Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers

Supporting Information for

Synthesis of Ferrocene-Functionalized Monomers for Biodegradable Polymer Formation

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Experimental Procedures

1-Bromoferrocene. Ferrocene (3.720 g, 20.0 mmol) and potassium *tert*-butoxide (1.615 g, 15.2 mmol) were weighed and added to a Schlenk flask along with 100 mL THF. The reaction was cooled to -78 °C and t-BuLi (25.0 mL, 40.0 mmol) was added dropwise over 30 minutes. The reaction was allowed to stir at -78 °C for 1 hour and then warmed to room temperature to stir for another hour. The reaction was cooled to -78 °C again and 1,1,2,2-tetrabromoethane (2.3 mL, 20.0 mmol) was added dropwise over 30 minutes. The reaction was allowed to stir at -78 °C for 1 hour and then warmed to room temperature to stir overnight. Volatiles were removed under reduced pressure and the residue was dissolved in dichloromethane. The organic phase was washed with water (2x50 mL), brine (2x50 mL), and dried over $MgSO_4$. The reaction was filtered and solvent was removed yielding a red-brown solid. The crude product contained ~10% of unreacted ferrocene and was used without further purification. Characterization was consistent with reported literature values.[1] Yield: 4.783 g, 90.3%

1-Azidoferrocene **(6)**. 1-bromoferrocene (4.783 g, 18.1 mmol) and CuCl (1.881 g, 19.0 mmol) were weighed and combined in 100 mL ethanol. Sodium azide (2.354 g, 36.2 mmol) was weighed, dissolved in water, and added dropwise to the reaction mixture. The reaction was shielded from light and allowed to stir at room temperature for 48 hours. After 48 hours, an additional 100 mL of water was added, the reaction was allowed to stir for 10 minutes, and the product was extracted into diethyl ether. The ether layer was dried over $MgSO_4$ and concentrated yielding an orange solid. Characterization was consistent with reported literature values.[1] Yield: 1.278 g, 31.2%

1-Methylazidoferrocene **(4)**. Ferrocene methanol (0.522 g, 2.4 mmol) and sodium azide (0.950 g, 14.6 mmol) were weighed and combined in glacial acetic acid (28 mL, 480 mmol). The reaction was heated to 50 °C under nitrogen for three hours. After three hours, the reaction was allowed to cool to room temperature and diluted with 200 mL dichloromethane. The reaction mixture was washed with saturated $NaHCO_3$ (3x100 mL) and water (1x100 mL). The organic layer was dried over $MgSO_4$, filtered and dried yielding a yellow solid. Characterization was consistent with reported literature values.[2] Yield: 0.521 g, 88.7%.

1-Azidoethylferrocene **(5)**. 1-hydroxyethylferrocene (1.018 g, 4.4 mmol) and sodium azide (1.730 g, 26.6 mmol) were weighed and combined in glacial acetic acid (50.6 mL, 885.5 mmol). The reaction was heated to 50 °C under nitrogen for three hours. After three hours, the reaction was allowed to cool to room temperature and diluted with 200 mL dichloromethane. The reaction mixture was washed with saturated $NaHCO_3$ (3x100 mL) and water (1x100 mL). The organic layer was dried over $MgSO_4$, filtered and dried yielding a yellow-orange solid. Yield: 0.863 g, 80.6% ^{1}H NMR (300 MHz, 25 °C, $CDCl_3$), δ (ppm): 4.38 (q, 1H, CH), 4.19 (m, 9 H, fc), 1.56 (d, 3H, CH_3).

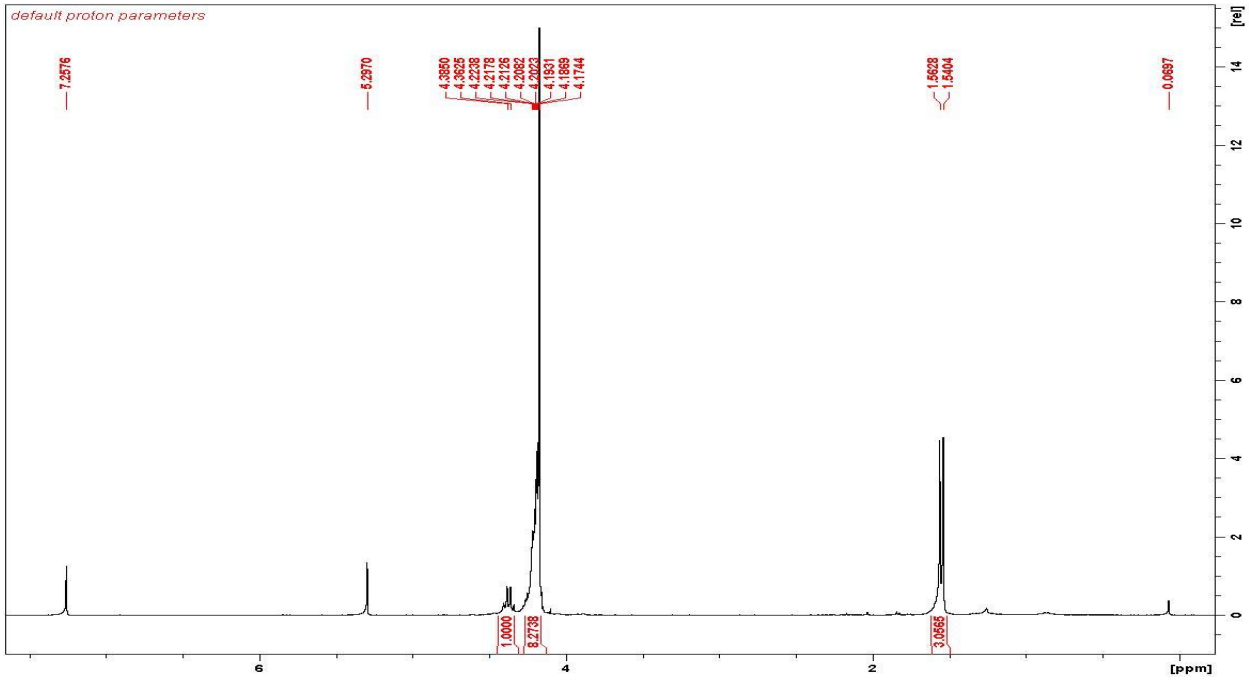
Dimethyl propargyl malonate. Dimethyl malonate (19.1 mL, 166.8 mmol), potassium carbonate (27.703 g, 200.4 mmol), and propargyl bromide (5.001 g, 33.6 mmol) were combined in 200 mL acetone. The reaction mixture was heated to reflux for 24 h. After 24 h, the reaction was filtered and solvent was removed yielding a yellow oil. The crude product contained approximately 10% impurities and was used without further purification. Characterization was consistent with reported literature values.[3] Yield: 19.200 g, 67.6%.

2-(Prop-2-yn-1-yl)propane-1,3-diol. Dimethyl propargyl malonate (19.200 g, 112.8 mmol) was weighed and added to a 1L Schlenk flask along with 400 mL diethyl ether. The reaction was cooled to 0 °C and lithium alumninum hydride (LAH) (9.423 g, 248.3 mmol) was added portionwise. The reaction was heated to reflux for 24 hours. After 24 hours, an additional portion of LAH (4.717 g, 124.3 mmol) was added and the reaction was heated to reflux for an additional 24 hours. The reaction was then cooled to 0 °C and quenched by the slow addition of $Na_2SO_4 \bullet 10H_2O$ until the reaction mixture becomes light grey in color.

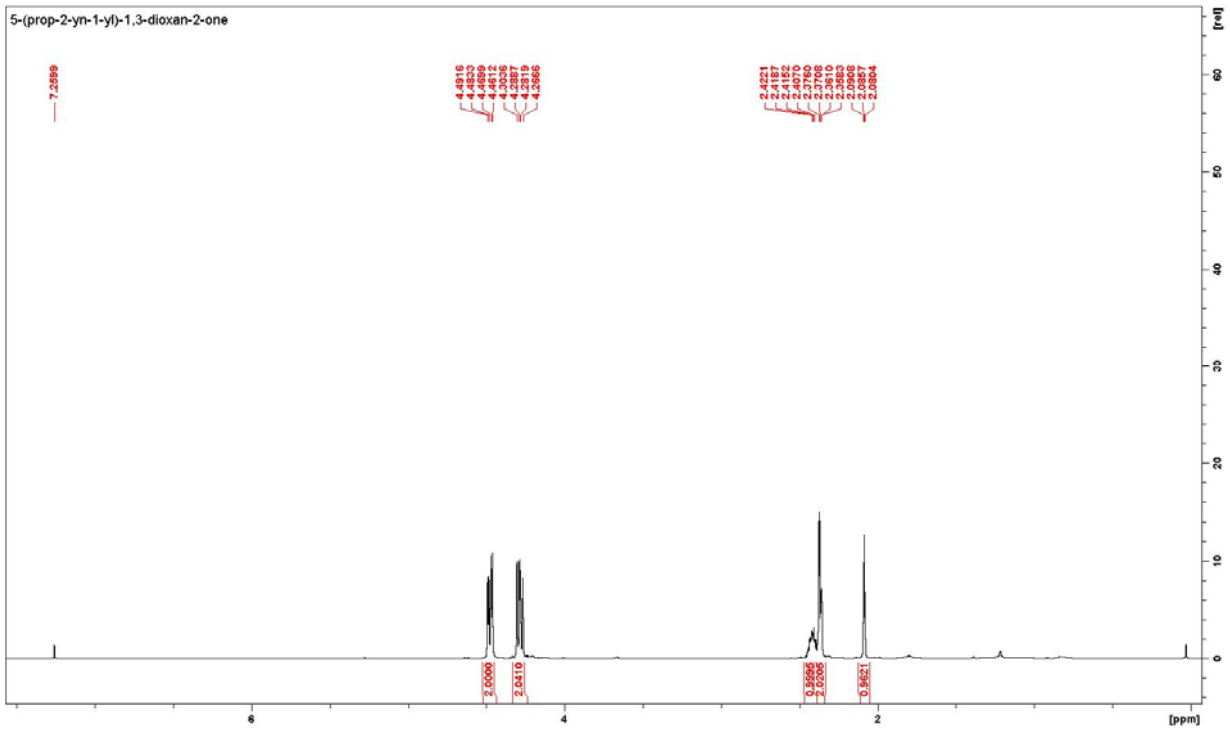
The reaction mixture was filtered through a fritted filter yielding a yellow filtrate. The solid was washed with an additional portion of diethyl ether and the combined organic layers were dried over $MgSO_4$. The solution was filtered and solvent was removed yielding a yellow oil. The crude product was purified via flash gradient column chromatography (60% ethyl acetate to 100 % ethyl acetate in hexanes), yielding a colorless oil. Characterization was consistent with reported literature values.[4] Yield: 3.253 g, 25.3%.

NMR Spectra

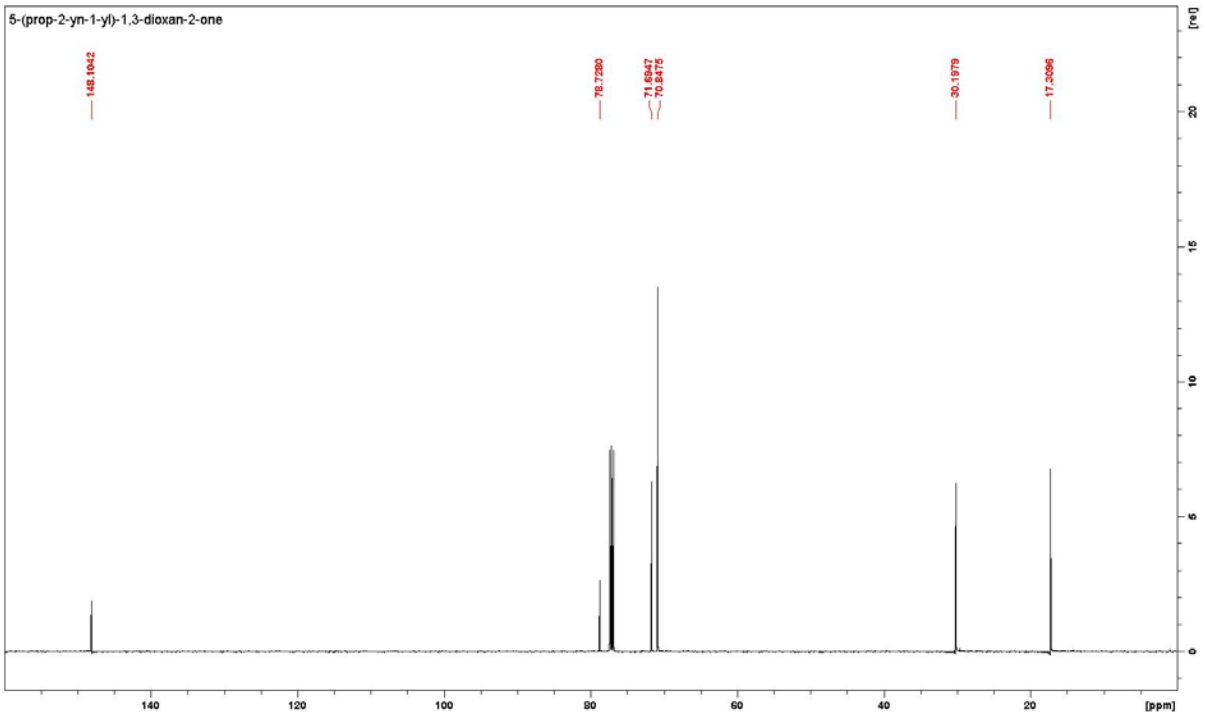
^{1}H spectrum of 1-azidoethylferrocene **(5)**



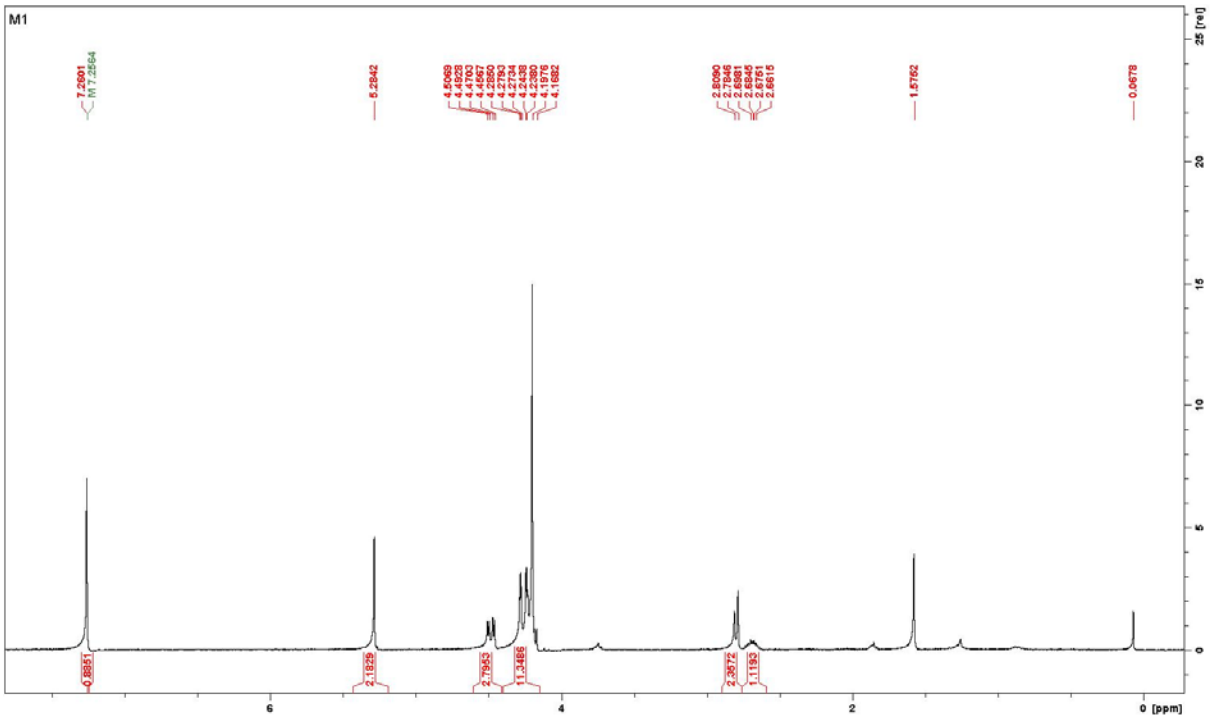
^{1}H spectrum of 5-(prop-2-yn-1-yl)-1,3-dioxan-2-one **(1)**



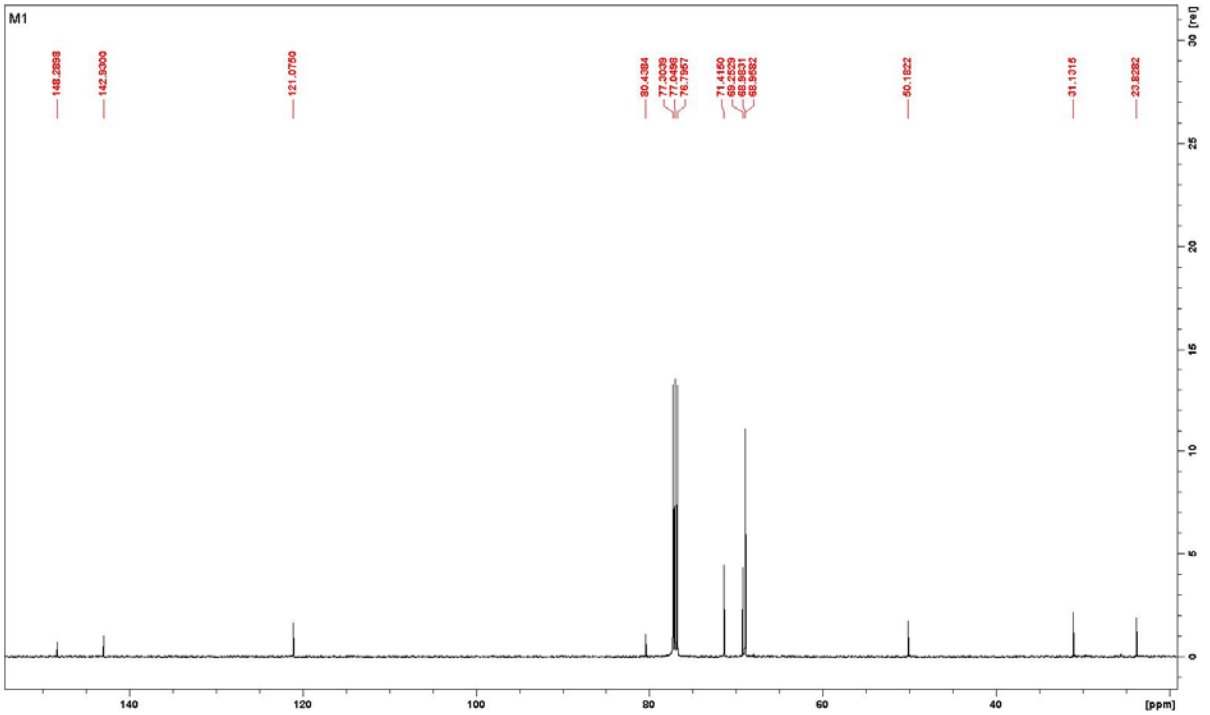
^{13}C spectrum of 5-(prop-2-yn-1-yl)-1,3-dioxan-2-one **(1)**



