000000080 |
| 135 | 1 | -0.000000337 | -0.000000195 | 0.000000242 |
| 136 | 1 | -0.000000098 | -0.000000146 | 0.000000202 |
| 137 | 1 | 0.000005556 | 0.000006290 | -0.000001215 |
| 138 | 1 | 0.000002610 | -0.000001787 | 0.000005277 |
| 139 | 1 | -0.000001275 | -0.000002404 | 0.000002259 |
| 140 | 1 | -0.000005249 | 0.000005730 | -0.000007951 |
| 141 | 1 | -0.000001700 | -0.000002356 | 0.000003083 |
| 142 | 1 | -0.000021841 | 0.000032395 | -0.000005273 |
| 143 | 1 | -0.000015124 | -0.000018247 | 0.000037041 |
| 144 | 1 | -0.000001105 | -0.000002065 | -0.000002572 |
| 145 | 8 | -0.000003614 | 0.000081497 | -0.000140127 |
| 146 | 1 | 0.000000432 | 0.000004314 | 0.000003990 |
| 147 | 1 | 0.000004191 | -0.000116795 | 0.000201314 |
| 148 | 8 | 0.000007290 | 0.000000056 | 0.000001137 |

| | | | | |
|---|---|---|---|---|
| 149 | 1 | -0.000001364 | 0.000001234 | 0.000001792 |
| 150 | 1 | -0.000006128 | -0.000007410 | -0.000005784 |
| 151 | 8 | 0.000002668 | -0.000000366 | -0.000002945 |
| 152 | 1 | 0.000000388 | 0.000000587 | 0.000001930 |
| 153 | 1 | 0.000000082 | 0.000006285 | 0.000004281 |
| 154 | 8 | 0.000011713 | 0.000000807 | 0.000000091 |
| 155 | 1 | -0.000039061 | -0.000002375 | -0.000011274 |
| 156 | 1 | -0.000001929 | 0.000005888 | -0.000021870 |
| 157 | 1 | 0.000003210 | 0.000030257 | -0.000006494 |
| 158 | 8 | 0.000002072 | -0.000038659 | 0.000016888 |
| 159 | 8 | 0.000018816 | 0.000003582 | -0.000017509 |
| 160 | 6 | 0.000013758 | 0.000008140 | -0.000016130 |
| 161 | 6 | -0.000014222 | 0.000019395 | -0.000002930 |
| 162 | 6 | 0.000017518 | -0.000018008 | 0.000017699 |
| 163 | 6 | -0.000008413 | -0.000001838 | -0.000001627 |
| 164 | 6 | -0.000002031 | -0.000000926 | -0.000000932 |
| 165 | 6 | -0.000021819 | 0.000008668 | 0.000002010 |
| 166 | 6 | -0.000000169 | -0.000001343 | 0.000002273 |
| 167 | 6 | 0.000000768 | 0.000002108 | -0.000002260 |
| 168 | 1 | -0.000001636 | -0.000003344 | 0.000005254 |
| 169 | 1 | 0.000000002 | 0.000003785 | 0.000000445 |
| 170 | 1 | 0.000000881 | 0.000001190 | -0.000001167 |
| 171 | 1 | -0.000000599 | 0.000000174 | 0.000000699 |
| 172 | 1 | 0.000000193 | -0.000000638 | 0.000000523 |
| 173 | 1 | -0.000000046 | -0.000000137 | 0.000000549 |
| 174 | 8 | -0.000009382 | -0.000003960 | 0.000003792 |
| 175 | 8 | 0.000002087 | 0.000003273 | 0.000003806 |
| 176 | 6 | -0.000000390 | -0.000003165 | -0.000006053 |
| 177 | 6 | 0.000002316 | -0.000000781 | 0.000001701 |
| 178 | 6 | 0.000008115 | 0.000003020 | 0.000007145 |
| 179 | 6 | -0.000010419 | -0.000003985 | -0.000006002 |
| 180 | 6 | 0.000005096 | 0.000001273 | 0.000002109 |
| 181 | 6 | -0.000002870 | -0.000004591 | -0.000006834 |
| 182 | 6 | -0.000000540 | 0.000000172 | -0.000000325 |
| 183 | 6 | -0.000000263 | -0.000001295 | 0.000000598 |
| 184 | 1 | -0.000000232 | 0.000000184 | 0.000000856 |
| 185 | 1 | 0.000000051 | 0.000001303 | 0.000000425 |
| 186 | 1 | -0.000001179 | -0.000000854 | 0.000000518 |
| 187 | 1 | 0.000000122 | 0.000000094 | 0.000000059 |
| 188 | 1 | 0.000000102 | 0.000000308 | 0.000000008 |
| 189 | 1 | 0.000000166 | -0.000000209 | -0.000000156 |
| 190 | 8 | 0.000020377 | -0.000023321 | 0.000013163 |
| 191 | 8 | -0.000001816 | 0.000002802 | -0.000002904 |
| 192 | 6 | -0.000000645 | 0.000002911 | -0.000005314 |
| 193 | 6 | 0.000002241 | 0.000007840 | 0.000006335 |
| 194 | 6 | -0.000002928 | -0.000007172 | 0.000001585 |
| 195 | 6 | -0.000003456 | -0.000001113 | -0.000001666 |
| 196 | 6 | 0.000007095 | 0.000007419 | -0.000001862 |
| 197 | 6 | -0.000002620 | -0.000001863 | -0.000000674 |
| 198 | 6 | 0.000005054 | 0.000000910 | 0.000002588 |
| 199 | 6 | -0.000000614 | -0.000001022 | 0.000000769 |
| 200 | 1 | -0.000002772 | -0.000000960 | -0.000003765 |
| 201 | 1 | -0.000001273 | -0.000000777 | 0.000001286 |
| 202 | 1 | 0.000001321 | 0.000000722 | -0.000000086 |
| 203 | 1 | -0.000000051 | -0.000000358 | 0.000000312 |
| 204 | 1 | -0.000000029 | 0.000000127 | 0.000001040 |
| 205 | 1 | -0.000000537 | -0.000000539 | 0.000001018 |
| 206 | 8 | -0.000001918 | -0.000000234 | -0.000001665 |
| 207 | 8 | 0.000010517 | -0.000013131 | 0.000013095 |
| 208 | 6 | -0.000005822 | 0.000005026 | -0.000008341 |
| 209 | 6 | -0.000002447 | -0.000002258 | 0.000002593 |
| 210 | 6 | 0.000005256 | 0.000005544 | 0.000000797 |
| 211 | 6 | 0.000001178 | 0.000002007 | -0.000008516 |
| 212 | 6 | -0.000001027 | 0.000002368 | 0.000000833 |
| 213 | 6 | 0.000011600 | 0.000000639 | 0.000009482 |
| 214 | 6 | 0.000002636 | 0.000000830 | -0.000000355 |
| 215 | 6 | 0.000001825 | -0.000001378 | -0.000000277 |
| 216 | 1 | 0.000001843 | 0.000000365 | 0.000001784 |
| 217 | 1 | 0.000000721 | 0.000000220 | -0.000001483 |
| 218 | 1 | 0.000003525 | -0.000007486 | 0.000000315 |
| 219 | 1 | -0.000000533 | 0.000000099 | 0.000000383 |
| 220 | 1 | -0.000000860 | 0.000000326 | 0.000000407 |
| 221 | 1 | -0.000000415 | 0.000000264 | -0.000000334 |

| | | | | |
|---|---|---|---|---|
| 222 | 1 | -0.000001896 | -0.000002065 | 0.000007858 |
| 223 | 1 | 0.000005503 | 0.000005105 | 0.000003016 |
| 224 | 1 | 0.000002121 | 0.000002117 | 0.000001355 |
| 225 | 1 | -0.000016232 | 0.000031475 | -0.000025627 |
| 226 | 1 | 0.000002935 | -0.000003140 | 0.000001500 |
| 227 | 1 | -0.000003585 | -0.000001274 | -0.000002374 |
| 228 | 1 | 0.000003647 | 0.000000465 | 0.000002599 |
| 229 | 1 | -0.000000813 | -0.000003092 | -0.000000710 |
| 230 | 1 | -0.000000472 | -0.000001705 | 0.000001615 |
| 231 | 1 | -0.000001697 | -0.000010509 | -0.000002066 |
| 232 | 8 | 0.000003519 | -0.000000423 | 0.000004755 |
| 233 | 8 | 0.000002567 | 0.000001176 | -0.000002430 |
| 234 | 6 | 0.000001168 | -0.000003431 | 0.000001588 |
| 235 | 6 | 0.000000196 | 0.000001426 | -0.000000068 |
| 236 | 6 | -0.000002256 | 0.000001359 | -0.000000961 |
| 237 | 6 | -0.000000017 | 0.000000655 | -0.000000030 |
| 238 | 6 | -0.000002568 | -0.000002759 | 0.000002075 |
| 239 | 6 | 0.000000100 | 0.000005631 | -0.000005270 |
| 240 | 6 | -0.000001321 | -0.000002997 | -0.000001799 |
| 241 | 6 | 0.000000341 | -0.000000246 | 0.000000455 |
| 242 | 1 | 0.000000525 | -0.000000120 | 0.000001361 |
| 243 | 1 | 0.000000478 | -0.000000106 | -0.000000351 |
| 244 | 1 | 0.000000714 | -0.000000796 | -0.000000925 |
| 245 | 1 | 0.000000196 | 0.000000463 | -0.000000037 |
| 246 | 1 | 0.000000229 | 0.000000071 | -0.000000325 |
| 247 | 1 | -0.000000004 | 0.000000175 | 0.000000092 |
| 248 | 8 | -0.000001338 | 0.000007443 | 0.000003296 |
| 249 | 8 | 0.000008702 | 0.000002254 | -0.000002293 |
| 250 | 6 | 0.000004157 | -0.000003976 | -0.000006045 |
| 251 | 6 | -0.000003401 | 0.000002691 | 0.000007604 |
| 252 | 6 | -0.000005712 | -0.000003784 | -0.000002374 |
| 253 | 6 | 0.000002734 | -0.000001997 | -0.000002758 |
| 254 | 6 | -0.000001100 | 0.000002828 | 0.000004222 |
| 255 | 6 | -0.000000448 | -0.000005846 | -0.000000834 |
| 256 | 6 | -0.000000777 | -0.000000053 | 0.000001382 |
| 257 | 6 | 0.000001122 | -0.000000136 | 0.000001519 |
| 258 | 1 | 0.000001926 | 0.000000421 | -0.000003223 |
| 259 | 1 | -0.000000480 | 0.000001687 | -0.000000893 |
| 260 | 1 | 0.000002280 | -0.000001196 | -0.000000296 |
| 261 | 1 | -0.000000341 | -0.000000403 | -0.000000288 |
| 262 | 1 | -0.000000643 | -0.000000157 | -0.000000269 |
| 263 | 1 | -0.000000078 | -0.000000085 | -0.000000268 |
| 264 | 8 | 0.000004838 | -0.000001653 | 0.000001357 |
| 265 | 8 | 0.000001841 | -0.000000107 | -0.000005740 |
| 266 | 6 | 0.000000024 | -0.000002638 | -0.000000255 |
| 267 | 6 | 0.000001155 | 0.000004741 | 0.000000458 |
| 268 | 6 | 0.000000756 | 0.000000152 | 0.000001246 |
| 269 | 6 | -0.000000706 | -0.000001889 | 0.000001445 |
| 270 | 6 | -0.000000427 | 0.000000199 | 0.000000484 |
| 271 | 6 | -0.000004788 | 0.000005662 | 0.000004454 |
| 272 | 6 | 0.000000372 | -0.000000216 | -0.000000045 |
| 273 | 6 | -0.000001083 | 0.000000459 | -0.000000744 |
| 274 | 1 | -0.000000395 | 0.000000221 | -0.000000081 |
| 275 | 1 | 0.000000190 | 0.000000360 | -0.000001078 |
| 276 | 1 | -0.000000549 | -0.000000391 | -0.000000627 |
| 277 | 1 | 0.000000417 | -0.000000296 | 0.000000276 |
| 278 | 1 | -0.000000158 | -0.000000182 | 0.000000079 |
| 279 | 1 | 0.000000363 | -0.000000178 | 0.000000350 |
| 280 | 8 | 0.000002985 | 0.000004915 | 0.000005520 |
| 281 | 8 | -0.000002899 | 0.000001558 | 0.000004379 |
| 282 | 6 | 0.000000638 | 0.000003104 | 0.000000105 |
| 283 | 6 | 0.000001929 | -0.000005506 | 0.000001707 |
| 284 | 6 | -0.000007493 | 0.000000509 | -0.000006313 |
| 285 | 6 | 0.000010785 | 0.000004887 | 0.000010016 |
| 286 | 6 | -0.000003843 | -0.000002433 | -0.000003310 |
| 287 | 6 | 0.000001509 | 0.000001432 | 0.000000972 |
| 288 | 6 | -0.000001368 | 0.000005520 | 0.000001950 |
| 289 | 6 | -0.000000565 | -0.000000135 | 0.000000029 |
| 290 | 1 | 0.000000128 | 0.000000896 | -0.000002609 |
| 291 | 1 | -0.000000893 | -0.000001028 | 0.000001076 |
| 292 | 1 | -0.000003007 | -0.000002792 | -0.000000238 |
| 293 | 1 | 0.000000043 | 0.000000116 | -0.000000632 |
| 294 | 1 | 0.000000670 | 0.000000012 | -0.000000172 |

| | | | | |
|---|---|---|---|---|
| 295 | 1 | 0.000000954 | -0.000000143 | -0.000000977 |
| 296 | 1 | 0.000000539 | 0.000003775 | 0.000000893 |
| 297 | 1 | -0.000003287 | 0.000001723 | 0.000004121 |
| 298 | 1 | -0.000004139 | 0.000013332 | -0.000001993 |
| 299 | 1 | 0.000003114 | -0.000002986 | 0.000000904 |
| 300 | 1 | -0.000000946 | -0.000002922 | -0.000001845 |
| 301 | 1 | -0.000008197 | -0.000000604 | -0.000006539 |
| 302 | 1 | -0.000014517 | 0.000000306 | -0.000004224 |
| 303 | 1 | -0.000002288 | 0.000008579 | -0.000004385 |
| 304 | 1 | 0.000015940 | -0.000021587 | -0.000022659 |
| 305 | 8 | 0.000005495 | -0.000023443 | -0.000003490 |
| 306 | 8 | 0.000013223 | 0.000003535 | 0.000000985 |
| 307 | 6 | 0.000007904 | 0.000002257 | 0.000011342 |
| 308 | 6 | -0.000001751 | 0.000000955 | -0.000000625 |
| 309 | 6 | -0.000003829 | -0.000003070 | -0.000000780 |
| 310 | 6 | 0.000003661 | 0.000007739 | -0.000000325 |
| 311 | 6 | 0.000000249 | -0.000004984 | 0.000001035 |
| 312 | 6 | -0.000003275 | 0.000005784 | -0.000001447 |
| 313 | 6 | 0.000002110 | -0.000000696 | 0.000001005 |
| 314 | 6 | -0.000000950 | -0.000000467 | 0.000000820 |
| 315 | 1 | 0.000000126 | 0.000000473 | 0.000001258 |
| 316 | 1 | -0.000000043 | -0.000000469 | -0.000000436 |
| 317 | 1 | 0.000000495 | -0.000000711 | -0.000000868 |
| 318 | 1 | -0.000000043 | 0.000000175 | 0.000000104 |
| 319 | 1 | -0.000000036 | 0.000000348 | 0.000000198 |
| 320 | 1 | -0.000000283 | 0.000000251 | -0.000000084 |
| 321 | 8 | 0.000001343 | -0.000037837 | 0.000015346 |
| 322 | 8 | -0.000004129 | 0.000010490 | 0.000018434 |
| 323 | 6 | 0.000009123 | 0.000015699 | -0.000001828 |
| 324 | 6 | 0.000002486 | 0.000004502 | -0.000004450 |
| 325 | 6 | -0.000008630 | -0.000007868 | 0.000007898 |
| 326 | 6 | 0.000002727 | 0.000007811 | -0.000003703 |
| 327 | 6 | 0.000003614 | 0.000001889 | -0.000002259 |
| 328 | 6 | -0.000013496 | 0.000001418 | 0.000011372 |
| 329 | 6 | -0.000001160 | -0.000004405 | 0.000000220 |
| 330 | 6 | 0.000000320 | -0.000003215 | 0.000002295 |
| 331 | 1 | -0.000002196 | -0.000001629 | -0.000000027 |
| 332 | 1 | -0.000001246 | -0.000000868 | -0.000000962 |
| 333 | 1 | 0.000002096 | -0.000000379 | 0.000000851 |
| 334 | 1 | -0.000000364 | 0.000000465 | -0.000000422 |
| 335 | 1 | -0.000000380 | 0.000000286 | -0.000000337 |
| 336 | 1 | 0.000000417 | 0.000000644 | -0.000000461 |
| 337 | 8 | 0.000001122 | -0.000012253 | -0.000001774 |
| 338 | 8 | 0.000012310 | 0.000004060 | -0.000005337 |
| 339 | 6 | -0.000011195 | 0.000008636 | 0.000002815 |
| 340 | 6 | 0.000001734 | 0.000000074 | -0.000003245 |
| 341 | 6 | 0.000003533 | -0.000001063 | 0.000005633 |
| 342 | 6 | -0.000008711 | -0.000000469 | -0.000002552 |
| 343 | 6 | -0.000000539 | 0.000000915 | -0.000000800 |
| 344 | 6 | 0.000007200 | -0.000005668 | 0.000001476 |
| 345 | 6 | 0.000000480 | 0.000004017 | -0.000006352 |
| 346 | 6 | 0.000002742 | -0.000001282 | 0.000000585 |
| 347 | 1 | 0.000000009 | -0.000001989 | 0.000000204 |
| 348 | 1 | 0.000003106 | 0.000001250 | -0.000001465 |
| 349 | 1 | 0.000002649 | -0.000001780 | 0.000003366 |
| 350 | 1 | -0.000000489 | 0.000000330 | -0.000000215 |
| 351 | 1 | -0.000000717 | 0.000000306 | 0.000000039 |
| 352 | 1 | -0.000000665 | 0.000000128 | -0.000000390 |
| 353 | 8 | -0.000004676 | 0.000001707 | 0.000014278 |
| 354 | 8 | -0.000002371 | -0.000000452 | 0.000000610 |
| 355 | 6 | 0.000004603 | 0.000001858 | 0.000000173 |
| 356 | 6 | 0.000001136 | -0.000000779 | -0.000003128 |
| 357 | 6 | -0.000003427 | -0.000003848 | 0.000005317 |
| 358 | 6 | 0.000003740 | 0.000006028 | -0.000004964 |
| 359 | 6 | -0.000000238 | -0.000000075 | 0.000001832 |
| 360 | 6 | -0.000002427 | -0.000000560 | -0.000001127 |
| 361 | 6 | 0.000003911 | -0.000004290 | 0.000000353 |
| 362 | 6 | -0.000002199 | 0.000001565 | 0.000001198 |
| 363 | 1 | -0.000001246 | -0.000000275 | 0.000001096 |
| 364 | 1 | -0.000000276 | -0.000000568 | 0.000000574 |
| 365 | 1 | 0.000000146 | 0.000002049 | -0.000001890 |
| 366 | 1 | -0.000000141 | -0.000000115 | -0.000000362 |
| 367 | 1 | 0.000000175 | -0.000000906 | -0.000000547 |

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|---|---|---|---|---|
| 368 | 1 | 0.000000728 | -0.000000406 | -0.000000343 |
| 369 | 1 | -0.000002393 | 0.000001943 | 0.000000948 |
| 370 | 1 | -0.000009433 | -0.000010922 | 0.000008437 |
| 371 | 1 | 0.000000302 | -0.000008664 | -0.000002720 |
| 372 | 1 | 0.000005847 | 0.000004025 | 0.000002301 |
| 373 | 1 | 0.000000795 | -0.000007509 | -0.000004472 |
| 374 | 1 | 0.000004049 | 0.000000747 | 0.000001678 |
| 375 | 1 | 0.000001496 | -0.000000176 | -0.000000704 |
| 376 | 1 | 0.000001359 | -0.000003051 | -0.000003408 |
| 377 | 8 | -0.000004647 | 0.000008925 | -0.000000247 |
| 378 | 8 | -0.000009157 | 0.000002377 | -0.000009230 |
| 379 | 6 | 0.000001185 | 0.000005334 | 0.000003567 |
| 380 | 6 | 0.000001424 | 0.000002136 | 0.000001934 |
| 381 | 6 | -0.000005092 | -0.000007870 | -0.000003880 |
| 382 | 6 | 0.000004288 | -0.000004055 | 0.000002279 |
| 383 | 6 | 0.000001282 | 0.000000060 | 0.000000758 |
| 384 | 6 | -0.000001836 | 0.000000365 | -0.000000795 |
| 385 | 6 | 0.000003347 | 0.000003408 | -0.000001712 |
| 386 | 6 | -0.000000457 | -0.000000368 | -0.000000541 |
| 387 | 1 | 0.000000512 | -0.000000233 | -0.000000076 |
| 388 | 1 | 0.000000753 | 0.000000102 | -0.000000917 |
| 389 | 1 | 0.000001972 | 0.000001256 | -0.000000154 |
| 390 | 1 | -0.000000151 | 0.000000211 | 0.000000086 |
| 391 | 1 | -0.000000190 | 0.000000113 | 0.000000436 |
| 392 | 1 | -0.000000223 | 0.000000197 | 0.000000402 |
| 393 | 8 | 0.000001869 | -0.000020361 | -0.000019170 |
| 394 | 8 | -0.000006531 | -0.000002724 | 0.000004212 |
| 395 | 6 | -0.000000816 | 0.000020635 | 0.000007573 |
| 396 | 6 | -0.000007826 | -0.000011878 | 0.000002221 |
| 397 | 6 | 0.000005949 | 0.000001430 | -0.000006709 |
| 398 | 6 | -0.000002612 | 0.000001145 | 0.000000855 |
| 399 | 6 | -0.000002853 | -0.000006638 | 0.000000586 |
| 400 | 6 | 0.000003533 | -0.000001404 | -0.000004108 |
| 401 | 6 | -0.000002097 | -0.000000294 | 0.000003549 |
| 402 | 6 | -0.000000873 | -0.000000100 | -0.000000345 |
| 403 | 1 | 0.000001849 | 0.000001720 | -0.000000423 |
| 404 | 1 | 0.000001035 | 0.000000194 | 0.000001053 |
| 405 | 1 | -0.000000698 | 0.000001157 | 0.000000299 |
| 406 | 1 | -0.000000224 | -0.000000185 | 0.000000157 |
| 407 | 1 | -0.000000051 | -0.000000138 | -0.000000230 |
| 408 | 1 | 0.000000210 | -0.000000208 | -0.000000208 |
| 409 | 8 | -0.000000986 | -0.000002835 | 0.000006961 |
| 410 | 8 | -0.000002987 | 0.000003012 | 0.000002031 |
| 411 | 6 | -0.000004155 | 0.000003873 | -0.000000912 |
| 412 | 6 | -0.000000499 | -0.000004331 | 0.000003230 |
| 413 | 6 | 0.000001907 | 0.000001667 | -0.000011978 |
| 414 | 6 | -0.000001821 | 0.000002889 | 0.000004577 |
| 415 | 6 | 0.000001378 | -0.000000233 | -0.000003042 |
| 416 | 6 | -0.000001346 | 0.000001518 | 0.000002494 |
| 417 | 6 | 0.000002176 | -0.000000829 | 0.000003407 |
| 418 | 6 | 0.000000921 | -0.000000419 | -0.000001538 |
| 419 | 1 | 0.000000533 | 0.000001036 | -0.000000055 |
| 420 | 1 | 0.000000178 | -0.000000904 | -0.000000073 |
| 421 | 1 | 0.000001796 | -0.000000797 | -0.000001146 |
| 422 | 1 | -0.000000355 | 0.000000196 | 0.000000109 |
| 423 | 1 | 0.000000027 | 0.000000159 | 0.000000216 |
| 424 | 1 | -0.000000350 | 0.000000373 | 0.000000458 |
| 425 | 8 | 0.000010889 | 0.000002570 | 0.000009487 |
| 426 | 8 | -0.000007668 | -0.000010509 | -0.000016593 |
| 427 | 6 | 0.000001883 | 0.000002744 | -0.000002477 |
| 428 | 6 | 0.000002040 | -0.000001064 | 0.000006124 |
| 429 | 6 | 0.000006468 | 0.000003368 | 0.000004551 |
| 430 | 6 | 0.000000393 | 0.000000127 | 0.000001832 |
| 431 | 6 | 0.000000177 | -0.000003679 | 0.000006483 |
| 432 | 6 | -0.000000302 | 0.000002145 | -0.000003401 |
| 433 | 6 | 0.000004622 | -0.000000485 | 0.000001343 |
| 434 | 6 | -0.000000979 | 0.000000452 | -0.000000448 |
| 435 | 1 | -0.000002081 | -0.000001678 | -0.000002155 |
| 436 | 1 | -0.000000632 | 0.000000245 | -0.000000502 |
| 437 | 1 | -0.000000027 | -0.000000842 | -0.000002099 |
| 438 | 1 | 0.000000028 | -0.000000290 | 0.000000457 |
| 439 | 1 | -0.000000152 | -0.000000298 | 0.000000401 |
| 440 | 1 | 0.000000119 | -0.000000241 | 0.000000052 |

