

Four-component zinc-porphyrin / zinc-salphen nanorotor

Electronic Supporting Information

Merve S. Özer, Anup Rana, Pronay K. Biswas and Michael Schmittel*

*Center for Micro- and Nanochemistry and Engineering, Organische Chemie I, Universität Siegen, D-57068
Siegen, Germany*

E-mail: schmittel@chemie.uni-siegen.de

Contents

Synthesis	2
NMR Spectra	3
Rate constant calculation by volume intensity of the ROESY cross peaks	10
ESI-MS	11
Computation	14

Synthesis

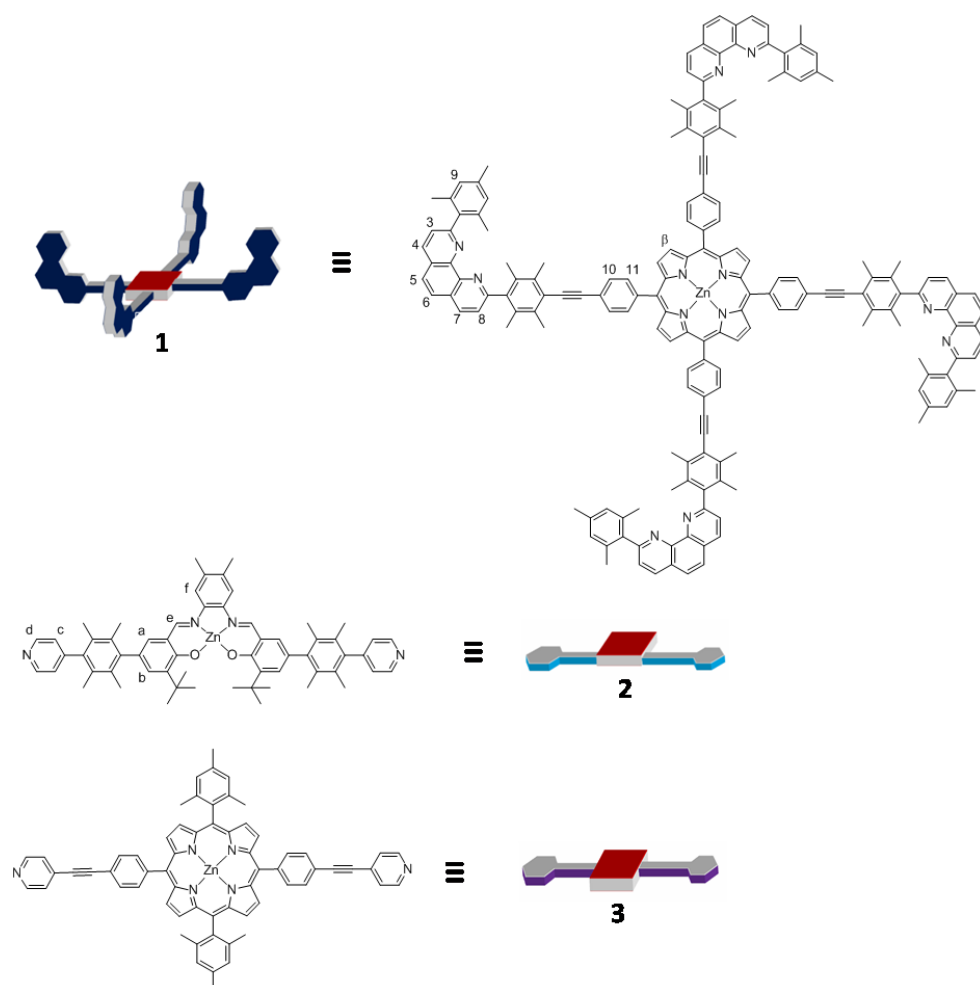


Table S1. ^1H NMR shifts of **1**, **1** + 4 equiv. of Cu^+ , **ROT-1** and **ROT-2** (**C** = complexed, **U** = uncomplexed, **Cu** = Cu^+ loaded) for comparison.

Protons	1 (δ/ppm)	1 + 4 equiv. of Cu^+ (δ/ppm)	ROT-1 (δ/ppm)		ROT-2 (δ/ppm)	
			C	U	C	Cu
[4 or 7]-H	8.40	8.74	8.81	8.40	8.81	8.74
[7 or 4]-H	8.36	8.70	8.79	8.37	8.78	8.69
[5 and 6]-H	7.93	8.18	8.26	7.94	8.25	8.18
[3 or 8]-H	7.61	7.99	8.07	7.60	8.07	7.98
[8 or 3]-H	7.59	7.94	8.02	7.59	8.02	7.93
9-H	6.99	7.06	7.07	6.99	7.07	7.05

NMR Spectra

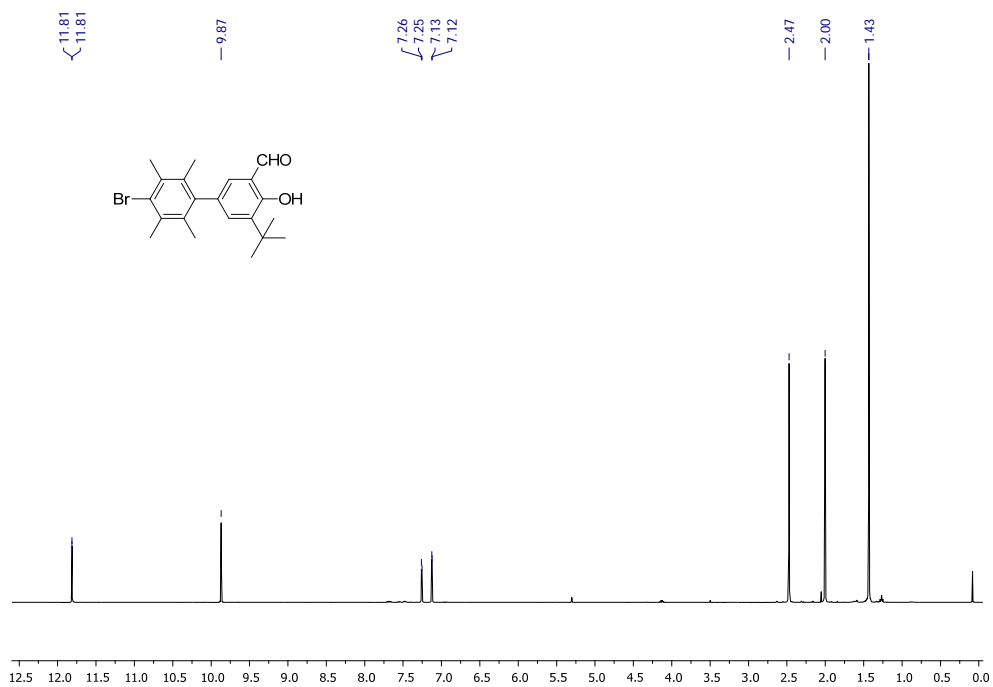


Figure S1. ^1H NMR (400 MHz, CDCl_3) of compound **9**.

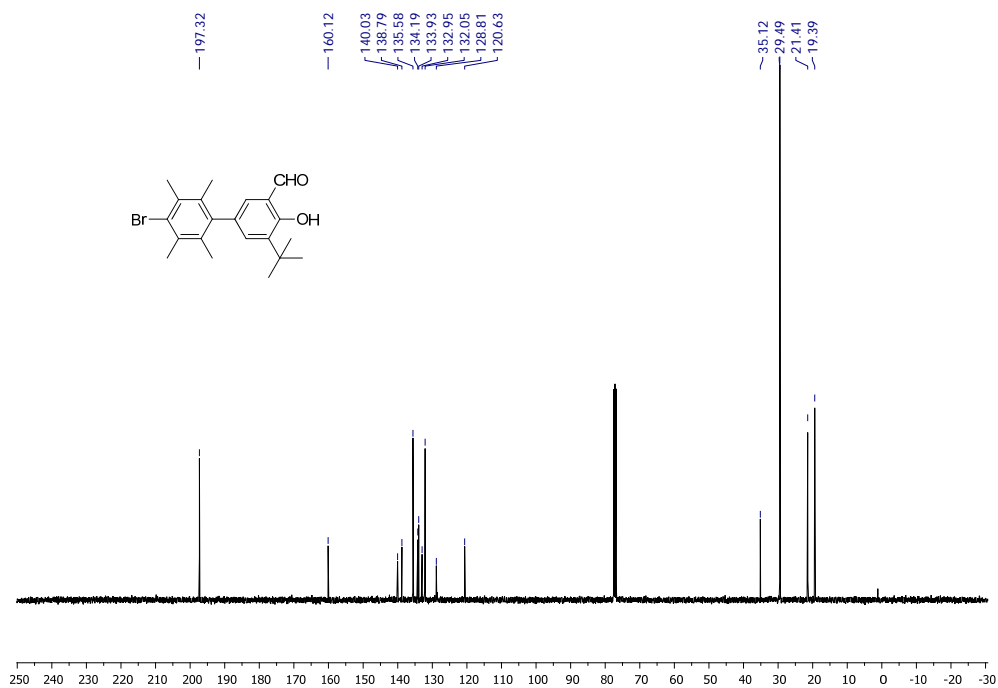


Figure S2. ^{13}C NMR (100 MHz, CDCl_3) of compound **9**.

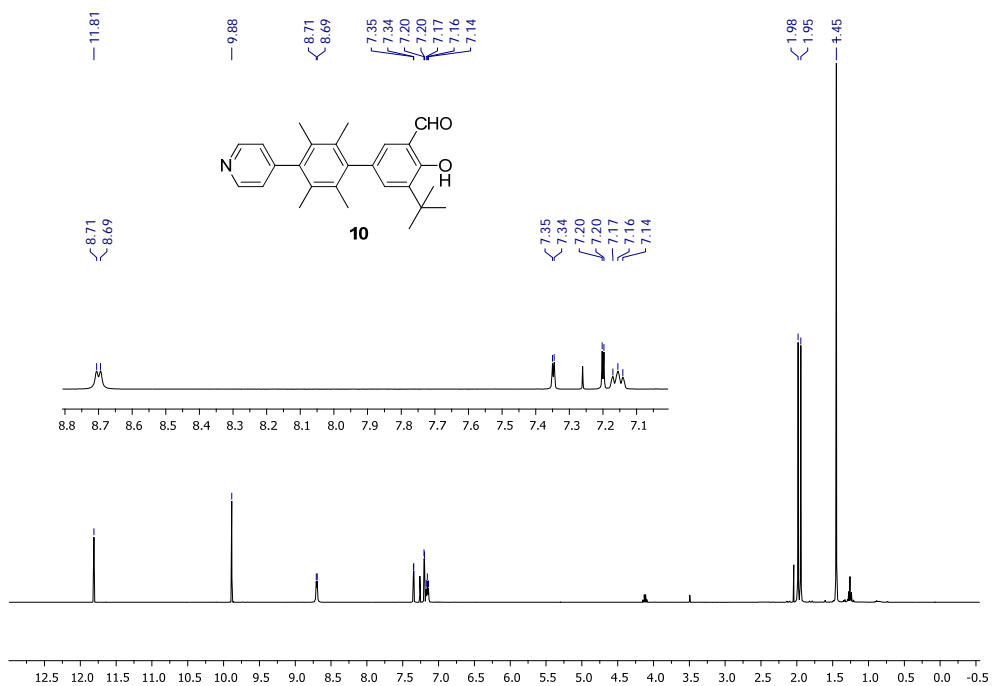


Figure S3. ^1H NMR (400 MHz, CDCl_3) of compound **10**.

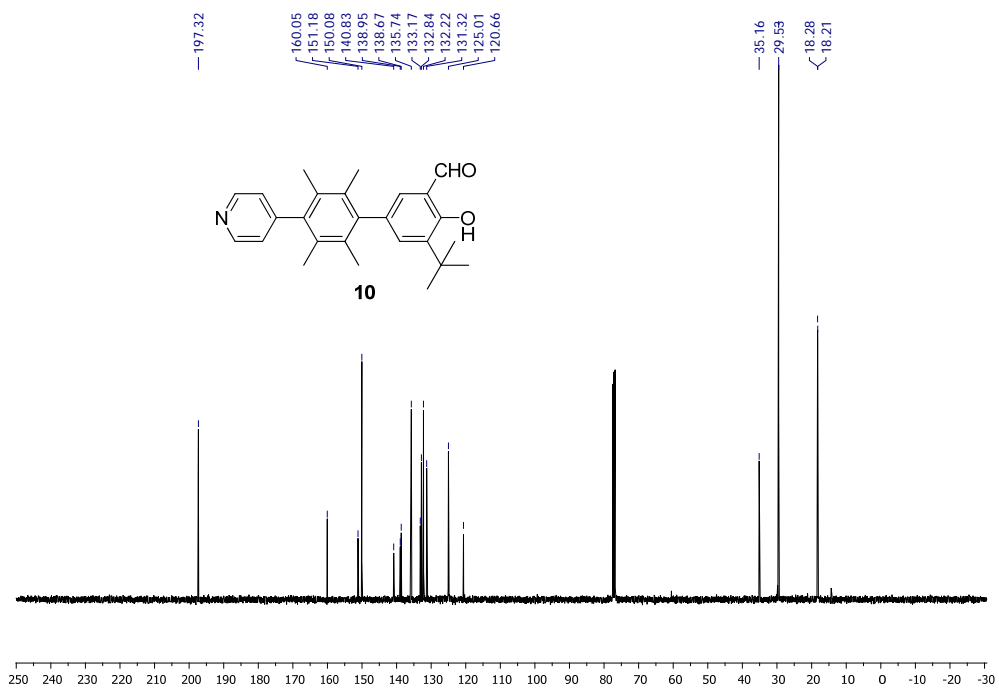


Figure S4. ^{13}C NMR (100 MHz, CDCl_3) of compound **10**.

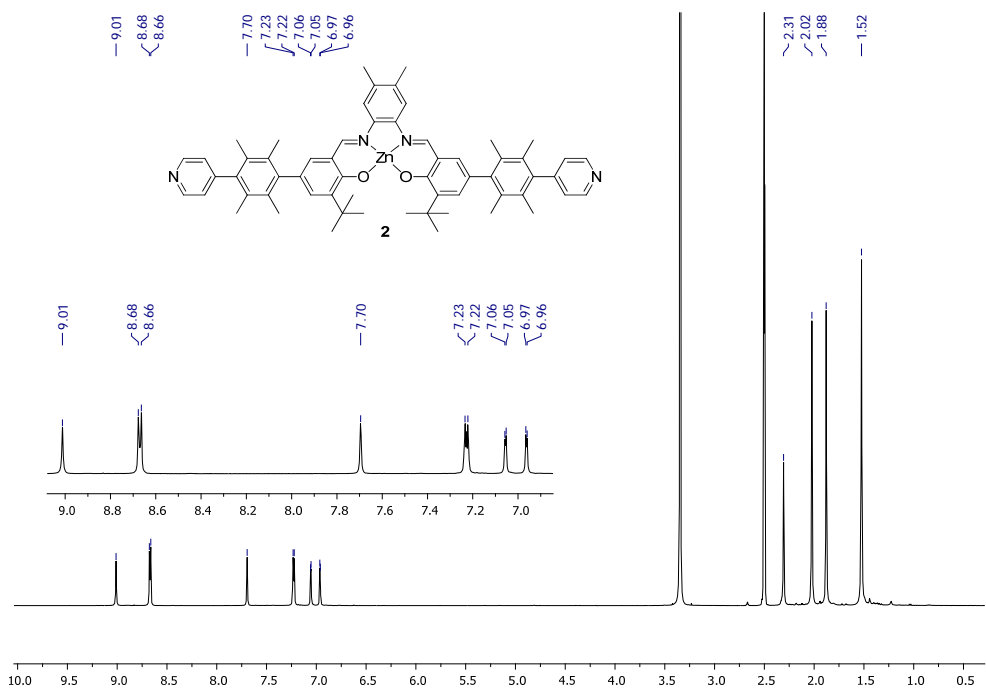


Figure S5. ^1H NMR (400 MHz, DMSO-d_6) of compound 2.

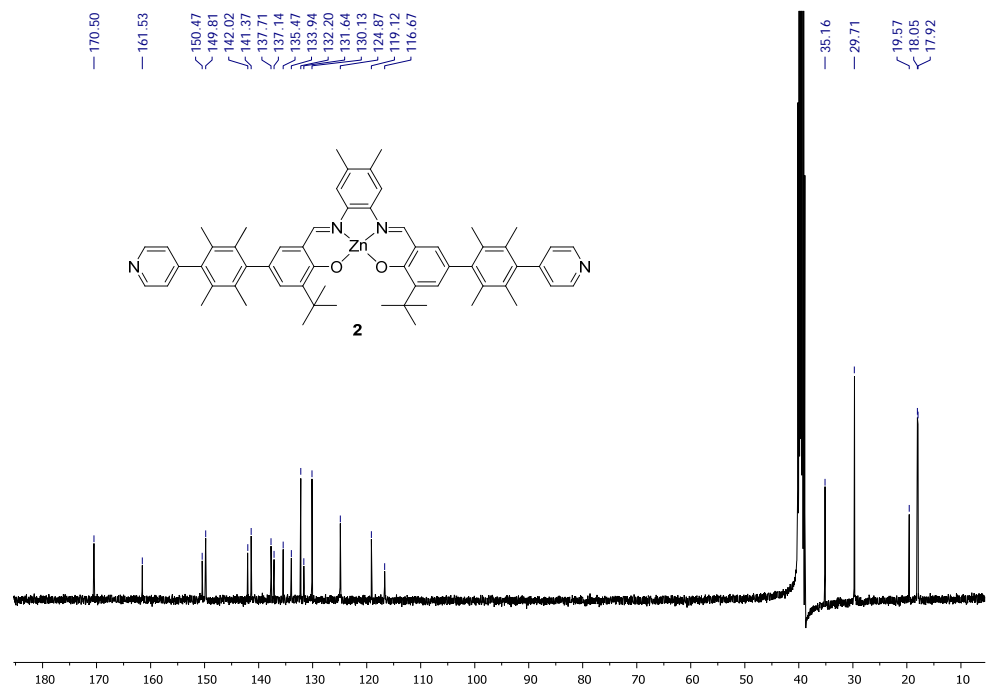


Figure S6. ^{13}C NMR (100 MHz, DMSO-d_6) of compound 2.

