

Supporting Information

Computer-Aided Rational Design of Fe(III)-Catalysts for the Selective Formation of Cyclic Carbonates from CO₂ and Internal Epoxides

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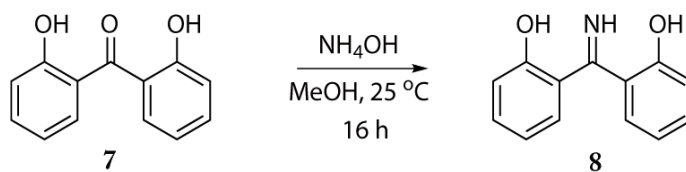
1. General experimental details

Commercially available reagents and carbon dioxide (99.99%) were used without further purification or drying. All of the CO₂/epoxide coupling reactions were conducted in a 80 mL stainless steel reactor with a magnetic stir bar. ¹H NMR (400 MHz) and ¹³C NMR (100 MHz) spectra were recorded on a Bruker Avance III HD spectrometer. Mass spectra were obtained on a Bruker Daltonik TOF-Q II high-resolution mass spectrometer (ESI) at the KAIST Analyst Center. (Mass spectra (ESI-MS) of **1c** and **1d** were collected on a Thermo Finnigan (San Jose, CA, USA) LCQTM Advantage MAX quadrupole ion trap instrument. UV-Vis spectra were recorded on an Agilent Cary 60 UV-Vis spectrophotometer using a 1cm two-window quartz spectrophotometer cell sealed with a screw-cap purchased from Sigma-Aldrich Co. LLC (Catalog number: Z276820). Infrared spectra were recorded in KBr pellets by a Bruker VECTOR 33. Elemental analyses were carried out at the KAIST Analysis Center on a Thermo Scientific FLASH 2000 series instrument. The diffraction data of **10d**, **1c** and **1d** were collected on a Bruker SMART APEX II. The diffraction data of **10c** was collected on a Bruker D8 QUEST. A suitable size and quality of crystal was coated with Paratone-*N* oil and mounted on a glass capillary. The data were collected with graphite-monochromated MoK α radiation ($\lambda = 0.71073$ Å) at 120 K. Cell parameters were determined and refined by SMART program.^[S1] Data reduction was performed using SAINT software.^[S2] An empirical absorption correction was applied using the SADABS program.^[S3]

2. Synthesis of ligands and catalysts

1b and **1e** were synthesized according to the reported procedures.^[S4] Aminotris(phenolate) ligands were prepared following the previously reported procedure.^{[S5],[S6]} Fe-salen-Cl were synthesized following the previously reported procedure.^{[S7]-[S9]}

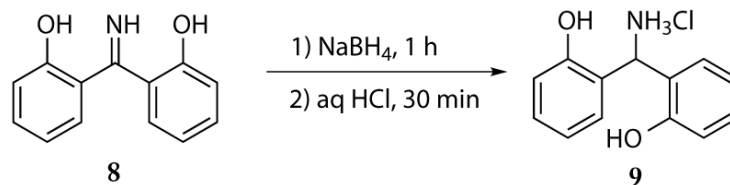
Preparation of **8**.



Aqueous ammonium hydroxide (38 mL, 560 mmol, 4 equiv.) was added to a solution of **7** (30 g, 140 mmol) in methanol (300 mL) at ambient temperature with continuous stirring. Yellow solids were precipitated out within 1 h and the opaque mixture was further stirred for 16 h. The crude ¹H NMR spectra in DMSO-*d*₆ was taken to confirm the complete conversion of **7** to **8**. The precipitate was filtered, washed with methanol and dried under vacuum to afford **8** as a yellow solid (90% yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 7.33 – 7.29 (ddd, *J* = 8.60, 7.20, 1.75 Hz, 2H), 7.06 – 7.05 (d, *J* = 7.49 Hz, 2H), 6.90 – 6.88 (d, *J* = 8.29 Hz, 2H), 6.76 – 6.72 (br, 2H). ¹³C

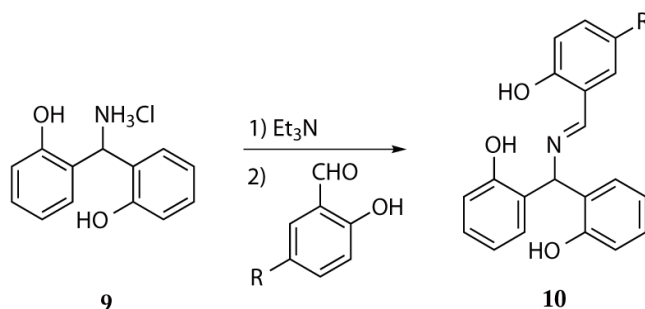
NMR (100 MHz, DMSO- d_6): δ 177.3, 132.4, 130.0, 117.8, 117.1; HRMS (ESI) calculated. for $C_{13}H_{12}NO_2[M+H]^+$: 214.0868, obtained: 214.0867.

Preparation of **9**.

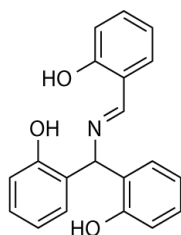


A solution of **8** (20 g, 94 mmol) in methanol (190 mL) was treated with $NaBH_4$ (6.4 g, 170 mmol, 1.8 equiv.) at ambient temperature. The reaction was monitored by 1H NMR in DMSO- d_6 . Almost complete conversion could be observed after an hour, indicating that the reduction was complete. 37% of aqueous HCl (24.3 mL, 28 mmol, 3 equiv.) was added to this at 0 °C and stirred for another 30 minutes. After that the solvent was evaporated and the product was redissolved in ethanol (200 mL). NaCl was precipitated out from the reaction mixture and it was removed by filtration. The remaining ethanolic solution was further concentrated and $CHCl_3$ (200 mL) was added to afford the product as a white solid. It was filtered and washed with $CHCl_3$ (50 mL X 3) and then dried in an oven (50 °C). Yield 91%. 1H NMR (400 MHz, DMSO- d_6): δ 10.32 (s, 2H), 8.65 (s, 3H), 7.32 – 7.29 (dd, J = 7.73, 1.64 Hz, 2H), 7.19 – 7.15 (m, 2H), 7.07 – 7.05 (dd, J = 8.17, 1.29 Hz, 2H), 6.83 – 6.79 (t, J = 7.77 Hz, 2H), 5.87 – 5.86 (d, J = 4.63 Hz, 1H). ^{13}C NMR (100 MHz, DMSO- d_6): δ 155.0, 129.4, 128.4, 123.4, 118.8, 115.7, 47.4. HRMS (ESI) calculated for $C_{13}H_{14}NO_2[M-Cl]^+$: 216.1019, obtained: 216.1002.

General procedure for synthesizing ligand, **10**.

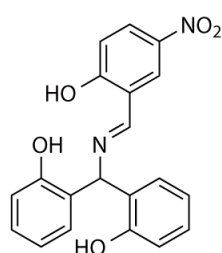


Triethylamine (2.3 mL, 16.7 mmol, 1.05 equiv.) and salicylaldehyde (1.8 mL, 16.7 mmol, 1.05 equiv.) were added to a methanolic solution of **9** (4 g, 15.9 mmol) and stirred. Yellow solid was precipitated in an hour. Completion of the reaction was confirmed by 1H NMR spectroscopy. The precipitate was filtered and washed with methanol (20 mL X 3) thoroughly and dried in a vacuum oven (50 °C).



10c

Yellow solid, 84% yield. ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 13.90 (s, 1H), 9.56 (s, 2H), 8.65 (s, 1H), 7.47 – 7.44 (dd, J = 8.02, 1.57 Hz, 1H), 7.34 – 7.30 (m, 1H), 7.14 – 7.08 (m, 4H), 6.89 – 6.84 (m, 4H), 6.82 – 6.78 (td, J = 7.44, 1.20 Hz, 2H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.8, 160.8, 154.8, 132.4, 131.8, 128.2, 128.1, 127.8, 118.8, 118.8, 118.5, 116.5, 115.3, 63.7. UV-Vis [THF, nm ($\text{Lmol}^{-1} \text{cm}^{-1}$)]: 259 (40000), ~285 (sh, 20000), 318 (10000). IR (KBr pellet, cm^{-1}): 3095, 2973, 2911, 2744, 2620, 2507, 1646, 1633, 1538, 1455, 1398, 1267, 1147, 1101, 1025, 916, 904, 842, 757. Crystals suitable for X-ray diffraction were obtained by slow diffusion of pentane into a saturated THF solution of **10c**. HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{18}\text{NO}_3[\text{M}+\text{H}]^+$: 320.1287, obtained: 320.1271.

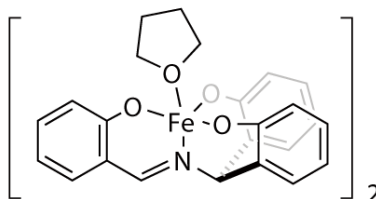


10d

Yellow solid, 87% yield. ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 15.15 (s, 1H), 10.02 (s, 2H), 8.94 (s, 1H), 8.51 – 8.50 (d, J = 3.06 Hz, 1H), 8.07 – 8.04 (dd, J = 9.62, 3.07 Hz, 1H), 7.20 – 7.10 (td, J = 8.00, 1.65 Hz, 2H), 7.13 – 7.10 (dd, J = 7.68, 1.38 Hz, 2H), 6.89 – 6.87 (dd, J = 8.07, 0.94 Hz, 2H), 6.84 – 6.80 (td, J = 7.59, 1.02 Hz, 2H), 6.65 – 6.53 (d, J = 9.63 Hz, 1H), 6.33 (s, 1H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 176.6, 165.9, 155.0, 134.5, 132.2, 129.2, 128.5, 124.5, 122.2, 119.1, 115.6, 114.0, 62.0. UV-Vis [THF, nm ($\text{L mol}^{-1} \text{cm}^{-1}$)]: 261 (20000), 321 (10000), 407 (5000). IR (KBr pellet, cm^{-1}): 3534, 3079, 2981, 2742, 2624, 1650, 1639, 1548, 1508, 1457, 1330, 1236, 1174, 1099, 1039, 950, 910, 842, 753. Crystals suitable for X-ray diffraction were obtained by slow diffusion of pentane into a saturated THF solution of **10d**. HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}_5[\text{M}+\text{H}]^+$: 365.1137, obtained: 365.1109.

Preparation of Fe complexes.

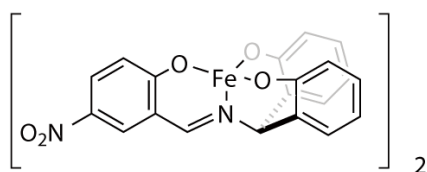
Synthesis of [**1c**(THF)]₂.



A solution of **10c** (0.122 g, 0.379 mmol) in 5 mL of THF treated with triethylamine (159 μL , 1.14 mmol) at room temperature and stirred. This was followed by the addition of FeCl_3 (0.064 g, 0.38 mmol) in 10 mL of THF. The solution changed its color from yellow to dark brown. The resulting reaction mixture was stirred for another 1 h at room temperature and then filtered through Celite. All volatiles were removed under vacuum. The product was washed

thoroughly with ethanol and dried under vacuum to obtain **1c** (0.124 g, 0.296 mmol, 78.1%) as a dark brown solid. UV-Vis [THF, nm ($\text{L mol}^{-1} \text{cm}^{-1}$)]: ~260 (sh, 40000), ~342(sh, 10000), 423(7000). IR (KBr pellet, cm^{-1}): 3465, 3064, 3045, 2996, 2894, 1627, 1616, 1546, 1481, 1479, 1401, 1295, 1151, 1114, 1037, 887, 823, 755. HRMS (ESI) calculated for $\text{C}_{40}\text{H}_{28}\text{FeN}_2\text{NaO}_6[\text{M}+\text{Na}-2\cdot\text{THF}]^+$: 767.05; obtained, 766.87. Anal. Calculated. for $\text{C}_{40}\text{H}_{28}\text{Fe}_2\text{N}_2\text{O}_6\cdot 2\text{EtOH}$: C, 63.18; H, 4.82; N, 3.35. Obtained: C, 63.18; H, 5.05; N, 3.21. single crystals were obtained by slow diffusion of diethyl ether into a saturated THF solution of **1c**, which proved to be having molecular formula $[(\mathbf{1c})(\text{THF})]_2$ according to X-ray diffraction analysis.

Synthesis of $[\mathbf{1d}]_2$.

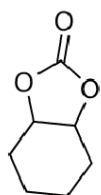


A solution of **10d** (0.158 g, 0.428 mmol) in 10 mL of THF was treated with triethylamine (180 μL , 1.28 mmol) at room temperature. After that a solution of FeCl_3 (0.072 g, 0.43 mmol) in 5 mL of THF was added to it, which led to a change in the color of the solution from yellow to dark brown. The resulting reaction mixture was stirred for another 1 h at room temperature and finally filtered through Celite. All volatiles were removed under vacuum and the remaining solid was dissolved in THF and EtOH was added to it, which resulted a dark brown precipitation. The supernatant was decanted off and the residue was thoroughly washed with ethanol and dried under vacuum to afford **1d** (0.110 g, 0.237 mmol, 55.3%) as a dark brown solid. UV-Vis [THF, nm ($\text{L mol}^{-1} \text{cm}^{-1}$)]: 276 (30000), 346 (30000), ~460(sh, 6000). IR (KBr pellet, cm^{-1}): 3471, 3075, 3006, 2902, 1637, 1610, 1587, 1482, 1473, 1394, 1319, 1101, 1035, 954, 894, 846, 755. HRMS (ESI) calculated for $\text{C}_{40}\text{H}_{26}\text{Fe}_2\text{N}_4\text{NaO}_{10}[\text{M}+\text{Na}]^+$: 857.02; obtained, 856.80. Anal. calculated. for $\text{C}_{40}\text{H}_{26}\text{Fe}_2\text{N}_4\text{O}_{10}\cdot 2\text{EtOH}$: C, 57.04; H, 4.13; N, 6.05. Obtained: C, 57.21; H, 4.27; N, 5.81. single crystals were obtained by slow evaporation of a saturated benzene solution of **1d**, which proved to be having molecular formula $[\mathbf{1d}]_2$ according to X-ray diffraction analysis.

3. Experimental section

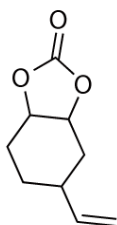
Substrate **11i** was synthesized following the reported procedure.^[S10] Cyclic carbonate synthesis was conducted as follows. To the 80 mL stainless steel reactor, 0.1 – 2.0 mol% of **1d**, 1.5 – 10 mol% of NBu_4Br and epoxide were charged. The reactor was charged and discharged with 5 bar of CO_2 twice and finally charged with 10 bar of CO_2 . The reactor was sealed and stirred at 100 $^\circ\text{C}$ for 12 - 18 h. At the end of the reaction, an aliquot of the reaction mixture was analyzed by ^1H NMR spectroscopy using CDCl_3 . The crude mixture was passed through silica using 10:1 mixture of chloroform and ethyl acetate as an eluent to remove catalyst and ammonium salt.

Solvent was removed under vacuum and yields were recorded. Cyclic carbonates were *cis* selective.



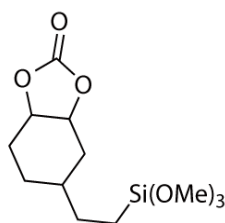
12g

Substrate: 9.9 mmol; **1d**: 0.2 mol%; [Br⁻]: 5.0 mol%; time: 12 h; conversion: >99%; yield: 91%. ¹H NMR (400 MHz, CDCl₃): δ 4.67 – 4.62 (m, 2H), 1.89 – 1.76 (m, 4H), 1.59 – 1.49 (m, 2H), 1.41 – 1.32 (m, 2H). ¹³C NMR (100 MHz, CDCl₃): δ 155.4, 75.8, 26.6, 19.0. The measured NMR data is in good agreement with the literature values.^[S10]



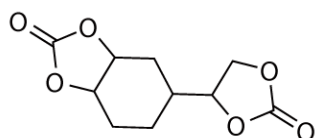
12h

Substrate: 7.7 mmol; **1d**: 0.2 mol%; [Br⁻]: 5.0 mol%; time: 18 h; conversion: >99%; yield: 90%, mixture of diastereomers. ¹H NMR (400 MHz, CDCl₃): δ 5.76 – 5.66 (m, 2H), 5.05 – 4.96 (m, 4H), 4.78 – 4.60 (m, 4H), 2.34 – 2.09 (m, 5H), 2.03 – 1.94 (m, 1H), 1.82 – 1.51 (m, 5H), 1.38 – 1.27 (m, 2H), 1.21 – 1.11 (m, 1H). ¹³C NMR (100 MHz, CDCl₃): δ 155.2, 155.2, 141.0, 140.9, 114.3, 114.0, 76.0, 75.7, 75.6, 75.2, 36.3, 33.9, 33.55, 31.7, 26.7, 25.8, 25.7, 25.1. The measured NMR data is in good agreement with the literature values.^[S10]



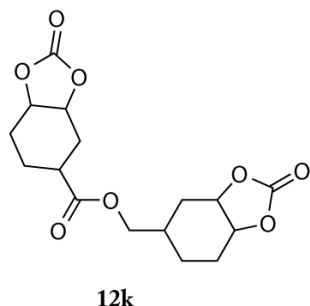
12i

Substrate: 4.3 mmol; **1d**: 0.2 mol%; [Br⁻]: 5.0 mol%; time: 18 h; conversion: >99%; yield: 77%, mixture of diastereomers. ¹H NMR (400 MHz, CDCl₃): δ 4.76 – 4.73 (m, 1H), 4.69 – 4.66 (m, 1H), 4.65 – 4.58 (m, 2H), 3.53 – 3.51 (m, 18H), 2.30 – 2.04 (m, 4H), 1.80 – 1.76 (m, 1H), 1.70 – 1.47 (m, 4H), 1.41 – 1.07 (m, 8H), 0.97 – 0.87 (m, 1H), 0.63 – 0.58 (m, 4H). ¹³C NMR (100 MHz, CDCl₃): δ 155.3, 155.3, 76.5, 76.1, 76.1, 75.6, 50.6, 35.30, 34.0, 32.4, 32.1, 29.1, 28.8, 26.9, 26.0, 25.6, 25.0, 6.37, 6.3. The measured NMR data is in good agreement with the literature values.^[S10]

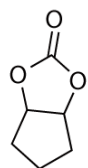


12j

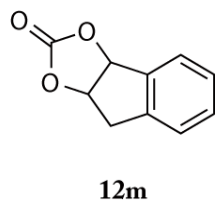
Substrate: 7.8 mmol; **1d**: 0.2 mol%; [Br⁻]: 5.0 mol%; time: 12 h; conversion: >99%; yield: 99%. ¹H NMR (400 MHz, CDCl₃): δ 4.92 – 4.69 (m, 2H), 4.63 – 4.16 (m, 3H), 2.44 – 2.35 (m, 1H), 2.21 – 1.86 (m, 2H), 1.82 – 1.69 (m, 2H), 1.67 – 1.24 (m, 2H). ¹³C NMR (100 MHz, CDCl₃): δ 154.8, 154.7, 154.7, 154.6, 154.6, 79.4, 79.1, 79.0, 79.0, 75.4, 75.2, 75.1, 75.0, 74.7, 74.6, 74.6, 67.6, 67.5, 67.4, 36.5, 36.4, 33.2, 33.1, 28.8, 28.4, 27.6, 26.4, 25.7, 25.1, 25.0, 21.0, 20.4, 19.6, 19.2. The measured NMR data is in good agreement with the literature values.^[S10]



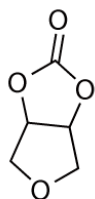
Substrate: 4.6 mmol; **1d**: 0.4 mol%; [Br⁻]: 10 mol%; time: 12 h; conversion: >99%; yield: 99%. ¹H NMR (400 MHz, CDCl₃): δ 4.91–4.66 (m, 8H), 4.08–3.91 (m, 4H), 2.75–2.68 (m, 1H), 2.43–2.23 (m, 6H), 2.16–1.95 (m, 7H), 1.91–1.71 (m, 7H), 1.71–1.57 (4H), 1.49–1.07 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 174.0, 174.0, 173.2, 173.2, 154.9, 154.9, 154.8, 154.7, 154.7, 75.6, 75.6, 75.5, 75.2, 75.1, 75.0, 75.0, 74.8, 74.6, 68.2, 68.2, 68.1, 37.4, 37.4, 37.3, 37.2, 35.6, 32.2, 30.6, 30.5, 30.5, 29.4, 29.3, 29.3, 29.3, 29.2, 28.8, 28.7, 28.0, 26.2, 26.1, 25.4, 25.4, 25.3, 25.2, 25.2, 25.2, 25.1, 25.1, 22.4, 21.9, 21.9, 21.9, 21.4, 21.4. HRMS (ESI) calculated for C₁₆H₂₀NaO₈[M+Na]⁺: 363.1056, obtained: 363.1075.



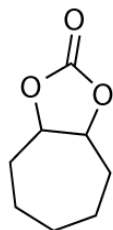
Substrate: 11.5 mmol; **1d**: 0.1 mol%; [Br⁻]: 1.5 mol%; time: 12 h; conversion: >99%; yield: 95%. ¹H NMR (400 MHz, CDCl₃): δ 5.07–5.06 (m, 2H), 2.11–2.04 (m, 2H), 1.81–1.58 (m, 4H). ¹³C NMR (100 MHz, CDCl₃): δ 155.5, 81.9, 33.1, 21.5. The measured NMR data is in good agreement with the literature values.^[S10]



Substrate: 8.5 mmol; **1d**: 0.1 mol%; [Br⁻]: 1.5 mol%; time: 12 h; conversion: >99%; yield: 94%. ¹H NMR (400 MHz, CDCl₃): δ 7.52–7.50 (d, *J* = 7.50 Hz, 1H), 7.44–7.40 (td, *J* = 7.44, 1.28 Hz, 1H), 7.37–7.31 (m, 2H), 6.01–5.99 (d, *J* = 6.38 Hz, 1H), 5.46–5.42 (m, 1H), 3.40–3.39 (m, 1H). ¹³C NMR (100 MHz, CDCl₃): δ 154.8, 140.2, 136.6, 131.2, 128.4, 126.6, 125.7, 83.7, 79.9, 38.2. The measured NMR data is in good agreement with the literature values.^[S10]



Substrate: 13.9 mmol; **1d**: 0.5 mol%; [Br⁻]: 5.0 mol%; time: 12 h; conversion: >99%; yield: 98%. ¹H NMR (400 MHz, CDCl₃): δ 5.20–5.19 (m, 2H), 4.24–4.21 (m, 2H), 3.57–3.53 (m, 2H). ¹³C NMR (100 MHz, CDCl₃): δ 154.5, 80.2, 73.1. The measured NMR data is in good agreement with the literature values.^[S10]



Substrate: 7.9 mmol; **1d**: 2.0 mol%; [Br⁻]: 10.0 mol%; time: 12 h; conversion: >99%; yield: 84%. ¹H NMR (400 MHz, CDCl₃): δ 4.84–4.78 (m, 2H), 1.99–1.86 (m, 4H), 7.84–1.74 (m, 2H), 1.66–1.57 (m, 1H), 1.52–1.42 (m, 1H), 1.35–1.25 (m, 2H). ¹³C NMR (100 MHz, CDCl₃): δ 154.7, 79.9, 30.2, 30.0, 23.6. The measured NMR data is in good agreement with the literature values.^[S10]

4. X-ray crystallography data

The diffraction data of **10c** was collected on a Bruker D8 QUEST. The diffraction data of **10d**, **[1c(THF)]₂**, and **[1d]₂** were collected on a Bruker SMART 1000. A suitable size and quality of crystal was coated with Paratone-*N* oil and mounted on a MiTeGen MicroLoop. The data were collected with graphite-monochromated Mo K α radiation ($\lambda = 0.71073$ Å) at 100 K or 120 K. Cell parameters were determined and refined by the SMART program.^[S11] Data reduction was performed using SAINT software.^[S12] An empirical absorption correction was applied using the SADABS program.^[S13] The structures were solved by direct methods, and all non-hydrogen atoms were subjected to anisotropic refinement by full-matrix least squares on F^2 by using the SHELXTL/PC package.^[S14] Unless otherwise noted, hydrogen atoms were placed at their geometrically calculated positions and refined riding on the corresponding carbon atoms with isotropic thermal parameters. Full crystallographic details can be obtained free of charge from the Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif (CCDC 1518349-1518352 for **10c**, **10d**, **[1c(THF)]₂**, and **[1d]₂**, respectively).

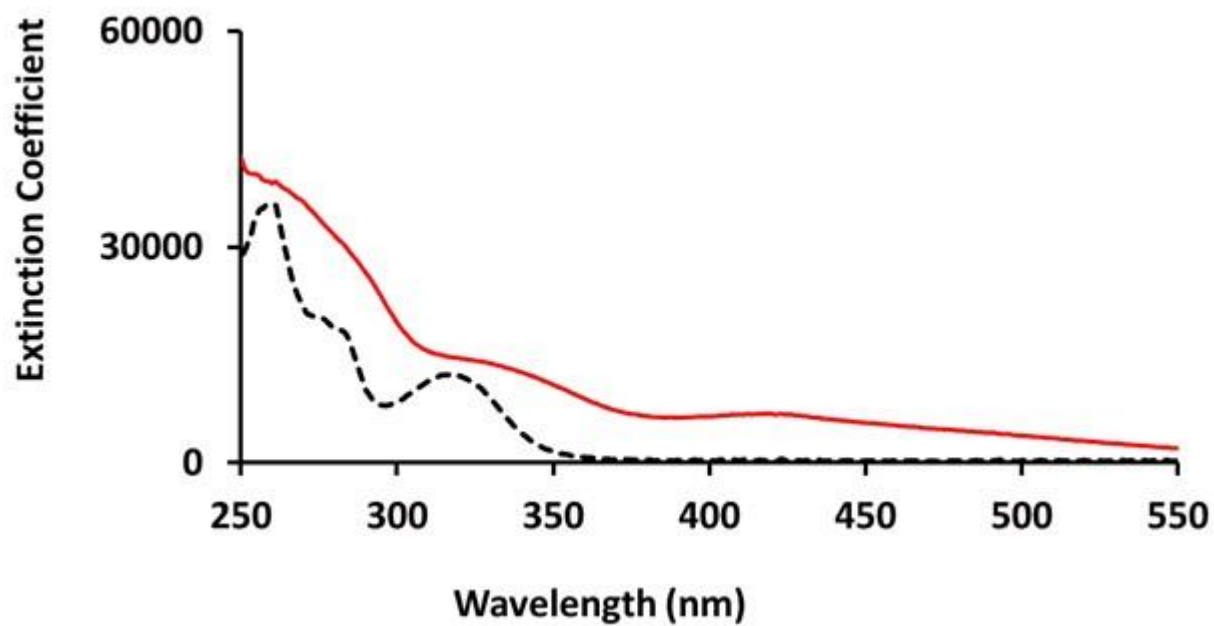


Figure S1. UV-Vis spectra of a N₁-O₃ ligand (**10c**, dotted black line) and [**1c**] (red line) in THF at room temperature.

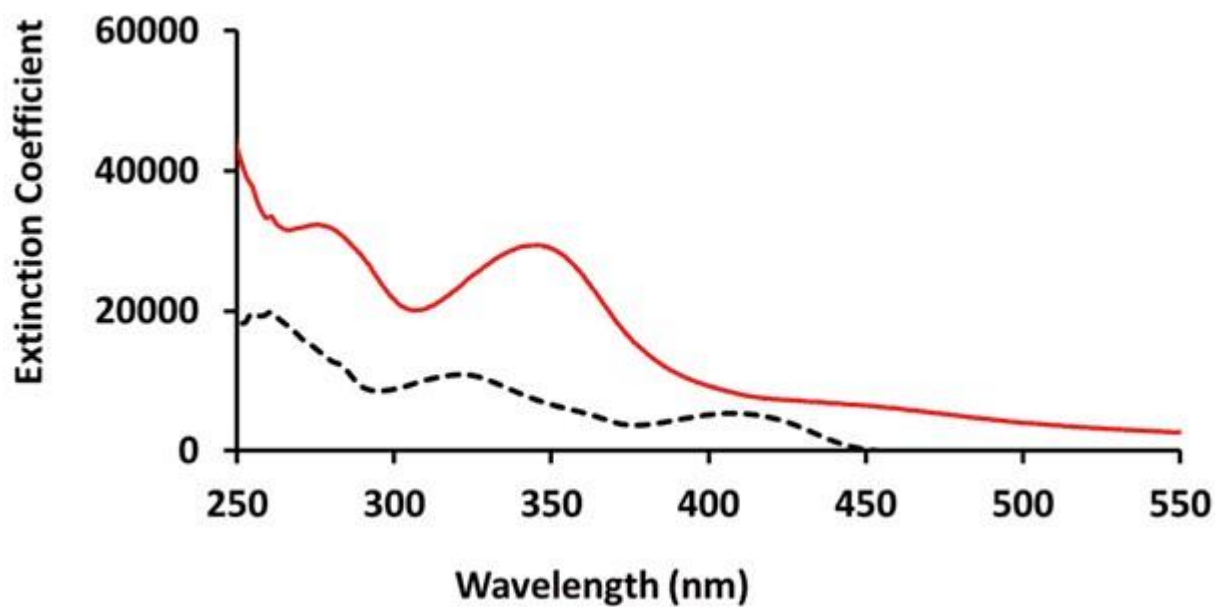


Figure S2. UV-Vis spectra of a ligand **10d** (dotted black line) and [**1d**] (red line) in THF at room temperature.

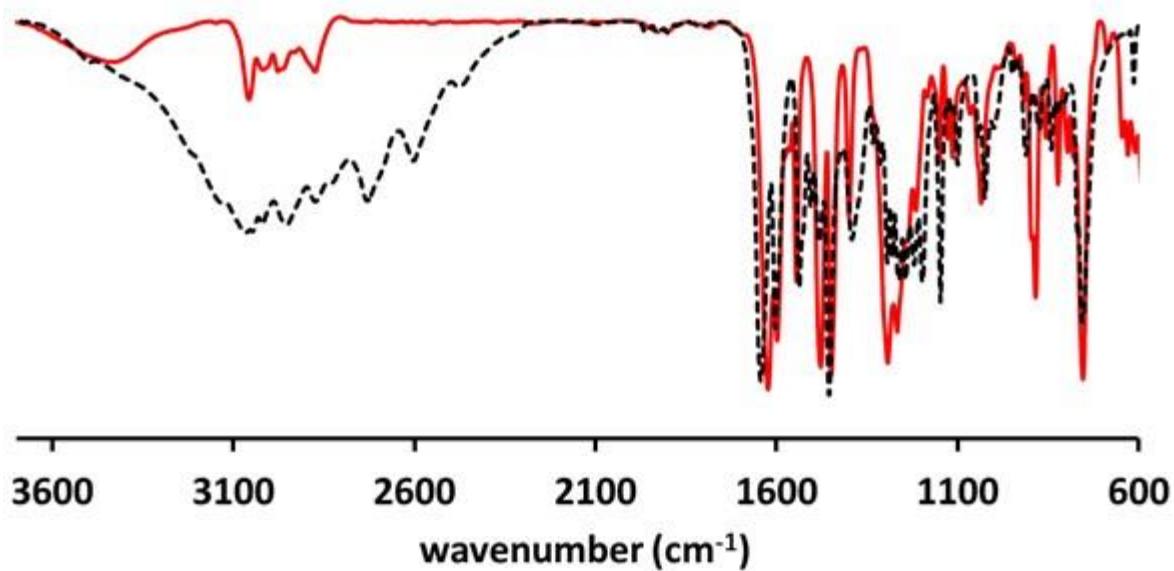


Figure S3. IR spectra of a N₁-O₃ ligand **10c** (dotted black line) and [**1c**] (red line) in KBr pellet.