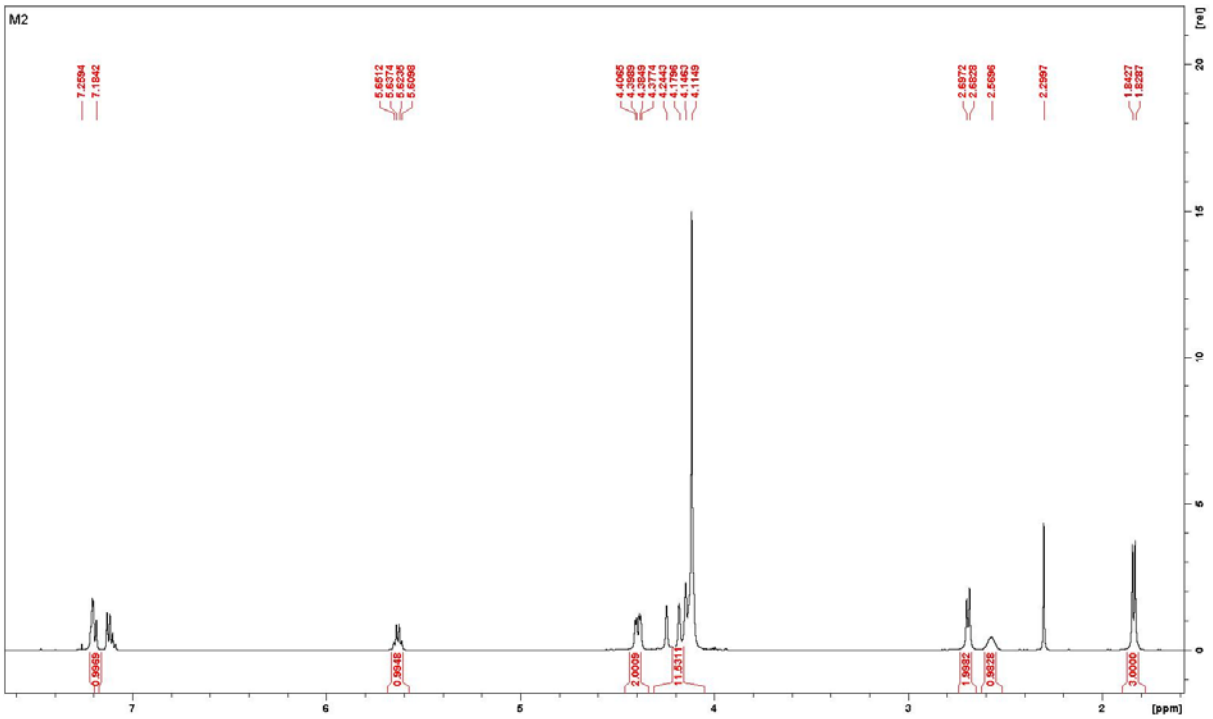
^{1}H spectrum of M_1



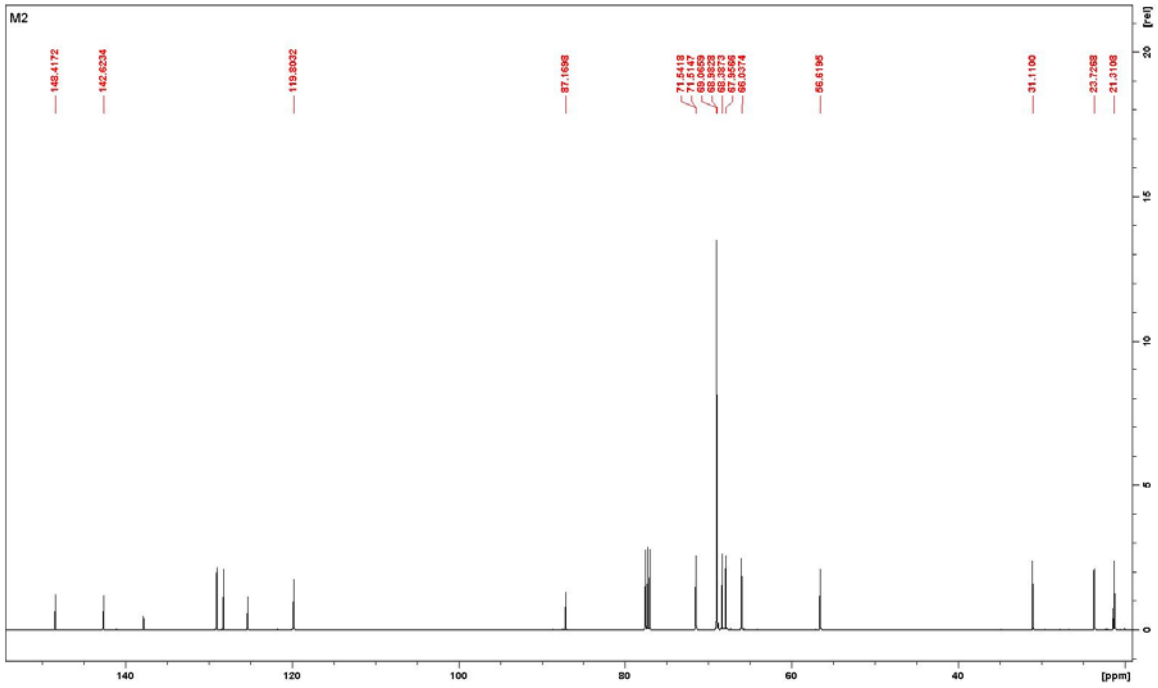
^{13}C spectrum of M_1



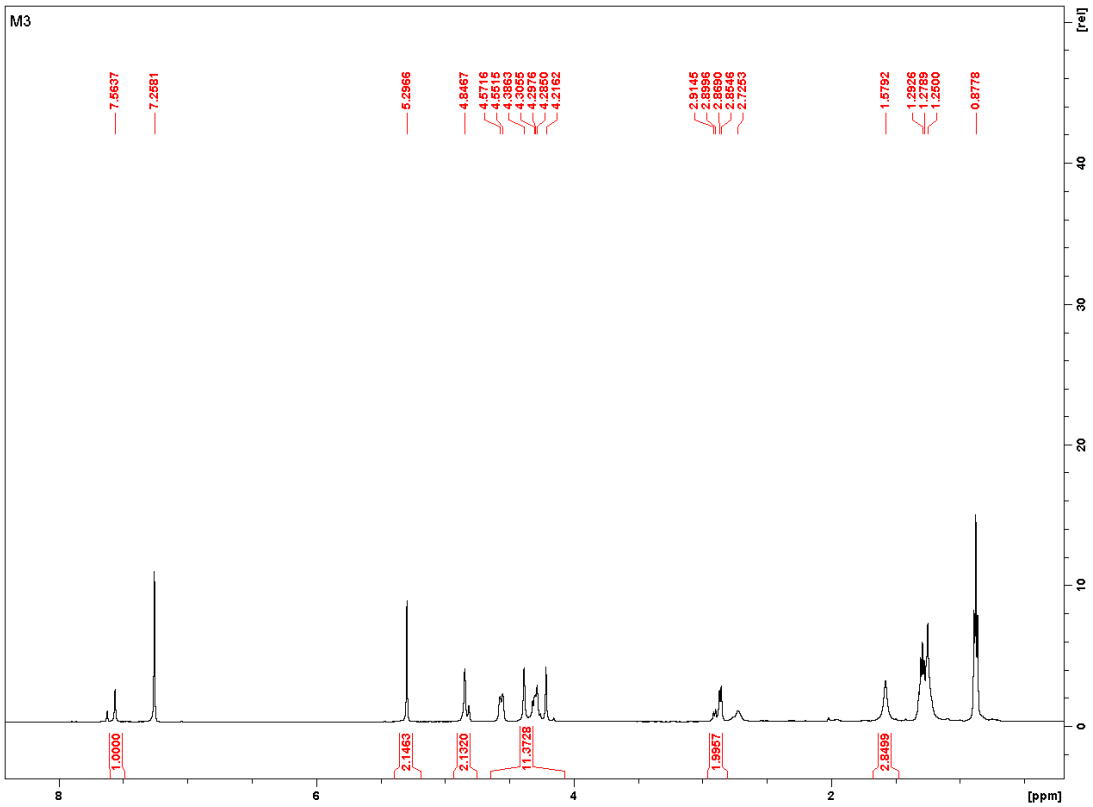
^{1}H spectrum of M_2



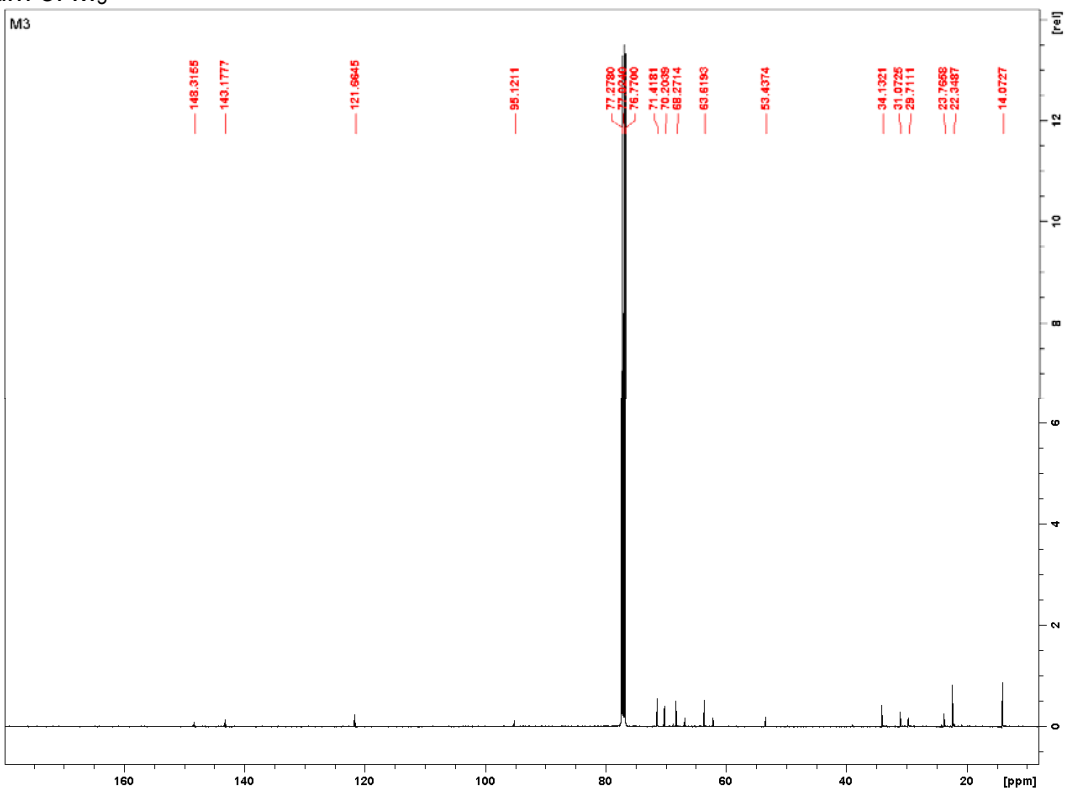
^{13}C spectrum of M_2



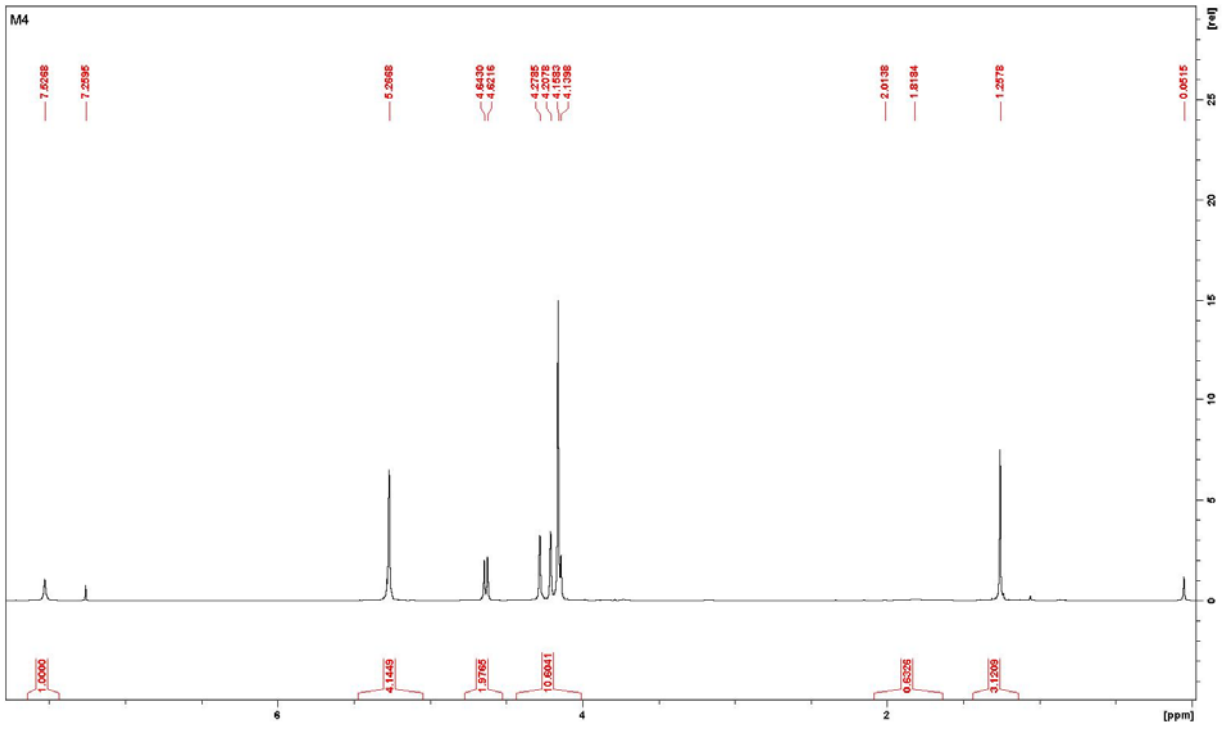
^{1}H spectrum of *M*$_3$



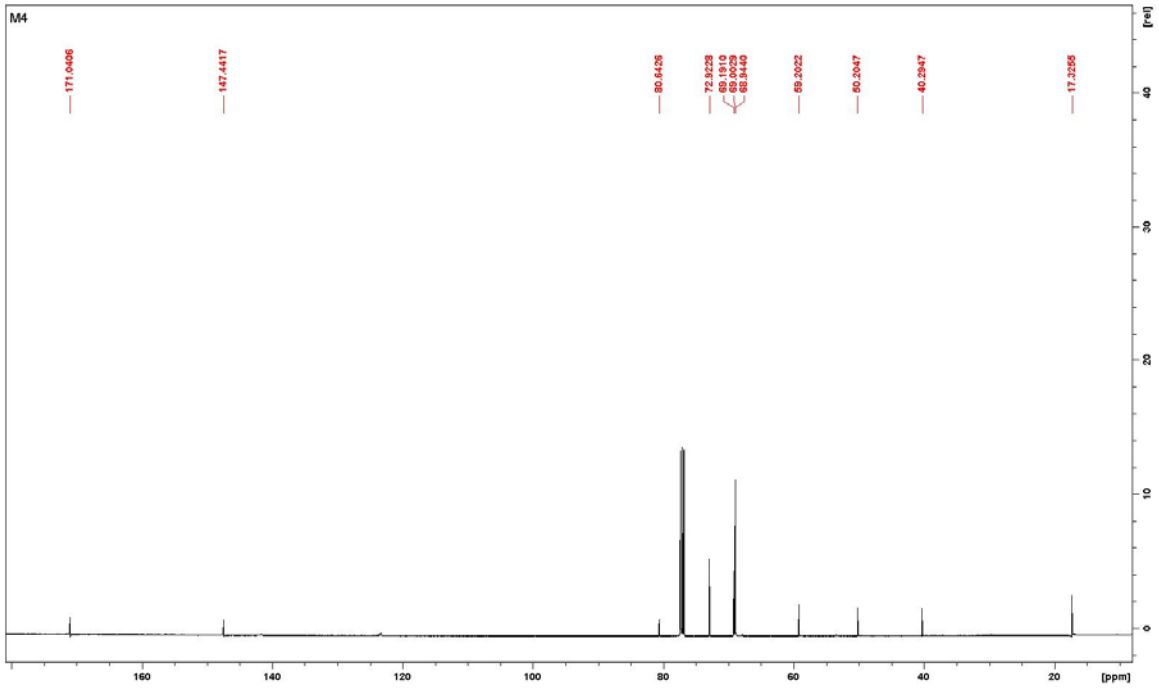
^{13}C spectrum of *M*$_3$