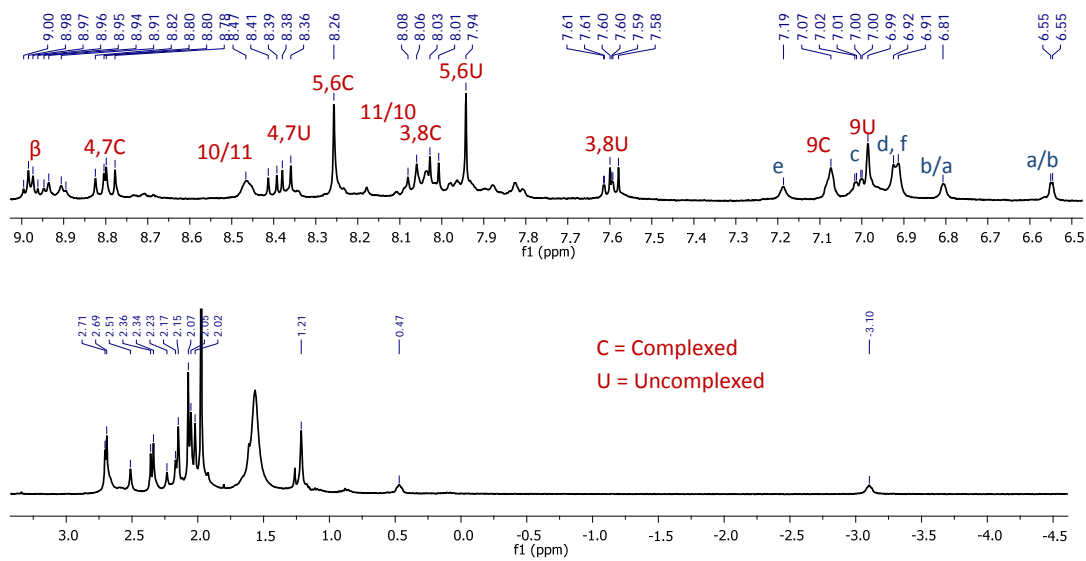


Figure S7. ^1H NMR (400 MHz, CD_2Cl_2) of ROT-1.

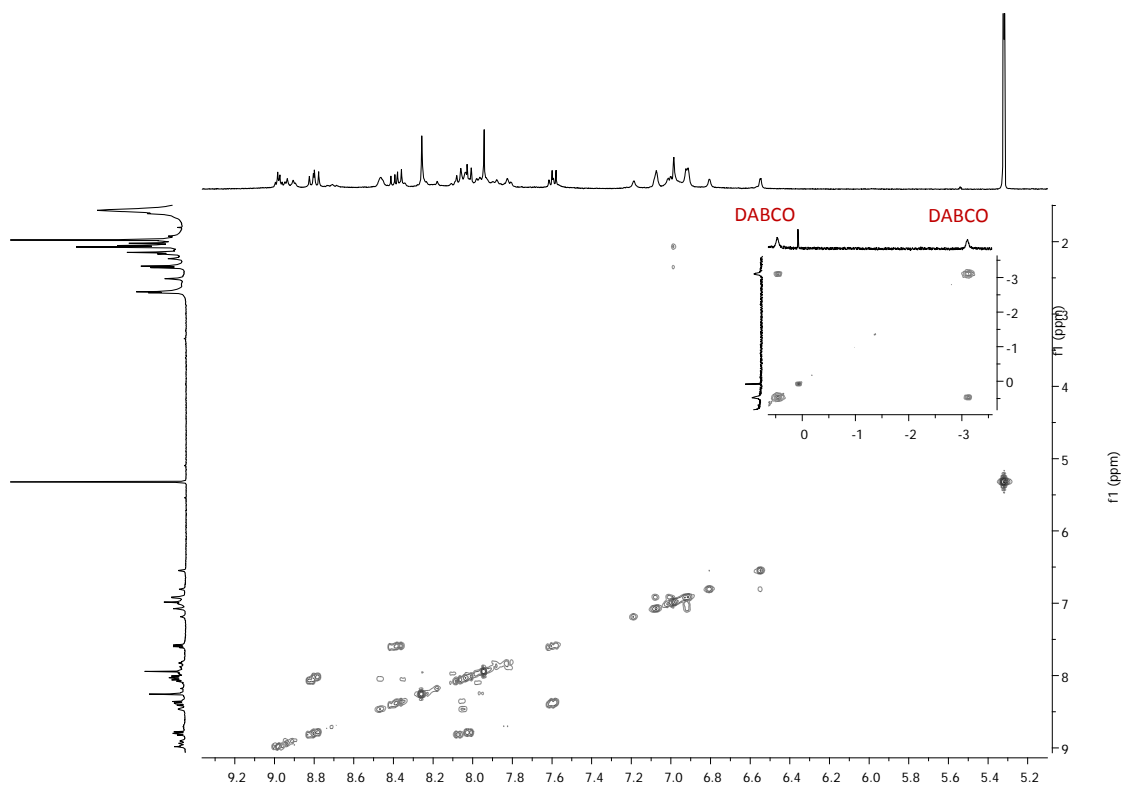


Figure S8. ^1H - ^1H COSY (400 MHz, CD_2Cl_2) of ROT-1.

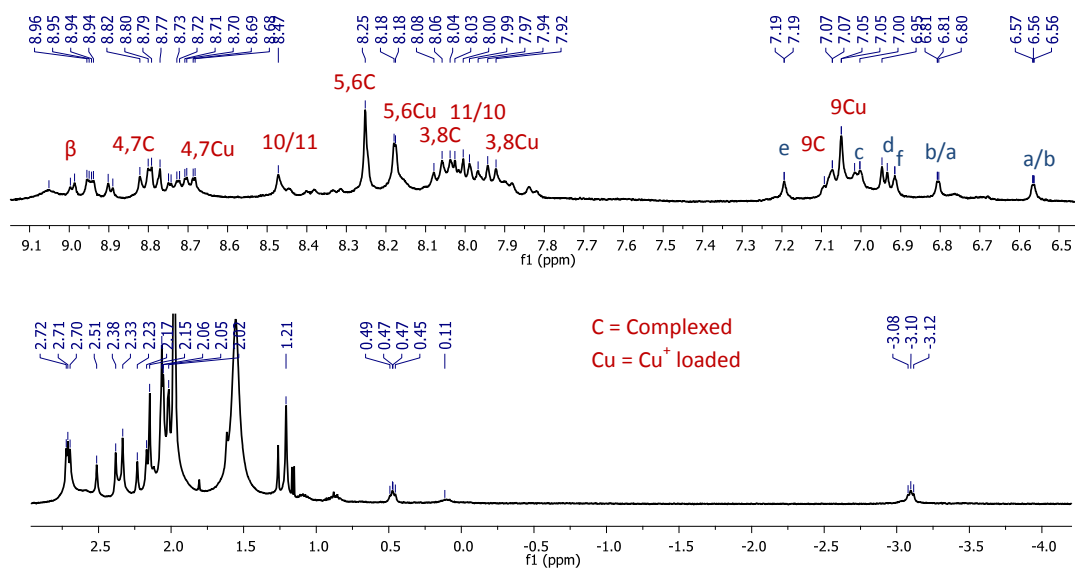


Figure S9. ^1H NMR (400 MHz, CD_2Cl_2) of ROT-2.

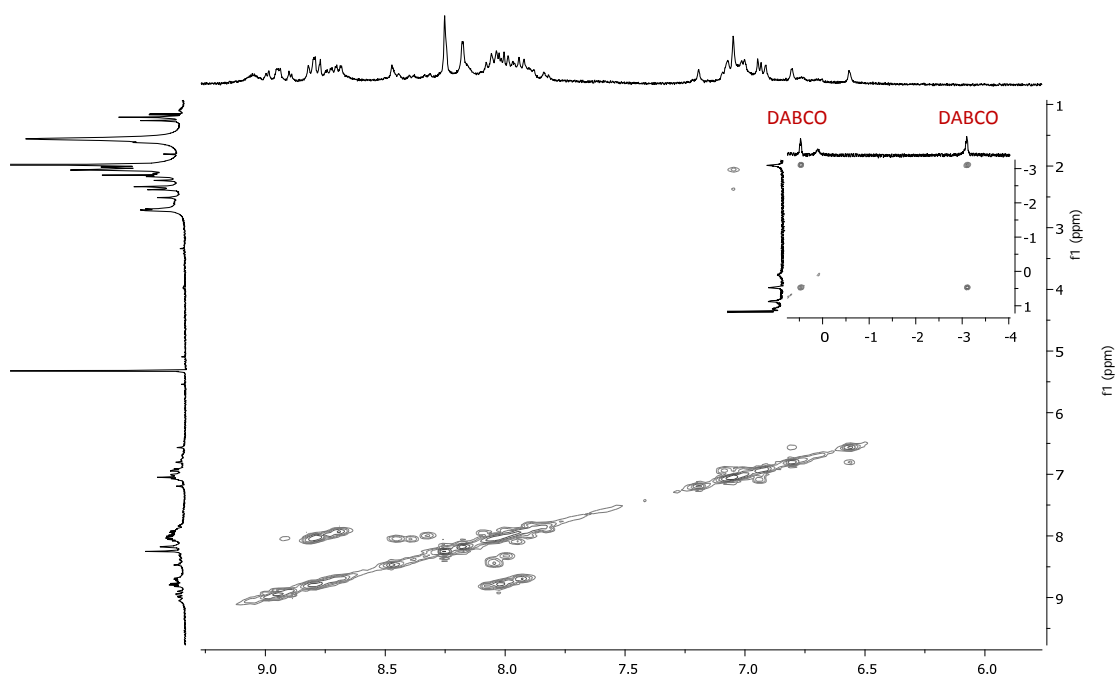


Figure S10. ^1H - ^1H COSY (400 MHz, CD_2Cl_2) of ROT-2.

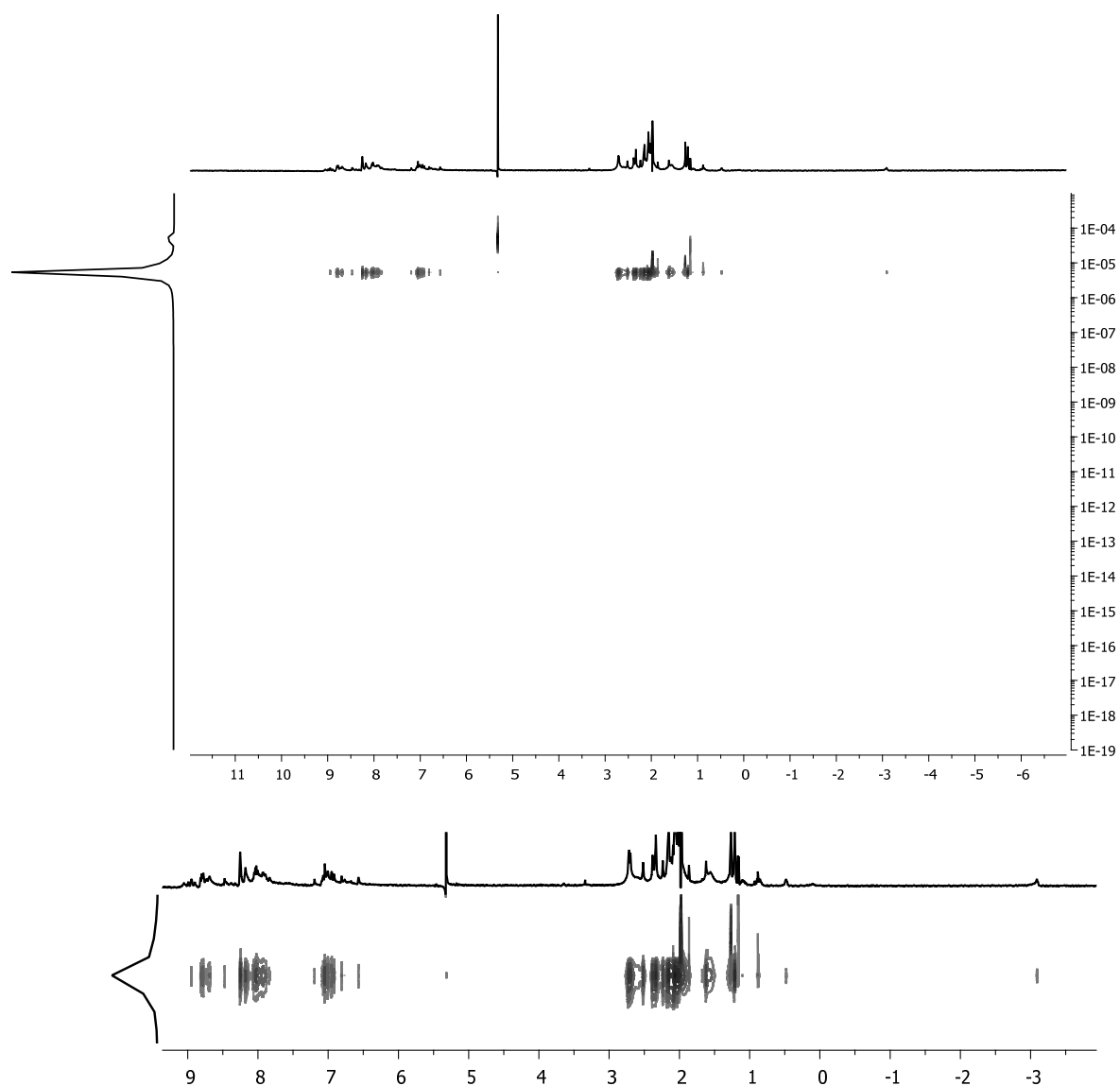


Figure S11. ^1H DOSY NMR (600 MHz, CD_2Cl_2) of **ROT-2**.

The hydrodynamic radius was calculated according to Stokes-Einstein Equation; $D = k_B T / 6\pi\eta R$

D = diffusion coefficient

k_B = Boltzmann constant

T = temperature

η = viscosity of the solution

R = hydrodynamic radius of the particle

$$D = 3.2 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$$

Then, hydrodynamic radius was calculated as $R = 17 \text{ \AA}$

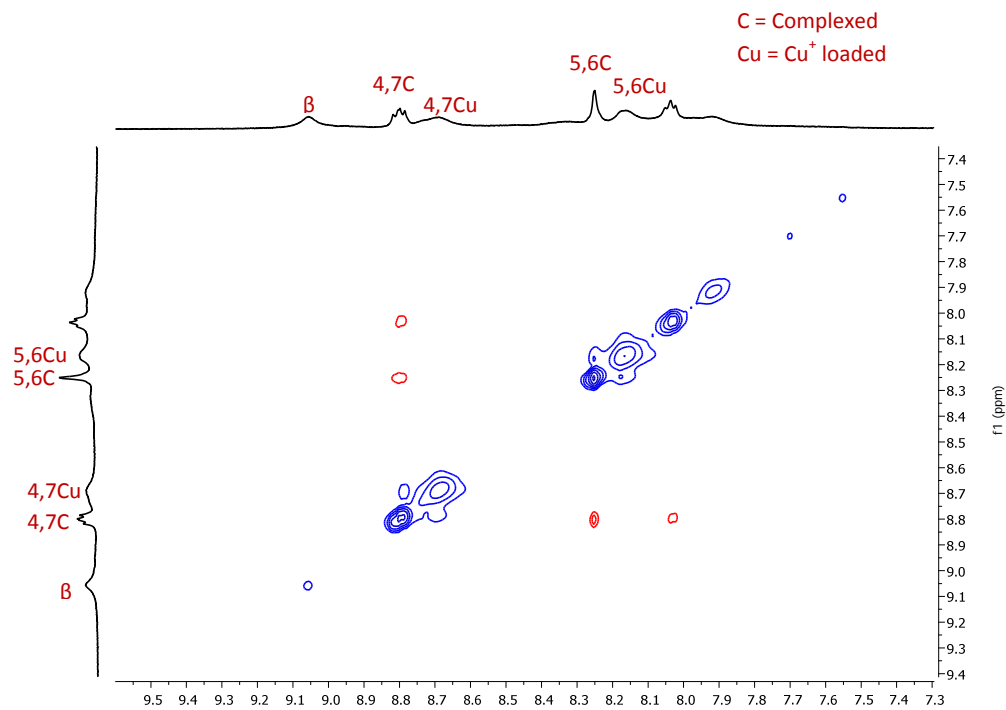


Figure S12. ^1H - ^1H ROESY (600 MHz, CD_2Cl_2) of ROT-2.

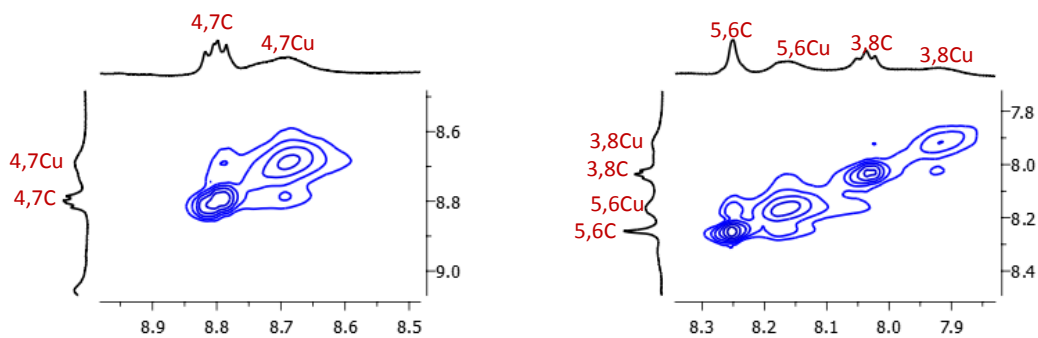


Figure S13. Partial ^1H - ^1H ROESY (600 MHz, CD_2Cl_2) of ROT-2.

Rate constant calculation by volume intensity of the ROESY cross peaks¹

$$I_D/I_C = (1 - kt_M)/kt_M \quad \text{or} \quad k = 1/[t_M(I_D/I_C + 1)]$$

Where I_D : intensity of diagonal peak

I_C : intensity of cross peak

t_M : mixing time (0.3 s)

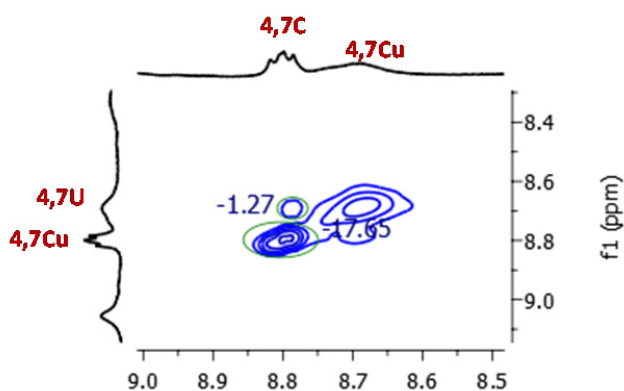


Figure S14. Partial ^1H - ^1H ROESY (600 MHz, CD_2Cl_2) of **ROT-2** with volume intensity of cross and diagonal peaks.