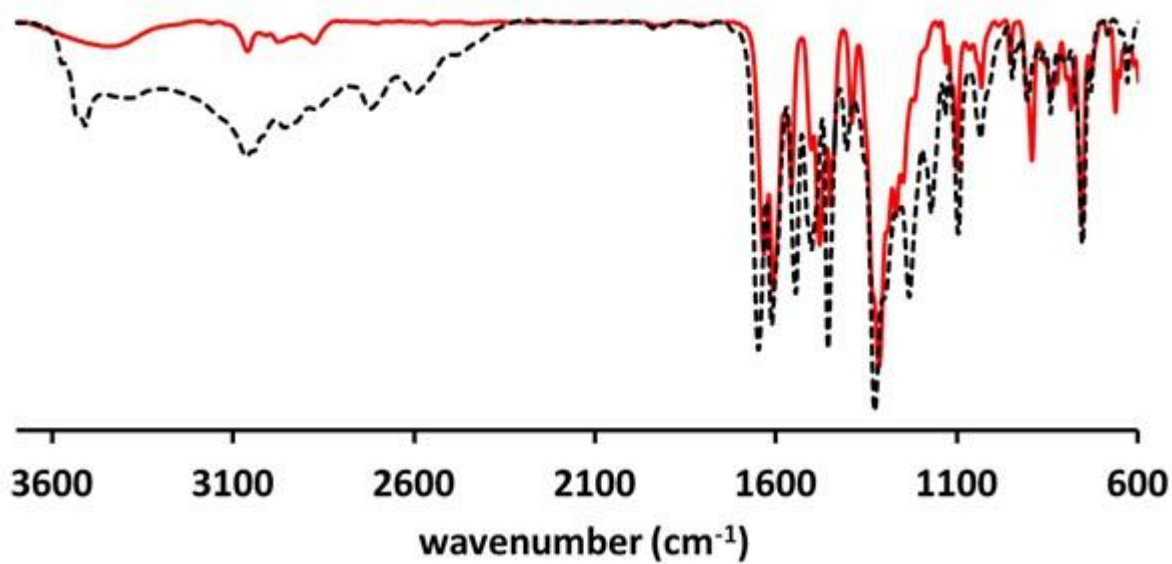


Figure S4. IR spectra of ligand **10d** (dotted black line) and [**1d**] (red line) in KBr pellet.

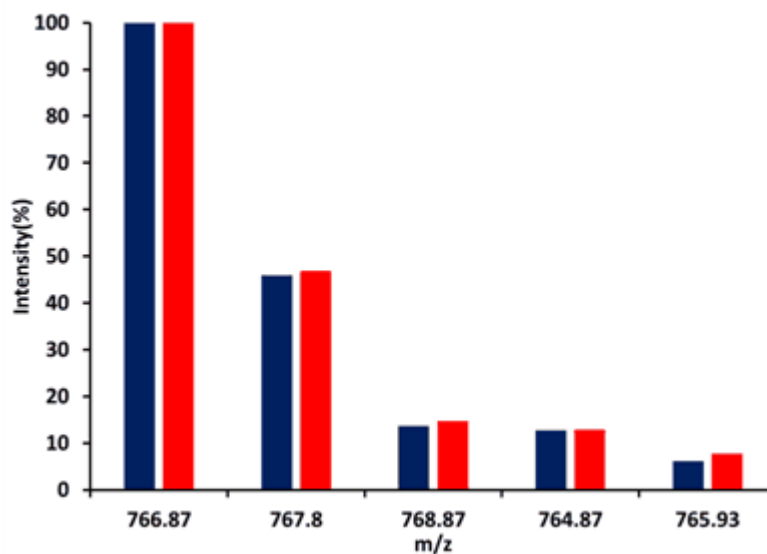


Figure S5. ESI mass data of $[1c(THF)]_2$: mass spectra of $\{1c\}_2(Na)^+$: m/z 766.87. Blue bars represent calculated values and red bars represent experimental values.

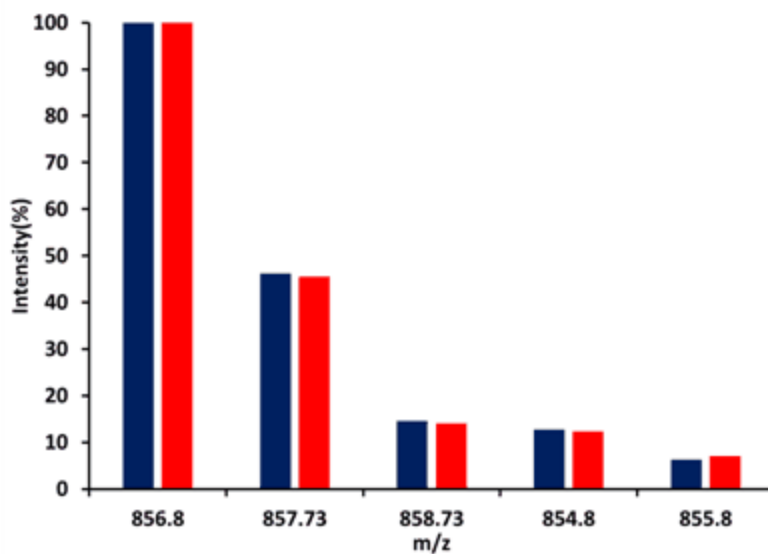


Figure S6. ESI mass data of $[1d]$: mass spectra of $\{1d\}_2(Na)^+$: m/z 856.80. Blue bars represent calculated values and red bars represent experimental values.

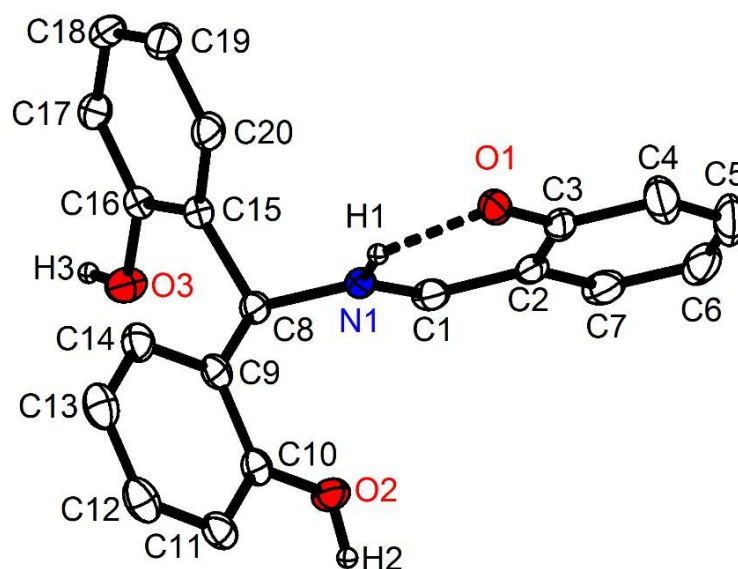


Figure S7. Solid state molecular structure of **10c**. All C–H hydrogen atoms are omitted for clarity. A dotted line denotes an intramolecular hydrogen bond. O–H and N–H hydrogen atoms were located on the Fourier difference map and their positions were freely refined.

Table S1. Selected bond distances and angles for **10c** (Å and °).

Distance	10c	Angle	10c
$d_{\text{N1-C1}}$	1.285(2)	$\angle\text{C1-N1-C8}$	124.7(1)
$d_{\text{N1-C8}}$	1.482(2)	$\angle\text{N1-C1-C2}$	124.0(1)
$d_{\text{N1-H1}}$	0.87(2)	$\angle\text{N1-C8-C9}$	109.62(9)
		$\angle\text{N1-C8-C15}$	108.50(9)
$d_{\text{O1}\cdots\text{H1}}$	1.89(2)	$\angle\text{N1-H1}\cdots\text{O1}$	139(1)

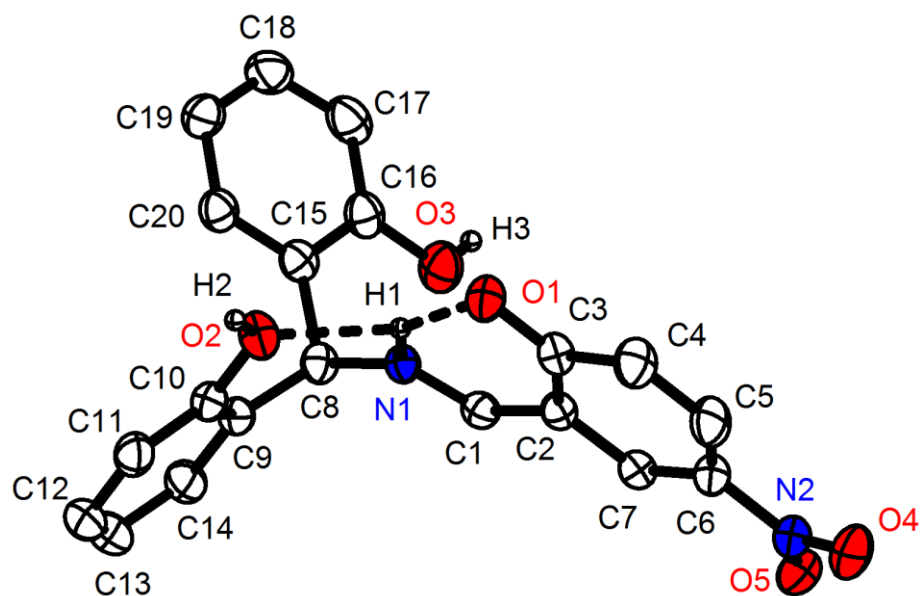


Figure S8. Solid state molecular structure of **10d**. Co-crystallized solvent molecule and all C–H hydrogen atoms are omitted for clarity. Dotted lines denote intramolecular hydrogen bonds. O–H and N–H hydrogen atoms were located on the Fourier difference map and their positions were freely refined.

Table S2. Selected bond distances and angles for **10d** (Å and °).

Distance	10d	Angle	10d
$d_{\text{N1-C1}}$	1.288(2)	$\angle\text{C1-N1-C8}$	124.8(1)
$d_{\text{N1-C8}}$	1.480(2)	$\angle\text{N1-C1-C2}$	123.2(1)
$d_{\text{N1-H1}}$	0.99(3)	$\angle\text{N1-C8-C9}$	110.4(1)
		$\angle\text{N1-C8-C15}$	108.4(1)
$d_{\text{O1}\cdots\text{H1}}$	1.83(3)	$\angle\text{N1-H1}\cdots\text{O1}$	134(3)
$d_{\text{O2}\cdots\text{H1}}$	2.16(3)	$\angle\text{N1-H1}\cdots\text{O2}$	112(2)

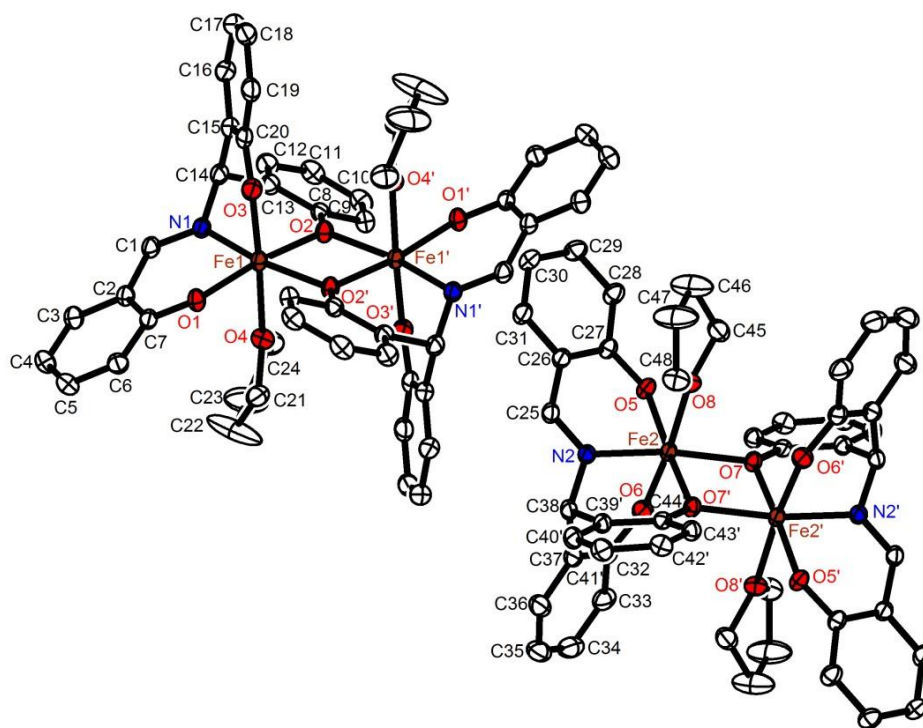


Figure S9. Solid state molecular structure of $[1c(THF)]_2$. All hydrogen atoms are omitted for clarity.

Table S3. Selected bond distances and angles for $[1c(THF)]_2$ (Å and °).

Distance	$[1c(THF)]_2$	Angle	$[1c(THF)]_2$	Angle	$[1c(THF)]_2$
d_{Fe1-N1}	2.070(1)	$\angle N1-Fe1-O2'$	164.55(5)	$\angle O1-Fe1-O4$	83.13(5)
d_{Fe2-N2}	2.068(1)	$\angle N2-Fe2-O7$	163.91(5)	$\angle O5-Fe2-O8$	82.50(5)
d_{Fe1-O1}	1.911(1)	$\angle N1-Fe1-O1$	88.71(5)	$\angle O2-Fe1-O2'$	77.23(5)
d_{Fe2-O5}	1.903(1)	$\angle N2-Fe2-O5$	89.29(5)	$\angle O7-Fe2-O7'$	77.15(4)
d_{Fe1-O2}	2.077(1)	$\angle N1-Fe1-O2$	87.49(5)	$\angle O2-Fe1-O3$	93.18(5)
$d_{Fe2-O7'}$	2.063(1)	$\angle N2-Fe2-O7'$	86.92(5)	$\angle O7'-Fe2-O6$	94.67(5)
$d_{Fe1-O2'}$	2.020(1)	$\angle N1-Fe1-O3$	86.07(5)	$\angle O2-Fe1-O4$	84.89(4)
d_{Fe2-O7}	2.012(1)	$\angle N2-Fe2-O6$	85.79(5)	$\angle O7'-Fe2-O8$	85.18(4)
d_{Fe1-O3}	1.909(1)	$\angle N1-Fe1-O4$	87.71(5)	$\angle O2'-Fe1-O3$	96.88(5)
d_{Fe2-O6}	1.909(1)	$\angle N2-Fe2-O8$	88.34(5)	$\angle O7-Fe2-O6$	97.61(5)
d_{Fe1-O4}	2.201(1)	$\angle O1-Fe1-O2$	167.56(5)	$\angle O2'-Fe1-O4$	88.69(5)
d_{Fe2-O8}	2.229(1)	$\angle O5-Fe2-O7'$	167.21(5)	$\angle O7-Fe2-O8$	88.09(4)
		$\angle O1-Fe1-O2'$	105.77(5)	$\angle O3-Fe1-O4$	173.56(5)
		$\angle O5-Fe2-O7$	105.77(4)	$\angle O6-Fe2-O8$	174.13(5)
		$\angle O1-Fe1-O3$	98.37(5)		
		$\angle O5-Fe2-O6$	97.24(5)		

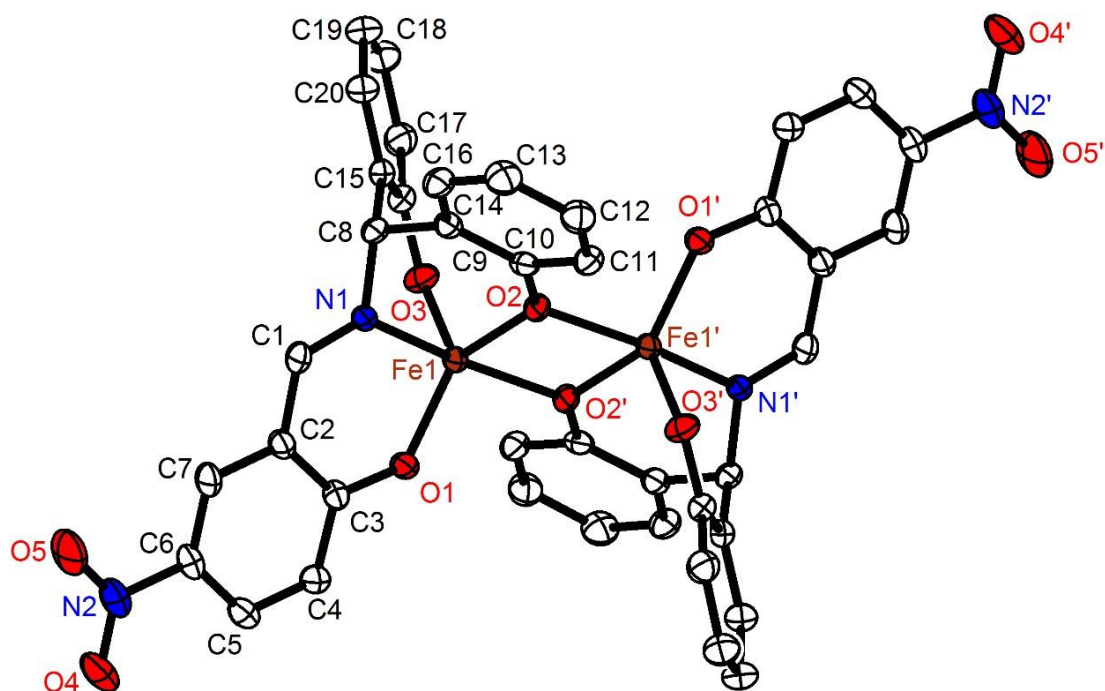


Figure S10. Solid state molecular structure of $[1\mathbf{d}]_2$. Co-crystallized solvent molecule and all hydrogen atoms are omitted for clarity.

Table S4. Selected bond distances and angles for $[1\mathbf{d}]_2$ (Å and °).

Distance	$[1\mathbf{d}]_2$	Angle	$[1\mathbf{d}]_2$
$d_{\text{Fe1-N1}}$	2.057(2)	$\angle \text{N1-Fe1-O2}$	87.16(8)
		$\angle \text{N1-Fe1-O2'}$	161.45(8)
$d_{\text{Fe1-O1}}$	1.887(2)	$\angle \text{N1-Fe1-O1}$	88.59(8)
		$\angle \text{N1-Fe1-O3}$	88.21(8)
$d_{\text{Fe1-O2}}$	1.977(2)	$\angle \text{O1-Fe1-O2}$	131.25(8)
		$\angle \text{O1-Fe1-O2'}$	96.10(7)
$d_{\text{Fe1-O2'}}$	2.029(2)	$\angle \text{O1-Fe1-O3}$	121.48(9)
$d_{\text{Fe1-O3}}$	1.845(2)	$\angle \text{O2-Fe1-O2'}$	76.24(7)
		$\angle \text{O2-Fe1-O3}$	106.90(8)
		$\angle \text{O2'-Fe1-O3}$	104.35(7)

5. Computational details

The energy components have been computed with the following protocol. The change in Gibbs free energy in solution phase $\Delta G(\text{Sol})$ has been calculated as follows:

$$\Delta G(\text{Sol}) = \Delta G(\text{gas}) + \Delta G^{\text{solv}} \quad (1)$$

$$\Delta G(\text{gas}) = \Delta H(\text{gas}) - T\Delta S(\text{gas}) \quad (2)$$

$$\Delta H(\text{gas}) = \Delta E(\text{SCF}) + \Delta \text{ZPE} + \Delta C_v T + \Delta PV \quad (3)$$

$$\Delta H(\text{gas}) \approx \Delta E(\text{SCF}) + \Delta \text{ZPE} \quad (4)$$

$G(\text{gas})$ is the Gibbs free energy in gas phase; $G(\text{solv})$ is the free energy of solvation as computed using the continuum solvation model; $H(\text{gas})$ is the enthalpy in gas phase; T is the temperature (298.15 K); $S(\text{gas})$ is the entropy in gas phase; $E(\text{SCF})$ is the self-consistent field energy, i.e. “raw” electronic energy as computed from the SCF procedure and ZPE is the zero point energy. Note that by entropy here we refer specifically to the vibrational/rotational/translational entropy of the solute(s); the entropy of the solvent is incorporated implicitly in the continuum solvation model. As the contributions from the last two terms in equation 3 are negligibly small, this equation can be essentially reduced to equation 4.

To locate transition states, the potential energy surface was first explored approximately using the linear synchronous transit (LST) method, followed by a quadratic synchronous transit (QST)¹⁶ search using the LST geometry as an initial guess.

References

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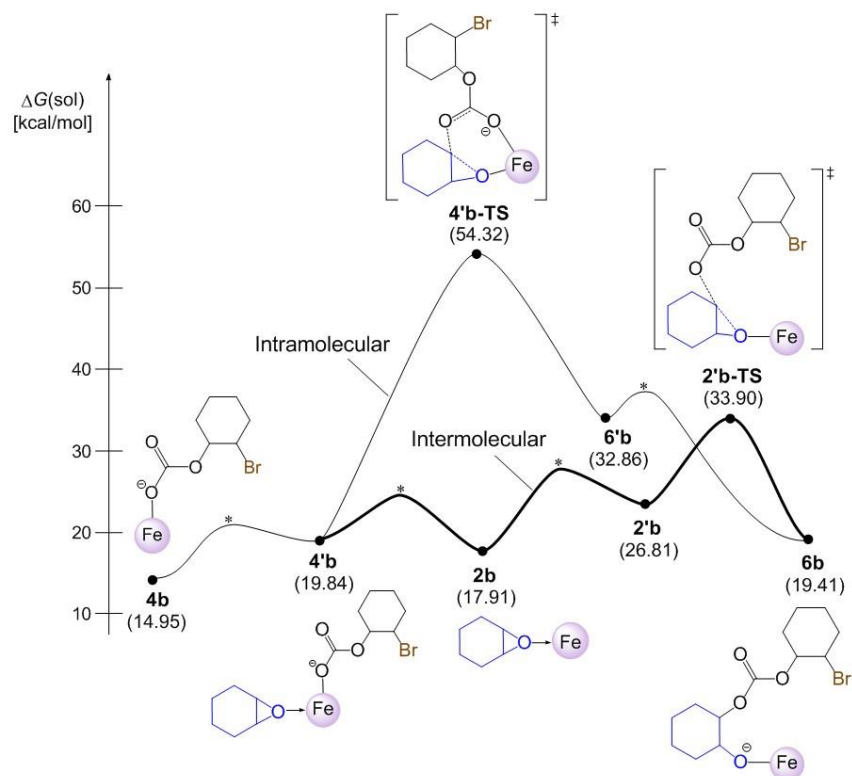


Figure S11. Free energy profile of the initial phase of the ring-opening polymerization reaction catalyzed by **1b**.

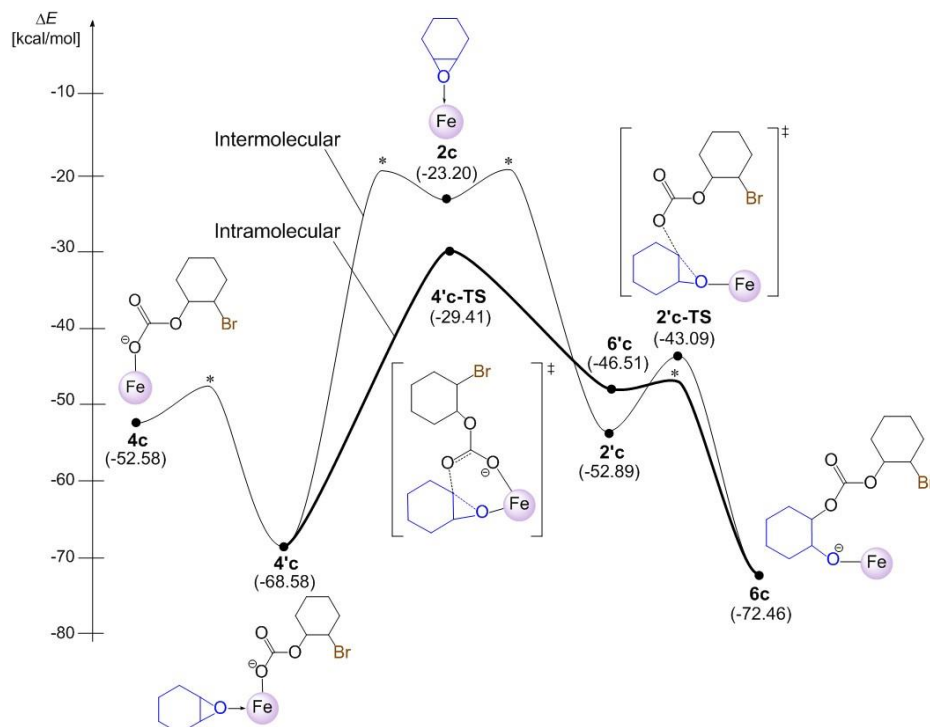


Figure S12. Electronic energy profile of the initial phase of the the ring-opening polymerization reaction catalyzed by **1c**.

In order to understand why the intermolecular path, where the unsaturated 15e complex **2c** is generated, is more favorable than the intramolecular path we analyzed the electronic energy profile of the reaction. The energy profile, depicted in Figure S1, reveals that the formation of the **2c** complex is a highly unfavorable process. It is even higher in energy than the intramolecular ring-opening transition state **4'c-TS**, which is the highest point on the free energy profile shown in Figure 5. The energy gap between **4'c** and **2c** is about 45 kcal/mol, but it drops to 5 kcal/mol on the free energy profile. This can be explained, first, by the gain in entropy of ~15 kcal/mol associated with liberation of the carbonate from **4'c**. Secondly, the higher total solvation energy of the more compact carbonate (-58.1 kcal/mol) and **2c** (-13.8) in comparison to **4'c** (-46.7) also contributes to the lowering of this gap by 25 kcal/mol. The overall effect is then estimated to be ~40 kcal/mol.

Table S5. Computed energy components for optimized structures.