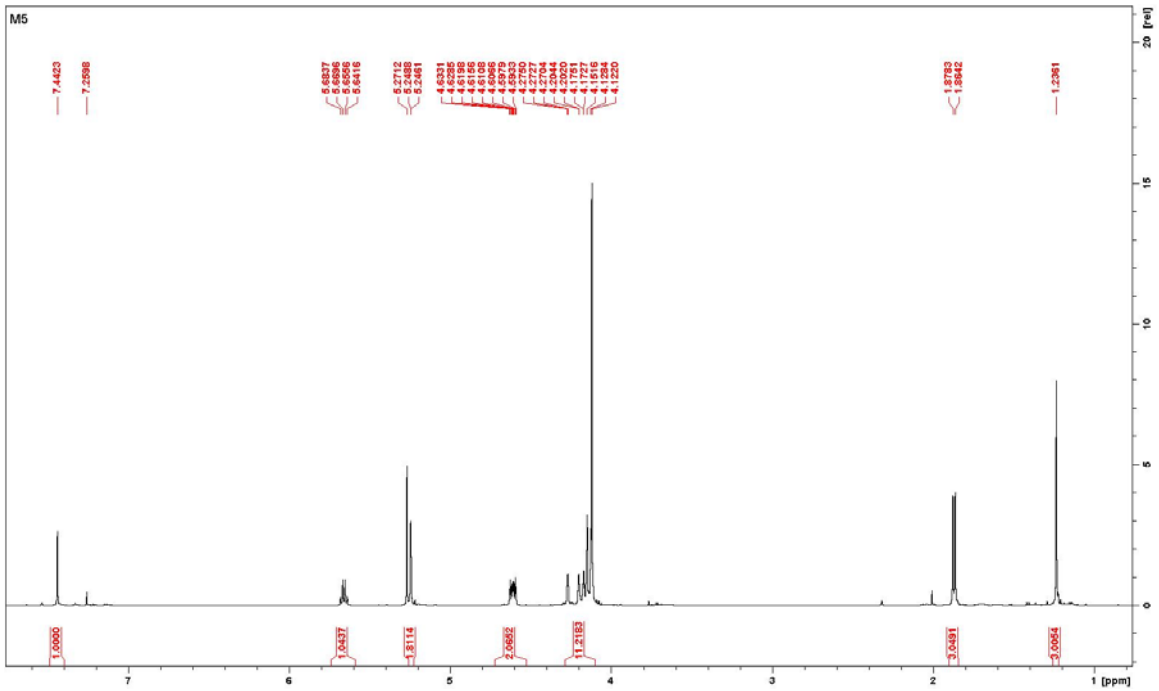
^{1}H spectrum of *M*$_{4}$



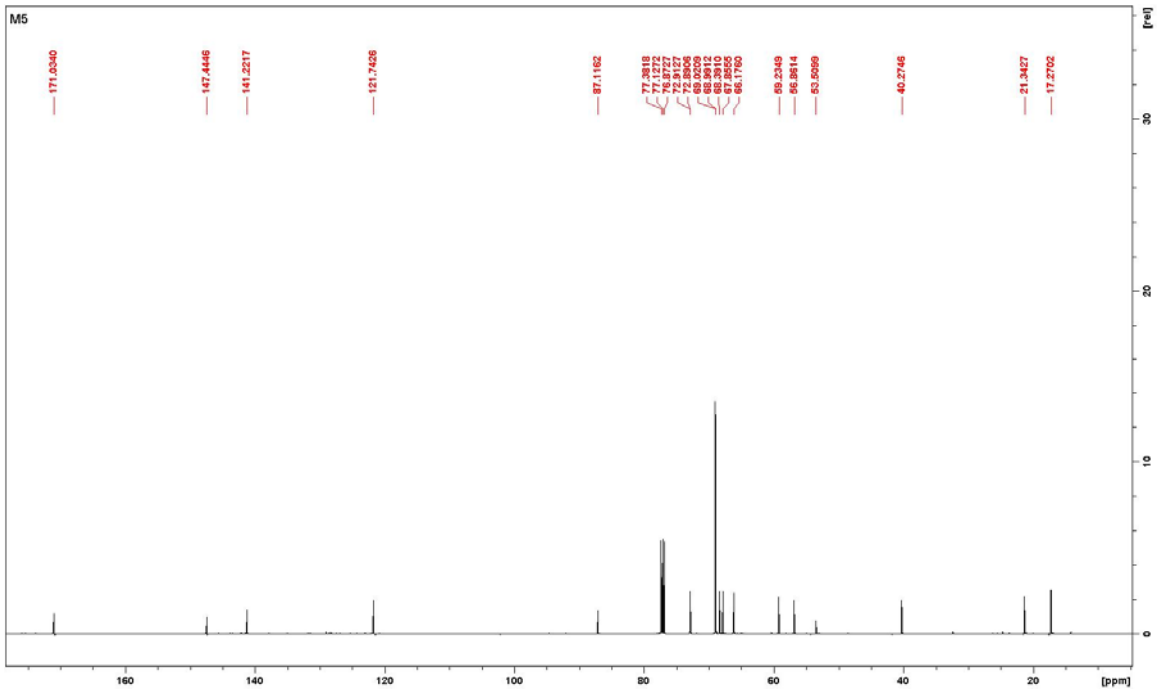
^{13}C spectrum of *M*$_{4}$



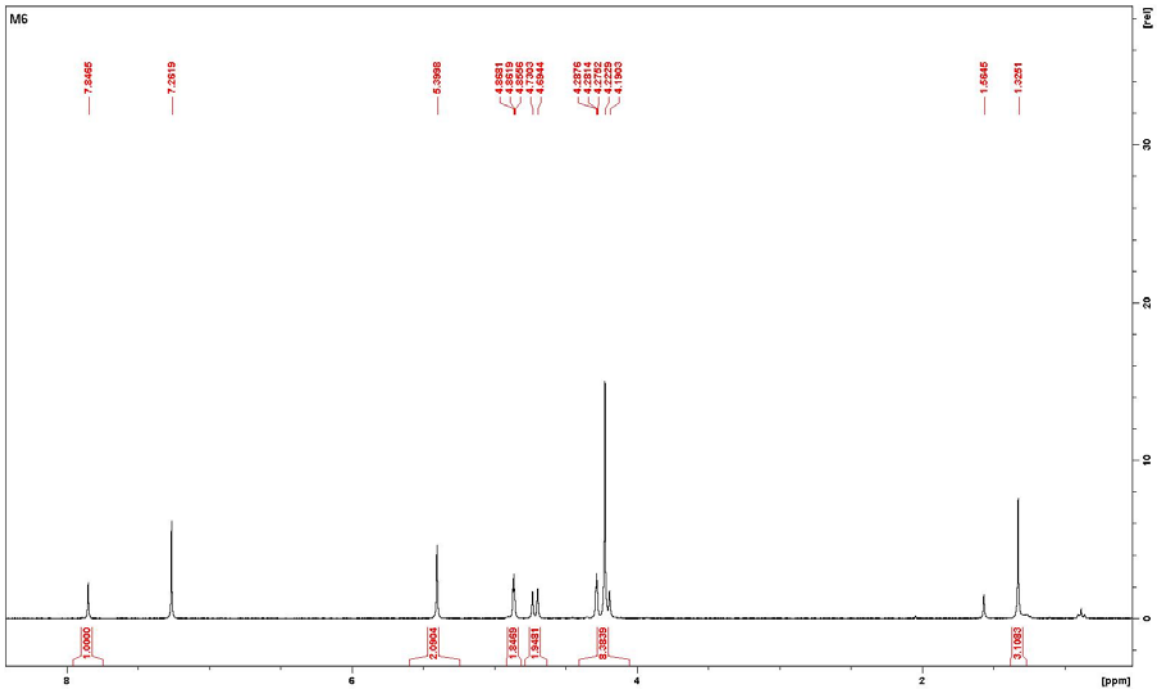
^{1}H spectrum of M_5



^{13}C spectrum of M_5



^{1}H spectrum of *M*$_{6}$



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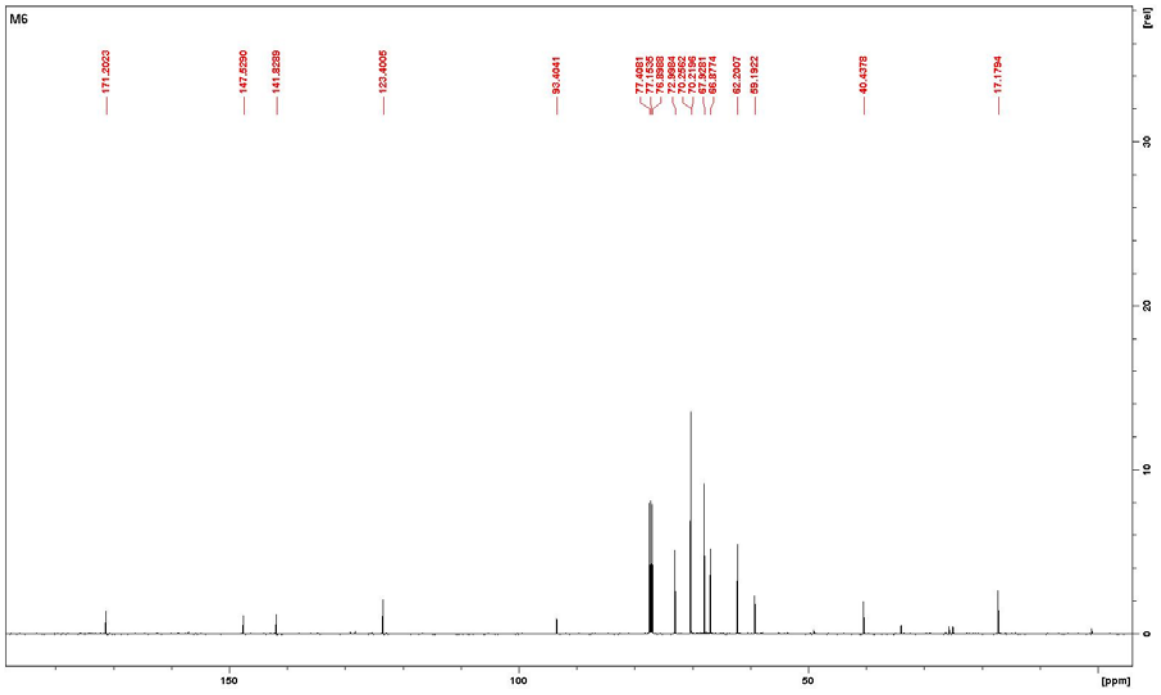
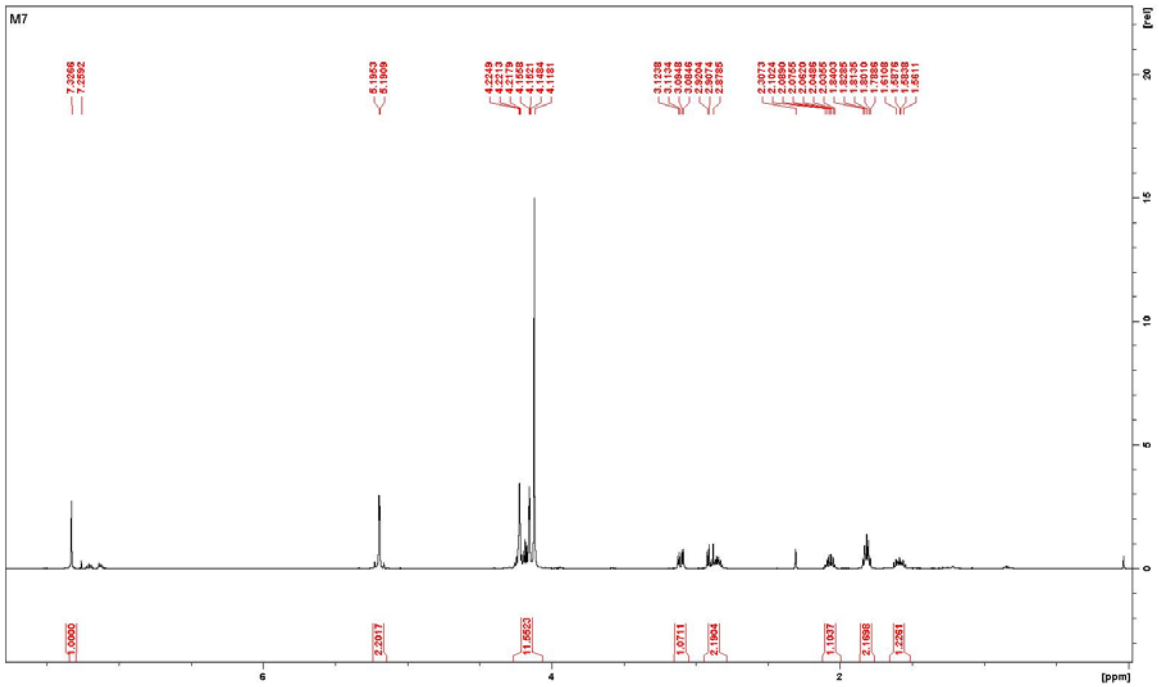
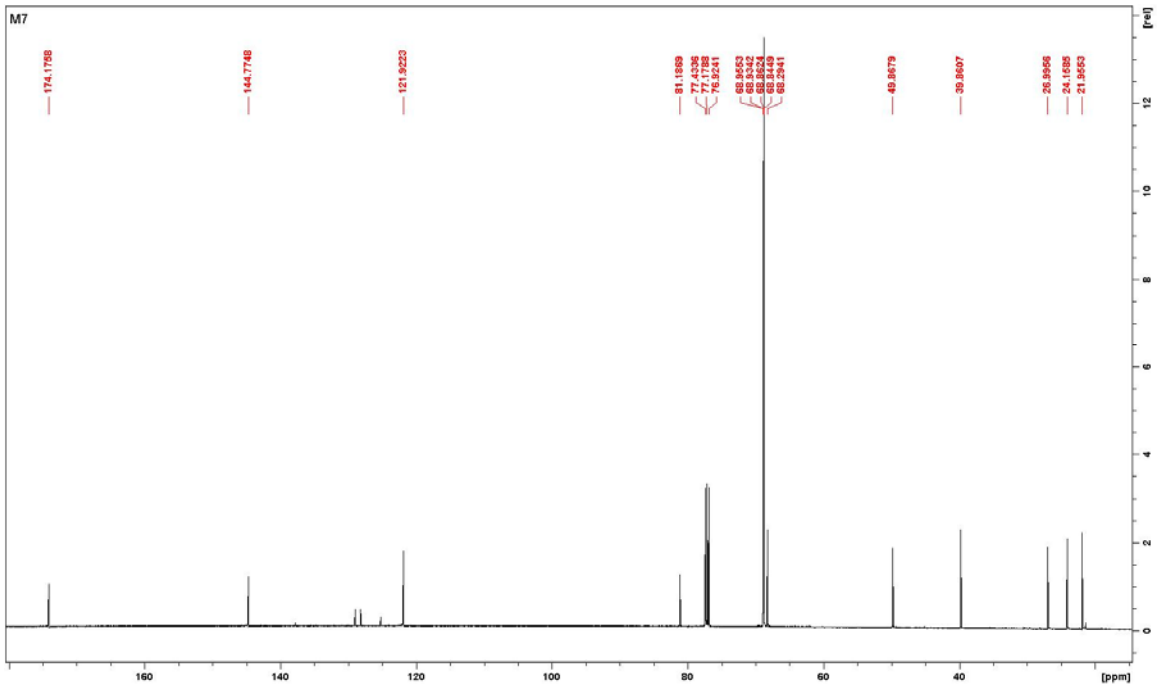


