

Supporting information for

Computational Analysis of a Non-heme Iron-Oxo Formation by Direct NO Release in Nitrite Reduction

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Table and Figure Captions

Table S1. The optimized molecular properties (ΔG (kcal/mol), bond distances (\AA), and spin,) of 1NHi-ONO (Fe (O)-nitrito-*trans*) and $P_{3\text{NHi-O}\dots\text{NO}}$ at triplet, quintet, and septet spin states, respectively.

Fig. S1 Schematic structures for the definition of n N-H bonds inward (nNHi) shown in the arm framework.

Fig. S2 The bond distances of (Fe) O \cdots H-N in the Fe (O)-nitrito-*trans* for the nNHi (n = 1-3) intermediates.

Fig. S3 Scanning (Fe)O-NO bond distance from the intermediate (${}^5\text{1NHi-ONO}$) to the product-complex (${}^5P_{\text{1NHi-O}\dots\text{NO-top}}$) at the B3LYP/6-31G (d) level.

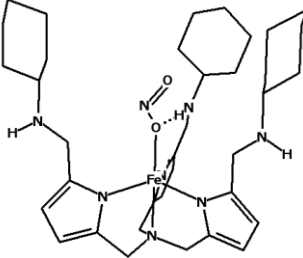
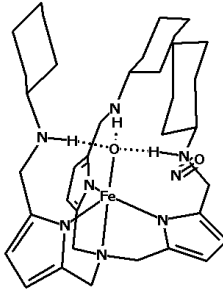
Fig. S4 The molecular structure of the transition state ${}^5\text{TS}_{\text{1NHi-O}\dots\text{NO}}$. The bond distance is in angstrom (\AA).

Fig. S5 Relative free energies (ΔG) and geometry profiles for NO release starting from 1NHi-ONO. The SCF energies (ΔE) including zero point energy and solvation (acetonitrile and water) corrections are listed in square brackets and parenthesis, respectively.

Fig. S6 Scanning potential energy surfaces for $0\text{NHi-ONO} \rightarrow 1\text{NHi-ONO}$, $P_{2\text{NHi-O}} \rightarrow P_{3\text{NHi-O}}$ and $P_{2\text{NHi-OH}} \rightarrow P_{3\text{NHi-OH}}$ calculated at the 6-31G (d) level.

Page S10-S25: Cartesian Coordinates of Intermediates, Transition States and Product-Complex.

Table S1. The optimized molecular properties (ΔG (kcal/mol), bond distances (\AA), and spin,) of 1NHi-ONO (Fe (O)-nitrito-*trans*) and $P_{3\text{NHi-O...NO}}$ at triplet, quintet, and septet spin states, respectively.

		triplet	quintet	septet	
	ΔG	16.48	0.00		
	Fe-O	1.960	2.078		
	(Fe)O-N	1.325	1.319		
	N-O	1.223	1.223		
	O-N-O	112.82	113.95		
	N-H...O	1.740	1.791		
	spin	Fe	1.92	3.72	
		ΔG	12.21	0.00	-9.06
Fe-O		1.754	1.745	1.780	
(Fe)O-N		3.639	3.883	3.908	
N-O		1.159	1.160	1.159	
O-N-O		89.06	89.95	90.11	
N-H...O		1.560	1.593	1.608	
			1.562	1.597	1.623
			1.583	1.633	1.638
spin		Fe	0.90	2.75	4.06
		(Fe)O	0.14	0.10	0.48
		N	0.78	0.73	0.73
		O	0.29	0.28	0.28

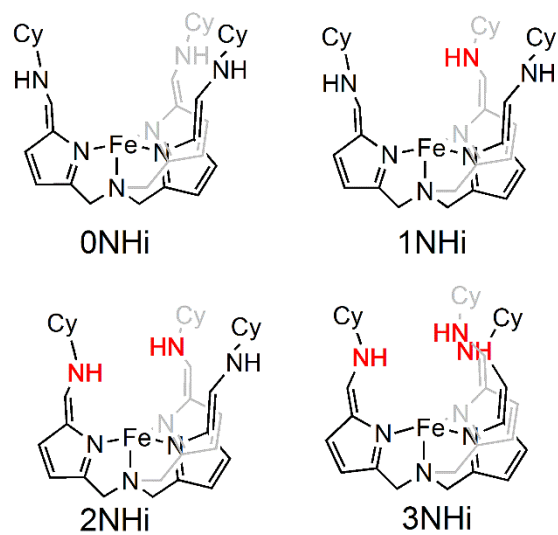


Fig. S1 Schematic structures for the definition of n N-H bonds inward (nNHi) shown in the arm framework.

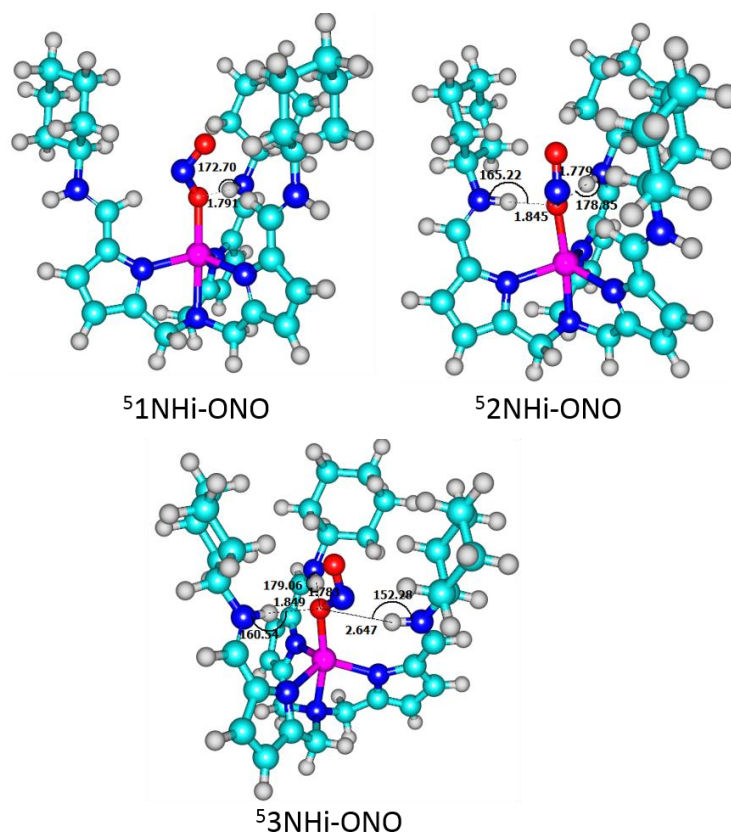


Fig. S2 The bond distances of (Fe) O ···H-N in the Fe (O)-nitrito-*trans* for the nNHi (n = 1-3) intermediates.

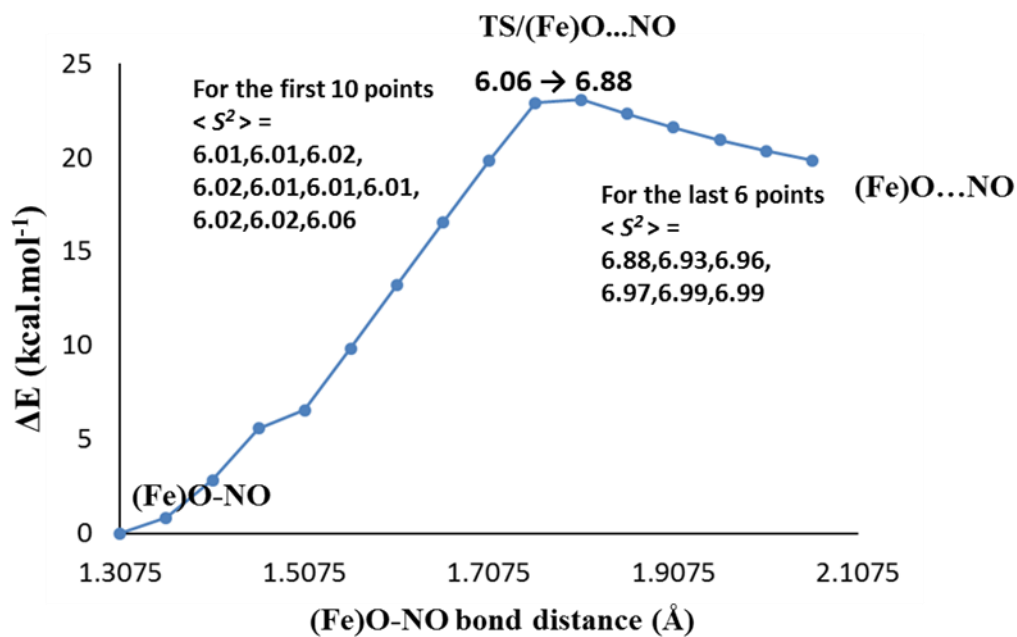


Fig. S3 Scanning (Fe)O-NO bond distance from the intermediate (⁵1NHi-ONO) to the product-complex (⁵P_{1NHi-O...NO-top}) at the B3LYP/6-31G (d) level.