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(eu)	G(sol)/(eV)
	cc-pVTZ(-f)/ LACV3P**	6- 31G**/LACVP* *	6-31G**/LACVP**	
2a	-48224.539	266.66	188.866	-48216.197
2a-TS	-48585.606	265.76	197.102	-48579.352
3a	-48586.301	266.63	195.252	-48579.588
3a-TS	-53718.853	276.04	204.123	-53712.129
4a	-53720.221	276.40	209.531	-53713.370
4a-TS	-53719.502	275.75	201.786	-53712.632
5a	-53358.587	277.71	196.321	-53350.141
2b	-41509.496	312.94	192.588	-41498.955
2b-TS	-41870.879	312.08	202.821	-41862.218
2'b	-55440.183	419.83	247.663	-55427.316
2'b-TS	-55440.050	418.59	242.645	-55427.008
3b	-41871.623	312.66	205.076	-41862.627
3b-TS	-47004.882	321.67	204.516	-46995.662
4b	-47005.351	322.28	211.868	-46996.215
4b-TS	-47004.556	322.00	209.076	-46995.461

4'b	-55440.759	420.21	240.630	-55427.618
4'b-TS	-55439.059	419.27	241.279	-55426.123
5b	-46643.515	323.62	197.712	-46632.851
6'b	-55440.328	420.72	237.753	-55427.054
6b	-55423.569	420.12	250.861	-55427.637
2c	-40406.148	280.02	186.623	-40397.015
2c-TS	-40767.495	279.03	200.071	-40760.463
3c	-40768.370	279.67	189.934	-40760.685
3c-TS	-45901.658	288.01	210.866	-45893.816
4c	-45902.207	289.39	205.854	-45894.497
4c-TS	-45901.315	288.82	202.683	-45893.700
5c	-45540.230	290.69	197.249	-45531.018
4'c	-54337.507	386.39	239.928	-54325.880
4'c-TS	-54335.809	385.56	228.421	-54324.287
2'c-TS	-54336.402	385.04	239.386	-54325.000
6'c	-54336.575	386.98	231.136	-54325.459
2'c	-54336.835	386.20	237.342	-54325.718
6c	-54337.675	387.37	240.699	-54326.092

6. References

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Appendix I. Cartesian Coordinates of the Optimized Geometries

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2a			
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C	-0.773519950000	2.246047982000	-0.856910344000
H	1.426545244000	-0.781527831000	3.686818162000
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C	-0.352817653000	-1.606387810000	2.725576230000
H	-1.025282077000	-1.583882037000	3.593513290000
N	1.442583089000	-0.432103441000	1.586116738000
C	2.721697654000	-0.272601620000	1.534247942000
C	3.503332272000	-0.107613851000	0.333636096000
C	2.914714332000	0.019106231000	-0.967817303000
C	3.781859115000	0.217248172000	-2.067561389000
C	5.154590451000	0.273079424000	-1.897537207000
C	5.733852256000	0.148604957000	-0.621579112000
C	4.907394911000	-0.032457863000	0.470924484000
O	1.618632519000	-0.010920842000	-1.173065840000
O	-1.269535240000	-0.861333977000	-1.283023730000
C	-2.556626133000	-0.983858558000	-1.078007165000
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C	-4.533756813000	-1.376102264000	0.327550230000
C	-5.373508115000	-1.224336395000	-0.760473926000
C	-4.808456944000	-0.955966562000	-2.019817030000
C	-3.437981404000	-0.838495925000	-2.176475432000
H	3.329142750000	0.306843170000	-3.050002367000
C	-2.340854188000	-1.452876261000	1.397463035000
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H	-2.995327239000	-0.638958895000	-3.147354520000
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H	-4.949824558000	-1.590986840000	1.309614058000
H	-5.454421437000	-0.841086955000	-2.886351981000
H	5.335003582000	-0.128486607000	1.466700899000
H	5.792665234000	0.413003845000	-2.766209105000
Cl	1.032417220000	-3.106022942000	-0.269610495000
C	0.306104168000	2.573114693000	0.093900190000
H	-0.493587617000	1.748146472000	-1.782675281000
H	1.324668628000	2.322909291000	-0.195157196000
C	0.139991694000	3.685754198000	1.105529627000
H	0.680824339000	4.562038566000	0.721398927000
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H	-1.391098829000	4.950054606000	1.968456549000
H	-1.820931985000	3.242674553000	1.913341455000
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H	-2.363330205000	3.246138361000	-1.880295219000
C	-2.069670449000	4.266233890000	0.019204031000
H	-1.563629084000	5.069638216000	-0.534018510000
H	-3.094178266000	4.610923075000	0.198130770000
Fe	0.257858876000	-0.894165497000	-0.154433739000

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2a-TS			
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C	0.525851895000	2.166874022000	-0.519651651000
H	0.156690722000	-2.327157018000	3.449770401000
C	-0.239566733000	-1.658141646000	2.670786468000
C	-1.680023007000	-2.050135815000	2.299218275000
H	-2.359485854000	-1.891318141000	3.150492404000
N	0.568233655000	-1.682337622000	1.463272502000
C	1.751990219000	-2.188127915000	1.455954062000
C	2.648504531000	-2.232912879000	0.325578052000

C	2.348983425000	-1.618295889000	-0.938316976000
C	3.341481617000	-1.686925782000	-1.950370442000
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C	4.834129234000	-2.943802560000	-0.502993036000
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O	-1.821282692000	-0.357397865000	-1.532574047000
C	-3.019219313000	0.107667001000	-1.342630629000
C	-3.764379735000	-0.062664166000	-0.123713039000
C	-5.068735279000	0.468076072000	-0.027323511000
C	-5.659172523000	1.161098748000	-1.069213213000
C	-4.932785656000	1.330071623000	-2.262348090000
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H	3.116404264000	-1.204846489000	-2.895937187000
C	-3.252725972000	-0.783477923000	1.019855229000
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Fe	-0.488882472000	-1.066114516000	-0.340766250000

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3a

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C	1.172153682000	2.220626450000	-0.350669977000
H	0.144430253000	-2.623258622000	3.433928614000
C	-0.269930640000	-1.911593766000	2.702277031000
C	-1.700606096000	-2.315973498000	2.305453683000
H	-2.376934499000	-2.258237961000	3.173167073000
N	0.530946774000	-1.835095970000	1.495388099000
C	1.700135382000	-2.364318331000	1.430481264000
C	2.574485800000	-2.351771231000	0.281768403000
C	2.268387448000	-1.644143254000	-0.933476752000
C	3.235876924000	-1.704298728000	-1.974879042000
C	4.415213189000	-2.410126434000	-1.833482956000
C	4.711718600000	-3.098659686000	-0.642197054000
C	3.793783361000	-3.054018046000	0.390849608000
O	1.190092885000	-0.944687629000	-1.114908605000
O	-1.980079335000	-0.372046583000	-1.407275310000
C	-3.178065772000	0.039307850000	-1.154997489000
C	-3.887628391000	-0.226722875000	0.072091866000
C	-5.203489922000	0.257164575000	0.234626272000
C	-5.845149877000	0.995806699000	-0.743273010000
C	-5.158728790000	1.256156669000	-1.945117589000
C	-3.874132604000	0.791058762000	-2.147711346000

H	3.002340287000	-1.172770943000	-2.892133058000
C	-3.332665586000	-1.013280011000	1.149319053000
N	-2.130579295000	-1.459833853000	1.215739297000
H	-3.342603622000	0.983930167000	-3.074829803000
H	5.640957350000	-3.650980539000	-0.536059576000
H	-6.856333539000	1.361853375000	-0.590315378000
H	-0.297895899000	-0.915342011000	3.163106893000
H	-1.683422512000	-3.345587133000	1.928046453000
H	-4.032348840000	-1.247013267000	1.967448984000
H	2.094854073000	-2.890144197000	2.314205786000
H	-5.717805478000	0.035037275000	1.169126565000
H	-5.646857737000	1.831020335000	-2.730215805000
H	4.001707326000	-3.577015303000	1.323597402000
H	5.124354018000	-2.432616453000	-2.658761431000
Cl	-0.860949727000	-3.404734246000	-0.904524184000
C	0.727644110000	1.486360167000	0.930129313000
H	1.407730005000	1.496686846000	-1.127299676000
H	1.555097983000	0.840834933000	1.267235280000
C	0.360171295000	2.480363214000	2.052240067000
H	1.266092202000	3.000840100000	2.389305128000
H	-0.025132301000	1.905179005000	2.903619022000
O	-0.393294034000	0.750636688000	0.561653190000
Br	3.071806690000	3.106476682000	-0.050402900000
C	-0.690768740000	3.495844040000	1.576479872000
H	-0.928481115000	4.204506390000	2.381616582000
H	-1.612738328000	2.953225645000	1.336507492000
C	0.188176957000	3.289601453000	-0.799024364000
H	-0.698048208000	2.731030129000	-1.129532966000
H	0.578609507000	3.828978179000	-1.668543560000
C	-0.208598120000	4.256394261000	0.328677247000
H	0.657045332000	4.880480124000	0.587989745000
H	-0.993333898000	4.935112848000	-0.030792881000
Fe	-0.555895812000	-1.002139913000	-0.220463099000

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H	1.990719031000	-3.540301103000	-2.429659270000
C	1.962173247000	-2.997447323000	-1.473080556000
C	0.983798624000	-3.681934771000	-0.519417676000
H	1.365860221000	-4.669267333000	-0.215797060000
N	1.550907897000	-1.610464269000	-1.653260480000
C	1.571500058000	-1.147066756000	-2.859360359000
C	1.134830178000	0.145853957000	-3.301215835000
C	0.511811298000	1.076867297000	-2.406340661000
C	0.090031591000	2.323974943000	-2.955962372000
C	0.276978367000	2.620515129000	-4.291398084000
C	0.887743356000	1.699078224000	-5.168453218000
C	1.301679433000	0.480594333000	-4.663628459000
O	0.331321613000	0.848459923000	-1.150997114000
O	-0.635486800000	-0.775646027000	1.787514211000
C	-0.544662786000	-1.440802974000	2.882601564000
C	0.074588249000	-2.735536421000	2.966966841000
C	0.099582085000	-3.430918543000	4.197320516000
C	-0.437677733000	-2.883669930000	5.346099717000
C	-1.047995003000	-1.611638834000	5.271282479000
C	-1.113037833000	-0.913625317000	4.083058222000
H	-0.380088508000	3.026266551000	-2.275170108000
C	0.548333357000	-3.383386389000	1.778698040000
N	0.738847159000	-2.819894135000	0.630484473000
H	-1.580647437000	0.063255641000	4.016171616000
H	1.025793667000	1.941751179000	-6.217906934000
H	-0.399891139000	-3.422734373000	6.288180295000
H	2.970785678000	-3.027219494000	-1.048962364000
H	0.023866723000	-3.812183624000	-1.031823209000
H	0.728253748000	-4.466014471000	1.865736651000
H	1.943412316000	-1.803283690000	-3.661018605000
H	0.557893664000	-4.418908891000	4.224223351000
H	-1.478179279000	-1.173053241000	6.169661049000
H	1.770315780000	-0.251292692000	-5.320501134000
H	-0.056950131000	3.582989418000	-4.674172809000

Cl	-1.589211989000	-1.571459209000	-1.092678410000
O	2.163334447000	0.265484311000	1.025787350000
Fe	0.378509843000	-0.644661285000	0.106795742000
O	0.376816441000	1.528748472000	1.343074536000
C	1.605010510000	1.582439362000	1.491525768000
O	2.425694589000	2.394577130000	1.898376875000
C	3.977920625000	0.173339638000	2.659487520000
C	3.617749090000	0.207252645000	1.157677005000
H	3.450916025000	0.965150084000	3.179095096000
H	3.989276174000	1.147791515000	0.750058433000
C	4.249566925000	-0.964467553000	0.399629388000
H	5.308609040000	-0.706893637000	0.272430936000
H	3.812650654000	-1.006862661000	-0.601759436000
Br	5.951741401000	0.858894112000	2.849542004000
C	4.157950621000	-2.329765712000	1.107998482000
H	4.744680360000	-3.069649050000	0.547051622000
H	3.121101049000	-2.671344845000	1.103259720000
C	3.867513862000	-1.184894778000	3.325256383000
H	2.793739159000	-1.426104500000	3.335901048000
H	4.187130115000	-1.118817611000	4.370170839000
C	4.628852640000	-2.278465166000	2.567559451000
H	5.705045513000	-2.072349450000	2.617239848000
H	4.465723671000	-3.250599624000	3.049841560000

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C	0.279505520000	4.646664652000	-0.608568713000
H	2.769310229000	-2.583796779000	-2.116188427000
C	2.272541182000	-1.942469799000	-1.371890992000
C	1.721443336000	-2.783864410000	-0.205447884000
H	2.542360130000	-3.273133674000	0.341014016000
N	1.174811364000	-1.184232148000	-1.942861193000
C	1.031104840000	-1.039204169000	-3.208376947000
C	-0.001510477000	-0.252860216000	-3.851790177000
C	-0.913556244000	0.588248249000	-3.126769392000
C	-1.861437567000	1.323628203000	-3.886813402000
C	-1.910274683000	1.239774773000	-5.267171254000
C	-1.011775843000	0.422161063000	-5.973961791000
C	-0.073765043000	-0.303142598000	-5.258757143000
O	-0.899009523000	0.731521922000	-1.830487083000
O	-1.086767177000	-0.010051568000	1.220431745000
C	-0.729249765000	-0.200208481000	2.455121191000
C	0.304737689000	-1.114311895000	2.859993133000
C	0.612366263000	-1.252179602000	4.229602055000
C	-0.048445702000	-0.530559665000	5.208829567000
C	-1.066418447000	0.357261014000	4.817219730000
C	-1.401603674000	0.514500980000	3.484406641000
H	-2.554775062000	1.951316630000	-3.335894538000
C	1.045434302000	-1.936939682000	1.926927417000
N	0.939254795000	-1.908720301000	0.649044183000
H	-2.186265703000	1.198048613000	3.175977701000
H	-1.051078118000	0.361299266000	-7.057593728000
H	0.212697640000	-0.648918431000	6.256326257000
H	2.997091743000	-1.221294816000	-0.975684309000
H	1.047297620000	-3.550591897000	-0.605278685000
H	1.752470877000	-2.644819610000	2.386263039000
H	1.736717452000	-1.540241356000	-3.888658341000
H	1.399878957000	-1.950204380000	4.510370408000
H	-1.599966999000	0.931542407000	5.572007513000
H	0.634199985000	-0.940892015000	-5.786083179000
H	-2.656263019000	1.816699820000	-5.809994094000
Cl	-1.674319838000	-2.287970133000	-1.061427832000
C	0.436646913000	4.008933212000	0.779280041000
H	1.109398002000	4.349906983000	-1.246398335000
H	1.399617489000	4.295113975000	1.208114462000
C	-0.733028027000	4.329949777000	1.713934661000
H	-0.682009608000	5.392757860000	1.980272191000
H	-0.602353705000	3.750554365000	2.634707557000
O	0.415658081000	2.593187005000	0.563460428000
Br	0.629097177000	6.708435814000	-0.446638599000

C	-2.090842933000	4.008793586000	1.064666180000
H	-2.905180523000	4.298921611000	1.741562480000
H	-2.161832116000	2.925195963000	0.916061053000
C	-1.082961695000	4.393922046000	-1.233657563000
H	-1.096001808000	3.318500232000	-1.461679871000
H	-1.171638049000	4.931222294000	-2.183487784000
C	-2.249951979000	4.723294877000	-0.288623001000
H	-2.296833486000	5.809553023000	-0.133106297000
H	-3.194296718000	4.428569888000	-0.763061438000
Fe	-0.204620540000	-0.406881625000	-0.437803637000
O	1.475552440000	0.728935041000	0.003099880000
C	1.623994399000	1.984481755000	0.196168569000
O	2.649875423000	2.653047254000	0.107208231000

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C	2.315779400000	3.046810178000	1.869361887000
H	2.827002250000	-2.012179750000	-2.245627183000
C	2.212842497000	-1.586261812000	-1.440346744000
C	2.094186226000	-2.566513656000	-0.262351367000
H	3.067376131000	-2.703434648000	0.229446901000
N	0.867902172000	-1.248241029000	-1.895804434000
C	0.654399042000	-0.948097127000	-3.132387280000
C	-0.594624853000	-0.505519532000	-3.693793190000
C	-1.763723572000	-0.277082005000	-2.894453033000
C	-2.923557353000	0.212892243000	-3.543314620000
C	-2.933827364000	0.453071842000	-4.905937874000
C	-1.788262259000	0.226773859000	-5.692343952000
C	-0.640396529000	-0.242511544000	-5.081462815000
O	-1.800184919000	-0.484132269000	-1.605298266000
O	-1.444454510000	-1.094042744000	1.265729141000
C	-0.919983631000	-0.798675895000	2.422840162000
C	0.424095714000	-1.141806282000	2.790769537000
C	0.888613596000	-0.841134497000	4.090385363000
C	0.094822371000	-0.179162317000	5.011119482000
C	-1.212321841000	0.187298418000	4.638418964000
C	-1.709729569000	-0.117770366000	3.383486875000
H	-3.800562284000	0.383943599000	-2.928150981000
C	1.339258787000	-1.771908880000	1.869735019000
N	1.088755601000	-2.021629958000	0.633714297000
H	-2.718373386000	0.153517433000	3.090241346000
H	-1.805750248000	0.420286572000	-6.760099054000
H	0.471692336000	0.050451964000	6.002749896000
H	2.690918200000	-0.668218344000	-1.077980188000
H	1.728005441000	-3.532880117000	-0.624503754000
H	2.330654099000	-2.021817726000	2.272542966000
H	1.493921944000	-1.008466677000	-3.838665445000
H	1.901195980000	-1.135149858000	4.359681384000
H	-1.845016674000	0.715066601000	5.347594621000
H	0.256464749000	-0.417177337000	-5.672557202000
H	-3.842020706000	0.823423340000	-5.374623701000
Cl	-1.194134938000	-3.650267025000	-1.005308262000
C	3.340797981000	2.140767735000	1.171827406000
H	2.558655979000	4.104339730000	1.742207037000
H	3.701403588000	2.619057929000	0.251952081000
C	4.513187521000	1.659747107000	2.013185910000
H	5.236812740000	2.484943735000	2.054268495000
H	5.006684602000	0.837079802000	1.484464117000
O	2.490298160000	1.033696433000	0.762010005000
C	4.111758945000	1.261679742000	3.438711869000
H	5.009665519000	1.010009156000	4.013077899000
H	3.487811035000	0.361127225000	3.403687617000
C	2.038085739000	2.688992129000	3.334291716000
H	1.405802291000	1.794977821000	3.355720694000
H	1.458775610000	3.494692563000	3.795233831000
C	3.328576278000	2.396505123000	4.114911676000
H	3.957859968000	3.296365891000	4.172014274000
H	3.071804474000	2.126833542000	5.144474032000
Fe	-0.697601929000	-1.473402856000	-0.435358374000
O	0.327615010000	0.904121784000	0.082557975000

C	1.226456801000	1.513509192000	0.594675310000
O	1.127753103000	2.771850340000	1.079867919000

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2b

N	-0.817954727000	0.718418943000	-2.739741361000
O	-1.224273538000	-0.254466507000	-0.004033795000
O	1.545203821000	1.123368447000	-0.999296527000
O	0.724002781000	-1.717571887000	-2.194700710000
C	-2.282838808000	0.485658019000	-2.546754076000
H	-2.433353048000	-0.596914447000	-2.615075448000
H	-2.828370502000	0.942812810000	-3.387481896000
C	-2.835690017000	1.007657834000	-1.246993595000
C	-2.276825138000	0.569908532000	-0.021220399000
C	-2.847150930000	1.005494338000	1.187238343000
C	-3.945744168000	1.860438143000	1.182996991000
H	-4.372126180000	2.188887588000	2.127323330000
C	-4.497957149000	2.299599584000	-0.022844246000
C	-3.935852536000	1.870035141000	-1.224694162000
H	-4.361889457000	2.203108178000	-2.169093038000
C	-0.510062453000	2.180617501000	-2.687921396000
H	-0.873208485000	2.534707330000	-1.717337058000
H	-1.099026490000	2.695654910000	-3.462952527000
C	0.948992878000	2.516261665000	-2.859161274000
C	1.907407589000	1.970085263000	-1.969333490000
C	3.256869378000	2.341818868000	-2.107781685000
C	3.650818501000	3.231993226000	-3.102756565000
H	4.699336280000	3.504034328000	-3.193125180000
C	2.710439514000	3.769970767000	-3.984478504000
C	1.370406102000	3.404618849000	-3.853530887000
H	0.628920219000	3.819399083000	-4.533598309000
C	-0.374960221000	0.133330148000	-4.042672499000
H	0.689346314000	0.370046707000	-4.139692850000
H	-0.901692903000	0.649432136000	-4.860728197000
C	-0.597398852000	-1.352461595000	-4.154448808000
C	0.000357816000	-2.217103949000	-3.204575210000
C	-0.160391694000	-3.606369321000	-3.340789264000
C	-0.904259052000	-4.129691752000	-4.395439109000
H	-1.021617061000	-5.206603968000	-4.485054614000
C	-1.503140681000	-3.281713799000	-5.330397271000
C	-1.345403568000	-1.901674338000	-5.199081495000
H	-1.807379087000	-1.233574368000	-5.923275873000
O	1.436442745000	-1.227562277000	0.596914286000
C	2.289621032000	-0.464573328000	1.498920315000
C	2.883598900000	-1.429203232000	0.548984176000
C	2.143914438000	-0.805727524000	2.962809532000
H	2.327913864000	0.588028111000	1.226789950000
H	3.313739623000	-1.028500293000	-0.367326655000
H	2.970846748000	-0.313141212000	3.493866575000
H	1.216417147000	-0.363346944000	3.345549706000
H	-2.088392652000	-3.689314616000	-6.149161501000
H	0.308776236000	-4.252611340000	-2.605229484000
H	3.015308313000	4.462099159000	-4.763528142000
H	3.978718285000	1.918360217000	-1.415464736000
H	-5.353021194000	2.968904810000	-0.027802950000
H	-2.407958304000	0.654140119000	2.115876196000
C	3.336592757000	-2.808226911000	0.992722669000
H	2.647751660000	-3.538947220000	0.550114497000
H	4.325294596000	-3.009420001000	0.562701781000
C	3.386961133000	-2.966016706000	2.524334475000
H	4.302571211000	-2.491946187000	2.904389835000
H	3.459173154000	-4.028834162000	2.780304569000
C	2.178538724000	-2.320661114000	3.219635996000
H	1.252188998000	-2.776236919000	2.851233280000
H	2.218898538000	-2.504072133000	4.298904140000
Fe	0.312329120000	-0.306263679000	-1.049713854000

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2b-TS

N	-2.405782186000	0.618942715000	-0.354555350000
O	-1.285532163000	-0.903319983000	1.933435262000
O	0.360612392000	1.337526123000	0.274301004000
O	-0.515471464000	-1.509314926000	-1.149868964000
C	-3.523887666000	0.044979860000	0.440734948000
H	-3.551955929000	-1.024869187000	0.209552983000
H	-4.480105064000	0.477977599000	0.096530917000
C	-3.387548292000	0.245680731000	1.927451767000
C	-2.247695068000	-0.273003047000	2.596710079000
C	-2.162703340000	-0.129362971000	3.996838671000
C	-3.170326928000	0.512069908000	4.711020157000
H	-3.078419281000	0.616003729000	5.790086546000
C	-4.290263702000	1.027993488000	4.052690504000
C	-4.383244102000	0.889030685000	2.666995480000
H	-5.249211854000	1.287662931000	2.140469285000
C	-2.324440197000	2.090176677000	-0.138181345000
H	-2.216677488000	2.236834495000	0.941379790000
H	-3.279407799000	2.557009470000	-0.438844154000
C	-1.185026160000	2.752982650000	-0.865314495000
C	0.138154403000	2.324913764000	-0.594178007000
C	1.217252874000	2.964806480000	-1.235518166000
C	0.977908954000	4.006592969000	-2.128052308000
H	1.821162931000	4.485663065000	-2.619989652000
C	-0.325707579000	4.434738332000	-2.399201742000
C	-1.395394159000	3.800848163000	-1.765464591000
H	-2.416162725000	4.121596061000	-1.969506314000
C	-2.595665690000	0.326651236000	-1.800746769000
H	-1.748915763000	0.785088893000	-2.322100259000
H	-3.510469230000	0.830513346000	-2.160533871000
C	-2.670521777000	-1.141402215000	-2.126636680000
C	-1.583349747000	-1.984697074000	-1.778505452000
C	-1.645118944000	-3.347920845000	-2.133674061000
C	-2.747536665000	-3.859079882000	-2.812240617000
H	-2.772768463000	-4.915007738000	-3.073128172000
C	-3.819474199000	-3.029507442000	-3.154199293000
C	-3.767445186000	-1.679496792000	-2.804083784000
H	-4.595709381000	-1.021241081000	-3.062370516000
O	1.452809059000	-1.185987360000	0.888193632000
C	2.611322140000	-0.402534691000	1.215062568000
C	2.880139189000	-0.712232082000	-0.190604766000
C	3.506022578000	-1.044720207000	2.262243543000
H	2.376699326000	0.643367264000	1.417470879000
H	2.419134427000	-0.079225054000	-0.933634471000
H	4.394619594000	-0.406636333000	2.349169969000
H	2.985935346000	-1.031028277000	3.228402395000
H	-4.682836286000	-3.427665746000	-3.680320953000
H	-0.805838709000	-3.980626948000	-1.860460701000
H	-0.507057167000	5.246664185000	-3.098646601000
H	2.229453327000	2.625469801000	-1.024989306000
H	-5.074830809000	1.535091739000	4.607662110000
H	-1.285578746000	-0.532095361000	4.494669807000
C	3.549858658000	-1.993835678000	-0.598723366000
H	2.756731156000	-2.729270853000	-0.790803769000
H	4.065115528000	-1.815802969000	-1.545989439000
C	4.530342978000	-2.510974426000	0.466991005000
H	5.421252435000	-1.872540124000	0.437820586000
H	4.843711804000	-3.531142103000	0.210548780000
C	3.922104036000	-2.474204379000	1.878360204000
H	3.043252867000	-3.129721005000	1.923991340000
H	4.646308524000	-2.855706233000	2.609588264000
Br	5.024788926000	1.014818878000	-0.686081348000
Fe	-0.324271619000	-0.419809912000	0.381438905000

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3b

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N	-2.368989387000	0.676260078000	-0.260281717000
O	-1.272085053000	-0.693494771000	2.136805210000
O	0.381733247000	1.563736940000	0.383501193000
O	-0.311421487000	-1.383182719000	-0.896675317000
C	-3.485545555000	0.034885194000	0.474469180000

H	-3.420737800000	-1.038362769000	0.265948507000
H	-4.451608984000	0.387272667000	0.066693648000
C	-3.459764429000	0.269425014000	1.962149810000
C	-2.322453647000	-0.132483540000	2.714054056000
C	-2.338171360000	0.057235428000	4.112033484000
C	-3.437274176000	0.630863700000	4.744517754000
H	-3.420351618000	0.772733278000	5.823279529000
C	-4.554322272000	1.029801654000	4.004967887000
C	-4.548768531000	0.845819292000	2.621331898000
H	-5.410107267000	1.157401027000	2.031822646000
C	-2.387260906000	2.143838972000	-0.047689709000
H	-2.317001051000	2.302458717000	1.033891230000
H	-3.359922251000	2.556608878000	-0.374582467000
C	-1.274510115000	2.877230347000	-0.748588529000
C	0.074794967000	2.527196779000	-0.472102013000
C	1.102088326000	3.247729921000	-1.118674900000
C	0.804090051000	4.278235127000	-2.005321923000
H	1.615697568000	4.812005720000	-2.495449058000
C	-0.523071530000	4.624311993000	-2.274689888000
C	-1.546234209000	3.914210960000	-1.644552348000
H	-2.585652315000	4.165603934000	-1.852106710000
C	-2.448898637000	0.359723193000	-1.706416132000
H	-1.598390177000	0.859368240000	-2.182106787000
H	-3.366925416000	0.802732747000	-2.136148308000
C	-2.415261579000	-1.113032635000	-2.021757930000
C	-1.308396105000	-1.898035405000	-1.596492782000
C	-1.277408714000	-3.262398336000	-1.958872702000
C	-2.299049556000	-3.829628396000	-2.714338742000
H	-2.249163868000	-4.884928650000	-2.975312995000
C	-3.385528300000	-3.056571956000	-3.133304419000
C	-3.428537080000	-1.707336898000	-2.778691939000
H	-4.269401794000	-1.092472535000	-3.097328257000
O	1.485323921000	-0.857920681000	1.251753109000
C	2.767019791000	-0.368789543000	1.006728217000
C	3.089076968000	-0.748004399000	-0.452458309000
C	3.760410832000	-1.015539916000	1.989160566000
H	2.798187208000	0.727635741000	1.101475970000
H	2.362433514000	-0.304392390000	-1.129647082000
H	4.753088182000	-0.567715044000	1.849030126000
H	3.431396862000	-0.776874157000	3.007304359000
H	-4.186875494000	-3.496279934000	-3.721522655000
H	-0.430236572000	-3.854284094000	-1.624527279000
H	-0.758016919000	5.425592248000	-2.970622866000
H	2.130374172000	2.966989562000	-0.910223289000
H	-5.411593308000	1.483639296000	4.495512415000
H	-1.462062662000	-0.252384899000	4.674170365000
C	3.243850145000	-2.243399863000	-0.665239890000
H	2.228798276000	-2.643020981000	-0.533333584000
H	3.541460031000	-2.453559610000	-1.698068044000
C	4.204222791000	-2.897595574000	0.340891864000
H	5.228668955000	-2.562908326000	0.128523344000
H	4.192898327000	-3.986797654000	0.201966464000
C	3.833881093000	-2.537619816000	1.790805353000
H	2.854505695000	-2.966905490000	2.034439169000
H	4.562051907000	-2.976182311000	2.486335047000
Br	4.850621419000	0.245308655000	-1.073380712000
Fe	-0.184288897000	-0.247011269000	0.646552877000

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3b-TS

N	-1.967807282000	0.388420098000	0.234054601000
O	-0.713634975000	-1.472438278000	2.100975679000
O	0.575460233000	1.597140173000	1.157133278000
O	0.524020034000	-0.991631796000	-0.602316190000
C	-2.997632350000	-0.508526180000	0.815057681000
H	-2.834260831000	-1.493624787000	0.368177902000
H	-4.003823215000	-0.168165230000	0.507992989000
C	-2.930717722000	-0.630944445000	2.313119949000
C	-1.741174128000	-1.142844561000	2.887646908000
C	-1.668024514000	-1.312899277000	4.282570658000

C	-2.759137034000	-0.990551204000	5.084130121000
H	-2.684384524000	-1.119215100000	6.161824544000
C	-3.939087271000	-0.492810858000	4.521887613000
C	-4.011446797000	-0.314060684000	3.139149891000
H	-4.922304133000	0.076432333000	2.687370950000
C	-2.218855870000	1.794487522000	0.638226404000
H	-2.198364110000	1.809557685000	1.733438397000
H	-3.235006754000	2.097985134000	0.325128133000
C	-1.212476635000	2.765709960000	0.077603739000
C	0.163954332000	2.575205267000	0.363455863000
C	1.102918697000	3.462700272000	-0.201108102000
C	0.689959653000	4.529897503000	-0.992851994000
H	1.433039154000	5.202016135000	-1.416982465000
C	-0.668106337000	4.735385043000	-1.252984631000
C	-1.601665379000	3.842600395000	-0.722372603000
H	-2.661002747000	3.977200280000	-0.936755426000
C	-1.943404168000	0.252160175000	-1.243923160000
H	-1.202339549000	0.966818577000	-1.614115539000
H	-2.921778959000	0.546087046000	-1.666868127000
C	-1.589985534000	-1.137134762000	-1.708406569000
C	-0.338975025000	-1.691308522000	-1.333118231000
C	-0.007468754000	-2.985900509000	-1.779745762000
C	-0.886234009000	-3.709137237000	-2.581028685000
H	-0.611142506000	-4.709243853000	-2.909077652000
C	-2.115412029000	-3.162466005000	-2.959254490000
C	-2.453216349000	-1.882914191000	-2.514594423000
H	-3.412000579000	-1.448488972000	-2.793895450000
O	2.319373391000	-0.679730534000	1.847319613000
C	3.567624281000	-1.152856904000	1.312777761000
C	4.685558069000	-0.352383414000	2.016453007000
C	3.613370536000	-0.951340545000	-0.207101551000
H	3.676288871000	-2.210310890000	1.573114914000
H	4.609652721000	-0.469335807000	3.092960019000
H	4.508341990000	-1.466381257000	-0.578663875000
H	2.739752900000	-1.429620942000	-0.651957049000
H	-2.804375826000	-3.726734241000	-3.581946441000
H	0.948589403000	-3.401838545000	-1.476079171000
H	-0.994164059000	5.567244688000	-1.871512391000
H	2.153264587000	3.266887643000	-0.004550607000
H	-4.786730254000	-0.237856295000	5.152736099000
H	-0.732439717000	-1.661397744000	4.703815365000
C	4.783657420000	1.097905224000	1.572552699000
H	3.864196999000	1.573205260000	1.945146385000
H	5.627446614000	1.588927315000	2.068748074000
C	4.847204876000	1.259826601000	0.047092946000
H	5.798285993000	0.854855416000	-0.322931145000
H	4.834224507000	2.326987930000	-0.210564133000
C	3.667569692000	0.532421333000	-0.615066794000
H	2.738011900000	1.034279573000	-0.320230518000
H	3.735991516000	0.606749260000	-1.707826144000
Br	6.508619751000	-1.322237457000	1.664432872000
Fe	0.346451667000	-0.268707308000	1.136441939000
C	2.087340416000	-0.884293253000	3.442431107000
O	2.847913603000	-1.700631036000	3.926119659000
O	1.172070618000	-0.140132184000	3.765528929000

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N	-2.164146213000	0.262288559000	0.511389222000
O	-1.376913752000	-1.151404599000	2.998130883000
O	0.118551076000	1.474886856000	1.967518028000
O	0.342142462000	-1.264219584000	0.218335048000
C	-3.285050755000	-0.610812313000	0.937809594000
H	-2.993599415000	-1.635818353000	0.684803417000
H	-4.189190086000	-0.374806728000	0.345950613000
C	-3.611181763000	-0.518661670000	2.406013723000
C	-2.604997561000	-0.816441394000	3.362849353000
C	-2.942225658000	-0.775027689000	4.732449393000
C	-4.231210230000	-0.448502548000	5.141591521000
H	-4.464135911000	-0.419793129000	6.204102268000