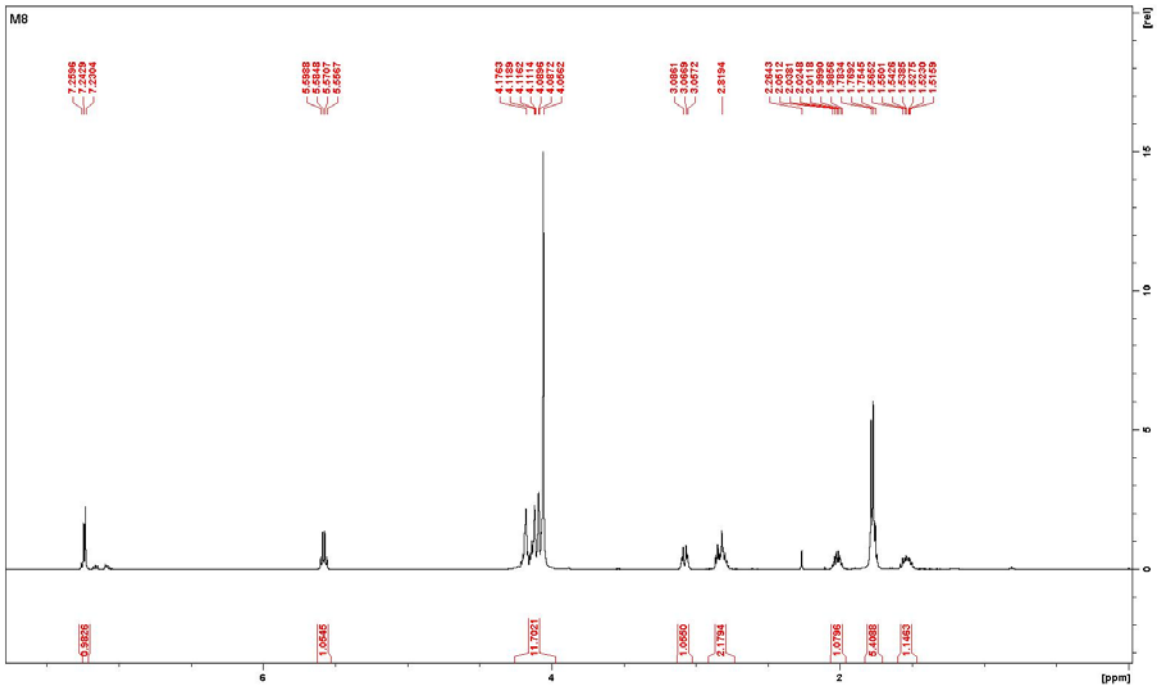
^{1}H spectrum of M_7



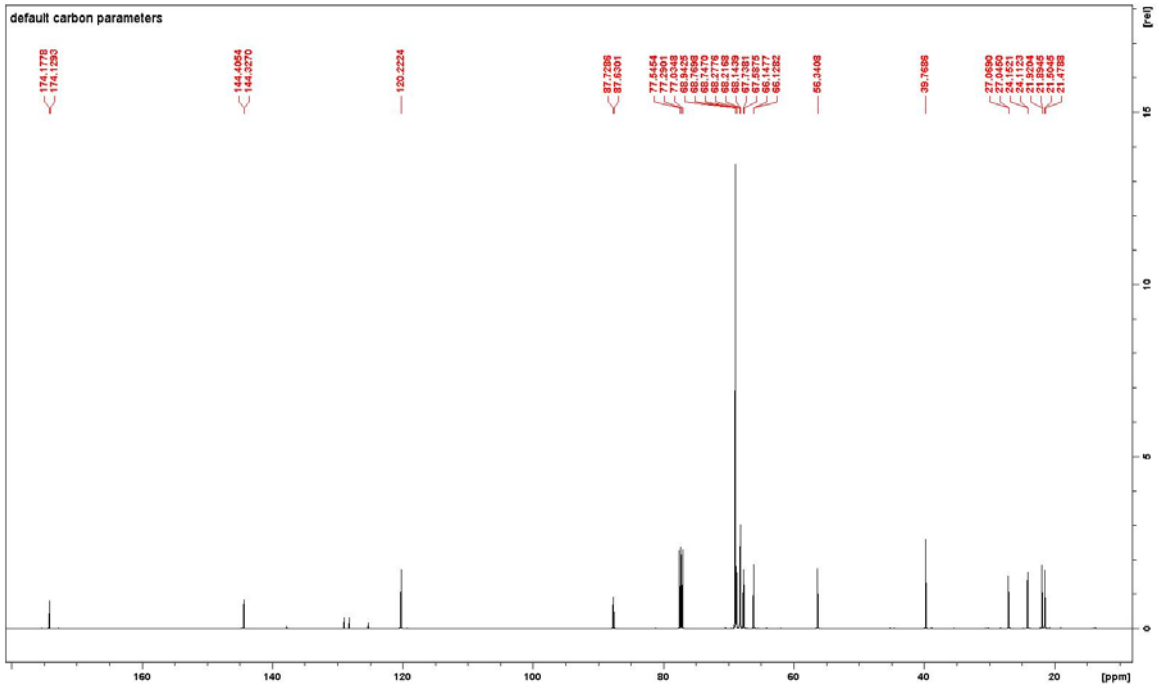
^{13}C spectrum of M_7



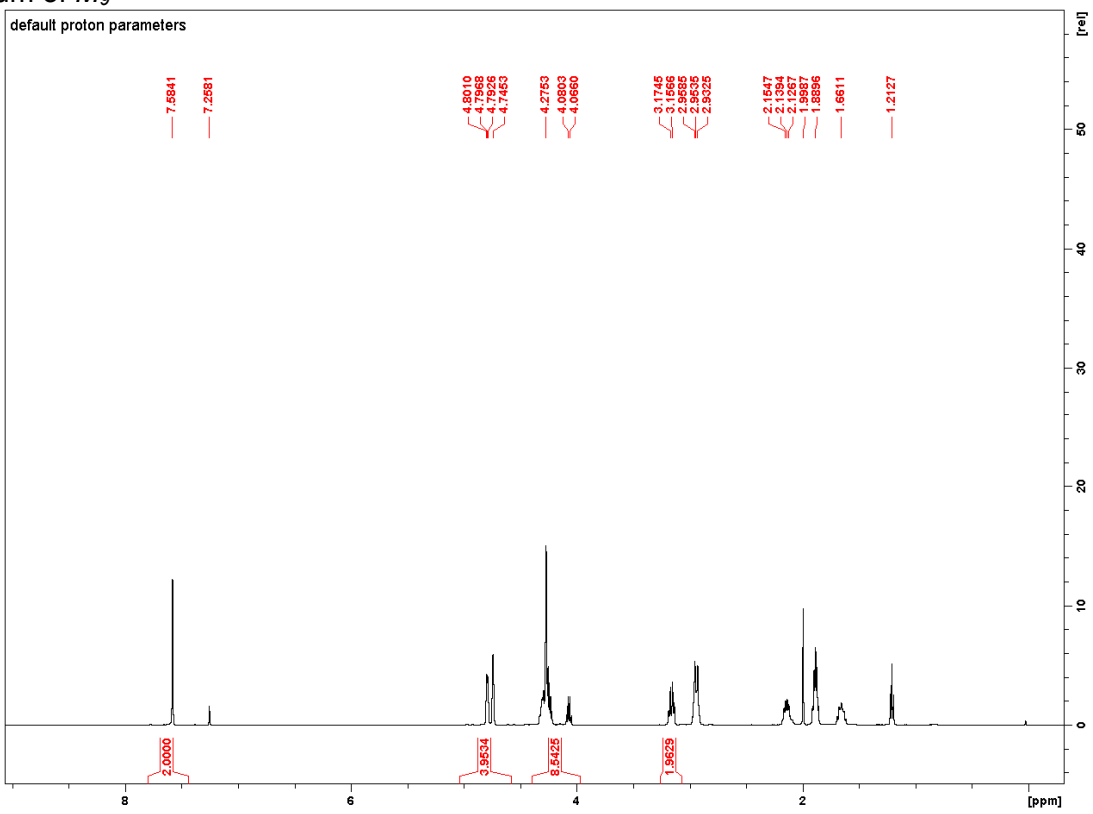
^{1}H spectrum of *M8*



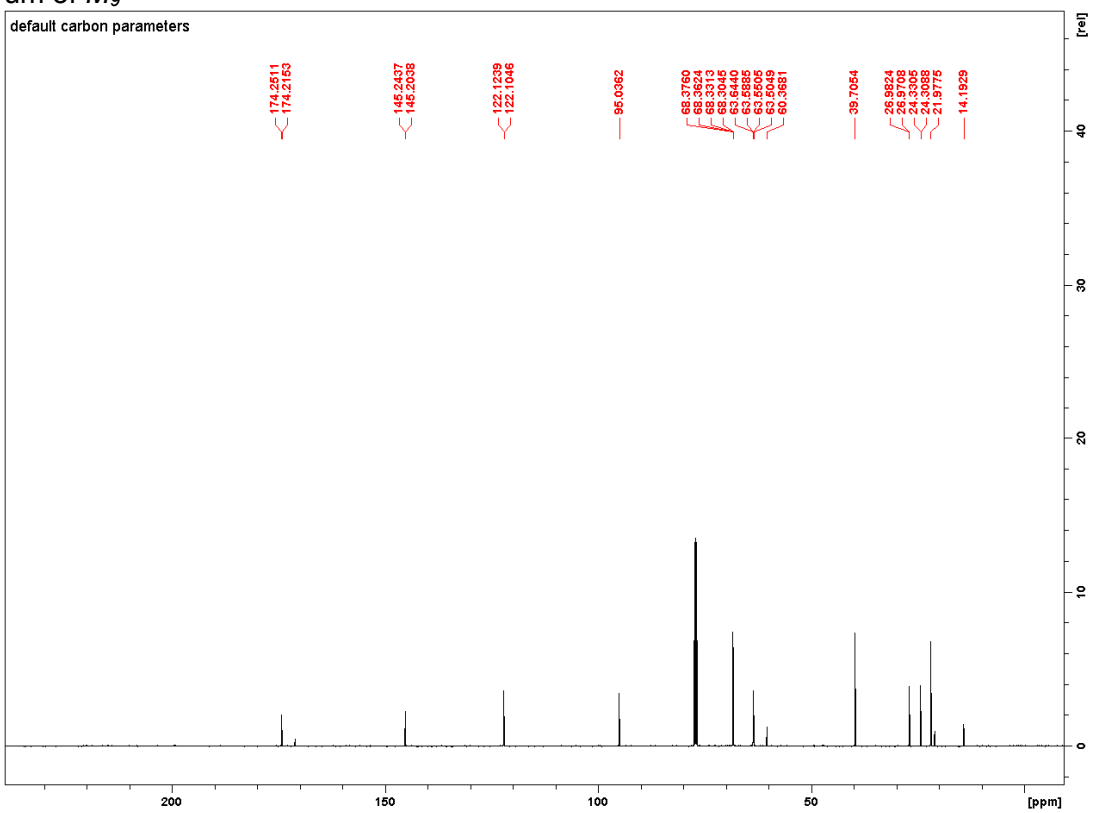
^{13}C spectrum of *M8*



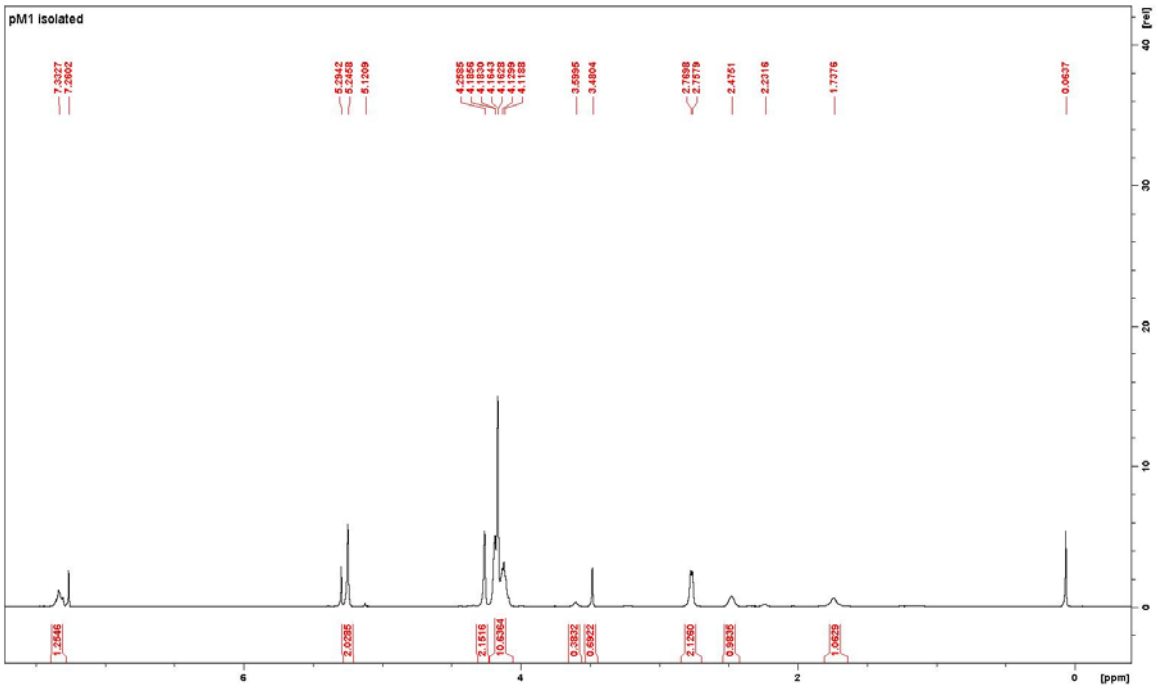
^{1}H spectrum of *M*$_{9}$



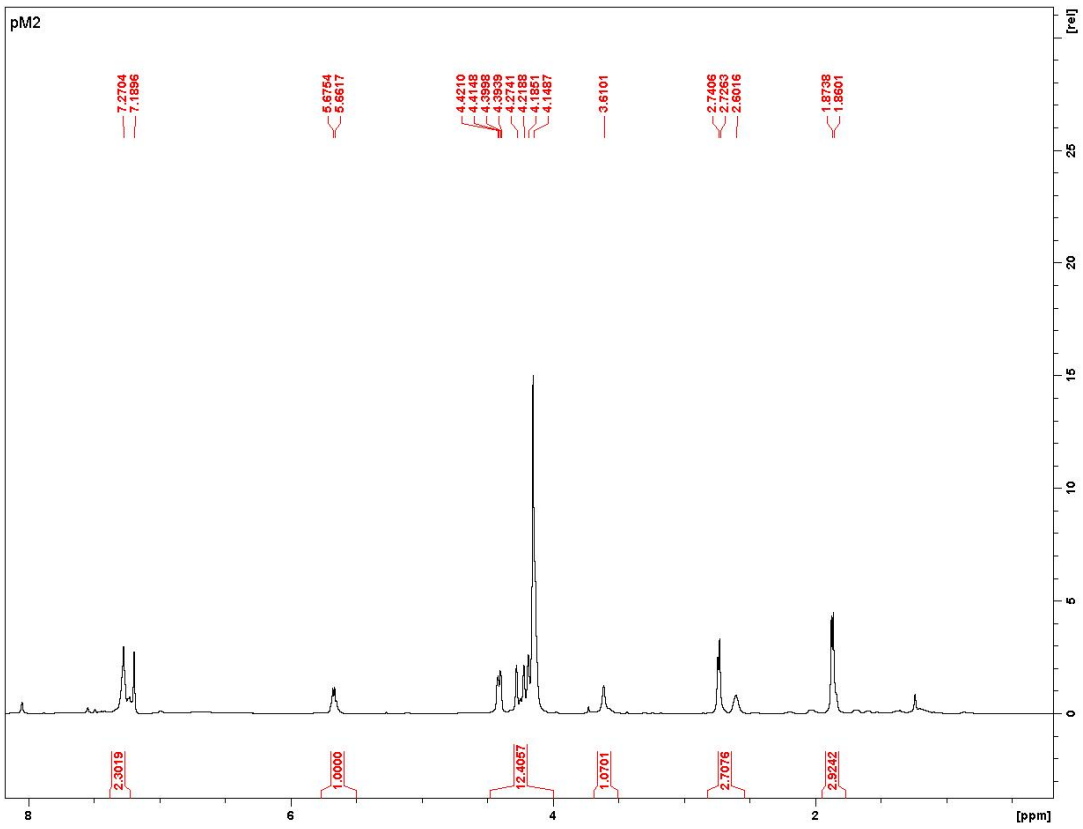
^{13}C spectrum of *M*$_{9}$



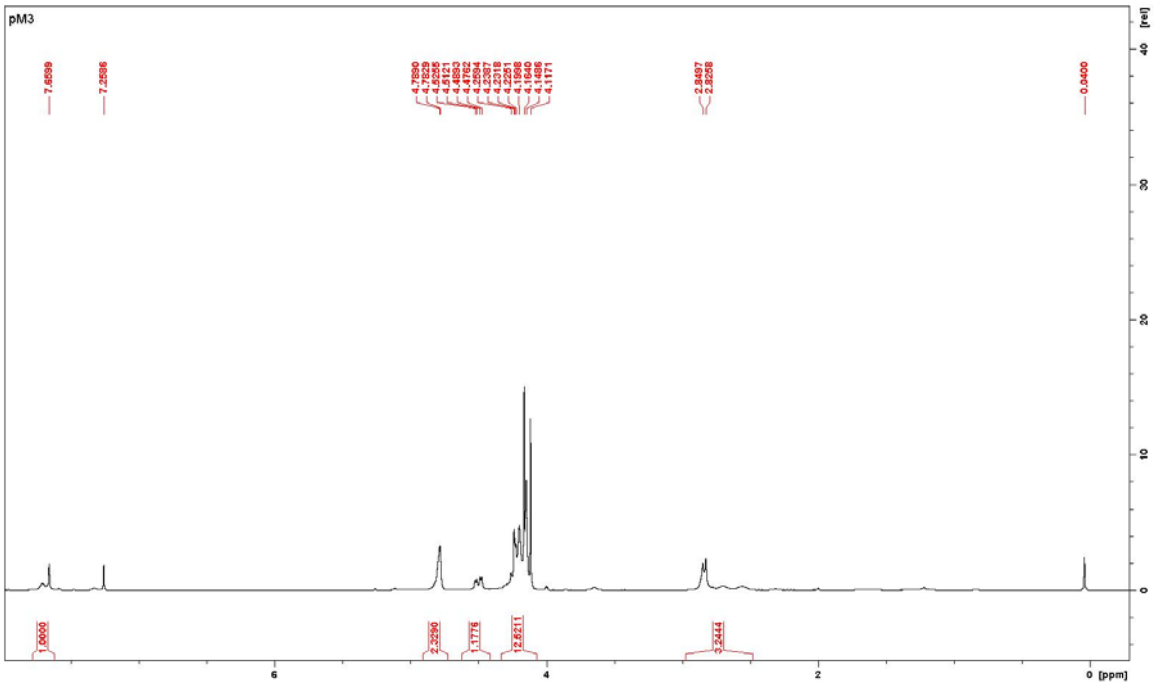
^{1}H spectrum of *pM*$_1$



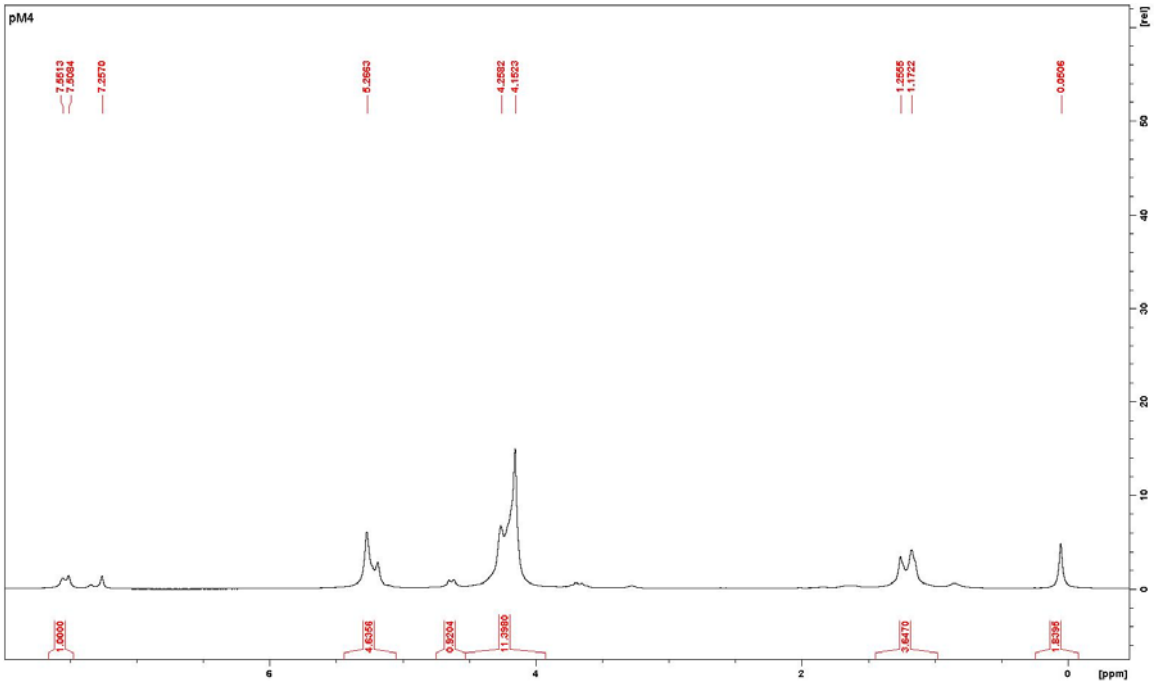