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|---|---|---|---|---|
| 441 | 1 | -0.000001047 | 0.000004955 | 0.000003215 |
| 442 | 1 | -0.000005732 | 0.000000974 | -0.000004541 |
| 443 | 1 | 0.000002409 | 0.000004151 | 0.000020545 |
| 444 | 1 | -0.000002051 | 0.000000202 | 0.000011122 |
| 445 | 8 | 0.000061361 | -0.000008172 | -0.000030673 |
| 446 | 1 | 0.000008246 | -0.000001476 | 0.000019045 |
| 447 | 1 | -0.000097830 | 0.000036353 | 0.000003465 |
| 448 | 8 | -0.000000742 | -0.000017295 | -0.000003726 |
| 449 | 1 | -0.000003256 | 0.000002343 | 0.000003926 |
| 450 | 1 | 0.000000181 | 0.000001366 | -0.000003664 |
| 451 | 8 | 0.000012391 | -0.000006403 | 0.000003315 |
| 452 | 1 | -0.000003827 | -0.000003513 | 0.000003489 |
| 453 | 1 | -0.000003308 | -0.000000363 | -0.000003863 |
| 454 | 8 | 0.000002569 | 0.000005763 | 0.000001638 |
| 455 | 1 | 0.000000707 | 0.000000593 | -0.000004938 |
| 456 | 1 | 0.000000118 | -0.000004092 | -0.000000246 |
| 457 | 6 | -0.000005784 | 0.000003147 | 0.000001078 |
| 458 | 6 | 0.000004753 | -0.000010910 | 0.000006987 |
| 459 | 6 | 0.000001228 | 0.000000968 | -0.000005894 |
| 460 | 7 | -0.000000734 | 0.000013288 | 0.000018261 |
| 461 | 6 | 0.000002533 | 0.000005780 | -0.000003202 |
| 462 | 6 | -0.000004990 | -0.000001304 | -0.000002277 |
| 463 | 6 | -0.000000032 | -0.000001547 | 0.000001126 |
| 464 | 6 | 0.000004541 | 0.000002502 | 0.000000271 |
| 465 | 6 | -0.000008764 | 0.000001892 | -0.000003529 |
| 466 | 8 | -0.000008132 | -0.000016490 | -0.000016448 |
| 467 | 8 | 0.000016614 | 0.000001325 | 0.000001920 |
| 468 | 1 | -0.000000653 | -0.000003963 | -0.000003396 |
| 469 | 1 | 0.000000297 | 0.000000693 | -0.000000214 |
| 470 | 1 | -0.000001729 | -0.000001363 | 0.000001251 |
| 471 | 1 | 0.000001452 | 0.000000617 | 0.000000792 |
| 472 | 1 | -0.000000208 | -0.000001087 | -0.000000199 |
| 473 | 1 | -0.000000203 | 0.000001667 | 0.000000120 |
| 474 | 1 | -0.000000357 | -0.000000680 | 0.000001908 |
| 475 | 6 | 0.000001039 | 0.000001819 | -0.000005030 |
| 476 | 6 | 0.000005222 | 0.000011676 | 0.000010090 |
| 477 | 7 | 0.000004166 | -0.000018928 | -0.000011236 |
| 478 | 6 | -0.000002004 | 0.000007496 | -0.000001850 |
| 479 | 6 | -0.000001665 | -0.000002176 | 0.000005111 |
| 480 | 6 | -0.000001941 | 0.000002045 | -0.000000130 |
| 481 | 1 | 0.000001449 | -0.000001587 | 0.000000453 |
| 482 | 1 | -0.000006801 | 0.000000765 | -0.000005825 |
| 483 | 1 | 0.000002976 | -0.000000641 | -0.000000467 |
| 484 | 1 | -0.000002253 | -0.000002531 | -0.000002620 |
| 485 | 1 | -0.000001070 | -0.000000698 | -0.000000386 |
| 486 | 1 | 0.000000439 | 0.000000430 | 0.000000445 |
| 487 | 1 | 0.000001499 | 0.000005084 | 0.000002358 |

Sum of electronic and thermal Free Energies = -1069.303724
ONIOM Total Energy = -1072.596211
0 imaginary frequency

**$\alpha$-4a@$C_R$**

| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | -0.000005843 | -0.000003282 | 0.000001623 |
| 2 | 8 | -0.000004210 | -0.000001206 | -0.000002503 |
| 3 | 6 | 0.000006583 | -0.000006452 | 0.000000817 |
| 4 | 6 | -0.000001197 | 0.000002441 | -0.000003763 |
| 5 | 6 | -0.000001850 | -0.000000540 | 0.000003672 |
| 6 | 6 | 0.000001627 | -0.000001615 | 0.000000840 |
| 7 | 6 | -0.000000842 | -0.000000239 | -0.000002263 |
| 8 | 6 | -0.000002439 | 0.000000232 | 0.000002790 |
| 9 | 6 | -0.000000237 | -0.000000731 | -0.000000254 |
| 10 | 6 | 0.000000247 | -0.000000630 | 0.000000188 |
| 11 | 1 | 0.000000220 | -0.000000428 | 0.000000339 |
| 12 | 1 | 0.000000220 | 0.000000220 | -0.000000277 |
| 13 | 1 | 0.000000160 | 0.000000812 | -0.000001100 |
| 14 | 1 | 0.000000148 | -0.000000158 | -0.000000741 |
| 15 | 1 | 0.000000162 | -0.000000133 | -0.000000175 |

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|---|---|---|---|---|
| 16 | 1 | 0.000000056 | -0.000000204 | -0.000000298 |
| 17 | 8 | -0.000006066 | -0.000004642 | 0.000016176 |
| 18 | 8 | -0.000012272 | 0.000015500 | 0.000029529 |
| 19 | 6 | 0.000005689 | -0.000020112 | 0.000004081 |
| 20 | 6 | 0.000013158 | -0.000000362 | 0.000005297 |
| 21 | 6 | -0.000017634 | 0.000023648 | -0.000009362 |
| 22 | 6 | -0.000001797 | 0.000003026 | -0.000005379 |
| 23 | 6 | 0.000001358 | -0.000003177 | 0.000004847 |
| 24 | 6 | -0.000008593 | -0.000007121 | -0.000003334 |
| 25 | 6 | 0.000001833 | -0.000002275 | 0.000017219 |
| 26 | 6 | -0.000002472 | 0.000001029 | -0.000004245 |
| 27 | 1 | 0.000000636 | 0.000001286 | -0.000000571 |
| 28 | 1 | 0.000000317 | 0.000000996 | 0.000001504 |
| 29 | 1 | 0.000000413 | -0.000001866 | 0.000005920 |
| 30 | 1 | 0.000000299 | -0.000000174 | -0.000000589 |
| 31 | 1 | 0.000000099 | -0.000000334 | -0.000000786 |
| 32 | 1 | 0.000000117 | 0.000000027 | -0.000000209 |
| 33 | 8 | 0.000002318 | 0.000004780 | 0.000000208 |
| 34 | 8 | 0.000023227 | 0.000015001 | -0.000018299 |
| 35 | 6 | -0.000002405 | -0.000000624 | -0.000001837 |
| 36 | 6 | 0.000008865 | 0.000004498 | -0.000002847 |
| 37 | 6 | -0.000019114 | -0.000001027 | -0.000012630 |
| 38 | 6 | 0.000007702 | -0.000007558 | 0.000004339 |
| 39 | 6 | 0.000004616 | 0.000003278 | -0.000000412 |
| 40 | 6 | -0.000000258 | -0.000001647 | 0.000004109 |
| 41 | 6 | 0.000000680 | 0.000007057 | 0.000006751 |
| 42 | 6 | -0.000001050 | -0.000000134 | 0.000000683 |
| 43 | 1 | -0.000001508 | -0.000001124 | -0.000000753 |
| 44 | 1 | 0.000000138 | 0.000000469 | -0.000000491 |
| 45 | 1 | -0.000001086 | 0.000003382 | 0.000002548 |
| 46 | 1 | 0.000000528 | 0.000000058 | -0.000000071 |
| 47 | 1 | 0.000000241 | 0.000000451 | 0.000000091 |
| 48 | 1 | -0.000000235 | 0.000000328 | -0.000000457 |
| 49 | 8 | 0.000027501 | -0.000009811 | -0.000016433 |
| 50 | 8 | 0.000012243 | 0.000010622 | -0.000004827 |
| 51 | 6 | -0.000014309 | -0.000020956 | -0.000012470 |
| 52 | 6 | 0.000002400 | -0.000004838 | -0.000004548 |
| 53 | 6 | 0.000002491 | 0.000005232 | 0.000008159 |
| 54 | 6 | -0.000000147 | -0.000000421 | -0.000006063 |
| 55 | 6 | -0.000000091 | -0.000002769 | 0.000002127 |
| 56 | 6 | 0.000012726 | 0.000018876 | 0.000003263 |
| 57 | 6 | -0.000001132 | -0.000001040 | -0.000001793 |
| 58 | 6 | 0.000000498 | 0.000001329 | -0.000000348 |
| 59 | 1 | 0.000000364 | 0.000001026 | 0.000000833 |
| 60 | 1 | -0.000001074 | -0.000002169 | -0.000000354 |
| 61 | 1 | -0.000001763 | 0.000000128 | -0.000000002 |
| 62 | 1 | -0.000000135 | 0.000000209 | -0.000000287 |
| 63 | 1 | 0.000000032 | 0.000000136 | -0.000000248 |
| 64 | 1 | 0.000000246 | 0.000000209 | -0.000000571 |
| 65 | 1 | -0.000009965 | -0.000008683 | 0.000007343 |
| 66 | 1 | -0.000002655 | 0.000000217 | 0.000000013 |
| 67 | 1 | 0.000004506 | 0.000004388 | 0.000001422 |
| 68 | 1 | -0.000014496 | -0.000003912 | -0.000003479 |
| 69 | 1 | -0.000004208 | -0.000014398 | -0.000033226 |
| 70 | 1 | 0.000000087 | -0.000003416 | 0.000002255 |
| 71 | 1 | -0.000009682 | 0.000007491 | -0.000004444 |
| 72 | 1 | -0.000004983 | -0.000001252 | 0.000000467 |
| 73 | 8 | 0.000000056 | -0.000014241 | -0.000006616 |
| 74 | 8 | -0.000021538 | 0.000037645 | 0.000046227 |
| 75 | 6 | -0.000009362 | -0.000003767 | 0.000001805 |
| 76 | 6 | 0.000001416 | 0.000002256 | 0.000007579 |
| 77 | 6 | 0.000013049 | -0.000000366 | 0.000007419 |
| 78 | 6 | 0.000008219 | -0.000012731 | -0.000009007 |
| 79 | 6 | 0.000000570 | -0.000001118 | -0.000004108 |
| 80 | 6 | 0.000007308 | -0.000021415 | -0.000013075 |
| 81 | 6 | -0.000000564 | -0.000001537 | 0.000004323 |
| 82 | 6 | 0.000001384 | -0.000001040 | -0.000000156 |
| 83 | 1 | -0.000002780 | 0.000003121 | -0.000001804 |
| 84 | 1 | -0.000001239 | 0.000004367 | -0.000001985 |
| 85 | 1 | -0.000000089 | 0.000005484 | 0.000001143 |
| 86 | 1 | -0.000000013 | -0.000000359 | -0.000000774 |
| 87 | 1 | -0.000000042 | -0.000000598 | -0.000001142 |
| 88 | 1 | 0.000000335 | -0.000001286 | -0.000000441 |

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| 89 | 8 | -0.000004280 | 0.000006701 | 0.000000653 |
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| 404 | 1 | 0.000000736 | 0.000000039 | 0.000000346 |
| 405 | 1 | 0.000004119 | 0.000003974 | 0.000003319 |
| 406 | 1 | -0.000000545 | 0.000000379 | 0.000000048 |
| 407 | 1 | -0.000000289 | 0.000000014 | 0.000000273 |
| 408 | 1 | -0.000000506 | -0.000000224 | 0.000000552 |
| 409 | 8 | 0.000000944 | -0.000002277 | 0.000005292 |
| 410 | 8 | 0.000008160 | 0.000006042 | 0.000008540 |
| 411 | 6 | -0.000001218 | 0.000000743 | 0.000002221 |
| 412 | 6 | -0.000002439 | -0.000001614 | 0.000001505 |
| 413 | 6 | -0.000004875 | 0.000001521 | -0.000002936 |
| 414 | 6 | 0.000003144 | 0.000005567 | -0.000001589 |
| 415 | 6 | 0.000000508 | -0.000001848 | -0.000000158 |
| 416 | 6 | 0.000001990 | 0.000001381 | -0.000001761 |
| 417 | 6 | 0.000005297 | -0.000000670 | -0.000000440 |
| 418 | 6 | -0.000000202 | 0.000000565 | 0.000000391 |
| 419 | 1 | 0.000001037 | 0.000000287 | -0.000000340 |
| 420 | 1 | -0.000000154 | -0.000000397 | 0.000000342 |
| 421 | 1 | -0.000000025 | -0.000003424 | 0.000003526 |
| 422 | 1 | -0.000000175 | -0.000000157 | -0.000000336 |
| 423 | 1 | -0.000000049 | 0.000000038 | -0.000000027 |
| 424 | 1 | -0.000000383 | -0.000000273 | 0.000000183 |
| 425 | 8 | 0.000005506 | -0.000007838 | 0.000010830 |
| 426 | 8 | 0.000011693 | 0.000009791 | 0.000000060 |
| 427 | 6 | 0.000001509 | -0.000001105 | -0.000004780 |
| 428 | 6 | -0.000002621 | -0.000002936 | -0.000000679 |
| 429 | 6 | 0.000011236 | 0.000000289 | 0.000006803 |
| 430 | 6 | -0.000007239 | -0.000001242 | -0.000001108 |
| 431 | 6 | -0.000003701 | 0.000000522 | -0.000002461 |
| 432 | 6 | 0.000002522 | -0.000000369 | 0.000002948 |
| 433 | 6 | -0.000002467 | -0.000001906 | -0.000000173 |
| 434 | 6 | 0.000001402 | -0.000000270 | 0.000001043 |
| 435 | 1 | 0.000000290 | -0.000001351 | 0.000001016 |
| 436 | 1 | -0.000000752 | 0.000000862 | -0.000001159 |
| 437 | 1 | -0.000003361 | 0.000000349 | 0.000000244 |
| 438 | 1 | 0.000000487 | -0.000000417 | 0.000000022 |
| 439 | 1 | 0.000000540 | 0.000000015 | 0.000000119 |
| 440 | 1 | 0.000000384 | -0.000000632 | -0.000000552 |
| 441 | 1 | -0.000004981 | 0.000000895 | 0.000006897 |
| 442 | 1 | 0.000000333 | 0.000006233 | -0.000001144 |
| 443 | 1 | -0.000007498 | -0.000008432 | 0.000001816 |
| 444 | 1 | 0.000001614 | -0.000004401 | 0.000006253 |
| 445 | 8 | 0.000019235 | -0.000031597 | -0.000015607 |
| 446 | 1 | -0.000019716 | 0.000002465 | -0.000002717 |
| 447 | 1 | 0.000013976 | 0.000018858 | -0.000026602 |
| 448 | 8 | -0.000001927 | -0.000006841 | 0.000002597 |
| 449 | 1 | 0.000000585 | 0.000005525 | 0.000000310 |
| 450 | 1 | -0.000002832 | 0.000000550 | 0.000001205 |
| 451 | 8 | 0.000005476 | 0.000029390 | 0.000037011 |
| 452 | 1 | -0.000002122 | 0.000008262 | -0.000018921 |
| 453 | 1 | -0.000009371 | 0.000005551 | -0.000001380 |

| | | | | |
|---|---|---|---|---|
| 454 | 8 | 0.000003434 | 0.000049962 | -0.000003588 |
| 455 | 1 | -0.000005946 | -0.000035916 | 0.000002496 |
| 456 | 1 | 0.000007984 | -0.000015086 | -0.000020594 |
| 457 | 6 | -0.000012947 | -0.000012720 | 0.000019555 |
| 458 | 6 | 0.000011134 | 0.000004048 | 0.000017678 |
| 459 | 6 | -0.000017599 | 0.000039251 | -0.000023417 |
| 460 | 7 | -0.000005762 | 0.000036782 | 0.000021864 |
| 461 | 6 | -0.000008759 | 0.000008975 | -0.000009604 |
| 462 | 6 | 0.000003978 | -0.000024172 | -0.000011138 |
| 463 | 6 | -0.000000949 | 0.000005163 | 0.000012093 |
| 464 | 6 | -0.000003541 | 0.000012548 | -0.000002709 |
| 465 | 6 | 0.000011941 | -0.000008393 | 0.000002820 |
| 466 | 8 | -0.000003949 | -0.000027034 | 0.000007561 |
| 467 | 8 | 0.000018377 | -0.000008557 | -0.000027309 |
| 468 | 1 | -0.000003163 | 0.000003709 | 0.000000872 |
| 469 | 1 | -0.000003819 | -0.000006076 | 0.000010319 |
| 470 | 1 | 0.000002060 | -0.000003785 | -0.000005840 |
| 471 | 1 | -0.000001370 | 0.000001761 | -0.000002210 |
| 472 | 1 | -0.000003375 | -0.000000215 | -0.000003536 |
| 473 | 1 | -0.000002466 | -0.000007773 | 0.000005599 |
| 474 | 1 | 0.000000616 | -0.000001558 | 0.000003066 |
| 475 | 6 | -0.000005239 | 0.000004204 | -0.000001028 |
| 476 | 6 | 0.000006412 | -0.000003422 | -0.000021532 |
| 477 | 7 | 0.000022570 | -0.000017137 | 0.000012323 |
| 478 | 6 | -0.000000439 | 0.000023424 | -0.000020297 |
| 479 | 6 | -0.000006324 | -0.000006397 | -0.000003645 |
| 480 | 6 | -0.000019792 | -0.000000692 | -0.000016261 |
| 481 | 1 | 0.000009879 | 0.000003171 | -0.000005396 |
| 482 | 1 | 0.000005422 | -0.000001286 | 0.000005791 |
| 483 | 1 | 0.000007364 | -0.000001728 | 0.000001388 |
| 484 | 1 | 0.000003537 | -0.000000838 | 0.000002419 |
| 485 | 1 | 0.000008454 | -0.000000671 | 0.000019661 |
| 486 | 1 | -0.000002683 | -0.000004102 | -0.000001290 |
| 487 | 1 | -0.000001116 | 0.000003091 | -0.000008907 |

Sum of electronic and thermal Free Energies = -1069.319901
ONIOM Total Energy = -1072.611506
0 imaginary frequency

**$\beta$-TS1@$C_R$**

| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | -0.000000074 | 0.000000001 | -0.000000061 |
| 2 | 8 | -0.000000079 | 0.000000020 | -0.000000023 |
| 3 | 6 | -0.000000090 | -0.000000020 | -0.000000022 |
| 4 | 6 | -0.000000104 | 0.000000019 | -0.000000089 |
| 5 | 6 | -0.000000045 | 0.000000044 | -0.000000042 |
| 6 | 6 | -0.000000084 | 0.000000046 | -0.000000013 |
| 7 | 6 | -0.000000071 | 0.000000047 | -0.000000060 |
| 8 | 6 | -0.000000008 | -0.000000016 | -0.000000047 |
| 9 | 6 | -0.000000066 | 0.000000062 | -0.000000012 |
| 10 | 6 | -0.000000080 | 0.000000064 | -0.000000008 |
| 11 | 1 | -0.000000081 | 0.000000010 | -0.000000060 |
| 12 | 1 | -0.000000058 | 0.000000027 | -0.000000023 |
| 13 | 1 | -0.000000090 | 0.000000067 | -0.000000017 |
| 14 | 1 | -0.000000081 | 0.000000045 | -0.000000021 |
| 15 | 1 | -0.000000094 | 0.000000058 | -0.000000032 |
| 16 | 1 | -0.000000085 | 0.000000067 | -0.000000013 |
| 17 | 8 | 0.000000038 | 0.000000071 | 0.000000002 |
| 18 | 8 | 0.000000047 | -0.000000021 | 0.000000075 |
| 19 | 6 | -0.000000004 | 0.000000080 | 0.000000070 |
| 20 | 6 | -0.000000012 | 0.000000017 | 0.000000016 |
| 21 | 6 | 0.000000017 | -0.000000015 | 0.000000046 |
| 22 | 6 | 0.000000004 | 0.000000039 | 0.000000056 |
| 23 | 6 | -0.000000036 | 0.000000035 | -0.000000031 |
| 24 | 6 | 0.000000067 | 0.000000006 | 0.000000035 |
| 25 | 6 | 0.000000016 | -0.000000008 | 0.000000010 |
| 26 | 6 | 0.000000008 | -0.000000001 | 0.000000026 |
| 27 | 1 | 0.000000020 | 0.000000027 | 0.000000064 |
| 28 | 1 | -0.000000011 | 0.000000036 | 0.000000004 |