C	-5.222471310000	-0.153656494000	4.200330736000
C	-4.897487667000	-0.191330443000	2.843406064000
H	-5.658387338000	0.038006424000	2.098454371000
C	-2.475230771000	1.683123177000	0.798096840000
H	-2.715096008000	1.739410656000	1.864741010000
H	-3.383774606000	1.986033910000	0.244390353000
C	-1.354181899000	2.638070171000	0.480235106000
C	-0.098527535000	2.473047998000	1.124463946000
C	0.918562008000	3.418663979000	0.871528061000
C	0.703075962000	4.485909341000	0.004184304000
H	1.505095358000	5.198658569000	-0.177607629000
C	-0.529746230000	4.643987762000	-0.635684941000
C	-1.543134213000	3.715834292000	-0.388400734000
H	-2.509677064000	3.827421612000	-0.878248662000
C	-1.883154800000	0.078385070000	-0.933119569000
H	-1.065454768000	0.763914206000	-1.179445165000
H	-2.761445190000	0.391463696000	-1.528272639000
C	-1.500014829000	-1.329450131000	-1.307032807000
C	-0.370071576000	-1.922772019000	-0.685401755000
C	0.009798452000	-3.224892665000	-1.073214409000
C	-0.704094993000	-3.914929628000	-2.048482138000
H	-0.392891142000	-4.919103308000	-2.329096038000
C	-1.815593788000	-3.330571789000	-2.662935977000
C	-2.200978168000	-2.043867508000	-2.281404558000
H	-3.066732972000	-1.577014479000	-2.749306587000
O	3.016775489000	-0.573848547000	1.345222381000
C	4.203038341000	-1.007718612000	0.660978878000
C	5.375252683000	-0.268379140000	1.320240688000
C	4.022708412000	-0.651720668000	-0.815655340000
H	4.325994909000	-2.082806485000	0.807960985000
H	5.407350006000	-0.511919160000	2.380070209000
H	4.848591942000	-1.101458730000	-1.380557753000
H	3.090863471000	-1.113195742000	-1.157534532000
H	-2.375969149000	-3.869174964000	-3.422461634000
H	0.873500792000	-3.666634002000	-0.584909104000
H	-0.698612552000	5.473283195000	-1.317578844000
H	1.870499376000	3.282893105000	1.376321318000
H	-6.229191143000	0.105837458000	4.517089373000
H	-2.160624541000	-1.005703113000	5.450377817000
C	5.378724456000	1.228195572000	1.039574628000
H	4.513851399000	1.626485284000	1.589767051000
H	6.273966872000	1.693845382000	1.464395111000
C	5.224061776000	1.560449313000	-0.452895951000
H	6.127787055000	1.240196463000	-0.988135839000
H	5.149031403000	2.647961408000	-0.579150314000
C	3.988976905000	0.867913018000	-1.051864155000
H	3.080357719000	1.280019079000	-0.596834520000
H	3.926088550000	1.074581096000	-2.127853359000
Br	7.167059814000	-1.112744599000	0.656516180000
Fe	-0.090974447000	-0.398869188000	1.843071414000
C	2.641104136000	-1.312570070000	2.468618475000
O	3.401817877000	-2.140779309000	2.951404615000
O	1.469108784000	-0.979462096000	2.884072899000

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N	-2.442093103000	0.525968601000	0.701132860000
O	-1.803898537000	-0.973357333000	3.154971378000
O	-0.214697276000	1.671399981000	2.240215642000
O	-0.031241454000	-1.125000370000	0.489175070000
C	-3.598508246000	-0.346202048000	1.038907147000
H	-3.307809854000	-1.365406575000	0.764558557000
H	-4.462490461000	-0.072785293000	0.407192176000
C	-4.000994391000	-0.301009220000	2.488969617000
C	-3.045830756000	-0.642953399000	3.481636174000
C	-3.447224562000	-0.652845604000	4.833225451000
C	-4.754039238000	-0.334048023000	5.189597401000
H	-5.040423359000	-0.346341612000	6.239074418000
C	-5.695638026000	0.004462637000	4.213200212000
C	-5.305447413000	0.019163183000	2.873186236000

H	-6.027912088000	0.281782655000	2.101748366000
C	-2.758492146000	1.944111162000	1.017385226000
H	-3.028419689000	1.972192831000	2.078180806000
H	-3.649269657000	2.258534883000	0.444620486000
C	-1.625307514000	2.899293817000	0.751467194000
C	-0.388406754000	2.697730655000	1.416656102000
C	0.653423040000	3.623772485000	1.207333821000
C	0.475281064000	4.714684541000	0.361676965000
H	1.294894737000	5.413965387000	0.210969282000
C	-0.741590796000	4.912783234000	-0.297392440000
C	-1.777918130000	3.999598562000	-0.095438058000
H	-2.730679860000	4.140616550000	-0.603752776000
C	-2.097696793000	0.387402664000	-0.739652545000
H	-1.241657753000	1.046685242000	-0.918117064000
H	-2.933525314000	0.764483852000	-1.355662594000
C	-1.760833214000	-1.019243579000	-1.157647802000
C	-0.705077799000	-1.699017242000	-0.497554270000
C	-0.360745675000	-2.997028677000	-0.926669617000
C	-1.042515475000	-3.602379053000	-1.977757177000
H	-0.759941466000	-4.605036197000	-2.290909094000
C	-2.085083746000	-2.935094778000	-2.627586207000
C	-2.433221277000	-1.650516518000	-2.206936495000
H	-3.244294527000	-1.119553845000	-2.703176348000
O	2.660143145000	-0.562996679000	1.630529164000
C	3.906251186000	-1.116858887000	1.129013733000
C	4.788376062000	-1.604341504000	2.283910699000
C	4.545031368000	0.017508924000	0.317517702000
H	3.653470061000	-1.965770469000	0.488015101000
H	4.796914230000	-2.640459001000	2.556970434000
H	5.338279644000	-0.409283796000	-0.300465878000
H	3.771392275000	0.422265947000	-0.344019101000
H	-2.620364529000	-3.408550458000	-3.446057909000
H	0.450547582000	-3.503564450000	-0.412611094000
H	-0.879509918000	5.761210804000	-0.962095478000
H	1.594045642000	3.454387308000	1.722673381000
H	-6.715497052000	0.256746292000	4.490593909000
H	-2.704243187000	-0.917127706000	5.579648438000
C	5.578472232000	-0.590089897000	3.072953404000
H	4.885348881000	-0.173546862000	3.814882914000
H	6.373990213000	-1.099052414000	3.623087326000
C	6.150773942000	0.554829283000	2.211400554000
H	7.009213404000	0.170714849000	1.651172298000
H	6.514656660000	1.348552483000	2.876166010000
C	5.108658512000	1.116414758000	1.231403036000
H	4.283569761000	1.582299728000	1.786305745000
H	5.561343351000	1.905260224000	0.617841334000
Br	6.695577508000	-2.619000134000	0.821297555000
Fe	-0.510283419000	-0.178339327000	2.042369960000
C	2.244870037000	-1.046267256000	2.831486505000
O	3.076504177000	-1.690722736000	3.513756884000
O	1.055709279000	-0.773135841000	3.166722504000

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N	-2.488655786000	0.597125308000	0.689543890000
O	-1.814442113000	-0.940726061000	3.093424911000
O	-0.133422007000	1.614253335000	2.102623089000
O	-0.136196883000	-1.136719293000	0.354371638000
C	-3.672602857000	-0.236196889000	1.065192718000
H	-3.436762987000	-1.260223059000	0.758591452000
H	-4.541014909000	0.090971788000	0.471404811000
C	-4.015526582000	-0.195300519000	2.530882966000
C	-3.040195544000	-0.580684809000	3.483667751000
C	-3.378686366000	-0.591073174000	4.848137559000
C	-4.657516472000	-0.226049234000	5.259841230000
H	-4.901776275000	-0.236544612000	6.319082145000
C	-5.622706518000	0.157507166000	4.324945576000
C	-5.290698627000	0.171198710000	2.970048528000
H	-6.034892938000	0.469080159000	2.233821622000
C	-2.733030470000	2.029042132000	1.042048675000

H	-2.961448475000	2.046344689000	2.112616493000
H	-3.632901519000	2.377791193000	0.510521942000
C	-1.577685907000	2.947135341000	0.741263566000
C	-0.314867753000	2.685675102000	1.328747375000
C	0.746512262000	3.578794716000	1.096588824000
C	0.562089029000	4.704424119000	0.298392714000
H	1.394047795000	5.383836374000	0.129628984000
C	-0.679714635000	4.963296584000	-0.287297572000
C	-1.736158137000	4.080039500000	-0.061080393000
H	-2.708107545000	4.273730099000	-0.510878737000
C	-2.202620479000	0.465113703000	-0.771613102000
H	-1.337729965000	1.105622972000	-0.973572100000
H	-3.052305034000	0.876231761000	-1.339850741000
C	-1.927868319000	-0.945840894000	-1.221574144000
C	-0.869058054000	-1.673681509000	-0.623916424000
C	-0.588744167000	-2.973614361000	-1.082584414000
C	-1.339124072000	-3.539757761000	-2.109357979000
H	-1.110702330000	-4.547955376000	-2.445946195000
C	-2.384796403000	-2.826198528000	-2.700410193000
C	-2.669437416000	-1.537556826000	-2.247862885000
H	-3.483793746000	-0.974018463000	-2.699209993000
O	2.717329829000	-0.220338875000	1.421506648000
C	4.035897653000	-0.728898820000	1.057205385000
C	4.530484066000	-1.231400382000	2.422431671000
C	4.879703091000	0.333080045000	0.365695017000
H	3.858498614000	-1.573187915000	0.380328051000
H	5.149820953000	-2.125755939000	2.328011619000
H	5.701085683000	-0.196914558000	-0.135610174000
H	4.276966960000	0.792658574000	-0.424623178000
H	-2.974271769000	-3.268834165000	-3.497695857000
H	0.220873314000	-3.520379177000	-0.608434736000
H	-0.823444747000	5.839070208000	-0.913041749000
H	1.705208217000	3.363769738000	1.558896115000
H	-6.618891177000	0.446273340000	4.646653715000
H	-2.617363615000	-0.888738243000	5.562437356000
C	5.195477732000	-0.161631936000	3.298466279000
H	4.409246473000	0.485511248000	3.706133173000
H	5.679261176000	-0.645276531000	4.153020944000
C	6.182335488000	0.703753801000	2.497818367000
H	7.010878431000	0.087432515000	2.120218398000
H	6.628059258000	1.451285220000	3.162232581000
C	5.462447852000	1.382047587000	1.322783435000
H	4.658452004000	2.022963088000	1.706223371000
H	6.149058783000	2.032796453000	0.770901903000
Fe	-0.662561716000	-0.159933325000	1.862852719000
C	2.288613258000	-0.915796531000	2.482853127000
O	3.273008122000	-1.645311246000	3.033760154000
O	1.153724192000	-0.897923623000	2.916064948000

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4'b

N	-1.892210051000	-0.209417101000	0.728688640000
O	-1.180647582000	-0.650629577000	3.465870404000
O	0.549141384000	1.090881546000	1.888042165000
O	0.716013151000	-1.372375758000	0.283879555000
C	-2.995123028000	-1.098246427000	1.163761913000
H	-2.652404062000	-2.119690033000	0.979037050000
H	-3.875373453000	-0.921744193000	0.519547336000
C	-3.416747455000	-0.952471394000	2.607620636000
C	-2.473513778000	-0.780719470000	3.663941678000
C	-2.966490374000	-0.728217022000	4.990014766000
C	-4.322304902000	-0.847695151000	5.269438067000
H	-4.663156066000	-0.807102013000	6.302118056000
C	-5.245199066000	-1.014566002000	4.232447753000
C	-4.775681080000	-1.055815416000	2.919208712000
H	-5.485138093000	-1.178188621000	2.101430262000
C	-2.199605262000	1.213437176000	1.042430550000
H	-2.300540525000	1.273956783000	2.128260634000
H	-3.174022503000	1.481749462000	0.599493370000
C	-1.143475097000	2.178980156000	0.575731879000

C	0.187540372000	2.057151057000	1.068426938000
C	1.134118785000	3.026751654000	0.665902759000
C	0.791500644000	4.049839851000	-0.211041882000
H	1.547812285000	4.773238755000	-0.509075896000
C	-0.509840030000	4.150678807000	-0.713547998000
C	-1.460129593000	3.212309113000	-0.308707612000
H	-2.479726408000	3.277988692000	-0.686292749000
C	-1.658410711000	-0.372960352000	-0.732078913000
H	-0.904266788000	0.371728103000	-1.001288617000
H	-2.584635402000	-0.126712086000	-1.279885141000
C	-1.156998662000	-1.732779019000	-1.127518051000
C	0.087932092000	-2.142906288000	-0.584888569000
C	0.642317678000	-3.368493031000	-1.005019366000
C	-0.030051177000	-4.165176058000	-1.929671042000
H	0.409816607000	-5.111518760000	-2.239006062000
C	-1.268023694000	-3.770653307000	-2.448564087000
C	-1.819435619000	-2.552504671000	-2.039458717000
H	-2.778712201000	-2.227523521000	-2.440386885000
O	3.315195868000	-0.826082750000	1.890668090000
C	4.381214493000	-1.037404498000	0.949342096000
C	5.289769784000	0.166366975000	1.218292491000
C	3.829404848000	-1.054978219000	-0.480058189000
H	4.892416417000	-1.974185570000	1.183697975000
H	5.606301271000	0.176494544000	2.260774402000
H	4.657102599000	-1.282001887000	-1.163941332000
H	3.101775957000	-1.865352791000	-0.546342161000
H	-1.793815422000	-4.399573052000	-3.162139393000
H	1.582299969000	-3.676332437000	-0.556710933000
H	-0.779501997000	4.943608926000	-1.405876013000
H	2.139053337000	2.940105721000	1.063467154000
H	-6.308375520000	-1.102059466000	4.439550302000
H	-2.234717997000	-0.595071605000	5.781520418000
C	4.665921521000	1.485696965000	0.789935381000
H	3.823381554000	1.622382155000	1.482298031000
H	5.369287386000	2.309430799000	0.950776407000
C	4.129823535000	1.461250546000	-0.649929162000
H	4.975454075000	1.389009257000	-1.346968978000
H	3.614576095000	2.405891152000	-0.859485694000
C	3.168631086000	0.280323132000	-0.853103426000
H	2.279778468000	0.412156851000	-0.229931605000
H	2.824383151000	0.243215380000	-1.894064048000
Br	7.100699981000	-0.130889369000	0.228800873000
Fe	0.027438436000	-0.749206453000	1.981773199000
C	2.596294967000	-1.937506500000	2.290413442000
O	2.987440235000	-3.071847763000	2.025881162000
O	1.542541344000	-1.598752278000	2.956352367000
C	-2.114335414000	-5.651522407000	1.848242683000
C	-0.619047229000	-5.440681268000	1.568184085000
C	-0.073044798000	-4.199470906000	2.238627838000
C	-0.779217249000	-3.603034966000	3.388817623000
C	-2.074131054000	-4.188558603000	3.929327883000
C	-2.399173840000	-5.579788857000	3.355150870000
H	0.993929772000	-4.006775702000	2.142167385000
H	-0.043707589000	-6.297348534000	1.950024610000
H	-0.429541062000	-5.377221763000	0.492281604000
H	-2.688843874000	-4.877163483000	1.325879868000
H	-2.434314474000	-6.618770477000	1.440984360000
H	-0.200025942000	-2.971203449000	4.056408090000
H	-2.014151056000	-4.232847602000	5.023302197000
H	-2.878351662000	-3.482037414000	3.695709050000
H	-1.785339982000	-6.339113634000	3.862139122000
H	-3.445928941000	-5.831670514000	3.566658181000
O	-0.883055568000	-3.003870033000	2.066638072000

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4' b-TS

N	-1.830916395000	-0.391762658000	0.687539242000
O	-1.351708055000	-0.606230142000	3.468345686000
O	0.354408173000	1.104458428000	1.962220142000
O	0.988181115000	-1.257796780000	0.464765770000

C	-2.853859430000	-1.416714648000	1.010129377000
H	-2.383629093000	-2.382594089000	0.811589680000
H	-3.703031477000	-1.294716512000	0.314366640000
C	-3.378599157000	-1.417809612000	2.430929658000
C	-2.570723332000	-1.096370564000	3.563107267000
C	-3.138032309000	-1.255969425000	4.849527766000
C	-4.442099615000	-1.704301557000	5.023916065000
H	-4.842763697000	-1.815430453000	6.029851446000
C	-5.237620513000	-2.001027949000	3.913771048000
C	-4.692178730000	-1.847302702000	2.638076839000
H	-5.303200794000	-2.079566040000	1.766134347000
C	-2.337731503000	0.980992703000	0.983219340000
H	-2.542455060000	1.000486633000	2.055608931000
H	-3.291369033000	1.131184069000	0.450647011000
C	-1.375687640000	2.083835261000	0.627510678000
C	-0.061123092000	2.072068959000	1.181001058000
C	0.799887311000	3.150233812000	0.868103012000
C	0.381990408000	4.190319670000	0.045701559000
H	1.068704059000	5.004986839000	-0.177507308000
C	-0.906312760000	4.194907623000	-0.500464278000
C	-1.765849253000	3.135230162000	-0.203650043000
H	-2.770712876000	3.121115058000	-0.624374274000
C	-1.424030634000	-0.502495435000	-0.741370623000
H	-0.743533513000	0.334201221000	-0.922292441000
H	-2.312254152000	-0.357466556000	-1.379573056000
C	-0.727294515000	-1.786779662000	-1.097785942000
C	0.518720492000	-2.062083340000	-0.467625048000
C	1.236782265000	-3.204492735000	-0.881239413000
C	0.723025241000	-4.059103386000	-1.853680278000
H	1.292191280000	-4.939668904000	-2.146650764000
C	-0.515787817000	-3.801041744000	-2.448242566000
C	-1.225682816000	-2.659832753000	-2.062528506000
H	-2.186618885000	-2.437251312000	-2.525054413000
H	-0.919944571000	-4.472461830000	-3.201176940000
H	2.195652866000	-3.398826412000	-0.408331038000
H	-1.233305359000	5.004441992000	-1.147681084000
H	1.798558431000	3.128506010000	1.294486449000
H	-6.262376932000	-2.341929882000	4.036339183000
H	-2.507184682000	-1.005222198000	5.697745572000
Fe	-0.060700429000	-0.770623478000	2.041729825000
C	4.138451330000	-1.868749379000	5.779319231000
H	3.584895841000	-2.710216852000	6.202042204000
O	3.259724388000	-1.080182164000	4.949975313000
C	4.523252337000	-0.868934888000	6.876384745000
H	3.629399663000	-0.494251233000	7.373471220000
C	5.346772074000	-2.362473203000	4.974883762000
H	5.959542449000	-2.995297169000	5.628200429000
H	4.969618805000	-2.991640139000	4.164602029000
Br	5.471034072000	-1.905869667000	8.404226728000
C	5.416674104000	0.255660522000	6.371422701000
H	5.724899673000	0.895776937000	7.203965422000
H	4.772620130000	0.856208036000	5.714014058000
C	6.625394272000	-0.253939554000	5.571739518000
H	7.181505839000	0.601392334000	5.169592197000
H	7.304556264000	-0.788655207000	6.248511918000
C	6.182023552000	-1.190983708000	4.435615108000
H	5.579057192000	-0.627551799000	3.713145216000
H	7.056291322000	-1.573432370000	3.895334855000
C	2.402403101000	-1.737884852000	4.094108612000
O	2.436146206000	-3.016523944000	4.141730633000
C	0.254458272000	-5.712661638000	1.763532622000
C	1.489173969000	-5.056885461000	2.432932063000
C	1.159682986000	-3.626323636000	2.727959061000
C	-0.170850341000	-3.338920242000	3.316160976000
C	-0.903373533000	-4.599478243000	3.787008076000
C	-1.009698041000	-5.653377954000	2.664540144000
H	1.570172457000	-2.869814039000	2.080263386000
H	1.715651502000	-5.561953185000	3.380182228000
H	2.369602635000	-5.134951676000	1.787661848000
H	0.065413973000	-5.175571045000	0.830777501000
H	0.503631209000	-6.748818928000	1.503930327000

H	-0.160893114000	-2.595232327000	4.125487600000
H	-0.364736965000	-5.005569892000	4.655594596000
H	-1.899965630000	-4.308014476000	4.134245342000
H	-1.206766087000	-6.635429223000	3.113664272000
H	-1.871400807000	-5.412599059000	2.035747560000
O	-0.635846108000	-2.866883822000	2.095885822000
O	1.716312207000	-0.985273079000	3.382043195000

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N	-1.495032082000	1.229142143000	-0.226290049000
O	-0.625001330000	-0.845660683000	1.709543878000
O	0.719175763000	2.187046982000	1.517758564000
O	1.158585391000	0.068239633000	-0.901970102000
C	-2.511638352000	0.151225044000	-0.204732068000
H	-2.087821508000	-0.687741017000	-0.767189090000
H	-3.417803188000	0.480417003000	-0.747652345000
C	-2.899434571000	-0.299801563000	1.179658624000
C	-1.898622327000	-0.790825250000	2.061948408000
C	-2.297123973000	-1.251720042000	3.336125739000
C	-3.632851606000	-1.224351878000	3.724826553000
H	-3.909952789000	-1.581351714000	4.714915203000
C	-4.615700790000	-0.738719339000	2.857292193000
C	-4.233039682000	-0.280885240000	1.595318224000
H	-4.986397421000	0.103473239000	0.908725087000
C	-1.978397630000	2.412865477000	0.524473636000
H	-2.189839813000	2.070270234000	1.543140285000
H	-2.937061532000	2.761564823000	0.096005793000
C	-1.005632199000	3.562735164000	0.561347738000
C	0.303128833000	3.362141360000	1.082277913000
C	1.170858575000	4.476932486000	1.146962983000
C	0.764288200000	5.734793687000	0.714551219000
H	1.457773889000	6.571622894000	0.774238327000
C	-0.522239007000	5.928546651000	0.202548548000
C	-1.388320119000	4.836260445000	0.131654677000
H	-2.393127756000	4.969613550000	-0.267661742000
C	-1.162145331000	1.600510508000	-1.621482437000
H	-0.416055294000	2.399797117000	-1.559826019000
H	-2.053593676000	2.029058823000	-2.117494654000
C	-0.626024720000	0.467173802000	-2.457144040000
C	0.544656305000	-0.221563905000	-2.036166179000
C	1.071923736000	-1.222814783000	-2.882991595000
C	0.456613657000	-1.541644208000	-4.089261970000
H	0.883579803000	-2.320638286000	-4.718131053000
C	-0.701721431000	-0.872297719000	-4.495552038000
C	-1.226214773000	0.124902134000	-3.671573616000
H	-2.124466323000	0.660627895000	-3.976483831000
O	2.183377666000	-0.272391859000	1.692431812000
C	3.438682972000	-0.061765637000	1.110743313000
C	3.825671171000	-1.437467317000	0.497209873000
C	4.422344618000	0.457486097000	2.177040674000
H	3.387496232000	0.664927581000	0.282126462000
H	2.904361220000	-1.813426351000	0.055963727000
H	5.350858045000	0.781565195000	1.695273681000
H	3.953791858000	1.333174245000	2.640499055000
H	-1.188014528000	-1.122159427000	-5.434929152000
H	1.979418033000	-1.726617405000	-2.562366642000
H	-0.843239783000	6.908946228000	-0.139686381000
H	2.167384373000	4.313399831000	1.547360744000
H	-5.659528896000	-0.711749381000	3.158914319000
H	-1.522593516000	-1.624738508000	4.000019025000
C	4.345259893000	-2.446793003000	1.529063278000
H	3.445562281000	-2.809188373000	2.042100657000
H	4.779578103000	-3.308745730000	1.006769460000
C	5.309787664000	-1.881246920000	2.586933266000
H	6.275393469000	-1.649670617000	2.126854795000
H	5.487756365000	-2.651321405000	3.350281790000
C	4.732773627000	-0.611423811000	3.235322132000
H	3.805625857000	-0.858559458000	3.767695713000

H	5.437089697000	-0.215093437000	3.978695770000
Fe	0.596487055000	0.372182310000	0.914677876000
O	6.168704543000	-0.803570198000	-2.153198400000
C	7.457970409000	-0.247050759000	-2.499769663000
C	7.301101477000	1.281336962000	-2.478953027000
C	7.802180396000	-0.795892063000	-3.886091817000
H	8.187397708000	-0.554919753000	-1.747569530000
H	6.987421961000	1.610524646000	-1.490747961000
H	8.831938279000	-0.501731266000	-4.119055525000
H	7.777888050000	-1.890207364000	-3.838565826000
C	6.410270930000	1.811819761000	-3.594662160000
H	5.390369988000	1.491505060000	-3.337428569000
H	6.409063361000	2.905853064000	-3.586134208000
C	6.782911848000	1.259814444000	-4.979050364000
H	7.754924556000	1.669410481000	-5.282504134000
H	6.048791406000	1.605261527000	-5.716477951000
C	6.844300100000	-0.276465851000	-4.971886110000
H	5.841773700000	-0.680733613000	-4.787256890000
H	7.162205785000	-0.648655170000	-5.953409756000
Br	9.195979805000	2.118044959000	-2.609249152000
C	5.852954380000	-0.832437613000	-0.823994395000
O	6.597049471000	-0.433155719000	0.050763935000
O	4.652233834000	-1.365611036000	-0.734552708000

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2'b-TS

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N	-1.624809865000	1.202299697000	0.027931285000
O	-0.679192125000	-0.873061469000	1.904198597000
O	0.614033193000	2.166596252000	1.716560448000
O	1.000083825000	0.046040735000	-0.718723609000
C	-2.630170200000	0.112079815000	0.071506151000
H	-2.212315283000	-0.719127112000	-0.506244405000
H	-3.553403216000	0.435021639000	-0.444536959000
C	-2.972848943000	-0.350723047000	1.464288659000
C	-1.938747770000	-0.835800663000	2.308959042000
C	-2.283088091000	-1.307822360000	3.593360353000
C	-3.604839647000	-1.297608500000	4.028265458000
H	-3.843103327000	-1.663257981000	5.025108851000
C	-4.622631199000	-0.819754417000	3.197668678000
C	-4.291310830000	-0.349926643000	1.925311420000
H	-5.073071499000	0.027718860000	1.267660181000
C	-2.103260515000	2.378202937000	0.794803462000
H	-2.289162877000	2.028525270000	1.816082118000
H	-3.073815913000	2.718105805000	0.388075819000
C	-1.141288036000	3.538115173000	0.817491562000
C	0.180508120000	3.347475260000	1.304200901000
C	1.041154853000	4.465719151000	1.362806527000
C	0.612872993000	5.724567305000	0.954132241000
H	1.299473012000	6.567041971000	1.007400041000
C	-0.686672105000	5.910630838000	0.473296938000
C	-1.545173182000	4.812251930000	0.409253555000
H	-2.559564991000	4.940839204000	0.033863316000
C	-1.330173882000	1.582284035000	-1.375176922000
H	-0.584597372000	2.383213865000	-1.329878004000
H	-2.235651939000	2.011155393000	-1.843606244000
C	-0.815764487000	0.454245247000	-2.230502629000
C	0.362083144000	-0.238449575000	-1.843385679000
C	0.874656174000	-1.231298310000	-2.705919430000
C	0.235004052000	-1.538190067000	-3.902763092000
H	0.651878851000	-2.307442002000	-4.549603589000
C	-0.932504465000	-0.866489922000	-4.277757069000
C	-1.441611744000	0.122873655000	-3.435187064000
H	-2.344726809000	0.661982474000	-3.718323708000
O	2.114762056000	-0.298199554000	1.837362641000
C	3.345340724000	-0.008041579000	1.230320052000
C	3.595930693000	-1.398229684000	0.677322560000
C	4.401036261000	0.476815315000	2.232550009000
H	3.252094338000	0.711779519000	0.403368720000
H	2.787850283000	-1.725598268000	0.037582482000
H	5.289536993000	0.771668006000	1.666387400000

H	3.996991806000	1.366420075000	2.731221425000
H	-1.436008146000	-1.106797512000	-5.210432270000
H	1.796322842000	-1.727600521000	-2.415736070000
H	-1.024088785000	6.891392783000	0.148827646000
H	2.048288267000	4.306437307000	1.737094815000
H	-5.655336992000	-0.808219914000	3.535886788000
H	-1.481485340000	-1.675453320000	4.227360302000
C	4.180567262000	-2.421255212000	1.600965758000
H	3.311283533000	-2.743537006000	2.197127466000
H	4.508367577000	-3.294638515000	1.028738199000
C	5.263555999000	-1.880603200000	2.550069602000
H	6.163640574000	-1.653108029000	1.971146596000
H	5.518469192000	-2.659016718000	3.281226098000
C	4.771358782000	-0.605241176000	3.258159674000
H	3.888619316000	-0.840244010000	3.867420140000
H	5.545231925000	-0.229975492000	3.939490962000
Fe	0.486990515000	0.376762263000	1.092976389000
O	6.231911203000	-0.874864525000	-2.256209488000
C	7.501818989000	-0.252296687000	-2.515724741000
C	7.247639294000	1.262342151000	-2.555441479000
C	7.995317330000	-0.806330401000	-3.855996008000
H	8.192699814000	-0.486117458000	-1.702268987000
H	6.853193752000	1.595368194000	-1.598429246000
H	9.017017051000	-0.444334724000	-4.020539483000
H	8.044425947000	-1.898334565000	-3.778313993000
C	6.398387868000	1.695962004000	-3.742098688000
H	5.391392523000	1.304459505000	-3.539797201000
H	6.315724025000	2.786876837000	-3.770058831000
C	6.905207399000	1.139632889000	-5.080992209000
H	7.859888135000	1.620347919000	-5.331610567000
H	6.198279377000	1.406626932000	-5.875987483000
C	7.092308433000	-0.386383605000	-5.029102785000
H	6.115207563000	-0.870135727000	-4.912064275000
H	7.517622786000	-0.747087292000	-5.973979746000
Br	9.087698246000	2.236588250000	-2.604248848000
C	5.783767905000	-0.868173682000	-0.934146530000
O	6.483761566000	-0.386699478000	-0.046285306000
O	4.622660172000	-1.417397780000	-0.896808852000

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2'b

N	-0.888629872	1.155228046	-0.398057240
O	-0.060044105	-0.827962040	1.603297159
O	0.869478782	2.285041145	1.665314205
O	1.879273313	0.359771000	-0.706705340
C	-1.781293260	-0.033650588	-0.495150207
H	-1.187564280	-0.824925441	-0.961975127
H	-2.621259069	0.194844299	-1.172376342
C	-2.301124083	-0.500027685	0.836453258
C	-1.369720320	-0.890542053	1.831834792
C	-1.850592959	-1.359022995	3.068144264
C	-3.219397838	-1.434250324	3.312634687
H	-3.571630938	-1.796317517	4.275882812
C	-4.139621211	-1.044645821	2.334977193
C	-3.668183535	-0.578201494	1.106562909
H	-4.372532933	-0.267014706	0.336888295
C	-1.593094936	2.286071842	0.266138572
H	-1.888786193	1.924069731	1.256011081
H	-2.515926134	2.519860730	-0.291003516
C	-0.744387332	3.520501115	0.401164629
C	0.472903530	3.435951109	1.123729975
C	1.256098520	4.595082158	1.273760580
C	0.844540537	5.805449752	0.721377815
H	1.468156245	6.687845353	0.844927919
C	-0.353826187	5.891453085	0.005814063
C	-1.133199667	4.743399395	-0.149306552
H	-2.064935091	4.791673874	-0.710427671
C	-0.406777133	1.557098188	-1.753709266
H	0.279155402	2.395169019	-1.598101970
H	-1.259209593	1.925168773	-2.348019214
C	0.288561333	0.436142797	-2.473757082