^{1}H spectrum of *pM*$_2$



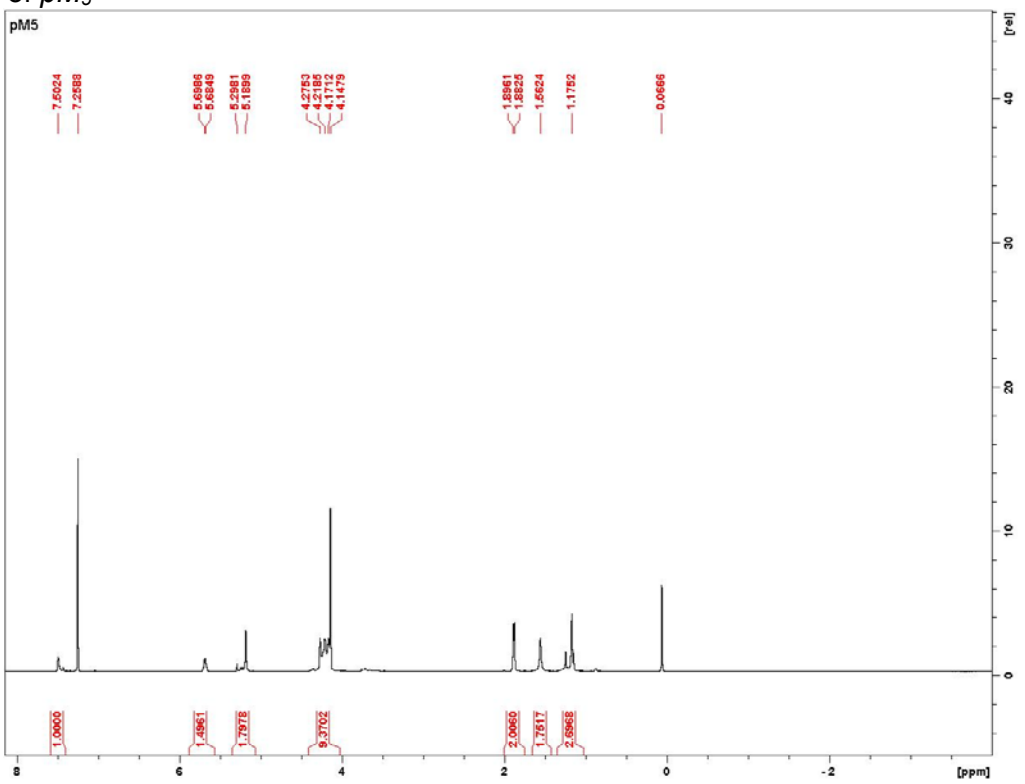
^{1}H spectrum of *pM*$_3$



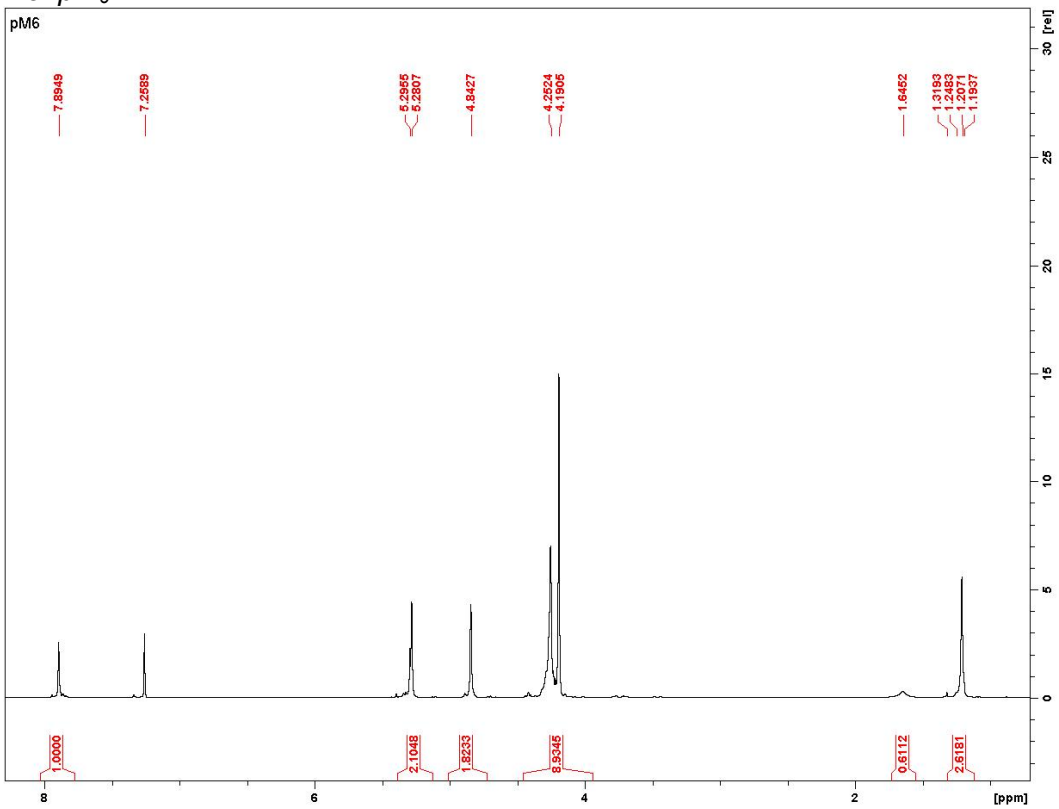
^{1}H spectrum of *pM*$_4$



^{1}H spectrum of *pM*$_5$



^{1}H spectrum of *pM*$_6$



Electrochemistry Data

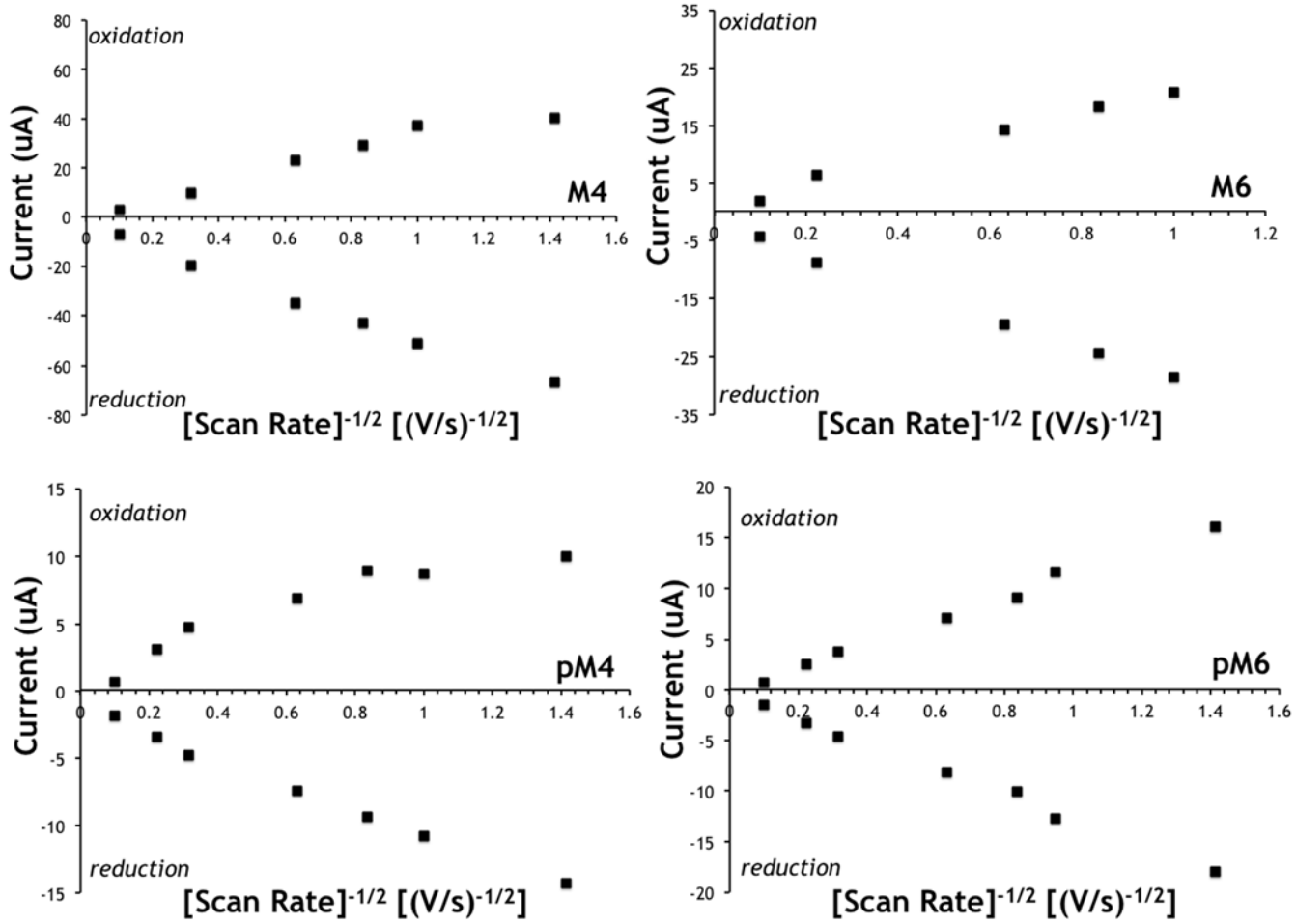


Figure S1. Current as a function of scan rate for cyclic carbonate monomers and polymers.

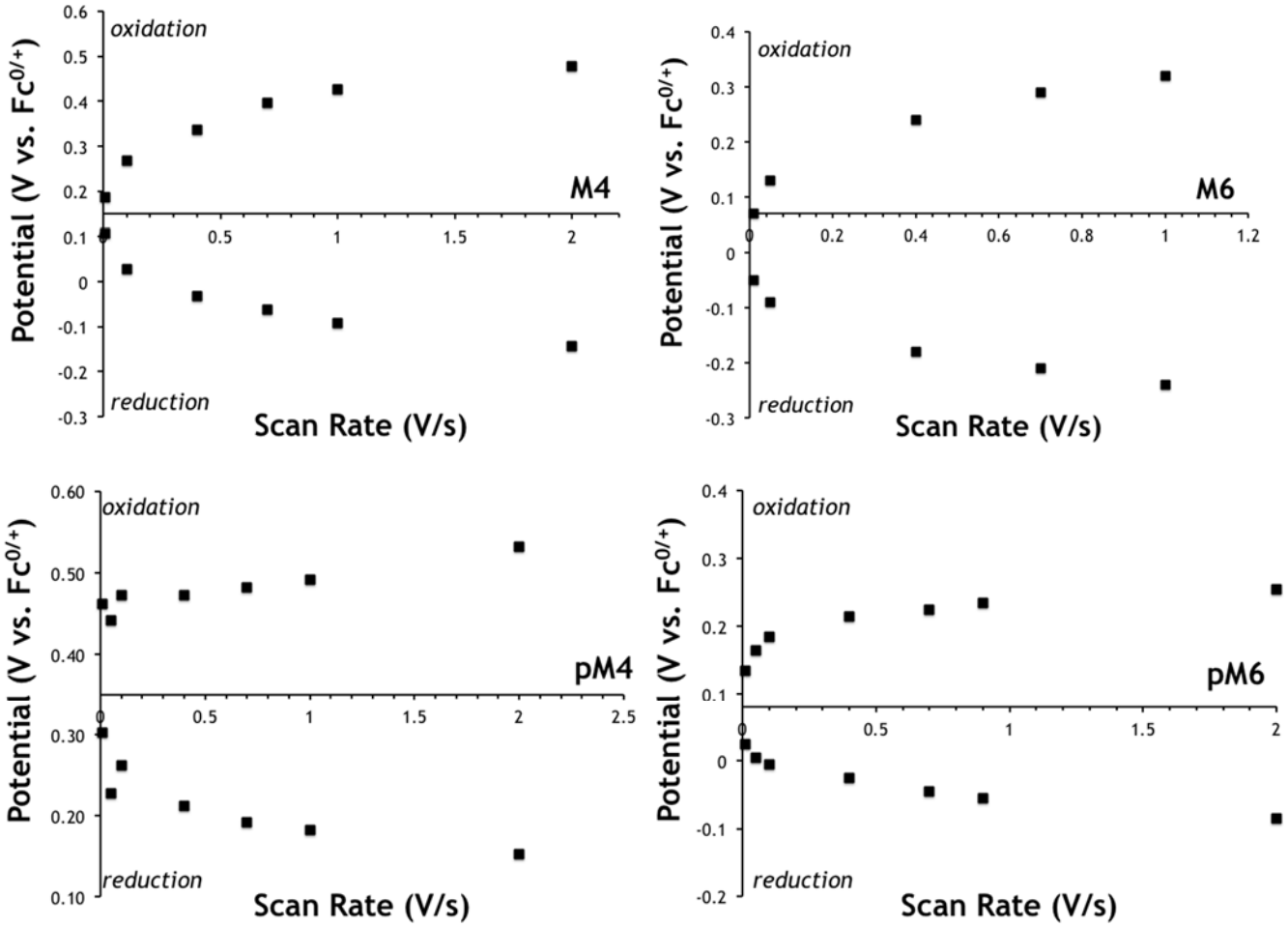


Figure S2. Potential as a function of scan rate for cyclic carbonate monomers and polymers.