Eyring Equation;

$$k = (k_B T/h) \exp(-\Delta G^\ddagger/RT)$$

k_B : Boltzmann constant

h : Planck's constant

$$k_{298} = 0.2 \text{ s}^{-1}$$

$$\Delta G^\ddagger_{298} = 77.0 \text{ kJ mol}^{-1}$$

ESI-MS

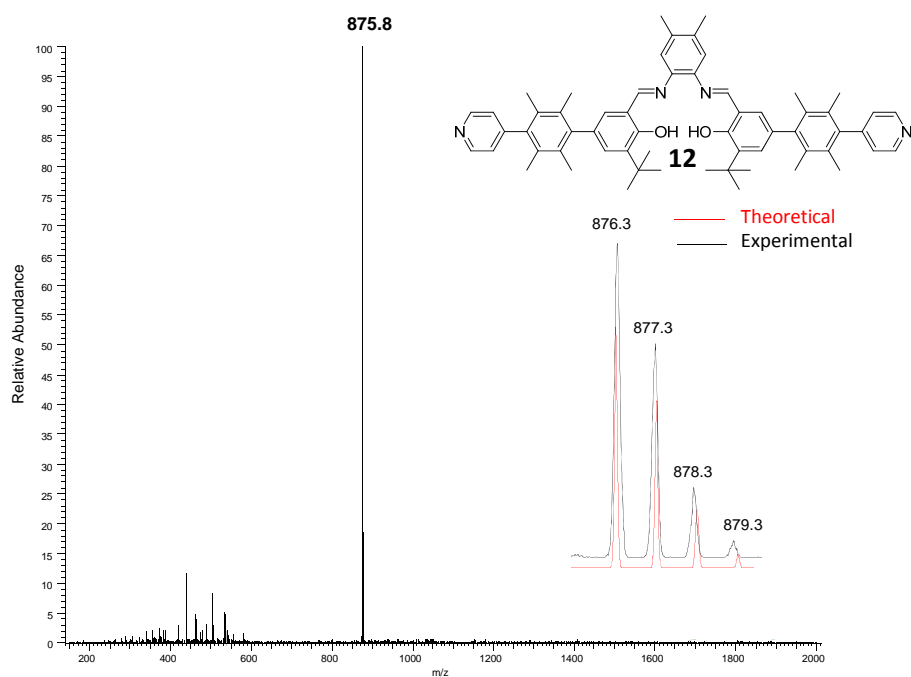


Figure S15. ESI-MS spectrum of **2** in the presence of $\text{CH}_3\text{CO}_2\text{H}$ in CH_2Cl_2 demonstrating demetallation.

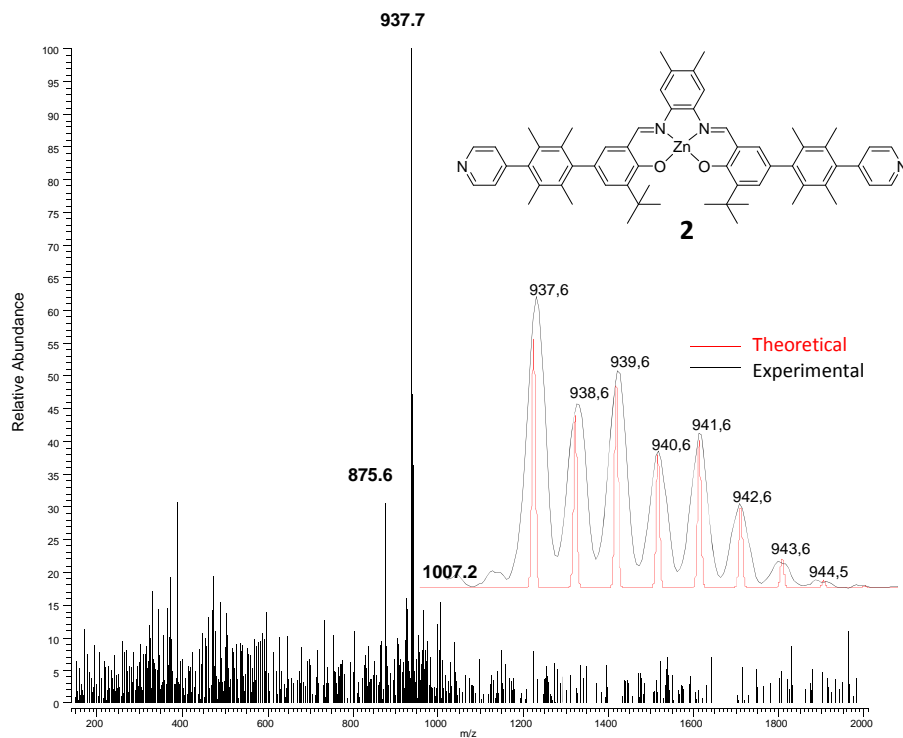


Figure S16. ESI-MS spectrum of $\text{Zn}^{\text{II}}(\text{Salphen})$ [**2** + H] $^+$ in THF.

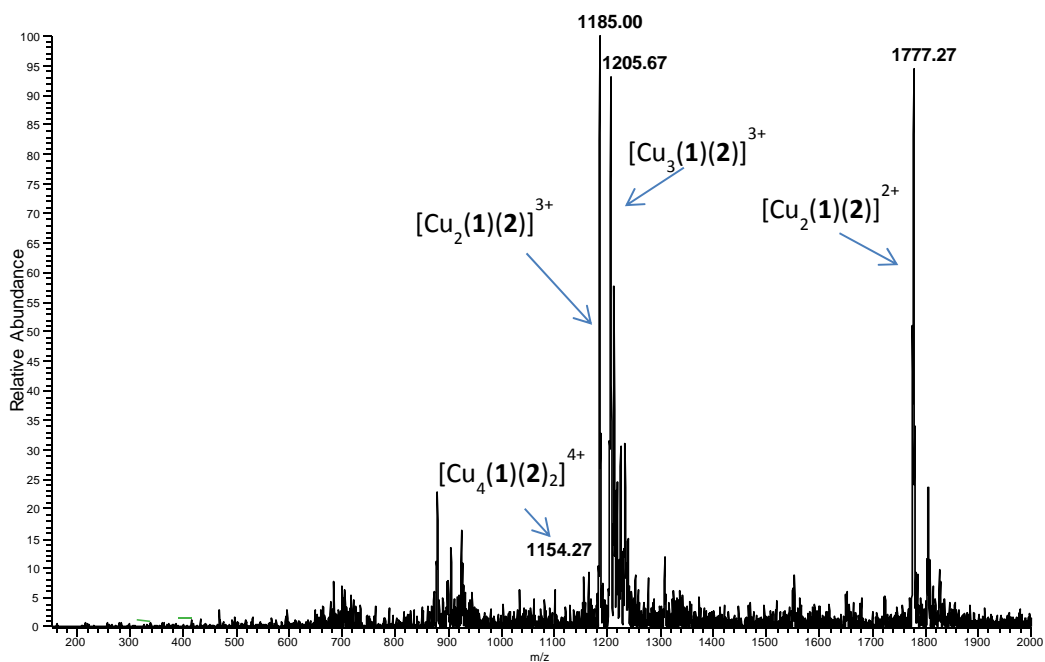


Figure S17. ESI-MS spectrum of rotor **ROT-1** in CH_2Cl_2 .

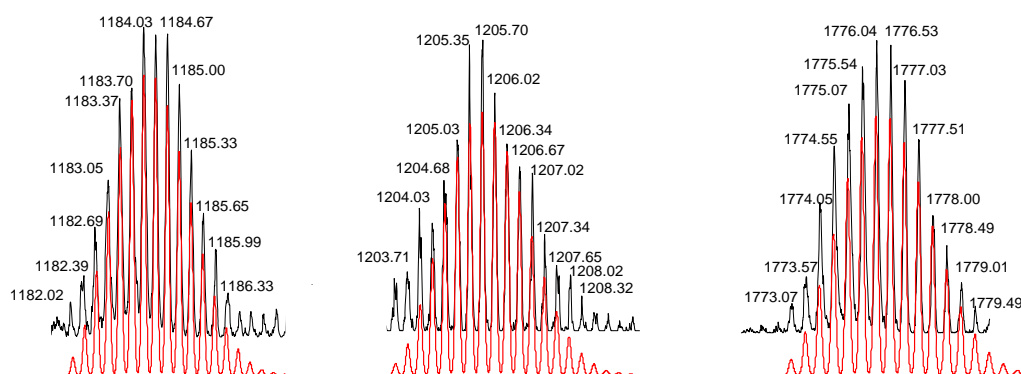


Figure S18. Experimental isotopic distribution (black lines) along with calculated isotopic distribution (red lines) of **ROT-1** for $[\text{Cu}_2(1)(2)]^{3+}$, $[\text{Cu}_3(1)(2)]^{3+}$, $[\text{Cu}_2(1)(2)]^{2+}$ in CH_2Cl_2 .

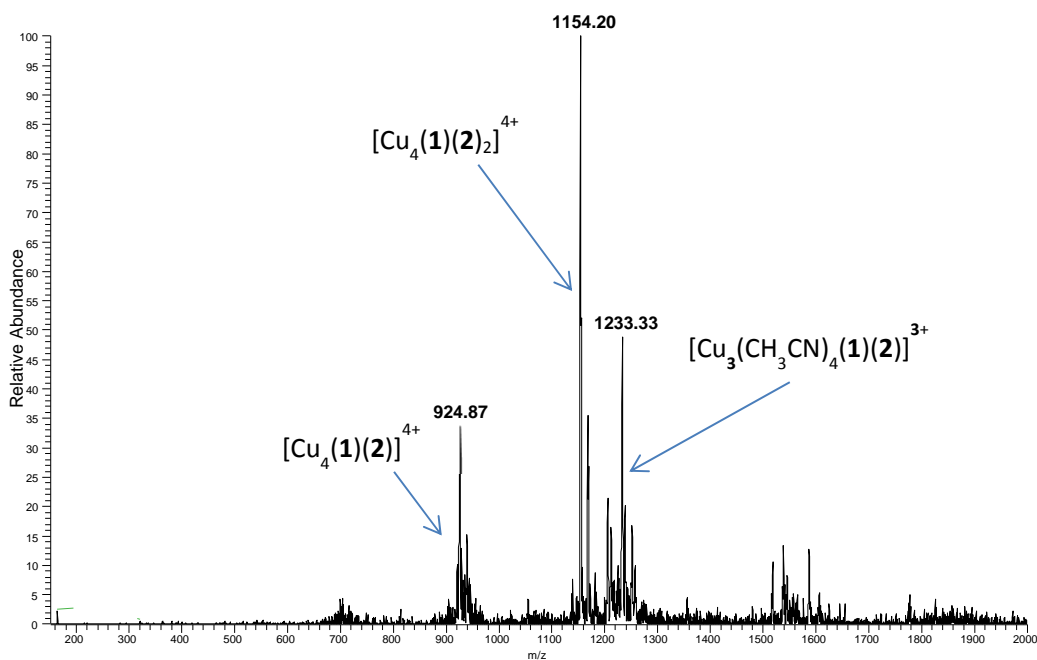


Figure S19. ESI-MS spectrum of rotor **ROT-2** in CH_2Cl_2 .

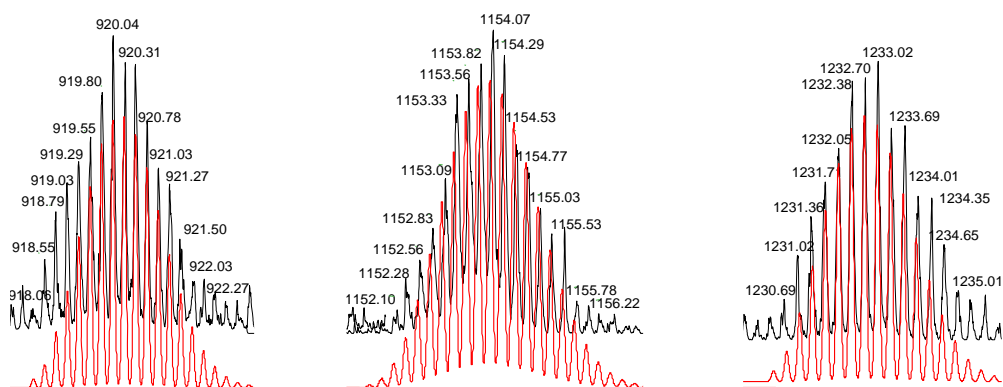


Figure S20. Experimental isotopic distribution (black lines) along with calculated isotopic distribution (red lines) of **ROT-2** for $[\text{Cu}_4(\mathbf{1})(\mathbf{2})]^{4+}$, $[\text{Cu}_4(\mathbf{1})(\mathbf{2})_2]^{4+}$ and $[\text{Cu}_3(\text{CH}_3\text{CN})_2(\mathbf{1})(\mathbf{2})]^{3+}$ in CH_2Cl_2 .

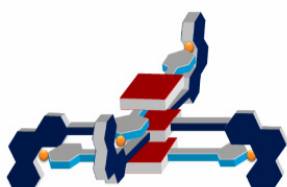


Figure S21. Proposed structure $[\text{Cu}_4(\mathbf{1})(\mathbf{2})_2]^{4+}$ of the common mass for **ROT-1** and **ROT-2** at $m/z = 1154$.

Computations

Construction of model systems **Conf-1_M** and **Conf-2_M**:

The GIAO (gauge-independent atomic orbital) method for PM6, which is integrated with DFT for the ONIOM computations, is not available in *Gaussian 09*. That is why to compute NMR, we first removed the low layer without disturbing the geometry of the high layer and then the removed connecting atoms were placed with hydrogen, keeping the C-H bond distance at 1.08 Å. The model systems constructed, from **Conf-1** and **Conf-2**, by this way are named as **Conf-1_M** and **Conf-2_M**.

Coordinates:

ROT-2'

C	-4.849987000	3.637435000	-0.607376000	H	-13.135253000	0.516343000	-1.735674000
C	-3.594775000	4.145591000	-0.770994000	H	-13.081048000	-0.647006000	2.217565000
C	-2.707805000	4.200228000	0.397350000	C	11.054178000	0.250927000	-1.414668000
C	-3.235729000	3.895875000	1.699093000	C	11.244912000	0.871908000	0.901092000
C	-4.572725000	3.411914000	1.799381000	C	12.336742000	-0.273814000	-1.327193000
H	-5.528078000	3.517176000	-1.455356000	H	10.516641000	0.212671000	-2.353528000
H	-4.968408000	3.156716000	2.782430000	C	12.518562000	0.319405000	0.895842000
C	-2.488646000	4.075599000	2.912763000	H	10.846676000	1.308116000	1.808503000
H	-3.092755000	4.139033000	3.838906000	N	13.074201000	-0.228802000	-0.201938000
N	-1.166740000	4.150211000	2.948915000	H	12.816683000	-0.716236000	-2.189808000
C	-0.437040000	4.388631000	4.158534000	H	13.135232000	0.320355000	1.784957000
C	0.994180000	4.442939000	4.036406000	Zn	0.064527000	3.935598000	1.328460000
C	-1.026721000	4.578239000	5.418736000	N	0.067599000	1.836629000	0.882118000
C	1.771909000	4.688130000	5.179539000	C	-1.181649000	1.466743000	0.108291000
C	-0.230703000	4.814015000	6.543019000	C	1.264300000	1.499763000	0.016062000
H	-2.111127000	4.552100000	5.526966000	C	0.121928000	0.937491000	2.101502000
C	1.161891000	4.869617000	6.423821000	C	-1.164331000	-0.014674000	-0.319501000
H	2.857682000	4.747477000	5.102341000	H	-1.259987000	2.139553000	-0.790311000
N	1.526949000	4.239831000	2.721327000	H	-2.080945000	1.679027000	0.730368000
C	2.827204000	4.243671000	2.470056000	C	1.275829000	0.013472000	-0.388100000
H	3.567346000	4.371628000	3.284432000	H	2.201617000	1.760930000	0.556996000
C	3.382102000	4.055082000	1.158085000	H	1.240714000	2.152068000	-0.903629000
C	4.732017000	3.611494000	1.066028000	C	0.119796000	-0.556222000	1.687629000
C	2.640470000	4.272390000	-0.055761000	H	1.032105000	1.178216000	2.691580000
H	5.289365000	3.422124000	1.983498000	H	-0.747197000	1.160427000	2.757417000
C	3.330124000	4.173723000	-1.346013000	H	-1.208375000	-0.091462000	-1.428604000
C	4.611402000	3.699231000	-1.359958000	H	-2.063976000	-0.544934000	0.067115000
H	5.143868000	3.542915000	-2.302146000	N	0.079947000	-0.717882000	0.181828000
O	-1.486770000	4.479984000	0.183669000	H	2.210343000	-0.481604000	-0.040769000
O	1.389987000	4.491144000	-0.072348000	H	1.273068000	-0.083607000	-1.498224000
C	-11.295834000	1.015758000	-0.719280000	H	1.023959000	-1.068311000	2.082678000
C	-11.259414000	0.322062000	1.585090000	H	-0.755156000	-1.084424000	2.129144000
C	-12.577187000	0.488172000	-0.809372000	Zn	0.093962000	-2.860223000	-0.448304000
H	-10.832089000	1.464995000	-1.588610000	N	-0.994045000	-2.600277000	-2.207113000
C	-12.540051000	-0.181667000	1.403363000	C	-0.474530000	-2.195373000	-3.439899000
H	-10.779919000	0.250604000	2.552642000	C	-2.385238000	-2.609578000	-2.335926000
N	-13.198812000	-0.099887000	0.230968000	C	0.881055000	-1.984561000	-3.725886000