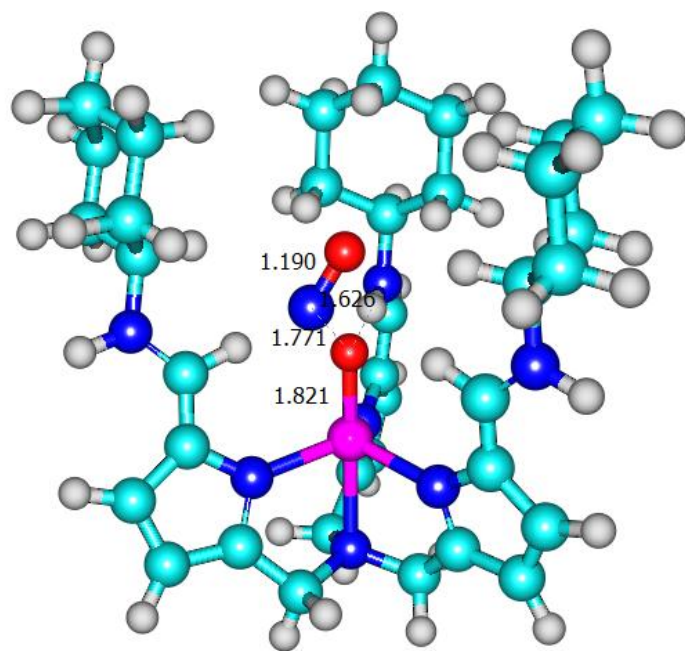


Fig. S4 The molecular structure of the transition state ${}^5\text{TS}_{1\text{NHi-O}\dots\text{NO}}$. The bond distance is in angstrom (\AA).

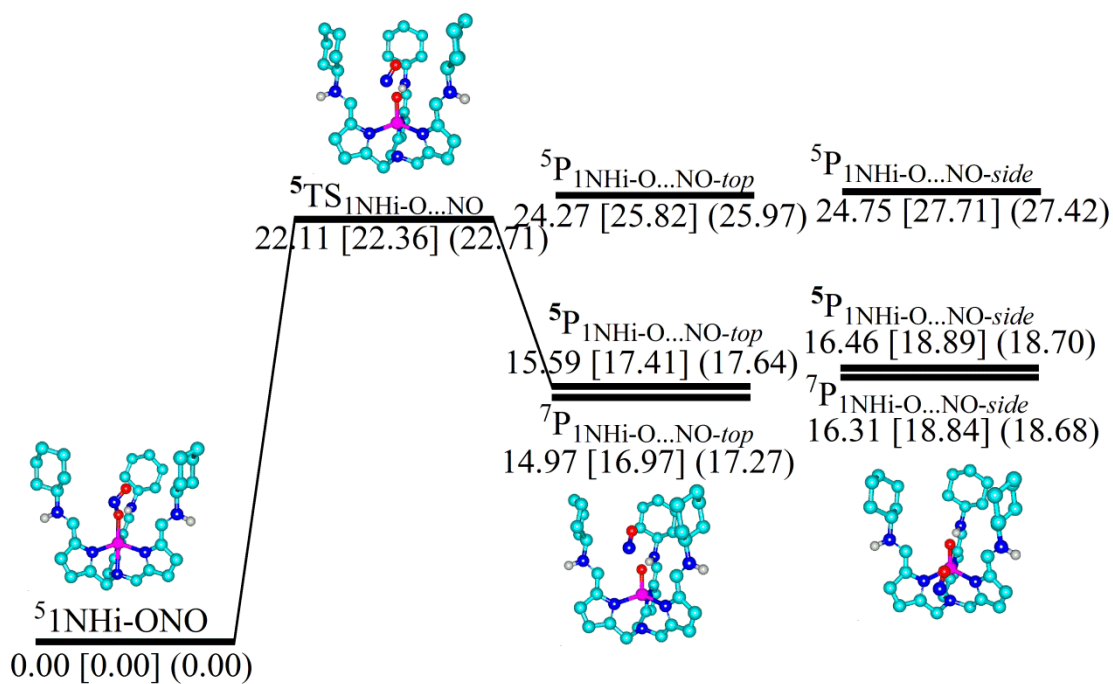


Fig. S5 Relative free energies (ΔG) and geometry profiles for NO release starting from 1NHi-ONO. The SCF energies (ΔE) including zero point energy and solvation (acetonitrile and water) corrections are listed in square brackets and parenthesis, respectively.

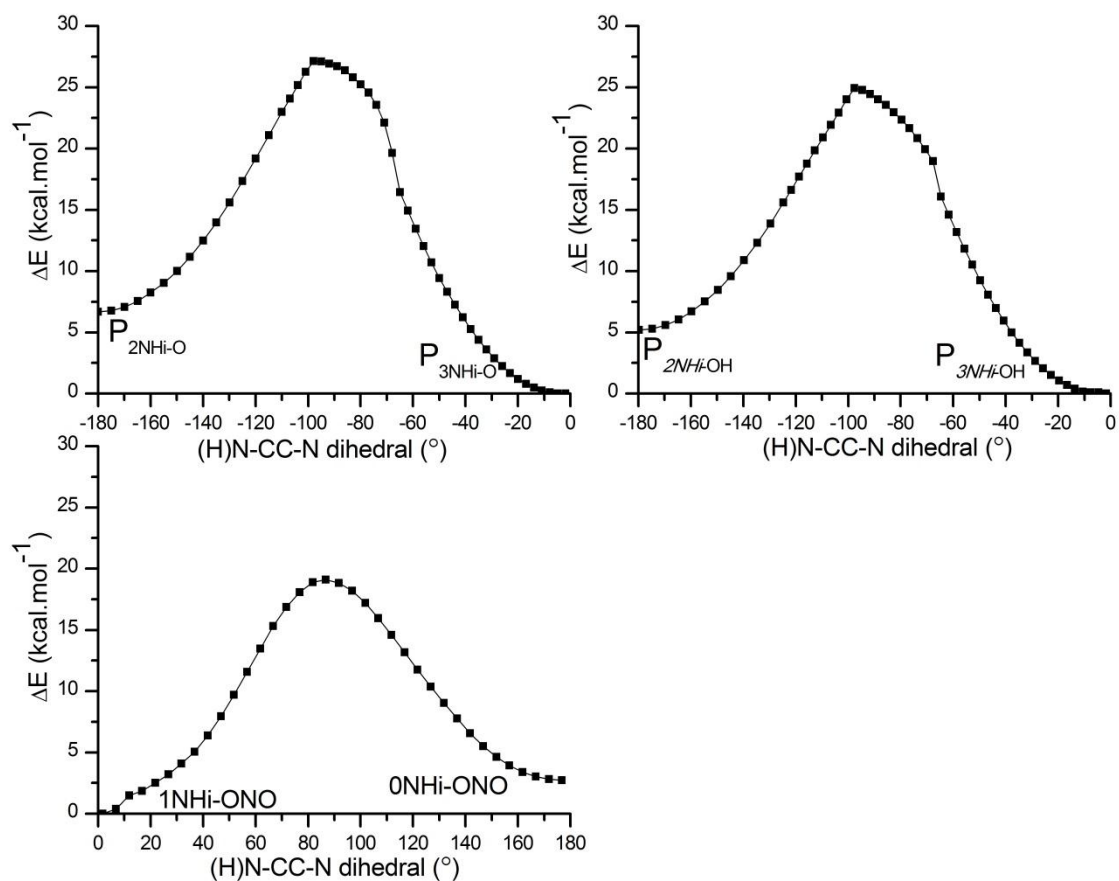


Fig. S6 Scanning potential energy surfaces for $0NH_i-ONO \rightarrow 1NH_i-ONO$, $P_{2NH_i-O} \rightarrow P_{3NH_i-O}$ and $P_{2NH_i-OH} \rightarrow P_{3NH_i-OH}$ calculated at the 6-31G (d) level.