C	1.427159499	-0.139928784	-1.866037468
C	2.086224944	-1.218804681	-2.479314368
C	1.617947030	-1.694257856	-3.702897473
H	2.135953933	-2.525664708	-4.174364674
C	0.501564140	-1.122062129	-4.322376324
C	-0.162145303	-0.065723819	-3.696236565
H	-1.044294442	0.376907369	-4.156247264
O	2.670921235	-0.040449995	1.997874797
C	3.997459772	0.060866376	1.349694628
C	3.342497439	-1.247269597	1.417563721
C	5.137065901	0.416630916	2.267452838
H	3.942716956	0.587623523	0.401930142
H	2.842783265	-1.591263598	0.522389785
H	6.041887599	0.280708608	1.663696212
H	5.063582351	1.474309610	2.551854548
H	0.145496685	-1.501161598	-5.276685701
H	2.951292616	-1.665296761	-1.993302651
H	-0.671670855	6.834013081	-0.430630345
H	2.186691564	4.510730271	1.826648351
H	-5.207516540	-1.099046669	2.527482861
H	-1.121633942	-1.653282571	3.816936746
C	3.767345652	-2.298002659	2.417157294
H	2.977178197	-2.389290611	3.174387972
H	3.832606329	-3.240704074	1.868132515
C	5.125742208	-1.972191219	3.060904891
H	5.900968282	-2.152754122	2.307003122
H	5.305225439	-2.642796156	3.910765410
C	5.202285158	-0.501301984	3.499730624
H	4.374942901	-0.266060031	4.183155822
H	6.135135054	-0.309456138	4.043758563
Fe	0.972656100	0.573344849	0.916956589
O	5.386841238	-1.283319799	-2.161918168
C	6.370625398	-0.326496977	-2.540090397
C	5.983396504	1.002301110	-1.875699179
C	6.325490416	-0.235615829	-4.069952774
H	7.357193051	-0.630759193	-2.176413678
H	6.016720448	0.885888010	-0.796100499
H	7.128312048	0.429139896	-4.411667452
H	6.522615689	-1.234732575	-4.474870107
C	4.677749171	1.578493931	-2.392853521
H	3.898235197	0.901677111	-2.024441339
H	4.488330525	2.558943926	-1.943879748
C	4.614689860	1.641800493	-3.927401647
H	5.317802694	2.406715537	-4.283468760
H	3.609692733	1.956195948	-4.235379289
C	4.962316917	0.282869651	-4.560079187
H	4.190843029	-0.445627829	-4.289222722
H	4.962683115	0.366643959	-5.655014996
Br	7.534393847	2.389893596	-2.180429155
C	5.457242887	-1.844809155	-0.829144690
O	6.344881752	-1.390013819	-0.079145156
O	4.566026722	-2.693339673	-0.650826807

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H	2.693913571000	1.018522639000	3.418586160000
C	2.180699927000	0.315395712000	2.746708403000
N	0.925678694000	0.929491742000	2.306910690000
C	3.124962543000	0.089525810000	1.557091456000
C	5.003976456000	-0.280638750000	-0.507545672000
C	2.681387621000	-0.183456606000	0.235195527000
C	4.500733033000	0.174655110000	1.798322470000
C	5.443999406000	-0.014594923000	0.790933784000
C	3.643591673000	-0.356551307000	-0.779749083000
H	4.839815754000	0.395727207000	2.808444394000
H	6.504191461000	0.054865913000	1.015531474000
H	3.280550172000	-0.554381606000	-1.783632019000
H	5.722090667000	-0.422455831000	-1.310958222000
C	1.893205530000	-0.942194162000	3.574594297000
C	1.477567738000	-3.213085524000	5.182577178000
C	0.834063649000	-1.838878696000	3.273118544000

C	2.704310039000	-1.206563636000	4.682734692000
C	2.517644001000	-2.331714180000	5.484039290000
C	0.645006633000	-2.965438785000	4.097048394000
H	3.504481734000	-0.509212901000	4.923036790000
H	3.168113912000	-2.510114944000	6.335109218000
H	-0.174792357000	-3.634090485000	3.852841003000
H	1.309152742000	-4.091758765000	5.799778732000
O	1.390715947000	-0.269992242000	-0.109742913000
O	-0.006728699000	-1.659856401000	2.248104313000
C	0.576086920000	2.098553862000	2.714431024000
H	1.242800734000	2.636171289000	3.402624511000
C	-0.636304653000	2.788910964000	2.344782086000
C	-2.934980431000	4.266720923000	1.731948158000
C	-0.845441369000	4.073606469000	2.892537803000
C	-1.613942687000	2.228921684000	1.459289344000
C	-2.761329244000	3.008842453000	1.177664149000
C	-1.974813983000	4.815340055000	2.598854745000
H	-0.088282741000	4.477568515000	3.561610946000
H	-3.503554257000	2.585069617000	0.508262284000
H	-2.116360212000	5.801413083000	3.029323994000
H	-3.829006054000	4.835988237000	1.490164180000
O	-1.497895743000	1.042522456000	0.902231571000
Fe	-0.117120707000	-0.312818212000	0.972235687000
C	-2.238364214000	-0.860508967000	-1.369587837000
H	-2.223217960000	0.226845853000	-1.332914742000
O	-1.357537990000	-1.455436484000	-0.367770661000
C	-2.811652246000	-1.566380608000	-0.206667135000
H	-3.169452535000	-0.949893989000	0.616345645000
C	-2.177156785000	-1.519293399000	-2.726346123000
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H	-1.250773115000	-1.218034985000	-3.230019108000
C	-3.351274788000	-2.979391862000	-0.316416206000
H	-4.322315192000	-3.021963920000	0.190191233000
H	-2.676187734000	-3.633802939000	0.248634351000
C	-3.487999198000	-3.465061439000	-1.772819635000
H	-3.611613917000	-4.553260044000	-1.783961286000
H	-4.403828208000	-3.042851931000	-2.209235314000
C	-2.290179561000	-3.050611420000	-2.640609173000
H	-1.364708917000	-3.460673380000	-2.219799057000
H	-2.392802572000	-3.463436423000	-3.649932374000

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6'b
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N	-1.202078893	-0.396797195	1.394043067
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O	0.883381412	-1.406424208	-0.352818193
C	-2.210156152	-1.339614012	1.944052445
H	-2.080314896	-2.266650377	1.376507752
H	-3.218281506	-0.949976511	1.719447076
C	-2.125079181	-1.637478071	3.425726782
C	-0.884855680	-1.742261762	4.120518704
C	-0.923127097	-2.138406506	5.480080339
C	-2.120755922	-2.407475369	6.129805500
H	-2.106214211	-2.703583212	7.177093495
C	-3.336257461	-2.290543698	5.448793806
C	-3.315836817	-1.903051064	4.109102766
H	-4.256355169	-1.807854864	3.566707461
C	-1.118091731	0.869049695	2.177605585
H	-0.879728388	0.579296494	3.200872423
H	-2.107746103	1.355103649	2.180524235
C	-0.072879802	1.833914843	1.672852656
C	1.297628731	1.435588375	1.609401966
C	2.245634165	2.406871094	1.205055274
C	1.865233562	3.701362490	0.868125090
H	2.621754890	4.418822723	0.555461240
C	0.519751631	4.081765775	0.920403740
C	-0.428142408	3.138421251	1.321743553
H	-1.479856982	3.419393109	1.369805769
C	-1.515148309	-0.099744085	-0.034466475

H	-0.785420766	0.652040335	-0.346703850
H	-2.520799142	0.349915013	-0.095415806
C	-1.411763737	-1.299598940	-0.931699701
C	-0.128100999	-1.898118854	-1.047143406
C	0.021163721	-3.008112093	-1.902580352
C	-1.069896981	-3.508158596	-2.608325647
H	-0.936178590	-4.372558069	-3.256716508
C	-2.335443391	-2.922948126	-2.485414266
C	-2.492497579	-1.819724981	-1.641594887
H	-3.470907709	-1.353410967	-1.530030578
H	-3.185306209	-3.322655073	-3.032797304
H	1.004230201	-3.463519780	-1.973926986
H	0.213770586	5.089686745	0.652596219
H	3.284614336	2.092509513	1.159891134
H	-4.279491572	-2.489813804	5.950767583
H	0.023206809	-2.213864620	6.005558092
Fe	0.774695604	-1.460089958	1.578259846
C	3.296429357	-1.495188052	5.383212343
H	2.783226150	-2.375561940	5.774668031
O	3.633223357	-1.701751077	3.981987073
C	2.369192475	-0.270512911	5.373786295
H	1.459651206	-0.496137958	4.813759767
C	4.628069975	-1.232359952	6.087511044
H	4.426444718	-1.109656732	7.157137906
H	5.267459848	-2.114660929	5.968422914
Br	1.678947910	-0.016203866	7.325623908
C	3.058356283	0.987479250	4.879587103
H	2.377966416	1.839419506	4.967317828
H	3.201459908	0.815261742	3.804131519
C	4.397541736	1.255770960	5.580792348
H	4.891918091	2.116347119	5.114317450
H	4.207754300	1.524313711	6.628462629
C	5.320374030	0.024585827	5.526299672
H	5.606267744	-0.166813596	4.485329455
H	6.245473482	0.213885899	6.085147258
C	2.972532580	-2.531565748	3.171829942
O	2.466981435	-3.607934634	3.767656207
C	1.565038322	-7.071213828	2.559587842
C	1.970947693	-5.952298942	3.553937839
C	1.840435646	-4.597607675	2.872817564
C	0.363559080	-4.238927600	2.579336071
C	-0.416998181	-5.533297824	2.197975229
C	0.494061457	-6.582432051	1.551394633
H	2.397238161	-4.568780355	1.932583165
H	1.318593851	-5.962016544	4.436098070
H	2.995249430	-6.096004539	3.914744899
H	2.450599923	-7.425140023	2.017076803
H	1.184452558	-7.929602254	3.126769213
H	-0.046703362	-3.864365753	3.528338193
H	-0.892032615	-5.961391571	3.091981772
H	-1.215765676	-5.225531344	1.517469558
H	-0.083944515	-7.434581350	1.173495833
H	0.977313662	-6.124037308	0.679650094
O	0.263576783	-3.298392649	1.566034668
O	2.930857394	-2.306019603	1.970921388

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H	3.571389855000	1.860907889000	0.275693132000
C	2.789978856000	1.094304305000	0.155834490000
N	1.511971624000	1.767418499000	-0.078100481000
C	3.203259403000	0.253899621000	-1.060013365000
C	4.162160785000	-1.222894080000	-3.257509828000
C	2.279835688000	-0.339528558000	-1.965834639000
C	4.573727646000	0.087108159000	-1.287728620000
C	5.068410979000	-0.645891795000	-2.364251063000
C	2.795886237000	-1.066876392000	-3.062290371000
H	5.273469365000	0.549276644000	-0.593265231000
H	6.140029227000	-0.756638817000	-2.506034408000
H	2.075172255000	-1.504073828000	-3.746866088000
H	4.522097623000	-1.793006533000	-4.111134532000

C	2.741423855000	0.322899605000	1.477106838000
C	2.753880521000	-1.040959254000	3.934473497000
C	1.586203420000	-0.392454821000	1.891927041000
C	3.863627297000	0.342140612000	2.310895028000
C	3.890758043000	-0.337297067000	3.528448102000
C	1.618530339000	-1.063606828000	3.133063494000
H	4.739071112000	0.907861873000	1.995259619000
H	4.779540653000	-0.307131728000	4.152967704000
H	0.721123292000	-1.592862621000	3.439345547000
H	2.747829607000	-1.568667459000	4.885389912000
O	0.957414238000	-0.243189527000	-1.855989068000
O	0.472151238000	-0.458031690000	1.169365606000
C	1.451612556000	3.051443194000	-0.060685991000
H	2.376083287000	3.621775655000	0.116774853000
C	0.259344840000	3.839165654000	-0.257073854000
C	-1.969440966000	5.497274902000	-0.609474995000
C	0.384181650000	5.244403501000	-0.219865102000
C	-1.026198058000	3.242420522000	-0.478411730000
C	-2.127991653000	4.123467923000	-0.651072144000
C	-0.705813652000	6.077736728000	-0.393842104000
H	1.372296728000	5.668325166000	-0.047071890000
H	-3.101512153000	3.672212772000	-0.815129672000
H	-0.589361471000	7.156888919000	-0.361929865000
H	-2.838353259000	6.137604905000	-0.745177364000
O	-1.228500593000	1.955346497000	-0.527751592000
Fe	-0.099756212000	0.369959571000	-0.428087345000
C	-2.896914921000	-0.638095523000	0.190117430000
H	-2.814592240000	0.166222589000	0.921677669000
O	-1.728602307000	-0.769900611000	-0.653537678000
C	-2.246923809000	-1.899078969000	0.529037310000
H	-1.471810149000	-1.880716617000	1.280278763000
C	-4.211371200000	-0.657364629000	-0.561064156000
H	-5.003393834000	-0.688844500000	0.197436663000
H	-4.314143765000	0.284382684000	-1.115182939000
Br	-3.771570019000	-2.502684013000	2.920058389000
C	-2.593985737000	-3.185026742000	-0.175895390000
H	-2.481624628000	-3.996794204000	0.546565724000
H	-1.852423932000	-3.338799307000	-0.971680760000
C	-4.018725165000	-3.175905418000	-0.753458458000
H	-4.150168545000	-4.038455444000	-1.419327042000
H	-4.715879308000	-3.289175712000	0.084986608000
C	-4.328342256000	-1.868764084000	-1.500367621000
H	-3.633609750000	-1.742819000000	-2.340906983000
H	-5.339603497000	-1.904623651000	-1.925156027000

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H	3.879466477000	1.255910304000	0.506787236000
C	3.119047103000	0.506418652000	0.234270973000
N	1.833547259000	1.188086126000	0.079133781000
C	3.586495306000	-0.097291862000	-1.095481684000
C	4.623935333000	-1.138377442000	-3.496206680000
C	2.691595995000	-0.596605340000	-2.085885451000
C	4.962929987000	-0.131722835000	-1.343422373000
C	5.498535210000	-0.649883718000	-2.521683510000
C	3.251745403000	-1.106870962000	-3.282509124000
H	5.636023811000	0.263880399000	-0.583723427000
H	6.574331985000	-0.662226838000	-2.677743051000
H	2.556923539000	-1.478414713000	-4.030102794000
H	5.014118846000	-1.541144640000	-4.429075037000
C	3.065937427000	-0.480872470000	1.405004066000
C	3.117869112000	-2.238890436000	3.601629055000
C	1.907975317000	-1.253608906000	1.709343445000
C	4.200570410000	-0.606479685000	2.213122105000
C	4.250617425000	-1.477948968000	3.301216203000
C	1.971492742000	-2.123804882000	2.824499299000
H	5.073471838000	0.002397376000	1.980316106000
H	5.151158147000	-1.552078892000	3.905661907000
H	1.080636818000	-2.703969207000	3.048133392000
H	3.126250783000	-2.920947983000	4.449970178000

O	1.374486118000	-0.606472279000	-1.965620959000
O	0.780820274000	-1.204623717000	1.020124990000
C	1.781664772000	2.458934582000	0.266353327000
H	2.708228253000	2.993799651000	0.529780527000
C	0.598904430000	3.278463927000	0.170673527000
C	-1.622027102000	4.980956720000	0.061340084000
C	0.730273681000	4.662581081000	0.411724372000
C	-0.687218427000	2.724841186000	-0.143520025000
C	-1.787057615000	3.629490223000	-0.181902332000
C	-0.355161534000	5.518658537000	0.359298216000
H	1.720555434000	5.051555070000	0.646467635000
H	-2.763354575000	3.210617728000	-0.406661170000
H	-0.233678477000	6.581546648000	0.548170974000
H	-2.488554781000	5.638278641000	0.022276066000
O	-0.892019131000	1.464896915000	-0.386086440000
Fe	0.219598749000	-0.190617377000	-0.508047897000
C	-2.671448093000	-0.918407689000	-0.980663229000
H	-2.885442190000	0.029289412000	-1.498115087000
O	-1.303432884000	-1.178745024000	-0.951011670000
C	-3.099750007000	-0.779584926000	0.493514011000
H	-2.562563851000	0.044478975000	0.957832375000
C	-3.400514337000	-2.083868710000	-1.675919724000
H	-4.468266758000	-1.844302770000	-1.768711597000
H	-2.992127940000	-2.179765719000	-2.689074926000
Br	-5.080004710000	-0.038549178000	0.593251332000
C	-3.000232728000	-2.081653904000	1.272328956000
H	-3.383954086000	-1.950051857000	2.289987077000
H	-1.921051623000	-2.275614785000	1.352513007000
C	-3.688096458000	-3.259134561000	0.561887992000
H	-3.488943179000	-4.186020475000	1.116699155000
H	-4.775781504000	-3.104665926000	0.582220518000
C	-3.212849561000	-3.395933986000	-0.895996449000
H	-2.147012775000	-3.654328727000	-0.907725885000
H	-3.752673858000	-4.213884183000	-1.392243615000

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H	4.026571159000	0.536703813000	-1.213506682000
C	3.200631686000	0.025993687000	-0.693265432000
N	2.131119427000	0.998664842000	-0.452135681000
C	2.730573903000	-1.096177367000	-1.634682464000
C	2.101781664000	-3.162059398000	-3.446272897000
C	1.373229948000	-1.500344841000	-1.798668221000
C	3.720797488000	-1.745243595000	-2.380750862000
C	3.433328639000	-2.772244996000	-3.276664902000
C	1.096299383000	-2.534490139000	-2.724854454000
H	4.755031962000	-1.431462838000	-2.246314013000
H	4.232236953000	-3.253593132000	-3.834514913000
H	0.054632165000	-2.817077695000	-2.845553280000
H	1.846669219000	-3.955690910000	-4.145594217000
C	3.761160477000	-0.478738402000	0.630451271000
C	4.814261737000	-1.435057087000	3.045168385000
C	2.877386181000	-0.918546275000	1.652204106000
C	5.138618315000	-0.515858549000	0.845917883000
C	5.680520610000	-0.996602921000	2.040624673000
C	3.435965082000	-1.392365989000	2.859112758000
H	5.802741492000	-0.162580226000	0.057782445000
H	6.757490862000	-1.020674390000	2.184840694000
H	2.7493201967000	-1.720289871000	3.633959719000
H	5.216101912000	-1.807247615000	3.985632589000
O	0.343764401000	-0.957378237000	-1.164566413000
O	1.567812336000	-0.908179770000	1.496182704000
C	2.283227110000	2.213996044000	-0.846125191000
H	3.239489153000	2.500153847000	-1.311146473000
C	1.297907091000	3.262274201000	-0.755904756000
C	-0.542299686000	5.373004656000	-0.705555652000
C	1.678872283000	4.568827047000	-1.127682653000
C	-0.055207156000	2.997885566000	-0.353476997000
C	-0.953612326000	4.103198143000	-0.347188329000
C	0.785273043000	5.624405285000	-1.102613953000

H	2.709624829000	4.734975434000	-1.438427725000
H	-1.977495883000	3.905143576000	-0.044937266000
H	1.098882898000	6.624644972000	-1.386826678000
H	-1.259808515000	6.191053350000	-0.682170531000
O	-0.489888470000	1.822093555000	-0.026506652000
Fe	0.358392000000	0.090924000000	0.421187000000
C	-2.331017890000	-1.279888165000	0.472188961000
H	-1.805927602000	-1.631301172000	-0.421889622000
O	-1.364797000000	-0.558051000000	1.229886000000
C	-3.431255488000	-0.299175041000	0.019081423000
H	-2.974255787000	0.612723176000	-0.361434072000
C	-2.898588711000	-2.512873963000	1.202414420000
H	-3.313938032000	-3.179757812000	0.434459225000
H	-2.055826256000	-3.039920058000	1.663573325000
Br	-4.321895735000	-1.065394946000	-1.733503292000
C	-1.378680000000	0.455022000000	2.829103000000
O	-0.297771000000	0.969975000000	2.740145000000
O	-2.398157728000	0.291676092000	3.426309989000
C	-4.529990478000	-0.039385760000	1.037039234000
H	-4.061163092000	0.550293194000	1.834356589000
H	-5.318413109000	0.577210631000	0.592037070000
C	-3.989018010000	-2.206347009000	2.242269082000
H	-4.414553946000	-3.148540504000	2.614408881000
H	-3.543711232000	-1.689651479000	3.096337028000
C	-5.103484927000	-1.327963296000	1.647761623000
H	-5.835474320000	-1.067173296000	2.423150047000
H	-5.646107567000	-1.884319448000	0.871803813000

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H	4.163330163000	1.170617121000	2.074669823000
C	3.509398537000	0.435917207000	1.578505949000
N	2.431042159000	1.157034532000	0.901580767000
C	4.394047618000	-0.294994868000	0.559301142000
C	6.179913512000	-1.580097245000	-1.196694848000
C	3.913935438000	-0.803369914000	-0.681737341000
C	5.748855946000	-0.444767726000	0.874233583000
C	6.648109119000	-1.083773131000	0.022963947000
C	4.842246756000	-1.437420326000	-1.541005198000
H	6.106759126000	-0.044651158000	1.821807966000
H	7.693292509000	-1.183665590000	0.303479698000
H	4.460309288000	-1.811693065000	-2.486162528000
H	6.862195822000	-2.075855221000	-1.884047965000
C	2.954443629000	-0.458325384000	2.685087875000
C	2.035334899000	-2.095072141000	4.774661716000
C	1.752284970000	-1.198201065000	2.516163643000
C	3.648134674000	-0.546578021000	3.894738085000
C	3.211457380000	-1.359386914000	4.941337874000
C	1.317384734000	-2.012355413000	3.587154027000
H	4.557730268000	0.039879609000	4.017790943000
H	3.774530435000	-1.409965729000	5.869469556000
H	0.398619377000	-2.573348842000	3.443222294000
H	1.671819439000	-2.732650109000	5.577961390000
O	2.658340135000	-0.706367695000	-1.095906517000
O	1.022394081000	-1.158504701000	1.414719886000
C	2.415606703000	2.441586967000	0.954123904000
H	3.195335125000	2.956362729000	1.537108952000
C	1.469836129000	3.301512769000	0.288132218000
C	-0.243772178000	5.091192508000	-1.015068234000
C	1.599014099000	4.694948441000	0.468577741000
C	0.442705987000	2.781139578000	-0.567757570000
C	-0.396964927000	3.731379716000	-1.216313643000
C	0.758249159000	5.593386253000	-0.163322575000
H	2.389697954000	5.056821304000	1.124534558000
H	-1.163792229000	3.342745466000	-1.879263267000
H	0.872121128000	6.662522549000	-0.010337357000
H	-0.909286570000	5.783091578000	-1.527254062000
O	0.247773046000	1.513556478000	-0.776700686000
Fe	1.077659914000	-0.179866338000	-0.207814144000
C	-3.071548441000	-0.691656129000	0.814481091000

H	-3.479037552000	-1.690415014000	0.641508348000
O	-1.739567991000	-0.631018553000	0.287216233000
C	-3.891340006000	0.341202178000	0.028174060000
H	-3.884915875000	0.083845493000	-1.028650037000
C	-2.968853140000	-0.359693874000	2.305715739000
H	-3.953233136000	-0.517009296000	2.762737205000
H	-2.271132729000	-1.068010181000	2.764906843000
Br	-5.914312431000	0.084053921000	0.490910959000
C	-3.469394960000	1.775340776000	0.304723606000
H	-4.126590789000	2.475010253000	-0.221788940000
H	-2.469305400000	1.868375467000	-0.140420763000
C	-3.383457401000	2.102417448000	1.804002445000
H	-2.982931676000	3.115735031000	1.930339915000
H	-4.393763271000	2.101799352000	2.234059227000
C	-2.499254993000	1.085827775000	2.546023234000
H	-1.463460366000	1.182845121000	2.201289270000
H	-2.497584175000	1.300534148000	3.622201545000
C	-1.478233389000	-1.342959533000	-0.890265452000
O	-0.240588412000	-1.233964013000	-1.219123147000
O	-2.371365416000	-1.953370767000	-1.460346865000

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H	-4.553452000000	0.318426000000	1.222652000000
C	-3.714151000000	-0.128731000000	0.671831000000
N	-2.688548000000	0.900518000000	0.472249000000
C	-3.159412000000	-1.246971000000	1.553512000000
C	-2.204549000000	-3.315464000000	3.200603000000
C	-1.863314000000	-1.781218000000	1.331966000000
C	-3.934468000000	-1.750700000000	2.602190000000
C	-3.477255000000	-2.783744000000	3.424226000000
C	-1.406811000000	-2.817508000000	2.173180000000
H	-4.919267000000	-1.323160000000	2.778960000000
H	-4.102136000000	-3.159170000000	4.229008000000
H	-0.411927000000	-3.214812000000	1.993476000000
H	-1.827769000000	-4.115864000000	3.832204000000
C	-4.292312000000	-0.622518000000	-0.664035000000
C	-5.548321000000	-1.576340000000	-3.003725000000
C	-3.597635000000	-0.585437000000	-1.904320000000
C	-5.596533000000	-1.134266000000	-0.640729000000
C	-6.231117000000	-1.616177000000	-1.784450000000
C	-4.257077000000	-1.065492000000	-3.059142000000
H	-6.128370000000	-1.153622000000	0.308188000000
H	-7.242122000000	-2.007419000000	-1.725164000000
H	-3.712625000000	-1.021917000000	-3.997835000000
H	-6.022985000000	-1.939256000000	-3.911622000000
O	-1.068095000000	-1.344276000000	0.356488000000
O	-2.360326000000	-0.106541000000	-2.055366000000
C	-2.861248000000	2.075296000000	0.975480000000
H	-3.777464000000	2.274234000000	1.546164000000
C	-1.943698000000	3.181800000000	0.855222000000
C	-0.257031000000	5.414731000000	0.688597000000
C	-2.267122000000	4.389178000000	1.514613000000
C	-0.739121000000	3.095235000000	0.084946000000
C	0.086386000000	4.247650000000	0.025335000000
C	-1.442289000000	5.498380000000	1.442784000000
H	-3.188710000000	4.432027000000	2.090751000000
H	0.998020000000	4.182372000000	-0.560403000000
H	-1.704634000000	6.416721000000	1.957700000000
H	0.400443000000	6.277730000000	0.622056000000
O	-0.378162000000	2.017608000000	-0.567017000000
Fe	-1.054812000000	0.207187000000	-0.729115000000
C	3.478888000000	-0.021273000000	0.118484000000
H	3.673817000000	1.045526000000	0.248410000000
O	2.073433000000	-0.150065000000	-0.239393000000
C	4.395649000000	-0.562366000000	-0.988646000000
H	4.760292000000	0.104199000000	-1.745980000000
C	3.626027000000	-0.780058000000	1.443652000000
H	4.560157000000	-0.468510000000	1.916430000000
H	2.801974000000	-0.468889000000	2.093896000000

Br	6.631460000000	0.280393000000	0.053194000000
C	1.785116000000	-0.335577000000	-1.552853000000
O	0.555036000000	-0.328924000000	-1.853734000000
O	2.738091000000	-0.521477000000	-2.344297000000
C	4.684167000000	-2.037575000000	-1.065938000000
H	5.594555000000	-2.202368000000	-1.647004000000
H	3.857201000000	-2.469881000000	-1.642927000000
C	3.616837000000	-2.300444000000	1.233547000000
H	2.649676000000	-2.604666000000	0.812874000000
H	3.709616000000	-2.803558000000	2.202403000000
C	4.755355000000	-2.740411000000	0.303401000000
H	5.717716000000	-2.509909000000	0.771299000000
H	4.722249000000	-3.823095000000	0.142093000000

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5c

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H	3.354720438000	1.162240130000	0.828171187000
C	2.689531287000	0.384060392000	0.426245333000
N	1.575912552000	1.040522131000	-0.263024932000
C	3.534150739000	-0.437818209000	-0.556556081000
C	5.248736219000	-1.892600653000	-2.250491161000
C	3.014911070000	-1.063144057000	-1.722266658000
C	4.901072237000	-0.557825585000	-0.282560221000
C	5.762056087000	-1.280339510000	-1.104755669000
C	3.898029622000	-1.779294830000	-2.555562598000
H	5.299067688000	-0.068623480000	0.604414119000
H	6.817375977000	-1.354783513000	-0.859122109000
H	3.480695237000	-2.239487287000	-3.445696135000
H	5.904413715000	-2.453264492000	-2.911612630000
C	2.174041859000	-0.411124619000	1.628212565000
C	1.329718429000	-1.843258976000	3.894801060000
C	0.960200883000	-1.146066903000	1.586904142000
C	2.921296719000	-0.404054961000	2.809512449000
C	2.521035624000	-1.116471364000	3.939501388000
C	0.557974382000	-1.851890155000	2.737826897000
H	3.842381623000	0.174836786000	2.843048474000
H	3.126210833000	-1.096532339000	4.841096341000
H	-0.374404501000	-2.406042594000	2.687281738000
H	0.996669257000	-2.400606773000	4.766739598000
O	1.730652802000	-0.992859470000	-2.092208675000
O	0.175892675000	-1.192115933000	0.507947292000
C	1.487933935000	2.323377488000	-0.303600772000
H	2.264399478000	2.918664754000	0.196632416000
C	0.449080052000	3.075705461000	-0.964820079000
C	-1.459091332000	4.683044050000	-2.238529617000
C	0.509971600000	4.483766053000	-0.884442468000
C	-0.610473735000	2.451887612000	-1.701600807000
C	-1.547780405000	3.304012645000	-2.338718253000
C	-0.427718396000	5.290878969000	-1.503190683000
H	1.323576758000	4.932831907000	-0.318091935000
H	-2.334004713000	2.835841106000	-2.922966290000
H	-0.363481067000	6.371630001000	-1.428035009000
H	-2.197246872000	5.302303716000	-2.742493167000
O	-0.746890358000	1.153892412000	-1.817496637000
Fe	0.265649308000	-0.352369803000	-1.153001232000
C	-4.369971540000	-0.741970885000	-0.547055901000
H	-4.606651853000	-1.677490172000	-0.025744056000
O	-2.914433583000	-0.672812257000	-0.613763137000
C	-4.711838491000	-0.858750097000	-2.039986843000
H	-5.586595903000	-1.487888604000	-2.214270939000
C	-4.951116217000	0.447622966000	0.205470474000
H	-5.983832193000	0.179549630000	0.467192912000
H	-4.408128878000	0.556594792000	1.150510154000
C	-4.801362408000	0.482899569000	-2.779885610000
H	-5.227741526000	0.317888572000	-3.774530887000
H	-3.780473746000	0.854578710000	-2.929106767000
C	-5.595488532000	1.530593899000	-1.981847313000
H	-5.624612815000	2.467094328000	-2.549086641000
H	-6.639422798000	1.207808701000	-1.859056047000
C	-4.951180789000	1.751317540000	-0.604820810000

H	-3.922993786000	2.111196647000	-0.734082048000
H	-5.489366019000	2.523546390000	-0.044614872000
C	-2.517814790000	-1.283169923000	-1.735723796000
O	-1.357098723000	-1.527200803000	-2.011849277000
O	-3.549083603000	-1.595132544000	-2.531730392000