Thermogravimetric Analysis

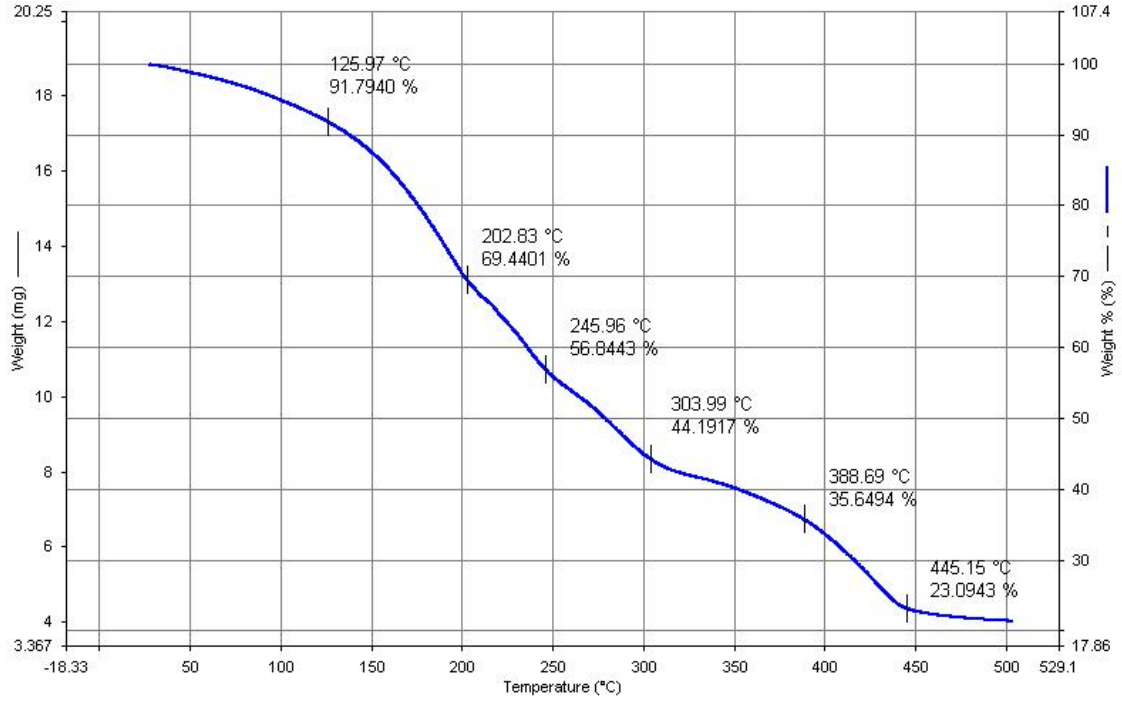


Figure S3: Thermogram for polymer *pM₁*

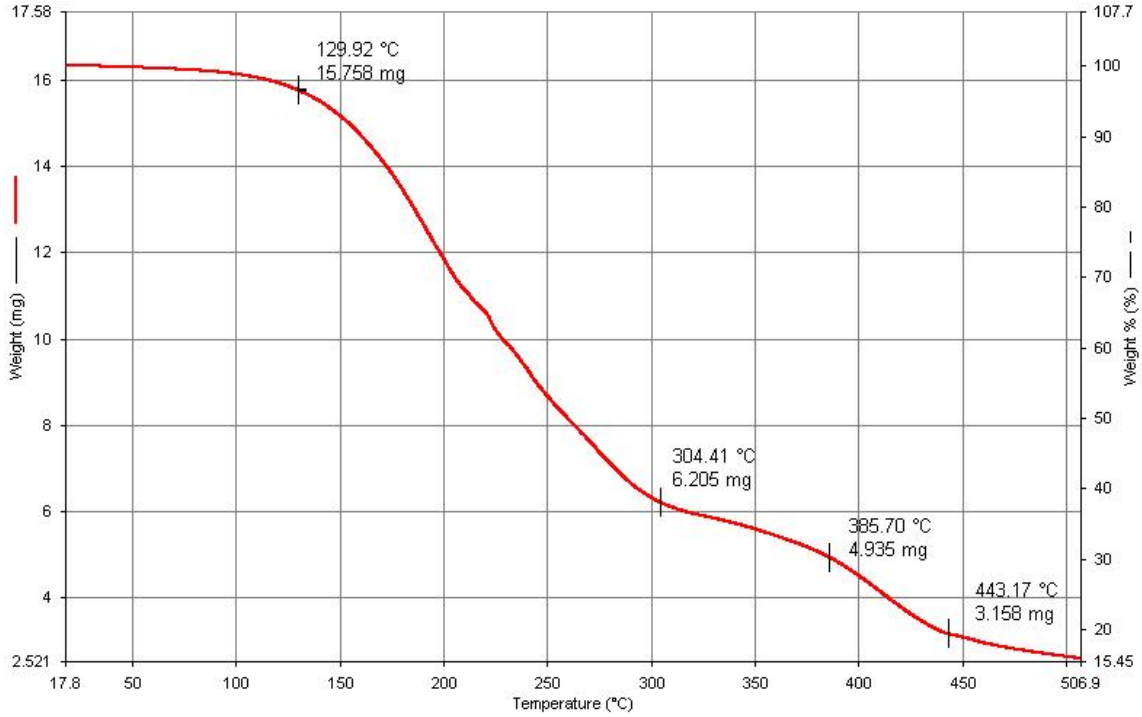


Figure S4: Thermogram for polymer *pM₂*

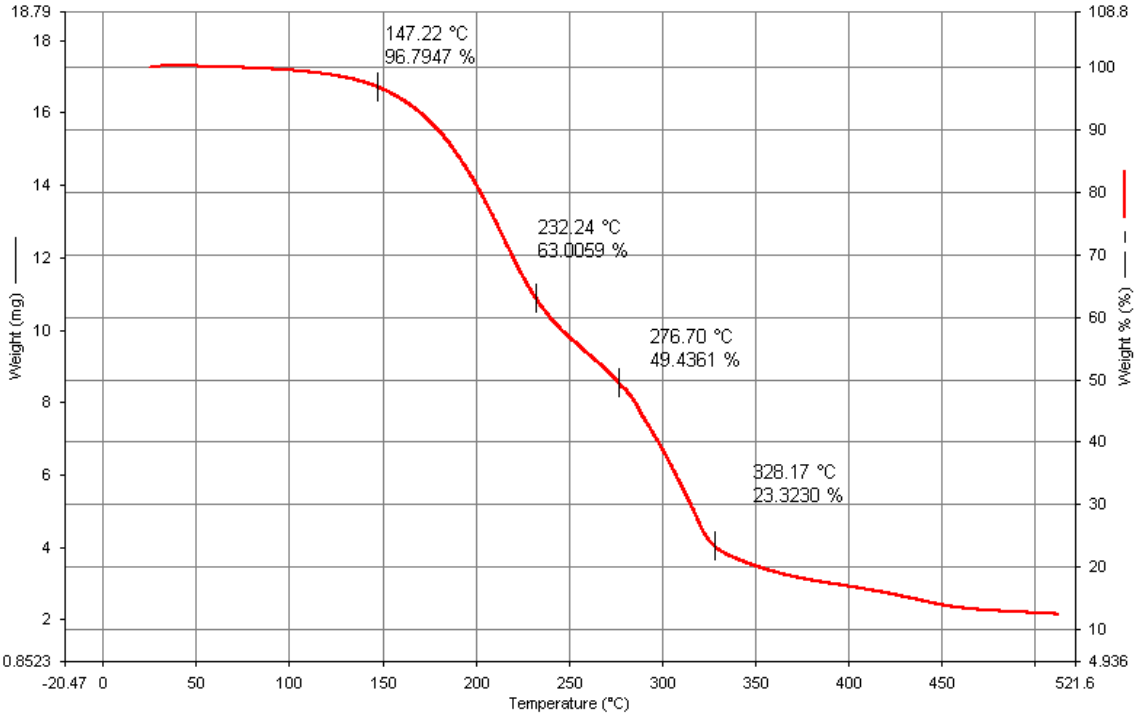


Figure S5: Thermogram for polymer *pM₃*

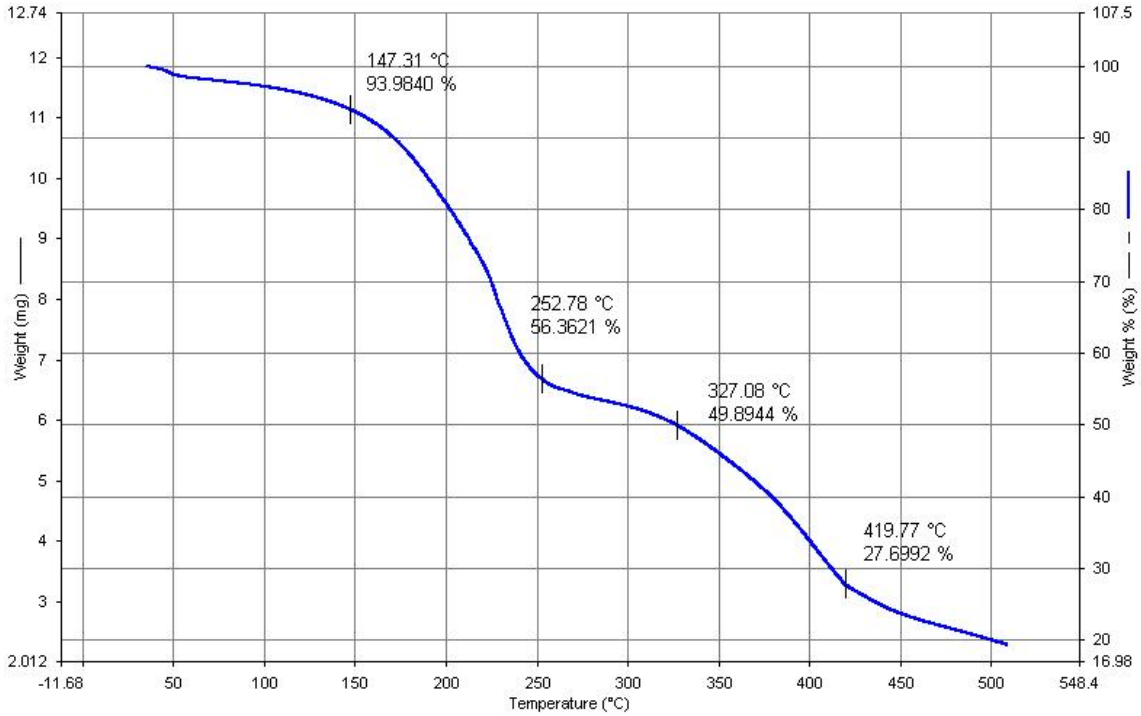


Figure S6: Thermogram for polymer *pM₄*

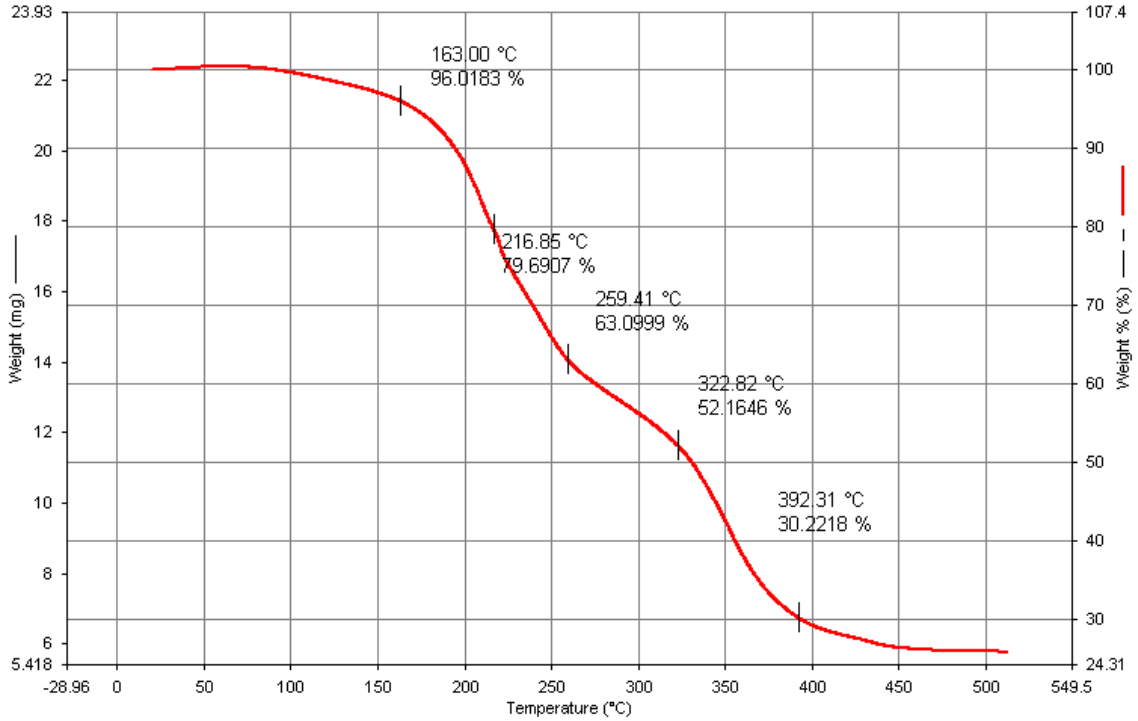


Figure S7: Thermogram for polymer *pM*$_5$

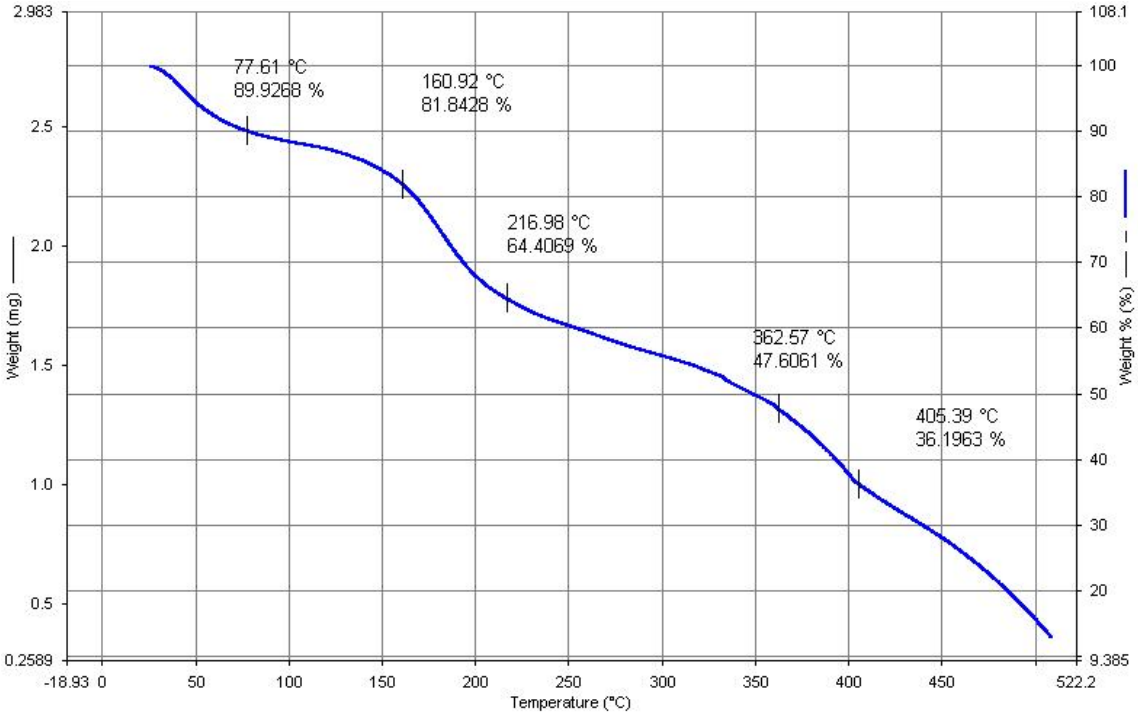


Figure S8: Thermogram for polymer *pM*$_6$

Computational Details

RCM = Ring closed monomer, ROM = Ring opened monomer
All structures were optimized using the B3LYP density functional with the 6-311+G* basis set in Gaussian 09. Vibrational frequency calculations confirmed structures were at minima by absence of imaginary frequencies. Frequency calculation results were also used to collect thermodynamic data for calculations on the change in Gibbs free energy of the ring opening reactions for each monomer.

Table S1. Thermodynamic favorability for ring-opened products as determined by DFT calculations.

Monomer	ΔG (kcal/mol)
M_1	0.70
M_2	0.70
M_3	0.28
M_4	0.44
M_5	0.03
M_6	0.34
M_7	4.21
M_8	3.22
M_9	6.89

Optimized coordinates

M1 RCM

C	-1.91763400	-0.92346100	-0.70211000
C	-1.85063400	0.18967600	0.19434000
N	0.12189200	1.64728300	-0.12574400
C	0.99439300	1.38349300	0.87698700
C	2.23641700	1.64117400	0.33694400
N	2.05297100	2.04317300	-0.95414400
N	0.77977800	2.04553400	-1.23046400
H	0.67570600	1.04112000	1.84793100
C	-2.41650000	-2.04469500	0.01876000
C	-2.65880600	-1.63601200	1.36300900
C	-2.30633000	-0.26071700	1.47490800
Fe	-3.79755700	-0.48663700	0.05663300
C	-5.56015500	-1.17349800	-0.80365400
C	-5.06882800	-0.04893100	-1.52934600
C	-5.00550900	1.05857600	-0.63373400
C	-5.45796100	0.61859700	0.64509800
C	-5.80072300	-0.76091700	0.53968200
H	-6.15684000	-1.38980000	1.34318900
H	-5.51305400	1.22000800	1.54145500
H	-4.66287000	2.05432100	-0.87827700
H	-4.77627500	-0.04253700	-2.56968200
H	-2.60748400	-3.02663800	-0.38996100
H	-5.70250400	-2.16988700	-1.19710100
H	-1.65127100	-0.90470900	-1.74973500
H	-3.06574500	-2.25321900	2.15118600
C	3.59930100	1.52277400	0.94653400
C	4.37383700	0.25994600	0.51801300
C	5.67164000	0.12887200	1.29644100
O	6.45685000	-0.99375500	0.84937300
C	6.41306300	-1.46233100	-0.42212900
O	5.53861700	-0.90401100	-1.28440900
C	4.75674600	0.26615000	-0.95213100
H	3.89797400	0.23576900	-1.61806200
H	3.75408800	-0.62336700	0.71450200
H	5.50451300	-0.04972500	2.35982500
O	7.11381600	-2.37138500	-0.75604700
H	5.34753400	1.15493800	-1.19961200
H	6.28268500	1.03267400	1.19114800
H	4.18219500	2.41296600	0.68530500
H	3.50464200	1.52321000	2.03727800
H	-2.39874000	0.34910900	2.36375700
C	-1.34597500	1.56156900	-0.13792800
H	-1.74107500	2.30234500	0.56195400
H	-1.63180200	1.86567700	-1.14452900

Sum of electronic and thermal Free Energies= **-2350.942233**

Sum of electronic and thermal Enthalpies= **-2350.862720**

M1 ROM

Fe	5.55477200	-1.14814800	0.18306800
C	4.12686800	-1.55054200	1.64304300
C	4.05777400	-0.18546000	1.24594500
C	3.78231400	-0.14207400	-0.15732400
C	3.67463100	-1.49374900	-0.61680000
C	3.89244400	-2.35962400	0.49268300
C	7.19387700	-2.37690800	-0.17416400
C	7.42304400	-1.57888000	0.98483300
C	7.36276000	-0.20856500	0.59599300
C	7.09604900	-0.16002300	-0.80361100
C	6.99135700	-1.50016700	-1.27975700
H	6.77716600	-1.79840100	-2.29618900
H	7.15606900	-3.45650300	-0.20460100
H	7.58919900	-1.94744700	1.98705500
H	7.47745400	0.64311000	1.25124900
H	6.98258400	0.73587000	-1.39764100
H	3.49353400	-1.80115100	-1.63804600
H	4.34967700	-1.91076300	2.63719800
H	4.20604200	0.67367900	1.88521400
H	3.90535600	-3.43972700	0.46203000
N	2.24685000	1.67222100	-0.83910500
N	2.10711500	2.95266200	-0.45883000
C	0.12149900	2.10029400	-0.79289900
N	0.82969400	3.21210300	-0.43146100
H	0.92307700	0.07504300	-1.36115500
C	-1.37425400	2.11062200	-0.85664500
C	-2.08754300	2.09239000	0.51753300
C	-1.55140700	3.16751700	1.48707100
C	-3.59408200	2.27815000	0.33954300
O	-1.46062800	4.45967100	0.90764300
H	-4.10915200	2.20477000	1.29736200
H	-3.81558700	3.24206700	-0.11783100
O	-4.17069300	1.30737900	-0.57272600
H	-1.68565400	3.00980600	-1.39760600
H	-1.72124100	1.26262600	-1.45048900
H	-2.22371600	3.25350900	2.34583200
H	-0.57657500	2.85291600	1.87435700
H	-1.91862500	1.11973600	0.99654600
C	-4.53312500	0.13314000	-0.04848200
C	1.03444200	1.10250800	-1.05636700
H	-0.61953100	4.49754100	0.42223600
O	-5.00695300	-0.63016400	-1.04393800
O	-4.44319000	-0.19090600	1.11220300
C	-5.52206200	-1.93866800	-0.66747800
C	-6.97629100	-1.88786500	-0.27780200
C	-7.35670800	-1.85747700	1.06759100
C	-8.70473200	-1.80848500	1.41901000
C	-9.68559600	-1.78573400	0.42908300
C	-9.31528800	-1.81370000	-0.91540600
C	-7.96835000	-1.86659000	-1.26450900
H	-6.59302400	-1.86074800	1.83783600
H	-8.98848100	-1.78635900	2.46637000
H	-10.73510300	-1.74787500	0.70337400
H	-10.07517700	-1.79813800	-1.69016200
H	-7.68294200	-1.88965200	-2.31242500
H	-5.37537100	-2.53631900	-1.56685700
H	-4.90607500	-2.33867700	0.13703000
C	3.59092600	1.09467600	-0.98248200
H	3.76689600	0.88578100	-2.04093400
H	4.26991600	1.89169900	-0.68080600

Sum of electronic and thermal Free Energies= **-2697.696986**

Sum of electronic and thermal Enthalpies= **-2697.598237**

M2 RCM

C	-1.67643600	-1.05649200	-0.30321200
C	-1.81294100	0.23982200	0.29040900
N	0.16845900	1.56919400	-0.25208500
C	0.99916500	1.25927500	0.77289200
C	2.26081300	1.55659300	0.30235000
N	2.12980100	2.03020300	-0.97018800
N	0.86831900	2.03842900	-1.30060700
H	0.64258500	0.85540800	1.70607600
C	-2.19969900	-2.02173000	0.60204900
C	-2.66500600	-1.33335600	1.76009900
C	-2.42326800	0.05857000	1.57390000
Fe	-3.67069800	-0.64936800	0.07508800
C	-5.23354800	-1.71356700	-0.78685300
C	-4.71820600	-0.76530400	-1.71813900
C	-4.86533300	0.53347500	-1.14974100
C	-5.47255900	0.38858700	0.13261300
C	-5.70015500	-1.00080700	0.35625100
H	-6.12911500	-1.43904700	1.24613400
H	-5.70424500	1.18864700	0.82125200
H	-4.56153800	1.46360500	-1.60913300
H	-4.27517300	-0.99247700	-2.67727400
H	-2.26399400	-3.08612900	0.42674200
H	-5.24528900	-2.78657900	-0.91466100
H	-1.25957100	-1.25978400	-1.27993800
H	-3.14401900	-1.78357700	2.61792200
C	3.59717700	1.39978100	0.96027200
C	4.38469600	0.15882100	0.49279900
C	5.63713200	-0.03890500	1.32865100
O	6.44215500	-1.13276700	0.84509600
C	6.45217200	-1.52522500	-0.45244200
O	5.62421200	-0.90588900	-1.31905100
C	4.84549000	0.25554200	-0.95134600
H	4.02283600	0.28683000	-1.66136600
H	3.74754600	-0.72785500	0.59726000
H	5.41077200	-0.29230100	2.36559100
O	7.15902800	-2.42149700	-0.80767900
H	5.46339400	1.14687400	-1.10686700
H	6.25790200	0.86443200	1.32307100
H	4.19291800	2.30032500	0.77446000
H	3.45698500	1.33894000	2.04446600
H	-2.69105800	0.84070500	2.26947200
C	-1.31074200	1.52362100	-0.31978800
H	-1.51332100	1.51548400	-1.39254300
C	-1.89863400	2.79869700	0.29080100
H	-1.50230100	3.67654600	-0.22216800

H	-1.65160300	2.88656800	1.35145200
H	-2.98549800	2.79901500	0.19162000

Sum of electronic and thermal Free Energies= **-2390.237443**

Sum of electronic and thermal Enthalpies= **-2390.156139**

M2 ROM

Fe	-5.35257300	-1.26579600	-0.25860400
C	-3.69223900	-1.88925400	-1.34396400
C	-3.66704100	-0.47763600	-1.16698900
C	-3.64640900	-0.19938000	0.23726400
C	-3.65554100	-1.45748400	0.92138200
C	-3.68931900	-2.49541700	-0.05408700
C	-7.05096500	-2.44357500	-0.02873500
C	-7.03964500	-1.84644500	-1.32325200
C	-7.03217000	-0.43059000	-1.15632100
C	-7.03821800	-0.15310000	0.24161100
C	-7.04952700	-1.39711000	0.93900600
H	-7.04186200	-1.52560400	2.01210300
H	-7.03837500	-3.50344700	0.18192000
H	-7.01578400	-2.37429700	-2.26602000
H	-7.00473200	0.30247600	-1.94978000
H	-7.02675700	0.82933800	0.69254200
H	-3.66904300	-1.60192700	1.99212100
H	-3.73944900	-2.40887100	-2.29036100
H	-3.67614300	0.26347000	-1.95413200
H	-3.73349400	-3.55553500	0.15102800
N	-2.18398700	1.72171300	0.64994700
N	-2.02728400	2.99323300	0.24944200
C	-0.05403800	2.12993400	0.62377800
N	-0.74642300	3.24076000	0.23179500
H	-0.88152100	0.12295400	1.21949800
C	1.44109900	2.12682900	0.70553100
C	2.17373700	2.07520200	-0.65758000
C	1.65499000	3.12948100	-1.65866900
C	3.67799400	2.26196300	-0.46252800
O	1.56418300	4.43541700	-1.11116500
H	4.20695200	2.16191000	-1.41029800
H	3.89480900	3.23738500	-0.02788800
O	4.23878000	1.31497400	0.48406400
H	1.75418900	3.03315400	1.23353500
H	1.77179900	1.28745900	1.32059600
H	2.33771100	3.19182800	-2.51134500
H	0.68305400	2.81064300	-2.04995100
H	2.00890300	1.09226500	-1.11670900
C	4.61074900	0.12801600	-0.00305100
C	-0.97979900	1.14596900	0.89623100
H	0.71807100	4.48848800	-0.63553300
O	5.06837400	-0.60840400	1.01997500
O	4.54083200	-0.22645900	-1.15626700
C	5.59118900	-1.92552400	0.68716700
C	7.05261800	-1.88283300	0.32422500
C	7.45791400	-1.87042300	-1.01421500
C	8.81220400	-1.82648100	-1.34128000
C	9.77470600	-1.79137600	-0.33382100
C	9.37962200	-1.80213500	1.00379900
C	8.02636400	-1.84957100	1.32866600
H	6.70854600	-1.88371600	-1.79824900
H	9.11521100	-1.81816400	-2.38343700
H	10.82913400	-1.75747600	-0.58910400
H	10.12509000	-1.77716700	1.79221200
H	7.72177000	-1.85900100	2.37139700
H	5.42782800	-2.50028400	1.59849800
H	4.99084700	-2.34657300	-0.11843200
C	-3.54904600	1.17976800	0.83929000
H	-4.17198900	1.86736600	0.26411700
C	-3.94167100	1.26747100	2.31677900
H	-3.86123800	2.29900000	2.66389500
H	-3.29405900	0.64931700	2.94293800
H	-4.97141700	0.93375100	2.45597100

Sum of electronic and thermal Free Energies= **-2736.992208**

Sum of electronic and thermal Enthalpies= **-2736.891392**

M3 RCM

C	-2.51689700	1.68082300	0.79600500
C	-1.64279200	0.99510300	-0.09653600
N	-0.41231200	0.40329900	0.27304100
C	0.44334900	-0.34054400	-0.47751100
C	1.47070600	-0.66548400	0.37966800
N	1.19199500	-0.10799500	1.59461100
N	0.06229200	0.53381200	1.53282600
H	0.25560500	-0.57749300	-1.51119600
C	-3.59042200	2.19969600	0.01784400
C	-3.38197600	1.82941300	-1.34178800
C	-2.17307900	1.07784000	-1.41966100
Fe	-3.52195200	0.12986500	-0.16007100
C	-5.33304500	-0.64368000	0.50460900
C	-4.26287300	-1.15063500	1.29877800
C	-3.37056500	-1.85393100	0.43828000
C	-3.88939000	-1.78169600	-0.88814500
C	-5.10232400	-1.03299300	-0.84730300
H	-5.72371000	-0.78330200	-1.69549000
H	-3.43465700	-2.20377600	-1.77331600
H	-2.44923700	-2.33367900	0.73746400
H	-4.13492100	-1.00452200	2.36174800
H	-4.43152000	2.75763600	0.40281400
H	-6.16013000	-0.04621600	0.86076500
H	-2.37343600	1.77590900	1.86055000
H	-4.03219800	2.05886400	-2.17338500
C	2.72310600	-1.44953500	0.13807200
C	3.94436600	-0.58755500	-0.24029500
C	5.13577900	-1.46104700	-0.59272000
O	6.31889700	-0.68093400	-0.85398900
C	6.54401500	0.52994700	-0.28727800
O	5.58224400	1.06297800	0.49593200
C	4.40185100	0.32572600	0.88429700
H	3.66673300	1.08308700	1.14700800
H	3.69061200	0.03121400	-1.10974500
H	4.97362800	-2.04088800	-1.50274000

O	7.55876100	1.12157800	-0.50664500
H	4.63568900	-0.24941500	1.78684800
H	5.36339300	-2.15745400	0.22238700
H	2.94923600	-2.02612600	1.04125100
H	2.54717900	-2.17777000	-0.66047200
H	-1.74339500	0.65597300	-2.31627700