**Cartesian Coordinates of
Intermediates, Transition States and
Product-Complex**

⁵
ONHi-ONO

				H	-0.922984000	-2.353354000	0.366109000
				C	0.444716000	1.680762000	-2.561521000
				H	0.550628000	0.830297000	-1.890310000
				N	0.997284000	1.920648000	3.514337000
				N	1.509679000	1.918193000	-3.315936000
				N	-1.349601000	-4.340861000	0.149585000
				H	-2.009531000	-5.047653000	-0.158941000
				H	0.791918000	2.519320000	4.306458000
				H	1.516558000	2.718356000	-3.938902000
Fe	-1.878561000	0.525128000	-0.114653000	C	2.410304000	1.579522000	3.259677000
N	-4.073221000	1.417357000	-0.250818000	C	3.019564000	2.498994000	2.186238000
C	-4.798659000	0.467220000	-1.114780000	C	3.213353000	1.631955000	4.564104000
H	-5.889834000	0.546051000	-0.993269000	H	2.417364000	0.548244000	2.883038000
H	-4.569854000	0.734900000	-2.153465000	C	4.488967000	2.131554000	1.927612000
C	-4.547492000	1.440455000	1.147864000	H	2.947508000	3.539893000	2.530788000
H	-5.407786000	2.112520000	1.283734000	H	2.430192000	2.424336000	1.264081000
H	-4.883781000	0.427449000	1.397482000	C	4.688215000	1.276755000	4.307685000
C	-3.947144000	2.764251000	-0.839281000	H	3.152437000	2.648900000	4.980688000
H	-4.869579000	3.080145000	-1.349030000	H	2.773273000	0.949702000	5.300876000
H	-3.781527000	3.471909000	-0.018022000	C	5.308777000	2.176286000	3.226720000
C	-3.409866000	1.820199000	2.058923000	H	4.913053000	2.811163000	1.179891000
C	-3.423905000	2.534284000	3.290707000	H	4.537740000	1.121228000	1.497574000
N	-2.169305000	1.432600000	1.741922000	H	5.251546000	1.356085000	5.243471000
C	-2.110527000	2.576667000	3.736271000	H	4.753799000	0.226798000	3.990024000
H	-4.295057000	2.953919000	3.776478000	H	6.343341000	1.871983000	3.033163000
C	-1.330587000	1.883799000	2.765011000	H	5.347969000	3.211417000	3.594106000
H	-1.751620000	3.037299000	4.648189000	C	0.023854000	-4.797962000	0.434514000
C	-2.765603000	2.832294000	-1.767375000	C	-0.004277000	-6.083239000	1.270942000
C	-2.505698000	3.773424000	-2.802715000	C	0.807401000	-4.987158000	-0.876102000
N	-1.734628000	1.993217000	-1.603816000	H	0.500076000	-3.995429000	1.009264000
C	-1.234935000	3.491964000	-3.279402000	C	1.423944000	-6.585963000	1.545784000
H	-3.177214000	4.551605000	-3.141059000	H	-0.559099000	-6.857070000	0.718490000
C	-0.756134000	2.380502000	-2.528827000	H	-0.543080000	-5.905402000	2.208877000
H	-0.715447000	4.004176000	-4.079616000	C	2.232582000	-5.484915000	-0.589995000
C	-4.330357000	-0.939474000	-0.857692000	H	0.276635000	-5.717191000	-1.504732000
C	-5.026289000	-2.163190000	-1.047295000	H	0.832056000	-4.035998000	-1.418257000
N	-3.074477000	-1.156846000	-0.440024000	C	2.216741000	-6.775625000	0.242868000
C	-4.130334000	-3.176926000	-0.737562000	H	1.379838000	-7.523141000	2.111289000
H	-6.053721000	-2.270028000	-1.369399000	H	1.943315000	-5.857526000	2.184339000
C	-2.915401000	-2.544081000	-0.351808000	H	2.763819000	-5.642641000	-1.535261000
H	-4.326235000	-4.241604000	-0.761624000	H	2.779428000	-4.701333000	-0.047830000
C	0.023768000	1.577602000	2.681350000	H	3.240346000	-7.094689000	0.469198000
H	0.326919000	0.959632000	1.837811000	H	1.758093000	-7.582782000	-0.346065000
C	-1.691424000	-3.064522000	0.069897000	C	2.769843000	1.164393000	-3.157345000

C	3.607064000	1.255380000	-4.437713000	H	5.405580000	-2.309829000	0.960085000
C	3.556248000	1.657887000	-1.929938000	H	4.974572000	-0.613545000	0.705965000
H	2.486167000	0.118339000	-2.988905000	N	2.349823000	-1.266313000	1.870243000
C	4.926283000	0.479224000	-4.279858000	C	3.636915000	-1.657994000	2.005225000
H	3.832165000	2.312980000	-4.644027000	C	3.928358000	-2.059738000	3.329599000
H	3.031009000	0.871934000	-5.288063000	C	2.746967000	-1.909426000	4.044216000
C	4.869824000	0.875739000	-1.775408000	H	2.576996000	-2.126509000	5.091382000
H	3.767907000	2.729678000	-2.052150000	C	1.772417000	-1.419523000	3.130159000
H	2.931859000	1.548200000	-1.035233000	H	4.881968000	-2.417141000	3.694198000
C	5.719460000	0.956494000	-3.053222000	C	0.436409000	-1.181944000	3.474105000
H	5.524718000	0.585514000	-5.190938000	H	0.159083000	-1.408915000	4.502311000
H	4.701542000	-0.591232000	-4.174206000	C	3.464997000	-3.354678000	-0.558511000
H	5.429136000	1.261409000	-0.916229000	H	3.439752000	-3.793582000	0.445853000
H	4.635654000	-0.174869000	-1.553988000	H	4.231742000	-3.899757000	-1.127549000
H	6.631294000	0.359677000	-2.940129000	N	1.172197000	-2.572343000	-0.990353000
H	6.040524000	1.996138000	-3.210547000	C	1.578180000	-4.625560000	-1.895488000
N	0.906885000	-0.759579000	-0.542625000	H	2.119841000	-5.518040000	-2.179851000
O	1.561495000	-1.731964000	-0.198060000	C	0.244546000	-4.335341000	-2.141326000
O	-0.056854000	-0.430910000	0.288987000	H	-0.466999000	-4.963113000	-2.663099000
				C	-0.006943000	-3.056248000	-1.568340000
				C	2.105030000	-3.516714000	-1.179432000
				C	-1.179998000	-2.312605000	-1.457603000
				H	-1.129037000	-1.376608000	-0.910616000
				N	1.835034000	4.079238000	-0.870738000
				H	2.442396000	4.592303000	-1.500941000
				C	0.677790000	4.811087000	-0.324432000
				C	1.091353000	6.238221000	0.057587000
				C	-0.498406000	4.802845000	-1.316735000
				H	0.376727000	4.273513000	0.583679000
				C	-0.107845000	7.025153000	0.613269000
				H	1.473546000	6.748791000	-0.839473000
				H	1.909439000	6.206818000	0.786590000
				C	-1.691883000	5.589827000	-0.750891000
				H	-0.165926000	5.261026000	-2.259234000
				H	-0.777678000	3.766542000	-1.535682000
				C	-1.289259000	7.022737000	-0.369418000
				H	0.201933000	8.050435000	0.842470000
				H	-0.423616000	6.573763000	1.564561000
				H	-2.505800000	5.599033000	-1.484014000
				H	-2.077446000	5.069225000	0.137471000
				H	-2.142469000	7.553896000	0.066955000
				H	-1.006486000	7.573639000	-1.277673000
				C	-3.591031000	-1.822574000	-1.749167000
				C	-4.138720000	-1.361053000	-3.108604000

5
1NH_i-ONO

Fe	1.803006000	-0.784684000	-0.096249000
N	3.799694000	-1.923329000	-0.413902000
N	3.035632000	0.619044000	-1.054657000
N	-0.536314000	-0.724074000	2.711328000
H	-0.343176000	-0.435878000	1.742198000
N	-2.375697000	-2.633628000	-1.928531000
H	-2.481833000	-3.499831000	-2.446795000
O	0.030519000	0.273749000	0.141290000
N	-0.705971000	1.111566000	-0.563124000
O	-1.908835000	0.910115000	-0.474837000
C	4.392375000	-1.343450000	-1.633949000
H	3.914223000	-1.830534000	-2.492463000
H	5.471966000	-1.545481000	-1.705566000
C	4.115547000	0.132945000	-1.682357000
C	4.832383000	1.163381000	-2.347922000
H	5.743450000	1.042112000	-2.918802000
C	4.135202000	2.339457000	-2.113170000
H	4.402782000	3.329270000	-2.461221000
C	3.020099000	1.996001000	-1.297446000
C	2.019373000	2.775815000	-0.723979000
H	1.301274000	2.269876000	-0.088283000
C	4.559423000	-1.621705000	0.817306000

C	-4.644689000	-2.606770000	-0.951417000	H	4.364590000	-3.702722000	0.825376000
H	-3.286550000	-0.941679000	-1.174798000	H	3.568547000	-2.728298000	2.063339000
C	-5.420123000	-0.530851000	-2.923152000	C	3.708132000	-0.099709000	2.060759000
H	-4.359062000	-2.245422000	-3.725057000	C	4.065795000	0.314870000	3.364550000
H	-3.370515000	-0.782205000	-3.633629000	N	2.399703000	0.124701000	1.797948000
C	-5.922301000	-1.770561000	-0.770677000	C	2.904977000	0.814273000	3.938874000
H	-4.887534000	-3.533031000	-1.492902000	H	5.047730000	0.239245000	3.811884000
H	-4.224973000	-2.900729000	0.017275000	C	1.877886000	0.696469000	2.960419000
C	-6.480984000	-1.303604000	-2.123645000	H	2.782210000	1.218530000	4.935935000
H	-5.813321000	-0.238235000	-3.902764000	C	2.221337000	-3.541831000	0.634665000
H	-5.169250000	0.398585000	-2.393142000	C	1.758765000	-4.874983000	0.804209000
H	-6.670716000	-2.354671000	-0.223645000	N	1.259034000	-2.742787000	0.150509000
H	-5.692663000	-0.892894000	-0.150774000	C	0.430692000	-4.879667000	0.410885000
H	-7.367854000	-0.678891000	-1.970254000	H	2.341373000	-5.711285000	1.167368000
H	-6.807887000	-2.178625000	-2.703040000	C	0.122427000	-3.551937000	0.000199000
C	-1.924655000	-0.527869000	3.147246000	H	-0.236221000	-5.732609000	0.393849000
C	-2.304064000	0.961464000	3.056019000	C	4.012266000	-0.715764000	-1.952480000
C	-2.869473000	-1.396339000	2.296532000	C	4.778937000	-0.202104000	-3.023153000
H	-1.985012000	-0.852525000	4.194331000	N	2.957933000	0.077404000	-1.656652000
C	-3.774622000	1.184261000	3.445445000	C	4.166645000	0.986405000	-3.394282000
H	-2.147496000	1.293487000	2.022071000	H	5.671416000	-0.647922000	-3.440830000
H	-1.635316000	1.547361000	3.697673000	C	3.045705000	1.160083000	-2.534356000
C	-4.335437000	-1.168128000	2.697918000	H	4.479150000	1.677587000	-4.166925000
H	-2.729292000	-1.118410000	1.243947000	C	0.555047000	1.092940000	3.186079000
H	-2.590777000	-2.451726000	2.400601000	H	0.318705000	1.423879000	4.196201000
C	-4.714042000	0.317048000	2.593068000	C	2.282384000	2.331458000	-2.505721000
H	-4.025995000	2.245119000	3.336674000	H	2.566034000	3.107293000	-3.214507000
H	-3.914438000	0.936216000	4.507234000	C	-1.048469000	-2.998674000	-0.504594000
H	-4.991235000	-1.779147000	2.068522000	H	-1.011098000	-1.959512000	-0.818022000
H	-4.488196000	-1.511099000	3.730909000	N	-0.446357000	1.117729000	2.328587000
H	-5.754293000	0.465809000	2.903652000	N	-2.224563000	-3.588809000	-0.667016000
H	-4.644171000	0.635574000	1.543448000	N	1.283432000	2.633067000	-1.700373000
				H	0.915497000	1.908100000	-1.078172000
				H	-0.270707000	0.885923000	1.341416000
				H	-2.339678000	-4.555116000	-0.379295000
5				C	-1.839801000	1.439010000	2.667155000
² NHi-ONO				C	-2.308992000	2.686390000	1.898615000
Fe	1.779604000	-0.691142000	-0.061479000	C	-2.734648000	0.224736000	2.356828000
N	3.795380000	-1.718420000	0.249892000	H	-1.871850000	1.642195000	3.745459000
C	4.274803000	-1.943162000	-1.127333000	C	-3.791490000	2.986562000	2.171397000
H	5.342862000	-2.206468000	-1.156675000	H	-2.165929000	2.499817000	0.827605000
H	3.715123000	-2.796654000	-1.528113000	H	-1.681279000	3.542117000	2.173602000
C	4.585700000	-0.733842000	1.016826000	C	-4.214450000	0.534726000	2.630807000
H	5.475751000	-1.186375000	1.477401000	H	-2.608580000	-0.024482000	1.295376000
H	4.934305000	0.030746000	0.314451000				
C	3.561888000	-2.969571000	0.993877000				