| | | | | |
|---|---|---|---|---|
| 29 | 1 | 0.000000023 | -0.000000008 | 0.000000011 |
| 30 | 1 | -0.000000006 | 0.000000015 | -0.000000005 |
| 31 | 1 | 0.000000002 | -0.000000009 | -0.000000003 |
| 32 | 1 | 0.000000006 | 0.000000006 | 0.000000011 |
| 33 | 8 | -0.000000052 | 0.000000070 | 0.000000008 |
| 34 | 8 | -0.000000051 | 0.000000047 | 0.000000042 |
| 35 | 6 | -0.000000033 | 0.000000122 | 0.000000029 |
| 36 | 6 | -0.000000028 | 0.000000044 | -0.000000002 |
| 37 | 6 | -0.000000068 | 0.000000049 | 0.000000050 |
| 38 | 6 | -0.000000087 | 0.000000092 | 0.000000003 |
| 39 | 6 | -0.000000033 | 0.000000027 | -0.000000026 |
| 40 | 6 | -0.000000060 | 0.000000050 | 0.000000044 |
| 41 | 6 | -0.000000039 | 0.000000048 | -0.000000001 |
| 42 | 6 | -0.000000034 | 0.000000064 | 0.000000049 |
| 43 | 1 | -0.000000050 | 0.000000072 | 0.000000024 |
| 44 | 1 | -0.000000055 | 0.000000046 | 0.000000004 |
| 45 | 1 | -0.000000022 | 0.000000071 | 0.000000048 |
| 46 | 1 | -0.000000039 | 0.000000053 | 0.000000022 |
| 47 | 1 | -0.000000029 | 0.000000058 | 0.000000042 |
| 48 | 1 | -0.000000042 | 0.000000081 | 0.000000033 |
| 49 | 8 | 0.000000001 | -0.000000020 | 0.000000016 |
| 50 | 8 | 0.000000143 | 0.000000139 | -0.000000340 |
| 51 | 6 | 0.000000078 | -0.000000014 | -0.000000005 |
| 52 | 6 | -0.000000026 | 0.000000000 | 0.000000006 |
| 53 | 6 | -0.000000070 | -0.000000078 | -0.000000071 |
| 54 | 6 | 0.000000050 | 0.000000021 | -0.000000023 |
| 55 | 6 | -0.000000048 | 0.000000044 | -0.000000012 |
| 56 | 6 | -0.000000048 | -0.000000038 | -0.000000046 |
| 57 | 6 | -0.000000028 | -0.000000017 | -0.000000077 |
| 58 | 6 | -0.000000050 | 0.000000003 | -0.000000030 |
| 59 | 1 | 0.000000007 | -0.000000031 | -0.000000027 |
| 60 | 1 | -0.000000028 | 0.000000014 | -0.000000033 |
| 61 | 1 | -0.000000047 | -0.000000011 | -0.000000066 |
| 62 | 1 | -0.000000056 | 0.000000002 | -0.000000060 |
| 63 | 1 | -0.000000049 | -0.000000014 | -0.000000052 |
| 64 | 1 | -0.000000048 | 0.000000003 | -0.000000045 |
| 65 | 1 | 0.000000026 | -0.000000007 | -0.000000000 |
| 66 | 1 | -0.000000064 | -0.000000029 | -0.000000093 |
| 67 | 1 | -0.000000107 | 0.000000101 | -0.000000015 |
| 68 | 1 | -0.000000039 | 0.000000016 | 0.000000138 |
| 69 | 1 | 0.000000029 | -0.000000008 | 0.000000027 |
| 70 | 1 | -0.000000088 | 0.000000048 | -0.000000022 |
| 71 | 1 | -0.000000015 | 0.000000071 | 0.000000067 |
| 72 | 1 | -0.000000087 | -0.000000040 | -0.000000021 |
| 73 | 8 | 0.000000063 | -0.000000056 | -0.000000233 |
| 74 | 8 | -0.000000056 | -0.000000305 | -0.000000228 |
| 75 | 6 | -0.000000189 | -0.000000037 | -0.000000064 |
| 76 | 6 | -0.000000014 | 0.000000165 | 0.000000249 |
| 77 | 6 | 0.000000399 | 0.000000097 | -0.000000109 |
| 78 | 6 | -0.000000215 | -0.000000085 | -0.000000049 |
| 79 | 6 | 0.000000026 | 0.000000087 | 0.000000275 |
| 80 | 6 | 0.000000274 | -0.000000031 | -0.000000072 |
| 81 | 6 | 0.000000003 | -0.000000002 | -0.000000020 |
| 82 | 6 | 0.000000022 | 0.000000010 | 0.000000041 |
| 83 | 1 | 0.000000039 | 0.000000030 | 0.000000062 |
| 84 | 1 | 0.000000042 | -0.000000024 | 0.000000030 |
| 85 | 1 | 0.000000002 | 0.000000032 | 0.000000038 |
| 86 | 1 | 0.000000001 | 0.000000015 | 0.000000022 |
| 87 | 1 | 0.000000027 | 0.000000012 | 0.000000020 |
| 88 | 1 | 0.000000014 | 0.000000014 | 0.000000004 |
| 89 | 8 | -0.000000026 | -0.000000110 | -0.000000153 |
| 90 | 8 | -0.000000023 | -0.000000100 | -0.000000062 |
| 91 | 6 | 0.000000017 | 0.000000025 | -0.000000035 |
| 92 | 6 | 0.000000019 | -0.000000039 | -0.000000021 |
| 93 | 6 | 0.000000026 | -0.000000097 | -0.000000059 |
| 94 | 6 | 0.000000025 | -0.000000047 | -0.000000117 |
| 95 | 6 | 0.000000014 | -0.000000041 | 0.000000037 |
| 96 | 6 | -0.000000006 | -0.000000068 | -0.000000010 |
| 97 | 6 | 0.000000065 | -0.000000050 | 0.000000011 |
| 98 | 6 | 0.000000079 | -0.000000079 | -0.000000033 |
| 99 | 1 | 0.000000013 | -0.000000068 | -0.000000058 |
| 100 | 1 | 0.000000023 | -0.000000057 | -0.000000016 |
| 101 | 1 | 0.000000065 | -0.000000075 | -0.000000024 |

| | | | | |
|---|---|---|---|---|
| 102 | 1 | 0.000000062 | -0.000000073 | -0.000000024 |
| 103 | 1 | 0.000000063 | -0.000000066 | -0.000000017 |
| 104 | 1 | 0.000000068 | -0.000000076 | -0.000000014 |
| 105 | 8 | 0.000000015 | -0.000000016 | -0.000000081 |
| 106 | 8 | 0.000000232 | -0.000000061 | 0.000000055 |
| 107 | 6 | 0.000000106 | -0.000000109 | -0.000000024 |
| 108 | 6 | 0.000000012 | -0.000000052 | 0.000000020 |
| 109 | 6 | 0.000000028 | -0.000000121 | 0.000000059 |
| 110 | 6 | 0.000000051 | 0.000000024 | 0.000000028 |
| 111 | 6 | 0.000000043 | 0.000000005 | 0.000000011 |
| 112 | 6 | 0.000000086 | -0.000000097 | 0.000000088 |
| 113 | 6 | 0.000000090 | -0.000000037 | 0.000000071 |
| 114 | 6 | 0.000000069 | -0.000000036 | 0.000000027 |
| 115 | 1 | 0.000000081 | -0.000000051 | -0.000000005 |
| 116 | 1 | 0.000000072 | -0.000000021 | 0.000000012 |
| 117 | 1 | 0.000000085 | -0.000000016 | 0.000000056 |
| 118 | 1 | 0.000000093 | -0.000000044 | 0.000000039 |
| 119 | 1 | 0.000000058 | -0.000000025 | 0.000000023 |
| 120 | 1 | 0.000000079 | -0.000000009 | 0.000000059 |
| 121 | 8 | 0.000000119 | 0.000000103 | 0.000000251 |
| 122 | 8 | -0.000000082 | 0.000000121 | -0.000000042 |
| 123 | 6 | 0.000000007 | -0.000000014 | -0.000000021 |
| 124 | 6 | -0.000000068 | 0.000000043 | 0.000000097 |
| 125 | 6 | -0.000000036 | 0.000000002 | -0.000000046 |
| 126 | 6 | 0.000000046 | -0.000000128 | -0.000000041 |
| 127 | 6 | -0.000000022 | -0.000000007 | -0.000000057 |
| 128 | 6 | -0.000000036 | -0.000000038 | -0.000000070 |
| 129 | 6 | -0.000000068 | -0.000000036 | -0.000000104 |
| 130 | 6 | -0.000000012 | -0.000000037 | -0.000000022 |
| 131 | 1 | -0.000000035 | 0.000000024 | -0.000000002 |
| 132 | 1 | 0.000000028 | 0.000000005 | -0.000000019 |
| 133 | 1 | -0.000000027 | -0.000000031 | -0.000000046 |
| 134 | 1 | 0.000000002 | -0.000000042 | -0.000000053 |
| 135 | 1 | 0.000000021 | -0.000000036 | -0.000000029 |
| 136 | 1 | -0.000000009 | -0.000000026 | -0.000000032 |
| 137 | 1 | 0.000000157 | -0.000000046 | 0.000000034 |
| 138 | 1 | 0.000000089 | -0.000000089 | -0.000000010 |
| 139 | 1 | 0.000000039 | -0.000000019 | 0.000000043 |
| 140 | 1 | -0.000000084 | 0.000000038 | 0.000000005 |
| 141 | 1 | 0.000000010 | -0.000000047 | -0.000000039 |
| 142 | 1 | 0.000000060 | 0.000000122 | 0.000000482 |
| 143 | 1 | -0.000000123 | 0.000000377 | 0.000000730 |
| 144 | 1 | -0.000000023 | -0.000000041 | -0.000000067 |
| 145 | 8 | 0.000000368 | -0.000000140 | 0.000000131 |
| 146 | 1 | 0.000000036 | -0.000000062 | 0.000000020 |
| 147 | 1 | -0.000000205 | 0.000000182 | -0.000000002 |
| 148 | 8 | 0.000000219 | 0.000000345 | -0.000000484 |
| 149 | 1 | 0.000000010 | -0.000000045 | -0.000000118 |
| 150 | 1 | -0.000000372 | -0.000000626 | 0.000000668 |
| 151 | 8 | -0.000000162 | -0.000000023 | 0.000000068 |
| 152 | 1 | -0.000000017 | 0.000000089 | 0.000000056 |
| 153 | 1 | -0.000000010 | 0.000000065 | 0.000000056 |
| 154 | 8 | 0.000000023 | 0.000000834 | -0.000000909 |
| 155 | 1 | -0.000000166 | -0.000000081 | 0.000000060 |
| 156 | 1 | -0.000000579 | -0.000001062 | 0.000001392 |
| 157 | 1 | 0.000000055 | 0.000000034 | -0.000000210 |
| 158 | 8 | -0.000000250 | -0.000000068 | 0.000000026 |
| 159 | 8 | -0.000000069 | 0.000000182 | 0.000000166 |
| 160 | 6 | 0.000000031 | 0.000000147 | -0.000000018 |
| 161 | 6 | -0.000000013 | -0.000000001 | 0.000000048 |
| 162 | 6 | 0.000000044 | -0.000000064 | 0.000000056 |
| 163 | 6 | -0.000000099 | 0.000000100 | 0.000000054 |
| 164 | 6 | 0.000000003 | 0.000000056 | 0.000000052 |
| 165 | 6 | -0.000000092 | 0.000000080 | 0.000000001 |
| 166 | 6 | -0.000000020 | 0.000000137 | 0.000000031 |
| 167 | 6 | -0.000000087 | 0.000000124 | 0.000000052 |
| 168 | 1 | -0.000000028 | 0.000000031 | 0.000000048 |
| 169 | 1 | -0.000000087 | 0.000000101 | 0.000000012 |
| 170 | 1 | -0.000000051 | 0.000000104 | 0.000000071 |
| 171 | 1 | -0.000000092 | 0.000000119 | 0.000000041 |
| 172 | 1 | -0.000000077 | 0.000000136 | 0.000000057 |
| 173 | 1 | -0.000000069 | 0.000000118 | 0.000000060 |
| 174 | 8 | -0.000000124 | 0.000000095 | 0.000000021 |

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|---|---|---|---|---|
| 175 | 8 | -0.000000116 | 0.000000035 | -0.000000010 |
| 176 | 6 | -0.000000120 | 0.000000165 | -0.000000054 |
| 177 | 6 | 0.000000007 | 0.000000061 | -0.000000026 |
| 178 | 6 | -0.000000133 | -0.000000000 | 0.000000078 |
| 179 | 6 | -0.000000122 | 0.000000149 | -0.000000079 |
| 180 | 6 | -0.000000003 | 0.000000069 | -0.000000053 |
| 181 | 6 | -0.000000162 | 0.000000053 | 0.000000095 |
| 182 | 6 | -0.000000156 | 0.000000061 | -0.000000036 |
| 183 | 6 | -0.000000116 | 0.000000088 | -0.000000033 |
| 184 | 1 | -0.000000086 | 0.000000062 | -0.000000020 |
| 185 | 1 | -0.000000113 | 0.000000089 | -0.000000006 |
| 186 | 1 | -0.000000119 | 0.000000064 | -0.000000048 |
| 187 | 1 | -0.000000146 | 0.000000101 | -0.000000028 |
| 188 | 1 | -0.000000123 | 0.000000110 | -0.000000008 |
| 189 | 1 | -0.000000135 | 0.000000090 | -0.000000035 |
| 190 | 8 | -0.000000197 | -0.000000083 | 0.000000005 |
| 191 | 8 | -0.000000310 | -0.000000146 | 0.000000097 |
| 192 | 6 | -0.000000081 | 0.000000028 | 0.000000183 |
| 193 | 6 | -0.000000033 | 0.000000247 | 0.000000014 |
| 194 | 6 | -0.000000029 | -0.000000032 | -0.000000066 |
| 195 | 6 | -0.000000175 | 0.000000073 | 0.000000166 |
| 196 | 6 | -0.000000034 | 0.000000279 | -0.000000009 |
| 197 | 6 | -0.000000002 | -0.000000038 | -0.000000003 |
| 198 | 6 | -0.000000112 | 0.000000093 | 0.000000025 |
| 199 | 6 | -0.000000122 | 0.000000121 | 0.000000028 |
| 200 | 1 | -0.000000042 | 0.000000100 | 0.000000082 |
| 201 | 1 | -0.000000080 | 0.000000105 | 0.000000044 |
| 202 | 1 | -0.000000094 | 0.000000104 | 0.000000032 |
| 203 | 1 | -0.000000110 | 0.000000128 | 0.000000041 |
| 204 | 1 | -0.000000113 | 0.000000136 | 0.000000029 |
| 205 | 1 | -0.000000106 | 0.000000127 | 0.000000016 |
| 206 | 8 | -0.000000019 | -0.000000043 | -0.000000040 |
| 207 | 8 | 0.000000187 | 0.000000531 | -0.000000716 |
| 208 | 6 | -0.000000046 | 0.000000070 | 0.000000062 |
| 209 | 6 | -0.000000030 | -0.000000048 | -0.000000083 |
| 210 | 6 | -0.000000184 | 0.000000078 | -0.000000204 |
| 211 | 6 | -0.000000099 | 0.000000067 | 0.000000111 |
| 212 | 6 | -0.000000104 | -0.000000014 | 0.000000023 |
| 213 | 6 | -0.000000199 | 0.000000183 | -0.000000149 |
| 214 | 6 | -0.000000053 | 0.000000104 | 0.000000064 |
| 215 | 6 | -0.000000095 | 0.000000081 | 0.000000001 |
| 216 | 1 | -0.000000065 | 0.000000018 | -0.000000053 |
| 217 | 1 | -0.000000106 | 0.000000087 | 0.000000020 |
| 218 | 1 | -0.000000089 | 0.000000041 | 0.000000009 |
| 219 | 1 | -0.000000098 | 0.000000098 | -0.000000016 |
| 220 | 1 | -0.000000097 | 0.000000089 | -0.000000011 |
| 221 | 1 | -0.000000096 | 0.000000094 | 0.000000019 |
| 222 | 1 | -0.000000069 | 0.000000060 | 0.000000019 |
| 223 | 1 | -0.000000080 | 0.000000064 | 0.000000020 |
| 224 | 1 | -0.000000102 | 0.000000058 | -0.000000045 |
| 225 | 1 | 0.000000282 | 0.000000457 | 0.000000133 |
| 226 | 1 | 0.000000316 | 0.000000418 | 0.000000017 |
| 227 | 1 | -0.000000125 | 0.000000055 | -0.000000053 |
| 228 | 1 | -0.000000106 | 0.000000014 | 0.000000117 |
| 229 | 1 | 0.000000032 | -0.000000066 | -0.000000030 |
| 230 | 1 | 0.000000080 | -0.000000026 | 0.000000034 |
| 231 | 1 | 0.000000114 | -0.000000099 | -0.000000010 |
| 232 | 8 | 0.000000046 | -0.000000014 | -0.000000003 |
| 233 | 8 | 0.000000104 | -0.000000057 | 0.000000059 |
| 234 | 6 | 0.000000028 | -0.000000059 | -0.000000009 |
| 235 | 6 | 0.000000025 | -0.000000077 | 0.000000040 |
| 236 | 6 | 0.000000091 | -0.000000027 | 0.000000015 |
| 237 | 6 | 0.000000037 | -0.000000039 | -0.000000019 |
| 238 | 6 | 0.000000113 | -0.000000101 | -0.000000022 |
| 239 | 6 | 0.000000082 | -0.000000060 | 0.000000000 |
| 240 | 6 | 0.000000090 | -0.000000088 | 0.000000029 |
| 241 | 6 | 0.000000122 | -0.000000071 | 0.000000026 |
| 242 | 1 | 0.000000050 | -0.000000033 | 0.000000022 |
| 243 | 1 | 0.000000105 | -0.000000080 | -0.000000015 |
| 244 | 1 | 0.000000106 | -0.000000056 | 0.000000043 |
| 245 | 1 | 0.000000120 | -0.000000088 | 0.000000009 |
| 246 | 1 | 0.000000128 | -0.000000085 | 0.000000038 |
| 247 | 1 | 0.000000127 | -0.000000085 | 0.000000031 |

| | | | | |
|---|---|---|---|---|
| 248 | 8 | 0.000000054 | 0.000000003 | -0.000000009 |
| 249 | 8 | 0.000000064 | -0.000000151 | -0.000000068 |
| 250 | 6 | 0.000000058 | -0.000000102 | 0.000000066 |
| 251 | 6 | 0.000000046 | -0.000000186 | -0.000000029 |
| 252 | 6 | 0.000000054 | -0.000000047 | -0.000000107 |
| 253 | 6 | 0.000000003 | -0.000000065 | 0.000000044 |
| 254 | 6 | 0.000000166 | -0.000000150 | -0.000000009 |
| 255 | 6 | 0.000000133 | -0.000000053 | -0.000000059 |
| 256 | 6 | 0.000000062 | -0.000000123 | -0.000000059 |
| 257 | 6 | 0.000000081 | -0.000000118 | -0.000000060 |
| 258 | 1 | 0.000000053 | -0.000000095 | -0.000000051 |
| 259 | 1 | 0.000000117 | -0.000000095 | -0.000000021 |
| 260 | 1 | 0.000000060 | -0.000000119 | -0.000000061 |
| 261 | 1 | 0.000000093 | -0.000000131 | -0.000000040 |
| 262 | 1 | 0.000000089 | -0.000000135 | -0.000000065 |
| 263 | 1 | 0.000000091 | -0.000000131 | -0.000000062 |
| 264 | 8 | 0.000000032 | -0.000000091 | -0.000000058 |
| 265 | 8 | 0.000000027 | -0.000000086 | -0.000000063 |
| 266 | 6 | 0.000000053 | -0.000000104 | -0.000000055 |
| 267 | 6 | 0.000000037 | -0.000000085 | -0.000000058 |
| 268 | 6 | 0.000000044 | -0.000000043 | -0.000000027 |
| 269 | 6 | 0.000000077 | -0.000000121 | -0.000000040 |
| 270 | 6 | 0.000000071 | -0.000000088 | -0.000000047 |
| 271 | 6 | 0.000000050 | -0.000000078 | -0.000000079 |
| 272 | 6 | 0.000000057 | -0.000000083 | -0.000000019 |
| 273 | 6 | 0.000000073 | -0.000000093 | -0.000000037 |
| 274 | 1 | 0.000000017 | -0.000000078 | -0.000000070 |
| 275 | 1 | 0.000000079 | -0.000000100 | -0.000000037 |
| 276 | 1 | 0.000000058 | -0.000000082 | -0.000000034 |
| 277 | 1 | 0.000000099 | -0.000000112 | -0.000000031 |
| 278 | 1 | 0.000000092 | -0.000000092 | -0.000000020 |
| 279 | 1 | 0.000000075 | -0.000000112 | -0.000000043 |
| 280 | 8 | 0.000000078 | -0.000000025 | 0.000000067 |
| 281 | 8 | 0.000000127 | -0.000000050 | 0.000000034 |
| 282 | 6 | 0.000000112 | -0.000000003 | -0.000000036 |
| 283 | 6 | 0.000000025 | -0.000000071 | 0.000000082 |
| 284 | 6 | 0.000000161 | -0.000000095 | 0.000000093 |
| 285 | 6 | 0.000000122 | -0.000000050 | -0.000000083 |
| 286 | 6 | 0.000000026 | -0.000000118 | 0.000000043 |
| 287 | 6 | 0.000000188 | -0.000000053 | 0.000000069 |
| 288 | 6 | 0.000000103 | -0.000000099 | 0.000000004 |
| 289 | 6 | 0.000000124 | -0.000000099 | 0.000000001 |
| 290 | 1 | 0.000000097 | -0.000000038 | 0.000000046 |
| 291 | 1 | 0.000000109 | -0.000000090 | 0.000000004 |
| 292 | 1 | 0.000000104 | -0.000000089 | 0.000000009 |
| 293 | 1 | 0.000000118 | -0.000000112 | 0.000000002 |
| 294 | 1 | 0.000000132 | -0.000000125 | -0.000000013 |
| 295 | 1 | 0.000000140 | -0.000000100 | 0.000000014 |
| 296 | 1 | 0.000000022 | -0.000000092 | -0.000000074 |
| 297 | 1 | 0.000000042 | -0.000000072 | -0.000000026 |
| 298 | 1 | 0.000000111 | -0.000000033 | 0.000000054 |
| 299 | 1 | 0.000000094 | -0.000000075 | 0.000000010 |
| 300 | 1 | 0.000000035 | -0.000000084 | -0.000000067 |
| 301 | 1 | 0.000000087 | -0.000000003 | 0.000000099 |
| 302 | 1 | 0.000000029 | 0.000000003 | 0.000000050 |
| 303 | 1 | -0.000000004 | 0.000000038 | 0.000000075 |
| 304 | 1 | -0.000000166 | 0.000000268 | 0.000000119 |
| 305 | 8 | 0.000000081 | -0.000000032 | 0.000000055 |
| 306 | 8 | 0.000000086 | 0.000000024 | 0.000000087 |
| 307 | 6 | 0.000000079 | -0.000000083 | 0.000000098 |
| 308 | 6 | 0.000000148 | 0.000000062 | 0.000000031 |
| 309 | 6 | -0.000000041 | 0.000000045 | 0.000000081 |
| 310 | 6 | 0.000000079 | -0.000000059 | 0.000000155 |
| 311 | 6 | 0.000000144 | 0.000000103 | 0.000000101 |
| 312 | 6 | 0.000000033 | 0.000000009 | 0.000000054 |
| 313 | 6 | 0.000000065 | 0.000000056 | 0.000000113 |
| 314 | 6 | 0.000000071 | 0.000000045 | 0.000000115 |
| 315 | 1 | 0.000000070 | -0.000000006 | 0.000000054 |
| 316 | 1 | 0.000000076 | 0.000000043 | 0.000000134 |
| 317 | 1 | 0.000000051 | 0.000000038 | 0.000000103 |
| 318 | 1 | 0.000000087 | 0.000000042 | 0.000000128 |
| 319 | 1 | 0.000000079 | 0.000000055 | 0.000000130 |
| 320 | 1 | 0.000000064 | 0.000000067 | 0.000000131 |

| | | | | |
|---|---|---|---|---|
| 321 | 8 | -0.000000111 | -0.000000017 | 0.000000062 |
| 322 | 8 | 0.000000073 | 0.000000050 | -0.000000235 |
| 323 | 6 | -0.000000053 | 0.000000103 | 0.000000077 |
| 324 | 6 | 0.000000020 | 0.000000157 | 0.000000077 |
| 325 | 6 | -0.000000011 | 0.000000064 | 0.000000096 |
| 326 | 6 | -0.000000010 | 0.000000042 | 0.000000170 |
| 327 | 6 | 0.000000080 | 0.000000114 | 0.000000140 |
| 328 | 6 | 0.000000049 | 0.000000028 | 0.000000161 |
| 329 | 6 | 0.000000085 | 0.000000077 | 0.000000152 |
| 330 | 6 | 0.000000063 | 0.000000053 | 0.000000121 |
| 331 | 1 | 0.000000001 | 0.000000060 | 0.000000072 |
| 332 | 1 | 0.000000067 | 0.000000057 | 0.000000142 |
| 333 | 1 | 0.000000047 | 0.000000057 | 0.000000112 |
| 334 | 1 | 0.000000058 | 0.000000079 | 0.000000137 |
| 335 | 1 | 0.000000071 | 0.000000050 | 0.000000129 |
| 336 | 1 | 0.000000077 | 0.000000054 | 0.000000145 |
| 337 | 8 | 0.000000079 | -0.000000044 | -0.000000085 |
| 338 | 8 | 0.000000121 | 0.000000046 | 0.000000270 |
| 339 | 6 | 0.000000022 | 0.000000010 | -0.000000059 |
| 340 | 6 | 0.000000141 | -0.000000053 | 0.000000052 |
| 341 | 6 | 0.000000047 | -0.000000040 | 0.000000078 |
| 342 | 6 | 0.000000041 | 0.000000003 | 0.000000062 |
| 343 | 6 | 0.000000103 | 0.000000100 | 0.000000106 |
| 344 | 6 | 0.000000058 | 0.000000146 | 0.000000132 |
| 345 | 6 | 0.000000072 | 0.000000036 | 0.000000099 |
| 346 | 6 | 0.000000100 | 0.000000005 | 0.000000119 |
| 347 | 1 | 0.000000089 | -0.000000029 | 0.000000067 |
| 348 | 1 | 0.000000078 | 0.000000072 | 0.000000125 |
| 349 | 1 | 0.000000105 | 0.000000002 | 0.000000096 |
| 350 | 1 | 0.000000121 | 0.000000012 | 0.000000123 |
| 351 | 1 | 0.000000118 | 0.000000011 | 0.000000125 |
| 352 | 1 | 0.000000096 | 0.000000033 | 0.000000129 |
| 353 | 8 | 0.000000073 | 0.000000079 | 0.000000039 |
| 354 | 8 | -0.000000043 | 0.000000083 | 0.000000059 |
| 355 | 6 | 0.000000023 | -0.000000134 | -0.000000023 |
| 356 | 6 | 0.000000012 | 0.000000077 | 0.000000269 |
| 357 | 6 | 0.000000026 | 0.000000283 | 0.000000040 |
| 358 | 6 | 0.000000054 | -0.000000115 | -0.000000037 |
| 359 | 6 | 0.000000045 | 0.000000028 | 0.000000339 |
| 360 | 6 | 0.000000012 | 0.000000283 | -0.000000014 |
| 361 | 6 | 0.000000030 | 0.000000098 | 0.000000141 |
| 362 | 6 | 0.000000026 | 0.000000089 | 0.000000123 |
| 363 | 1 | -0.000000011 | 0.000000060 | 0.000000076 |
| 364 | 1 | 0.000000061 | 0.000000059 | 0.000000119 |
| 365 | 1 | 0.000000005 | 0.000000092 | 0.000000105 |
| 366 | 1 | 0.000000027 | 0.000000109 | 0.000000135 |
| 367 | 1 | 0.000000026 | 0.000000098 | 0.000000132 |
| 368 | 1 | 0.000000042 | 0.000000084 | 0.000000141 |
| 369 | 1 | -0.000000010 | 0.000000065 | 0.000000198 |
| 370 | 1 | 0.000000097 | -0.000000146 | -0.000000144 |
| 371 | 1 | 0.000000034 | 0.000000009 | 0.000000093 |
| 372 | 1 | -0.000000041 | 0.000000114 | 0.000000067 |
| 373 | 1 | -0.000000105 | -0.000000001 | -0.000000072 |
| 374 | 1 | -0.000000091 | 0.000000042 | -0.000000083 |
| 375 | 1 | 0.000000001 | -0.000000068 | -0.000000059 |
| 376 | 1 | -0.000000070 | -0.000000002 | -0.000000090 |
| 377 | 8 | -0.000000104 | -0.000000001 | -0.000000092 |
| 378 | 8 | -0.000000097 | -0.000000003 | -0.000000098 |
| 379 | 6 | -0.000000118 | 0.000000029 | -0.000000095 |
| 380 | 6 | -0.000000091 | 0.000000021 | -0.000000091 |
| 381 | 6 | -0.000000077 | -0.000000007 | -0.000000084 |
| 382 | 6 | -0.000000110 | -0.000000025 | -0.000000102 |
| 383 | 6 | -0.000000086 | 0.000000002 | -0.000000129 |
| 384 | 6 | -0.000000078 | -0.000000038 | -0.000000070 |
| 385 | 6 | -0.000000082 | -0.000000017 | -0.000000130 |
| 386 | 6 | -0.000000101 | -0.000000040 | -0.000000122 |
| 387 | 1 | -0.000000087 | 0.000000023 | -0.000000063 |
| 388 | 1 | -0.000000088 | -0.000000037 | -0.000000118 |
| 389 | 1 | -0.000000094 | -0.000000016 | -0.000000110 |
| 390 | 1 | -0.000000101 | -0.000000040 | -0.000000137 |
| 391 | 1 | -0.000000104 | -0.000000017 | -0.000000135 |
| 392 | 1 | -0.000000095 | -0.000000036 | -0.000000123 |
| 393 | 8 | -0.000000046 | -0.000000090 | -0.000000079 |