Sum of electronic and thermal Free Energies= **-2311.642805**

Sum of electronic and thermal Enthalpies= **-2311.566753**

M3 ROM

Fe	-5.59292200	-0.75679500	-0.01130000
C	-5.94555700	-0.65520500	-2.05647800
C	-5.02212000	0.35854000	-1.67187400
C	-3.89497800	-0.29594300	-1.09508900
C	-4.11777700	-1.70648300	-1.11225200
C	-5.39031000	-1.92324900	-1.71791600
C	-6.90388100	-1.69156800	1.30402900
C	-7.37788100	-0.38505400	0.98584700
C	-6.38453000	0.55496000	1.38974300
C	-5.29741500	-0.16986200	1.95842800
C	-5.61798000	-1.55812500	1.90619800
H	-4.98731000	-2.36920600	2.24197400
H	-7.41808000	-2.62063900	1.10243900
H	-8.31416500	-0.15050200	0.49970700
H	-6.42979300	1.62650100	1.25884000
H	-4.37873000	0.25952500	2.33219800
H	-3.45447300	-2.46775200	-0.72863900
H	-6.91237900	-0.48521200	-2.50758000
H	-5.13830600	1.42592400	-1.77663900
H	-5.85871600	-2.88518600	-1.86726900
N	-2.72288300	0.35024900	-0.63516500
N	-2.73517100	1.65994200	-0.31179300
C	-0.71258100	0.87975800	-0.00608200
N	-1.52937100	1.97445500	0.06485600
H	-1.24241100	-1.19903500	-0.67730200
C	0.73107200	0.95097000	0.38328200
C	1.65145300	1.67447200	-0.63040100
C	1.09960400	3.04560900	-1.07421500
C	3.04847500	1.84846900	-0.04801000
O	0.70405800	3.87626000	0.00548900
H	3.72436800	2.31250600	-0.76943200
H	3.03221800	2.46640200	0.85168300
O	3.56451100	0.53494800	0.28634400
H	0.79743500	1.47370900	1.34290100
H	1.11657400	-0.05587700	0.55202900
H	1.87284000	3.59087500	-1.62362800
H	0.26353900	2.89225500	-1.76477000
H	1.73542200	1.05537700	-1.53384000
C	4.78108600	0.50830300	0.83941900
C	-1.47679200	-0.17046800	-0.46106500
H	-0.19886700	3.61739100	0.25328300
O	5.08606100	-0.77117500	1.10026200
O	5.47495600	1.46850100	1.07096900
C	6.40641000	-1.01868200	1.66304100
C	7.45394400	-1.20247600	0.59608900
C	8.27093400	-0.13698600	0.20376100
C	9.23409700	-0.31422700	-0.78807100
C	9.38882700	-1.55732300	-1.39950600
C	8.57815300	-2.62514700	-1.01506600
C	7.61833300	-2.44702300	-0.02181300
H	8.14111800	0.83352800	0.67029600
H	9.86365300	0.51914700	-1.08318200
H	10.14009000	-1.69506500	-2.17074500
H	8.69717300	-3.59618300	-1.48515400
H	6.99034500	-3.28139200	0.27769200
H	6.65790200	-0.19933300	2.33523000
H	6.26831300	-1.93143000	2.24191100

Sum of electronic and thermal Free Energies= **-2658.398232**

Sum of electronic and thermal Enthalpies= **-2658.303547**

M4 RCM

C	-3.59749400	-1.06745700	1.04860700
C	-2.81360000	-0.22205600	0.20113600
N	-0.66475600	-1.21978700	-0.50205000
C	0.30361000	-0.64549600	0.24447300
C	1.27479300	-1.61755700	0.35808100
N	0.84803500	-2.72308200	-0.31700600
N	-0.32051500	-2.48460500	-0.83302400
H	0.22842600	0.35942600	0.62652400
C	-4.21729900	-0.25232300	2.03704300
C	-3.81986200	1.09811200	1.81162000
C	-2.95051000	1.11896100	0.68411400
Fe	-4.79554500	0.35392200	0.13164300
C	-6.86611700	0.22140100	0.02336200
C	-6.27094400	-0.62843800	-0.95453500
C	-5.48424200	0.18393800	-1.82259200
C	-5.59374500	1.53576300	-1.38184800
C	-6.44802700	1.55860400	-0.24097600
H	-6.71121700	2.43254900	0.33775500
H	-5.10096000	2.39023000	-1.82360500
H	-4.89785000	-0.16548700	-2.66100400
H	-6.37978000	-1.70200800	-1.01400900
H	-4.89524600	-0.59394500	2.80616800
H	-7.50272000	-0.09559300	0.83710500
H	-3.71024300	-2.13717800	0.93997000
H	-4.14199200	1.95887000	2.38012300
C	2.58702000	-1.57826300	1.04841100
C	5.78154200	-0.31192700	-0.45811900
C	6.82063200	0.59799500	0.18673900
O	6.27182800	1.87518500	0.57740800
C	5.21423700	2.45252300	-0.03249400
O	4.57248100	1.75589000	-1.00009600
C	5.10093600	0.52682800	-1.53312100
H	5.82111200	0.77457100	-2.32002000
H	7.63933500	0.78722000	-0.51378800
O	4.82840200	3.53395700	0.29890000
H	4.24953400	0.02109300	-1.98165000
H	7.22265700	0.16938100	1.10232300

H	2.57165100	-0.94857600	1.93811400
H	-2.49920300	1.99876100	0.24523800
H	2.90240900	-2.58146900	1.33518900
C	-1.95677500	-0.67204300	-0.94341700
H	-1.76339900	0.15199300	-1.63467700
H	-2.42238400	-1.48096000	-1.50574600
C	6.46817300	-1.53861700	-1.09065200
H	7.19268400	-1.22780500	-1.84803200
H	5.73560000	-2.19185100	-1.56978600
H	6.99585000	-2.12075700	-0.33240100
O	3.57770500	-1.03097300	0.12276900
C	4.80651500	-0.83203000	0.61569000
O	5.13427200	-1.08101400	1.74963500

Sum of electronic and thermal Free Energies= **-2578.841993**

Sum of electronic and thermal Enthalpies= **-2578.753522**

M4 ROM

Fe	4.24021000	-1.01749200	-0.52065300
C	3.96802600	-3.08110300	-0.53661300
C	3.29459300	-2.50221300	0.57561200
C	2.33949800	-1.55972600	0.07965700
C	2.42576000	-1.57208400	-1.34934900
C	3.43183700	-2.50679000	-1.72643900
C	5.79918600	-0.12269700	-1.56226900
C	6.27221600	-0.63548700	-0.31876800
C	5.54879000	0.00889700	0.72763400
C	4.62749100	0.91937100	0.13083000
C	4.78283600	0.83775500	-1.28435400
H	4.21305200	1.39015800	-2.01792900
H	6.13359700	-0.42844700	-2.54343600
H	7.02845100	-1.39713900	-0.19213300
H	5.66365600	-0.17699900	1.78615800
H	3.92358400	1.55079500	0.65450700
H	1.84772300	-0.95467900	-2.02362000
H	4.76734900	-3.80673800	-0.48651900
H	3.48197500	-2.71741800	1.61840200
H	3.75224900	-2.72103700	-2.73610700
N	0.16247100	-1.49027800	1.25241600
N	-0.14001900	-1.73232200	2.54795700
C	-1.71491100	-2.55365800	1.29674100
N	-1.27243900	-2.37091200	2.57449400
H	-0.76087400	-1.90888000	-0.63326100
C	-3.01215900	-3.22267700	1.00907400
C	-5.27303500	-0.67433200	-0.58489500
C	-5.80098500	-0.22787300	0.78961200
C	-4.70936600	0.51858000	-1.36338700
O	-6.80381700	0.76695900	0.56268400
H	-4.36322000	0.21049900	-2.34911900
H	-5.46037200	1.30024600	-1.46332200
O	-3.58093400	1.03351100	-0.61392600
H	-2.95326800	-3.88396800	0.14585800
H	-3.34360900	-3.77617700	1.88474300
H	-6.22371100	-1.08671000	1.31914100
H	-4.98377000	0.17873600	1.39174600
C	-2.94186100	2.07152900	-1.15633100
C	-0.79241000	-1.99063600	0.43977800
H	-7.11576500	1.09883300	1.41133100
O	-1.89047700	2.36085200	-0.37201500
O	-3.24470700	2.64950800	-2.17026000
C	-1.11403700	3.50847400	-0.77348500
C	0.06008200	3.65880800	0.15985700
C	-0.00969800	3.26571800	1.49986200
C	1.07536700	3.47022400	2.35085400
C	2.23850700	4.07592300	1.87666100
C	2.31503500	4.46854200	0.54118000
C	1.23392100	4.25418700	-0.31204500
H	-0.90916900	2.79005100	1.87296200
H	1.00903900	3.15697000	3.38789000
H	3.07990400	4.23955100	2.54236200
H	3.21797300	4.93523900	0.16073400
H	1.30444500	4.55674700	-1.35340700
H	-0.78788700	3.38039000	-1.80744400
H	-1.76236800	4.38975700	-0.74284100
O	-4.08279500	-2.25462200	0.77296100
C	-4.15447200	-1.71798000	-0.45557300
O	-3.43407900	-2.03727400	-1.37249600
C	1.38654200	-0.75185500	0.90880700
H	1.82351600	-0.47625000	1.86798200
H	1.09594300	0.16800300	0.39668600
C	-6.40938800	-1.30209200	-1.42251800
H	-7.21082300	-0.57696800	-1.56787200
H	-6.83140500	-2.17009900	-0.90956300
H	-6.04147200	-1.62740400	-2.39740700

Sum of electronic and thermal Free Energies= **-2925.597168**

Sum of electronic and thermal Enthalpies= **-2925.487603**

M5 RCM

C	3.63657200	-1.33039300	0.33725700
C	3.02620100	-0.10410100	-0.08232500
N	0.88372900	0.11391300	1.08373300
C	0.08140000	-0.61445000	0.27605400
C	-1.00330500	-0.93606400	1.06500100
N	-0.80545600	-0.39051600	2.29905200
N	0.32946400	0.24309900	2.30863300
H	0.34378800	-0.85402700	-0.74114400
C	4.29560500	-1.90911700	-0.78328400
C	4.10246600	-1.04751600	-1.90205100
C	3.31556000	0.06105400	-1.47561500
Fe	5.07385400	-0.02353900	-0.37637300
C	7.10798700	-0.25239800	-0.01941500
C	6.47047100	0.30131300	1.12916400
C	5.87033100	1.53615500	0.74636100
C	6.13749700	1.74645000	-0.63871100
C	6.90258100	0.64049900	-1.11156400
H	7.24551500	0.49276500	-2.12569200
H	5.80501300	2.58741900	-1.23073700
H	5.30482000	2.19232100	1.39309000
H	6.43058300	-0.14705800	2.11162200

H	4.87075100	-2.82395600	-0.77769700
H	7.63354300	-1.19571500	-0.06080800
H	3.61039100	-1.73507600	1.33964400
H	4.50512000	-1.19351500	-2.89423000
C	-2.21589100	-1.72958600	0.74846100
C	-5.45698100	-0.31643600	-0.45865500
C	-5.49192000	0.85598000	0.52632500
O	-6.57306400	1.76170600	0.22774500
C	-7.75136000	1.35637100	-0.30111800
O	-7.86382500	0.07067700	-0.70251900
C	-6.85868700	-0.92459900	-0.42214900
H	-6.99796000	-1.69345300	-1.17951800
H	-4.58949200	1.46174400	0.48190600
O	-8.65023000	2.12848100	-0.45287900
H	-7.07074900	-1.36495300	0.55479600
H	-5.62142300	0.50134700	1.55353800
H	-2.03488100	-2.47117100	-0.03054500
H	3.02370400	0.89801300	-2.09323600
H	-2.58608400	-2.24141500	1.63634100
C	2.17560300	0.78054400	0.79333700
H	2.64005100	0.86926700	1.77737200
O	-3.25851300	-0.81898900	0.27620300
C	-4.45600400	-1.36883400	0.01896100
O	-4.70145500	-2.54526500	0.13476400
C	-5.06937700	0.14240500	-1.88022900
H	-5.78386500	0.87133400	-2.26573600
H	-5.05564600	-0.70610700	-2.56897200
H	-4.08053100	0.60334400	-1.88070800
C	1.92075600	2.18211200	0.23293300
H	1.32404100	2.76457000	0.93659600
H	1.38134600	2.14189700	-0.71637600
H	2.86724800	2.69974600	0.06732300

Sum of electronic and thermal Free Energies= **-2618.136846**

Sum of electronic and thermal Enthalpies= **-2618.045527**

M5 ROM

Fe	-3.82395843	-2.44303997	-1.35408397
C	-3.87568245	-0.53869789	-2.18752529
C	-3.01787251	-0.55822544	-1.05219673
C	-1.97431670	-1.50922210	-1.29149924
C	-2.19868650	-2.07050253	-2.58935435
C	-3.37138007	-1.47512109	-3.13634729
C	-5.19139028	-3.94823378	-1.77755306
C	-5.77719340	-2.98927093	-0.89983148
C	-4.99445216	-2.94563233	0.29103236
C	-3.92499672	-3.87712327	0.14858243
C	-4.04565381	-4.49706358	-1.13029606
H	-3.37263374	-5.23371289	-1.54544403
H	-5.54004432	-4.19611692	-2.77009265
H	-6.64689939	-2.38330690	-1.11053995
H	-5.16804061	-2.30326265	1.14263757
H	-3.15069556	-4.06816764	0.87827757
H	-1.60194566	-2.83638337	-3.06297826
H	-4.77007267	0.05805102	-2.29701207
H	-3.13634601	0.03106122	-0.15331006
H	-3.81567684	-1.71371199	-4.09220774
N	0.16909000	-0.67929329	-0.45032981
N	0.81542127	-0.27307857	0.66417574
C	1.62492096	0.79913263	-1.04291037
N	1.69373440	0.61881236	0.30734651
H	0.27411070	-0.20325807	-2.53522445
C	2.52924384	1.74681572	-1.74812667
C	4.56171731	-0.14183945	-4.28064631
C	5.51940405	-0.68282287	-3.20343687
C	4.07308580	-1.26804033	-5.19332543
O	6.59001717	-1.35184965	-3.87565957
H	3.37535772	-0.88791010	-5.93823989
H	4.91629698	-1.74527434	-5.68878156
O	3.38925094	-2.25068289	-4.37671812
H	2.00012415	2.35822976	-2.47788158
H	3.03195822	2.38099580	-1.02131849
H	5.89977565	0.14521071	-2.59958320
H	4.98651420	-1.37502105	-2.54440206
C	2.94742711	-3.32849753	-5.02801738
C	0.64363759	-0.03509059	-1.53835561
H	7.19404299	-1.71704307	-3.22029095
O	2.30898366	-4.11731471	-4.14682802
O	3.09140976	-3.56223143	-6.20257351
C	1.82166183	-5.36888490	-4.69283550
C	1.16530445	-6.15644965	-3.59159223
C	-0.10977169	-6.69458102	-3.77898501
C	-0.70677817	-7.47316260	-2.78677595
C	-0.03581532	-7.70999201	-1.58965567
C	1.23525883	-7.16815298	-1.39084636
C	1.83346456	-6.40132487	-2.38643364
H	-0.64054892	-6.50925316	-4.70853613
H	-1.69479998	-7.89162383	-2.95052501
H	-0.49780791	-8.31391895	-0.81526135
H	1.76268254	-7.34878094	-0.45963098
H	2.82066804	-5.98034412	-2.22643915
H	1.12341060	-5.15739328	-5.50422010
H	2.67211801	-5.90625468	-5.12101345
O	3.61903556	1.05659889	-2.43697318
C	3.34429637	0.54816400	-3.65051843
O	2.27426809	0.66379370	-4.20013133
C	-0.82059364	-1.77859637	-0.36019531
H	-1.17280657	-1.72167461	0.67177657
C	-0.11327255	-3.11901680	-0.57839190
H	0.68454291	-3.24059854	0.15622951
H	0.33343762	-3.18330086	-1.57271542
H	-0.81764710	-3.94435257	-0.46563530
C	5.28165881	0.90585647	-5.16186230
H	6.16057490	0.45861368	-5.62734923
H	5.61328597	1.75342988	-4.55764964
H	4.61952711	1.28234207	-5.94476758

Sum of electronic and thermal Free Energies= **-2964.892682**

Sum of electronic and thermal Enthalpies= **-2964.780255**

M6 RCM

C	-3.23336100	1.46916600	1.10563600
C	-2.57101700	0.80955400	0.02884600
N	-1.50113500	-0.10892400	0.16117200
C	-0.46082400	-0.31104200	-0.68394000
C	0.30994600	-1.26985700	-0.06443900
N	-0.29201800	-1.59751400	1.11520900
N	-1.38121400	-0.90583800	1.25427000
H	-0.34650000	0.23746100	-1.60389500
C	-4.17809100	2.36558000	0.52966300
C	-4.09480400	2.26000900	-0.88943300
C	-3.10184300	1.28872500	-1.20798500
Fe	-4.59284300	0.41785300	-0.06427000
C	-6.51847100	-0.05516100	0.55416000
C	-5.57718800	-0.93185200	1.16949800
C	-4.88385400	-1.62874000	0.13813000
C	-5.39644700	-1.18391400	-1.11556500
C	-6.40644000	-0.20996000	-0.85884200
H	-6.97079600	0.33222700	-1.60417600
H	-5.06262200	-1.51026700	-2.09037600
H	-4.08403500	-2.34011800	0.28665500
H	-5.39542800	-1.02951100	2.23008300
H	-4.85694000	3.00096500	1.07978700
H	-7.18230400	0.62614700	1.06715300
H	-3.04690700	1.29717400	2.15446900
H	-4.69720500	2.80034800	-1.60507500
C	1.59384100	-1.88522000	-0.48272100
C	4.97033900	-0.42115100	0.15913200
C	4.64446100	0.99236100	-0.33342100
O	5.71475400	1.91269300	-0.04952800
C	7.01899600	1.54699100	-0.03921800
O	7.31423500	0.23271900	-0.14058800
C	6.32532300	-0.76848400	-0.45710800
H	6.72999100	-1.70179300	-0.07071700
H	3.76952100	1.40901900	0.16104300
O	7.87940200	2.36271300	0.10477400
H	6.25403500	-0.85145800	-1.54410200
H	4.47200300	0.99898300	-1.41479500
H	1.73550900	-2.84668000	0.01018000
H	-2.81530300	0.96391100	-2.19764400
H	1.65646100	-2.03417600	-1.56134900
O	2.68143000	-0.99411900	-0.08260800
C	3.92791200	-1.40820200	-0.36644000
O	4.18433500	-2.43474000	-0.94718600
C	5.00437600	-0.49506200	1.70035600
H	5.76272200	0.17559500	2.10742200
H	5.24338000	-1.50826900	2.03246900
H	4.03853200	-0.21439500	2.12255600

Sum of electronic and thermal Free Energies= **-2539.540701**

Sum of electronic and thermal Enthalpies= **-2539.456675**

M6 ROM

Fe	-5.592922	-0.756795	-0.011300
C	-5.945526	-0.655204	-2.056471
C	-5.022089	0.358541	-1.671867
C	-3.894947	-0.295942	-1.095082
C	-4.117746	-1.706482	-1.112245
C	-5.390279	-1.923248	-1.717909
C	-6.903881	-1.691568	1.304029
C	-7.377881	-0.385054	0.985847
C	-6.384530	0.554960	1.389743
C	-5.297415	-0.169862	1.958428
C	-5.617980	-1.558125	1.906198
H	-4.987310	-2.369206	2.241974
H	-7.418080	-2.620639	1.102439
H	-8.314165	-0.150502	0.499707
H	-6.429793	1.626501	1.258840
H	-4.378730	0.259525	2.332198
H	-3.454442	-2.467751	-0.728632
H	-6.912348	-0.485211	-2.507573
H	-5.138275	1.425925	-1.776632
H	-5.858685	-2.885185	-1.867262
N	-2.722852	0.350250	-0.635158
N	-2.735140	1.659943	-0.311786
C	-0.712550	0.879759	-0.006075
N	-1.529340	1.974456	0.064863
H	-1.242380	-1.199034	-0.677295
C	0.796403	0.922366	0.350389
C	2.883088	-1.482585	2.359748
C	2.222125	-2.842413	2.050680
C	4.398967	-1.634166	2.343655
O	2.577304	-3.372828	0.783910
H	4.730262	-2.387432	3.061599
H	4.761331	-1.921602	1.354905
O	4.983636	-0.359179	2.712428
H	1.359370	0.393558	-0.425471
H	1.146594	1.955811	0.336798
H	2.532652	-3.578558	2.798160
H	1.134574	-2.742300	2.131910
C	6.319335	-0.309230	2.720819
C	-1.476761	-0.170467	-0.461058
H	2.015056	-4.149542	0.628096
O	6.681927	0.936730	3.058787
O	7.063849	-1.222831	2.459888
C	8.112513	1.183912	3.175522
C	8.423064	2.645187	3.369750
C	8.643996	3.166328	4.648914
C	8.925438	4.520675	4.820264
C	8.986494	5.368278	3.715310
C	8.766908	4.857421	2.436232
C	8.488761	3.503390	2.266619
H	8.583132	2.509098	5.509582
H	9.096945	4.913666	5.817304
H	9.207204	6.422561	3.849303
H	8.817191	5.512279	1.572118
H	8.321127	3.107717	1.268828
H	8.505352	0.578427	3.991294
O	1.116687	0.350346	1.598713
C	2.373732	-0.259509	1.408937
O	3.121270	0.139299	0.521845