C	-1.592281000	-1.987345000	-4.390523000	C	-0.980048000	-3.623590000	5.133989000
C	-3.299088000	-2.868095000	-1.301852000	C	-1.425144000	-5.875087000	4.328431000
C	-2.744228000	-2.248191000	-3.726980000	C	-10.127861000	-2.470422000	-2.205717000
C	1.947636000	-2.290377000	-2.854779000	H	3.943158000	-4.482499000	2.860426000
C	1.218592000	-1.351090000	-5.025600000	C	6.836043000	-2.493070000	1.733944000
H	-1.445499000	-1.693944000	-5.415223000	H	4.811376000	-1.786233000	1.966192000
C	-2.942634000	-3.215827000	0.019623000	C	7.137892000	-4.363788000	0.195373000
C	-4.745908000	-2.769889000	-1.606930000	H	5.338151000	-5.103929000	-0.745647000
H	-3.756481000	-2.225814000	-4.088650000	H	1.631420000	-4.893229000	4.226693000
N	1.830937000	-2.773930000	-1.548401000	C	-1.301278000	-4.029335000	6.431788000
C	3.360262000	-2.133198000	-3.191372000	H	-0.683295000	-2.596547000	4.936126000
C	1.554467000	-2.131093000	-6.140061000	C	-1.743093000	-6.272610000	5.629412000
C	1.204908000	0.049701000	-5.119809000	H	-1.472843000	-6.587357000	3.505096000
N	-1.642837000	-3.382211000	0.504451000	C	-11.551653000	-2.479763000	-2.294306000
C	-3.897070000	-3.477864000	1.095919000	C	7.683520000	-3.410194000	1.077718000
C	-5.537375000	-3.932249000	-1.603867000	H	7.258280000	-1.768549000	2.428914000
C	-5.335538000	-1.520300000	-1.861259000	H	7.789921000	-5.091052000	-0.286993000
C	3.132051000	-2.926855000	-1.062130000	C	-1.681593000	-5.352087000	6.680871000
C	4.086013000	-2.524394000	-2.095038000	H	-2.038353000	-7.303141000	5.824396000
H	3.718221000	-1.780314000	-4.139895000	C	-12.190062000	-1.670228000	-3.258063000
C	1.877115000	-1.506157000	-7.348020000	C	-12.285348000	-3.306885000	-1.414899000
H	1.563310000	-3.217381000	-6.059010000	C	9.081419000	-3.336738000	1.275482000
C	1.533477000	0.665884000	-6.328934000	C	-13.595683000	-1.685059000	-3.340949000
H	0.938533000	0.648912000	-4.251522000	C	-11.397585000	-0.744150000	-4.162678000
C	-1.761046000	-3.783319000	1.837960000	C	-13.686920000	-3.344990000	-1.525360000
C	-3.173671000	-3.830366000	2.207036000	C	-11.601061000	-4.121432000	-0.331412000
H	-4.961673000	-3.402454000	0.994406000	C	10.279274000	-3.234364000	1.422412000
C	-6.912803000	-3.841194000	-1.804829000	C	-14.323748000	-2.530120000	-2.480179000
H	-5.068027000	-4.903661000	-1.437508000	C	-14.291664000	-0.738740000	-4.306215000
C	-6.713611000	-1.422928000	-2.060283000	H	-11.663925000	0.304852000	-3.973591000
H	-4.716881000	-0.623463000	-1.891139000	H	-10.319943000	-0.851907000	-3.999449000
C	3.486382000	-3.373705000	0.227863000	H	-11.603446000	-0.951022000	-5.218827000
H	5.151606000	-2.549019000	-1.981104000	C	-14.496643000	-4.217461000	-0.582625000
H	2.135585000	-2.109637000	-8.217518000	H	-11.797290000	-5.192713000	-0.455797000
C	1.868659000	-0.110890000	-7.443451000	H	-10.516629000	-3.970340000	-0.340956000
H	1.528073000	1.752650000	-6.402816000	H	-11.976417000	-3.823480000	0.656217000
C	-0.697671000	-4.121185000	2.701181000	C	11.685546000	-3.121172000	1.628427000
H	-3.533647000	-4.102824000	3.180868000	C	-15.811115000	-2.378831000	-2.429481000
C	-7.512232000	-2.581577000	-2.013105000	H	-14.065667000	0.305848000	-4.049127000
H	-7.529244000	-4.739853000	-1.799234000	H	-13.946457000	-0.902779000	-5.333508000
H	-7.175467000	-0.450288000	-2.230405000	H	-15.376457000	-0.857940000	-4.288229000
C	2.570114000	-3.748540000	1.225092000	H	-15.545928000	-4.265537000	-0.884026000
C	4.929492000	-3.426407000	0.558062000	H	-14.099570000	-5.237929000	-0.554691000
C	0.659153000	-4.091773000	2.353592000	H	-14.460543000	-3.807651000	0.433671000
C	-1.041594000	-4.548778000	4.081189000	C	12.153242000	-2.376092000	2.733531000
C	-8.919269000	-2.501497000	-2.138222000	C	12.572177000	-3.757905000	0.731373000
C	2.930128000	-4.292296000	2.554988000	C	-16.716954000	-3.013130000	-3.310709000
N	1.181078000	-3.654874000	1.131073000	N	-16.228934000	-1.522646000	-1.497518000
C	5.467056000	-2.502157000	1.471953000	C	13.540884000	-2.260639000	2.941649000
C	5.766931000	-4.370116000	-0.060698000	C	11.196105000	-1.661244000	3.670391000
C	1.777369000	-4.499297000	3.236148000	C	13.956873000	-3.664581000	0.960684000

C	12.066287000	-4.508218000	-0.487381000	C	-14.536677000	1.904002000	3.743276000
C	-18.066114000	-2.712990000	-3.232954000	C	-16.825190000	0.828427000	3.964577000
H	-16.335299000	-3.714102000	-4.042344000	C	20.043859000	0.120956000	1.440151000
C	-17.539845000	-1.194420000	-1.438381000	H	20.540571000	-1.377780000	2.870987000
C	14.422526000	-2.908042000	2.053584000	C	19.224750000	1.834093000	-0.225878000
C	14.050710000	-1.392656000	4.080673000	Cu	15.024803000	-0.757167000	-0.224494000
H	10.153146000	-1.832936000	3.384585000	C	16.938295000	1.628138000	-0.982638000
H	11.327148000	-2.001507000	4.703698000	H	-13.013827000	3.364210000	1.085582000
H	11.373923000	-0.577875000	3.651009000	C	-13.540718000	2.557754000	3.007907000
C	14.931494000	-4.332937000	0.006678000	H	-15.184154000	1.893670000	-0.996796000
H	12.346109000	-5.567507000	-0.445949000	H	-16.183671000	3.298284000	-0.597993000
H	10.976159000	-4.447064000	-0.570195000	H	-14.426680000	3.491124000	-0.802660000
H	12.502054000	-4.082815000	-1.400677000	H	-14.354112000	1.654023000	4.784114000
C	-18.518296000	-1.757935000	-2.290103000	H	-17.685642000	1.477745000	4.162961000
H	-18.777827000	-3.185838000	-3.900692000	H	-17.190040000	-0.045686000	3.412989000
C	-17.916450000	-0.173548000	-0.489230000	H	-16.422863000	0.500001000	4.928092000
C	15.876792000	-2.565557000	2.125042000	H	21.023382000	0.584580000	1.461651000
H	15.139340000	-1.411722000	4.156354000	C	18.178485000	2.308571000	-0.997967000
H	13.742620000	-0.347415000	3.937134000	H	20.183385000	2.340746000	-0.221116000
H	13.635984000	-1.723927000	5.039567000	C	15.732500000	2.044170000	-1.759574000
H	14.643247000	-5.372562000	-0.182193000	C	-12.217370000	2.930730000	3.648527000
H	14.946601000	-3.801768000	-0.952382000	H	18.286529000	3.196838000	-1.607603000
H	15.948837000	-4.327196000	0.406033000	C	14.618315000	2.550747000	-1.059446000
C	-19.883713000	-1.319177000	-2.166528000	C	15.652776000	1.767169000	-3.135039000
C	-19.258987000	0.265197000	-0.414735000	H	-11.434837000	3.033541000	2.882311000
N	-16.927105000	0.351324000	0.261820000	H	-12.301229000	3.884491000	4.182567000
C	16.815474000	-3.167248000	2.993567000	H	-11.896776000	2.167767000	4.366141000
N	16.219086000	-1.565305000	1.312842000	C	13.426900000	2.761998000	-1.753389000
C	-20.238416000	-0.350237000	-1.270770000	C	14.711207000	2.837652000	0.429594000
H	-20.629066000	-1.767035000	-2.813679000	C	14.438867000	1.984541000	-3.797951000
C	-19.532503000	1.312469000	0.499170000	C	16.860309000	1.212457000	-3.874604000
Cu	-15.093411000	-0.746133000	0.100578000	H	12.551711000	3.126432000	-1.212479000
C	-17.190050000	1.353420000	1.098265000	C	13.316224000	2.473935000	-3.118887000
C	18.112474000	-2.684777000	3.032785000	H	14.911197000	1.911742000	0.979765000
H	16.499135000	-3.989354000	3.623060000	H	15.529633000	3.534822000	0.642330000
C	17.474766000	-1.067152000	1.364208000	H	13.776261000	3.266758000	0.799406000
H	-21.268232000	-0.019692000	-1.199096000	H	14.370132000	1.779172000	-4.862696000
C	-18.503060000	1.860248000	1.246008000	H	17.682222000	1.936646000	-3.881797000
H	-20.544958000	1.689136000	0.593594000	H	17.227289000	0.301918000	-3.385871000
C	-15.984918000	1.876686000	1.809243000	H	16.608763000	0.980722000	-4.913670000
C	18.476753000	-1.585528000	2.218091000	C	12.007911000	2.722585000	-3.844499000
H	18.848518000	-3.128920000	3.693751000	H	11.156509000	2.507403000	-3.188116000
C	17.760387000	0.077391000	0.531401000	H	11.935502000	3.771395000	-4.156070000
H	-18.680024000	2.679726000	1.931093000	H	11.923634000	2.097439000	-4.739204000
C	-14.994781000	2.536136000	1.051874000	C	-10.612630000	0.943521000	0.505800000
C	-15.761814000	1.560457000	3.161313000	C	-5.344604000	3.235266000	0.679330000
C	19.775940000	-0.966695000	2.222019000	C	-6.700066000	2.642935000	0.738539000
C	19.037678000	0.684491000	0.579640000	C	-7.825912000	3.490338000	0.673260000
N	16.753455000	0.537188000	-0.240747000	C	-6.848891000	1.245005000	0.822418000
C	-13.789745000	2.875352000	1.668655000	C	-9.114567000	2.927099000	0.636617000
C	-15.209513000	2.828496000	-0.423857000	C	-8.140869000	0.679287000	0.773918000

C	-9.259713000	1.524084000	0.648152000	C	5.489478000	0.555025000	-0.679449000
C	-7.627667000	4.972174000	0.624616000	H	4.645679000	0.952955000	-0.099691000
H	-8.510975000	5.530572000	0.966941000	H	5.180083000	0.555114000	-1.735539000
H	-6.780623000	5.293887000	1.250065000	H	5.616484000	-0.497859000	-0.380727000
H	-7.404536000	5.305210000	-0.400084000	C	8.118643000	-0.719002000	-0.840940000
C	-10.332434000	3.795881000	0.589539000	H	8.251576000	-0.892161000	-1.917536000
H	-10.779598000	3.804651000	-0.413274000	H	8.955174000	-1.199323000	-0.316044000
H	-11.101568000	3.459448000	1.308163000	H	7.209291000	-1.272787000	-0.547806000
H	-10.105101000	4.844979000	0.843032000	C	7.693729000	5.007025000	0.087787000
C	-8.330684000	-0.801683000	0.861646000	H	6.746495000	5.408116000	-0.306142000
H	-8.546860000	-1.109682000	1.893314000	H	7.724378000	5.258911000	1.157102000
H	-9.149189000	-1.162480000	0.223313000	H	8.500664000	5.564397000	-0.408473000
H	-7.428130000	-1.355216000	0.547867000	C	10.316880000	3.740932000	-0.018784000
C	-5.637329000	0.378696000	0.971383000	H	10.558109000	3.911135000	1.039692000
H	-4.782597000	0.764129000	0.397583000	H	11.202258000	3.288183000	-0.497719000
H	-5.324268000	0.324837000	2.023458000	H	10.190701000	4.734785000	-0.479267000
H	-5.811727000	-0.655436000	0.632497000	H	-1.254020000	-3.314262000	7.251482000
C	-3.054410000	4.606330000	-2.128000000	H	-1.928713000	-5.666155000	7.693789000
C	-4.182180000	4.738590000	-3.174016000	H	2.121556000	0.371432000	-8.386379000
H	-4.689213000	3.788409000	-3.360988000	H	1.776343000	5.061485000	7.303668000
H	-4.931477000	5.473338000	-2.862377000	H	-0.700223000	4.961804000	7.515788000
H	-3.779511000	5.081075000	-4.133821000	C	15.168593000	-1.652051000	-3.295186000
C	-2.375997000	5.979609000	-1.978744000	C	-15.555110000	-2.295105000	2.932232000
H	-3.041564000	6.709959000	-1.511502000	C	-15.849954000	-2.839981000	4.257357000
H	-1.474867000	5.911060000	-1.343380000	H	-14.931641000	-3.206573000	4.729006000
H	-2.055217000	6.381555000	-2.942635000	H	-16.287452000	-2.058172000	4.887455000
C	-2.033638000	3.560651000	-2.626841000	H	-16.560601000	-3.669519000	4.173595000
H	-1.271319000	3.366018000	-1.850749000	C	15.087770000	-1.718770000	-4.753227000
H	-2.516714000	2.617107000	-2.887575000	H	16.088509000	-1.832979000	-5.182761000
H	-1.495954000	3.922425000	-3.508461000	H	14.468164000	-2.567344000	-5.062574000
C	2.584204000	4.482438000	-2.648517000	H	14.643018000	-0.790595000	-5.129510000
C	1.574294000	5.626930000	-2.474510000	N	15.218381000	-1.567391000	-2.140762000
H	0.737026000	5.335245000	-1.813309000	N	-15.330741000	-1.854543000	1.884754000
H	2.035651000	6.505873000	-2.014808000	ROT-3'			
H	1.136141000	5.933859000	-3.426615000	N	1.495558000	0.826719000	-4.796337000
C	1.845946000	3.191635000	-3.073389000	C	1.343231000	2.191808000	-5.046665000
H	2.546965000	2.388388000	-3.314992000	C	2.862490000	0.603631000	-4.602516000
H	1.185380000	2.843185000	-2.261720000	C	2.652716000	2.835484000	-5.026455000
H	1.217657000	3.367738000	-3.951038000	C	3.581293000	1.867478000	-4.731889000
C	3.574018000	4.889834000	-3.762142000	H	2.811211000	3.881431000	-5.212464000
H	4.143493000	5.780377000	-3.474951000	H	4.641387000	1.979423000	-4.624033000
H	4.286538000	4.095062000	-3.999902000	N	-1.396618000	0.926448000	-4.876696000
H	3.041775000	5.132920000	-4.687671000	C	-2.770568000	0.794305000	-4.702984000
C	10.490137000	0.863836000	-0.284749000	C	-1.144879000	2.280980000	-5.139666000
C	5.314625000	3.374104000	-0.154396000	C	-3.418265000	2.104943000	-4.912430000
C	6.651392000	2.746215000	-0.254951000	C	-2.439442000	2.999489000	-5.200806000
C	7.812942000	3.530184000	-0.117742000	H	-4.480070000	2.255368000	-4.857397000
C	6.738072000	1.358470000	-0.487732000	H	-2.516346000	4.046812000	-5.435555000
C	9.078448000	2.911393000	-0.159970000	N	-1.482727000	-1.941855000	-4.564428000
C	8.004708000	0.741560000	-0.545419000	C	-1.330271000	-3.329209000	-4.537149000
C	9.163981000	1.515171000	-0.337039000				

C	-2.849647000	-1.684978000	-4.416329000	H	5.812384000	-0.205992000	-5.667547000
C	-2.641249000	-3.956518000	-4.406291000	C	6.282720000	-0.905635000	-1.858606000
C	-3.570264000	-2.949453000	-4.309289000	H	4.147599000	-1.167912000	-1.801522000
H	-2.800534000	-5.018632000	-4.391421000	C	7.399547000	-0.603342000	-2.664795000
H	-4.631674000	-3.037526000	-4.192783000	H	8.095141000	-0.142474000	-4.665543000
N	1.410902000	-2.049851000	-4.568356000	H	6.418513000	-1.114472000	-0.797002000
C	2.787091000	-1.886846000	-4.434655000	C	8.676514000	-0.538366000	-2.058812000
C	1.159546000	-3.429028000	-4.565765000	C	9.744840000	-0.475481000	-1.493378000
C	3.434339000	-3.213373000	-4.391477000	C	-8.606275000	-0.013398000	-2.007607000
C	2.454184000	-4.146473000	-4.489979000	C	-9.674226000	0.059416000	-1.442632000
H	4.496773000	-3.351103000	-4.317490000	C	10.976959000	-0.379559000	-0.791126000
H	2.530233000	-5.219654000	-4.513081000	C	12.136956000	0.102553000	-1.418915000
C	0.116591000	2.874930000	-5.224745000	C	11.045811000	-0.735716000	0.564653000
C	-3.434354000	-0.402264000	-4.356284000	C	13.294136000	0.234372000	-0.660874000
C	-0.101313000	-4.030369000	-4.545394000	H	12.130469000	0.388132000	-2.463795000
C	3.453593000	-0.647277000	-4.323833000	C	12.256237000	-0.589930000	1.231350000
Zn	0.003697000	-0.538038000	-4.462114000	H	10.170759000	-1.096553000	1.093336000
C	-1.042065000	-1.204827000	-1.577383000	H	14.206166000	0.628840000	-1.093545000
C	1.328160000	-0.621375000	-1.638159000	H	12.355658000	-0.856461000	2.276283000
C	-0.361818000	1.126071000	-1.845634000	C	-10.912507000	0.144264000	-0.749420000
C	-1.046124000	-1.026794000	-0.042479000	C	-10.998722000	0.846961000	0.462487000
H	-0.817576000	-2.259690000	-1.851957000	C	-12.065058000	-0.488572000	-1.242720000
H	-2.049747000	-0.989490000	-1.997558000	C	-12.220441000	0.887629000	1.123513000
C	1.326706000	-0.451614000	-0.103326000	C	-13.234395000	-0.411527000	-0.495501000
H	2.092511000	0.044104000	-2.100724000	H	-12.335207000	1.425227000	2.056821000
H	1.603846000	-1.663730000	-1.910314000	H	-14.141998000	-0.907412000	-0.819374000
H	0.373526000	1.813710000	-2.322467000	N	-13.320536000	0.268260000	0.662106000
H	-1.356131000	1.394924000	-2.263765000	N	13.362245000	-0.107996000	0.638780000
C	-0.359589000	1.304326000	-0.310997000	C	-0.153554000	-5.509053000	-4.454217000
H	-0.822089000	-1.994665000	0.458450000	C	-0.167901000	-6.134745000	-3.191003000
H	-2.053416000	-0.714820000	0.311909000	C	-0.192189000	-6.288529000	-5.629580000
H	2.098703000	0.285342000	0.210122000	C	-0.211236000	-7.531588000	-3.109342000
H	1.594294000	-1.411328000	0.393597000	C	-0.235303000	-7.684142000	-5.530462000
H	0.377456000	2.081725000	-0.011849000	C	-0.244687000	-8.309800000	-4.275339000
H	-1.351970000	1.666460000	0.039856000	H	-0.222928000	-8.015900000	-2.136868000
N	-0.024812000	-0.297563000	-2.234538000	H	-0.263645000	-8.287840000	-6.434764000
N	-0.027723000	0.005664000	0.395455000	C	0.171653000	4.338220000	-5.456615000
C	-4.803212000	-0.282900000	-3.804671000	C	0.161251000	5.229224000	-4.364817000
C	-4.938021000	0.214871000	-2.493662000	C	0.238265000	4.837758000	-6.775005000
C	-5.940310000	-0.664822000	-4.530247000	C	0.207937000	6.609654000	-4.594712000
C	-6.196158000	0.312644000	-1.907928000	C	0.284998000	6.220314000	-6.987663000
H	-4.052135000	0.524691000	-1.939694000	C	0.269925000	7.109505000	-5.903057000
C	-7.204676000	-0.574129000	-3.945374000	H	0.199735000	7.297583000	-3.753756000
H	-5.830597000	-1.032719000	-5.552159000	H	0.335333000	6.607955000	-8.002670000
C	-7.337595000	-0.092996000	-2.629580000	C	-0.141191000	-5.312950000	-1.940223000
H	-6.303260000	0.701666000	-0.894737000	H	0.757886000	-4.681911000	-1.898972000
H	-8.089388000	-0.875831000	-4.506257000	H	-1.015030000	-4.644930000	-1.894705000
C	4.836407000	-0.662942000	-3.793736000	H	-0.155752000	-5.926696000	-1.030853000
C	5.950786000	-0.392211000	-4.600738000	C	-0.183803000	-5.627238000	-6.967458000
C	5.011595000	-0.934488000	-2.422515000	H	-0.994603000	-4.885506000	-7.053002000
C	7.229099000	-0.359304000	-4.040004000	H	0.757696000	-5.082302000	-7.137492000