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|---|---|---|---|---|
| 394 | 8 | 0.000000032 | -0.000000060 | -0.000000078 |
| 395 | 6 | -0.000000028 | -0.000000252 | -0.000000155 |
| 396 | 6 | 0.000000009 | 0.000000001 | -0.000000220 |
| 397 | 6 | -0.000000113 | -0.000000020 | 0.000000050 |
| 398 | 6 | 0.000000006 | -0.000000262 | -0.000000110 |
| 399 | 6 | 0.000000088 | 0.000000019 | -0.000000188 |
| 400 | 6 | -0.000000092 | -0.000000002 | 0.000000019 |
| 401 | 6 | -0.000000016 | -0.000000075 | -0.000000138 |
| 402 | 6 | -0.000000038 | -0.000000076 | -0.000000130 |
| 403 | 1 | 0.000000003 | -0.000000078 | -0.000000080 |
| 404 | 1 | -0.000000027 | -0.000000070 | -0.000000105 |
| 405 | 1 | -0.000000020 | -0.000000076 | -0.000000116 |
| 406 | 1 | -0.000000047 | -0.000000100 | -0.000000127 |
| 407 | 1 | -0.000000056 | -0.000000078 | -0.000000142 |
| 408 | 1 | -0.000000045 | -0.000000077 | -0.000000126 |
| 409 | 8 | -0.000000105 | -0.000000041 | -0.000000061 |
| 410 | 8 | -0.000000011 | -0.000000080 | -0.000000031 |
| 411 | 6 | -0.000000093 | -0.000000024 | 0.000000004 |
| 412 | 6 | -0.000000078 | -0.000000142 | -0.000000145 |
| 413 | 6 | 0.000000060 | 0.000000012 | -0.000000111 |
| 414 | 6 | -0.000000106 | 0.000000004 | -0.000000032 |
| 415 | 6 | -0.000000116 | -0.000000071 | -0.000000219 |
| 416 | 6 | 0.000000046 | -0.000000030 | -0.000000094 |
| 417 | 6 | -0.000000048 | -0.000000075 | -0.000000120 |
| 418 | 6 | -0.000000052 | -0.000000086 | -0.000000144 |
| 419 | 1 | -0.000000041 | -0.000000048 | -0.000000072 |
| 420 | 1 | -0.000000071 | -0.000000029 | -0.000000128 |
| 421 | 1 | -0.000000029 | -0.000000090 | -0.000000113 |
| 422 | 1 | -0.000000038 | -0.000000090 | -0.000000138 |
| 423 | 1 | -0.000000045 | -0.000000084 | -0.000000130 |
| 424 | 1 | -0.000000052 | -0.000000087 | -0.000000134 |
| 425 | 8 | 0.000000005 | -0.000000028 | -0.000000073 |
| 426 | 8 | -0.000000516 | -0.000000055 | -0.000000022 |
| 427 | 6 | -0.000000066 | 0.000000025 | -0.000000164 |
| 428 | 6 | 0.000000021 | 0.000000052 | -0.000000015 |
| 429 | 6 | -0.000000095 | -0.000000200 | -0.000000097 |
| 430 | 6 | -0.000000105 | 0.000000045 | -0.000000196 |
| 431 | 6 | -0.000000035 | 0.000000004 | -0.000000008 |
| 432 | 6 | -0.000000058 | -0.000000177 | -0.000000085 |
| 433 | 6 | -0.000000099 | -0.000000005 | -0.000000103 |
| 434 | 6 | -0.000000107 | -0.000000031 | -0.000000112 |
| 435 | 1 | -0.000000046 | -0.000000021 | -0.000000073 |
| 436 | 1 | -0.000000076 | -0.000000053 | -0.000000110 |
| 437 | 1 | -0.000000102 | -0.000000009 | -0.000000095 |
| 438 | 1 | -0.000000094 | -0.000000031 | -0.000000132 |
| 439 | 1 | -0.000000112 | -0.000000022 | -0.000000125 |
| 440 | 1 | -0.000000102 | -0.000000034 | -0.000000133 |
| 441 | 1 | -0.000000003 | -0.000000111 | -0.000000133 |
| 442 | 1 | -0.000000018 | -0.000000079 | -0.000000063 |
| 443 | 1 | 0.000000727 | 0.000000007 | -0.000000293 |
| 444 | 1 | 0.000000007 | -0.000000064 | -0.000000099 |
| 445 | 8 | 0.000000131 | -0.000000258 | -0.000000224 |
| 446 | 1 | 0.000000005 | 0.000000050 | 0.000000071 |
| 447 | 1 | -0.000000104 | 0.000000075 | 0.000000119 |
| 448 | 8 | -0.000000097 | 0.000000010 | -0.000000078 |
| 449 | 1 | -0.000000106 | 0.000000058 | -0.000000046 |
| 450 | 1 | -0.000000079 | 0.000000035 | -0.000000044 |
| 451 | 8 | 0.000000093 | 0.000000034 | 0.000000065 |
| 452 | 1 | 0.000000039 | -0.000000029 | 0.000000038 |
| 453 | 1 | 0.000000070 | -0.000000015 | 0.000000048 |
| 454 | 8 | -0.000000086 | 0.000000072 | -0.000000084 |
| 455 | 1 | 0.000000074 | -0.000000102 | -0.000000086 |
| 456 | 1 | 0.000000034 | -0.000000334 | -0.000000117 |
| 457 | 6 | 0.000000042 | -0.000000487 | -0.000000119 |
| 458 | 6 | -0.000000235 | 0.000000117 | -0.000000062 |
| 459 | 6 | 0.000000011 | 0.000000359 | -0.000000004 |
| 460 | 7 | 0.000000059 | -0.000000228 | 0.000000238 |
| 461 | 6 | 0.000000051 | -0.000000180 | -0.000000057 |
| 462 | 6 | 0.000000107 | -0.000000121 | -0.000000304 |
| 463 | 6 | 0.000000236 | -0.000000222 | 0.000000470 |
| 464 | 6 | -0.000000103 | 0.000000160 | -0.000000038 |
| 465 | 6 | 0.000000058 | -0.000000057 | 0.000000027 |
| 466 | 8 | 0.000000020 | 0.000000105 | -0.000000205 |

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|---|---|---|---|---|
| 467 | 8 | -0.000000123 | -0.000000000 | 0.000000197 |
| 468 | 1 | -0.000000281 | 0.000000384 | -0.000000050 |
| 469 | 1 | -0.000000036 | -0.000000060 | -0.000000016 |
| 470 | 1 | -0.000000100 | -0.000000142 | -0.000000207 |
| 471 | 1 | 0.000000003 | -0.000000165 | -0.000000020 |
| 472 | 1 | 0.000000042 | 0.000000172 | 0.000000079 |
| 473 | 1 | 0.000000151 | -0.000000011 | 0.000000089 |
| 474 | 1 | 0.000000190 | 0.000000230 | 0.000000027 |
| 475 | 6 | 0.000000429 | -0.000000201 | -0.000000016 |
| 476 | 6 | -0.000000522 | 0.000000213 | 0.000000321 |
| 477 | 7 | -0.000000063 | -0.000000007 | -0.000000140 |
| 478 | 6 | 0.000000279 | -0.000000598 | -0.000000154 |
| 479 | 6 | -0.000000032 | 0.000000309 | 0.000000192 |
| 480 | 6 | 0.000000179 | -0.000000188 | -0.000000229 |
| 481 | 1 | -0.000000070 | 0.000000179 | 0.000000036 |
| 482 | 1 | 0.000000297 | 0.000000279 | -0.000000153 |
| 483 | 1 | -0.000000014 | 0.000000176 | 0.000000219 |
| 484 | 1 | -0.000000051 | -0.000000071 | -0.000000004 |
| 485 | 1 | 0.000000283 | -0.000000219 | 0.000000206 |
| 486 | 1 | 0.000000091 | 0.000000100 | 0.000000107 |
| 487 | 1 | 0.000000072 | 0.000000101 | 0.000000152 |

Sum of electronic and thermal Free Energies = -1069.253660
ONIOM Total Energy = -1072.546647
1 imaginary frequency = -392.77

**$\beta$-I1@$C_R$**

| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | 0.000080891 | -0.000006691 | 0.000005929 |
| 2 | 8 | 0.000075344 | 0.000074860 | -0.000045888 |
| 3 | 6 | 0.000015147 | 0.000008008 | -0.000040722 |
| 4 | 6 | -0.000032948 | 0.000010699 | -0.000029024 |
| 5 | 6 | 0.000077202 | -0.000004639 | 0.000109601 |
| 6 | 6 | -0.000008685 | -0.000001949 | 0.000031909 |
| 7 | 6 | 0.000006549 | -0.000012597 | 0.000016639 |
| 8 | 6 | -0.000018427 | 0.000000906 | -0.000019427 |
| 9 | 6 | -0.000044771 | 0.000029402 | -0.000015912 |
| 10 | 6 | 0.000010814 | -0.000003851 | -0.000000377 |
| 11 | 1 | -0.000018224 | -0.000006634 | 0.000001396 |
| 12 | 1 | 0.000000683 | 0.000013235 | -0.000004898 |
| 13 | 1 | -0.000024979 | 0.000015838 | -0.000008406 |
| 14 | 1 | 0.000005195 | -0.000004291 | -0.000001215 |
| 15 | 1 | 0.000000075 | -0.000003083 | 0.000000144 |
| 16 | 1 | 0.000006616 | -0.000002997 | -0.000001095 |
| 17 | 8 | -0.000006317 | 0.000015750 | 0.000001373 |
| 18 | 8 | 0.000203562 | -0.000955554 | 0.000183415 |
| 19 | 6 | -0.000031040 | -0.000056920 | -0.000086906 |
| 20 | 6 | 0.000009454 | 0.000015631 | 0.000071460 |
| 21 | 6 | -0.000248398 | 0.000046290 | -0.000299854 |
| 22 | 6 | 0.000027086 | -0.000026524 | 0.000040352 |
| 23 | 6 | -0.000008627 | -0.000001593 | -0.000063620 |
| 24 | 6 | 0.000021894 | 0.000035184 | 0.000024768 |
| 25 | 6 | 0.000027909 | 0.000020436 | 0.000035767 |
| 26 | 6 | -0.000017492 | -0.000022822 | -0.000007782 |
| 27 | 1 | -0.000006219 | -0.000008074 | -0.000027476 |
| 28 | 1 | 0.000000888 | -0.000007175 | 0.000005763 |
| 29 | 1 | 0.000014669 | 0.000041513 | 0.000010776 |
| 30 | 1 | -0.000001495 | -0.000004837 | -0.000005516 |
| 31 | 1 | 0.000000179 | -0.000003438 | 0.000003540 |
| 32 | 1 | 0.000004673 | -0.000002949 | -0.000001449 |
| 33 | 8 | -0.000079291 | -0.000105865 | 0.000012856 |
| 34 | 8 | -0.000362615 | -0.000261923 | -0.000516152 |
| 35 | 6 | 0.000023141 | -0.000007528 | -0.000024213 |
| 36 | 6 | -0.000058551 | 0.000107930 | 0.000035002 |
| 37 | 6 | -0.000038654 | -0.000159834 | 0.000106530 |
| 38 | 6 | -0.000042374 | 0.000031819 | 0.000004292 |
| 39 | 6 | -0.000013427 | -0.000008148 | -0.000009909 |
| 40 | 6 | 0.000001960 | -0.000010753 | 0.000012728 |
| 41 | 6 | 0.000035408 | -0.000027077 | -0.000028448 |

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|---|---|---|---|---|
| 42 | 6 | -0.000025283 | 0.000005837 | 0.000017887 |
| 43 | 1 | 0.000076909 | -0.000125128 | -0.000088797 |
| 44 | 1 | 0.000007760 | -0.000006232 | 0.000002819 |
| 45 | 1 | 0.000031041 | -0.000003987 | -0.000003075 |
| 46 | 1 | 0.000001066 | 0.000000155 | 0.000000707 |
| 47 | 1 | 0.000003896 | 0.000002570 | -0.000000740 |
| 48 | 1 | 0.000003194 | 0.000003792 | 0.000002339 |
| 49 | 8 | -0.000120723 | -0.000065044 | 0.000094671 |
| 50 | 8 | -0.000080866 | 0.000062111 | -0.000053656 |
| 51 | 6 | -0.000023476 | 0.000004960 | 0.000021447 |
| 52 | 6 | 0.000031189 | 0.000009463 | 0.000056707 |
| 53 | 6 | 0.000011484 | 0.000063969 | -0.000042361 |
| 54 | 6 | 0.000009719 | -0.000028027 | -0.000008101 |
| 55 | 6 | 0.000029494 | 0.000007370 | 0.000036444 |
| 56 | 6 | -0.000019130 | -0.000056717 | -0.000049001 |
| 57 | 6 | 0.000030743 | 0.000010050 | 0.000031854 |
| 58 | 6 | 0.000002319 | 0.000007099 | -0.000005241 |
| 59 | 1 | 0.000002947 | -0.000014745 | -0.000023135 |
| 60 | 1 | -0.000002839 | -0.000002072 | -0.000004988 |
| 61 | 1 | -0.000019372 | -0.000011915 | 0.000004732 |
| 62 | 1 | -0.000001684 | -0.000000525 | 0.000000286 |
| 63 | 1 | 0.000001832 | -0.000000823 | -0.000002714 |
| 64 | 1 | 0.000001410 | -0.000000158 | -0.000004726 |
| 65 | 1 | 0.000133581 | 0.000025053 | -0.000026989 |
| 66 | 1 | 0.000014053 | -0.000082777 | -0.000039020 |
| 67 | 1 | 0.000051485 | -0.000036242 | -0.000055206 |
| 68 | 1 | 0.000031451 | 0.000120227 | 0.000018893 |
| 69 | 1 | 0.000071661 | 0.000259732 | 0.000152436 |
| 70 | 1 | 0.000004557 | 0.000038391 | -0.000038261 |
| 71 | 1 | 0.000150468 | 0.000011615 | -0.000024922 |
| 72 | 1 | -0.000010933 | -0.000030737 | 0.000012643 |
| 73 | 8 | 0.000381757 | 0.000061692 | -0.000243014 |
| 74 | 8 | 0.000130328 | -0.000058685 | -0.000180465 |
| 75 | 6 | 0.000318953 | -0.000284119 | 0.000399898 |
| 76 | 6 | -0.000098932 | 0.000024441 | -0.000155133 |
| 77 | 6 | 0.000225789 | 0.000012210 | -0.000119773 |
| 78 | 6 | -0.000092216 | 0.000100438 | -0.000021517 |
| 79 | 6 | -0.000154255 | -0.000087701 | 0.000198826 |
| 80 | 6 | -0.000136591 | 0.000073634 | -0.000139570 |
| 81 | 6 | -0.000012950 | -0.000029595 | -0.000045239 |
| 82 | 6 | 0.000005152 | 0.000041640 | 0.000017427 |
| 83 | 1 | -0.000055523 | 0.000028093 | 0.000042574 |
| 84 | 1 | 0.000012492 | -0.000011289 | -0.000024637 |
| 85 | 1 | 0.000040392 | -0.000013372 | 0.000017750 |
| 86 | 1 | -0.000000055 | -0.000002723 | -0.000004770 |
| 87 | 1 | -0.000005516 | -0.000008317 | -0.000001207 |
| 88 | 1 | -0.000001823 | -0.000008690 | -0.000000139 |
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| 392 | 1 | 0.000004116 | -0.000001027 | -0.000006195 |
| 393 | 8 | 0.000199920 | -0.000073576 | -0.000155921 |
| 394 | 8 | -0.000008124 | 0.000195453 | -0.000022910 |
| 395 | 6 | -0.000091400 | 0.000177372 | 0.000129001 |
| 396 | 6 | 0.000030596 | -0.000128594 | -0.000031003 |
| 397 | 6 | -0.000069584 | -0.000109645 | 0.000210705 |
| 398 | 6 | 0.000108959 | -0.000117579 | -0.000030618 |
| 399 | 6 | -0.000042083 | -0.000000801 | -0.000052685 |
| 400 | 6 | -0.000065339 | 0.000024812 | -0.000066103 |
| 401 | 6 | -0.000076943 | -0.000019767 | -0.000136335 |
| 402 | 6 | -0.000017730 | 0.000039194 | 0.000051831 |
| 403 | 1 | 0.000046438 | 0.000060377 | -0.000032608 |
| 404 | 1 | 0.000013334 | 0.000005118 | 0.000016876 |
| 405 | 1 | -0.000020513 | 0.000071283 | -0.000065910 |
| 406 | 1 | 0.000000997 | -0.000004873 | 0.000000555 |

| | | | | |
|---|---|---|---|---|
| 407 | 1 | 0.000002210 | 0.000009365 | 0.000010061 |
| 408 | 1 | 0.000008564 | -0.000005742 | 0.000000140 |
| 409 | 8 | -0.000130417 | 0.000051143 | 0.000206872 |
| 410 | 8 | 0.000015347 | -0.000152493 | 0.000006528 |
| 411 | 6 | -0.000060042 | -0.000033822 | -0.000038569 |
| 412 | 6 | 0.000032774 | 0.000029174 | -0.000010905 |
| 413 | 6 | -0.000034863 | 0.000092328 | -0.000031772 |
| 414 | 6 | 0.000038127 | 0.000042398 | -0.000003388 |
| 415 | 6 | 0.000009214 | 0.000037865 | -0.000019807 |
| 416 | 6 | 0.000015284 | -0.000012988 | 0.000002716 |
| 417 | 6 | -0.000005174 | -0.000049946 | 0.000036218 |
| 418 | 6 | 0.000032323 | 0.000000115 | -0.000007978 |
| 419 | 1 | -0.000035233 | -0.000009954 | -0.000009810 |
| 420 | 1 | -0.000001311 | -0.000022724 | -0.000005611 |
| 421 | 1 | -0.000001237 | -0.000007392 | 0.000021187 |
| 422 | 1 | 0.000001632 | -0.000000117 | -0.000002964 |
| 423 | 1 | -0.000002303 | -0.000002005 | 0.000002210 |
| 424 | 1 | 0.000004685 | -0.000001939 | 0.000005845 |
| 425 | 8 | 0.000045891 | 0.000189391 | -0.000154458 |
| 426 | 8 | 0.000084139 | -0.000013548 | 0.000122398 |
| 427 | 6 | -0.000106972 | 0.000048123 | 0.000095931 |
| 428 | 6 | 0.000052187 | 0.000058894 | 0.000013976 |
| 429 | 6 | -0.000142029 | -0.000092411 | -0.000134316 |
| 430 | 6 | 0.000011595 | 0.000045246 | 0.000001341 |
| 431 | 6 | 0.000058359 | -0.000036978 | -0.000062677 |
| 432 | 6 | -0.000046960 | -0.000128341 | 0.000104637 |
| 433 | 6 | 0.000012989 | -0.000029472 | 0.000015672 |
| 434 | 6 | -0.000024743 | 0.000043604 | -0.000015821 |
| 435 | 1 | 0.000006024 | 0.000024878 | -0.000000010 |
| 436 | 1 | -0.000008229 | 0.000022659 | 0.000005004 |
| 437 | 1 | 0.000018857 | -0.000048726 | -0.000008231 |
| 438 | 1 | -0.000005707 | 0.000006299 | -0.000001284 |
| 439 | 1 | -0.000000528 | -0.000001075 | 0.000006709 |
| 440 | 1 | 0.000002494 | 0.000003218 | 0.000001257 |
| 441 | 1 | 0.000016241 | 0.000012773 | 0.000073208 |
| 442 | 1 | 0.000058934 | -0.000077842 | -0.000019639 |
| 443 | 1 | 0.000026186 | 0.000041230 | 0.000084860 |
| 444 | 1 | 0.000006069 | 0.000014725 | 0.000003373 |
| 445 | 8 | -0.001426917 | -0.001006793 | 0.000605311 |
| 446 | 1 | 0.001863992 | 0.001198278 | 0.000075628 |
| 447 | 1 | -0.000155625 | -0.000073582 | -0.000185363 |
| 448 | 8 | -0.000085187 | 0.000056916 | 0.000074161 |
| 449 | 1 | 0.000047190 | -0.000025827 | 0.000028673 |
| 450 | 1 | 0.000049248 | 0.000044910 | 0.000000442 |
| 451 | 8 | -0.000749656 | 0.000344681 | 0.000592502 |
| 452 | 1 | 0.000277277 | -0.000010034 | -0.000413610 |
| 453 | 1 | 0.000123595 | 0.000415912 | -0.000712571 |
| 454 | 8 | 0.000286804 | 0.000325755 | 0.000393161 |
| 455 | 1 | -0.000341710 | -0.000123200 | 0.000208006 |
| 456 | 1 | -0.000399428 | -0.000360014 | 0.000370135 |
| 457 | 6 | -0.000053648 | 0.002790761 | 0.000716863 |
| 458 | 6 | 0.000231292 | -0.000252353 | -0.000085253 |
| 459 | 6 | -0.001288969 | -0.000839072 | -0.001707703 |
| 460 | 7 | 0.001161628 | 0.002847123 | 0.001186270 |
| 461 | 6 | -0.000123852 | 0.000335700 | -0.000523240 |
| 462 | 6 | 0.000096342 | -0.000092281 | 0.000557481 |
| 463 | 6 | 0.000203719 | 0.000074638 | -0.000181784 |
| 464 | 6 | -0.000086187 | -0.000359021 | 0.000147723 |
| 465 | 6 | -0.000238121 | -0.000210732 | -0.000035368 |
| 466 | 8 | -0.000685405 | -0.000974539 | -0.000418573 |
| 467 | 8 | -0.000209604 | -0.001032984 | 0.000597504 |
| 468 | 1 | -0.000165043 | -0.001675599 | 0.000654021 |
| 469 | 1 | 0.000331739 | -0.000352212 | 0.000020109 |
| 470 | 1 | 0.000063754 | -0.000216232 | 0.000219839 |
| 471 | 1 | 0.000041976 | 0.000078623 | -0.000052638 |
| 472 | 1 | 0.000361995 | 0.000777119 | -0.000421535 |
| 473 | 1 | -0.000043472 | -0.000068283 | -0.000175997 |
| 474 | 1 | 0.000170347 | 0.000271038 | -0.000093848 |
| 475 | 6 | 0.002160688 | -0.005596877 | -0.000412287 |
| 476 | 6 | 0.000342582 | 0.000669015 | -0.001123353 |
| 477 | 7 | -0.000049092 | -0.000973420 | 0.000792734 |
| 478 | 6 | 0.000169378 | 0.000526879 | -0.000424783 |
| 479 | 6 | -0.002051684 | 0.000826428 | 0.000182118 |

| | | | | |
|---|---|---|---|---|
| 480 | 6 | -0.000303097 | 0.000481273 | -0.000129991 |
| 481 | 1 | -0.000489929 | 0.003105800 | -0.000175574 |
| 482 | 1 | -0.000162537 | 0.000740142 | 0.000063642 |
| 483 | 1 | 0.000045470 | -0.000268335 | 0.000226874 |
| 484 | 1 | 0.000416340 | -0.000313708 | 0.000287720 |
| 485 | 1 | -0.000312000 | -0.000302826 | -0.000129428 |
| 486 | 1 | -0.000004642 | -0.000302152 | -0.000013676 |
| 487 | 1 | 0.000174501 | -0.000019655 | -0.000058218 |