H	8.513418	0.815922	2.224168
C	2.462041	-1.094021	3.779501
H	2.910865	-0.129357	4.042553
H	2.803822	-1.860372	4.484559
H	1.370019	-1.014171	3.827752

Sum of electronic and thermal Free Energies= **-2886.296039**

Sum of electronic and thermal Enthalpies= **-2886.189788**

M7 RCM

C	5.28538000	-1.12847700	1.18670100
C	6.05571800	-0.02224000	0.72311900
C	6.00568100	-0.01649300	-0.70166500
C	5.20501400	-1.11965800	-1.11967200
C	4.75960600	-1.80676900	0.04755000
Fe	4.08883300	0.16209300	0.07756300
H	6.47205200	0.71109400	-1.35047200
H	4.96119600	-1.37661900	-2.14063500
H	4.12499900	-2.68195000	0.06553600
H	5.11385300	-1.39441000	2.22016300
H	6.56729900	0.70012900	1.34316200
C	2.02109200	0.17880900	0.08228300
C	2.52090900	0.81602000	1.26269000
C	3.32040400	1.92559700	0.86490000
C	3.31210900	1.98545600	-0.55943900
C	2.51260400	0.91219900	-1.04313100
H	2.31899300	0.67717600	-2.08044100
H	3.86093900	2.58831600	1.52557400
H	2.34797500	0.48905700	2.27930700
C	1.09861400	-1.00267600	0.02841400
H	1.15179700	-1.58068400	0.95465500
H	1.34500900	-1.66891100	-0.79793900
N	-0.29967200	-0.61920800	-0.20358100
N	-0.93685300	-1.04069500	-1.31140700
H	-4.16751200	-1.83971900	0.30410400
C	-2.30474400	0.20133000	-0.15395500
C	-1.11949800	0.15684700	0.54841800
H	-0.80152000	0.61150000	1.47236000
C	-3.57451300	0.94072700	0.14649400
H	-3.59288200	1.88448400	-0.40364000
H	-3.59886000	1.20906500	1.20809700
C	-4.83916600	0.14359400	-0.21993600
H	-4.75888400	-0.11742000	-1.28401700
C	-6.07380300	1.04727700	-0.15017600
O	-6.02902900	2.23194400	-0.35990200
O	-7.28833600	0.47777800	0.06445600
C	-7.45042000	-0.84733800	0.62198700
C	-6.33914700	-1.80671200	0.24140300
C	-4.99037500	-1.16934700	0.56089300
H	-4.91829900	-0.97572500	1.63973300
H	-6.48015000	-2.74334700	0.79098100
H	-6.39830200	-2.04984500	-0.82547300
H	-8.42692000	-1.17851300	0.26696200
H	-7.50700000	-0.73255000	1.71029100
N	-2.14383600	-0.54791100	-1.28291300
H	3.84521500	2.70249300	-1.16734300

Sum of electronic and thermal Free Energies= **-2314.995790**

Sum of electronic and thermal Enthalpies= **-2314.917526**

M7 ROM

C	6.92443700	-0.22248500	1.36609800
C	6.57413600	1.00267900	0.72656600
C	6.96888600	0.91550300	-0.64102700
C	7.56314600	-0.36370800	-0.84660800
C	7.53516500	-1.06708100	0.39323400
Fe	5.60101400	-0.58631300	-0.19516800
C	3.91697300	-1.52033000	0.57507100
C	3.55873400	-0.29104500	-0.06228900
C	3.95308000	-0.38747100	-1.43503900
C	4.55762700	-1.66130900	-1.63641500
C	4.53298000	-2.36093500	-0.39429500
C	2.85602300	0.86609900	0.58334700
N	1.40650600	0.66484000	0.69811200
C	0.48121000	0.45208400	-0.27025000
C	-0.71421400	0.33357600	0.40517400
N	-0.45447600	0.47984900	1.73721600
N	0.82069400	0.67960100	1.91165700
C	-2.09507000	0.07767000	-0.11376500
C	-3.10041400	1.21184600	0.22841600
C	-2.74844300	2.53777600	-0.46047700
C	-3.62036700	3.71238900	-0.00413700
C	-3.24699900	5.01453700	-0.69241900
O	-4.10298600	6.04251000	-0.18926000
C	-4.48393100	0.73446000	-0.18653200
O	-5.16433100	0.22447300	0.86200500
C	-6.47743700	-0.34846900	0.59419800
C	-6.39131000	-1.80745500	0.22802300
C	-6.42140100	-2.21339000	-1.11017900
C	-6.33812100	-3.56501200	-1.44046700
C	-6.21956200	-4.52503200	-0.43674700
C	-6.18684600	-4.12954900	0.90028300
C	-6.27397000	-2.77878500	1.22851900
O	-4.91814200	0.77223900	-1.31465300
H	7.89292800	-2.07299000	0.56079000
H	6.73967100	-0.47510100	2.40047700
H	6.08419200	1.84549100	1.19406300
H	6.82484200	1.67726000	-1.39411300
H	7.94533900	-0.74334500	-1.78357400
H	3.76000300	-1.75646500	1.61833000
H	4.98465200	-2.02270200	-2.56107800
H	3.84158100	0.38809300	-2.18099600
H	3.03620200	1.78877000	0.02531800
H	3.19598200	1.02236500	1.60687900
H	-1.69673500	2.76086400	-0.25161900
H	0.73708700	0.38817800	-1.31517400
H	-2.46340200	-0.86043000	0.31400100
H	-2.06225800	-0.06146300	-1.19835600
H	-3.09517500	1.34086200	1.31331500
H	-2.83633600	2.40401600	-1.54442200

H	4.93806500	-3.34622800	-0.21270300
H	-3.52819300	3.85321400	1.07839500
H	-4.67681700	3.50943900	-0.20844500
H	-3.89456000	6.87583200	-0.62676300
H	-3.36634400	4.91450000	-1.78054900
H	-2.19433000	5.26162100	-0.49183100
H	-6.95732600	0.23429000	-0.19101500
H	-7.01574100	-0.20703900	1.53098000
H	-6.50022800	-1.46515200	-1.89151200
H	-6.36557600	-3.86818500	-2.48234900
H	-6.25119300	-2.47450900	2.27111700
H	-6.09808700	-4.87270000	1.68633600
H	-6.15587500	-5.57753800	-0.69445600

Sum of electronic and thermal Free Energies= **-2661.744950**

Sum of electronic and thermal Enthalpies= **-2661.642396**

M8 RCM

N	-2.18427400	-0.53410500	-1.36446700
N	-0.98299100	-1.04099800	-1.41805800
N	-0.31303700	-0.61558200	-0.33205100
C	-1.10659700	0.17223300	0.43598300
C	-2.30826700	0.22527200	-0.23824800
C	1.07915200	-1.06123800	-0.11083400
C	1.94840000	0.11774800	0.25267200
C	2.52775800	0.42378700	1.52594800
C	3.21553700	1.66696300	1.41589500
C	3.05876400	2.14153600	0.08134300
C	2.28178000	1.18951800	-0.63592300
Fe	4.00639000	0.29013900	0.07501500
C	4.78261800	-1.49073200	-0.66707900
C	5.36235300	-1.19777500	0.60265900
C	6.02798300	0.05876500	0.50254300
C	5.85933500	0.54208300	-0.82810600
C	5.09001300	-0.41593400	-1.55156700
C	-3.55763700	0.99143800	0.08180100
C	-4.84408200	0.22600700	-0.27548600
C	-6.05656700	1.15797100	-0.19312300
O	-7.28242200	0.61576000	0.02861200
C	-7.47028800	-0.70583800	0.58629100
C	-6.38517500	-1.69034800	0.19457300
C	-5.01906200	-1.08518800	0.50321300
O	-5.98635500	2.34194800	-0.39990500
H	6.22804300	1.48186900	-1.21378500
H	4.77578500	-0.33147900	-2.58208200
H	4.20210800	-2.36849300	-0.91462400
H	5.29635800	-1.81188500	1.48968000
H	6.54778700	0.56761800	1.30188300
H	1.99660000	1.25318700	-1.67686300
H	3.77901700	2.15059300	2.20115300
H	2.48632500	-0.19438000	2.41108600
C	1.11305700	-2.21238300	0.89789100
H	1.37662500	-1.43892700	-1.09094500
H	-4.21445400	-1.77374700	0.23702800
H	-0.75931700	0.63454000	1.34530900
H	-3.56110400	1.93917800	-0.46180200
H	-3.56409100	1.25327100	1.14532200
H	-4.77930400	-0.03403000	-1.34090400
H	-4.93254500	-0.89627300	1.58182400
H	-6.54341100	-2.62442600	0.74385900
H	-6.45937400	-1.92996600	-0.87217400
H	-8.45744400	-1.01365600	0.23976900
H	-7.51441700	-0.59122600	1.67521300
H	3.48255000	3.04920300	-0.32415400
H	0.48871900	-3.03616900	0.54756800
H	2.13453500	-2.57836000	1.01958300
H	0.74273400	-1.90022500	1.87735600

Sum of electronic and thermal Free Energies= **-2354.290703**

Sum of electronic and thermal Enthalpies= **-2354.210508**

M8 ROM

C	-6.24371900	-2.89977800	1.24229500
C	-6.38832600	-1.92614500	0.24765400
C	-6.40746800	-2.32489300	-1.09296100
C	-6.28760500	-3.67178100	-1.43119700
C	-6.14277300	-4.63417900	-0.43318400
C	-6.12004900	-4.24576600	0.90612400
C	-6.51650800	-0.47248300	0.62270400
O	-5.22041200	0.13910100	0.88714600
C	-4.56066200	0.67358900	-0.16277600
O	-5.00230700	0.70272700	-1.28824900
C	-3.18924700	1.18829400	0.24772700
C	-2.85974500	2.50566700	-0.46747200
C	-3.75152300	3.67366700	-0.03300800
C	-3.40326900	4.96798000	-0.74855800
O	-4.27451000	5.99135000	-0.26215400
C	-2.16020200	0.06672700	-0.06292600
C	-0.78533900	0.36472700	0.45079500
C	0.41661700	0.43223900	-0.22063300
N	1.33456700	0.70565000	0.73963100
N	0.73783200	0.80987900	1.94254200
N	-0.53765300	0.60237000	1.77134700
C	2.78997800	0.93495900	0.62252800
C	3.43374600	-0.19089000	-0.14867100
C	3.61067700	-1.52255200	0.34600500
C	4.18462900	-2.31300800	-0.68872200
C	4.36947800	-1.47886700	-1.82941900
C	3.90338100	-0.17275600	-1.50131000
Fe	5.43721700	-0.72261300	-0.21590300
C	7.26215000	-1.52163900	0.37577400
C	6.70345700	-0.74663700	1.43402300
C	6.54158800	0.58876500	0.96266900
C	6.99997600	0.63942300	-0.38686000
C	7.44589900	-0.66516700	-0.74904700
H	7.48469600	-2.57855000	0.41224400
H	6.43038100	-1.11219000	2.41363200
H	6.13270600	1.41459600	1.52782500
H	6.99426300	1.50930300	-1.02842800
H	7.83158000	-0.95915800	-1.71482800

H	3.35995800	-1.85994000	1.34217900
H	4.81187100	-1.77548700	-2.76977800
H	3.93433100	0.68710100	-2.15499800
C	3.05825500	2.33266200	0.05794100
H	3.12993700	0.89812200	1.65928600
H	-1.81207500	2.75052600	-0.26310500
H	0.68172600	0.29004300	-1.25535700
H	-2.51162200	-0.86710800	0.38809500
H	-2.12116700	-0.10063100	-1.14344200
H	-3.19197600	1.34086000	1.32961000
H	-2.94552200	2.34967600	-1.54854600
H	4.46247800	-3.35450100	-0.61124400
H	-3.65889000	3.83808900	1.04618200
H	-4.80458900	3.44753800	-0.23012700
H	-4.08304400	6.81870600	-0.71833500
H	-3.52535400	4.84435000	-1.83394900
H	-2.35415300	5.23679100	-0.55755100
H	-7.01818100	0.09974200	-0.15664800
H	-7.05409600	-0.35301200	1.56294800
H	-6.50662100	-1.57435000	-1.86974300
H	-6.30728600	-3.96942800	-2.47485600
H	-6.22910400	-2.60113900	2.28667000
H	-6.01085000	-4.99084300	1.68778200
H	-6.05092500	-5.68305600	-0.69712900
H	2.58459200	3.08786200	0.68772300
H	4.13142600	2.52911400	0.02644800
H	2.66208100	2.44125900	-0.95462700

Sum of electronic and thermal Free Energies= **-2701.041449**

Sum of electronic and thermal Enthalpies= **-2700.935673**

M9 RCM

C	-1.64166500	0.35790100	0.93049500
C	-2.39875600	-0.52922800	1.74989300
C	-3.56548600	0.17419200	2.16613600
C	-3.52578100	1.48448900	1.60591900
C	-2.33562300	1.60220600	0.82957300
Fe	-3.50868600	0.06143400	0.09362100
C	-3.99806200	-1.64982600	-0.97397400
C	-5.18545700	-0.97897300	-0.55769700
C	-5.17310100	0.33022600	-1.12281700
C	-3.97820900	0.46658600	-1.88963800
C	-3.25190800	-0.75682500	-1.79627500
H	-5.94786600	-1.38208200	0.09370800
H	-5.92488000	1.09297100	-0.97703300
H	-3.66717300	1.35100300	-2.42748200
H	-2.28688600	-0.96270200	-2.23677400
H	-3.69631500	-2.64760100	-0.68981900
H	-2.12625500	-1.54625400	1.98541800
H	-4.35523900	-0.22888300	2.78344900
H	-4.27797500	2.25120000	1.72222500
H	-2.02545300	2.46466500	0.25807700
N	-0.37955200	0.06930800	0.36043300
C	0.61869300	0.93148400	0.03060400
C	1.62710100	0.13479200	-0.46537700
N	1.19459400	-1.16079100	-0.40823900
N	-0.00827500	-1.20310700	0.08639000
C	2.97621700	0.52585300	-0.98305600
H	0.54075000	1.99524700	0.18119200
C	4.13618900	0.20335900	-0.01483800
H	3.15753000	0.01750000	-1.93616800
H	2.98867500	1.59572200	-1.19305500
C	5.38126800	1.02242900	-0.38760000
H	3.86248700	0.59704200	0.97558300
O	6.60435400	0.54137500	-0.05506600
C	6.84449600	-0.84476000	0.29010300
C	5.66831900	-1.51001200	0.97783300
H	7.09527700	-1.36678300	-0.63960600
H	7.73733100	-0.82055500	0.91571200
C	4.41108000	-1.29858500	0.14040700
H	5.89048800	-2.57499400	1.10139300
H	5.53380800	-1.09359500	1.98311300
H	4.54457900	-1.75207200	-0.85006300
H	3.54147000	-1.78898700	0.58053000
O	5.31292300	2.11764300	-0.88403000

Sum of electronic and thermal Free Energies= **-2275.696252**

Sum of electronic and thermal Enthalpies= **-2275.622900**

M9 ROM

C	3.09676800	-0.17932600	0.89963000
C	4.11024200	0.64787800	1.46586400
C	4.97855800	-0.20036700	2.21108000
C	4.50044900	-1.53954900	2.10614800
C	3.33484400	-1.53387200	1.28551200
Fe	4.94876100	-0.79141700	0.22035500
C	5.96651100	0.20620000	-1.28777100
C	6.87013800	-0.61249900	-0.54824100
C	6.42630200	-1.96368100	-0.65236900
C	5.24923600	-1.97866100	-1.45818800
C	4.96520800	-0.63747300	-1.84972900
N	1.99677200	0.27474000	0.13442200
C	0.73291600	-0.22609200	0.10040700
C	0.05079800	0.59502800	-0.77104000
N	0.92713000	1.54389300	-1.21462300
N	2.09586100	1.35448000	-0.67528400
C	-1.37457500	0.55681100	-1.22909900
C	-2.40584900	0.86736200	-0.10804100
C	-3.83032700	0.67434000	-0.62140300
O	-3.99899500	-0.57135000	-1.12621600
C	-2.22221100	2.23340300	0.57501600
C	-2.17053100	3.44755900	-0.36145400
C	-2.24209600	4.76599600	0.39191300
O	-1.12790600	4.84717900	1.28696400
H	-1.17418800	5.67441500	1.77916500
C	-5.32425700	-0.92791100	-1.61607500
C	-6.16083700	-1.57615900	-0.54369500
C	-7.02947000	-0.81551500	0.24677200
C	-6.07111600	-2.95393300	-0.31822700
C	-7.79139900	-1.42263400	1.24328300

C	-6.83067700	-3.56235600	0.67840400
C	-7.69303600	-2.79617000	1.46177900
O	-4.71452100	1.49601200	-0.57644600
H	4.19236200	1.71515400	1.32911800
H	5.86111100	0.11807700	2.74688500
H	4.95546900	-2.41509800	2.54623800
H	2.74902700	-2.39359700	0.99430700
H	6.00804000	1.28195700	-1.37885200
H	7.72538200	-0.26709100	0.01509800
H	6.88689400	-2.82186000	-0.18364700
H	4.66140100	-2.85125800	-1.70608800
H	4.11752200	-0.30613900	-2.43218700
H	0.43638000	-1.07667900	0.69131400
H	-1.60440200	-0.42518600	-1.64781300
H	-1.47893200	1.27781300	-2.04329900
H	-2.28349900	0.09190600	0.66016800
H	-1.30243100	2.20501000	1.16347100
H	-3.03943900	2.36477800	1.29190700
H	-3.01179600	3.42353300	-1.06125800
H	-1.24874500	3.43348400	-0.95090600
H	-3.18546800	4.82699300	0.95354300
H	-2.21898100	5.60169300	-0.32056300
H	-5.12440400	-1.62181000	-2.43242600
H	-5.80084900	-0.03168600	-2.01071200
H	-7.09891600	0.25447900	0.08269700
H	-5.40385700	-3.55480400	-0.92989600
H	-8.46361000	-0.82282000	1.84857500
H	-6.75369600	-4.63283300	0.84046900
H	-8.28867000	-3.26839700	2.23658700

Sum of electronic and thermal Free Energies= **-2622.441146**

Sum of electronic and thermal Enthalpies= **-2622.343602**

BnOH

C	-0.45591400	0.00008200	-0.28853100
C	0.24475100	1.20316000	-0.16387200
C	1.61652500	1.20587400	0.08009500
C	2.30562100	-0.00009900	0.20160400
C	1.61648400	-1.20595600	0.07987600
C	0.24455700	-1.20301200	-0.16375200
H	-0.28936300	2.14467000	-0.25412300
H	2.14771800	2.14786300	0.17341100
H	3.37473900	-0.00004600	0.38911200
H	2.14745300	-2.14807000	0.17307300
H	-0.28949100	-2.14456800	-0.25392100
C	-1.94269000	0.00003500	-0.52086100
O	-2.60511100	-0.00007600	0.75175500
H	-2.23333800	0.88741200	-1.09804600
H	-2.23312000	-0.88729200	-1.09820100
H	-3.55972600	0.00012900	0.60731000

Sum of electronic and thermal Free Energies= **-346.755876**

Sum of electronic and thermal Enthalpies= **-346.714914**

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