H	-0.304154000	-6.334293000	-7.797472000	H	-7.375930000	-1.384732000	0.648893000
C	0.093224000	4.710484000	-2.962678000	C	4.879090000	1.066984000	2.639002000
H	-0.897457000	4.282652000	-2.753015000	C	5.493794000	1.035489000	1.375833000
H	0.840021000	3.919876000	-2.793730000	C	5.643322000	1.332068000	3.786741000
H	0.280958000	5.492159000	-2.215103000	C	6.860162000	1.290390000	1.255497000
C	0.255714000	3.895916000	-7.932557000	H	4.896860000	0.821899000	0.489811000
H	1.074083000	3.163288000	-7.840323000	C	7.009014000	1.588796000	3.672016000
H	-0.678251000	3.315499000	-7.989354000	H	5.159578000	1.342396000	4.764603000
H	0.382535000	4.402206000	-8.897350000	C	7.623529000	1.580824000	2.403509000
Zn	-0.024906000	0.257024000	2.607335000	H	7.337864000	1.277510000	0.276000000
N	1.187034000	1.945058000	2.648675000	H	7.601561000	1.808115000	4.559370000
C	0.760377000	3.264698000	2.465181000	C	-9.054448000	-1.361855000	2.732489000
C	2.582352000	1.963875000	2.646550000	C	-10.229405000	-1.654277000	2.708177000
C	1.947603000	4.145177000	2.367036000	C	8.998890000	1.892532000	2.286263000
C	3.046898000	3.361125000	2.478904000	C	10.169132000	2.190279000	2.193386000
H	1.880768000	5.210927000	2.236375000	C	15.733086000	3.121298000	1.603770000
H	4.084955000	3.640012000	2.462673000	C	16.585805000	4.246385000	1.533066000
N	-1.681265000	1.466325000	2.690939000	C	17.939553000	4.062510000	1.299889000
C	-3.014397000	1.053163000	2.757761000	H	16.165695000	5.235888000	1.662436000
C	-1.701183000	2.851205000	2.503265000	C	17.521097000	1.693893000	1.213571000
C	-3.890471000	2.216367000	2.617509000	C	18.451096000	2.754322000	1.118176000
C	-3.085989000	3.316294000	2.462153000	H	18.610731000	4.912563000	1.246243000
H	-4.961073000	2.171779000	2.647576000	C	17.953708000	0.333016000	1.000441000
H	-3.372643000	4.343737000	2.341657000	C	19.828091000	2.442805000	0.833953000
N	-1.232646000	-1.367426000	3.086976000	C	19.306982000	0.056955000	0.697924000
C	-0.806802000	-2.691953000	3.230267000	C	20.237491000	1.154171000	0.633605000
C	-2.628576000	-1.385455000	3.100598000	H	20.539192000	3.258654000	0.773567000
C	-1.993617000	-3.567712000	3.369534000	C	19.638067000	-1.299701000	0.460370000
C	-3.092745000	-2.779128000	3.294961000	C	17.322021000	-1.892533000	0.810804000
H	-1.925937000	-4.632182000	3.510167000	H	21.276306000	0.937627000	0.412521000
H	-4.130440000	-3.051422000	3.363199000	C	18.649249000	-2.270420000	0.509958000
N	1.632878000	-0.896903000	2.988776000	H	20.662439000	-1.567286000	0.226224000
C	2.966814000	-0.480892000	2.943186000	H	18.872197000	-3.310928000	0.309589000
C	1.653405000	-2.285690000	3.142406000	C	-15.805835000	-2.569688000	2.256369000
C	3.842804000	-1.643514000	3.089267000	C	-16.691616000	-3.657797000	2.428524000
C	3.038329000	-2.747737000	3.209182000	C	-18.034132000	-3.499235000	2.123423000
H	4.913513000	-1.593199000	3.104497000	H	-16.305118000	-4.599698000	2.796968000
H	3.324855000	-3.774013000	3.339710000	C	-17.540731000	-1.228892000	1.494538000
C	0.524862000	-3.129960000	3.209081000	C	-18.500909000	-2.258578000	1.624735000
C	3.416686000	0.839418000	2.754240000	H	-18.730407000	-4.320379000	2.253422000
C	-0.572775000	3.685621000	2.353669000	C	-17.926677000	0.052310000	0.951645000
C	-3.463342000	-0.271543000	2.917104000	C	-19.861337000	-1.989636000	1.236512000
C	-4.925984000	-0.518837000	2.867157000	C	-19.263967000	0.281288000	0.553198000
C	-5.698097000	-0.430191000	4.036400000	C	-20.226480000	-0.775909000	0.725015000
C	-5.533598000	-0.854687000	1.645433000	H	-20.595665000	-2.778636000	1.351312000
C	-7.066371000	-0.695608000	3.990843000	C	-19.548055000	1.549078000	-0.011229000
H	-5.219003000	-0.158933000	4.978315000	C	-17.222922000	2.151043000	0.251880000
C	-6.902403000	-1.117719000	1.593500000	H	-21.253057000	-0.592370000	0.429474000
H	-4.928814000	-0.917842000	0.741436000	C	-18.531116000	2.478359000	-0.168009000
C	-7.674885000	-1.050194000	2.770128000	H	-20.558492000	1.777733000	-0.331369000
H	-7.665543000	-0.640836000	4.898860000	H	-18.717378000	3.445176000	-0.618633000

N	-16.240235000	-1.385695000	1.821844000	H	12.020845000	-5.331138000	0.565434000
N	-16.950254000	0.972032000	0.812204000	C	16.767235000	-3.448322000	3.211603000
N	17.004061000	-0.622427000	1.063844000	H	17.739548000	-3.861537000	2.923474000
N	16.208325000	1.882837000	1.465880000	H	16.929738000	-2.418064000	3.553004000
C	-0.812396000	5.107917000	2.002080000	H	16.380064000	-4.038479000	4.047709000
C	-0.761691000	6.108500000	2.982054000	C	15.591115000	-2.005078000	-1.499229000
C	-1.082944000	5.440778000	0.664929000	H	15.882451000	-0.971834000	-1.281829000
C	-0.977223000	7.441308000	2.620412000	H	16.443289000	-2.495805000	-1.983555000
C	-1.294275000	6.775179000	0.311769000	H	14.751695000	-1.990907000	-2.199623000
C	-1.240710000	7.775899000	1.288216000	Cu	-15.091360000	0.391592000	1.655925000
H	-0.939415000	8.221378000	3.380234000	Cu	15.100094000	0.095041000	1.677067000
H	-1.502634000	7.036656000	-0.724832000	C	-14.282740000	2.495501000	3.864218000
C	0.761748000	-4.595820000	3.219505000	C	-13.813622000	3.608765000	4.685242000
C	0.943914000	-5.265962000	1.999269000	H	-14.642409000	4.022237000	5.270344000
C	0.796952000	-5.305866000	4.427355000	H	-13.027747000	3.272967000	5.370974000
C	1.156293000	-6.646266000	1.992118000	H	-13.411197000	4.393255000	4.034732000
C	1.011371000	-6.686816000	4.411032000	N	-14.654472000	1.629159000	3.191656000
C	1.189342000	-7.357348000	3.196611000	C	14.248054000	-1.403337000	4.326258000
H	1.297819000	-7.169576000	1.047602000	C	13.771699000	-2.286304000	5.387888000
H	1.039509000	-7.241634000	5.348367000	H	12.960920000	-1.806869000	5.947646000
C	-16.002605000	3.005488000	0.109727000	H	13.400479000	-3.217098000	4.944712000
C	-15.057403000	2.647850000	-0.875223000	H	14.588912000	-2.522260000	6.078261000
C	-15.688554000	3.948417000	1.099845000	N	14.625572000	-0.725294000	3.466898000
C	-13.785358000	3.217379000	-0.827363000	H	-1.405311000	8.816015000	1.011045000
C	-14.407786000	4.516650000	1.106104000	H	1.354264000	-8.433701000	3.188734000
C	-13.439994000	4.140147000	0.169407000	H	-10.129854000	1.335477000	0.888874000
H	-13.039195000	2.915222000	-1.556952000	H	-12.044775000	-1.041724000	-2.173788000
H	-14.159885000	5.257696000	1.860813000	C	11.547116000	2.542581000	2.074787000
C	-12.032214000	4.704832000	0.215240000	C	12.023793000	3.038022000	0.841853000
H	-11.878013000	5.321275000	1.106138000	C	12.399658000	2.382018000	3.190436000
H	-11.300399000	3.887230000	0.225302000	C	13.398443000	3.318811000	0.704243000
H	-11.831911000	5.323455000	-0.667104000	C	13.758865000	2.717554000	3.064131000
C	-16.695971000	4.268993000	2.191109000	C	14.249370000	3.143621000	1.811928000
H	-17.638681000	4.631689000	1.768072000	C	-11.612930000	-2.000562000	2.660791000
H	-16.917038000	3.365642000	2.773665000	C	-12.083866000	-2.788509000	1.588562000
H	-16.308515000	5.036421000	2.868054000	C	-12.477797000	-1.537685000	3.678009000
C	-15.417359000	1.628301000	-1.941543000	C	-13.464245000	-3.059676000	1.494308000
H	-15.732781000	0.687326000	-1.478547000	C	-13.843392000	-1.863437000	3.612228000
H	-16.247521000	1.989916000	-2.559399000	C	-14.327161000	-2.582527000	2.498963000
H	-14.560368000	1.427106000	-2.589901000	C	0.321408000	8.581573000	-6.150597000
C	16.127233000	-2.792554000	0.853401000	H	1.241239000	8.864314000	-6.684238000
C	15.211831000	-2.727640000	-0.218579000	H	-0.524124000	8.913202000	-6.771359000
C	15.795504000	-3.456034000	2.043843000	H	0.292822000	9.173438000	-5.226897000
C	13.950137000	-3.300713000	-0.062844000	C	-0.291410000	-9.800294000	-4.190583000
C	14.527789000	-4.041670000	2.157802000	H	-1.193718000	-10.199800000	-4.677378000
C	13.587115000	-3.945740000	1.127315000	H	0.573476000	-10.257021000	-4.694275000
H	13.224218000	-3.216156000	-0.866634000	H	-0.294159000	-10.171667000	-3.157914000
H	14.267821000	-4.570325000	3.070671000	H	-1.130344000	4.656913000	-0.087499000
C	12.188165000	-4.514625000	1.277136000	H	-0.558016000	5.842783000	4.018746000
H	12.021098000	-4.902294000	2.286737000	H	0.921952000	-4.706680000	1.066646000
H	11.443574000	-3.734215000	1.074949000	H	0.659583000	-4.778465000	5.370619000

C	11.888044000	1.830941000	4.509639000	H	2.472779000	4.927243000	-0.348000000
H	12.460822000	0.938157000	4.791670000	N	1.337582000	2.396327000	-0.118605000
H	11.997810000	2.565220000	5.316244000	C	2.656792000	2.243504000	-0.044421000
H	10.829814000	1.554593000	4.444534000	H	3.325105000	3.127471000	-0.078138000
C	11.092689000	3.264148000	-0.335657000	C	3.304727000	0.979315000	0.098866000
H	11.073203000	4.324120000	-0.615460000	C	4.734671000	0.964366000	0.010559000
H	11.419872000	2.690223000	-1.208932000	C	2.623120000	-0.253901000	0.368428000
H	10.068118000	2.955871000	-0.100000000	H	5.256969000	1.900625000	-0.187170000
C	13.930329000	3.761944000	-0.647876000	C	3.391715000	-1.494872000	0.505405000
H	15.011997000	3.910212000	-0.633801000	C	4.751719000	-1.433107000	0.410768000
H	13.699167000	3.010879000	-1.413625000	H	5.373276000	-2.326705000	0.506564000
H	13.459504000	4.701710000	-0.960218000	O	-1.355871000	-0.343971000	-0.524840000
C	14.688008000	2.586114000	4.259593000	O	1.355903000	-0.343840000	0.525067000
H	14.853462000	1.531313000	4.504146000	C	-11.893052000	-1.488820000	0.054312000
H	15.660890000	3.041753000	4.060637000	C	-11.915115000	0.903497000	0.304841000
H	14.256144000	3.076935000	5.138807000	C	-13.284924000	-1.452836000	0.136162000
C	-13.985161000	-3.824430000	0.289577000	H	-11.371615000	-2.429760000	-0.073523000
H	-13.702096000	-3.314290000	-0.639780000	C	-13.305910000	0.826167000	0.374062000
H	-13.551322000	-4.831002000	0.252926000	H	-11.411052000	1.859503000	0.377275000
H	-15.072500000	-3.922745000	0.305071000	N	-13.996925000	-0.323761000	0.293271000
C	-11.140650000	-3.333171000	0.531325000	H	-13.860991000	-2.371542000	0.072993000
H	-10.108039000	-3.017130000	0.715870000	H	-13.898688000	1.727433000	0.500768000
H	-11.164065000	-4.429156000	0.518854000	C	11.893035000	-1.488825000	-0.053867000
H	-11.423477000	-2.977459000	-0.465221000	C	11.915125000	0.903350000	-0.305745000
C	-11.972673000	-0.673625000	4.819702000	C	13.284901000	-1.452915000	-0.135831000
H	-12.534235000	0.268702000	4.853579000	H	11.371588000	-2.429684000	0.074524000
H	-12.103955000	-1.174685000	5.785965000	C	13.305915000	0.825952000	-0.375018000
H	-10.909388000	-0.437120000	4.701894000	H	11.411079000	1.859326000	-0.378682000
C	-14.785367000	-1.416870000	4.718352000	N	13.996913000	-0.323942000	-0.293629000
H	-14.921928000	-0.330460000	4.694616000	H	13.860955000	-2.371596000	-0.072183000
H	-15.768733000	-1.881791000	4.616025000	H	13.898701000	1.727136000	-0.502277000
H	-14.380541000	-1.688655000	5.699666000	Zn	-0.000015000	0.928561000	0.000048000
2				C	-11.186610000	-0.281997000	0.140768000
C	-4.751682000	-1.433253000	-0.410501000	C	-5.441476000	-0.196593000	-0.168878000
C	-3.391675000	-1.495007000	-0.505123000	C	-6.920815000	-0.217390000	-0.088058000
C	-2.623106000	-0.254006000	-0.368276000	C	-7.678378000	-0.155351000	-1.274121000
C	-3.304734000	0.979227000	-0.098914000	C	-7.544909000	-0.306807000	1.171531000
C	-4.734679000	0.964278000	-0.010643000	C	-9.085248000	-0.175604000	-1.198822000
H	-5.373218000	-2.326880000	-0.506160000	C	-8.951794000	-0.327429000	1.247210000
H	-5.256993000	1.900558000	0.186927000	C	-9.707036000	-0.260257000	0.061224000
C	-2.656825000	2.243457000	0.044203000	C	-6.974253000	-0.085272000	-2.592745000
H	-3.325158000	3.127417000	0.077655000	H	-7.627764000	0.273747000	-3.401343000
N	-1.337631000	2.396300000	0.118543000	H	-6.103997000	0.585775000	-2.556242000
C	-0.713471000	3.688113000	0.088840000	H	-6.601511000	-1.077219000	-2.887324000
C	0.713401000	3.688122000	-0.089016000	C	-9.932576000	-0.121683000	-2.430950000
C	-1.394121000	4.909067000	0.193628000	H	-10.351236000	-1.112345000	-2.660620000
C	1.394019000	4.909090000	-0.193863000	H	-10.778207000	0.571245000	-2.317255000
C	-0.691536000	6.114727000	0.100755000	H	-9.366861000	0.205612000	-3.316624000
H	-2.472879000	4.927205000	0.347776000	C	-9.660433000	-0.409308000	2.562584000
C	0.691405000	6.114736000	-0.101058000	H	-10.081305000	0.567366000	2.841661000
				H	-10.492420000	-1.127357000	2.535805000

H	-8.994032000	-0.723121000	3.380574000	C	9.660291000	-0.410240000	-2.562656000
C	-6.702220000	-0.370753000	2.406674000	H	10.081056000	0.566344000	-2.842207000
H	-5.821119000	-1.014296000	2.265722000	H	10.492347000	-1.128202000	-2.535615000
H	-6.331943000	0.627263000	2.679655000	H	8.993861000	-0.724483000	-3.380456000
H	-7.254461000	-0.765282000	3.272541000	H	1.229733000	7.058682000	-0.183969000
C	-2.630008000	-2.809692000	-0.702619000	H	-1.229885000	7.058664000	0.183616000
C	-3.584221000	-4.018353000	-0.810796000				
H	-4.181566000	-4.148507000	0.096603000	3			
H	-4.264646000	-3.925490000	-1.662331000	N	-1.452692000	1.453520000	-0.002775000
H	-3.016940000	-4.944280000	-0.954602000	C	-1.248514000	2.840753000	0.003162000
C	-1.803539000	-2.725705000	-1.999692000	C	-2.834092000	1.255773000	0.000084000
H	-2.436382000	-2.523687000	-2.866906000	C	-2.558547000	3.524883000	0.013888000
H	-1.059457000	-1.915022000	-1.938519000	C	-3.517733000	2.567396000	0.013362000
H	-1.252767000	-3.651141000	-2.184646000	H	-2.659647000	4.596065000	0.021489000
C	-1.708948000	-3.020196000	0.514710000	H	-4.587225000	2.674986000	0.023427000
H	-0.921731000	-2.246737000	0.550848000	N	1.429371000	1.424660000	-0.004731000
H	-2.262521000	-2.966665000	1.454769000	C	2.817216000	1.225966000	-0.007541000
H	-1.200065000	-3.986115000	0.475299000	C	1.236021000	2.813890000	-0.006818000
C	2.630068000	-2.809550000	0.703046000	C	3.497544000	2.521241000	-0.015813000
C	1.708990000	-3.020191000	-0.514245000	C	2.528548000	3.490666000	-0.014326000
H	0.921726000	-2.246782000	-0.550424000	H	4.563990000	2.641933000	-0.024434000
H	2.262535000	-2.966703000	-1.454324000	H	2.646548000	4.558449000	-0.018580000
H	1.200157000	-3.986135000	-0.474750000	N	1.452775000	-1.454663000	-0.008340000
C	1.803616000	-2.725440000	2.000123000	C	1.248709000	-2.841919000	-0.007888000
H	2.436466000	-2.523309000	2.867308000	C	2.834172000	-1.256889000	-0.005320000
H	1.059513000	-1.914783000	1.938873000	C	2.558831000	-3.525987000	-0.001102000
H	1.252874000	-3.650871000	2.185193000	C	3.517970000	-2.568439000	0.001420000
C	3.584302000	-4.018186000	0.811323000	H	2.660018000	-4.597186000	0.001848000
H	4.181649000	-4.148405000	-0.096066000	H	4.587484000	-2.675932000	0.009356000
H	4.264727000	-3.925241000	1.662849000	N	-1.429324000	-1.425724000	-0.010161000
H	3.017039000	-4.944111000	0.955207000	C	-2.817176000	-1.227077000	-0.013192000
C	11.186608000	-0.282037000	-0.140958000	C	-1.235839000	-2.814925000	-0.017948000
C	5.441488000	-0.196468000	0.168946000	C	-3.497321000	-2.522370000	-0.028385000
C	6.920824000	-0.217281000	0.088072000	C	-2.528264000	-3.491745000	-0.029869000
C	7.544854000	-0.307153000	-1.171529000	H	-4.563729000	-2.643179000	-0.039618000
C	7.678443000	-0.154816000	1.274066000	H	-2.646189000	-4.559501000	-0.039001000
C	8.951728000	-0.327834000	-1.247275000	C	-0.005304000	3.484830000	-0.001121000
C	9.085320000	-0.175099000	1.198699000	C	3.479991000	-0.011215000	-0.005554000
C	9.707038000	-0.260234000	-0.061341000	C	0.005494000	-3.485922000	-0.013911000
C	6.974385000	-0.084292000	2.592700000	C	-3.480138000	0.010125000	-0.005671000
H	6.104162000	0.586788000	2.556028000	Zn	0.000048000	-0.000572000	-0.006700000
H	6.601595000	-1.076131000	2.887590000	C	4.963945000	-0.006641000	-0.002514000
H	7.627951000	0.274932000	3.401161000	C	5.667775000	-0.223544000	-1.197639000
C	9.932724000	-0.120675000	2.430751000	C	5.660918000	0.213873000	1.195995000
H	10.351727000	-1.111152000	2.660587000	C	7.062045000	-0.221904000	-1.196510000
H	10.778122000	0.572504000	2.316828000	H	5.118801000	-0.389364000	-2.124612000
H	9.366986000	0.206616000	3.316411000	C	7.055134000	0.215685000	1.202247000
C	6.702103000	-0.371490000	-2.406608000	H	5.106151000	0.384991000	2.118722000
H	5.820919000	-1.014857000	-2.265372000	C	7.763300000	-0.002994000	0.004856000
H	6.331944000	0.626467000	-2.679968000	H	7.612132000	-0.387766000	-2.122290000
H	7.254256000	-0.766441000	-3.272338000	H	7.599896000	0.385736000	2.130431000