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4'c
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H	4.048931027000	1.460764982000	1.910264568000
C	3.439645295000	0.678820453000	1.429175860000
N	2.339863360000	1.317313573000	0.709546573000
C	4.367079308000	-0.068966320000	0.465027403000
C	6.264850555000	-1.381522110000	-1.145390032000
C	3.973095715000	-0.566793090000	-0.812844176000
C	5.685789472000	-0.254867964000	0.891658569000
C	6.640647173000	-0.905739723000	0.114070226000
C	4.962355438000	-1.212260343000	-1.594800545000
H	5.964858855000	0.123234226000	1.874492357000
H	7.655773506000	-1.032469263000	0.480871851000
H	4.656845973000	-1.579716665000	-2.569287071000
H	6.990604187000	-1.886589029000	-1.779541020000
C	2.890468488000	-0.203308163000	2.541275730000
C	1.924834662000	-1.852955541000	4.588746321000
C	1.914985303000	-1.192335269000	2.235703620000
C	3.342730428000	-0.054906219000	3.850469805000
C	2.874147847000	-0.871739189000	4.884464788000
C	1.449797560000	-2.010252227000	3.288725349000
H	4.082494979000	0.715513816000	4.065494051000
H	3.242549217000	-0.740848490000	5.898495434000
H	0.704580878000	-2.762174604000	3.045198139000
H	1.545265608000	-2.497784238000	5.379058169000
O	2.760225503000	-0.451641330000	-1.334015169000
O	1.453569199000	-1.361674467000	1.014168888000
C	2.170227983000	2.585931858000	0.797944759000
H	2.849381720000	3.165520752000	1.442704179000
C	1.157686760000	3.351565003000	0.108729678000
C	-0.706136799000	4.971576225000	-1.217403770000
C	1.008975620000	4.712915403000	0.442044292000
C	0.350379166000	2.778311639000	-0.931801305000
C	-0.578457192000	3.641829983000	-1.578937920000
C	0.087246702000	5.526520537000	-0.196005620000
H	1.640408638000	5.122908089000	1.229413953000
H	-1.195518380000	3.204941201000	-2.357831650000
H	-0.016410154000	6.571385980000	0.081458090000
H	-1.434200576000	5.595575169000	-1.732063533000
O	0.438332255000	1.543115013000	-1.310503487000
Fe	1.120855854000	-0.101149863000	-0.405453896000
C	0.220719239000	-0.350163377000	-4.445776957000
H	-0.789514689000	-0.553736930000	-4.808656948000
O	0.328872290000	-0.793174171000	-3.086052656000
C	1.253035558000	-1.233077841000	-5.155245228000
H	1.010235198000	-2.285678196000	-5.013952848000
C	0.554701692000	1.143709878000	-4.535422959000
H	0.385490457000	1.471647498000	-5.568895927000
H	-0.147162081000	1.676312987000	-3.888757755000
Br	1.010179747000	-1.020273356000	-7.221146329000
C	2.679986375000	-0.905950018000	-4.751659300000
H	3.386344919000	-1.532770983000	-5.306449672000
H	2.734830332000	-1.179789517000	-3.688613418000
C	3.015512657000	0.587395737000	-4.881105843000
H	4.026467304000	0.758610089000	-4.491588751000
H	3.022688445000	0.869513654000	-5.942766455000
C	2.000281195000	1.440410017000	-4.103184772000
H	2.096609201000	1.224208564000	-3.036511366000
H	2.212311221000	2.508473503000	-4.240827953000
C	-0.817084716000	-0.850037162000	-2.299538003000
O	-0.483888258000	-1.071743392000	-1.070705625000
O	-1.934870823000	-0.709381103000	-2.772023059000
C	-2.081734221000	2.420223527000	2.859352783000
C	-2.426862416000	2.175757322000	1.381920383000

C	-1.789776614000	0.908282259000	0.858591352000
C	-1.373972424000	-0.166172619000	1.781788347000
C	-1.558670514000	-0.045960068000	3.283955092000
C	-2.401443807000	1.175625175000	3.701943881000
H	-1.975990642000	0.637381899000	-0.178653346000
H	-3.515922410000	2.084002420000	1.257888106000
H	-2.101711510000	3.016791870000	0.759324133000
H	-1.015109174000	2.660458895000	2.938736417000
H	-2.639546188000	3.288320640000	3.231522591000
H	-1.253440263000	-1.163272929000	1.364416468000
H	-2.017729906000	-0.967567077000	3.662386859000
H	-0.556556634000	0.001180033000	3.726184355000
H	-3.468830426000	0.940045079000	3.578450131000
H	-2.249211303000	1.380319453000	4.768979640000
O	-0.398841686000	0.755093008000	1.232289251000

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4'C-TS
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H	0.655521688000	0.911388951000	3.362527364000
C	1.112581358000	0.497018155000	2.449801955000
N	0.246473415000	0.795422726000	1.311897240000
C	2.480236469000	1.168192708000	2.279296865000
C	5.009860547000	2.396690490000	2.206384357000
C	3.033620385000	1.553225539000	1.018710781000
C	3.212412918000	1.401371940000	3.446788034000
C	4.468726125000	2.004003658000	3.434754989000
C	4.304841110000	2.179011114000	1.030465174000
H	2.778545302000	1.087135056000	4.395605778000
H	5.010573430000	2.165864868000	4.363002329000
H	4.709864030000	2.474076595000	0.066765476000
H	5.986871953000	2.874849444000	2.166875663000
C	1.204446656000	-1.012978678000	2.635458989000
C	1.401944533000	-3.784098298000	2.979175986000
C	1.661138303000	-1.817587637000	1.553666076000
C	0.850311314000	-1.606869317000	3.843839448000
C	0.946672880000	-2.989581793000	4.034209549000
C	1.752015973000	-3.211274370000	1.758193319000
H	0.494405050000	-0.973884223000	4.656302571000
H	0.668845471000	-3.434577404000	4.986197567000
H	2.102716985000	-3.818557770000	0.928467150000
H	1.481584332000	-4.862330197000	3.106793340000
O	2.437494227000	1.389555510000	-0.147865232000
O	2.009393556000	-1.282200307000	0.402260676000
C	-0.907714181000	1.328827835000	1.460180677000
H	-1.259166366000	1.555939508000	2.478517040000
C	-1.818607330000	1.671579393000	0.386209258000
C	-3.690555081000	2.396242124000	-1.573584459000
C	-3.128574771000	2.051653995000	0.733338973000
C	-1.418463918000	1.669560942000	-0.995577638000
C	-2.402966968000	2.048885012000	-1.949528239000
C	-4.071513672000	2.403057336000	-0.221113996000
H	-3.401569808000	2.053473709000	1.788010068000
H	-2.098081463000	2.052333468000	-2.992175263000
H	-5.080300192000	2.680035120000	0.071274010000
H	-4.414061088000	2.671411251000	-2.339005554000
O	-0.220802390000	1.371880330000	-1.403102568000
Fe	1.049820887000	0.121535734000	-0.538700673000
C	2.487808332000	-2.114474791000	-5.538001188000
H	1.944023896000	-3.044018360000	-5.354750509000
O	2.618087700000	-1.378023794000	-4.307233263000
C	3.951950104000	-2.399397921000	-5.891932338000
H	4.433331688000	-2.951032168000	-5.085332455000
C	1.774027956000	-1.262483578000	-6.593667611000
H	1.657378633000	-1.862878440000	-7.503765922000
H	0.773361485000	-1.038507431000	-6.214023131000

Br	3.997663363000	-3.771739061000	-7.448525245000
C	4.724624129000	-1.143854876000	-6.272381466000
H	5.738782257000	-1.405703382000	-6.589788239000
H	4.808511822000	-0.569619642000	-5.339348002000
C	4.002241321000	-0.294329128000	-7.329369039000
H	4.564807602000	0.632135576000	-7.495793813000
H	3.992311931000	-0.839380489000	-8.282178141000
C	2.559720486000	0.022609987000	-6.898850062000
H	2.577754619000	0.648674592000	-5.998590495000
H	2.048038316000	0.597503431000	-7.679971862000
C	1.518773986000	-1.297243395000	-3.478200945000
O	1.711236848000	-0.567756609000	-2.480919312000
O	0.486262626000	-1.949841316000	-3.827599058000
C	-0.332663604000	-2.303063262000	-1.189991646000
H	0.746297760000	-2.490914673000	-1.246223421000
O	-0.675674996000	-1.229793514000	-0.357250689000
C	-0.896412565000	-1.556544914000	-2.344602809000
H	-0.546759372000	-0.551441016000	-2.492607569000
C	-1.041571368000	-3.612121965000	-0.822036187000
H	-0.623365659000	-4.423166336000	-1.436968451000
H	-0.787070746000	-3.822733227000	0.222309517000
C	-2.287646137000	-1.801744650000	-2.839911457000
H	-2.287774103000	-1.605311289000	-3.919087645000
H	-2.900653073000	-1.007245096000	-2.389790036000
C	-2.860839876000	-3.183706210000	-2.495959995000
H	-3.939802780000	-3.192963143000	-2.695103516000
H	-2.409190624000	-3.941441324000	-3.151534238000
C	-2.558232616000	-3.540178045000	-1.032166577000
H	-2.971638426000	-2.768043804000	-0.371675231000
H	-3.031826758000	-4.492561024000	-0.762614210000

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2' c-TS
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H	2.553333501000	1.800233914000	2.109629113000
C	2.030186293000	0.919161469000	1.706532685000
N	0.800329754000	1.368962277000	1.053456377000
C	2.994370316000	0.277227745000	0.699086554000
C	4.924628991000	-0.807215531000	-1.044478576000
C	2.574898347000	-0.399760862000	-0.480933761000
C	4.364608620000	0.388239772000	0.961846706000
C	5.335721239000	-0.147478027000	0.117373082000
C	3.571035730000	-0.924585050000	-1.336390116000
H	4.676283622000	0.914411906000	1.862826177000
H	6.389920499000	-0.042525280000	0.358446921000
H	3.230684881000	-1.428472025000	-2.236194850000
H	5.660532866000	-1.226484317000	-1.726835908000
C	1.687064930000	0.039195712000	2.910914586000
C	1.127698607000	-1.505580548000	5.190838200000
C	0.629662034000	-0.909367115000	2.874459856000
C	2.422390553000	0.193302701000	4.089471735000
C	2.164906303000	-0.570765758000	5.227526590000
C	0.370278262000	-1.667572894000	4.036532074000
H	3.216596695000	0.937961796000	4.115155512000
H	2.755030929000	-0.428674541000	6.128791123000
H	-0.447437951000	-2.380992886000	3.996616734000
H	0.900402774000	-2.105153140000	6.069427129000
O	1.304222764000	-0.558794529000	-0.841047791000
O	-0.127683144000	-1.116589153000	1.802419103000
C	0.474770244000	2.613024268000	1.100032882000
H	1.145291766000	3.314072875000	1.619809085000
C	-0.714115833000	3.194080150000	0.529418472000
C	-2.991196881000	4.449039113000	-0.506647945000
C	-0.919685991000	4.581151931000	0.695836873000
C	-1.679930796000	2.409493388000	-0.182181879000
C	-2.820373519000	3.088331593000	-0.689335449000
C	-2.038273356000	5.217260100000	0.189107358000
H	-0.170130576000	5.149964674000	1.244054802000
H	-3.557394684000	2.492809506000	-1.218617144000
H	-2.182508722000	6.283970493000	0.331188086000
H	-3.881417754000	4.930639743000	-0.905285505000

O	-1.560175071000	1.126397114000	-0.383163317000
Fe	-0.284365975000	-0.256184324000	0.121111939000
C	-2.928473479000	-1.615318924000	-0.466857947000
H	-3.290919626000	-0.749219680000	0.082443680000
O	-1.499253038000	-1.624261686000	-0.676007977000
C	-2.421734730000	-2.721169418000	0.338991812000
H	-2.043014988000	-2.493485797000	1.323762683000
C	-3.742987077000	-1.934575358000	-1.704196403000
H	-4.788420262000	-2.009620151000	-1.378642340000
H	-3.676268719000	-1.086640571000	-2.397663223000
C	-2.246905137000	-4.102927103000	-0.231665761000
H	-2.378008379000	-4.815987386000	0.586221365000
H	-1.213499743000	-4.192657019000	-0.588545783000
C	-3.243085320000	-4.392451614000	-1.366460158000
H	-2.972600139000	-5.332734453000	-1.863776133000
H	-4.232949642000	-4.528817604000	-0.916135971000
C	-3.299627898000	-3.240453222000	-2.382965305000
H	-2.309751099000	-3.094593206000	-2.833914446000
H	-3.991062683000	-3.486284705000	-3.199161294000
C	-6.501339843000	-2.072128587000	3.820676096000
H	-6.902815401000	-1.342034278000	3.113270870000
O	-5.685746642000	-3.019648885000	3.128325013000
C	-5.589482899000	-1.346727094000	4.821854306000
H	-4.802902246000	-0.824366961000	4.283012026000
C	-7.611771982000	-2.867167219000	4.516606301000
H	-8.317392029000	-2.160991053000	4.970686442000
H	-8.157307867000	-3.434248361000	3.753792123000
Br	-6.638804867000	0.261550400000	5.663114348000
C	-5.075573050000	-2.251825491000	5.931375274000
H	-4.492934528000	-1.674938281000	6.656747969000
H	-4.381461787000	-2.945269505000	5.436121137000
C	-6.190778406000	-3.056841770000	6.618572567000
H	-5.746530557000	-3.759164587000	7.335746392000
H	-6.823528781000	-2.371184657000	7.197075308000
C	-7.050707691000	-3.814408333000	5.591692704000
H	-6.439775066000	-4.579559485000	5.098197989000
H	-7.872625382000	-4.335469883000	6.100206029000
C	-4.877188995000	-2.508490067000	2.063077753000
O	-4.241591510000	-3.434297522000	1.496129326000
O	-4.905281121000	-1.286344916000	1.856577302000

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6c

H	3.204414066000	1.341581367000	0.516103494000
C	2.548293997000	0.507332819000	0.220009919000
N	1.165591776000	0.984554506000	0.223603929000
C	2.980375146000	0.126148710000	-1.201403801000
C	3.926980265000	-0.444199634000	-3.789822158000
C	2.090562645000	-0.436108803000	-2.162981393000
C	4.304235111000	0.386065644000	-1.569849942000
C	4.796789745000	0.103949974000	-2.843346954000
C	2.603921642000	-0.703412394000	-3.455791326000
H	4.969072237000	0.830418880000	-0.830077654000
H	5.832492793000	0.319683748000	-3.092732849000
H	1.911941780000	-1.122537156000	-4.180774010000
H	4.280680530000	-0.663931592000	-4.795470423000
C	2.751681706000	-0.577748350000	1.282788635000
C	3.272599958000	-2.482339026000	3.290847497000
C	1.752105889000	-1.540107470000	1.608842386000
C	3.965817083000	-0.596240415000	1.976419612000
C	4.248412663000	-1.535100834000	2.968614125000
C	2.051816781000	-2.478969582000	2.627134611000
H	4.713832307000	0.156300277000	1.729492452000
H	5.205090351000	-1.518416184000	3.484244928000
H	1.280424917000	-3.204814773000	2.868853460000
H	3.461605040000	-3.221962468000	4.066474243000
O	0.819178571000	-0.714342257000	-1.932612968000
O	0.567666573000	-1.608743517000	1.027171367000
C	0.940089867000	2.217277984000	0.513926561000
H	1.795494446000	2.867872782000	0.757261977000

C	-0.352117966000	2.853199368000	0.553703777000
C	-2.801396722000	4.201165279000	0.685425673000
C	-0.410277321000	4.223393654000	0.888557608000
C	-1.559702409000	2.133176155000	0.270348149000
C	-2.782929933000	2.858701425000	0.354393170000
C	-1.611407009000	4.905532377000	0.955354847000
H	0.524790860000	4.742349897000	1.096983223000
H	-3.695556925000	2.305883112000	0.161628108000
H	-1.637513314000	5.960394139000	1.214019087000
H	-3.756264529000	4.720934809000	0.740183046000
O	-1.588437533000	0.873275094000	-0.048316640000
Fe	-0.269311297000	-0.576217256000	-0.373891592000
C	-3.005606156000	-1.882667459000	-0.530564588000
H	-3.560794279000	-1.080081847000	-1.042987863000
O	-1.642523697000	-1.775815818000	-0.773043339000
C	-3.246264808000	-1.722640691000	0.990986163000
H	-2.880694604000	-0.740256104000	1.295206329000
C	-3.508540613000	-3.259490659000	-1.010763495000
H	-4.599533313000	-3.315669590000	-0.885157493000
H	-3.294299337000	-3.346507371000	-2.082370095000
C	-2.608627388000	-2.855984195000	1.788410488000
H	-2.845274230000	-2.732613417000	2.852972871000
H	-1.524824244000	-2.742656793000	1.674782976000
C	-3.053685096000	-4.241870580000	1.285559042000
H	-2.508317735000	-5.021842560000	1.832792874000
H	-4.119685232000	-4.384894505000	1.511094683000
C	-2.825258516000	-4.393091543000	-0.228766250000
H	-1.750352674000	-4.353020072000	-0.439081333000
H	-3.190959201000	-5.370524705000	-0.571329967000
C	-7.578308011000	0.226323084000	1.479162373000
H	-7.435922166000	0.676165431000	0.494359407000
O	-6.650640798000	-0.878450381000	1.622864631000
C	-7.239929946000	1.256842150000	2.568664191000
H	-6.218647932000	1.609124874000	2.444291985000
C	-8.976208076000	-0.372144277000	1.641172821000
H	-9.707606694000	0.408925645000	1.405009982000
H	-9.098402238000	-1.169466107000	0.900195909000
Br	-8.319806498000	2.980680097000	2.177842992000
C	-7.533024072000	0.760049499000	3.977685387000
H	-7.353903799000	1.560036762000	4.702504849000
H	-6.787424303000	-0.023259776000	4.177021839000
C	-8.943296522000	0.168737794000	4.127672901000
H	-9.056438881000	-0.253826975000	5.133255981000
H	-9.682809149000	0.974378344000	4.036948739000
C	-9.214267827000	-0.908140983000	3.063546583000
H	-8.553663967000	-1.766653591000	3.235139414000
H	-10.243552660000	-1.276373680000	3.151505890000
C	-5.395326384000	-0.662040626000	1.132539724000
O	-4.695384389000	-1.769654094000	1.308227662000
O	-5.035172811000	0.387990936000	0.642460439000

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4'c

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H	4.048931027	1.460764982	1.910264568
C	3.439645295	0.678820453	1.429175860
N	2.339863360	1.317313573	0.709546573
C	4.367079308	-0.068966320	0.465027403
C	6.264850555	-1.381522110	-1.145390032
C	3.973095715	-0.566793090	-0.812844176
C	5.685789472	-0.254867964	0.891658569
C	6.640647173	-0.905739723	0.114070226
C	4.962355438	-1.212260343	-1.594800545
H	5.964858855	0.123234226	1.874492357
H	7.655773506	-1.032469263	0.480871851
H	4.656845973	-1.579716665	-2.569287071
H	6.990604187	-1.886589029	-1.779541020
C	2.890468488	-0.203308163	2.541275730
C	1.924834662	-1.852955541	4.588746321
C	1.914985303	-1.192335269	2.235703620
C	3.342730428	-0.054906219	3.850469805

C	2.874147847	-0.871739189	4.884464788
C	1.449797560	-2.010252227	3.288725349
H	4.082494979	0.715513816	4.065494051
H	3.242549217	-0.740848490	5.898495434
H	0.704580878	-2.762174604	3.045198139
H	1.545265608	-2.497784238	5.379058169
O	2.760225503	-0.451641330	-1.334015169
O	1.453569199	-1.361674467	1.014168888
C	2.170227983	2.585931858	0.797944759
H	2.849381720	3.165520752	1.442704179
C	1.157686760	3.351565003	0.108729678
C	-0.706136799	4.971576225	-1.217403770
C	1.008975620	4.712915403	0.442044292
C	0.350379166	2.778311639	-0.931801305
C	-0.578457192	3.641829983	-1.578937920
C	0.087246702	5.526520537	-0.196005620
H	1.640408638	5.122908089	1.229413953
H	-1.195518380	3.204941201	-2.357831650
H	-0.016410154	6.571385980	0.081458090
H	-1.434200576	5.595575169	-1.732063533
O	0.438332255	1.543115013	-1.310503487
Fe	1.120855854	-0.101149863	-0.405453896
C	0.220719239	-0.350163377	-4.445776957
H	-0.789514689	-0.553736930	-4.808656948
O	0.328872290	-0.793174171	-3.086052656
C	1.253035558	-1.233077841	-5.155245228
H	1.010235198	-2.285678196	-5.013952848
C	0.554701692	1.143709878	-4.535422959
H	0.385490457	1.471647498	-5.568895927
H	-0.147162081	1.676312987	-3.888757755
Br	1.010179747	-1.020273356	-7.221146329
C	2.679986375	-0.905950018	-4.751659300
H	3.386344919	-1.532770983	-5.306449672
H	2.734830332	-1.179789517	-3.688613418
C	3.015512657	0.587395737	-4.881105843
H	4.026467304	0.758610089	-4.491588751
H	3.022688445	0.869513654	-5.942766455
C	2.000281195	1.440410017	-4.103184772
H	2.096609201	1.224208564	-3.036511366
H	2.212311221	2.508473503	-4.240827953
C	-0.817084716	-0.850037162	-2.299538003
O	-0.483888258	-1.071743392	-1.070705625
O	-1.934870823	-0.709381103	-2.772023059
C	-2.081734221	2.420223527	2.859352783
C	-2.426862416	2.175757322	1.381920383
C	-1.789776614	0.908282259	0.858591352
C	-1.373972424	-0.166172619	1.781788347
C	-1.558670514	-0.045960068	3.283955092
C	-2.401443807	1.175625175	3.701943881
H	-1.975990642	0.637381899	-0.178653346
H	-3.515922410	2.084002420	1.257888106
H	-2.101711510	3.016791870	0.759324133
H	-1.015109174	2.660458895	2.938736417
H	-2.639546188	3.288320640	3.231522591
H	-1.253440263	-1.163272929	1.364416468
H	-2.017729906	-0.967567077	3.662386859
H	-0.556556634	0.001180033	3.726184355
H	-3.468830426	0.940045079	3.578450131
H	-2.249211303	1.380319453	4.768979640
O	-0.398841686	0.755093008	1.232289251

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2'c

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H	1.303733098	-0.848151393	3.106964622
C	1.067681030	-1.118220785	2.067143514
N	0.603463459	0.089434643	1.377511366
C	2.372637491	-1.613659352	1.432691087
C	4.816609664	-2.589571599	0.441110091
C	2.675687856	-1.467110210	0.048070764

C	3.297452316	-2.243462057	2.269647464
C	4.511005628	-2.739947861	1.796541517
C	3.918196553	-1.961426812	-0.412121134
H	3.049969733	-2.352348628	3.324368469
H	5.205655862	-3.227647164	2.474788288
H	4.141711439	-1.827103063	-1.466759205
H	5.761640045	-2.959519631	0.049222219
C	-0.014408975	-2.189692979	2.125695136
C	-1.921975100	-4.240984553	2.327173556
C	-0.798408669	-2.532918211	0.990938065
C	-0.204971911	-2.883886360	3.321356168
C	-1.145022545	-3.908728029	3.437930259
C	-1.752394281	-3.561884365	1.125079266
H	0.393999938	-2.609282650	4.187210651
H	-1.281122102	-4.420312791	4.386061580
H	-2.356776091	-3.799310349	0.254122849
H	-2.673962389	-5.022794258	2.400765120
O	1.877390028	-0.882107989	-0.832089442
O	-0.671485153	-1.921815985	-0.181593030
C	0.700251729	1.244844881	1.935891570
H	1.032529134	1.294083066	2.980773644
C	0.394855877	2.507959677	1.305954995
C	-0.155088888	5.033186142	0.229512217
C	0.237848122	3.634613535	2.140480664
C	0.288248938	2.654573230	-0.119855034
C	0.018592109	3.953130367	-0.619683523
C	-0.048014637	4.886120745	1.624042239
H	0.322963545	3.497423433	3.216597181
H	-0.062931572	4.060255742	-1.696863320
H	-0.189077659	5.736552677	2.283613240
H	-0.380168126	6.010570090	-0.191641752
O	0.460904950	1.666577806	-0.954502561
Fe	0.086839566	-0.208582337	-0.631104153
C	-4.531235684	1.790135306	-0.967747383
C	-4.379952223	0.269909317	-0.792311010
C	-3.180090955	-0.085378380	0.046274917
C	-2.618693157	0.880818583	0.981178784
C	-3.172537651	2.280487139	1.136957883
C	-4.508385554	2.489743981	0.400090533
H	-3.020616039	-1.139010017	0.255500645
H	-5.244740496	-0.131579717	-0.251859857
H	-4.311772962	-0.237114931	-1.765241250
H	-3.716099822	2.167509979	-1.599742657
H	-5.472877010	2.004058151	-1.489174494
H	-2.056501708	0.480346977	1.817803531
H	-3.312390595	2.446924722	2.207860450
H	-2.410654035	2.983493202	0.778728335
H	-5.303863335	2.064706573	1.019457187
H	-4.699316626	3.564537439	0.284045832
O	-1.940316155	0.617010218	-0.317363304
C	2.699946303	-0.486125617	-4.311034096
C	1.953899640	0.702465280	-3.684670796
C	0.480885417	0.767755917	-4.126900422
C	-0.264522894	-0.565049027	-4.003129400
C	0.527446734	-1.740652031	-4.588013510
C	1.957767607	-1.803299616	-4.031830181
H	3.719031950	-0.536819152	-3.908174601
H	2.794975392	-0.343909704	-5.399520675
H	2.442968095	1.648343237	-3.949249000
H	2.007463161	0.617232418	-2.598169949
H	-0.050748432	1.520258026	-3.535528223
H	0.420241391	1.064627669	-5.183483982
H	-1.237619202	-0.481881608	-4.507260112
H	-0.014158113	-2.677914995	-4.395273425
H	0.552308593	-1.615819221	-5.680188553
H	2.490612102	-2.653552033	-4.475337511
H	1.918636574	-1.960649035	-2.948333876
O	-0.540936420	-0.800720760	-2.600648023
H	-0.858621911	-1.702898567	-2.439031734
C	-3.650371899	1.003363004	5.295454072
H	-4.546259144	1.505756356	5.673392178

O	-3.788782211	0.726771322	3.909956014
C	-2.445461170	1.948382963	5.321761677
H	-2.633392887	2.828339624	4.707645207
C	-3.399779608	-0.282325645	6.097630246
H	-3.337895394	-0.035164140	7.165635980
H	-4.275916272	-0.918605667	5.947865227
Br	-2.254217587	2.813507950	7.227060663
C	-1.140603413	1.256967092	4.955879620
H	-0.297609331	1.950442667	5.055323385
H	-1.253473397	1.011735532	3.892443043
C	-0.901159233	-0.038960775	5.744743454
H	0.005250793	-0.530136858	5.366353656
H	-0.713590244	0.213199653	6.796841783
C	-2.111924690	-0.981558180	5.638870509
H	-2.233036835	-1.299363330	4.597909370
H	-1.934155286	-1.888542354	6.231248852
C	-5.135871541	0.240098316	3.476689035
O	-5.142955816	0.021355611	2.256888988
O	-5.974462355	0.145191667	4.378110559

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4' C-TS

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H	0.655521688	0.911388951	3.362527364
C	1.112581358	0.497018155	2.449801955
N	0.246473415	0.795422726	1.311897240
C	2.480236469	1.168192708	2.279296865
C	5.009860547	2.396690490	2.206384357
C	3.033620385	1.553225539	1.018710781
C	3.212412918	1.401371940	3.446788034
C	4.468726125	2.004003658	3.434754989
C	4.304841110	2.179011114	1.030465174
H	2.778545302	1.087135056	4.395605778
H	5.010573430	2.165864868	4.363002329
H	4.709864030	2.474076595	0.066765476
H	5.986871953	2.874849444	2.166875663
C	1.204446656	-1.012978678	2.635458989
C	1.401944533	-3.784098298	2.979175986
C	1.661138303	-1.817587637	1.553666076
C	0.850311314	-1.606869317	3.843839448
C	0.946672880	-2.989581793	4.034209549
C	1.752015973	-3.211274370	1.758193319
H	0.494405050	-0.973884223	4.656302571
H	0.668845471	-3.434577404	4.986197567
H	2.102716985	-3.818557770	0.928467150
H	1.481584332	-4.862330197	3.106793340
O	2.437494227	1.389555510	-0.147865232
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6'c