Sum of electronic and thermal Free Energies = -1069.254658
ONIOM Total Energy = -1072.550771
0 imaginary frequency

**$\beta$-TS2@$C_R$**

| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | 0.000000052 | 0.000000087 | 0.000000143 |
| 2 | 8 | -0.000000033 | 0.000000076 | 0.000000066 |
| 3 | 6 | -0.000000009 | 0.000000085 | 0.000000116 |
| 4 | 6 | -0.000000059 | 0.000000048 | 0.000000101 |
| 5 | 6 | -0.000000005 | 0.000000097 | 0.000000107 |
| 6 | 6 | 0.000000020 | 0.000000084 | 0.000000144 |
| 7 | 6 | 0.000000013 | 0.000000055 | 0.000000108 |
| 8 | 6 | 0.000000015 | 0.000000082 | 0.000000089 |
| 9 | 6 | -0.000000057 | 0.000000061 | 0.000000094 |
| 10 | 6 | -0.000000044 | 0.000000110 | 0.000000124 |
| 11 | 1 | -0.000000004 | 0.000000087 | 0.000000101 |
| 12 | 1 | 0.000000011 | 0.000000083 | 0.000000111 |
| 13 | 1 | -0.000000052 | 0.000000086 | 0.000000104 |
| 14 | 1 | -0.000000048 | 0.000000102 | 0.000000125 |
| 15 | 1 | -0.000000043 | 0.000000102 | 0.000000122 |
| 16 | 1 | -0.000000056 | 0.000000095 | 0.000000127 |
| 17 | 8 | -0.000000045 | 0.000000020 | 0.000000000 |
| 18 | 8 | 0.000000018 | 0.000000023 | 0.000000056 |
| 19 | 6 | -0.000000088 | 0.000000036 | 0.000000052 |
| 20 | 6 | -0.000000074 | 0.000000017 | 0.000000062 |
| 21 | 6 | 0.000000022 | -0.000000002 | 0.000000045 |
| 22 | 6 | -0.000000024 | 0.000000050 | 0.000000016 |
| 23 | 6 | -0.000000028 | 0.000000086 | 0.000000089 |
| 24 | 6 | 0.000000013 | 0.000000061 | 0.000000066 |
| 25 | 6 | -0.000000011 | 0.000000054 | 0.000000102 |
| 26 | 6 | 0.000000025 | 0.000000056 | 0.000000079 |
| 27 | 1 | -0.000000026 | 0.000000005 | 0.000000030 |
| 28 | 1 | -0.000000006 | 0.000000087 | 0.000000072 |
| 29 | 1 | 0.000000024 | 0.000000039 | 0.000000070 |
| 30 | 1 | 0.000000006 | 0.000000059 | 0.000000095 |
| 31 | 1 | 0.000000027 | 0.000000069 | 0.000000086 |
| 32 | 1 | 0.000000009 | 0.000000062 | 0.000000093 |
| 33 | 8 | -0.000000048 | 0.000000084 | 0.000000104 |
| 34 | 8 | -0.000000080 | 0.000000032 | 0.000000069 |
| 35 | 6 | 0.000000072 | 0.000000066 | 0.000000036 |
| 36 | 6 | -0.000000105 | 0.000000202 | 0.000000125 |
| 37 | 6 | -0.000000119 | -0.000000010 | 0.000000147 |
| 38 | 6 | 0.000000044 | 0.000000043 | 0.000000006 |
| 39 | 6 | -0.000000145 | 0.000000137 | 0.000000006 |
| 40 | 6 | -0.000000105 | -0.000000015 | 0.000000173 |
| 41 | 6 | -0.000000080 | 0.000000047 | 0.000000048 |
| 42 | 6 | -0.000000050 | 0.000000073 | 0.000000087 |
| 43 | 1 | -0.000000067 | 0.000000060 | 0.000000056 |
| 44 | 1 | -0.000000061 | 0.000000058 | 0.000000066 |
| 45 | 1 | -0.000000072 | 0.000000057 | 0.000000059 |
| 46 | 1 | -0.000000051 | 0.000000074 | 0.000000095 |
| 47 | 1 | -0.000000068 | 0.000000070 | 0.000000076 |
| 48 | 1 | -0.000000076 | 0.000000087 | 0.000000089 |
| 49 | 8 | 0.000000061 | 0.000000019 | 0.000000039 |
| 50 | 8 | 0.000000054 | 0.000000098 | 0.000000064 |
| 51 | 6 | 0.000000018 | -0.000000064 | 0.000000052 |
| 52 | 6 | -0.000000003 | 0.000000082 | -0.000000030 |
| 53 | 6 | 0.000000127 | 0.000000055 | 0.000000104 |
| 54 | 6 | 0.000000011 | -0.000000031 | 0.000000077 |

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|---|---|---|---|---|
| 55 | 6 | -0.000000049 | 0.000000119 | 0.000000112 |
| 56 | 6 | 0.000000081 | 0.000000096 | 0.000000114 |
| 57 | 6 | 0.000000017 | 0.000000070 | 0.000000136 |
| 58 | 6 | 0.000000029 | 0.000000092 | 0.000000121 |
| 59 | 1 | 0.000000062 | 0.000000036 | 0.000000057 |
| 60 | 1 | 0.000000009 | 0.000000078 | 0.000000130 |
| 61 | 1 | 0.000000042 | 0.000000076 | 0.000000121 |
| 62 | 1 | 0.000000028 | 0.000000097 | 0.000000143 |
| 63 | 1 | 0.000000045 | 0.000000079 | 0.000000129 |
| 64 | 1 | 0.000000013 | 0.000000088 | 0.000000120 |
| 65 | 1 | 0.000000025 | 0.000000040 | 0.000000055 |
| 66 | 1 | 0.000000020 | 0.000000072 | 0.000000101 |
| 67 | 1 | -0.000000032 | 0.000000069 | 0.000000108 |
| 68 | 1 | -0.000000075 | 0.000000025 | 0.000000027 |
| 69 | 1 | 0.000000004 | 0.000000015 | 0.000000026 |
| 70 | 1 | -0.000000055 | 0.000000072 | 0.000000077 |
| 71 | 1 | -0.000000070 | 0.000000057 | 0.000000033 |
| 72 | 1 | 0.000000056 | 0.000000053 | 0.000000105 |
| 73 | 8 | -0.000000151 | 0.000000175 | -0.000000439 |
| 74 | 8 | -0.000001804 | -0.000000893 | -0.000000260 |
| 75 | 6 | 0.000000246 | -0.000000118 | 0.000000221 |
| 76 | 6 | -0.000000922 | -0.000000014 | -0.000000235 |
| 77 | 6 | -0.000000841 | 0.000000789 | 0.000000878 |
| 78 | 6 | -0.000000080 | -0.000000116 | -0.000000097 |
| 79 | 6 | -0.000000066 | -0.000000071 | -0.000000205 |
| 80 | 6 | -0.000000017 | -0.000000304 | -0.000000116 |
| 81 | 6 | -0.000000024 | 0.000000003 | -0.000000173 |
| 82 | 6 | -0.000000037 | -0.000000130 | -0.000000062 |
| 83 | 1 | 0.000000176 | -0.000000033 | -0.000000147 |
| 84 | 1 | 0.000000027 | -0.000000021 | -0.000000108 |
| 85 | 1 | -0.000000040 | -0.000000034 | -0.000000101 |
| 86 | 1 | -0.000000050 | -0.000000054 | -0.000000102 |
| 87 | 1 | -0.000000046 | -0.000000066 | -0.000000139 |
| 88 | 1 | -0.000000004 | -0.000000061 | -0.000000125 |
| 89 | 8 | 0.000000128 | -0.000000103 | 0.000000089 |
| 90 | 8 | 0.000000051 | 0.000000099 | -0.000000224 |
| 91 | 6 | 0.000000089 | -0.000000024 | -0.000000052 |
| 92 | 6 | 0.000000151 | -0.000000041 | 0.000000071 |
| 93 | 6 | -0.000000077 | 0.000000000 | 0.000000111 |
| 94 | 6 | 0.000000084 | -0.000000072 | 0.000000023 |
| 95 | 6 | 0.000000073 | -0.000000168 | -0.000000027 |
| 96 | 6 | -0.000000113 | -0.000000014 | -0.000000140 |
| 97 | 6 | 0.000000054 | -0.000000067 | -0.000000082 |
| 98 | 6 | 0.000000073 | -0.000000074 | -0.000000107 |
| 99 | 1 | 0.000000095 | -0.000000052 | -0.000000043 |
| 100 | 1 | 0.000000048 | -0.000000088 | -0.000000087 |
| 101 | 1 | 0.000000094 | -0.000000084 | -0.000000079 |
| 102 | 1 | 0.000000096 | -0.000000089 | -0.000000087 |
| 103 | 1 | 0.000000061 | -0.000000074 | -0.000000091 |
| 104 | 1 | 0.000000081 | -0.000000093 | -0.000000113 |
| 105 | 8 | -0.000000008 | -0.000000035 | -0.000000172 |
| 106 | 8 | 0.000000109 | 0.000000001 | -0.000000287 |
| 107 | 6 | 0.000000084 | -0.000000000 | -0.000000176 |
| 108 | 6 | 0.000000098 | -0.000000127 | -0.000000204 |
| 109 | 6 | -0.000000118 | -0.000000117 | 0.000000115 |
| 110 | 6 | 0.000000031 | 0.000000078 | -0.000000200 |
| 111 | 6 | 0.000000096 | -0.000000217 | -0.000000168 |
| 112 | 6 | -0.000000055 | -0.000000097 | -0.000000001 |
| 113 | 6 | 0.000000051 | -0.000000052 | -0.000000030 |
| 114 | 6 | -0.000000024 | -0.000000116 | -0.000000184 |
| 115 | 1 | -0.000000022 | -0.000000088 | -0.000000118 |
| 116 | 1 | 0.000000029 | -0.000000079 | -0.000000102 |
| 117 | 1 | 0.000000004 | -0.000000091 | -0.000000108 |
| 118 | 1 | 0.000000033 | -0.000000094 | -0.000000138 |
| 119 | 1 | 0.000000029 | -0.000000092 | -0.000000110 |
| 120 | 1 | 0.000000006 | -0.000000093 | -0.000000130 |
| 121 | 8 | 0.000000848 | -0.000000310 | -0.000000190 |
| 122 | 8 | 0.000000007 | 0.000000041 | -0.000000019 |
| 123 | 6 | -0.000000179 | 0.000000147 | 0.000000013 |
| 124 | 6 | 0.000000187 | -0.000000080 | 0.000000043 |
| 125 | 6 | 0.000000027 | -0.000000026 | 0.000000008 |
| 126 | 6 | 0.000000024 | -0.000000077 | -0.000000140 |
| 127 | 6 | 0.000000042 | -0.000000027 | -0.000000078 |

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|---|---|---|---|---|
| 128 | 6 | -0.000000012 | -0.000000037 | -0.000000019 |
| 129 | 6 | 0.000000033 | 0.000000008 | -0.000000003 |
| 130 | 6 | 0.000000042 | -0.000000051 | -0.000000073 |
| 131 | 1 | -0.000000102 | -0.000000114 | -0.000000052 |
| 132 | 1 | -0.000000006 | -0.000000045 | -0.000000112 |
| 133 | 1 | 0.000000031 | -0.000000043 | -0.000000049 |
| 134 | 1 | 0.000000042 | -0.000000060 | -0.000000082 |
| 135 | 1 | 0.000000028 | -0.000000054 | -0.000000084 |
| 136 | 1 | 0.000000020 | -0.000000063 | -0.000000074 |
| 137 | 1 | 0.000000183 | -0.000000138 | -0.000000276 |
| 138 | 1 | 0.000000115 | -0.000000072 | -0.000000036 |
| 139 | 1 | -0.000000015 | -0.000000015 | 0.000000125 |
| 140 | 1 | -0.000000774 | 0.000000753 | -0.000000634 |
| 141 | 1 | 0.000000020 | -0.000000065 | -0.000000056 |
| 142 | 1 | 0.000000009 | -0.000000232 | -0.000000076 |
| 143 | 1 | 0.000002651 | -0.000000470 | -0.000001852 |
| 144 | 1 | -0.000000058 | 0.000000021 | -0.000000001 |
| 145 | 8 | -0.000000938 | -0.000000431 | -0.000000830 |
| 146 | 1 | 0.000000108 | -0.000000176 | -0.000000354 |
| 147 | 1 | -0.000000253 | -0.000000295 | 0.000000190 |
| 148 | 8 | 0.000000103 | 0.000000008 | 0.000000065 |
| 149 | 1 | 0.000000084 | 0.000000042 | 0.000000083 |
| 150 | 1 | 0.000000073 | 0.000000049 | 0.000000089 |
| 151 | 8 | -0.000000069 | 0.000000045 | 0.000000016 |
| 152 | 1 | -0.000000099 | 0.000000037 | 0.000000026 |
| 153 | 1 | -0.000000114 | 0.000000034 | 0.000000042 |
| 154 | 8 | -0.000000006 | 0.000000068 | -0.000000011 |
| 155 | 1 | -0.000000012 | -0.000000041 | -0.000000003 |
| 156 | 1 | -0.000000029 | -0.000000034 | 0.000000003 |
| 157 | 1 | -0.000000196 | -0.000000271 | 0.000000541 |
| 158 | 8 | -0.000000393 | 0.000000014 | -0.000000805 |
| 159 | 8 | 0.000000284 | -0.000000879 | -0.000001217 |
| 160 | 6 | 0.000000043 | 0.000000296 | 0.000000392 |
| 161 | 6 | -0.000000295 | -0.000000378 | -0.000000608 |
| 162 | 6 | -0.000000573 | 0.000000125 | 0.000001232 |
| 163 | 6 | -0.000000029 | -0.000000132 | 0.000000009 |
| 164 | 6 | -0.000000119 | 0.000000166 | -0.000000005 |
| 165 | 6 | -0.000000179 | -0.000000077 | -0.000000215 |
| 166 | 6 | -0.000000061 | 0.000000082 | -0.000000036 |
| 167 | 6 | -0.000000177 | -0.000000016 | -0.000000026 |
| 168 | 1 | -0.000000082 | 0.000000003 | -0.000000101 |
| 169 | 1 | -0.000000091 | 0.000000019 | -0.000000017 |
| 170 | 1 | -0.000000146 | 0.000000016 | -0.000000027 |
| 171 | 1 | -0.000000154 | 0.000000022 | -0.000000004 |
| 172 | 1 | -0.000000153 | 0.000000030 | -0.000000016 |
| 173 | 1 | -0.000000163 | 0.000000033 | -0.000000005 |
| 174 | 8 | -0.000000121 | 0.000000046 | 0.000000094 |
| 175 | 8 | -0.000000059 | 0.000000095 | 0.000000084 |
| 176 | 6 | -0.000000177 | 0.000000189 | 0.000000221 |
| 177 | 6 | -0.000000017 | -0.000000139 | 0.000000063 |
| 178 | 6 | 0.000000042 | 0.000000161 | -0.000000091 |
| 179 | 6 | -0.000000221 | 0.000000101 | 0.000000188 |
| 180 | 6 | -0.000000116 | -0.000000119 | 0.000000032 |
| 181 | 6 | -0.000000002 | 0.000000139 | -0.000000070 |
| 182 | 6 | -0.000000070 | 0.000000091 | 0.000000043 |
| 183 | 6 | -0.000000118 | 0.000000060 | 0.000000059 |
| 184 | 1 | -0.000000067 | 0.000000068 | 0.000000078 |
| 185 | 1 | -0.000000132 | 0.000000057 | 0.000000036 |
| 186 | 1 | -0.000000072 | 0.000000062 | 0.000000071 |
| 187 | 1 | -0.000000097 | 0.000000060 | 0.000000070 |
| 188 | 1 | -0.000000104 | 0.000000072 | 0.000000050 |
| 189 | 1 | -0.000000110 | 0.000000059 | 0.000000062 |
| 190 | 8 | 0.000000020 | -0.000000084 | 0.000000040 |
| 191 | 8 | -0.000000205 | -0.000000003 | 0.000000103 |
| 192 | 6 | -0.000000131 | 0.000000184 | -0.000000223 |
| 193 | 6 | -0.000000351 | 0.000000014 | -0.000000001 |
| 194 | 6 | 0.000000089 | -0.000000109 | 0.000000087 |
| 195 | 6 | -0.000000051 | 0.000000154 | -0.000000111 |
| 196 | 6 | -0.000000322 | 0.000000049 | 0.000000043 |
| 197 | 6 | -0.000000051 | -0.000000082 | 0.000000183 |
| 198 | 6 | -0.000000160 | 0.000000082 | 0.000000032 |
| 199 | 6 | -0.000000151 | 0.000000051 | 0.000000056 |
| 200 | 1 | -0.000000123 | 0.000000021 | -0.000000003 |

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|---|---|---|---|---|
| 201 | 1 | -0.000000125 | 0.000000053 | 0.000000044 |
| 202 | 1 | -0.000000135 | 0.000000055 | 0.000000055 |
| 203 | 1 | -0.000000166 | 0.000000061 | 0.000000045 |
| 204 | 1 | -0.000000132 | 0.000000057 | 0.000000042 |
| 205 | 1 | -0.000000144 | 0.000000086 | 0.000000065 |
| 206 | 8 | -0.000000075 | 0.000000068 | 0.000000092 |
| 207 | 8 | -0.000000219 | 0.000000043 | -0.000000064 |
| 208 | 6 | -0.000000107 | -0.000000106 | -0.000000153 |
| 209 | 6 | 0.000000097 | 0.000000105 | -0.000000026 |
| 210 | 6 | -0.000000041 | 0.000000184 | 0.000000188 |
| 211 | 6 | -0.000000234 | -0.000000072 | -0.000000098 |
| 212 | 6 | 0.000000172 | 0.000000016 | 0.000000021 |
| 213 | 6 | -0.000000209 | 0.000000182 | 0.000000267 |
| 214 | 6 | -0.000000039 | -0.000000039 | -0.000000026 |
| 215 | 6 | -0.000000135 | 0.000000053 | -0.000000023 |
| 216 | 1 | -0.000000028 | 0.000000010 | 0.000000021 |
| 217 | 1 | -0.000000095 | 0.000000012 | 0.000000047 |
| 218 | 1 | -0.000000081 | 0.000000001 | 0.000000001 |
| 219 | 1 | -0.000000087 | 0.000000013 | -0.000000005 |
| 220 | 1 | -0.000000115 | 0.000000035 | 0.000000012 |
| 221 | 1 | -0.000000124 | -0.000000005 | 0.000000002 |
| 222 | 1 | -0.000000176 | 0.000000968 | 0.000000030 |
| 223 | 1 | -0.000000072 | 0.000000065 | 0.000000057 |
| 224 | 1 | -0.000000054 | 0.000000044 | 0.000000066 |
| 225 | 1 | -0.000000150 | 0.000000068 | -0.000000102 |
| 226 | 1 | -0.000000115 | 0.000000070 | -0.000000010 |
| 227 | 1 | -0.000000033 | 0.000000040 | 0.000000049 |
| 228 | 1 | 0.000000053 | -0.000000119 | 0.000000021 |
| 229 | 1 | 0.000000077 | 0.000000023 | 0.000000053 |
| 230 | 1 | 0.000000085 | -0.000000017 | -0.000000030 |
| 231 | 1 | 0.000000078 | -0.000000097 | -0.000000012 |
| 232 | 8 | 0.000000040 | 0.000000024 | 0.000000039 |
| 233 | 8 | -0.000000025 | -0.000000024 | -0.000000024 |
| 234 | 6 | 0.000000078 | -0.000000201 | -0.000000168 |
| 235 | 6 | -0.000000144 | 0.000000181 | 0.000000061 |
| 236 | 6 | 0.000000314 | -0.000000018 | 0.000000137 |
| 237 | 6 | 0.000000038 | -0.000000205 | -0.000000173 |
| 238 | 6 | -0.000000103 | 0.000000145 | 0.000000039 |
| 239 | 6 | 0.000000314 | 0.000000017 | 0.000000140 |
| 240 | 6 | 0.000000080 | -0.000000041 | -0.000000020 |
| 241 | 6 | 0.000000086 | -0.000000053 | -0.000000025 |
| 242 | 1 | 0.000000043 | 0.000000002 | 0.000000030 |
| 243 | 1 | 0.000000112 | -0.000000024 | -0.000000013 |
| 244 | 1 | 0.000000067 | -0.000000036 | -0.000000029 |
| 245 | 1 | 0.000000122 | -0.000000039 | -0.000000040 |
| 246 | 1 | 0.000000092 | -0.000000049 | -0.000000042 |
| 247 | 1 | 0.000000098 | -0.000000020 | -0.000000021 |
| 248 | 8 | 0.000000139 | -0.000000055 | -0.000000095 |
| 249 | 8 | 0.000000131 | 0.000000152 | 0.000000019 |
| 250 | 6 | 0.000000088 | -0.000000093 | -0.000000045 |
| 251 | 6 | 0.000000026 | -0.000000051 | -0.000000062 |
| 252 | 6 | 0.000000061 | -0.000000188 | -0.000000113 |
| 253 | 6 | 0.000000172 | -0.000000033 | 0.000000015 |
| 254 | 6 | 0.000000106 | -0.000000051 | -0.000000014 |
| 255 | 6 | 0.000000144 | 0.000000019 | -0.000000017 |
| 256 | 6 | 0.000000169 | -0.000000010 | 0.000000024 |
| 257 | 6 | 0.000000132 | -0.000000039 | -0.000000011 |
| 258 | 1 | 0.000000097 | -0.000000040 | 0.000000030 |
| 259 | 1 | 0.000000142 | -0.000000022 | -0.000000022 |
| 260 | 1 | 0.000000141 | -0.000000023 | 0.000000008 |
| 261 | 1 | 0.000000150 | -0.000000038 | 0.000000004 |
| 262 | 1 | 0.000000175 | -0.000000015 | 0.000000001 |
| 263 | 1 | 0.000000174 | -0.000000054 | -0.000000031 |
| 264 | 8 | 0.000000130 | 0.000000043 | 0.000000024 |
| 265 | 8 | 0.000000048 | -0.000000019 | 0.000000027 |
| 266 | 6 | -0.000000036 | -0.000000024 | -0.000000087 |
| 267 | 6 | 0.000000222 | 0.000000119 | 0.000000068 |
| 268 | 6 | 0.000000183 | -0.000000104 | 0.000000200 |
| 269 | 6 | -0.000000040 | 0.000000029 | -0.000000072 |
| 270 | 6 | 0.000000249 | 0.000000116 | 0.000000014 |
| 271 | 6 | 0.000000166 | -0.000000204 | 0.000000066 |
| 272 | 6 | 0.000000098 | -0.000000009 | 0.000000039 |
| 273 | 6 | 0.000000121 | -0.000000010 | 0.000000020 |