C	-4.963985000	0.005690000	-0.002553000	H	0.900383000	-4.333372000	2.618210000
C	-5.661077000	-0.252673000	1.188380000	H	-0.861484000	-4.226237000	2.554898000
C	-5.668137000	0.260768000	-1.190014000	H	-0.088823000	-5.591527000	3.373991000
C	-7.055323000	-0.254643000	1.194713000	C	-0.001044000	-4.927615000	-2.532817000
H	-5.106443000	-0.452816000	2.105374000	H	-0.852500000	-4.230871000	-2.594609000
C	-7.062427000	0.260198000	-1.188598000	H	0.910936000	-4.320457000	-2.638685000
H	-5.119516000	0.455309000	-2.111614000	H	-0.057519000	-5.587543000	-3.406418000
C	-7.763479000	0.002959000	0.005181000	C	0.015853000	4.924911000	2.517976000
H	-7.600003000	-0.454014000	2.117127000	H	-0.900681000	4.326114000	2.632592000
H	-7.612595000	0.455730000	-2.108554000	H	0.861296000	4.220279000	2.570173000
C	-9.180202000	0.002789000	0.009226000	H	0.087211000	5.583325000	3.391637000
C	-10.389826000	0.002874000	0.012559000	C	0.002266000	4.931823000	-2.516607000
C	9.179790000	-0.002010000	0.008749000	H	0.855803000	4.237844000	-2.580796000
C	10.389469000	-0.001189000	0.012132000	H	-0.907933000	4.322046000	-2.622676000
C	-11.815686000	0.003137000	0.016299000	H	0.055663000	5.593742000	-3.388893000
C	-12.533647000	0.830784000	-0.858661000	C	0.028226000	9.269251000	0.015686000
C	-12.529577000	-0.824072000	0.894963000	H	-0.001124000	9.703607000	-0.991787000
C	-13.927814000	0.791026000	-0.811706000	H	-0.836569000	9.669289000	0.564182000
H	-12.024055000	1.487011000	-1.554668000	H	0.932384000	9.657075000	0.507143000
C	-13.923958000	-0.783454000	0.855248000	C	-0.027522000	-9.270371000	-0.009639000
H	-12.016748000	-1.480816000	1.588141000	H	-0.929757000	-9.659584000	0.484204000
H	-14.516040000	1.419471000	-1.475004000	H	-0.001575000	-9.702605000	-1.018119000
H	-14.509110000	-1.411629000	1.521524000	H	0.839396000	-9.671209000	0.534941000
C	11.815140000	-0.000153000	0.016176000				
C	12.527566000	0.427818000	1.145604000	Conf-1			
C	12.534642000	-0.427135000	-1.109133000	C	-4.934470000	3.526156000	-1.318134000
C	13.921980000	0.408032000	1.094208000	C	-3.620512000	3.939328000	-1.437715000
H	12.013510000	0.766634000	2.037585000	C	-2.761043000	3.836657000	-0.276917000
C	13.928712000	-0.405461000	-1.049687000	C	-3.338311000	3.378282000	0.971230000
H	12.026221000	-0.766341000	-2.004175000	C	-4.694667000	2.959710000	1.013471000
H	14.506051000	0.732977000	1.951058000	H	-5.592329000	3.583652000	-2.178971000
H	14.518154000	-0.729481000	-1.903198000	H	-5.102077000	2.589844000	1.953393000
N	14.626089000	0.001702000	0.024300000	C	-2.618879000	3.331487000	2.213055000
N	-14.626673000	0.004039000	0.023621000	H	-3.234296000	3.049614000	3.075727000
C	0.004478000	4.966706000	0.000437000	N	-1.347808000	3.574589000	2.393679000
C	0.007215000	5.672638000	-1.219725000	C	-0.730412000	3.587898000	3.656544000
C	0.014247000	5.670051000	1.223549000	C	0.698235000	3.614441000	3.670855000
C	0.013425000	7.073710000	-1.209307000	C	-1.423710000	3.623106000	4.878801000
C	0.020372000	7.069617000	1.216375000	C	1.361913000	3.668810000	4.908823000
C	0.019883000	7.774606000	0.003596000	C	-0.744012000	3.652598000	6.091112000
H	0.015068000	7.618251000	-2.149630000	H	-2.508430000	3.655585000	4.882020000
H	0.027275000	7.613681000	2.157025000	C	0.654753000	3.674489000	6.105847000
C	-0.004316000	-4.967799000	-0.015863000	H	2.444862000	3.730978000	4.940025000
C	-0.006583000	-5.671144000	-1.237499000	N	1.340305000	3.622423000	2.417900000
C	-0.014465000	-5.673738000	1.205773000	C	2.632480000	3.494531000	2.268223000
C	-0.012689000	-7.072247000	-1.230024000	H	3.252316000	3.299891000	3.150927000
C	-0.020505000	-7.073273000	1.195659000	C	3.376427000	3.562540000	1.041943000
C	-0.019525000	-7.775701000	-0.018616000	C	4.763192000	3.268006000	1.135849000
H	-0.013874000	-7.614795000	-2.171502000	C	2.796863000	3.908960000	-0.239848000
H	-0.027637000	-7.619326000	2.135150000	H	5.181913000	2.997430000	2.103944000
C	-0.016477000	-4.931319000	2.501772000	C	3.667671000	3.992458000	-1.393762000

C	5.005889000	3.686989000	-1.226957000	C	1.481367000	-3.258540000	-3.028473000
H	5.675449000	3.728291000	-2.079590000	C	0.288686000	-2.837331000	-5.135987000
O	-1.509551000	4.140668000	-0.384624000	H	-2.387393000	-2.950355000	-4.892639000
O	1.531429000	4.130278000	-0.385477000	C	-2.743595000	-3.911204000	0.863664000
C	-11.925135000	1.855682000	-0.860109000	C	-4.812175000	-3.652615000	-0.432731000
C	-11.340836000	0.063125000	0.643887000	H	-4.366225000	-3.251726000	-3.076029000
C	-13.257622000	1.439767000	-0.778107000	N	1.648792000	-3.502764000	-1.685864000
H	-11.644585000	2.706723000	-1.480269000	C	2.779935000	-3.095529000	-3.650010000
C	-12.690749000	-0.299667000	0.671586000	C	0.223193000	-3.867856000	-6.084599000
H	-10.602570000	-0.509648000	1.205687000	C	0.396213000	-1.501121000	-5.550773000
N	-13.664009000	0.383051000	-0.008475000	N	-1.394056000	-3.939491000	1.114626000
H	-14.039424000	1.972608000	-1.335261000	C	-3.465452000	-4.132428000	2.101408000
H	-13.017596000	-1.171334000	1.258237000	C	-5.543696000	-4.730378000	-0.954813000
C	11.967506000	2.289466000	-0.979771000	C	-5.480960000	-2.526474000	0.072975000
C	11.704548000	1.136471000	1.125487000	C	2.991511000	-3.492241000	-1.434110000
C	13.295114000	1.855046000	-1.007481000	C	3.713040000	-3.238989000	-2.664804000
H	11.570889000	2.918932000	-1.775951000	H	2.942592000	-2.902446000	-4.705001000
C	13.038565000	0.730205000	1.024201000	C	0.268474000	-3.558752000	-7.446471000
H	11.101119000	0.857332000	1.988103000	H	0.135909000	-4.903024000	-5.755559000
N	13.837256000	1.051592000	-0.039064000	C	0.439456000	-1.200957000	-6.914331000
H	13.962853000	2.154257000	-1.829464000	H	0.443133000	-0.705007000	-4.810950000
H	13.492661000	0.113453000	1.811664000	C	-1.233192000	-4.173108000	2.451868000
Zn	0.012485000	3.547904000	0.740274000	C	-2.531569000	-4.296694000	3.081970000
N	0.038771000	1.335776000	0.427728000	H	-4.544993000	-4.173909000	2.193094000
C	-1.093525000	0.930460000	-0.450363000	C	-6.937133000	-4.684445000	-0.971992000
C	1.318700000	0.934016000	-0.219164000	H	-5.017376000	-5.604356000	-1.343976000
C	-0.080997000	0.618489000	1.725019000	C	-6.874310000	-2.476861000	0.060680000
C	-1.064259000	-0.603043000	-0.685812000	H	-4.909606000	-1.690881000	0.476865000
H	-1.007500000	1.493842000	-1.381866000	C	3.576976000	-3.662299000	-0.159012000
H	-2.018077000	1.247531000	0.035487000	H	4.791110000	-3.181206000	-2.754821000
C	1.340273000	-0.599387000	-0.455195000	H	0.218470000	-4.357964000	-8.185484000
H	2.133817000	1.257350000	0.431228000	C	0.376475000	-2.227753000	-7.862200000
H	1.407075000	1.494586000	-1.150728000	H	0.521359000	-0.164784000	-7.239617000
C	-0.057876000	-0.915904000	1.490141000	C	0.010798000	-4.265121000	3.116221000
H	0.743184000	0.951113000	2.361668000	H	-2.693515000	-4.491976000	4.136853000
H	-1.010670000	0.944074000	2.196975000	C	-7.609018000	-3.555790000	-0.465913000
H	-0.953649000	-0.853714000	-1.743421000	H	-7.508410000	-5.521117000	-1.375152000
H	-1.976184000	-1.090001000	-0.331307000	H	-7.394919000	-1.603548000	0.456322000
N	0.080479000	-1.207177000	0.041604000	C	2.903213000	-3.879712000	1.062375000
H	2.169785000	-1.086303000	0.064253000	C	5.056646000	-3.617223000	-0.084966000
H	1.432059000	-0.847357000	-1.515204000	C	1.289063000	-4.157786000	2.545610000
H	0.775837000	-1.400658000	2.004059000	C	-0.041507000	-4.502002000	4.582660000
H	-0.975732000	-1.397548000	1.835425000	C	-9.024080000	-3.499568000	-0.503845000
Zn	0.122292000	-3.441320000	-0.250891000	C	3.541127000	-4.122186000	2.343779000
N	-1.299753000	-3.538297000	-1.794512000	N	1.545102000	-3.902441000	1.218652000
C	-1.045457000	-3.291122000	-3.116631000	C	5.693857000	-2.539977000	0.555657000
C	-2.659965000	-3.539315000	-1.633695000	C	5.828958000	-4.658015000	-0.628329000
C	0.241646000	-3.156317000	-3.684557000	C	2.545224000	-4.294752000	3.257654000
C	-2.297026000	-3.144085000	-3.829199000	C	0.028360000	-3.415522000	5.467843000
C	-3.327243000	-3.707213000	-0.400941000	C	-0.160989000	-5.808369000	5.079549000
C	-3.296116000	-3.297281000	-2.911474000	C	-10.231506000	-3.439278000	-0.560873000

H	4.611830000	-4.174131000	2.507196000	C	-17.779127000	-1.496047000	-0.691968000
C	7.081933000	-2.512835000	0.673934000	C	14.615500000	-3.087009000	0.887112000
H	5.094924000	-1.729302000	0.967955000	C	14.341338000	-2.001608000	3.132769000
C	7.218068000	-4.632029000	-0.521254000	H	10.651135000	-1.586622000	2.296387000
H	5.331157000	-5.494079000	-1.122375000	H	10.838335000	-3.073415000	3.232278000
H	2.636428000	-4.509533000	4.317444000	H	11.883135000	-1.686149000	3.569174000
C	-0.019327000	-3.639812000	6.845991000	C	15.087521000	-4.376014000	-1.213364000
H	0.117869000	-2.404854000	5.077714000	H	12.055262000	-5.918831000	-1.082029000
C	-0.207303000	-6.023931000	6.458941000	H	11.198851000	-4.544453000	-1.778570000
H	-0.217610000	-6.647388000	4.386716000	H	12.847220000	-4.925510000	-2.312051000
C	-11.644139000	-3.341892000	-0.639889000	C	-18.639979000	-2.535957000	-1.109427000
C	7.853053000	-3.562030000	0.137888000	H	-18.705102000	-4.644362000	-1.662214000
H	7.571383000	-1.684504000	1.186037000	C	-18.328641000	-0.160356000	-0.463773000
H	7.814850000	-5.444920000	-0.934065000	C	16.065297000	-2.771320000	0.985988000
C	-0.136388000	-4.941974000	7.342656000	H	14.983298000	-1.140888000	2.899789000
H	-0.298797000	-7.038232000	6.846350000	H	13.572802000	-1.654695000	3.842886000
C	-12.245365000	-2.871486000	-1.826304000	H	14.960308000	-2.729546000	3.681188000
C	-12.424959000	-3.701591000	0.486115000	H	15.558574000	-5.299870000	-0.842948000
C	9.260838000	-3.545102000	0.281813000	H	14.598075000	-4.633794000	-2.165930000
C	-13.648936000	-2.728760000	-1.877759000	H	15.894029000	-3.669693000	-1.456335000
C	-11.414667000	-2.511461000	-3.014858000	C	-20.047122000	-2.270870000	-1.288709000
C	-13.822747000	-3.558101000	0.430894000	C	-19.704625000	0.069507000	-0.690338000
C	-11.733363000	-4.216509000	1.706209000	N	-17.450446000	0.836905000	-0.050973000
C	10.462965000	-3.524101000	0.423252000	C	16.978248000	-3.737335000	1.512074000
C	-14.416198000	-3.056102000	-0.745570000	N	16.463294000	-1.541782000	0.591031000
C	-14.312566000	-2.206933000	-3.112148000	C	-20.555135000	-1.024457000	-1.093217000
H	-11.409422000	-1.423939000	-3.179351000	H	-20.689275000	-3.100793000	-1.592552000
H	-10.366189000	-2.830373000	-2.925550000	C	-20.191354000	1.397253000	-0.516272000
H	-11.799018000	-2.981835000	-3.933408000	Cu	-15.614222000	0.017052000	0.350415000
C	-14.695943000	-3.909836000	1.592423000	C	-17.944579000	2.086342000	0.094446000
H	-11.200992000	-5.157173000	1.489242000	C	18.309533000	-3.414880000	1.644363000
H	-10.981390000	-3.505057000	2.076833000	H	16.595336000	-4.717734000	1.801286000
H	-12.424680000	-4.427451000	2.536545000	C	17.801780000	-1.209100000	0.766575000
C	11.865671000	-3.451535000	0.608893000	H	-21.618405000	-0.819379000	-1.237401000
C	-15.890729000	-2.878485000	-0.809861000	C	-19.322451000	2.394241000	-0.140268000
H	-14.360843000	-1.107524000	-3.088359000	H	-21.249642000	1.607663000	-0.690467000
H	-13.774671000	-2.490671000	-4.029383000	C	-17.019686000	3.165391000	0.508689000
H	-15.338787000	-2.576741000	-3.239385000	C	18.759353000	-2.112956000	1.280311000
H	-15.306681000	-3.054347000	1.915604000	H	19.027751000	-4.140024000	2.035305000
H	-15.383271000	-4.731806000	1.342134000	C	18.205830000	0.158534000	0.441595000
H	-14.119229000	-4.243334000	2.471032000	H	-19.656204000	3.425970000	-0.013948000
C	12.365661000	-2.776907000	1.749723000	C	-16.186183000	3.788147000	-0.446975000
C	12.739889000	-4.034450000	-0.334281000	C	-16.990358000	3.591686000	1.852996000
C	-16.705154000	-3.983677000	-1.216737000	C	20.129374000	-1.685673000	1.434674000
N	-16.408465000	-1.666722000	-0.518346000	C	19.546436000	0.551253000	0.649142000
C	13.754631000	-2.624780000	1.905442000	N	17.223011000	1.026066000	-0.026484000
C	11.397248000	-2.249265000	2.758499000	C	-15.278247000	4.769455000	-0.035884000
C	14.129331000	-3.825804000	-0.206630000	C	-16.288737000	3.428271000	-1.893261000
C	12.186016000	-4.881002000	-1.434070000	C	-16.084561000	4.586011000	2.244076000
C	-18.062207000	-3.815350000	-1.355877000	C	-17.925098000	3.005181000	2.859665000
H	-16.222952000	-4.943207000	-1.415424000	C	20.504774000	-0.413163000	1.134032000