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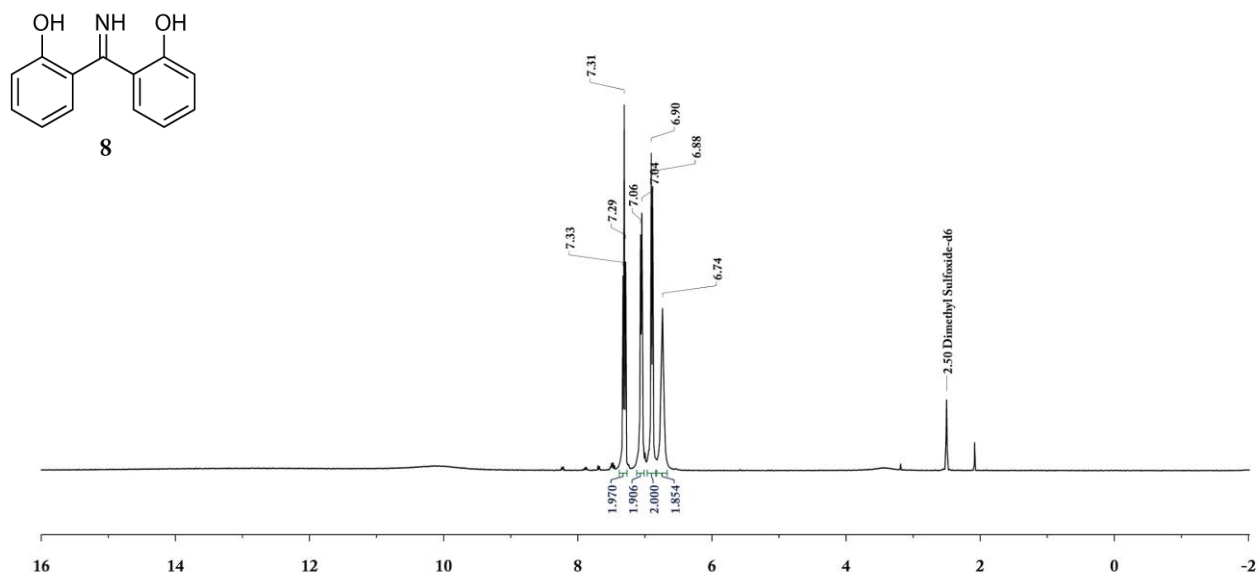
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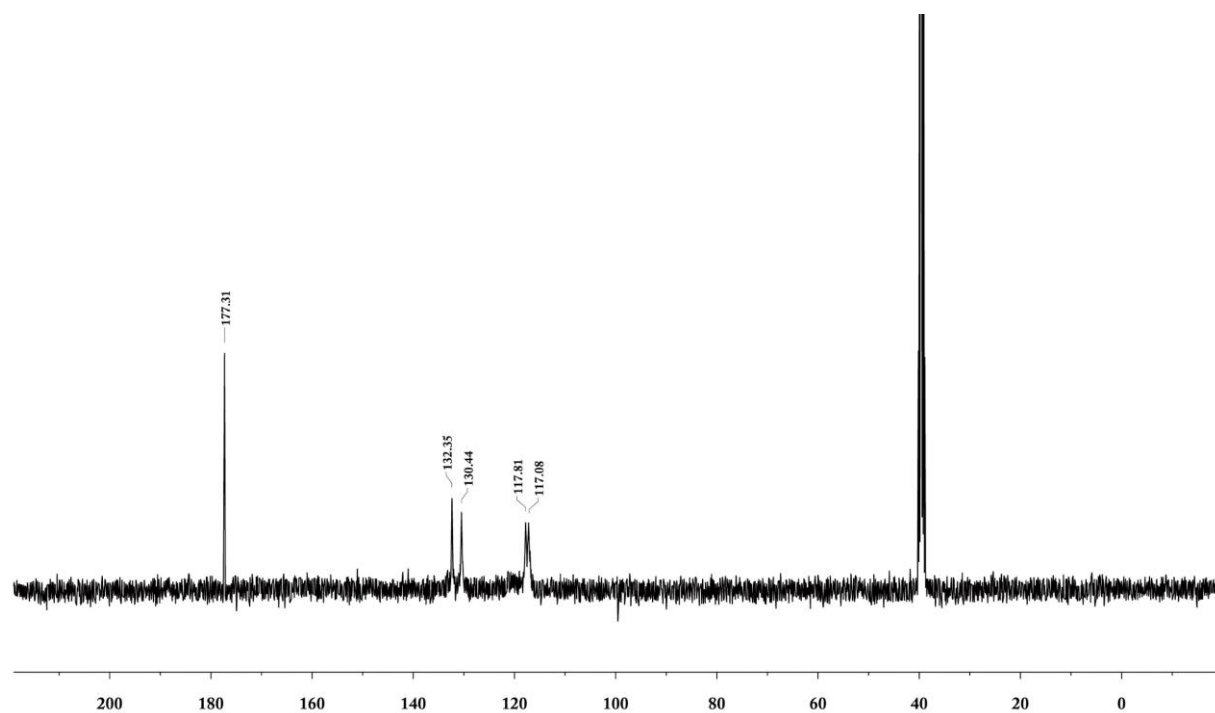
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C	3.965817083	-0.596240415	1.976419612
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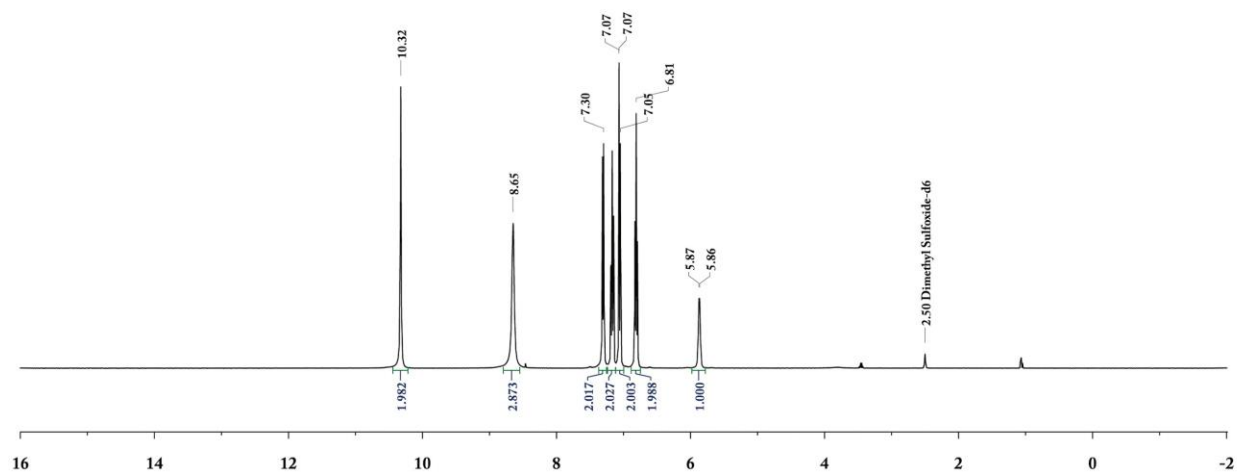
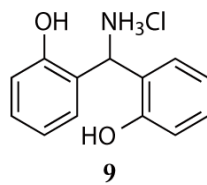
Appendix II. Spectral copies of ^1H and ^{13}C NMR data obtained in this study



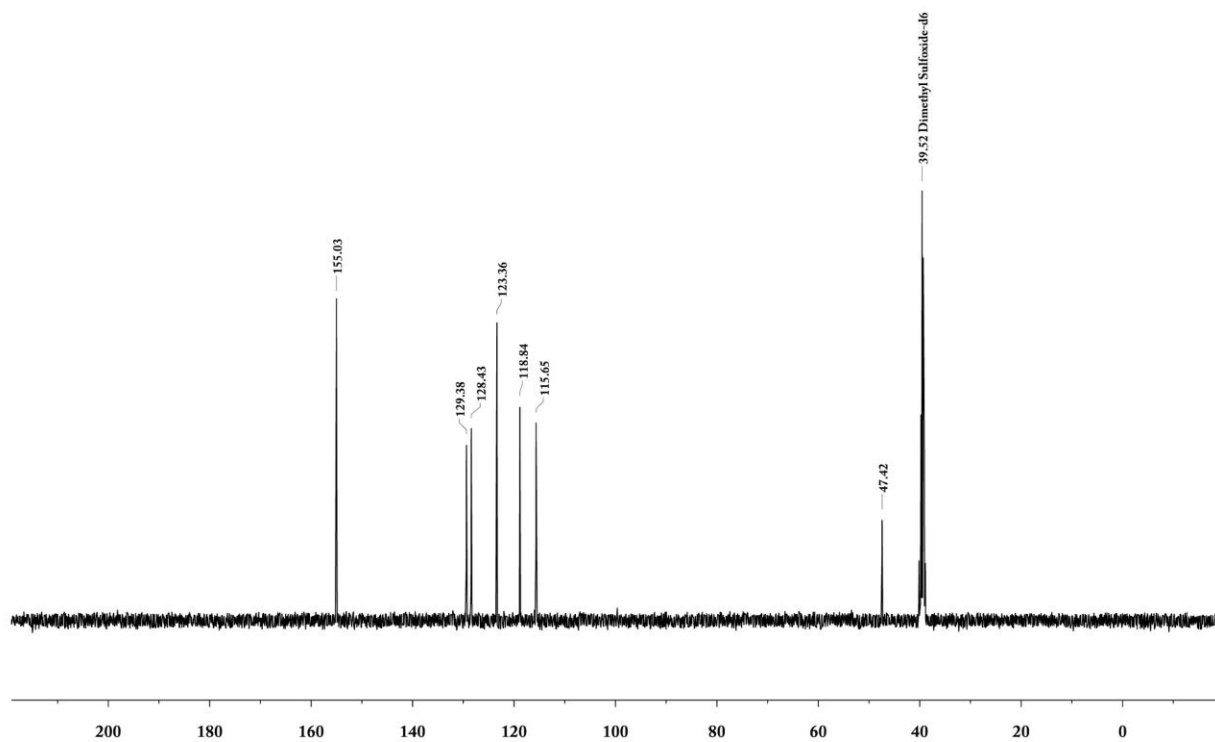
^1H NMR (400 MHz, DMSO-d_6)



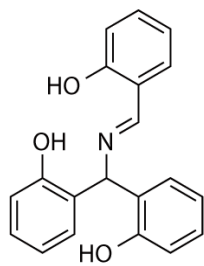
^{13}C NMR (100 MHz, DMSO-d_6)



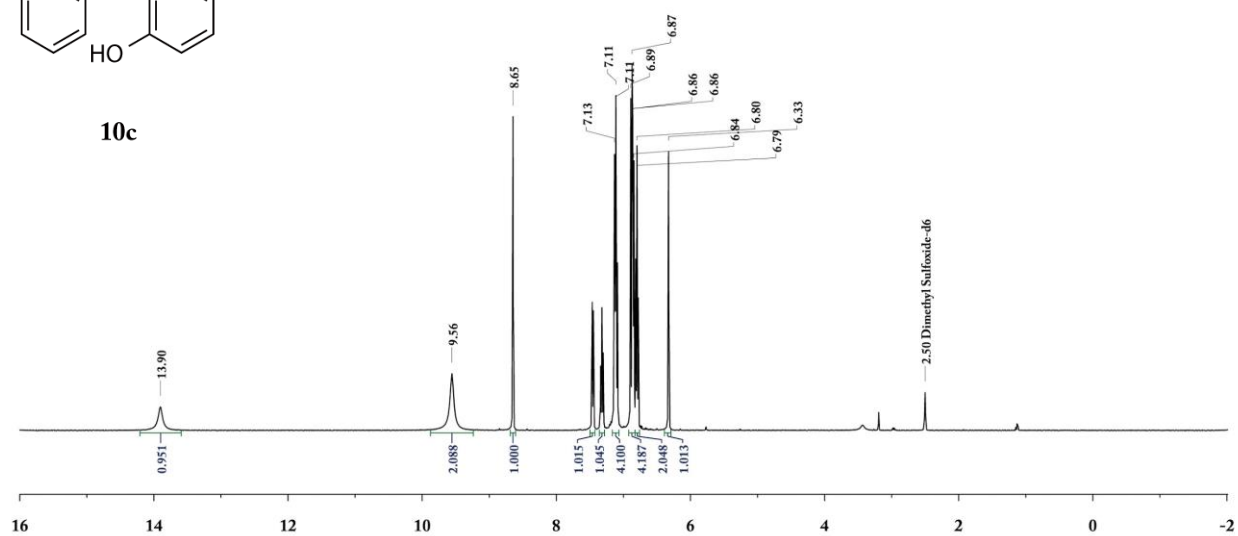
¹H NMR (400 MHz, DMSO-d₆)



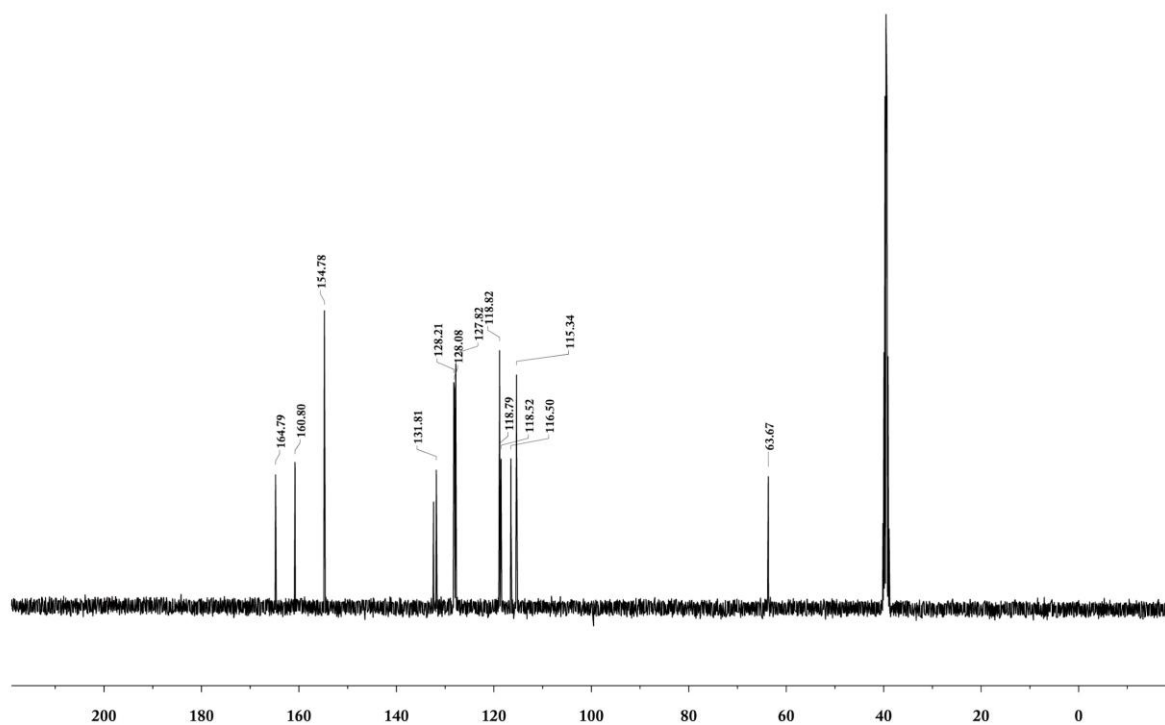
¹³C NMR (100 MHz, DMSO-d₆)



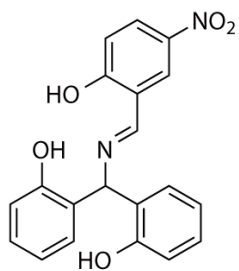
10c



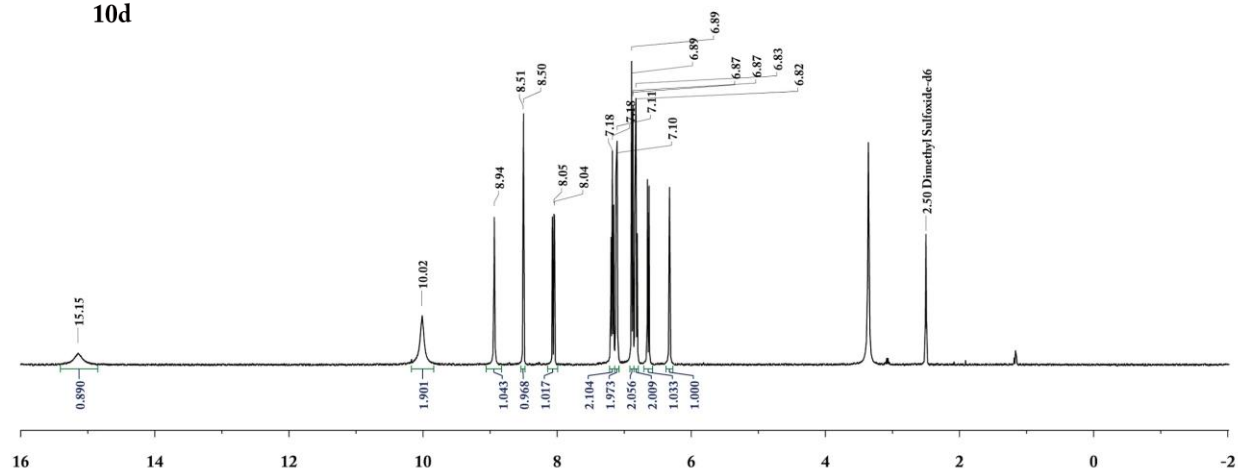
^1H NMR (400 MHz, DMSO-d_6)



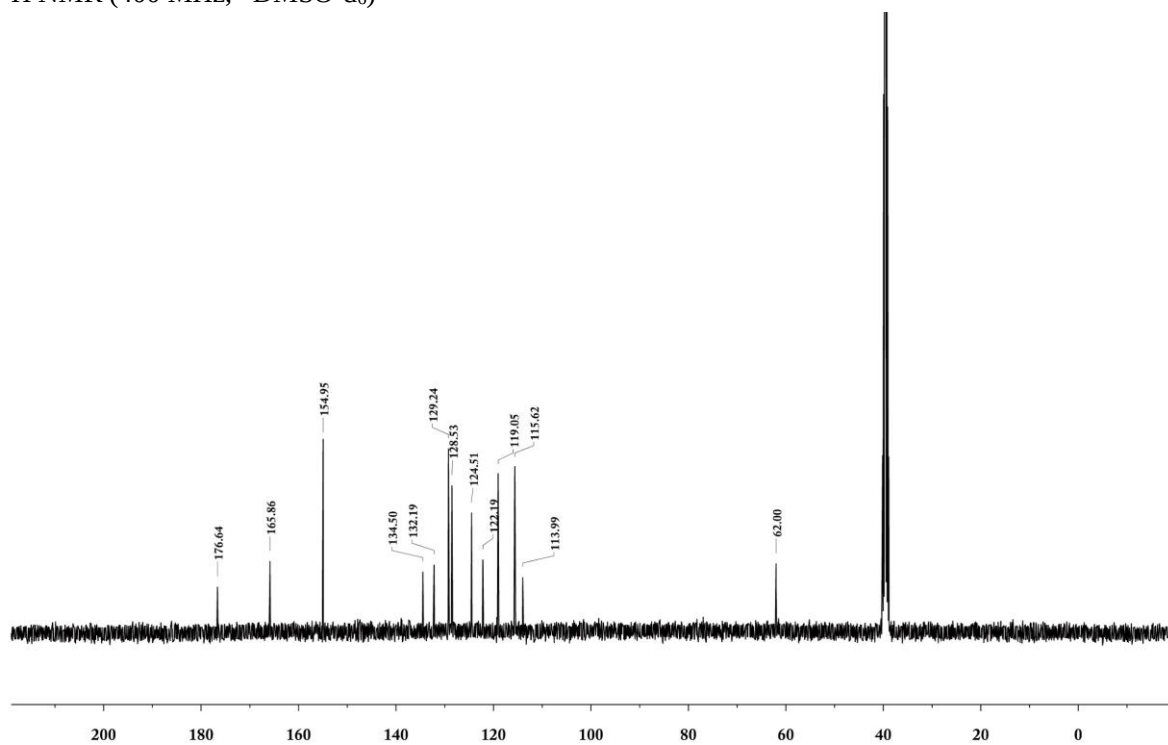
^{13}C NMR (100 MHz, DMSO-d_6)



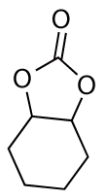
10d



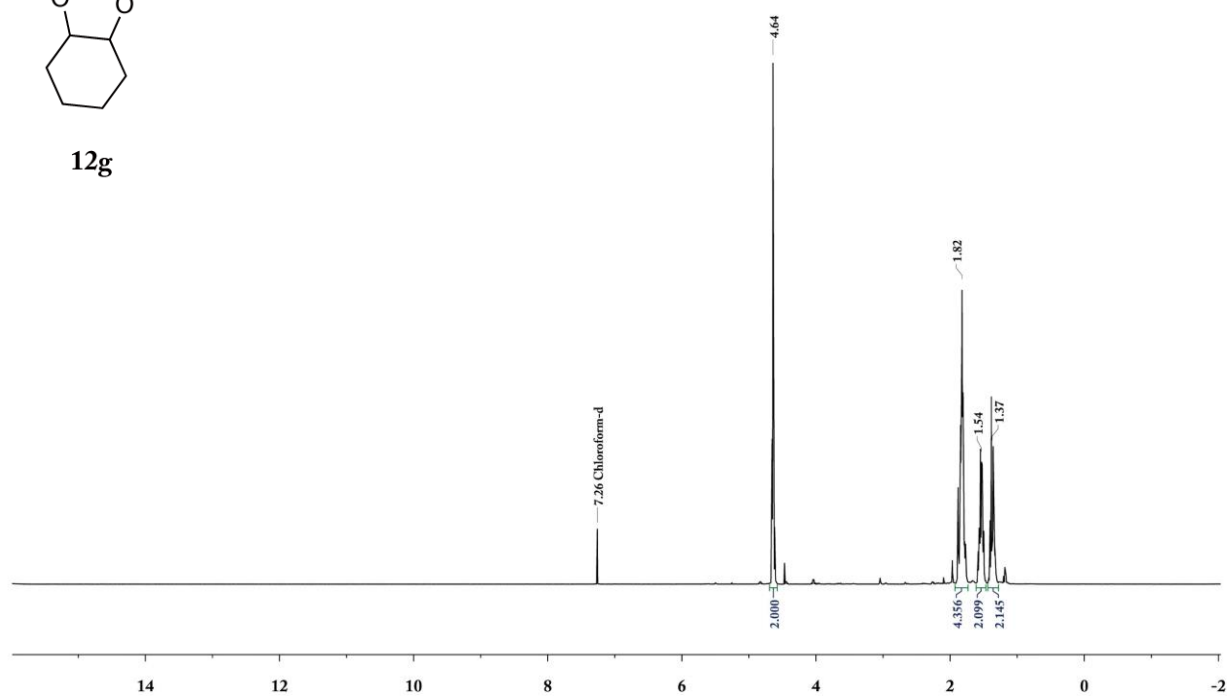
^1H NMR (400 MHz, DMSO-d_6)



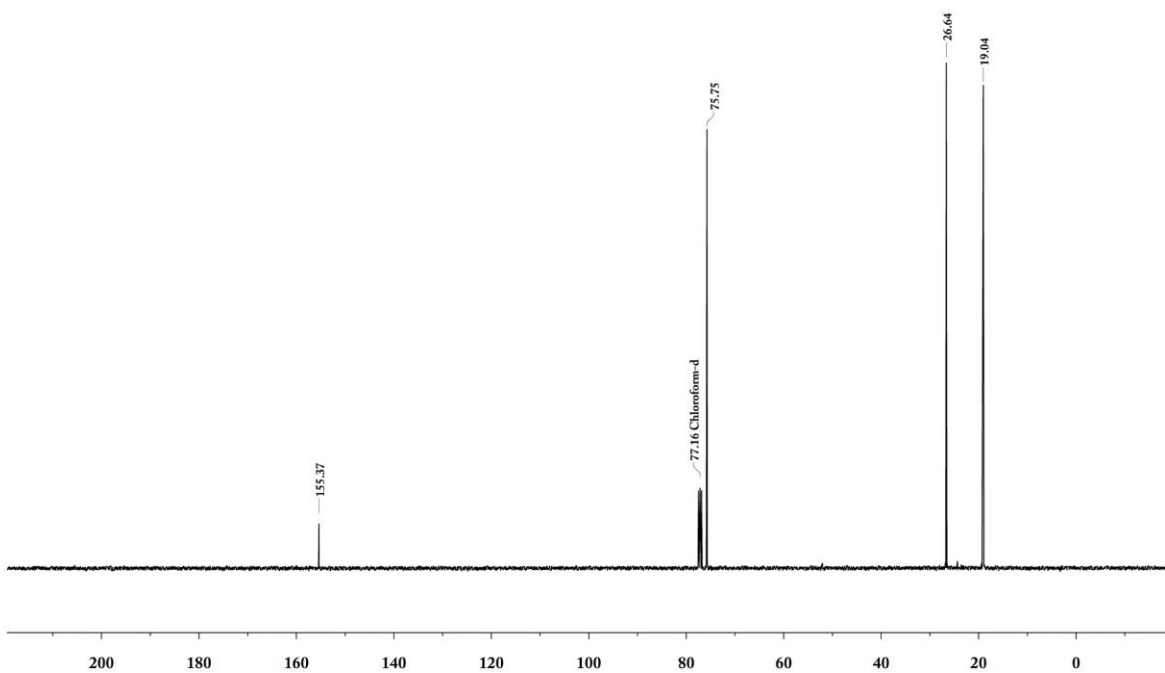
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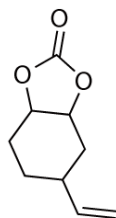
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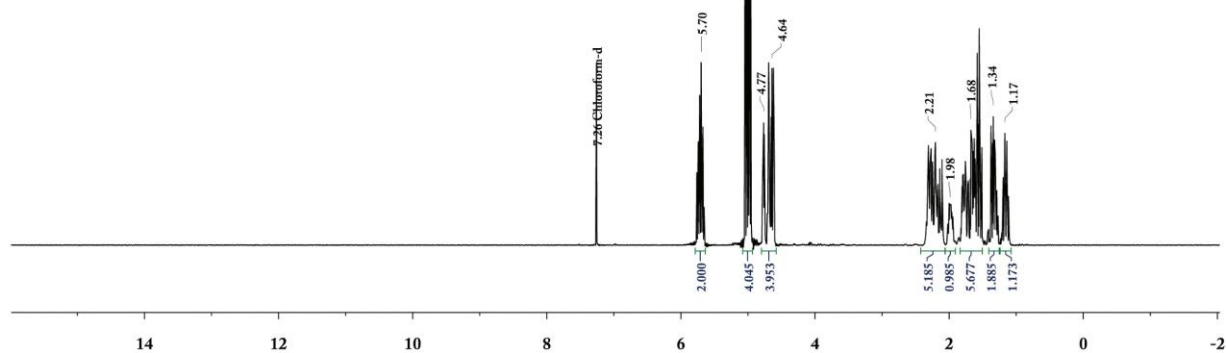
^1H NMR (400 MHz, CDCl_3)



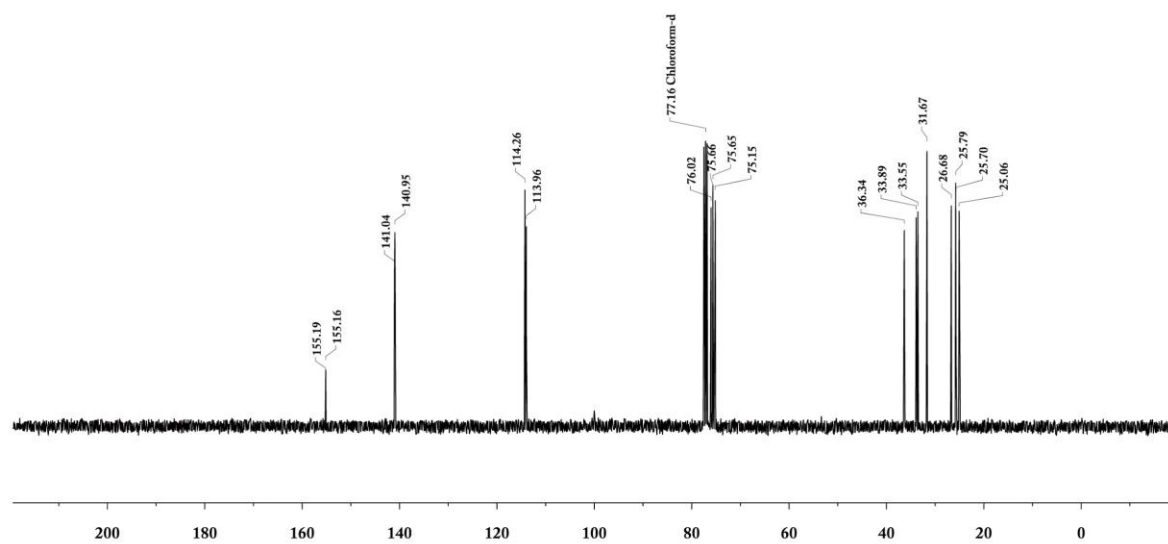
^{13}C NMR (100 MHz, CDCl_3)



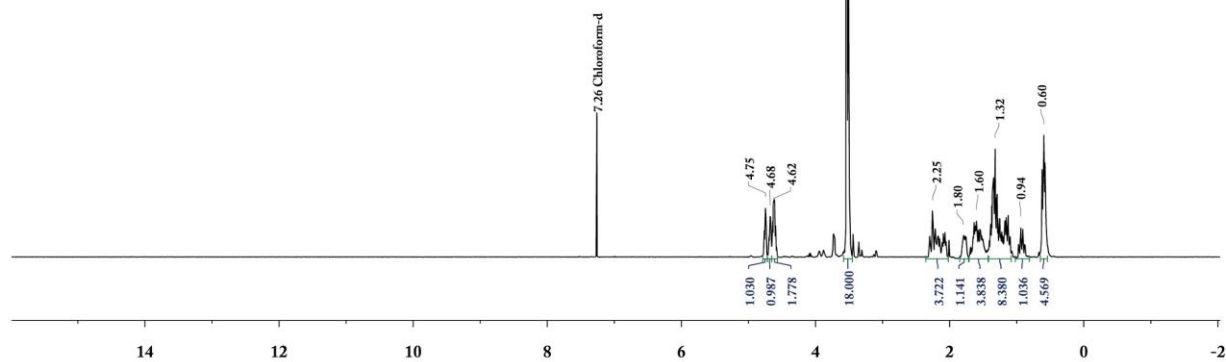
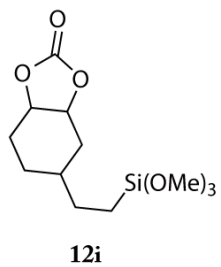
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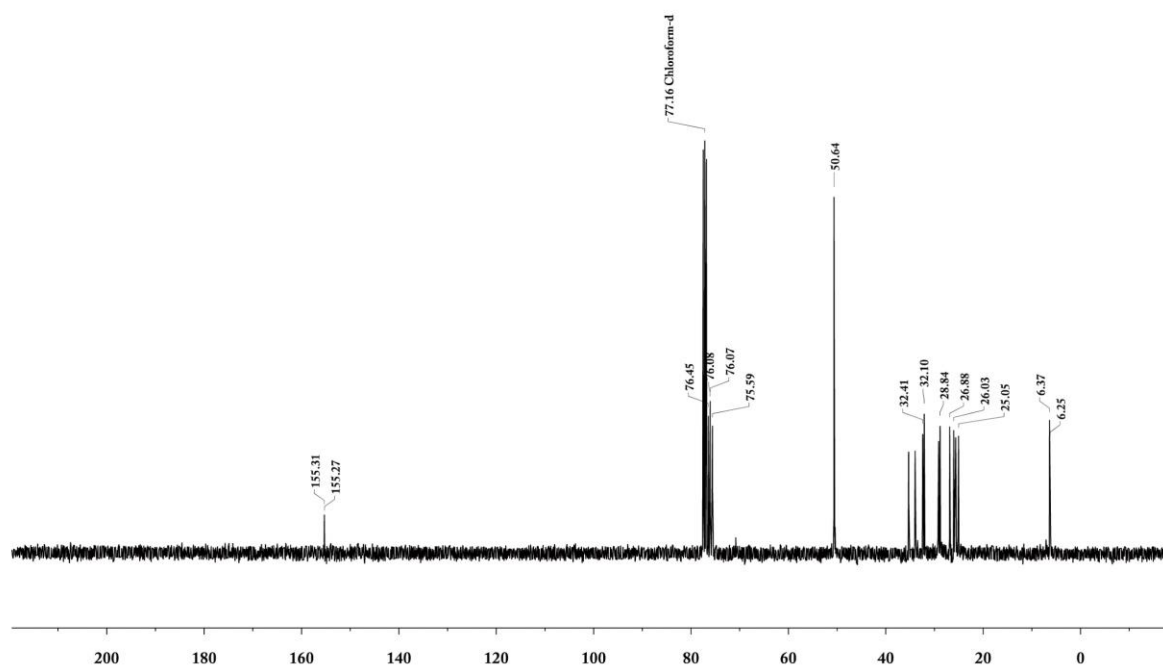
¹H NMR (400 MHz, CDCl₃)



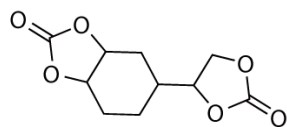
¹³C NMR (100 MHz, CDCl₃)