| | | | | |
|---|---|---|---|---|
| 274 | 1 | 0.000000097 | 0.000000016 | 0.000000046 |
| 275 | 1 | 0.000000134 | -0.000000031 | -0.000000012 |
| 276 | 1 | 0.000000110 | 0.000000005 | 0.000000043 |
| 277 | 1 | 0.000000137 | -0.000000009 | 0.000000006 |
| 278 | 1 | 0.000000144 | -0.000000006 | 0.000000032 |
| 279 | 1 | 0.000000143 | -0.000000010 | 0.000000033 |
| 280 | 8 | -0.000000017 | -0.000000143 | -0.000000023 |
| 281 | 8 | 0.000000112 | 0.000000010 | -0.000000005 |
| 282 | 6 | 0.000000072 | 0.000000004 | -0.000000058 |
| 283 | 6 | 0.000000094 | -0.000000009 | 0.000000143 |
| 284 | 6 | 0.000000103 | -0.000000113 | -0.000000162 |
| 285 | 6 | -0.000000025 | -0.000000051 | 0.000000008 |
| 286 | 6 | 0.000000108 | 0.000000013 | -0.000000044 |
| 287 | 6 | 0.000000084 | -0.000000045 | -0.000000066 |
| 288 | 6 | 0.000000119 | -0.000000072 | -0.000000053 |
| 289 | 6 | 0.000000133 | -0.000000064 | -0.000000053 |
| 290 | 1 | 0.000000039 | -0.000000054 | -0.000000155 |
| 291 | 1 | 0.000000102 | -0.000000045 | -0.000000067 |
| 292 | 1 | 0.000000102 | -0.000000075 | -0.000000071 |
| 293 | 1 | 0.000000127 | -0.000000067 | -0.000000054 |
| 294 | 1 | 0.000000128 | -0.000000072 | -0.000000073 |
| 295 | 1 | 0.000000120 | -0.000000072 | -0.000000071 |
| 296 | 1 | 0.000000131 | -0.000000021 | 0.000000034 |
| 297 | 1 | 0.000000103 | 0.000000032 | 0.000000043 |
| 298 | 1 | 0.000000035 | -0.000000004 | -0.000000077 |
| 299 | 1 | 0.000000045 | -0.000000142 | -0.000000086 |
| 300 | 1 | 0.000000115 | -0.000000063 | -0.000000035 |
| 301 | 1 | -0.000000037 | 0.000000069 | -0.000000226 |
| 302 | 1 | -0.000000008 | -0.000000028 | -0.000000001 |
| 303 | 1 | -0.000000174 | -0.000000021 | -0.000000023 |
| 304 | 1 | 0.000000278 | 0.000003512 | 0.000001061 |
| 305 | 8 | -0.000000219 | -0.000000306 | -0.000000119 |
| 306 | 8 | -0.000000059 | 0.000000026 | -0.000000031 |
| 307 | 6 | 0.000000367 | 0.000000337 | -0.000000004 |
| 308 | 6 | -0.000000216 | -0.000000127 | -0.000000096 |
| 309 | 6 | 0.000000049 | 0.000000049 | 0.000000092 |
| 310 | 6 | -0.000000023 | -0.000000019 | -0.000000129 |
| 311 | 6 | -0.000000096 | -0.000000037 | -0.000000084 |
| 312 | 6 | -0.000000083 | -0.000000024 | -0.000000074 |
| 313 | 6 | -0.000000036 | -0.000000013 | 0.000000006 |
| 314 | 6 | -0.000000087 | -0.000000020 | -0.000000059 |
| 315 | 1 | 0.000000022 | -0.000000032 | -0.000000010 |
| 316 | 1 | -0.000000066 | -0.000000016 | -0.000000079 |
| 317 | 1 | -0.000000053 | -0.000000003 | -0.000000018 |
| 318 | 1 | -0.000000069 | -0.000000023 | -0.000000051 |
| 319 | 1 | -0.000000084 | -0.000000025 | -0.000000056 |
| 320 | 1 | -0.000000094 | -0.000000004 | -0.000000040 |
| 321 | 8 | 0.000000046 | -0.000000002 | 0.000000086 |
| 322 | 8 | -0.000000510 | -0.000001587 | -0.000002718 |
| 323 | 6 | -0.000000248 | -0.000000112 | -0.000000088 |
| 324 | 6 | 0.000000022 | 0.000000068 | 0.000000031 |
| 325 | 6 | -0.000000420 | -0.000000028 | 0.000000988 |
| 326 | 6 | -0.000000093 | -0.000000068 | -0.000000099 |
| 327 | 6 | -0.000000005 | 0.000000020 | -0.000000111 |
| 328 | 6 | -0.000000222 | 0.000000061 | -0.000000056 |
| 329 | 6 | -0.000000054 | -0.000000043 | -0.000000055 |
| 330 | 6 | -0.000000115 | -0.000000052 | -0.000000148 |
| 331 | 1 | -0.000000082 | -0.000000040 | -0.000000045 |
| 332 | 1 | -0.000000089 | -0.000000053 | -0.000000073 |
| 333 | 1 | -0.000000086 | -0.000000066 | -0.000000081 |
| 334 | 1 | -0.000000117 | -0.000000062 | -0.000000093 |
| 335 | 1 | -0.000000092 | -0.000000044 | -0.000000089 |
| 336 | 1 | -0.000000101 | -0.000000073 | -0.000000113 |
| 337 | 8 | -0.000000080 | 0.000000231 | -0.000000480 |
| 338 | 8 | 0.000000072 | -0.000000313 | -0.000000430 |
| 339 | 6 | -0.000000726 | 0.000000006 | 0.000000468 |
| 340 | 6 | -0.000000022 | 0.000000098 | -0.000000562 |
| 341 | 6 | -0.000000395 | -0.000000040 | 0.000000384 |
| 342 | 6 | -0.000000005 | 0.000000078 | 0.000000017 |
| 343 | 6 | -0.000000051 | 0.000000024 | -0.000000276 |
| 344 | 6 | -0.000000158 | -0.000000059 | -0.000000091 |
| 345 | 6 | -0.000000001 | -0.000000047 | -0.000000113 |
| 346 | 6 | -0.000000047 | -0.000000076 | -0.000000107 |

| | | | | |
|---|---|---|---|---|
| 347 | 1 | -0.000000066 | -0.000000087 | -0.000000031 |
| 348 | 1 | -0.000000086 | -0.000000029 | -0.000000082 |
| 349 | 1 | -0.000000028 | -0.000000045 | -0.000000095 |
| 350 | 1 | -0.000000057 | -0.000000073 | -0.000000120 |
| 351 | 1 | -0.000000031 | -0.000000051 | -0.000000096 |
| 352 | 1 | -0.000000068 | -0.000000058 | -0.000000075 |
| 353 | 8 | -0.000000106 | 0.000000045 | 0.000000032 |
| 354 | 8 | -0.000000108 | 0.000000045 | -0.000000084 |
| 355 | 6 | 0.000000120 | -0.000000074 | 0.000000149 |
| 356 | 6 | 0.000000031 | 0.000000099 | -0.000000218 |
| 357 | 6 | -0.000000320 | 0.000000055 | 0.000000126 |
| 358 | 6 | 0.000000045 | -0.000000102 | 0.000000127 |
| 359 | 6 | -0.000000071 | -0.000000019 | -0.000000252 |
| 360 | 6 | -0.000000246 | 0.000000067 | -0.000000004 |
| 361 | 6 | -0.000000099 | -0.000000022 | -0.000000063 |
| 362 | 6 | -0.000000120 | 0.000000015 | -0.000000053 |
| 363 | 1 | -0.000000093 | 0.000000032 | 0.000000014 |
| 364 | 1 | -0.000000112 | -0.000000043 | -0.000000054 |
| 365 | 1 | -0.000000128 | 0.000000007 | -0.000000039 |
| 366 | 1 | -0.000000149 | -0.000000022 | -0.000000067 |
| 367 | 1 | -0.000000149 | -0.000000003 | -0.000000047 |
| 368 | 1 | -0.000000123 | -0.000000036 | -0.000000065 |
| 369 | 1 | 0.000000029 | -0.000000159 | 0.000000057 |
| 370 | 1 | -0.000000232 | 0.000000268 | -0.000000132 |
| 371 | 1 | -0.000000033 | -0.000000005 | -0.000000010 |
| 372 | 1 | -0.000000105 | 0.000000023 | 0.000000005 |
| 373 | 1 | 0.000000004 | 0.000000022 | 0.000000061 |
| 374 | 1 | 0.000000005 | 0.000000070 | 0.000000094 |
| 375 | 1 | 0.000000013 | -0.000000011 | 0.000000019 |
| 376 | 1 | 0.000000058 | 0.000000066 | 0.000000138 |
| 377 | 8 | 0.000000008 | 0.000000055 | 0.000000037 |
| 378 | 8 | 0.000000001 | 0.000000067 | 0.000000094 |
| 379 | 6 | -0.000000013 | -0.000000020 | 0.000000015 |
| 380 | 6 | 0.000000079 | 0.000000098 | 0.000000087 |
| 381 | 6 | -0.000000008 | 0.000000047 | 0.000000149 |
| 382 | 6 | 0.000000017 | 0.000000015 | 0.000000063 |
| 383 | 6 | 0.000000078 | 0.000000098 | 0.000000053 |
| 384 | 6 | 0.000000025 | 0.000000079 | 0.000000135 |
| 385 | 6 | 0.000000022 | 0.000000076 | 0.000000069 |
| 386 | 6 | 0.000000058 | 0.000000067 | 0.000000123 |
| 387 | 1 | -0.000000001 | 0.000000042 | 0.000000070 |
| 388 | 1 | 0.000000049 | 0.000000052 | 0.000000073 |
| 389 | 1 | 0.000000037 | 0.000000075 | 0.000000105 |
| 390 | 1 | 0.000000068 | 0.000000067 | 0.000000121 |
| 391 | 1 | 0.000000064 | 0.000000079 | 0.000000119 |
| 392 | 1 | 0.000000075 | 0.000000063 | 0.000000124 |
| 393 | 8 | 0.000000145 | 0.000000029 | 0.000000046 |
| 394 | 8 | -0.000000024 | -0.000000032 | 0.000000012 |
| 395 | 6 | -0.000000154 | 0.000000013 | -0.000000067 |
| 396 | 6 | 0.000000272 | 0.000000183 | -0.000000196 |
| 397 | 6 | 0.000000203 | -0.000000258 | 0.000000283 |
| 398 | 6 | -0.000000141 | 0.000000090 | 0.000000087 |
| 399 | 6 | 0.000000370 | 0.000000194 | -0.000000093 |
| 400 | 6 | 0.000000129 | -0.000000223 | 0.000000251 |
| 401 | 6 | 0.000000110 | 0.000000044 | 0.000000048 |
| 402 | 6 | 0.000000119 | 0.000000006 | 0.000000048 |
| 403 | 1 | 0.000000107 | -0.000000020 | 0.000000014 |
| 404 | 1 | 0.000000111 | 0.000000035 | 0.000000077 |
| 405 | 1 | 0.000000113 | 0.000000000 | 0.000000017 |
| 406 | 1 | 0.000000117 | -0.000000003 | 0.000000051 |
| 407 | 1 | 0.000000108 | 0.000000008 | 0.000000050 |
| 408 | 1 | 0.000000107 | 0.000000014 | 0.000000049 |
| 409 | 8 | -0.000000035 | -0.000000004 | 0.000000041 |
| 410 | 8 | 0.000000139 | 0.000000020 | 0.000000187 |
| 411 | 6 | 0.000000022 | 0.000000106 | 0.000000100 |
| 412 | 6 | 0.000000067 | 0.000000125 | 0.000000096 |
| 413 | 6 | 0.000000074 | -0.000000009 | 0.000000043 |
| 414 | 6 | 0.000000132 | 0.000000018 | 0.000000022 |
| 415 | 6 | 0.000000094 | 0.000000090 | 0.000000087 |
| 416 | 6 | 0.000000086 | 0.000000045 | 0.000000140 |
| 417 | 6 | 0.000000165 | 0.000000078 | 0.000000091 |
| 418 | 6 | 0.000000120 | 0.000000038 | 0.000000094 |
| 419 | 1 | 0.000000046 | 0.000000040 | 0.000000101 |

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|---|---|---|---|---|
| 420 | 1 | 0.000000109 | 0.000000023 | 0.000000083 |
| 421 | 1 | 0.000000124 | 0.000000030 | 0.000000086 |
| 422 | 1 | 0.000000154 | 0.000000027 | 0.000000080 |
| 423 | 1 | 0.000000133 | 0.000000040 | 0.000000121 |
| 424 | 1 | 0.000000102 | 0.000000040 | 0.000000086 |
| 425 | 8 | 0.000000194 | -0.000000035 | 0.000000032 |
| 426 | 8 | -0.000000006 | 0.000000022 | 0.000000007 |
| 427 | 6 | 0.000000123 | 0.000000020 | -0.000000083 |
| 428 | 6 | 0.000000017 | 0.000000061 | 0.000000017 |
| 429 | 6 | 0.000000070 | -0.000000018 | 0.000000019 |
| 430 | 6 | 0.000000040 | 0.000000005 | 0.000000096 |
| 431 | 6 | 0.000000032 | 0.000000002 | 0.000000045 |
| 432 | 6 | -0.000000037 | 0.000000035 | 0.000000018 |
| 433 | 6 | 0.000000023 | 0.000000018 | 0.000000069 |
| 434 | 6 | 0.000000056 | 0.000000051 | 0.000000070 |
| 435 | 1 | 0.000000040 | -0.000000001 | -0.000000005 |
| 436 | 1 | 0.000000078 | -0.000000003 | 0.000000066 |
| 437 | 1 | 0.000000025 | 0.000000039 | 0.000000055 |
| 438 | 1 | 0.000000064 | 0.000000040 | 0.000000083 |
| 439 | 1 | 0.000000037 | 0.000000040 | 0.000000084 |
| 440 | 1 | 0.000000048 | 0.000000039 | 0.000000061 |
| 441 | 1 | 0.000000101 | 0.000000071 | 0.000000055 |
| 442 | 1 | 0.000000092 | -0.000000026 | -0.000000003 |
| 443 | 1 | 0.000000012 | 0.000000011 | 0.000000033 |
| 444 | 1 | 0.000000108 | 0.000000002 | 0.000000056 |
| 445 | 8 | -0.000000153 | 0.000002521 | -0.000000621 |
| 446 | 1 | -0.000001174 | -0.000002603 | -0.000001387 |
| 447 | 1 | -0.000000144 | 0.000000613 | 0.000000137 |
| 448 | 8 | -0.000000049 | 0.000000071 | 0.000000129 |
| 449 | 1 | -0.000000037 | 0.000000071 | 0.000000073 |
| 450 | 1 | -0.000000019 | 0.000000068 | 0.000000071 |
| 451 | 8 | 0.000000001 | 0.000000006 | -0.000000020 |
| 452 | 1 | 0.000000028 | -0.000000003 | 0.000000027 |
| 453 | 1 | 0.000000034 | 0.000000004 | 0.000000016 |
| 454 | 8 | 0.000000992 | -0.000000141 | -0.000000066 |
| 455 | 1 | 0.000000090 | -0.000000069 | -0.000000043 |
| 456 | 1 | -0.000000805 | 0.000000435 | -0.000000116 |
| 457 | 6 | -0.000000782 | -0.000000932 | -0.000000229 |
| 458 | 6 | -0.000001748 | 0.000001070 | -0.000000790 |
| 459 | 6 | -0.000000096 | 0.000000837 | 0.000001238 |
| 460 | 7 | -0.000001747 | 0.000002138 | -0.000003832 |
| 461 | 6 | -0.000000111 | -0.000000475 | -0.000000069 |
| 462 | 6 | -0.000000597 | 0.000001460 | 0.000000341 |
| 463 | 6 | 0.000002188 | -0.000001284 | 0.000000205 |
| 464 | 6 | -0.000000569 | 0.000000427 | 0.000000212 |
| 465 | 6 | 0.000001088 | -0.000001258 | -0.000000368 |
| 466 | 8 | 0.000002817 | -0.000002333 | 0.000003058 |
| 467 | 8 | 0.000000533 | -0.000003841 | 0.000002986 |
| 468 | 1 | 0.000000892 | -0.000000239 | -0.000000059 |
| 469 | 1 | 0.000000044 | -0.000000123 | -0.000000245 |
| 470 | 1 | -0.000000069 | -0.000000767 | -0.000000295 |
| 471 | 1 | 0.000000156 | -0.000000380 | 0.000000375 |
| 472 | 1 | -0.000000165 | 0.000000009 | 0.000000708 |
| 473 | 1 | 0.000000211 | 0.000000408 | 0.000000445 |
| 474 | 1 | -0.000000071 | 0.000000042 | -0.000000399 |
| 475 | 6 | -0.000001426 | 0.000000436 | 0.000000650 |
| 476 | 6 | 0.000001145 | -0.000001740 | 0.000003100 |
| 477 | 7 | -0.000001213 | -0.000000051 | 0.000000276 |
| 478 | 6 | -0.000000116 | 0.000000387 | -0.000001378 |
| 479 | 6 | 0.000000045 | -0.000000616 | -0.000001816 |
| 480 | 6 | 0.000001829 | -0.000000480 | 0.000000969 |
| 481 | 1 | 0.000001129 | 0.000002575 | 0.000000346 |
| 482 | 1 | 0.000000488 | -0.000000172 | -0.000000547 |
| 483 | 1 | 0.000000518 | 0.000000134 | -0.000000257 |
| 484 | 1 | 0.000000351 | 0.000000398 | -0.000000209 |
| 485 | 1 | 0.000000062 | -0.000000102 | 0.000000212 |
| 486 | 1 | -0.000000128 | 0.000000341 | -0.000000121 |
| 487 | 1 | 0.000000209 | 0.000000088 | -0.000000114 |

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Sum of electronic and thermal Free Energies = -1069.254232
ONIOM Total Energy = -1072.5472518
1 imaginary frequency = -349.62

$\beta$-I2@$C_R$

| Center Number | Atomic Number | Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | -0.000000096 | -0.000001849 | -0.000002661 |
| 2 | 8 | -0.000000083 | -0.000002987 | -0.000001064 |
| 3 | 6 | -0.000000800 | -0.000001062 | -0.000000159 |
| 4 | 6 | -0.000000015 | -0.000000228 | -0.000000494 |
| 5 | 6 | -0.000000254 | 0.000003810 | -0.000001772 |
| 6 | 6 | 0.000000488 | -0.000000945 | -0.000001087 |
| 7 | 6 | 0.000000120 | 0.000001109 | -0.000000685 |
| 8 | 6 | 0.000000476 | -0.000001049 | -0.000001422 |
| 9 | 6 | 0.000000150 | -0.000000654 | 0.000000535 |
| 10 | 6 | 0.000000522 | 0.000000221 | -0.000000627 |
| 11 | 1 | 0.000000244 | -0.000000299 | -0.000000715 |
| 12 | 1 | 0.000000053 | -0.000000147 | -0.000000383 |
| 13 | 1 | 0.000000497 | -0.000000092 | -0.000000041 |
| 14 | 1 | 0.000000151 | -0.000000330 | -0.000000675 |
| 15 | 1 | 0.000000105 | -0.000000315 | -0.000000720 |
| 16 | 1 | 0.000000176 | -0.000000165 | -0.000000754 |
| 17 | 8 | -0.000001727 | -0.000000734 | -0.000003895 |
| 18 | 8 | 0.000005305 | 0.000000758 | -0.000003229 |
| 19 | 6 | -0.000002302 | -0.000001470 | 0.000002284 |
| 20 | 6 | -0.000000242 | -0.000001567 | -0.000000057 |
| 21 | 6 | 0.000000848 | -0.000000399 | 0.000000949 |
| 22 | 6 | 0.000001105 | 0.000002287 | -0.000000806 |
| 23 | 6 | 0.000001140 | -0.000001996 | 0.000000211 |
| 24 | 6 | 0.000000602 | 0.000001610 | -0.000000199 |
| 25 | 6 | 0.000001085 | -0.000000567 | -0.000001171 |
| 26 | 6 | 0.000000686 | -0.000000817 | -0.000000475 |
| 27 | 1 | 0.000001009 | 0.000000719 | 0.000000436 |
| 28 | 1 | 0.000000243 | 0.000000048 | -0.000000753 |
| 29 | 1 | 0.000000761 | -0.000000137 | -0.000000905 |
| 30 | 1 | -0.000000041 | -0.000000101 | -0.000000692 |
| 31 | 1 | 0.000000065 | -0.000000254 | -0.000000498 |
| 32 | 1 | 0.000000184 | -0.000000104 | -0.000000648 |
| 33 | 8 | -0.000001222 | 0.000000044 | 0.000003050 |
| 34 | 8 | -0.000001572 | -0.000001231 | -0.000002171 |
| 35 | 6 | -0.000000709 | 0.000000428 | -0.000001995 |
| 36 | 6 | 0.000000758 | -0.000000108 | -0.000001127 |
| 37 | 6 | 0.000000557 | -0.000000154 | 0.000000729 |
| 38 | 6 | -0.000000259 | 0.000000450 | 0.000000739 |
| 39 | 6 | 0.000001530 | -0.000000650 | -0.000001750 |
| 40 | 6 | 0.000000652 | 0.000000218 | 0.000000645 |
| 41 | 6 | 0.000000965 | -0.000000286 | -0.000001716 |
| 42 | 6 | 0.000000554 | 0.000000115 | -0.000000326 |
| 43 | 1 | 0.000000275 | -0.000000310 | -0.000000006 |
| 44 | 1 | 0.000000166 | -0.000000011 | -0.000000329 |
| 45 | 1 | 0.000000073 | -0.000000365 | -0.000000093 |
| 46 | 1 | 0.000000533 | 0.000000043 | -0.000000571 |
| 47 | 1 | 0.000000560 | 0.000000115 | -0.000000582 |
| 48 | 1 | 0.000000505 | 0.000000070 | -0.000000641 |
| 49 | 8 | -0.000000015 | -0.000009558 | -0.000002518 |
| 50 | 8 | 0.000001451 | 0.000002272 | -0.000002984 |
| 51 | 6 | 0.000001357 | 0.000000335 | -0.000002820 |
| 52 | 6 | 0.000001845 | -0.000000893 | 0.000001048 |
| 53 | 6 | -0.000001604 | -0.000000380 | 0.000001115 |
| 54 | 6 | 0.000000777 | 0.000000564 | -0.000001261 |
| 55 | 6 | -0.000000618 | 0.000000387 | 0.000000498 |
| 56 | 6 | -0.000000680 | 0.000000627 | -0.000000767 |
| 57 | 6 | -0.000000474 | 0.000000185 | 0.000000733 |
| 58 | 6 | 0.000000581 | -0.000000521 | -0.000000878 |
| 59 | 1 | 0.000000165 | 0.000000417 | -0.000000549 |
| 60 | 1 | 0.000000353 | -0.000000001 | -0.000000689 |
| 61 | 1 | -0.000000006 | -0.000000099 | -0.000001324 |
| 62 | 1 | 0.000000261 | -0.000000126 | -0.000000695 |
| 63 | 1 | 0.000000313 | 0.000000000 | -0.000000652 |
| 64 | 1 | 0.000000344 | -0.000000121 | -0.000000499 |
| 65 | 1 | -0.000001036 | 0.000005217 | 0.000002214 |
| 66 | 1 | 0.000000447 | 0.000000390 | 0.000001690 |
| 67 | 1 | 0.000002401 | 0.000001402 | 0.000001319 |