H	-2.395784000	-0.638916000	2.941340000	O	0.042015000	0.452003000	-0.355223000
C	-4.675836000	1.772691000	1.846842000				
H	-4.100788000	3.857328000	1.582329000				
H	-3.923076000	3.260720000	3.227787000				
H	-4.826964000	-0.336095000	2.371243000	Fe	1.788056000	-0.342536000	-0.032914000
H	-4.358132000	0.708030000	3.706603000	N	4.012762000	-0.609991000	0.114900000
H	-5.724305000	1.995754000	2.073481000	C	4.430902000	-0.840628000	-1.282195000
H	-4.618890000	1.560147000	0.769996000	H	5.521470000	-0.764767000	-1.406082000
C	0.554048000	3.909953000	-1.700429000	H	4.140322000	-1.865081000	-1.542424000
C	-0.811075000	3.755327000	-2.392459000	C	4.514629000	0.650219000	0.702771000
C	0.403918000	4.404857000	-0.252278000	H	5.539133000	0.543128000	1.087077000
H	1.164667000	4.627536000	-2.263454000	H	4.538204000	1.403329000	-0.091670000
C	-1.618103000	5.061248000	-2.324959000	C	4.237224000	-1.767069000	0.994895000
H	-1.367350000	2.954790000	-1.890874000	H	5.236703000	-2.204230000	0.852029000
H	-0.658762000	3.439328000	-3.431400000	H	4.188851000	-1.409964000	2.030390000
C	-0.429801000	5.694863000	-0.181171000	C	3.577656000	1.089162000	1.793880000
H	-0.090793000	3.616996000	0.329701000	C	3.895273000	1.748008000	3.004668000
H	1.396215000	4.555288000	0.188635000	N	2.252794000	0.838913000	1.684328000
C	-1.792336000	5.528213000	-0.872009000	C	2.694170000	1.900164000	3.683852000
H	-2.593088000	4.913387000	-2.802128000	H	4.882196000	2.051271000	3.327255000
H	-1.103030000	5.844036000	-2.899875000	C	1.680818000	1.339898000	2.856782000
H	-0.560375000	5.987179000	0.867076000	H	2.536647000	2.354575000	4.654047000
H	0.123844000	6.511613000	-0.665113000	C	3.173289000	-2.802906000	0.788797000
H	-2.348956000	6.471384000	-0.839002000	C	3.270192000	-4.172048000	1.122459000
H	-2.390361000	4.786571000	-0.323859000	N	1.953483000	-2.470161000	0.301430000
C	-3.440170000	-2.874265000	-1.094739000	C	2.032580000	-4.718823000	0.833047000
C	-4.183890000	-3.662661000	-2.180696000	H	4.143055000	-4.670740000	1.521439000
C	-4.348411000	-2.583311000	0.112365000	C	1.222980000	-3.667957000	0.313098000
H	-3.099731000	-1.921025000	-1.516265000	H	1.723252000	-5.750682000	0.943814000
C	-5.455182000	-2.913474000	-2.617630000	C	3.728198000	0.150455000	-2.166132000
H	-4.460960000	-4.649280000	-1.779660000	C	4.192243000	0.748158000	-3.360145000
H	-3.518833000	-3.834333000	-3.034513000	N	2.528131000	0.641959000	-1.784447000
C	-5.610677000	-1.825971000	-0.329618000	C	3.228800000	1.680555000	-3.717774000
H	-4.633324000	-3.536185000	0.581674000	H	5.124993000	0.531567000	-3.862935000
H	-3.786531000	-2.012529000	0.859367000	C	2.208121000	1.623116000	-2.726372000
C	-6.367678000	-2.599279000	-1.421094000	H	3.247355000	2.358209000	-4.562154000
H	-5.992354000	-3.507108000	-3.364991000	C	0.326441000	1.299955000	3.204371000
H	-5.165405000	-1.975087000	-3.110902000	H	0.067188000	1.622193000	4.211498000
H	-6.257890000	-1.648902000	0.536677000	C	1.195375000	2.582635000	-2.623031000
H	-5.319429000	-0.837830000	-0.712976000	H	1.180061000	3.352626000	-3.392238000
H	-7.240386000	-2.026659000	-1.753740000	C	-0.061061000	-3.938001000	-0.168308000
H	-6.749896000	-3.539429000	-0.998748000	H	-0.405212000	-4.957914000	-0.004315000
N	-0.970535000	0.078533000	-1.135073000	N	-0.679093000	0.915909000	2.443246000
O	-1.945420000	0.797977000	-1.055970000	N	-0.915801000	-3.166098000	-0.808740000

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3NH₂-ONO

N	0.288302000	2.705134000	-1.674363000	H	-3.056711000	-3.361757000	0.836811000
H	0.195100000	1.953665000	-0.986933000	C	-4.041752000	-3.553250000	-2.990868000
H	-0.492765000	0.682654000	1.461998000	H	-2.508812000	-2.054162000	-2.680078000
H	-0.690139000	-2.187290000	-1.006464000	H	-1.880879000	-3.585190000	-3.305562000
C	-2.071534000	0.731183000	2.872210000	C	-5.068100000	-2.992494000	-1.993851000
C	-3.008558000	1.619948000	2.035560000	H	-5.445529000	-2.985561000	0.152800000
C	-2.433312000	-0.760519000	2.738356000	H	-4.843854000	-4.517753000	-0.470442000
H	-2.132303000	1.026662000	3.927383000	H	-4.263632000	-3.207462000	-4.006230000
C	-4.485205000	1.345061000	2.361968000	H	-4.114937000	-4.649985000	-3.010545000
H	-2.826405000	1.413646000	0.973216000	H	-6.077645000	-3.319841000	-2.265744000
H	-2.761503000	2.673676000	2.210030000	H	-5.062799000	-1.894769000	-2.048640000
C	-3.915982000	-1.023412000	3.042672000	N	-1.063462000	-0.316738000	-1.023879000
H	-2.214145000	-1.071874000	1.709201000	O	-2.134290000	0.244523000	-1.124745000
H	-1.784734000	-1.351753000	3.395390000	O	-0.185237000	0.299679000	-0.252469000
C	-4.828809000	-0.140679000	2.178647000				
H	-5.120705000	1.969486000	1.724191000				
H	-4.694634000	1.641985000	3.399382000	Fe	-1.965460000	0.158951000	-0.028935000
H	-4.138396000	-2.084391000	2.881124000	N	-4.351311000	0.330361000	-0.149568000
H	-4.113014000	-0.821455000	4.104756000	N	-2.576268000	-1.340503000	-1.322999000
H	-5.879441000	-0.321369000	2.431247000	N	0.428116000	-0.278095000	2.554152000
H	-4.704112000	-0.412640000	1.120879000	H	0.217839000	-0.113621000	1.535677000
C	-0.684927000	3.803997000	-1.571321000	N	0.777053000	3.951876000	-1.202521000
C	-2.016935000	3.441917000	-2.250605000	H	0.486985000	4.905340000	-1.394048000
C	-0.880221000	4.144734000	-0.084949000	O	-0.146701000	0.068015000	-0.038194000
H	-0.245017000	4.670956000	-2.081574000	N	1.107679000	-0.236893000	-1.250107000
C	-3.053955000	4.559996000	-2.059695000	O	2.143700000	0.230790000	-0.896438000
H	-2.389399000	2.510323000	-1.810307000	C	-4.703537000	-0.151525000	-1.501974000
H	-1.841443000	3.246962000	-3.315654000	H	-4.542482000	0.680492000	-2.197984000
C	-1.936527000	5.243997000	0.106646000	H	-5.763089000	-0.438682000	-1.575590000
H	-1.204538000	3.234192000	0.435473000	C	-3.801467000	-1.297987000	-1.865984000
H	0.079532000	4.442245000	0.353663000	C	-4.007673000	-2.399748000	-2.734999000
C	-3.264644000	4.871789000	-0.570003000	H	-4.907548000	-2.612043000	-3.296932000
H	-3.999114000	4.266234000	-2.529279000	C	-2.833476000	-3.145787000	-2.712273000
H	-2.716675000	5.469595000	-2.577085000	H	-2.643095000	-4.065743000	-3.250564000
H	-2.084925000	5.425327000	1.177425000	C	-1.945211000	-2.483674000	-1.822839000
H	-1.562473000	6.185614000	-0.319034000	C	-0.667131000	-2.779624000	-1.349750000
H	-3.990346000	5.683813000	-0.450024000	H	-0.253368000	-2.081433000	-0.628037000
H	-3.690528000	3.988155000	-0.073081000	C	-4.816741000	-0.562964000	0.931248000
C	-2.281163000	-3.582523000	-1.176097000	H	-5.845868000	-0.332506000	1.241946000
C	-3.306431000	-3.019707000	-0.174801000	H	-4.820785000	-1.584398000	0.533686000
C	-2.607619000	-3.145421000	-2.612916000	N	-2.547110000	-0.331404000	1.891639000
H	-2.299614000	-4.679188000	-1.124777000	C	-3.875770000	-0.507997000	2.102213000
C	-4.737252000	-3.427197000	-0.557576000	C	-4.157389000	-0.721890000	3.465971000
H	-3.230158000	-1.926313000	-0.181338000	C	-2.929600000	-0.690032000	4.124219000