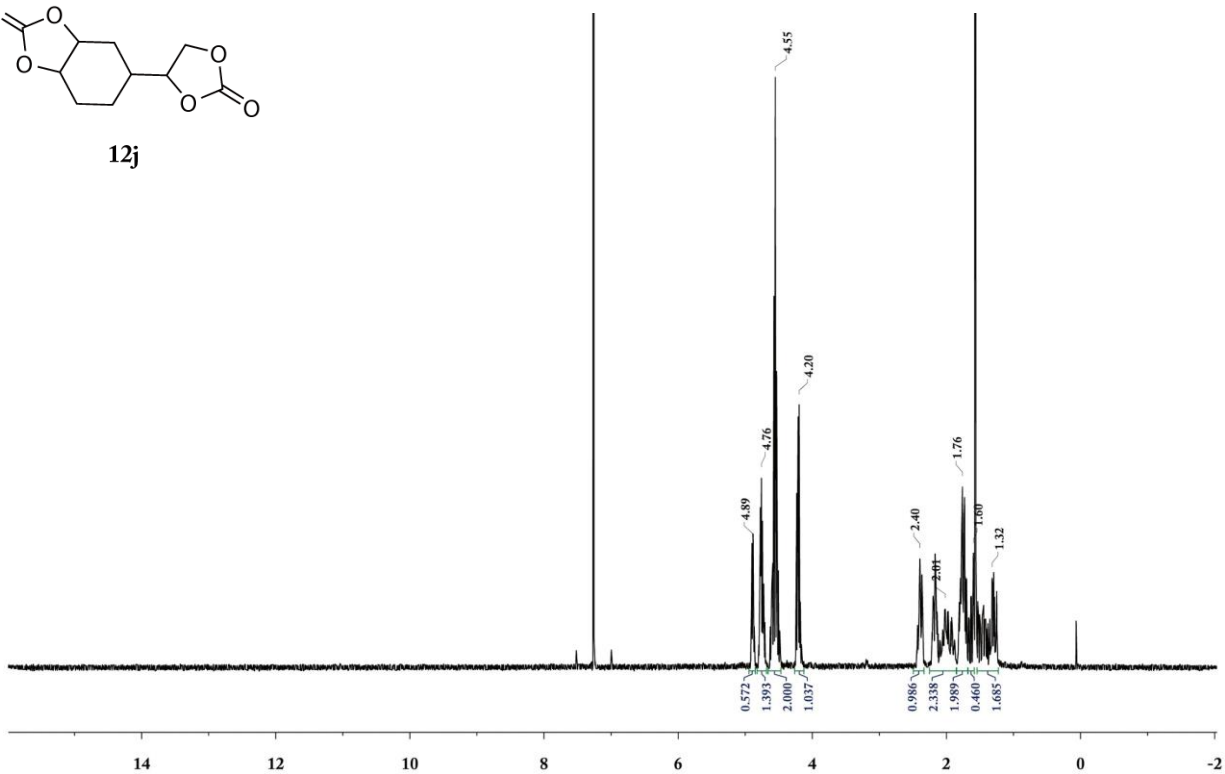
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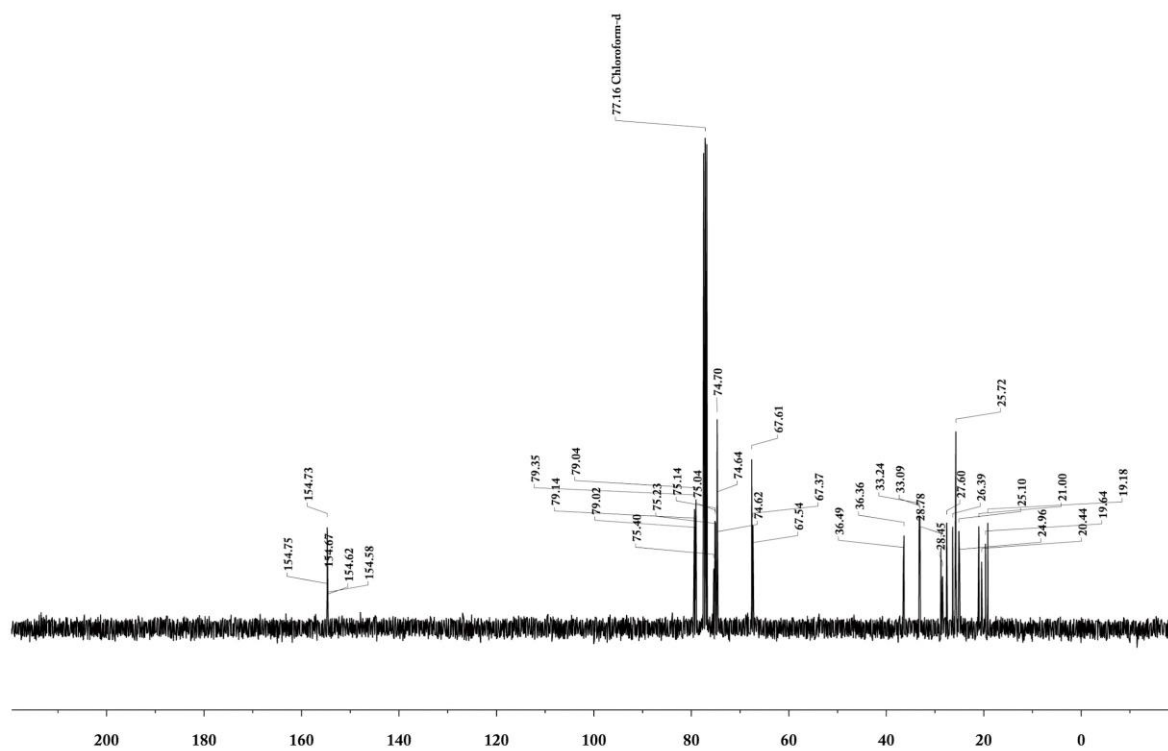
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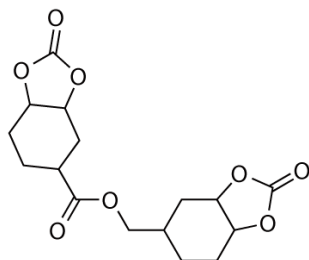
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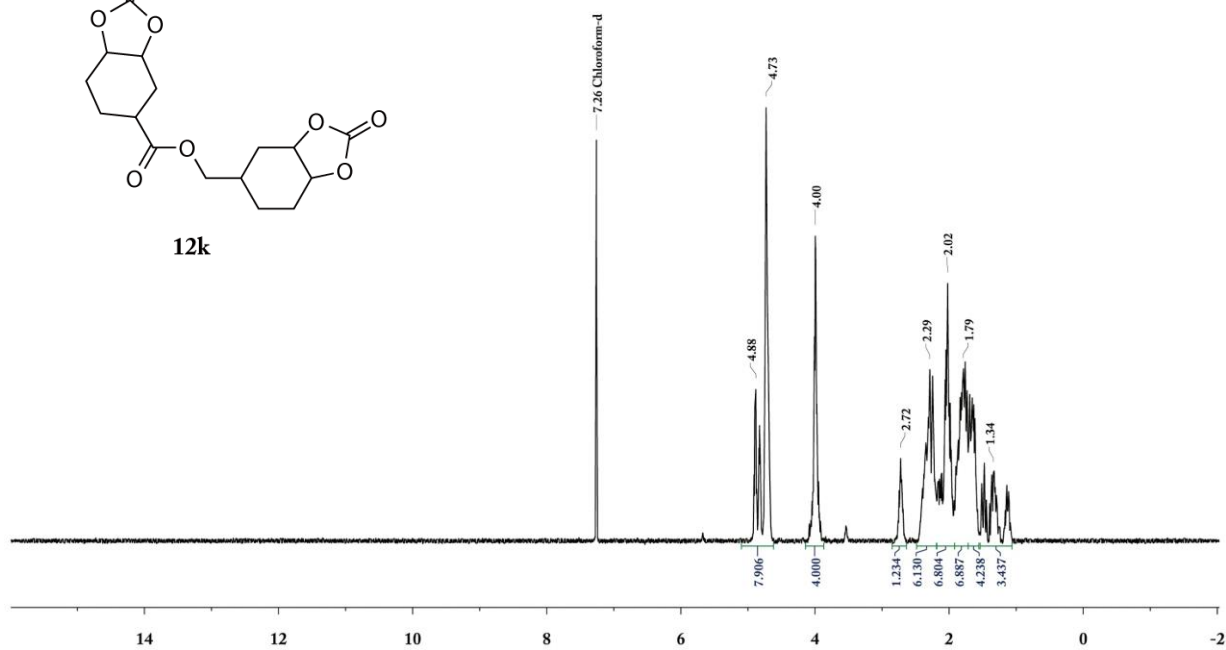
¹H NMR (400 MHz, CDCl₃)



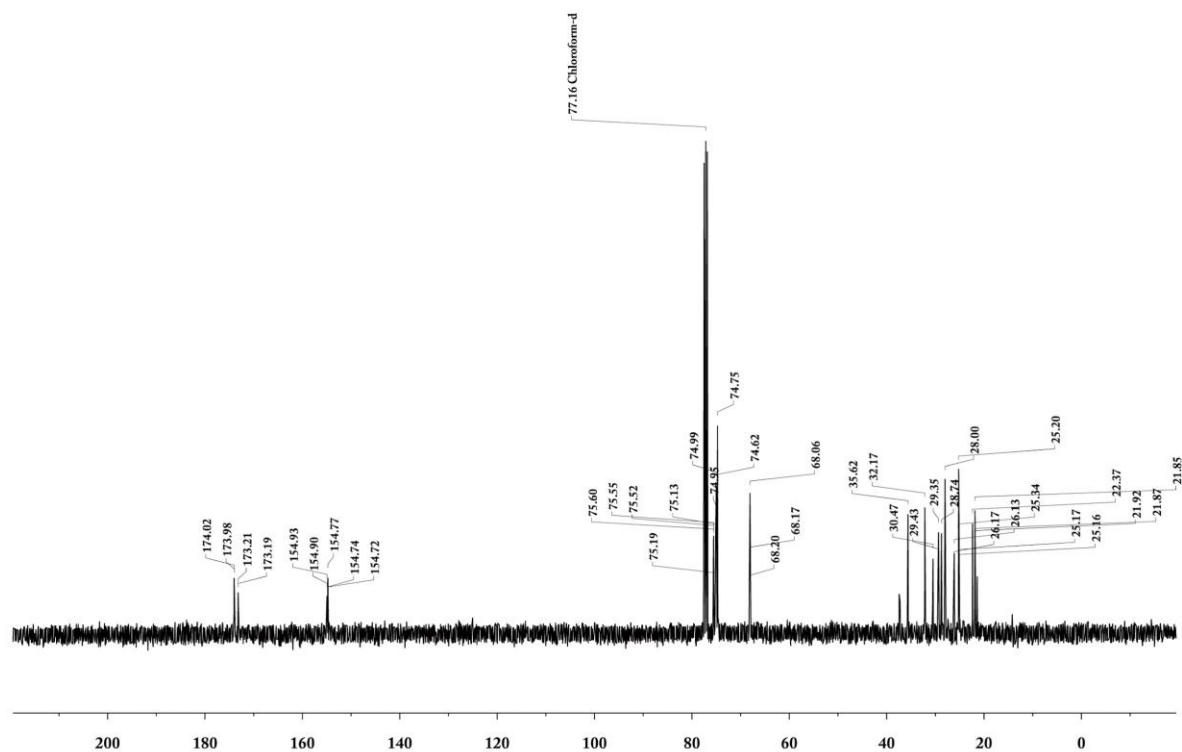
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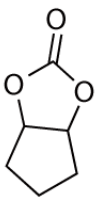
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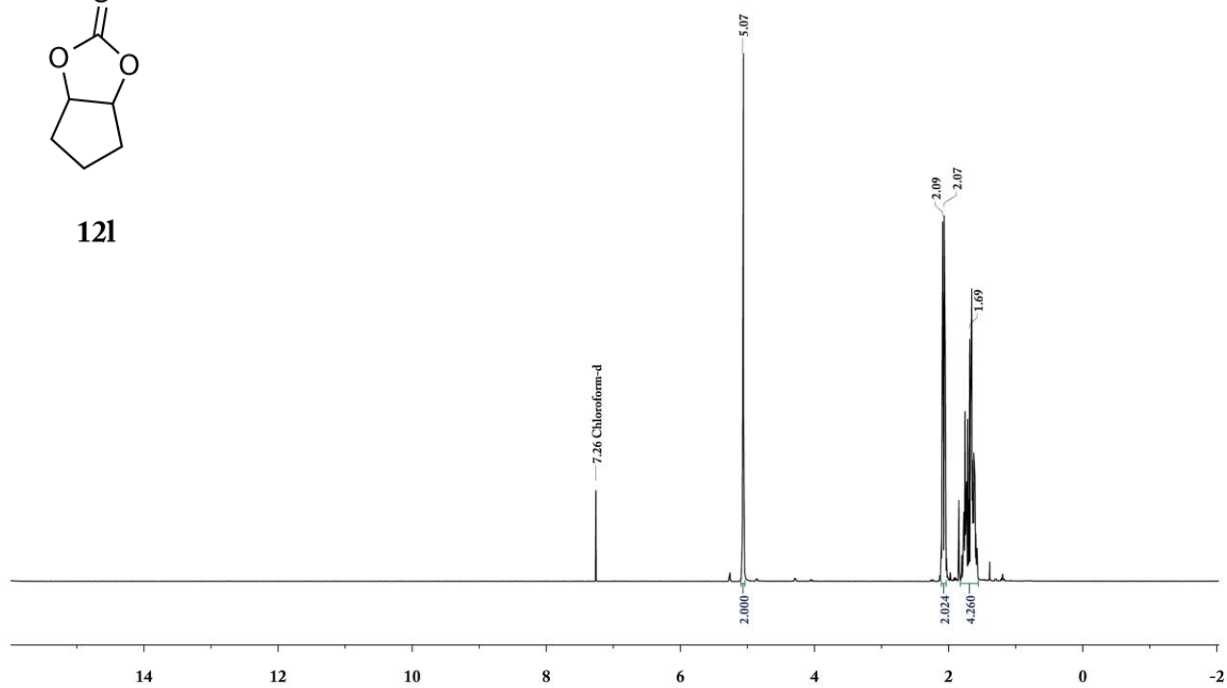
¹H NMR (400 MHz, CDCl₃)



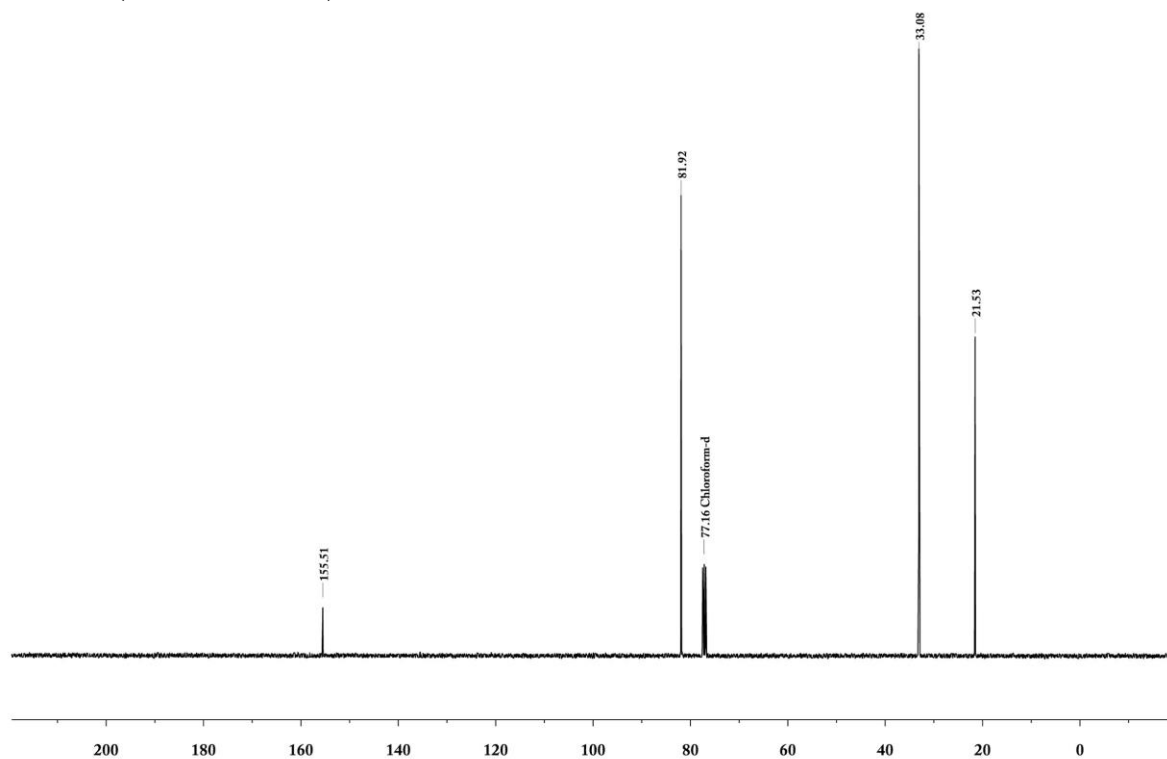
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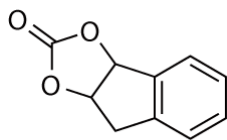
121



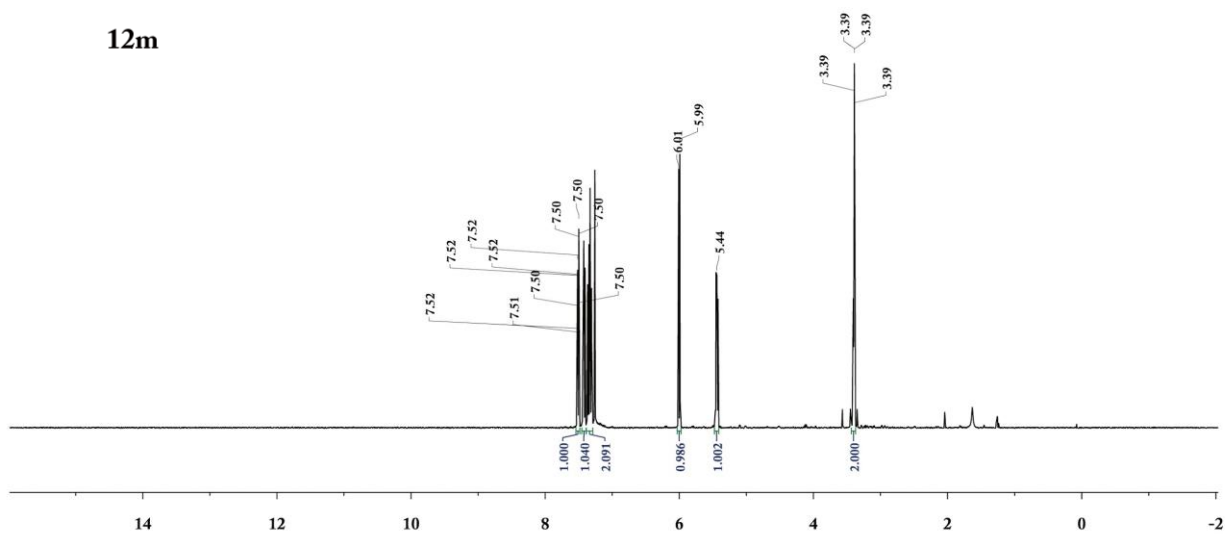
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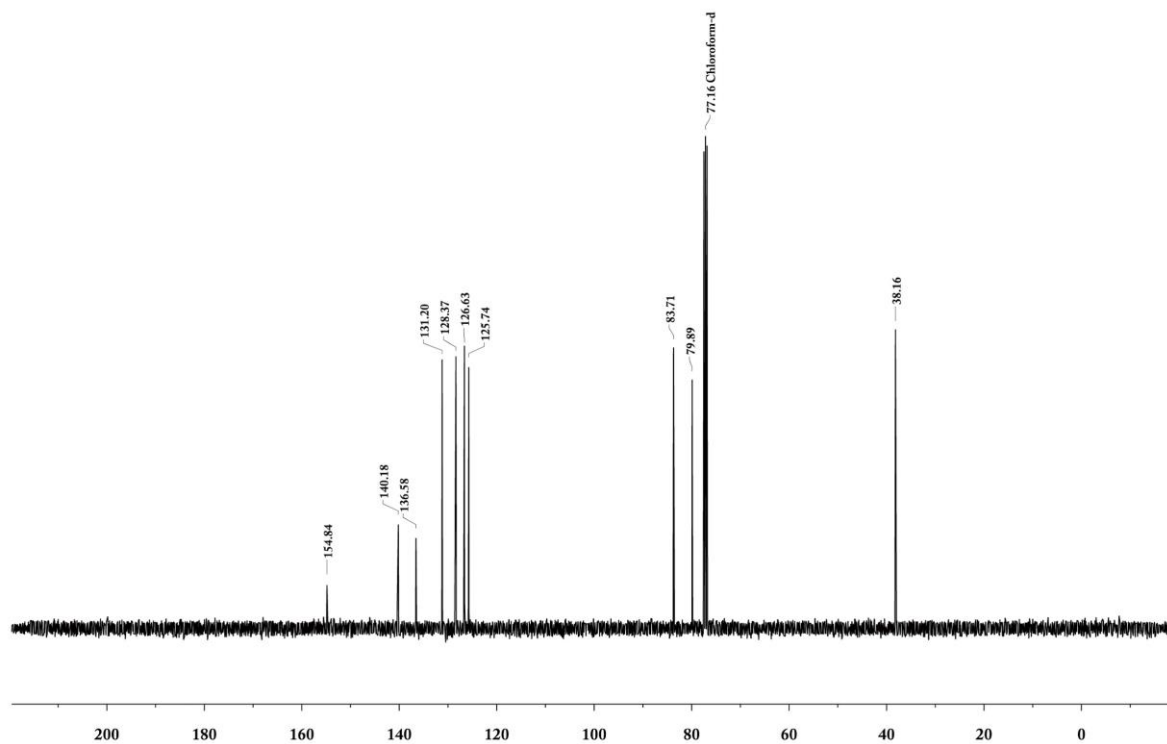
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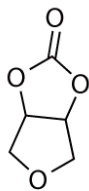
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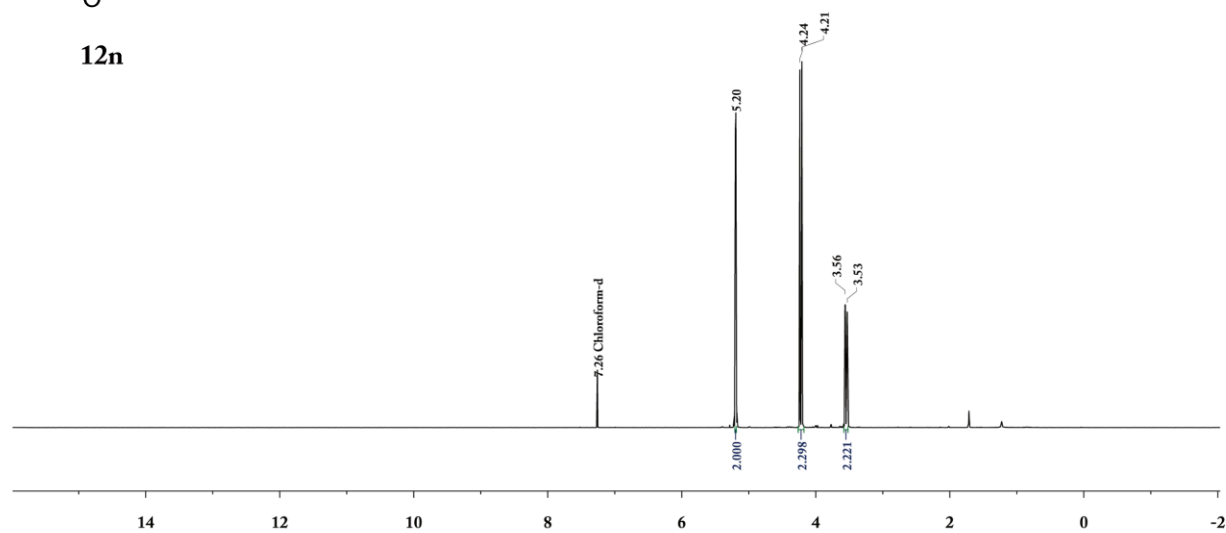
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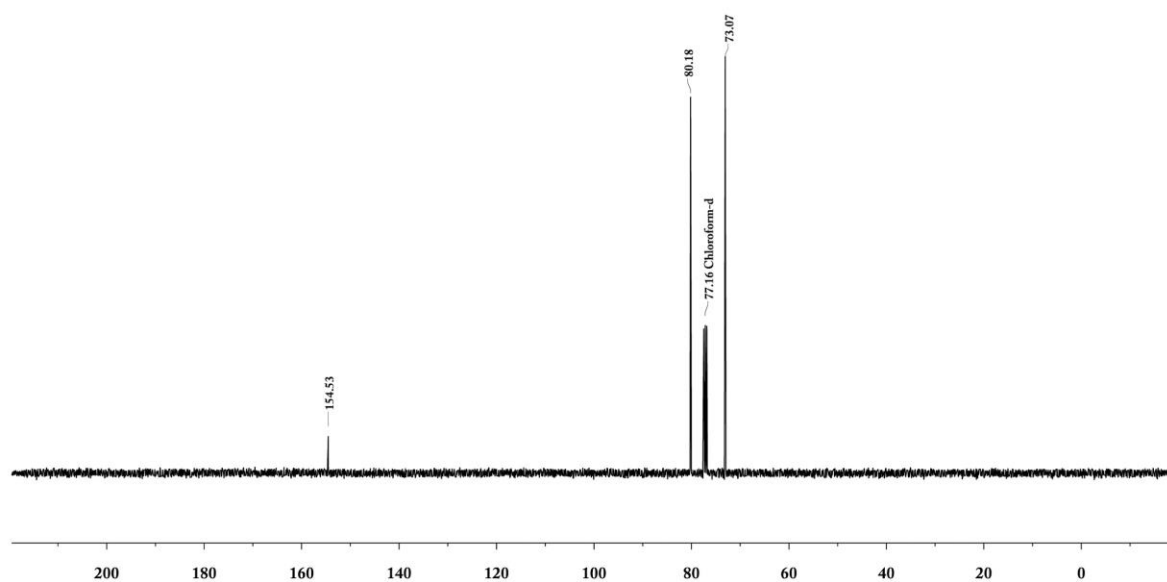
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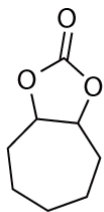
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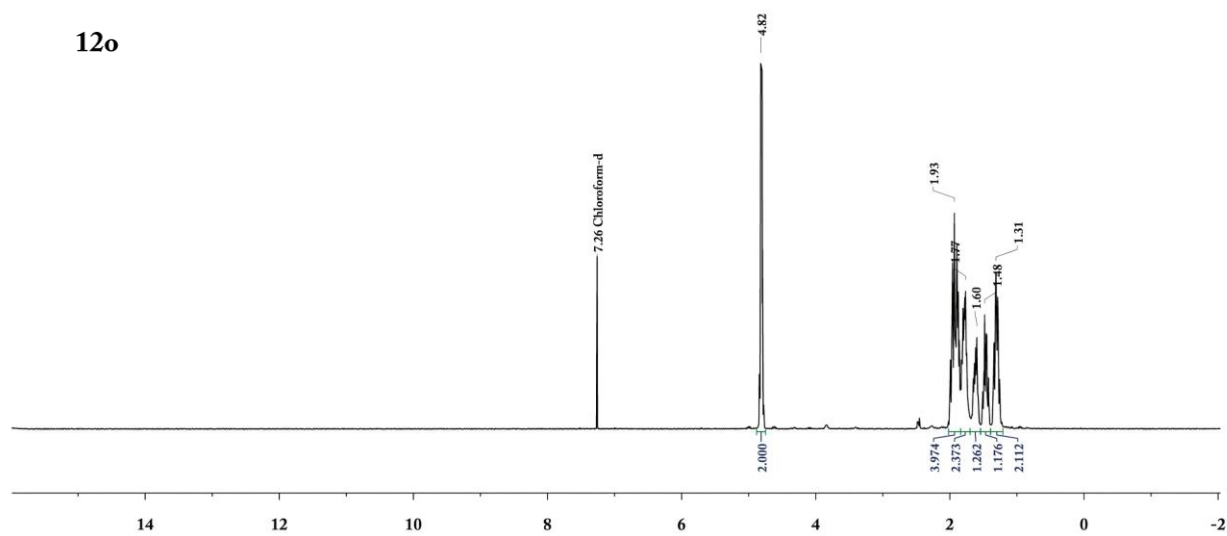
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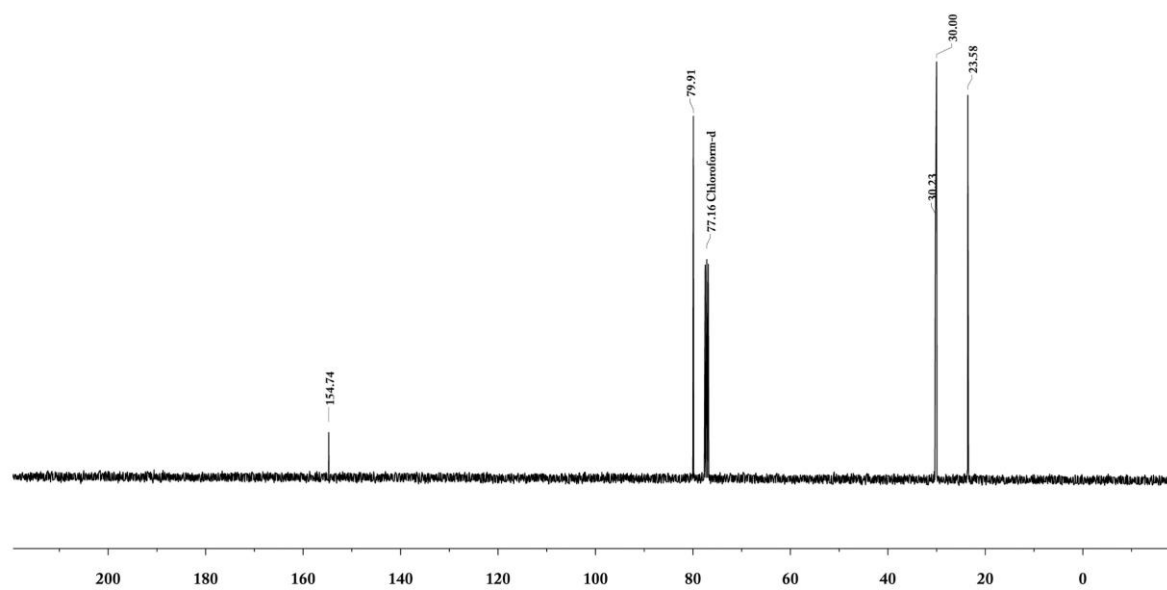
^{13}C NMR (100 MHz, CDCl_3)



12o



^1H NMR (400 MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3)