H	20.853464000	-2.414561000	1.805524000	H	-6.557298000	4.936415000	0.995203000
C	19.885272000	1.909436000	0.379559000	H	-8.261502000	5.289803000	1.218652000
Cu	15.520068000	-0.016456000	-0.419482000	C	-10.238439000	3.484179000	1.452928000
C	17.568739000	2.315931000	-0.231691000	H	-10.611402000	4.369104000	0.916586000
H	-14.627636000	5.245161000	-0.767277000	H	-11.105741000	2.855026000	1.686092000
C	-15.217414000	5.168256000	1.308643000	H	-9.838506000	3.828515000	2.417185000
H	-16.224290000	2.344367000	-2.064147000	C	-8.989422000	-0.203871000	-1.724611000
H	-17.257059000	3.756578000	-2.307515000	H	-9.695129000	-0.872092000	-1.211460000
H	-15.514373000	3.904951000	-2.509783000	H	-9.474057000	0.151059000	-2.645052000
H	-16.076291000	4.932569000	3.275013000	H	-8.138566000	-0.832693000	-2.034436000
H	-18.933291000	3.439952000	2.752639000	C	-6.173140000	0.645660000	-1.597595000
H	-18.036056000	1.916809000	2.753713000	H	-5.997056000	1.106916000	-2.580720000
H	-17.615765000	3.199605000	3.894934000	H	-5.210614000	0.646243000	-1.066614000
H	21.540293000	-0.087067000	1.256076000	H	-6.440511000	-0.407112000	-1.778635000
C	18.909803000	2.781676000	-0.042020000	C	-3.052731000	4.469360000	-2.770345000
H	20.916472000	2.242649000	0.520896000	C	-4.126584000	4.520445000	-3.874107000
C	16.515640000	3.271208000	-0.642376000	H	-4.529854000	3.527713000	-4.107335000
C	-14.241751000	6.215641000	1.728002000	H	-4.961737000	5.179033000	-3.606696000
H	19.128121000	3.833574000	-0.237863000	H	-3.680206000	4.916507000	-4.793853000
C	15.699599000	3.873103000	0.342509000	C	-2.503820000	5.903049000	-2.579311000
C	16.328401000	3.589342000	-2.003589000	H	-3.302864000	6.583729000	-2.260897000
H	-13.221205000	5.986521000	1.389313000	H	-1.708181000	5.924629000	-1.833377000
H	-14.506201000	7.195793000	1.296294000	H	-2.100296000	6.279023000	-3.528596000
H	-14.198606000	6.357257000	2.816010000	C	-1.916870000	3.542442000	-3.267719000
C	14.686880000	4.756781000	-0.044770000	H	-1.088058000	3.533108000	-2.560247000
C	15.898467000	3.556307000	1.788437000	H	-2.283952000	2.517584000	-3.407328000
C	15.308528000	4.476076000	-2.371982000	H	-1.537220000	3.897812000	-4.234402000
C	17.200985000	2.978630000	-3.049726000	C	3.089111000	4.387480000	-2.768252000
H	14.055614000	5.219418000	0.710803000	C	2.436223000	5.787856000	-2.687323000
C	14.481887000	5.057927000	-1.400171000	H	1.621668000	5.803350000	-1.962111000
H	15.626123000	2.511253000	2.003688000	H	3.177540000	6.543186000	-2.398973000
H	16.945515000	3.691600000	2.097664000	H	2.033603000	6.070364000	-3.668818000
H	15.291777000	4.189686000	2.450111000	C	2.033009000	3.348659000	-3.217631000
H	15.166506000	4.726954000	-3.421276000	H	2.476672000	2.347119000	-3.286325000
H	18.235028000	3.350591000	-2.972943000	H	1.195331000	3.322684000	-2.520890000
H	17.243755000	1.883001000	-2.963458000	H	1.643010000	3.611960000	-4.209187000
H	16.865503000	3.205446000	-4.071519000	C	4.177772000	4.440343000	-3.857450000
C	13.378920000	5.982166000	-1.793089000	H	4.957371000	5.175584000	-3.624753000
H	12.413649000	5.668924000	-1.368915000	H	4.656518000	3.466309000	-4.014191000
H	13.571454000	7.005225000	-1.430876000	H	3.721946000	4.738002000	-4.809097000
H	13.245095000	6.056614000	-2.880868000	C	11.145114000	1.905408000	0.092477000
C	-10.944616000	1.173923000	-0.119233000	C	5.568791000	3.312212000	0.019978000
C	-5.484796000	3.012643000	-0.114615000	C	7.007636000	2.956381000	0.082492000
C	-6.890246000	2.538462000	-0.101952000	C	7.948411000	3.890997000	0.545531000
C	-7.868349000	3.248346000	0.621132000	C	7.407803000	1.674959000	-0.361728000
C	-7.231946000	1.384939000	-0.840554000	C	9.319854000	3.546883000	0.562399000
C	-9.196822000	2.774713000	0.642553000	C	8.770197000	1.334093000	-0.350060000
C	-8.571237000	0.951013000	-0.872239000	C	9.713796000	2.278065000	0.111959000
C	-9.539536000	1.639296000	-0.115068000	C	6.367065000	0.717516000	-0.851192000
C	-7.506527000	4.503843000	1.350760000	H	5.528595000	0.639506000	-0.144586000
H	-7.390395000	4.322698000	2.427402000	H	5.943754000	1.052789000	-1.809868000

H	6.757542000	-0.299902000	-1.007891000
C	9.252143000	0.002481000	-0.838152000
H	9.884948000	0.115182000	-1.727762000
H	9.836984000	-0.527201000	-0.073434000
H	8.421190000	-0.667828000	-1.117954000
C	7.512141000	5.242071000	1.014654000
H	6.470270000	5.471236000	0.740975000
H	7.577990000	5.322794000	2.108415000
H	8.126126000	6.044693000	0.583681000
C	10.332071000	4.530632000	1.059567000
H	10.213357000	4.698823000	2.140774000
H	11.370378000	4.216819000	0.897286000
H	10.215329000	5.507862000	0.567493000
H	0.034640000	-2.798737000	7.535068000
H	-0.172569000	-5.114145000	8.417127000
H	0.410383000	-1.990669000	-8.924662000
H	1.191982000	3.720907000	7.049528000
H	-1.302263000	3.683549000	7.023062000
C	13.632528000	-1.290516000	-2.362854000
C	-15.124501000	1.063700000	3.168202000
C	-14.713900000	1.896855000	4.266048000
H	-14.672669000	2.964601000	3.967199000
H	-15.410829000	1.825401000	5.123047000
H	-13.710097000	1.622548000	4.641800000
C	12.376297000	-1.718736000	-2.915093000
H	12.494868000	-2.585065000	-3.593434000
H	11.670978000	-2.030515000	-2.115875000
H	11.883632000	-0.915647000	-3.494476000
N	14.638748000	-0.934159000	-1.904015000
N	-15.456354000	0.399344000	2.275777000

Conf-2

C	-4.832837000	-3.524928000	1.038556000
C	-3.518936000	-3.947684000	1.119195000
C	-2.673541000	-3.782246000	-0.044725000
C	-3.262436000	-3.247792000	-1.257305000
C	-4.618689000	-2.826841000	-1.260541000
H	-5.480931000	-3.631612000	1.902179000
H	-5.036784000	-2.405876000	-2.173999000
C	-2.555082000	-3.142131000	-2.503493000
H	-3.177670000	-2.824305000	-3.348616000
N	-1.282358000	-3.361075000	-2.698458000
C	-0.659562000	-3.286060000	-3.955059000
C	0.770200000	-3.264701000	-3.962690000
C	-1.349038000	-3.273737000	-5.179946000
C	1.435541000	-3.202891000	-5.199559000
C	-0.667096000	-3.203482000	-6.389018000
H	-2.431838000	-3.346528000	-5.187363000
C	0.731183000	-3.162410000	-6.397675000
H	2.520007000	-3.198409000	-5.233870000
N	1.409031000	-3.329363000	-2.706188000

C	2.707361000	-3.297722000	-2.555643000
H	3.340851000	-3.165286000	-3.439380000
C	3.449063000	-3.398757000	-1.330203000
C	4.851242000	-3.193180000	-1.433201000
C	2.856286000	-3.685525000	-0.041216000
H	5.283674000	-2.974270000	-2.408275000
C	3.718223000	-3.754733000	1.120083000
C	5.072574000	-3.538482000	0.943653000
H	5.738608000	-3.579050000	1.799169000
O	-1.424850000	-4.106207000	0.027207000
O	1.584282000	-3.864019000	0.107189000
C	-11.842393000	-1.969153000	0.762719000
C	-11.315594000	-0.042420000	-0.588792000
C	-13.185592000	-1.582771000	0.723199000
H	-11.535348000	-2.860992000	1.308523000
C	-12.674530000	0.286446000	-0.577952000
H	-10.596406000	0.594842000	-1.103865000
N	-13.625143000	-0.477649000	0.045246000
H	-13.949022000	-2.179670000	1.239286000
H	-13.028098000	1.196794000	-1.084947000
C	12.031867000	-2.461375000	0.842788000
C	11.975144000	-1.549593000	-1.391859000
C	13.373820000	-2.079834000	0.925752000
H	11.548195000	-2.981229000	1.669355000
C	13.317367000	-1.192148000	-1.232496000
H	11.450681000	-1.348566000	-2.324466000
N	14.020618000	-1.409398000	-0.079852000
H	13.968259000	-2.308607000	1.822821000
H	13.864901000	-0.693363000	-2.053093000
Zn	0.063438000	-3.348991000	-1.043348000
N	-0.017620000	-1.163495000	-0.597270000
C	-0.823893000	-0.923439000	0.631801000
C	1.370907000	-0.680910000	-0.362983000
C	-0.616464000	-0.382725000	-1.712974000
C	-0.882186000	0.597010000	0.937301000
H	-0.361402000	-1.486229000	1.445037000
H	-1.817323000	-1.345281000	0.468939000
C	1.354587000	0.812305000	0.051649000
H	1.933606000	-0.850187000	-1.284438000
H	1.812381000	-1.310125000	0.409546000
C	-0.549033000	1.136346000	-1.397461000
H	-0.077169000	-0.641416000	-2.629347000
H	-1.647633000	-0.722068000	-1.829744000
H	-0.524281000	0.822567000	1.944183000
H	-1.896884000	0.994396000	0.855893000
N	-0.029608000	1.343559000	-0.023182000
H	1.983533000	1.430191000	-0.593548000
H	1.703825000	0.952354000	1.076941000
H	0.111023000	1.677622000	-2.081481000
H	-1.532685000	1.607899000	-1.457081000
Zn	-0.007988000	3.549777000	0.452477000

N	-1.397752000	3.486689000	2.027182000	N	1.382942000	4.160604000	-0.992907000
C	-1.116395000	3.105488000	3.311098000	C	5.511940000	2.745151000	-0.595285000
C	-2.760859000	3.484143000	1.890021000	C	5.735128000	4.686377000	0.850023000
C	0.182481000	2.908589000	3.833347000	C	2.339463000	4.763444000	-3.001425000
C	-2.352502000	2.869817000	4.026471000	C	-0.178011000	4.066059000	-5.241123000
C	-3.452627000	3.765764000	0.691986000	C	-0.446644000	6.402541000	-4.624025000
C	-3.370281000	3.102858000	3.146962000	C	-10.347873000	3.358702000	0.913760000
C	1.408330000	3.077160000	3.164260000	H	4.421001000	4.602750000	-2.302573000
C	0.259719000	2.421950000	5.235918000	C	6.894527000	2.696458000	-0.750213000
H	-2.420662000	2.563003000	5.064639000	H	4.879617000	2.011767000	-1.093385000
C	-2.895831000	4.102956000	-0.556025000	C	7.121584000	4.634218000	0.709857000
C	-4.935764000	3.683509000	0.741023000	H	5.273556000	5.466811000	1.457255000
H	-4.436474000	3.025196000	3.324272000	H	2.407860000	5.082311000	-4.036452000
N	1.548431000	3.468682000	1.853673000	C	-0.254320000	4.418386000	-6.590953000
C	2.719358000	2.847197000	3.736472000	H	-0.046445000	3.026826000	-4.950685000
C	0.141505000	3.324251000	6.302606000	C	-0.521016000	6.746380000	-5.975859000
C	0.448643000	1.053766000	5.485849000	H	-0.522510000	7.169455000	-3.853712000
N	-1.551980000	4.174992000	-0.827127000	C	-11.756351000	3.216511000	0.997112000
C	-3.644213000	4.425590000	-1.755336000	C	7.709380000	3.640512000	-0.094204000
C	-5.675208000	4.685285000	1.388000000	H	7.350658000	1.934943000	-1.382516000
C	-5.595224000	2.608817000	0.123189000	H	7.750828000	5.368864000	1.211136000
C	2.886120000	3.492188000	1.575293000	C	-0.424951000	5.756613000	-6.959636000
C	3.632303000	3.103253000	2.755122000	H	-0.653894000	7.788912000	-6.263563000
H	2.903757000	2.538198000	4.759848000	C	-12.328704000	2.606158000	2.133078000
C	0.215468000	2.855821000	7.616958000	C	-12.561079000	3.669575000	-0.077041000
H	-0.008019000	4.384833000	6.101677000	C	9.111248000	3.575653000	-0.273016000
C	0.519252000	0.593872000	6.802854000	C	-13.726442000	2.415261000	2.181643000
H	0.537886000	0.356561000	4.655468000	C	-11.471923000	2.145890000	3.267233000
C	-1.420138000	4.526473000	-2.141127000	C	-13.952896000	3.475032000	-0.026130000
C	-2.731361000	4.689508000	-2.733883000	C	-11.900197000	4.333931000	-1.240614000
H	-4.725724000	4.460463000	-1.823585000	C	10.303295000	3.482431000	-0.462539000
C	-7.067577000	4.615121000	1.418076000	C	-14.516306000	2.832556000	1.095397000
H	-5.156322000	5.520051000	1.863677000	C	-14.360244000	1.747307000	3.360005000
C	-6.987130000	2.535916000	0.147413000	H	-11.404003000	1.048195000	3.290030000
H	-5.017482000	1.831876000	-0.377452000	H	-10.444130000	2.533810000	3.220202000
C	3.444479000	3.803291000	0.314853000	H	-11.876651000	2.470860000	4.238479000
H	4.711909000	3.037085000	2.816879000	C	-14.849946000	3.916327000	-1.137788000
H	0.125413000	3.555569000	8.447406000	H	-11.387339000	5.258045000	-0.927022000
C	0.403692000	1.492973000	7.868279000	H	-11.137068000	3.687282000	-1.697122000
H	0.663819000	-0.467435000	7.000022000	H	-12.608710000	4.618006000	-2.033868000
C	-0.190717000	4.687958000	-2.818799000	C	11.685295000	3.319106000	-0.726271000
H	-2.915708000	4.975460000	-3.764115000	C	-15.982138000	2.591244000	1.148192000
C	-7.729879000	3.538420000	0.799299000	H	-14.390290000	0.656632000	3.214720000
H	-7.645151000	5.393055000	1.918216000	H	-13.811546000	1.937254000	4.295051000
H	-7.500354000	1.703090000	-0.335405000	H	-15.390160000	2.082408000	3.542097000
C	2.744181000	4.141706000	-0.863836000	H	-15.425700000	3.076122000	-1.552400000
C	4.920652000	3.745802000	0.197917000	H	-15.569946000	4.674436000	-0.795110000
C	1.099173000	4.539277000	-2.284419000	H	-14.295289000	4.370569000	-1.975561000
C	-0.273299000	5.060100000	-4.255479000	C	12.068361000	2.476133000	-1.798743000
C	-9.142983000	3.452084000	0.849064000	C	12.650733000	3.976328000	0.066738000
C	3.354466000	4.517948000	-2.126164000	C	-16.839281000	3.613546000	1.667614000

N	-16.450799000	1.394361000	0.736539000	C	19.524025000	-0.533595000	-0.801222000
C	13.434696000	2.275747000	-2.061961000	N	17.307556000	-0.987875000	0.176733000
C	11.003793000	1.814433000	-2.611897000	C	-15.044151000	-4.900555000	-0.378850000
C	14.017929000	3.702843000	-0.146972000	C	-16.114999000	-3.803239000	1.600807000
C	12.215874000	4.962165000	1.101722000	C	-15.861134000	-4.525873000	-2.631423000
C	-18.187384000	3.374601000	1.791271000	C	-17.773249000	-2.977098000	-3.090926000
H	-16.396498000	4.567296000	1.962530000	C	20.367510000	0.353985000	-1.564379000
C	-17.811734000	1.148924000	0.894447000	H	20.517559000	2.194241000	-2.645351000
C	14.391116000	2.835006000	-1.189803000	C	19.994627000	-1.772315000	-0.275369000
C	13.894681000	1.491792000	-3.250002000	Cu	15.512619000	-0.088821000	0.391619000
H	10.406269000	1.119470000	-1.985699000	C	17.780509000	-2.162990000	0.645285000
H	10.301071000	2.552372000	-3.030334000	H	-14.371027000	-5.416625000	0.303112000
H	11.401102000	1.236683000	-3.458168000	C	-14.966143000	-5.157933000	-1.756598000
C	15.073074000	4.319237000	0.713737000	H	-16.100832000	-2.740489000	1.881101000
H	12.122765000	5.966018000	0.652617000	H	-17.066985000	-4.216230000	1.975291000
H	11.235003000	4.725616000	1.535513000	H	-15.319228000	-4.304039000	2.169052000
H	12.932540000	5.050499000	1.931835000	H	-15.838599000	-4.766365000	-3.691900000
C	-18.712948000	2.103878000	1.416490000	H	-18.760524000	-3.465607000	-3.031152000
H	-18.862411000	4.140257000	2.181851000	H	-17.933297000	-1.910991000	-2.876575000
C	-18.305222000	-0.179150000	0.532968000	H	-17.456879000	-3.052278000	-4.139503000
C	15.827328000	2.509633000	-1.397383000	H	21.407117000	0.059368000	-1.725321000
H	14.310140000	0.511824000	-2.951998000	C	19.135556000	-2.577482000	0.432362000
H	13.079529000	1.296250000	-3.965681000	H	21.033393000	-2.066585000	-0.444979000
H	14.677491000	2.024634000	-3.809571000	C	16.870653000	-3.056717000	1.395351000
H	15.571771000	5.150996000	0.192450000	C	-13.941163000	-6.108980000	-2.276140000
H	14.667538000	4.734665000	1.649853000	H	19.456847000	-3.536446000	0.844776000
H	15.849827000	3.596589000	1.001933000	C	16.129859000	-4.040525000	0.702643000
C	-20.106795000	1.762389000	1.568755000	C	16.769743000	-2.954348000	2.798898000
C	-19.669201000	-0.488894000	0.735517000	H	-12.929537000	-5.850278000	-1.931983000
N	-17.387104000	-1.091518000	0.022429000	H	-14.142215000	-7.135685000	-1.926417000
C	16.635331000	3.404127000	-2.168264000	H	-13.909204000	-6.155588000	-3.372720000
N	16.314272000	1.369964000	-0.860671000	C	15.284422000	-4.896974000	1.415956000
C	-20.562883000	0.521893000	1.247640000	C	16.235024000	-4.159214000	-0.782054000
H	-20.781869000	2.529142000	1.955824000	C	15.915090000	-3.818118000	3.494279000
C	-20.099911000	-1.811812000	0.428174000	C	17.566414000	-1.932835000	3.541582000
Cu	-15.588060000	-0.156593000	-0.294278000	H	14.716510000	-5.659163000	0.886471000
C	-17.828231000	-2.340185000	-0.247311000	C	15.173915000	-4.793050000	2.811132000
C	17.958834000	3.105754000	-2.389621000	H	15.880645000	-3.241973000	-1.278446000
H	16.178093000	4.311937000	-2.566611000	H	17.273322000	-4.326227000	-1.105088000
C	17.651702000	1.067611000	-1.101235000	H	15.642368000	-4.991225000	-1.186238000
H	-21.615949000	0.258579000	1.370605000	H	15.839981000	-3.744730000	4.577507000
C	-19.190976000	-2.728196000	-0.045844000	H	18.647590000	-2.082187000	3.396717000
H	-21.147682000	-2.083493000	0.579685000	H	17.331716000	-0.911483000	3.206815000
C	-16.858336000	-3.331477000	-0.765121000	H	17.391050000	-1.961206000	4.626309000
C	18.506642000	1.903700000	-1.855838000	C	14.276054000	-5.721356000	3.557132000
H	18.597963000	3.774119000	-2.972075000	H	13.309725000	-5.862492000	3.053441000
C	18.177175000	-0.184339000	-0.556621000	H	14.736114000	-6.719922000	3.646703000
H	-19.481340000	-3.755170000	-0.275618000	H	14.061237000	-5.383340000	4.580014000
C	-15.996449000	-4.009154000	0.125905000	C	-10.885642000	-1.203938000	0.073925000
C	-16.811392000	-3.618676000	-2.145279000	C	-5.396471000	-2.944252000	-0.128073000
C	19.881390000	1.520161000	-2.067396000	C	-6.806735000	-2.485161000	-0.097390000