⁵TS_{INH-O...NO}

H	-2.746968000	-0.824652000	5.182997000	H	2.639675000	5.149571000	0.382624000
C	-1.937003000	-0.451607000	3.139896000	H	2.298171000	3.528501000	0.995607000
H	-5.134720000	-0.887696000	3.898682000	C	5.056263000	4.515774000	-0.908787000
C	-0.555433000	-0.436848000	3.407847000	H	4.940852000	4.711304000	-3.075143000
H	-0.270898000	-0.599362000	4.447213000	H	4.624319000	3.086761000	-2.477093000
C	-4.700372000	1.746264000	0.076351000	H	4.742383000	4.090149000	1.204761000
H	-4.809971000	1.893506000	1.157473000	H	4.487621000	2.708565000	0.141721000
H	-5.664242000	2.010440000	-0.382037000	H	6.123704000	4.269111000	-0.894792000
N	-2.339207000	2.165834000	-0.450990000	H	4.981651000	5.601611000	-0.755017000
C	-3.639120000	4.007875000	-0.775499000	C	1.853445000	-0.382972000	2.881057000
H	-4.525125000	4.626389000	-0.830709000	C	2.462326000	-1.576901000	2.118601000
C	-2.327749000	4.388681000	-1.029327000	C	2.573142000	0.929022000	2.521832000
H	-1.989148000	5.372117000	-1.330927000	H	1.938734000	-0.561526000	3.961481000
C	-1.518632000	3.238298000	-0.822316000	C	3.978080000	-1.679393000	2.348006000
C	-3.595334000	2.636647000	-0.415687000	H	2.267479000	-1.428846000	1.049686000
C	-0.138553000	3.047524000	-0.893444000	H	1.954835000	-2.500360000	2.423744000
H	0.225724000	2.049612000	-0.657203000	C	4.087001000	0.815477000	2.760909000
N	0.119580000	-3.792497000	-1.672275000	H	2.384559000	1.141330000	1.462587000
H	-0.177851000	-4.454984000	-2.381140000	H	2.143486000	1.751714000	3.105686000
C	1.496307000	-3.920021000	-1.162549000	C	4.686431000	-0.365740000	1.981825000
C	1.785443000	-5.353519000	-0.699876000	H	4.381030000	-2.511809000	1.758894000
C	2.520436000	-3.441285000	-2.204064000	H	4.174337000	-1.919134000	3.402554000
H	1.550813000	-3.254571000	-0.293490000	H	4.573929000	1.753142000	2.472563000
C	3.213942000	-5.453436000	-0.135677000	H	4.279530000	0.679804000	3.834647000
H	1.680992000	-6.036335000	-1.556100000	H	5.760562000	-0.446741000	2.182653000
H	1.047224000	-5.658554000	0.050808000	H	4.573188000	-0.182785000	0.904260000
C	3.944566000	-3.538088000	-1.632358000				
H	2.436912000	-4.069794000	-3.102395000				
H	2.284151000	-2.413428000	-2.497517000	⁵⁵ P _{INHI-O...NO-top}			
C	4.259487000	-4.962913000	-1.149903000	Fe	1.938103000	-0.202694000	-0.034056000
H	3.420720000	-6.486803000	0.162612000	N	4.346842000	-0.567173000	-0.265601000
H	3.279393000	-4.844071000	0.777438000	N	2.612365000	1.218747000	-1.377920000
H	4.668872000	-3.217641000	-2.389009000	N	-0.270187000	-0.003344000	2.643180000
H	4.038390000	-2.835757000	-0.791502000	H	-0.096754000	0.033334000	1.580301000
H	5.260528000	-5.000447000	-0.705781000	N	-1.158714000	-3.578508000	-1.285273000
H	4.273349000	-5.642678000	-2.013511000	H	-0.983664000	-4.535139000	-1.576651000
C	2.227141000	3.691610000	-1.161629000	O	0.196896000	0.064801000	0.082402000
C	2.934107000	4.423914000	-2.309266000	N	-1.623843000	0.323190000	-1.603984000
C	2.818793000	4.079655000	0.204310000	O	-2.615961000	0.435255000	-1.003066000
H	2.346159000	2.611652000	-1.299376000	C	4.698478000	-0.040935000	-1.598220000
C	4.448148000	4.152012000	-2.272604000	H	4.482949000	-0.827655000	-2.331250000
H	2.756342000	5.505623000	-2.209674000	H	5.769307000	0.197760000	-1.682174000
H	2.506433000	4.110514000	-3.268535000	C	3.846956000	1.161209000	-1.897861000
C	4.328554000	3.792070000	0.234883000	C	4.109081000	2.298587000	-2.703970000
				H	5.025231000	2.503540000	-3.241869000

C	2.962588000	3.084782000	-2.662574000	H	-3.861596000	6.286513000	-1.915269000
H	2.810851000	4.030513000	-3.167619000	H	-4.056839000	4.542844000	-1.785716000
C	2.029175000	2.405320000	-1.833899000	H	-4.571895000	5.593461000	0.399916000
C	0.725894000	2.696196000	-1.430956000	H	-3.011542000	6.408211000	0.415264000
H	0.238315000	1.935525000	-0.817579000	C	-2.563788000	-3.142481000	-1.267003000
C	4.913422000	0.224893000	0.844120000	C	-3.138183000	-3.103205000	-2.691751000
H	5.937347000	-0.087631000	1.096561000	C	-3.398981000	-4.037514000	-0.339351000
H	4.968628000	1.266323000	0.505314000	H	-2.558890000	-2.125956000	-0.862411000
N	2.671960000	0.074038000	1.875707000	C	-4.610658000	-2.659948000	-2.675437000
C	4.016781000	0.146849000	2.047195000	H	-3.061713000	-4.107165000	-3.134543000
C	4.356986000	0.198391000	3.411426000	H	-2.531325000	-2.430666000	-3.308660000
C	3.151275000	0.157636000	4.113410000	C	-4.870641000	-3.589332000	-0.333449000
H	3.015020000	0.174997000	5.187496000	H	-3.334193000	-5.078099000	-0.689769000
C	2.114042000	0.082746000	3.152392000	H	-2.976303000	-4.010182000	0.671755000
H	5.356961000	0.257928000	3.819457000	C	-5.454568000	-3.554069000	-1.753928000
C	0.741295000	0.024080000	3.473095000	H	-5.009577000	-2.670768000	-3.695534000
H	0.503630000	0.003712000	4.537350000	H	-4.668427000	-1.619612000	-2.325057000
C	4.561126000	-2.019463000	-0.126961000	H	-5.455754000	-4.255969000	0.309508000
H	4.682380000	-2.237062000	0.940941000	H	-4.937627000	-2.585967000	0.109325000
H	5.481533000	-2.352367000	-0.628274000	H	-6.490555000	-3.198688000	-1.726815000
N	2.155385000	-2.183142000	-0.593575000	H	-5.481698000	-4.574380000	-2.161720000
C	3.251903000	-4.116594000	-1.069802000	C	-1.673821000	-0.108838000	3.041269000
H	4.068071000	-4.815991000	-1.194077000	C	-2.456358000	1.100400000	2.497223000
C	1.900574000	-4.350929000	-1.296500000	C	-2.257921000	-1.433674000	2.512999000
H	1.456183000	-5.276787000	-1.640130000	H	-1.722468000	-0.108715000	4.139128000
C	1.217766000	-3.141812000	-0.993605000	C	-3.959473000	0.979389000	2.790540000
C	3.359961000	-2.771880000	-0.630113000	H	-2.294267000	1.152860000	1.413788000
C	-0.134053000	-2.795738000	-0.986634000	H	-2.046427000	2.021600000	2.927421000
H	-0.366652000	-1.772260000	-0.683150000	C	-3.759026000	-1.543476000	2.818158000
N	0.014290000	3.774997000	-1.713923000	H	-2.096158000	-1.466855000	1.427406000
H	0.425292000	4.516606000	-2.270197000	H	-1.703769000	-2.274471000	2.946549000
C	-1.373295000	3.962217000	-1.238164000	C	-4.529895000	-0.341704000	2.250886000
C	-1.428724000	4.086077000	0.294250000	H	-4.487624000	1.834251000	2.353464000
C	-1.996287000	5.184147000	-1.921283000	H	-4.126210000	1.030276000	3.875758000
H	-1.934025000	3.067857000	-1.537163000	H	-4.151655000	-2.482096000	2.411552000
C	-2.879119000	4.277371000	0.763780000	H	-3.907494000	-1.590350000	3.906050000
H	-0.817459000	4.946124000	0.599925000	H	-5.594992000	-0.423686000	2.494971000
H	-0.989115000	3.194612000	0.755287000	H	-4.451866000	-0.346096000	1.154216000
C	-3.444606000	5.389628000	-1.445132000				
H	-1.400460000	6.075103000	-1.672462000				
H	-1.964627000	5.061410000	-3.011059000	⁷ P _{INH_i-O...NO-<i>top</i>}	1.995707000	-0.094829000	-0.042079000
C	-3.526748000	5.494877000	0.086096000	Fe	4.409365000	-0.244656000	-0.344014000
H	-2.902615000	4.384609000	1.853941000	N	2.497628000	1.398391000	-1.375663000
H	-3.457248000	3.373368000	0.525504000	N	-0.177772000	0.110539000	2.659098000