| | | | | |
|---|---|---|---|---|
| 68 | 1 | 0.000006937 | 0.000004528 | 0.000000954 |
| 69 | 1 | -0.000006279 | 0.000000734 | 0.000001851 |
| 70 | 1 | -0.000000046 | -0.000000690 | -0.000000243 |
| 71 | 1 | 0.000000825 | 0.000000455 | 0.000000752 |
| 72 | 1 | 0.000000375 | -0.000000737 | -0.000000100 |
| 73 | 8 | -0.000014709 | -0.000009340 | 0.000007341 |
| 74 | 8 | -0.000006048 | -0.000004064 | -0.000003424 |
| 75 | 6 | 0.000002495 | -0.000002248 | -0.000000298 |
| 76 | 6 | 0.000000707 | 0.000002574 | -0.000000091 |
| 77 | 6 | -0.000000466 | -0.000000620 | 0.000000260 |
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| 400 | 6 | 0.000000768 | -0.000001876 | -0.000002453 |
| 401 | 6 | -0.000000041 | -0.000000486 | 0.000000631 |
| 402 | 6 | -0.000000602 | -0.000000180 | 0.000000024 |
| 403 | 1 | 0.000000037 | -0.000000178 | -0.000000403 |
| 404 | 1 | -0.000000938 | -0.000000441 | -0.000000072 |
| 405 | 1 | -0.000000927 | -0.000000198 | 0.000000093 |
| 406 | 1 | -0.000000602 | -0.000000207 | -0.000000137 |
| 407 | 1 | -0.000000585 | -0.000000423 | -0.000000150 |
| 408 | 1 | -0.000000751 | -0.000000317 | -0.000000195 |
| 409 | 8 | -0.000002221 | 0.000001470 | -0.000000467 |
| 410 | 8 | -0.000001310 | 0.000001120 | -0.000000585 |
| 411 | 6 | 0.000000255 | -0.000001274 | 0.000000322 |
| 412 | 6 | -0.000001933 | 0.000002549 | -0.000002080 |
| 413 | 6 | 0.000001648 | -0.000002522 | 0.000001689 |
| 414 | 6 | -0.000000907 | 0.000001396 | -0.000000160 |
| 415 | 6 | -0.000001638 | 0.000000905 | -0.000001656 |
| 416 | 6 | -0.000001176 | -0.000000149 | -0.000000566 |
| 417 | 6 | -0.000001104 | -0.000000199 | 0.000000681 |
| 418 | 6 | -0.000000255 | -0.000001013 | -0.000000481 |
| 419 | 1 | 0.000000430 | -0.000000068 | -0.000000969 |
| 420 | 1 | -0.000000360 | -0.000000624 | -0.000000185 |
| 421 | 1 | -0.000000218 | -0.000001243 | -0.000000664 |
| 422 | 1 | -0.000000566 | -0.000000213 | -0.000000300 |
| 423 | 1 | -0.000000465 | -0.000000314 | -0.000000424 |
| 424 | 1 | -0.000000541 | -0.000000075 | -0.000000255 |
| 425 | 8 | -0.000010351 | -0.000006156 | -0.000002494 |
| 426 | 8 | 0.000003754 | -0.000006701 | 0.000003587 |
| 427 | 6 | 0.000001966 | 0.000000861 | -0.000000475 |
| 428 | 6 | -0.000001897 | 0.000000629 | 0.000000534 |
| 429 | 6 | 0.000002137 | 0.000002816 | -0.000003247 |
| 430 | 6 | -0.000000184 | 0.000000359 | -0.000000270 |
| 431 | 6 | -0.000001655 | 0.000000674 | -0.000000635 |
| 432 | 6 | -0.000000275 | -0.000000678 | -0.000000809 |

| | | | | |
|---|---|---|---|---|
| 433 | 6 | -0.000000029 | -0.000000170 | -0.000000913 |
| 434 | 6 | -0.000000788 | -0.000000421 | 0.000000261 |
| 435 | 1 | -0.000001030 | 0.000000643 | 0.000001038 |
| 436 | 1 | -0.000000495 | -0.000000470 | -0.000000472 |
| 437 | 1 | -0.000000344 | -0.000000926 | -0.000000195 |
| 438 | 1 | -0.000000719 | -0.000000343 | -0.000000172 |
| 439 | 1 | -0.000000718 | -0.000000291 | -0.000000200 |
| 440 | 1 | -0.000000716 | -0.000000318 | -0.000000040 |
| 441 | 1 | -0.000000597 | -0.000003491 | -0.000002301 |
| 442 | 1 | 0.000002200 | 0.000001349 | 0.000002196 |
| 443 | 1 | -0.000009250 | 0.000002486 | -0.000002138 |
| 444 | 1 | -0.000005173 | -0.000002092 | 0.000001108 |
| 445 | 8 | 0.000013251 | 0.000003952 | -0.000011070 |
| 446 | 1 | 0.000003332 | -0.000004813 | -0.000015727 |
| 447 | 1 | -0.000020209 | -0.000003720 | 0.000004517 |
| 448 | 8 | 0.000001186 | -0.000000369 | -0.000001570 |
| 449 | 1 | -0.000000232 | 0.000000079 | -0.000000035 |
| 450 | 1 | -0.000002844 | -0.000001625 | -0.000000108 |
| 451 | 8 | 0.000007097 | -0.000001140 | -0.000007961 |
| 452 | 1 | -0.000000798 | 0.000000599 | 0.000002511 |
| 453 | 1 | -0.000000732 | 0.000001490 | 0.000001631 |
| 454 | 8 | -0.000001569 | 0.000011951 | -0.000003194 |
| 455 | 1 | 0.000008828 | 0.000002748 | 0.000001427 |
| 456 | 1 | -0.000002817 | -0.000002613 | 0.000005472 |
| 457 | 6 | 0.000003369 | 0.000008722 | -0.000004812 |
| 458 | 6 | 0.000002130 | 0.000004148 | 0.000004758 |
| 459 | 6 | -0.000009072 | -0.000008090 | -0.000006508 |
| 460 | 7 | -0.000007601 | 0.000002728 | 0.000003965 |
| 461 | 6 | 0.000004537 | -0.000003803 | -0.000008917 |
| 462 | 6 | -0.000002346 | 0.000000952 | 0.000000623 |
| 463 | 6 | 0.000000000 | 0.000000292 | 0.000001260 |
| 464 | 6 | -0.000006601 | 0.000004850 | 0.000011148 |
| 465 | 6 | 0.000000002 | -0.000004976 | -0.000008790 |
| 466 | 8 | -0.000001311 | -0.000002234 | 0.000006688 |
| 467 | 8 | 0.000013337 | 0.000002434 | 0.000002361 |
| 468 | 1 | -0.000002891 | -0.000001728 | 0.000000367 |
| 469 | 1 | 0.000003220 | -0.000000261 | 0.000000173 |
| 470 | 1 | -0.000003329 | 0.000004149 | 0.000005963 |
| 471 | 1 | 0.000000977 | -0.000000934 | 0.000000525 |
| 472 | 1 | 0.000000829 | 0.000002471 | -0.000001363 |
| 473 | 1 | 0.000001313 | -0.000000874 | 0.000000491 |
| 474 | 1 | 0.000000127 | 0.000002433 | -0.000000099 |
| 475 | 6 | 0.000008322 | -0.000007200 | 0.000016481 |
| 476 | 6 | -0.000008963 | 0.000010136 | 0.000010642 |
| 477 | 7 | 0.000008943 | -0.000007825 | -0.000012685 |
| 478 | 6 | 0.000004320 | 0.000005337 | 0.000008812 |
| 479 | 6 | -0.000004496 | -0.000009297 | -0.000009867 |
| 480 | 6 | -0.000003348 | 0.000005510 | 0.000003049 |
| 481 | 1 | -0.000002989 | 0.000002342 | -0.000007676 |
| 482 | 1 | 0.000001977 | -0.000004949 | -0.000000387 |
| 483 | 1 | -0.000004987 | 0.000001316 | -0.000005320 |
| 484 | 1 | 0.000002244 | -0.000000144 | 0.000002003 |
| 485 | 1 | 0.000001290 | 0.000002726 | 0.000000545 |
| 486 | 1 | -0.000000072 | -0.000001942 | -0.000001016 |
| 487 | 1 | -0.000004018 | -0.000000443 | -0.000001159 |

Sum of electronic and thermal Free Energies = -1069.302106
ONIOM Total Energy = -1072.583130
0 imaginary frequency

***β*-4a@C$_R$**

| Center Number | Atomic Number | Integrated Forces (Hartrees/Bohr) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | 0.000001754 | -0.000000602 | -0.000000854 |
| 2 | 8 | 0.000001471 | -0.000000159 | 0.000002193 |
| 3 | 6 | 0.000000094 | 0.000000480 | 0.000000165 |
| 4 | 6 | -0.000000132 | -0.000000595 | -0.000000263 |
| 5 | 6 | -0.000001070 | 0.000000546 | 0.000000265 |
| 6 | 6 | -0.000000222 | -0.000001596 | -0.000000666 |
| 7 | 6 | -0.000000792 | 0.000000956 | -0.000000007 |

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|---|---|---|---|---|
| 8 | 6 | 0.000001290 | -0.000000852 | 0.000000613 |
| 9 | 6 | 0.000001196 | 0.000001594 | 0.000001538 |
| 10 | 6 | 0.000000014 | 0.000000307 | -0.000000455 |
| 11 | 1 | 0.000000281 | -0.000000083 | -0.000000025 |
| 12 | 1 | -0.000000096 | 0.000000204 | 0.000000280 |
| 13 | 1 | 0.000000097 | 0.000000287 | 0.000000301 |
| 14 | 1 | -0.000000104 | -0.000000083 | 0.000000009 |
| 15 | 1 | -0.000000020 | -0.000000011 | -0.000000008 |
| 16 | 1 | -0.000000034 | -0.000000125 | -0.000000169 |
| 17 | 8 | -0.000000234 | 0.000001349 | -0.000001183 |
| 18 | 8 | 0.000007924 | 0.000004529 | -0.000001727 |
| 19 | 6 | 0.000000650 | -0.000004054 | 0.000001350 |
| 20 | 6 | -0.000000566 | 0.000002473 | 0.000000459 |
| 21 | 6 | -0.000004188 | -0.000005344 | -0.000002019 |
| 22 | 6 | 0.000002836 | -0.000002774 | 0.000000780 |
| 23 | 6 | -0.000000157 | 0.000001523 | -0.000000573 |
| 24 | 6 | -0.000001324 | -0.000000889 | 0.000000103 |
| 25 | 6 | -0.000000228 | -0.000001032 | -0.000003067 |
| 26 | 6 | -0.000000274 | 0.000000460 | 0.000000849 |
| 27 | 1 | 0.000000008 | 0.000000069 | -0.000000096 |
| 28 | 1 | 0.000000059 | 0.000000144 | 0.000000030 |
| 29 | 1 | 0.000000489 | 0.000002196 | -0.000001205 |
| 30 | 1 | -0.000000153 | 0.000000204 | 0.000000157 |
| 31 | 1 | 0.000000058 | -0.000000113 | 0.000000340 |
| 32 | 1 | -0.000000015 | 0.000000015 | -0.000000038 |
| 33 | 8 | -0.000002296 | -0.000000231 | -0.000001090 |
| 34 | 8 | -0.000001376 | 0.000002592 | -0.000003200 |
| 35 | 6 | -0.000001481 | 0.000000357 | -0.000000739 |
| 36 | 6 | -0.000000695 | 0.000000126 | -0.000000855 |
| 37 | 6 | -0.000002903 | -0.000000563 | -0.000002444 |
| 38 | 6 | 0.000001819 | 0.000000275 | 0.000002310 |
| 39 | 6 | -0.000000017 | 0.000000657 | 0.000000015 |
| 40 | 6 | -0.000001163 | -0.000001759 | 0.000001025 |
| 41 | 6 | -0.000000623 | -0.000000362 | -0.000000555 |
| 42 | 6 | 0.000000181 | -0.000000467 | 0.000000373 |
| 43 | 1 | 0.000000143 | 0.000000149 | 0.000000513 |
| 44 | 1 | 0.000000057 | 0.000000035 | -0.000000311 |
| 45 | 1 | 0.000000222 | 0.000000211 | -0.000000135 |
| 46 | 1 | -0.000000018 | 0.000000010 | 0.000000085 |
| 47 | 1 | 0.000000058 | 0.000000075 | 0.000000116 |
| 48 | 1 | -0.000000056 | 0.000000076 | -0.000000036 |
| 49 | 8 | -0.000009865 | -0.000000892 | 0.000003400 |
| 50 | 8 | 0.000002152 | -0.000001065 | 0.000000409 |
| 51 | 6 | 0.000003450 | 0.000002831 | 0.000003140 |
| 52 | 6 | 0.000001084 | 0.000002360 | 0.000003296 |
| 53 | 6 | -0.000000954 | -0.000001647 | -0.000001586 |
| 54 | 6 | 0.000001376 | 0.000000761 | 0.000000135 |
| 55 | 6 | 0.000000129 | -0.000000382 | -0.000000286 |
| 56 | 6 | -0.000002950 | -0.000003892 | -0.000003082 |
| 57 | 6 | -0.000001247 | -0.000000103 | -0.000000998 |
| 58 | 6 | -0.000000268 | 0.000000069 | -0.000000061 |
| 59 | 1 | -0.000000329 | -0.000000500 | -0.000000934 |
| 60 | 1 | 0.000000029 | 0.000000784 | 0.000000308 |
| 61 | 1 | 0.000000120 | -0.000000597 | -0.000000176 |
| 62 | 1 | -0.000000009 | -0.000000011 | 0.000000061 |
| 63 | 1 | 0.000000100 | -0.000000096 | 0.000000243 |
| 64 | 1 | -0.000000109 | 0.000000121 | 0.000000135 |
| 65 | 1 | 0.000001721 | 0.000002503 | -0.000000378 |
| 66 | 1 | -0.000002593 | -0.000000241 | 0.000002201 |
| 67 | 1 | 0.000001357 | -0.000000462 | -0.000005381 |
| 68 | 1 | 0.000004803 | -0.000001049 | 0.000003287 |
| 69 | 1 | -0.000002413 | -0.000000902 | -0.000000854 |
| 70 | 1 | 0.000000519 | 0.000001486 | -0.000000246 |
| 71 | 1 | 0.000000138 | 0.000001054 | -0.000001388 |
| 72 | 1 | -0.000002326 | 0.000002636 | 0.000000722 |
| 73 | 8 | -0.000000883 | 0.000003167 | -0.000017206 |
| 74 | 8 | -0.000003960 | -0.000003271 | -0.000002847 |
| 75 | 6 | -0.000000700 | 0.000000355 | 0.000003698 |
| 76 | 6 | 0.000005742 | 0.000003430 | -0.000003800 |
| 77 | 6 | -0.000001501 | 0.000005571 | 0.000012728 |
| 78 | 6 | 0.000005001 | -0.000004188 | -0.000004488 |
| 79 | 6 | -0.000003284 | 0.000000942 | -0.000000849 |
| 80 | 6 | -0.000003316 | 0.000000966 | 0.000000723 |

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|---|---|---|---|---|
| 81 | 6 | 0.000003231 | 0.000003666 | -0.000002210 |
| 82 | 6 | 0.000000852 | -0.000001125 | 0.000002539 |
| 83 | 1 | -0.000006541 | -0.000000193 | 0.000000010 |
| 84 | 1 | -0.000000991 | 0.000000679 | 0.000000204 |
| 85 | 1 | 0.000002093 | -0.000001503 | -0.000000335 |
| 86 | 1 | -0.000000049 | -0.000000091 | -0.000000065 |
| 87 | 1 | -0.000000499 | -0.000000151 | -0.000000112 |
| 88 | 1 | -0.000000471 | -0.000000568 | -0.000000360 |
| 89 | 8 | 0.000000759 | 0.000004006 | 0.000001131 |
| 90 | 8 | -0.000013410 | -0.000002293 | 0.000001649 |
| 91 | 6 | -0.000004082 | -0.000007815 | 0.000004753 |
| 92 | 6 | 0.000001247 | 0.000007016 | -0.000003326 |
| 93 | 6 | -0.000003130 | -0.000005623 | -0.000000623 |
| 94 | 6 | 0.000005952 | 0.000000140 | 0.000001885 |
| 95 | 6 | -0.000000361 | -0.000000270 | -0.000000053 |
| 96 | 6 | 0.000002132 | 0.000004806 | -0.000004184 |
| 97 | 6 | -0.000001330 | 0.000000210 | 0.000001325 |
| 98 | 6 | 0.000001044 | 0.000000883 | 0.000000299 |
| 99 | 1 | 0.000001121 | -0.000000485 | -0.000000422 |
| 100 | 1 | 0.000000251 | 0.000000415 | 0.000000236 |
| 101 | 1 | -0.000000316 | 0.000001534 | 0.000000421 |
| 102 | 1 | -0.000000103 | -0.000000189 | -0.000000466 |
| 103 | 1 | -0.000000244 | -0.000000178 | -0.000000645 |
| 104 | 1 | -0.000000521 | -0.000000363 | 0.000000133 |
| 105 | 8 | 0.000005945 | -0.000003313 | 0.000003743 |
| 106 | 8 | 0.000009169 | -0.000006224 | -0.000006390 |
| 107 | 6 | -0.000004271 | 0.000005134 | -0.000008127 |
| 108 | 6 | 0.000014543 | -0.000007292 | 0.000000204 |
| 109 | 6 | -0.000011980 | 0.000003116 | 0.000009613 |
| 110 | 6 | -0.000000758 | 0.000000028 | -0.000006435 |
| 111 | 6 | 0.000000917 | 0.000000235 | -0.000000263 |
| 112 | 6 | -0.000002064 | -0.000001197 | 0.000002306 |
| 113 | 6 | -0.000000617 | -0.000002499 | 0.000001598 |
| 114 | 6 | 0.000000296 | 0.000000703 | -0.000001920 |
| 115 | 1 | -0.000002332 | 0.000001680 | 0.000001130 |
| 116 | 1 | 0.000000637 | -0.000000724 | 0.000001396 |
| 117 | 1 | 0.000001037 | -0.000000023 | -0.000000815 |
| 118 | 1 | 0.000000263 | -0.000000156 | 0.000000442 |
| 119 | 1 | -0.000000410 | -0.000000294 | 0.000001094 |
| 120 | 1 | 0.000000217 | -0.000000183 | 0.000000177 |
| 121 | 8 | -0.000002828 | -0.000000129 | 0.000007376 |
| 122 | 8 | -0.000004631 | 0.000001859 | 0.000000284 |
| 123 | 6 | -0.000009991 | -0.000004936 | -0.000010168 |
| 124 | 6 | -0.000001429 | 0.000000824 | -0.000003847 |
| 125 | 6 | 0.000004282 | -0.000007156 | -0.000004470 |
| 126 | 6 | 0.000005504 | 0.000000136 | 0.000001962 |
| 127 | 6 | -0.000001168 | 0.000001926 | 0.000001904 |
| 128 | 6 | 0.000000176 | 0.000013476 | 0.000007509 |
| 129 | 6 | 0.000002222 | 0.000001980 | 0.000003313 |
| 130 | 6 | -0.000001039 | -0.000002517 | -0.000000176 |
| 131 | 1 | 0.000001972 | 0.000001313 | 0.000004147 |
| 132 | 1 | -0.000000288 | 0.000000278 | -0.000000880 |
| 133 | 1 | -0.000003153 | -0.000001165 | 0.000000702 |
| 134 | 1 | 0.000000255 | -0.000000179 | -0.000000294 |
| 135 | 1 | 0.000000198 | -0.000000260 | -0.000000152 |
| 136 | 1 | 0.000000418 | -0.000000089 | 0.000000025 |
| 137 | 1 | 0.000005696 | 0.000005223 | -0.000000016 |
| 138 | 1 | -0.000001439 | 0.000001316 | -0.000001637 |
| 139 | 1 | -0.000003304 | 0.000001549 | 0.000001315 |
| 140 | 1 | 0.000001835 | -0.000005856 | -0.000003019 |
| 141 | 1 | -0.000000058 | 0.000000359 | -0.000000786 |
| 142 | 1 | 0.000004146 | 0.000009164 | 0.000013753 |
| 143 | 1 | 0.000010095 | -0.000011094 | 0.000002793 |
| 144 | 1 | -0.000000143 | -0.000000050 | -0.000001259 |
| 145 | 8 | 0.000007920 | 0.000008973 | 0.000003779 |
| 146 | 1 | -0.000002099 | -0.000005191 | -0.000004221 |
| 147 | 1 | -0.000005719 | -0.000004495 | 0.000000383 |
| 148 | 8 | -0.000001819 | 0.000005081 | -0.000002217 |
| 149 | 1 | 0.000001347 | -0.000000519 | 0.000000153 |
| 150 | 1 | 0.000003685 | -0.000002737 | 0.000001001 |
| 151 | 8 | 0.000001636 | -0.000000281 | 0.000005494 |
| 152 | 1 | 0.000001609 | 0.000001393 | 0.000001274 |
| 153 | 1 | 0.000001372 | -0.000002867 | -0.000001934 |

| | | | | |
|---|---|---|---|---|
| 154 | 8 | -0.000007733 | 0.000003636 | 0.000003180 |
| 155 | 1 | -0.000001028 | -0.000002252 | -0.000000200 |
| 156 | 1 | 0.000015181 | 0.000001755 | -0.000007676 |
| 157 | 1 | 0.000000737 | -0.000007342 | -0.000006018 |
| 158 | 8 | -0.000002158 | 0.000009322 | 0.000006108 |
| 159 | 8 | 0.000010716 | -0.000005229 | 0.000009195 |
| 160 | 6 | 0.000000731 | -0.000003990 | -0.000002705 |
| 161 | 6 | 0.000003309 | 0.000000160 | 0.000003045 |
| 162 | 6 | -0.000005682 | -0.000007743 | -0.000001249 |
| 163 | 6 | -0.000007768 | 0.000001663 | 0.000001394 |
| 164 | 6 | 0.000003132 | 0.000004550 | -0.000002402 |
| 165 | 6 | -0.000003476 | -0.000003144 | -0.000001776 |
| 166 | 6 | -0.000001164 | 0.000001950 | 0.000003942 |
| 167 | 6 | 0.000000837 | -0.000001322 | -0.000000337 |
| 168 | 1 | 0.000000021 | -0.000001186 | -0.000001667 |
| 169 | 1 | 0.000001035 | -0.000000621 | 0.000000836 |
| 170 | 1 | 0.000000217 | 0.000000478 | 0.000001120 |
| 171 | 1 | 0.000000414 | 0.000000594 | -0.000000409 |
| 172 | 1 | -0.000000057 | 0.000000492 | -0.000000183 |
| 173 | 1 | 0.000000254 | 0.000000038 | -0.000000190 |
| 174 | 8 | -0.000001937 | 0.000000715 | -0.000001757 |
| 175 | 8 | -0.000002328 | -0.000003652 | 0.000000030 |
| 176 | 6 | 0.000000691 | 0.000000019 | 0.000000263 |
| 177 | 6 | -0.000001023 | -0.000000634 | -0.000000597 |
| 178 | 6 | 0.000000701 | 0.000000228 | 0.000000966 |
| 179 | 6 | 0.000001057 | 0.000000440 | 0.000000056 |
| 180 | 6 | 0.000000285 | 0.000000143 | -0.000000474 |
| 181 | 6 | 0.000000053 | -0.000001790 | 0.000000815 |
| 182 | 6 | -0.000000202 | -0.000001109 | 0.000000823 |
| 183 | 6 | -0.000000562 | -0.000000380 | 0.000000133 |
| 184 | 1 | 0.000000345 | 0.000000580 | 0.000000281 |
| 185 | 1 | -0.000000014 | 0.000000312 | -0.000000074 |
| 186 | 1 | 0.000000143 | -0.000000257 | 0.000000209 |
| 187 | 1 | 0.000000064 | 0.000000235 | 0.000000031 |
| 188 | 1 | 0.000000014 | 0.000000165 | -0.000000089 |
| 189 | 1 | 0.000000072 | 0.000000069 | -0.000000192 |
| 190 | 8 | -0.000003411 | -0.000002594 | 0.000012174 |
| 191 | 8 | -0.000003393 | 0.000002122 | 0.000004220 |
| 192 | 6 | 0.000003477 | 0.000004967 | -0.000008742 |
| 193 | 6 | -0.000002998 | -0.000003673 | -0.000000305 |
| 194 | 6 | 0.000005990 | 0.000008648 | -0.000002835 |
| 195 | 6 | -0.000001665 | -0.000002476 | -0.000000163 |
| 196 | 6 | -0.000002959 | -0.000003289 | 0.000001260 |
| 197 | 6 | 0.000003834 | 0.000001563 | -0.000001684 |
| 198 | 6 | -0.000000633 | 0.000000197 | 0.000000402 |
| 199 | 6 | 0.000000414 | 0.000000004 | 0.000000297 |
| 200 | 1 | -0.000001069 | -0.000000554 | 0.000000780 |
| 201 | 1 | -0.000001796 | 0.000000088 | 0.000000941 |
| 202 | 1 | 0.000000060 | 0.000000026 | -0.000000634 |
| 203 | 1 | 0.000000024 | -0.000000091 | 0.000000161 |
| 204 | 1 | 0.000000067 | -0.000000135 | 0.000000124 |
| 205 | 1 | -0.000000000 | -0.000000062 | -0.000000003 |
| 206 | 8 | 0.000000225 | 0.000000715 | -0.000000134 |
| 207 | 8 | -0.000002100 | -0.000000151 | 0.000002405 |
| 208 | 6 | -0.000000089 | -0.000000623 | -0.000000179 |
| 209 | 6 | 0.000000688 | -0.000000023 | 0.000000687 |
| 210 | 6 | -0.000000053 | -0.000003398 | 0.000000066 |
| 211 | 6 | -0.000001342 | 0.000006227 | 0.000002182 |
| 212 | 6 | 0.000000968 | -0.000000597 | 0.000000998 |
| 213 | 6 | -0.000001828 | 0.000000761 | -0.000002172 |
| 214 | 6 | 0.000001324 | 0.000000399 | 0.000001257 |
| 215 | 6 | -0.000000571 | -0.000000024 | 0.000000306 |
| 216 | 1 | -0.000001224 | 0.000000800 | -0.000000522 |
| 217 | 1 | 0.000000202 | -0.000001267 | -0.000001175 |
| 218 | 1 | 0.000000824 | -0.000001339 | -0.000001570 |
| 219 | 1 | 0.000000155 | 0.000000115 | -0.000000064 |
| 220 | 1 | 0.000000039 | -0.000000273 | 0.000000089 |
| 221 | 1 | 0.000000215 | 0.000000122 | 0.000000214 |
| 222 | 1 | 0.000000198 | 0.000001165 | -0.000008001 |
| 223 | 1 | 0.000002260 | -0.000001467 | 0.000001572 |
| 224 | 1 | 0.000000800 | 0.000000511 | 0.000000155 |
| 225 | 1 | -0.000000609 | 0.000000656 | -0.000010624 |
| 226 | 1 | 0.000003469 | -0.000005455 | -0.000000649 |