C	-7.782477000	-3.153745000	-0.862689000	C	7.570614000	-1.679185000	-0.086945000
C	-7.158618000	-1.396944000	0.729972000	C	9.402398000	-3.741763000	-0.713174000
C	-9.118157000	-2.701933000	-0.834121000	C	8.948491000	-1.409731000	-0.097616000
C	-8.505543000	-0.993413000	0.813816000	C	9.854351000	-2.453403000	-0.392471000
C	-9.471441000	-1.636994000	0.015905000	C	6.567815000	-0.619041000	0.243671000
C	-7.411261000	-4.345781000	-1.688028000	H	5.945453000	-0.380794000	-0.630093000
H	-7.299349000	-4.081044000	-2.747599000	H	5.882090000	-0.948623000	1.039106000
H	-6.457761000	-4.796303000	-1.367828000	H	7.029019000	0.318310000	0.590110000
H	-8.158648000	-5.146609000	-1.615888000	C	9.478938000	-0.041211000	0.197341000
C	-10.157249000	-3.362279000	-1.688411000	H	10.317092000	-0.067008000	0.903245000
H	-10.512765000	-4.291141000	-1.218746000	H	9.836816000	0.453131000	-0.727893000
H	-11.035411000	-2.729749000	-1.865153000	H	8.711721000	0.621652000	0.631463000
H	-9.761517000	-3.625041000	-2.679637000	C	7.520601000	-5.384346000	-1.033979000
C	-8.932011000	0.077329000	1.766046000	H	6.428857000	-5.482766000	-0.930391000
H	-9.676649000	0.758325000	1.330926000	H	7.765762000	-5.665755000	-2.067217000
H	-9.372039000	-0.364978000	2.671054000	H	7.962029000	-6.139322000	-0.368501000
H	-8.091829000	0.709657000	2.097237000	C	10.371181000	-4.831167000	-1.048072000
C	-6.103408000	-0.694779000	1.526375000	H	10.138274000	-5.284088000	-2.023700000
H	-5.918483000	-1.212465000	2.479290000	H	11.413223000	-4.494049000	-1.099828000
H	-5.143367000	-0.653088000	0.992641000	H	10.331693000	-5.637671000	-0.300606000
H	-6.380751000	0.342382000	1.771505000	H	-0.180714000	3.649106000	-7.357755000
C	-2.939924000	-4.569566000	2.406521000	H	-0.483084000	6.028689000	-8.012299000
C	-3.994493000	-4.657514000	3.526345000	H	0.459429000	1.131512000	8.894128000
H	-4.368322000	-3.669794000	3.821891000	H	1.272115000	-3.118255000	-7.339359000
H	-4.850572000	-5.280023000	3.239332000	H	-1.221592000	-3.198734000	-7.323699000
H	-3.541616000	-5.115685000	4.413384000	C	13.364390000	1.262779000	2.065412000
C	-2.439330000	-6.003978000	2.114073000	C	-15.050419000	-0.906331000	-3.198774000
H	-3.265137000	-6.639522000	1.771576000	C	-14.605841000	-1.605565000	-4.374107000
H	-1.660176000	-6.000944000	1.350310000	H	-14.518309000	-2.695326000	-4.184738000
H	-2.027679000	-6.451353000	3.028306000	H	-15.306406000	-1.477711000	-5.221539000
C	-1.765109000	-3.711964000	2.938056000	H	-13.615284000	-1.251747000	-4.717154000
H	-0.944448000	-3.690951000	2.221949000	C	12.117505000	1.750334000	2.587983000
H	-2.092083000	-2.683795000	3.139493000	H	12.258461000	2.637667000	3.234755000
H	-1.389425000	-4.134484000	3.879001000	H	11.429281000	2.059281000	1.771767000
C	3.113047000	-4.026406000	2.512705000	H	11.591652000	0.986304000	3.190705000
C	2.379227000	-5.388440000	2.525735000	N	14.367798000	0.864623000	1.638979000
H	1.569772000	-5.409819000	1.795279000	N	-15.409378000	-0.350428000	-2.244888000
H	3.077328000	-6.203801000	2.299699000				
H	1.955475000	-5.575504000	3.521116000				
C	2.118580000	-2.897054000	2.879424000				
H	2.620022000	-1.920626000	2.882099000				
H	1.290223000	-2.871201000	2.171598000				
H	1.705642000	-3.067167000	3.881828000				
C	4.192041000	-4.064964000	3.611998000				
H	4.928253000	-4.858763000	3.437359000				
H	4.726498000	-3.111749000	3.703447000				
H	3.716376000	-4.268085000	4.578570000				
C	11.303960000	-2.163098000	-0.322325000				
C	5.655693000	-3.253635000	-0.317205000				
C	7.112907000	-2.983158000	-0.387213000				
C	8.013182000	-4.010544000	-0.709812000				

Conf-1_M							
C	-3.022779000	-4.944077000	-1.362965000				
C	-3.410741000	-3.623221000	-1.490931000				
C	-3.300940000	-2.760932000	-0.332861000				
C	-2.862486000	-3.341361000	0.920941000				
C	-2.469234000	-4.705032000	0.971822000				
H	-3.085998000	-5.604283000	-2.221620000				
H	-2.113857000	-5.115246000	1.916091000				
C	-2.811652000	-2.617785000	2.160254000				
H	-2.547512000	-3.234668000	3.027405000				
N	-3.032658000	-1.341695000	2.333921000				
C	-3.043943000	-0.718911000	3.594094000				
C	-3.044263000	0.709982000	3.602552000				

C	-3.100935000	-1.406361000	4.818874000	N	4.128667000	1.507434000	-1.704671000
C	-3.095604000	1.379709000	4.837333000	C	3.756791000	2.637650000	-3.676292000
C	-3.126897000	-0.721201000	6.028177000	N	4.488579000	-1.531305000	1.111225000
H	-3.153407000	-2.490259000	4.826191000	C	4.636033000	-3.601779000	2.107759000
C	-3.123169000	0.677815000	6.037090000	C	4.140907000	2.851138000	-1.458357000
H	-3.138100000	2.463789000	4.863713000	C	3.910137000	3.572044000	-2.693806000
N	-3.031177000	1.346907000	2.346956000	H	3.574529000	2.799482000	-4.733352000
C	-2.878423000	2.635906000	2.193023000	C	4.715197000	-1.369165000	2.449577000
H	-2.678991000	3.255692000	3.074654000	C	4.810224000	-2.666986000	3.085798000
C	-2.923649000	3.375826000	0.963268000	H	4.656988000	-4.681469000	2.204106000
C	-2.604390000	4.757361000	1.053792000	C	4.312308000	3.438710000	-0.184385000
C	-3.271257000	2.797464000	-0.318646000	H	3.872847000	4.650640000	-2.788569000
H	-2.333306000	5.175042000	2.022196000	C	4.825147000	-0.124314000	3.109540000
C	-3.330181000	3.664847000	-1.476729000	H	4.994700000	-2.828059000	4.142770000
C	-3.001358000	4.997892000	-1.313031000	C	4.508231000	2.766114000	1.041305000
H	-3.024024000	5.664488000	-2.168601000	C	4.745607000	1.153358000	2.533019000
O	-3.581062000	-1.504619000	-0.447861000	C	4.752935000	3.404774000	2.321907000
O	-3.514715000	1.535647000	-0.460908000	N	4.504786000	1.408488000	1.203229000
Zn	-2.968703000	0.011000000	0.675311000	C	4.900417000	2.409679000	3.241068000
N	-0.754240000	-0.004630000	0.379154000	H	4.823312000	4.475010000	2.481385000
C	-0.363352000	-1.147823000	-0.491333000	H	5.108910000	2.501325000	4.301968000
C	-0.324187000	1.264974000	-0.269865000	C	-2.528310000	-5.498710000	-0.153457000
C	-0.048886000	-0.132190000	1.682251000	C	-3.920429000	-3.051325000	-2.829729000
C	1.172126000	-1.147771000	-0.715378000	C	-3.983006000	-4.128686000	-3.929553000
H	-0.918065000	-1.055365000	-1.427356000	H	-2.996195000	-4.551116000	-4.153702000
H	-0.700894000	-2.064418000	-0.004103000	H	-4.658818000	-4.950431000	-3.663729000
C	1.211055000	1.257428000	-0.494480000	H	-4.364009000	-3.678914000	-4.854076000
H	-0.637342000	2.088573000	0.374818000	C	-5.345063000	-2.475399000	-2.651659000
H	-0.876157000	1.359782000	-1.205877000	H	-6.042686000	-3.260533000	-2.335147000
C	1.487376000	-0.138251000	1.458737000	H	-5.357543000	-1.676443000	-1.909146000
H	-0.370970000	0.700619000	2.313128000	H	-5.706541000	-2.069011000	-3.605358000
H	-0.395018000	-1.053784000	2.155537000	C	-2.969036000	-1.934819000	-3.324747000
H	1.432640000	-1.046091000	-1.771511000	H	-2.949727000	-1.103396000	-2.620535000
H	1.639631000	-2.066980000	-0.353584000	H	-1.950158000	-2.321255000	-3.455205000
N	1.791884000	-0.011247000	0.011910000	H	-3.310227000	-1.552677000	-4.295595000
H	1.709275000	2.079998000	0.025307000	C	-3.725575000	3.087890000	-2.851807000
H	1.468540000	1.340250000	-1.552957000	C	-5.138310000	2.461162000	-2.778654000
H	1.983613000	0.688534000	1.972991000	H	-5.174157000	1.650105000	-2.050322000
H	1.949442000	-1.063298000	1.811314000	H	-5.881958000	3.217400000	-2.498991000
Zn	4.028478000	-0.011701000	-0.264046000	H	-5.420897000	2.059742000	-3.760612000
N	4.110722000	-1.441746000	-1.801148000	C	-2.703082000	2.011032000	-3.289079000
C	3.878032000	-1.188447000	-3.126071000	H	-1.693009000	2.435972000	-3.352073000
C	4.085509000	-2.801055000	-1.634878000	H	-2.697654000	1.175899000	-2.588843000
C	3.771140000	0.098539000	-3.700232000	H	-2.966167000	1.621815000	-4.281044000
C	3.713312000	-2.439988000	-3.834713000	C	-3.750276000	4.172839000	-3.945739000
C	4.231979000	-3.466096000	-0.398185000	H	-4.472812000	4.966773000	-3.721678000
C	3.841311000	-3.437909000	-2.911884000	H	-2.766502000	4.632915000	-4.097076000
C	3.891272000	1.338970000	-3.048376000	H	-4.049262000	3.718532000	-4.897697000
H	3.525857000	-2.531234000	-4.899159000	C	-2.625504000	5.558992000	-0.065537000
C	4.437316000	-2.881089000	0.865548000	H	-3.166662000	1.219694000	6.978249000
H	3.777252000	-4.507666000	-3.072417000	H	-3.174959000	-1.274960000	6.962157000

H	-2.202068000	-6.528134000	-0.137588000
H	-2.347590000	6.601727000	-0.022312000
H	4.172635000	-4.544296000	-0.417250000
H	4.298885000	4.517499000	-0.135045000
H	3.547896000	0.132620000	-4.756358000
H	4.988654000	-0.161039000	4.176459000

Conf-2_M

C	-2.905110000	-4.923328000	-1.381383000
C	-3.337711000	-3.616594000	-1.511350000
C	-3.287661000	-2.759363000	-0.345415000
C	-2.854171000	-3.330315000	0.915095000
C	-2.415925000	-4.680100000	0.968209000
H	-2.925917000	-5.579963000	-2.244877000
H	-2.071480000	-5.084409000	1.919176000
C	-2.868995000	-2.611388000	2.159034000
H	-2.618297000	-3.222264000	3.034706000
N	-3.122374000	-1.340557000	2.321944000
C	-3.167496000	-0.706491000	3.574331000
C	-3.167111000	0.723483000	3.570303000
C	-3.253566000	-1.385630000	4.801899000
C	-3.224242000	1.399685000	4.801502000
C	-3.300110000	-0.692932000	6.005993000
H	-3.311395000	-2.469301000	4.813162000
C	-3.279755000	0.705850000	6.005095000
H	-3.238155000	2.484374000	4.825835000
N	-3.129613000	1.350990000	2.307024000
C	-3.103134000	2.648449000	2.147567000
H	-3.058308000	3.291034000	3.033585000
C	-3.106096000	3.378550000	0.911084000
C	-2.930284000	4.784359000	1.018588000
C	-3.269388000	2.771052000	-0.392531000
H	-2.804521000	5.228009000	2.005072000
C	-3.247943000	3.622335000	-1.563486000
C	-3.067381000	4.981206000	-1.381487000
H	-3.041687000	5.639535000	-2.243477000
O	-3.621703000	-1.516272000	-0.457388000
O	-3.416042000	1.495360000	-0.544092000
Zn	-2.983184000	-0.008252000	0.661643000
N	-0.765903000	-0.060209000	0.410933000
C	-0.406774000	-0.872815000	-0.784539000
C	-0.284215000	1.333394000	0.207027000
C	-0.078300000	-0.638266000	1.596753000
C	1.135341000	-0.910871000	-0.954180000
H	-0.902039000	-0.425416000	-1.648536000
H	-0.827296000	-1.871050000	-0.650124000
C	1.239851000	1.336037000	-0.074080000
H	-0.542197000	1.900987000	1.104554000
H	-0.848911000	1.759135000	-0.622090000
C	1.461522000	-0.550643000	1.415841000
H	-0.424542000	-0.095447000	2.481536000

H	-0.412038000	-1.673338000	1.692782000
H	1.443907000	-0.557852000	-1.940588000
H	1.538334000	-1.918822000	-0.828478000
N	1.782025000	-0.039413000	0.060344000
H	1.789380000	1.979335000	0.617046000
H	1.465008000	1.678929000	-1.086274000
H	1.930881000	0.122923000	2.138663000
H	1.939904000	-1.526666000	1.526081000
Zn	4.021093000	0.011283000	-0.219091000
N	4.117032000	-1.392085000	-1.780039000
C	3.846783000	-1.126880000	-3.095155000
C	4.121637000	-2.753909000	-1.630753000
C	3.678395000	0.164636000	-3.644916000
C	3.692733000	-2.372150000	-3.816866000
C	4.306186000	-3.431541000	-0.406104000
C	3.861632000	-3.379156000	-2.910672000
C	3.769858000	1.398227000	-2.975244000
H	3.479827000	-2.453381000	-4.877291000
C	4.523908000	-2.859617000	0.861466000
H	3.815011000	-4.447807000	-3.084070000
N	4.042036000	1.554832000	-1.636600000
C	3.572747000	2.701039000	-3.577842000
N	4.552633000	-1.512728000	1.125173000
C	4.749882000	-3.593319000	2.091552000
C	4.021897000	2.894957000	-1.369843000
C	3.728198000	3.625628000	-2.586332000
H	3.352763000	2.872460000	-4.626102000
C	4.784787000	-1.364891000	2.463752000
C	4.913350000	-2.668737000	3.080961000
H	4.793932000	-4.673585000	2.172862000
C	4.212505000	3.468192000	-0.092238000
H	3.652426000	4.703579000	-2.663911000
C	4.868359000	-0.127736000	3.141430000
H	5.109815000	-2.840345000	4.134065000
C	4.455354000	2.782651000	1.118268000
C	4.749183000	1.155402000	2.583854000
C	4.709889000	3.408767000	2.403117000
N	4.482062000	1.422882000	1.261367000
C	4.891478000	2.404712000	3.306095000
H	4.763757000	4.477818000	2.576251000
H	5.116699000	2.486299000	4.364597000
C	-2.421908000	-5.468767000	-0.162754000
C	-3.851612000	-3.057457000	-2.853891000
C	-3.825304000	-4.122339000	-3.967082000
H	-2.810157000	-4.483731000	-4.170873000
H	-4.458529000	-4.985281000	-3.728045000
H	-4.209725000	-3.683578000	-4.895372000
C	-5.313181000	-2.575987000	-2.693884000
H	-5.964686000	-3.408375000	-2.400998000
H	-5.388600000	-1.790732000	-1.940170000
H	-5.683866000	-2.178579000	-3.647824000

C	-2.967138000	-1.874340000	-3.318833000
H	-3.021114000	-1.047612000	-2.611345000
H	-1.920638000	-2.187566000	-3.425664000
H	-3.310156000	-1.512672000	-4.296833000
C	-3.386969000	3.001819000	-2.968853000
C	-4.731962000	2.247664000	-3.095013000
H	-4.806326000	1.444010000	-2.361745000
H	-5.573947000	2.935316000	-2.948409000
H	-4.824384000	1.813121000	-4.098995000
C	-2.215717000	2.021455000	-3.225120000
H	-1.249997000	2.537354000	-3.146408000
H	-2.240704000	1.199327000	-2.510012000
H	-2.290740000	1.597808000	-4.234676000
C	-3.343599000	4.071132000	-4.077401000
H	-4.160071000	4.796884000	-3.980450000
H	-2.393621000	4.619058000	-4.089398000
H	-3.453765000	3.584693000	-5.053619000
C	-2.903262000	5.578750000	-0.105929000
H	-3.326678000	1.255001000	6.941870000
H	-3.370037000	-1.239667000	6.942662000
H	-2.072468000	-6.490533000	-0.145851000
H	-2.726757000	6.642643000	-0.047821000
H	4.147995000	4.543917000	-0.021152000
H	4.265038000	-4.510324000	-0.436678000
H	3.415452000	0.207128000	-4.691556000
H	5.046280000	-0.175200000	4.205615000

1. H. Günther *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley-VHC: Weinheim, 3rd Ed.; 2013; Chapter 13, p 516.