H	-0.014483000	0.074615000	1.592690000	C	-1.905063000	4.937719000	-0.111845000
N	-0.847006000	-3.722843000	-1.147120000	C	-2.769435000	3.695160000	-2.153796000
H	-0.609802000	-4.675798000	-1.404552000	H	-1.824184000	2.811663000	-0.436795000
O	0.240364000	0.021102000	0.103087000	C	-3.324805000	4.946585000	0.480559000
N	-1.570220000	0.143663000	-1.637947000	H	-1.740895000	5.858448000	-0.690391000
O	-2.575761000	0.226357000	-1.054426000	H	-1.149208000	4.914871000	0.681629000
C	4.669078000	0.316396000	-1.685200000	C	-4.187381000	3.704936000	-1.557920000
H	4.499050000	-0.484484000	-2.414848000	H	-2.633294000	4.577016000	-2.796847000
H	5.711970000	0.646938000	-1.802075000	H	-2.612332000	2.809162000	-2.778803000
C	3.706832000	1.441626000	-1.952433000	C	-4.395262000	4.905799000	-0.621456000
C	3.829196000	2.588307000	-2.778100000	H	-3.455708000	5.831306000	1.112932000
H	4.697932000	2.869084000	-3.358709000	H	-3.442854000	4.071318000	1.135681000
C	2.618922000	3.270169000	-2.690146000	H	-4.927273000	3.713661000	-2.365590000
H	2.362734000	4.195278000	-3.191179000	H	-4.342650000	2.772009000	-0.997541000
C	1.789707000	2.522898000	-1.811510000	H	-5.395131000	4.867982000	-0.174889000
C	0.490659000	2.695351000	-1.330882000	H	-4.347681000	5.834695000	-1.207010000
H	0.126901000	1.906951000	-0.668269000	C	-2.279356000	-3.390543000	-1.093809000
C	4.938898000	0.590727000	0.753147000	C	-2.928764000	-3.590785000	-2.472073000
H	5.988610000	0.356524000	0.982450000	C	-2.994942000	-4.202901000	-0.003366000
H	4.908273000	1.632255000	0.411833000	H	-2.332425000	-2.329581000	-0.830828000
N	2.737726000	0.290825000	1.840856000	C	-4.427430000	-3.249554000	-2.425094000
C	4.078167000	0.458198000	1.978591000	H	-2.801260000	-4.640024000	-2.777005000
C	4.441843000	0.571931000	3.332955000	H	-2.408473000	-2.973043000	-3.212838000
C	3.255280000	0.478829000	4.062839000	C	-4.492888000	-3.853915000	0.033360000
H	3.140071000	0.526208000	5.138485000	H	-2.872970000	-5.275176000	-0.214793000
C	2.205424000	0.308178000	3.128411000	H	-2.522378000	-4.008422000	0.966445000
H	5.443471000	0.710553000	3.717051000	C	-5.152188000	-4.059233000	-1.338943000
C	0.839631000	0.217393000	3.474639000	H	-4.877441000	-3.430144000	-3.407237000
H	0.615379000	0.255522000	4.541403000	H	-4.543650000	-2.176382000	-2.216769000
C	4.760591000	-1.672379000	-0.221233000	H	-4.993417000	-4.458171000	0.797964000
H	4.951938000	-1.878058000	0.838833000	H	-4.608912000	-2.803713000	0.335536000
H	5.683663000	-1.919159000	-0.765565000	H	-6.209090000	-3.773745000	-1.296082000
N	2.363727000	-2.049302000	-0.600092000	H	-5.124088000	-5.126495000	-1.600212000
C	3.604188000	-3.891227000	-1.082832000	C	-1.581172000	0.038935000	3.063159000
H	4.472185000	-4.521112000	-1.226192000	C	-2.356700000	1.193179000	2.397982000
C	2.270438000	-4.244340000	-1.254696000	C	-2.167120000	-1.327454000	2.657236000
H	1.895440000	-5.210867000	-1.567670000	H	-1.635504000	0.144275000	4.155672000
C	1.497453000	-3.091817000	-0.948927000	C	-3.863791000	1.105294000	2.681900000
C	3.612169000	-2.533738000	-0.670420000	H	-2.181292000	1.136016000	1.316467000
C	0.122685000	-2.855311000	-0.906094000	H	-1.947908000	2.150973000	2.741818000
H	-0.180748000	-1.844264000	-0.623572000	C	-3.670825000	-1.402907000	2.960442000
N	-0.355994000	3.677698000	-1.588133000	H	-1.998320000	-1.462536000	1.580268000
H	-0.080414000	4.433652000	-2.207003000	H	-1.619489000	-2.125627000	3.171999000
C	-1.718936000	3.723767000	-1.034108000	C	-4.432960000	-0.261641000	2.269686000

H	-4.384155000	1.913255000	2.154231000	C	0.262642000	-2.055736000	-1.458518000
H	-4.044715000	1.265560000	3.753995000	H	0.409074000	-1.195885000	-0.798782000
H	-4.062763000	-2.376162000	2.645301000	N	0.155010000	2.523129000	-1.443980000
H	-3.828113000	-1.341369000	4.046418000	N	1.345979000	-2.747479000	-1.770120000
H	-5.500555000	-0.316509000	2.510294000	N	0.330075000	0.228992000	2.653988000
H	-4.344298000	-0.375061000	1.179602000	H	0.126562000	0.349526000	1.603915000
				H	0.023542000	1.684508000	-0.789839000
				H	1.270714000	-3.556318000	-2.378765000
⁷ P _{2NHi-O...NO-side}				C	1.538726000	2.851348000	-1.791954000
Fe	-1.968983000	0.131258000	-0.030082000	C	2.273551000	3.415696000	-0.562585000
N	-4.294044000	-0.365012000	-0.285933000	C	2.245001000	1.592186000	-2.328657000
C	-4.631935000	-1.274789000	0.824440000	H	1.520484000	3.615105000	-2.581490000
H	-5.704255000	-1.249936000	1.066790000	C	3.755864000	3.682676000	-0.864919000
H	-4.398579000	-2.294986000	0.496419000	H	2.188127000	2.681634000	0.247969000
C	-4.949453000	0.955306000	-0.183365000	H	1.769750000	4.327973000	-0.222733000
H	-5.973495000	0.941837000	-0.583630000	C	3.725461000	1.870701000	-2.630924000
H	-5.019070000	1.199313000	0.883488000	H	2.162328000	0.805038000	-1.566453000
C	-4.436681000	-0.996977000	-1.615971000	H	1.720314000	1.230730000	-3.220790000
H	-5.348062000	-1.607673000	-1.684855000	C	4.452368000	2.419799000	-1.394119000
H	-4.527727000	-0.194383000	-2.357314000	H	4.256406000	4.051739000	0.037265000
C	-4.108212000	1.983583000	-0.883116000	H	3.837660000	4.482420000	-1.614049000
C	-4.499852000	3.138746000	-1.583491000	H	4.211107000	0.955806000	-2.986757000
N	-2.757740000	1.850401000	-0.861853000	H	3.799246000	2.599989000	-3.449481000
C	-3.320383000	3.744014000	-2.019688000	H	5.500385000	2.633554000	-1.631447000
H	-5.514645000	3.474973000	-1.747651000	H	4.456140000	1.651395000	-0.607000000
C	-2.246952000	2.938220000	-1.567187000	C	1.701063000	0.507294000	3.093040000
H	-3.224146000	4.652409000	-2.601095000	C	2.685767000	-0.028134000	2.038643000
C	-3.205616000	-1.806661000	-1.920007000	C	1.902857000	2.014110000	3.336121000
C	-3.021107000	-2.936292000	-2.758593000	H	1.868335000	-0.027275000	4.038884000
N	-2.038677000	-1.414541000	-1.390545000	C	4.140152000	0.293511000	2.414012000
C	-1.662118000	-3.234002000	-2.728829000	H	2.438666000	0.431531000	1.072590000
H	-3.792736000	-3.456560000	-3.310439000	H	2.539857000	-1.108343000	1.923488000
C	-1.050403000	-2.277773000	-1.873566000	C	3.358346000	2.322040000	3.721068000
H	-1.167474000	-4.040310000	-3.255902000	H	1.631067000	2.554305000	2.420261000
C	-3.794664000	-0.965816000	2.031216000	H	1.212466000	2.350525000	4.118686000
C	-4.070834000	-1.235203000	3.384757000	C	4.341912000	1.796146000	2.664357000
N	-2.542843000	-0.470891000	1.867328000	H	4.810488000	-0.053313000	1.618340000
C	-2.913547000	-0.906397000	4.087976000	H	4.415463000	-0.266720000	3.318442000
H	-4.995031000	-1.632425000	3.782062000	H	3.483472000	3.401734000	3.858574000
C	-1.967634000	-0.440935000	3.141087000	H	3.583357000	1.855518000	4.690559000
H	-2.744136000	-0.993334000	5.153846000	H	5.374034000	1.991282000	2.976027000
C	-0.890332000	3.203839000	-1.843373000	H	4.188490000	2.343202000	1.724833000
H	-0.696896000	4.076039000	-2.468570000	C	2.683429000	-2.418714000	-1.253125000
C	-0.636930000	-0.112070000	3.467931000	C	3.241764000	-3.567221000	-0.399314000
H	-0.379936000	-0.198474000	4.524136000				