| | | | | |
|---|---|---|---|---|
| 227 | 1 | 0.000000687 | -0.000000769 | 0.000000759 |
| 228 | 1 | 0.000000910 | -0.000000652 | -0.000000031 |
| 229 | 1 | 0.000002319 | -0.000000246 | -0.000000205 |
| 230 | 1 | -0.000000627 | -0.000004414 | -0.000003860 |
| 231 | 1 | 0.000002552 | 0.000001640 | 0.000000638 |
| 232 | 8 | -0.000006568 | 0.000000361 | -0.000002817 |
| 233 | 8 | -0.000000309 | 0.000004668 | 0.000000856 |
| 234 | 6 | -0.000002089 | 0.000009823 | 0.000004995 |
| 235 | 6 | 0.000006332 | -0.000000875 | -0.000000605 |
| 236 | 6 | -0.000004368 | 0.000001402 | 0.000010660 |
| 237 | 6 | 0.000000795 | 0.000001962 | -0.000003434 |
| 238 | 6 | 0.000003548 | -0.000000859 | -0.000002487 |
| 239 | 6 | 0.000003732 | -0.000006419 | -0.000004108 |
| 240 | 6 | 0.000001164 | -0.000004066 | 0.000002772 |
| 241 | 6 | 0.000000215 | -0.000001131 | 0.000000386 |
| 242 | 1 | 0.000000538 | -0.000000132 | -0.000002057 |
| 243 | 1 | -0.000000500 | -0.000001198 | 0.000002789 |
| 244 | 1 | -0.000001629 | -0.000000220 | -0.000004579 |
| 245 | 1 | -0.000000745 | 0.000000749 | 0.000000558 |
| 246 | 1 | -0.000000980 | -0.000000177 | -0.000000158 |
| 247 | 1 | 0.000000306 | 0.000000400 | -0.000000177 |
| 248 | 8 | -0.000005208 | -0.000002190 | -0.000006792 |
| 249 | 8 | 0.000007362 | -0.000009938 | 0.000013953 |
| 250 | 6 | 0.000006597 | -0.000001219 | 0.000011542 |
| 251 | 6 | 0.000000485 | 0.000000014 | -0.000003258 |
| 252 | 6 | -0.000000383 | -0.000000989 | 0.000004700 |
| 253 | 6 | 0.000001799 | 0.000002593 | -0.000003917 |
| 254 | 6 | 0.000002636 | -0.000000783 | -0.000000329 |
| 255 | 6 | -0.000000319 | 0.000003922 | -0.000005934 |
| 256 | 6 | 0.000002294 | 0.000003884 | 0.000001593 |
| 257 | 6 | -0.000000852 | 0.000000040 | -0.000001068 |
| 258 | 1 | 0.000001835 | 0.000000365 | -0.000001196 |
| 259 | 1 | -0.000000639 | -0.000000033 | 0.000001647 |
| 260 | 1 | -0.000000944 | 0.000000352 | 0.000000234 |
| 261 | 1 | -0.000000161 | -0.000000451 | 0.000000372 |
| 262 | 1 | 0.000000268 | -0.000000220 | 0.000000308 |
| 263 | 1 | -0.000000045 | -0.000000298 | 0.000000165 |
| 264 | 8 | -0.000008228 | -0.000002875 | -0.000000804 |
| 265 | 8 | -0.000007291 | -0.000003687 | 0.000003307 |
| 266 | 6 | 0.000004945 | -0.000000778 | -0.000007162 |
| 267 | 6 | -0.000002665 | 0.000001127 | 0.000001614 |
| 268 | 6 | 0.000001196 | -0.000002363 | -0.000000955 |
| 269 | 6 | 0.000001265 | 0.000000268 | 0.000002800 |
| 270 | 6 | 0.000000158 | -0.000000093 | -0.000003015 |
| 271 | 6 | -0.000003597 | -0.000003576 | 0.000002251 |
| 272 | 6 | -0.000002251 | 0.000001348 | 0.000000316 |
| 273 | 6 | -0.000000059 | 0.000000248 | -0.000000863 |
| 274 | 1 | 0.000000855 | 0.000000561 | -0.000000510 |
| 275 | 1 | 0.000000518 | 0.000000745 | -0.000000573 |
| 276 | 1 | -0.000000835 | 0.000000966 | -0.000000424 |
| 277 | 1 | 0.000000168 | -0.000000162 | 0.000000038 |
| 278 | 1 | 0.000000015 | -0.000000069 | 0.000000057 |
| 279 | 1 | -0.000000026 | 0.000000101 | -0.000000098 |
| 280 | 8 | 0.000011558 | -0.000008798 | 0.000003479 |
| 281 | 8 | -0.000001280 | 0.000001233 | 0.000004841 |
| 282 | 6 | -0.000001377 | 0.000003051 | 0.000004734 |
| 283 | 6 | 0.000001077 | -0.000006877 | 0.000006694 |
| 284 | 6 | 0.000003060 | 0.000003293 | -0.000008746 |
| 285 | 6 | 0.000002131 | 0.000004016 | 0.000000988 |
| 286 | 6 | -0.000003111 | 0.000000262 | 0.000004999 |
| 287 | 6 | -0.000002441 | 0.000003793 | -0.000003659 |
| 288 | 6 | -0.000002198 | -0.000006732 | 0.000001587 |
| 289 | 6 | 0.000001424 | -0.000002167 | -0.000000862 |
| 290 | 1 | -0.000005935 | 0.000004202 | -0.000003807 |
| 291 | 1 | 0.000001512 | -0.000000301 | -0.000001577 |
| 292 | 1 | -0.000000552 | -0.000002925 | 0.000001310 |
| 293 | 1 | -0.000000412 | 0.000000597 | -0.000001416 |
| 294 | 1 | -0.000000298 | 0.000000461 | -0.000000286 |
| 295 | 1 | 0.000000025 | 0.000000278 | -0.000000676 |
| 296 | 1 | 0.000004407 | 0.000004330 | 0.000000759 |
| 297 | 1 | 0.000001422 | 0.000000637 | -0.000001894 |
| 298 | 1 | -0.000006407 | 0.000008456 | -0.000002141 |
| 299 | 1 | -0.000003506 | -0.000001401 | 0.000001321 |

| | | | | |
|---|---|---|---|---|
| 300 | 1 | -0.000003234 | 0.000001338 | 0.000001154 |
| 301 | 1 | 0.000002115 | -0.000003435 | 0.000000363 |
| 302 | 1 | 0.000005584 | 0.000000945 | 0.000001399 |
| 303 | 1 | -0.000000166 | 0.000000569 | 0.000002931 |
| 304 | 1 | -0.000004746 | -0.000003976 | -0.000006670 |
| 305 | 8 | -0.000001499 | 0.000001884 | -0.000002712 |
| 306 | 8 | -0.000000708 | -0.000002129 | 0.000002132 |
| 307 | 6 | -0.000000991 | -0.000000010 | -0.000002748 |
| 308 | 6 | 0.000005280 | -0.000002519 | -0.000002412 |
| 309 | 6 | -0.000004931 | 0.000006212 | -0.000001955 |
| 310 | 6 | 0.000000698 | -0.000003264 | -0.000001388 |
| 311 | 6 | -0.000000673 | -0.000002262 | 0.000001827 |
| 312 | 6 | 0.000000162 | 0.000000054 | 0.000005355 |
| 313 | 6 | -0.000002952 | 0.000001602 | 0.000002989 |
| 314 | 6 | 0.000001357 | -0.000000028 | -0.000000353 |
| 315 | 1 | -0.000000690 | -0.000000226 | 0.000000561 |
| 316 | 1 | 0.000000660 | 0.000000827 | -0.000000864 |
| 317 | 1 | -0.000000523 | 0.000000089 | 0.000000031 |
| 318 | 1 | -0.000000084 | -0.000000018 | 0.000000044 |
| 319 | 1 | 0.000000276 | 0.000000182 | -0.000000076 |
| 320 | 1 | 0.000000106 | 0.000000185 | -0.000000155 |
| 321 | 8 | -0.000000467 | -0.000000010 | 0.000000727 |
| 322 | 8 | 0.000001937 | 0.000012426 | 0.000005915 |
| 323 | 6 | 0.000002423 | 0.000002255 | -0.000000987 |
| 324 | 6 | -0.000007178 | -0.000005256 | -0.000006495 |
| 325 | 6 | 0.000001441 | -0.000006922 | 0.000010027 |
| 326 | 6 | 0.000007479 | 0.000002094 | -0.000001420 |
| 327 | 6 | -0.000003201 | 0.000003106 | -0.000002546 |
| 328 | 6 | -0.000005190 | -0.000002743 | 0.000002785 |
| 329 | 6 | -0.000004028 | -0.000000951 | -0.000001120 |
| 330 | 6 | -0.000000948 | 0.000000954 | 0.000000487 |
| 331 | 1 | 0.000002561 | 0.000001006 | -0.000001844 |
| 332 | 1 | 0.000002781 | -0.000000982 | -0.000000555 |
| 333 | 1 | -0.000000689 | 0.000000126 | 0.000002079 |
| 334 | 1 | 0.000000635 | 0.000000375 | -0.000000362 |
| 335 | 1 | 0.000000353 | 0.000000338 | -0.000000634 |
| 336 | 1 | 0.000000580 | 0.000000481 | -0.000000184 |
| 337 | 8 | 0.000001637 | -0.000012608 | -0.000001493 |
| 338 | 8 | 0.000012092 | -0.000010148 | 0.000001866 |
| 339 | 6 | -0.000001090 | 0.000004218 | -0.000003865 |
| 340 | 6 | -0.000003674 | 0.000010522 | 0.000004064 |
| 341 | 6 | -0.000012616 | 0.000010291 | -0.000004995 |
| 342 | 6 | -0.000001602 | 0.000005042 | -0.000005090 |
| 343 | 6 | 0.000004933 | 0.000001805 | -0.000002209 |
| 344 | 6 | 0.000004520 | -0.000002209 | -0.000004828 |
| 345 | 6 | -0.000001037 | -0.000004790 | -0.000000644 |
| 346 | 6 | 0.000001376 | 0.000000026 | -0.000000053 |
| 347 | 1 | -0.000000942 | -0.000001794 | -0.000001029 |
| 348 | 1 | -0.000003052 | 0.000000546 | 0.000000056 |
| 349 | 1 | -0.000002363 | -0.000001194 | 0.000002501 |
| 350 | 1 | -0.000000230 | -0.000000178 | -0.000000135 |
| 351 | 1 | -0.000000041 | -0.000000166 | -0.000000042 |
| 352 | 1 | -0.000000382 | 0.000000354 | -0.000000036 |
| 353 | 8 | -0.000003958 | 0.000005254 | -0.000003965 |
| 354 | 8 | 0.000005436 | 0.000002976 | 0.000002690 |
| 355 | 6 | 0.000001053 | -0.000005314 | 0.000002866 |
| 356 | 6 | -0.000001488 | 0.000004002 | -0.000003852 |
| 357 | 6 | -0.000003523 | -0.000009469 | 0.000003603 |
| 358 | 6 | 0.000001853 | 0.000006147 | -0.000003606 |
| 359 | 6 | 0.000002141 | -0.000000921 | -0.000000538 |
| 360 | 6 | 0.000003371 | 0.000000909 | -0.000002604 |
| 361 | 6 | 0.000004012 | 0.000000048 | -0.000000393 |
| 362 | 6 | -0.000000802 | -0.000001365 | 0.000001161 |
| 363 | 1 | -0.000000360 | 0.000000331 | 0.000000523 |
| 364 | 1 | -0.000000989 | 0.000001133 | 0.000001704 |
| 365 | 1 | -0.000001010 | -0.000002327 | 0.000000558 |
| 366 | 1 | -0.000000108 | 0.000000252 | -0.000000344 |
| 367 | 1 | 0.000000052 | -0.000000110 | -0.000000359 |
| 368 | 1 | 0.000000230 | 0.000000289 | -0.000000123 |
| 369 | 1 | -0.000001478 | -0.000002216 | 0.000003214 |
| 370 | 1 | 0.000000024 | -0.000005917 | -0.000001634 |
| 371 | 1 | 0.000000294 | 0.000001092 | 0.000001484 |
| 372 | 1 | -0.000005614 | 0.000000690 | -0.000000803 |

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|---|---|---|---|---|
| 373 | 1 | 0.000000420 | -0.000001586 | 0.000001901 |
| 374 | 1 | -0.000001745 | 0.000002052 | -0.000000182 |
| 375 | 1 | 0.000001425 | 0.000001069 | -0.000000215 |
| 376 | 1 | -0.000000668 | -0.000000062 | -0.000000173 |
| 377 | 8 | -0.000000349 | -0.000001127 | -0.000004165 |
| 378 | 8 | 0.000000951 | -0.000001713 | -0.000000151 |
| 379 | 6 | 0.000002139 | -0.000000914 | -0.000000680 |
| 380 | 6 | -0.000001022 | 0.000000180 | -0.000000233 |
| 381 | 6 | 0.000001249 | 0.000000755 | -0.000000113 |
| 382 | 6 | -0.000000688 | 0.000000008 | -0.000000200 |
| 383 | 6 | -0.000000450 | -0.000000429 | -0.000000121 |
| 384 | 6 | -0.000001356 | 0.000001518 | -0.000000863 |
| 385 | 6 | 0.000000183 | 0.000000258 | 0.000000156 |
| 386 | 6 | 0.000000093 | 0.000000311 | -0.000000292 |
| 387 | 1 | 0.000000076 | -0.000000034 | 0.000000028 |
| 388 | 1 | 0.000000181 | -0.000000048 | 0.000000115 |
| 389 | 1 | 0.000000448 | 0.000000008 | 0.000000330 |
| 390 | 1 | 0.000000025 | 0.000000012 | 0.000000110 |
| 391 | 1 | -0.000000059 | -0.000000127 | 0.000000098 |
| 392 | 1 | -0.000000054 | 0.000000008 | 0.000000005 |
| 393 | 8 | -0.000002024 | -0.000000039 | -0.000001206 |
| 394 | 8 | 0.000002762 | 0.000002031 | -0.000001205 |
| 395 | 6 | -0.000001793 | -0.000002487 | -0.000000568 |
| 396 | 6 | -0.000000258 | 0.000000704 | -0.000001504 |
| 397 | 6 | -0.000001762 | -0.000000784 | 0.000001782 |
| 398 | 6 | -0.000002617 | -0.000001650 | -0.000000493 |
| 399 | 6 | 0.000000279 | 0.000000386 | -0.000000917 |
| 400 | 6 | 0.000000459 | 0.000000452 | 0.000000962 |
| 401 | 6 | -0.000001309 | -0.000000404 | -0.000001265 |
| 402 | 6 | 0.000000441 | -0.000000300 | -0.000000180 |
| 403 | 1 | 0.000000396 | 0.000000343 | 0.000000265 |
| 404 | 1 | 0.000000399 | 0.000000143 | -0.000000012 |
| 405 | 1 | 0.000000671 | 0.000001154 | 0.000001066 |
| 406 | 1 | 0.000000089 | 0.000000040 | -0.000000028 |
| 407 | 1 | 0.000000178 | 0.000000090 | 0.000000110 |
| 408 | 1 | 0.000000023 | -0.000000090 | -0.000000056 |
| 409 | 8 | 0.000002154 | -0.000000510 | -0.000000241 |
| 410 | 8 | 0.000001664 | 0.000001993 | 0.000002126 |
| 411 | 6 | 0.000000033 | 0.000002046 | -0.000000797 |
| 412 | 6 | -0.000000358 | -0.000000896 | 0.000000467 |
| 413 | 6 | 0.000000355 | -0.000000633 | -0.000002432 |
| 414 | 6 | -0.000000971 | 0.000000886 | 0.000000602 |
| 415 | 6 | 0.000000126 | -0.000001033 | 0.000000662 |
| 416 | 6 | 0.000000116 | 0.000000391 | 0.000000083 |
| 417 | 6 | 0.000000450 | -0.000000496 | 0.000000404 |
| 418 | 6 | 0.000000136 | -0.000000228 | -0.000000136 |
| 419 | 1 | -0.000000398 | -0.000000070 | 0.000000207 |
| 420 | 1 | 0.000000005 | -0.000000099 | -0.000000083 |
| 421 | 1 | 0.000000198 | 0.000000144 | -0.000000276 |
| 422 | 1 | 0.000000017 | 0.000000065 | 0.000000049 |
| 423 | 1 | 0.000000051 | 0.000000006 | 0.000000098 |
| 424 | 1 | 0.000000060 | 0.000000086 | -0.000000076 |
| 425 | 8 | 0.000000862 | -0.000004943 | 0.000000793 |
| 426 | 8 | 0.000000906 | 0.000005574 | 0.000001477 |
| 427 | 6 | -0.000001572 | -0.000000994 | -0.000002115 |
| 428 | 6 | -0.000001375 | -0.000001896 | -0.000000390 |
| 429 | 6 | 0.000000510 | 0.000001778 | 0.000000145 |
| 430 | 6 | 0.000000469 | -0.000000730 | 0.000001263 |
| 431 | 6 | -0.000002048 | -0.000001311 | -0.000001051 |
| 432 | 6 | 0.000001596 | 0.000002616 | 0.000001162 |
| 433 | 6 | -0.000000859 | -0.000000127 | 0.000000338 |
| 434 | 6 | -0.000000163 | 0.000000290 | 0.000000381 |
| 435 | 1 | 0.000001743 | 0.000000237 | 0.000000847 |
| 436 | 1 | 0.000000435 | -0.000000055 | -0.000000176 |
| 437 | 1 | -0.000000504 | -0.000000486 | 0.000000139 |
| 438 | 1 | 0.000000225 | -0.000000095 | 0.000000078 |
| 439 | 1 | 0.000000175 | 0.000000059 | 0.000000048 |
| 440 | 1 | 0.000000042 | -0.000000035 | -0.000000037 |
| 441 | 1 | -0.000000728 | -0.000001144 | 0.000001194 |
| 442 | 1 | -0.000000133 | 0.000003540 | 0.000000780 |
| 443 | 1 | -0.000000555 | -0.000006000 | 0.000001829 |
| 444 | 1 | -0.000000531 | -0.000002549 | 0.000000371 |
| 445 | 8 | -0.000032389 | 0.000033256 | 0.000010717 |

| | | | | |
|---|---|---|---|---|
| 446 | 1 | 0.000016590 | -0.000010962 | -0.000024918 |
| 447 | 1 | 0.000004816 | -0.000008231 | -0.000006833 |
| 448 | 8 | -0.000008946 | -0.000007059 | 0.000003416 |
| 449 | 1 | 0.000004047 | 0.000005874 | -0.000002740 |
| 450 | 1 | 0.000005452 | 0.000004021 | 0.000001454 |
| 451 | 8 | -0.000000299 | -0.000003820 | 0.000005399 |
| 452 | 1 | -0.000000784 | 0.000001391 | -0.000000926 |
| 453 | 1 | 0.000003474 | -0.000001103 | -0.000004276 |
| 454 | 8 | 0.000009711 | -0.000005154 | -0.000011137 |
| 455 | 1 | -0.000003437 | 0.000002930 | -0.000001416 |
| 456 | 1 | -0.000008310 | 0.000007711 | 0.000004819 |
| 457 | 6 | -0.000011550 | 0.000014835 | 0.000013838 |
| 458 | 6 | -0.000016536 | -0.000014100 | 0.000014222 |
| 459 | 6 | 0.000016192 | -0.000017543 | -0.000018313 |
| 460 | 7 | 0.000001281 | 0.000044954 | 0.000033937 |
| 461 | 6 | 0.000029982 | 0.000005453 | -0.000006916 |
| 462 | 6 | -0.000000352 | 0.000001266 | -0.000004090 |
| 463 | 6 | 0.000006953 | 0.000003882 | -0.000005520 |
| 464 | 6 | -0.000007251 | -0.000008699 | -0.000005263 |
| 465 | 6 | -0.000000505 | 0.000005225 | 0.000005161 |
| 466 | 8 | 0.000010590 | -0.000017387 | 0.000023198 |
| 467 | 8 | -0.000012435 | -0.000022999 | -0.000012656 |
| 468 | 1 | -0.000002434 | -0.000009150 | -0.000003940 |
| 469 | 1 | -0.000003867 | 0.000004818 | -0.000007457 |
| 470 | 1 | -0.000010549 | 0.000004191 | -0.000000180 |
| 471 | 1 | 0.000000515 | -0.000002077 | 0.000000110 |
| 472 | 1 | 0.000001310 | 0.000001243 | 0.000004903 |
| 473 | 1 | 0.000003198 | 0.000002906 | 0.000000950 |
| 474 | 1 | 0.000002908 | 0.000001512 | -0.000002288 |
| 475 | 6 | 0.000005790 | 0.000026207 | -0.000009561 |
| 476 | 6 | 0.000011411 | -0.000025440 | 0.000021492 |
| 477 | 7 | -0.000015491 | 0.000016660 | -0.000038282 |
| 478 | 6 | 0.000009216 | 0.000002967 | 0.000002808 |
| 479 | 6 | -0.000002742 | -0.000010859 | 0.000018311 |
| 480 | 6 | 0.000000254 | 0.000010899 | 0.000008172 |
| 481 | 1 | -0.000002381 | -0.000008926 | -0.000002144 |
| 482 | 1 | 0.000001492 | 0.000001828 | -0.000000840 |
| 483 | 1 | -0.000003498 | -0.000006238 | -0.000002084 |
| 484 | 1 | 0.000000017 | 0.000001366 | 0.000001845 |
| 485 | 1 | -0.000001698 | -0.000000057 | 0.000001815 |
| 486 | 1 | -0.000001384 | -0.000007089 | -0.000002532 |
| 487 | 1 | 0.000000976 | 0.000001544 | -0.000003578 |

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Sum of electronic and thermal Free Energies = -1069.319090
ONIOM Total Energy = -1072.610990
0 imaginary frequency