C	3.640151000	-2.043812000	-2.393923000	H	2.310111000	3.884779000	-3.507802000
H	2.542957000	-1.541762000	-0.610632000	C	3.482142000	0.544517000	2.158106000
C	4.631473000	-3.205020000	0.152189000	C	3.682491000	0.767082000	3.533055000
H	3.316967000	-4.470981000	-1.021475000	N	2.213540000	0.130882000	1.902761000
H	2.542989000	-3.789922000	0.414440000	C	2.472036000	0.461128000	4.153069000
C	5.021814000	-1.671068000	-1.831060000	H	4.600136000	1.096261000	4.001072000
H	3.738797000	-2.899882000	-3.076764000	C	1.567858000	0.068078000	3.133509000
H	3.212194000	-1.217135000	-2.971481000	H	2.248441000	0.497869000	5.211879000
C	5.600696000	-2.806445000	-0.971804000	C	0.198459000	-3.025474000	-1.983510000
H	5.031754000	-4.048630000	0.724583000	H	-0.099041000	-3.850728000	-2.630399000
H	4.528806000	-2.368533000	0.857230000	C	0.261531000	-0.395049000	3.380025000
H	5.702583000	-1.422895000	-2.652651000	H	-0.005900000	-0.503933000	4.430993000
H	4.924945000	-0.762653000	-1.219123000	C	0.276029000	2.782374000	-1.860302000
H	6.565560000	-2.505714000	-0.548807000	H	-0.007031000	3.682834000	-2.404652000
H	5.795463000	-3.679191000	-1.610606000	N	-0.697572000	-2.089350000	-1.779876000
N	-0.887445000	-2.954647000	1.796364000	N	-0.649545000	2.254291000	-1.092628000
O	0.237003000	-2.740548000	1.601918000	N	-0.659614000	-0.733291000	2.510195000
O	-0.233418000	0.465783000	0.129162000	H	-0.484950000	-0.559097000	1.477530000
				H	-0.484034000	-1.298331000	-1.103402000
				H	-0.457376000	1.337412000	-0.604005000
⁷ P _{3NHi-O...NO-side}				C	-2.000279000	-2.036159000	-2.450093000
Fe	1.693807000	-0.191309000	-0.077535000	C	-3.134321000	-2.148196000	-1.418739000
N	4.049113000	-0.236332000	-0.066495000	C	-2.103841000	-0.731239000	-3.262467000
C	4.442897000	0.688591000	1.014121000	H	-2.057956000	-2.889808000	-3.138877000
H	5.478259000	0.521934000	1.344897000	C	-4.513997000	-1.996880000	-2.076903000
H	4.386835000	1.707157000	0.612891000	H	-2.993358000	-1.362246000	-0.666660000
C	4.387460000	-1.649494000	0.200800000	H	-3.055608000	-3.107507000	-0.894498000
H	5.428633000	-1.882870000	-0.063964000	C	-3.488352000	-0.585811000	-3.913671000
H	4.277753000	-1.815081000	1.278713000	H	-1.917070000	0.112781000	-2.585554000
C	4.457205000	0.220100000	-1.408890000	H	-1.310652000	-0.711134000	-4.018657000
H	5.497064000	0.576669000	-1.425677000	C	-4.615769000	-0.687657000	-2.874501000
H	4.397989000	-0.642464000	-2.082779000	H	-5.294221000	-2.042422000	-1.308512000
C	3.427734000	-2.527897000	-0.549919000	H	-4.690120000	-2.847092000	-2.750642000
C	3.624475000	-3.801211000	-1.116191000	H	-3.543504000	0.368017000	-4.450339000
N	2.161281000	-2.086343000	-0.754055000	H	-3.619353000	-1.374776000	-4.667541000
C	2.411341000	-4.152319000	-1.708675000	H	-5.591761000	-0.620692000	-3.367645000
H	4.541477000	-4.374393000	-1.099567000	H	-4.554101000	0.164624000	-2.182980000
C	1.510500000	-3.082786000	-1.477780000	C	-1.922134000	-1.378639000	2.891373000
H	2.185398000	-5.059175000	-2.255476000	C	-3.128774000	-0.536140000	2.452899000
C	3.511296000	1.285172000	-1.880155000	C	-1.982130000	-2.794071000	2.287044000
C	3.736381000	2.337954000	-2.788525000	H	-1.928424000	-1.462209000	3.986551000
N	2.230783000	1.275450000	-1.436058000	C	-4.450175000	-1.230744000	2.816136000
C	2.522357000	3.009955000	-2.906022000	H	-3.076475000	-0.396862000	1.367807000
H	4.671107000	2.569377000	-3.280848000	H	-3.069035000	0.458944000	2.909068000
C	1.594508000	2.346080000	-2.062036000				

C	-3.311594000	-3.487413000	2.628635000	H	5.744660000	0.695864000	-1.720989000
H	-1.871393000	-2.709185000	1.198605000	C	3.735123000	1.470629000	-1.913947000
H	-1.131041000	-3.381671000	2.650000000	C	3.856669000	2.624808000	-2.724756000
C	-4.522008000	-2.639267000	2.206654000	H	4.729962000	2.919875000	-3.290950000
H	-5.292775000	-0.619219000	2.473787000	C	2.638599000	3.295065000	-2.644267000
H	-4.538550000	-1.300249000	3.909390000	H	2.380064000	4.222295000	-3.140002000
H	-3.345168000	-4.472024000	2.148798000	C	1.803293000	2.533204000	-1.786267000
H	-3.356837000	-3.667815000	3.711822000	C	0.495442000	2.699655000	-1.324307000
H	-5.452362000	-3.135014000	2.504769000	H	0.115310000	1.899602000	-0.688058000
H	-4.544615000	-2.556355000	1.111486000	C	4.919612000	0.641199000	0.815757000
C	-1.967888000	2.884062000	-0.894611000	H	5.972534000	0.427391000	1.045817000
C	-2.867140000	1.911291000	-0.127915000	H	4.865298000	1.680183000	0.469849000
C	-1.850634000	4.219256000	-0.135070000	N	2.692122000	0.304190000	1.845002000
H	-2.404609000	3.076837000	-1.886006000	C	4.049019000	0.465495000	2.024236000
C	-4.256401000	2.508649000	0.128753000	C	4.361584000	0.536954000	3.376282000
H	-2.378460000	1.686183000	0.827382000	C	3.135632000	0.427292000	4.069882000
H	-2.943123000	0.966613000	-0.674233000	H	2.989682000	0.447413000	5.142531000
C	-3.239220000	4.830257000	0.112095000	C	2.121270000	0.286720000	3.114858000
H	-1.348247000	4.026135000	0.821955000	H	5.347778000	0.665617000	3.801958000
H	-1.217835000	4.918549000	-0.694665000	C	0.718056000	0.183275000	3.429534000
C	-4.155371000	3.853063000	0.866038000	H	0.502709000	0.198088000	4.507164000
H	-4.860365000	1.797528000	0.704600000	C	4.789722000	-1.629767000	-0.160221000
H	-4.774149000	2.653817000	-0.830075000	H	4.958717000	-1.827412000	0.904969000
H	-3.135198000	5.767114000	0.670012000	H	5.727238000	-1.859574000	-0.685277000
H	-3.699139000	5.089229000	-0.852275000	N	2.407569000	-2.023300000	-0.588731000
H	-5.151115000	4.290724000	0.996996000	C	3.667873000	-3.859575000	-1.039494000
H	-3.749434000	3.682209000	1.873416000	H	4.541227000	-4.485883000	-1.163327000
N	1.720968000	2.970852000	1.449462000	C	2.338518000	-4.219974000	-1.234365000
O	0.892212000	3.068231000	2.254367000	H	1.974626000	-5.189664000	-1.550397000
O	-0.086027000	-0.156646000	-0.043360000	C	1.552268000	-3.072674000	-0.949004000
				C	3.661742000	-2.503011000	-0.632492000
				C	0.173121000	-2.853418000	-0.932339000
⁷ P _{INH_i-OH...NO-top}				H	-0.151226000	-1.845314000	-0.669059000
Fe	2.067927000	-0.081659000	-0.014999000	N	-0.342720000	3.689961000	-1.570973000
N	4.416654000	-0.206204000	-0.294433000	H	-0.052626000	4.464174000	-2.160166000
N	2.515966000	1.408421000	-1.354054000	C	-1.713416000	3.731064000	-1.032068000
N	-0.250053000	0.099050000	2.583943000	C	-1.897179000	4.909277000	-0.064322000
H	-0.041351000	0.055517000	1.030280000	C	-2.747005000	3.761305000	-2.167526000
N	-0.781928000	-3.734311000	-1.175814000	H	-1.837267000	2.797826000	-0.471969000
H	-0.531841000	-4.690050000	-1.409973000	C	-3.325827000	4.912240000	0.507034000
O	0.239398000	0.017868000	0.036561000	H	-1.712609000	5.850193000	-0.602736000
N	-1.750332000	0.176108000	-1.783992000	H	-1.154391000	4.843283000	0.738822000
O	-2.725264000	0.220166000	-1.155622000	C	-4.173556000	3.766349000	-1.592165000
C	4.703068000	0.355521000	-1.632521000	H	-2.589886000	4.666740000	-2.771784000
H	4.557338000	-0.446599000	-2.365951000				

H	-2.591923000	2.899837000	-2.826804000				
C	-4.379603000	4.931664000	-0.611853000	${}^6\text{P}_{\text{INH}i\text{-OH}}$			
H	-3.454153000	5.772042000	1.173243000	Fe	2.042346000	0.069928000	0.007535000
H	-3.464867000	4.012757000	1.123666000	N	4.318730000	-0.026549000	-0.570508000
H	-4.900567000	3.817146000	-2.409874000	N	2.434101000	1.907841000	-0.842129000
H	-4.349928000	2.814706000	-1.071023000	N	0.088982000	-1.000750000	2.685877000
H	-5.386528000	4.889569000	-0.182118000	H	0.087233000	-0.252278000	1.223092000
H	-4.310489000	5.882522000	-1.158678000	N	-1.215978000	-2.580032000	-2.264915000
C	-2.219528000	-3.419518000	-1.129199000	H	-1.094926000	-3.337152000	-2.932420000
C	-2.865530000	-3.648143000	-2.504336000	O	0.226930000	0.208053000	0.329323000
C	-2.925011000	-4.223114000	-0.025896000	C	4.545531000	0.951634000	-1.655418000
H	-2.284689000	-2.355357000	-0.881125000	H	4.385179000	0.434395000	-2.607827000
C	-4.367644000	-3.320728000	-2.461630000	H	5.581163000	1.316512000	-1.659902000
H	-2.727937000	-4.700724000	-2.792537000	C	3.560529000	2.081443000	-1.553261000
H	-2.351671000	-3.037239000	-3.255372000	C	3.550514000	3.340299000	-2.201688000
C	-4.426253000	-3.887858000	0.006215000	H	4.339565000	3.737791000	-2.826994000
H	-2.792518000	-5.296946000	-0.222449000	C	2.334667000	3.943484000	-1.884422000
H	-2.454813000	-4.008433000	0.940423000	H	1.979311000	4.916218000	-2.200523000
C	-5.084325000	-4.119863000	-1.362365000	C	1.641022000	3.047535000	-1.033659000
H	-4.815895000	-3.520856000	-3.440734000	C	0.380181000	3.084328000	-0.428218000
H	-4.494272000	-2.245630000	-2.269899000	H	0.151440000	2.246320000	0.225710000
H	-4.919709000	-4.486109000	0.779854000	C	4.996637000	0.337505000	0.694618000
H	-4.551903000	-2.835124000	0.295064000	H	6.055554000	0.047385000	0.685438000
H	-6.143529000	-3.842740000	-1.323379000	H	4.955839000	1.430158000	0.768969000
H	-5.047342000	-5.190607000	-1.607649000	N	2.902579000	-0.392358000	1.797530000
C	-1.633237000	0.019586000	3.031660000	C	4.269959000	-0.285173000	1.851345000
C	-2.435716000	1.170191000	2.390314000	C	4.752318000	-0.763429000	3.068215000
C	-2.227538000	-1.343583000	2.622922000	C	3.621545000	-1.179760000	3.805198000
H	-1.695534000	0.113109000	4.130106000	H	3.605817000	-1.608248000	4.800406000
C	-3.934991000	1.076654000	2.710241000	C	2.493246000	-0.946891000	3.007178000
H	-2.289192000	1.119660000	1.302649000	H	5.790630000	-0.798016000	3.373478000
H	-2.022725000	2.129884000	2.724232000	C	1.133208000	-1.233479000	3.399716000
C	-3.722961000	-1.434330000	2.960125000	H	1.034497000	-1.676196000	4.400343000
H	-2.083835000	-1.466500000	1.539724000	C	4.582058000	-1.421567000	-0.990513000
H	-1.663360000	-2.146060000	3.112886000	H	4.792729000	-2.000682000	-0.084444000
C	-4.509758000	-0.289709000	2.302846000	H	5.467730000	-1.493387000	-1.634188000
H	-4.474410000	1.886207000	2.203530000	N	2.153186000	-1.520727000	-1.296005000
H	-4.088390000	1.226782000	3.787918000	C	3.224837000	-3.041128000	-2.592061000
H	-4.118850000	-2.406053000	2.643502000	H	4.036405000	-3.593509000	-3.048048000
H	-3.853930000	-1.385852000	4.050060000	C	1.856213000	-3.220993000	-2.795404000
H	-5.570492000	-0.352026000	2.571452000	H	1.377535000	-3.940683000	-3.447568000
H	-4.451809000	-0.393364000	1.209008000	C	1.191774000	-2.269645000	-1.982770000
				C	3.361333000	-1.988001000	-1.657822000
				C	-0.161570000	-1.988288000	-1.749456000

H	-0.360337000	-1.185798000	-1.039725000	C	-3.385327000	-2.557159000	2.570663000
N	-0.590572000	3.959045000	-0.584978000	H	-1.847879000	-1.906431000	1.191593000
H	-0.483101000	4.726914000	-1.241626000	H	-1.345094000	-3.248197000	2.222589000
C	-1.915055000	3.755519000	0.041768000	C	-4.177679000	-1.242147000	2.597150000
C	-2.760190000	5.027004000	-0.070422000	H	-4.085008000	0.714544000	3.547517000
C	-2.641109000	2.544326000	-0.576164000	H	-3.608343000	-0.626475000	4.590899000
H	-1.731677000	3.546465000	1.103279000	H	-3.828282000	-3.257995000	1.852733000
C	-4.131991000	4.819348000	0.592016000	H	-3.444231000	-3.033869000	3.559952000
H	-2.898400000	5.269331000	-1.133869000	H	-5.222326000	-1.430435000	2.875725000
H	-2.230994000	5.868823000	0.392160000	H	-4.189490000	-0.807212000	1.586678000
C	-4.006536000	2.335493000	0.094217000				
H	-2.774304000	2.726616000	-1.651540000				
H	-2.021295000	1.646784000	-0.469638000	⁶ P _{2NH_i-OH}			
C	-4.868183000	3.604103000	0.005789000	Fe	-2.029908000	-0.020575000	-0.037368000
H	-4.736390000	5.726679000	0.474576000	N	-4.271386000	0.581994000	-0.173601000
H	-3.989306000	4.668937000	1.671683000	C	-4.655923000	0.451682000	-1.591542000
H	-4.519900000	1.485942000	-0.374031000	H	-5.737651000	0.304724000	-1.705636000
H	-3.852246000	2.069104000	1.150380000	H	-4.401815000	1.395114000	-2.087675000
H	-5.821821000	3.453673000	0.526963000	C	-4.948022000	-0.402294000	0.701882000
H	-5.107267000	3.802106000	-1.049189000	H	-5.965847000	-0.082812000	0.961001000
C	-2.596804000	-2.202238000	-1.929596000	H	-5.029585000	-1.330317000	0.124411000
C	-3.321061000	-1.630403000	-3.157494000	C	-4.370492000	1.974587000	0.319030000
C	-3.355078000	-3.394877000	-1.329140000	H	-5.271472000	2.473426000	-0.058973000
H	-2.518497000	-1.416502000	-1.170088000	H	-4.454837000	1.931332000	1.410267000
C	-4.759341000	-1.229999000	-2.792640000	C	-4.111596000	-0.616901000	1.926316000
H	-3.337202000	-2.392379000	-3.949841000	C	-4.486951000	-0.857270000	3.246550000
H	-2.761645000	-0.768808000	-3.540924000	N	-2.745646000	-0.588097000	1.803815000
C	-4.796317000	-2.994421000	-0.976606000	C	-3.287489000	-0.980549000	3.979091000
H	-3.367029000	-4.215380000	-2.060613000	H	-5.501329000	-0.925648000	3.618961000
H	-2.823754000	-3.752565000	-0.439510000	C	-2.226629000	-0.807905000	3.078206000
C	-5.533913000	-2.412244000	-2.191187000	H	-3.180461000	-1.162169000	5.042058000
H	-5.272840000	-0.844721000	-3.681772000	C	-3.121844000	2.721225000	-0.052448000
H	-4.726966000	-0.408622000	-2.061318000	C	-2.890459000	4.101999000	-0.247269000
H	-5.333242000	-3.863995000	-0.578491000	N	-1.974257000	2.029276000	-0.174406000
H	-4.771518000	-2.242643000	-0.176170000	C	-1.524540000	4.247597000	-0.493864000
H	-6.544109000	-2.095421000	-1.903219000	H	-3.639121000	4.882587000	-0.206368000
H	-5.649381000	-3.194727000	-2.955374000	C	-0.957771000	2.950532000	-0.445941000
C	-1.249989000	-1.300282000	3.170205000	H	-0.987505000	5.167506000	-0.688518000
C	-2.063690000	0.009814000	3.214041000	C	-3.880585000	-0.654698000	-2.240874000
C	-1.913565000	-2.309546000	2.212409000	C	-4.219809000	-1.417867000	-3.371479000
H	-1.218849000	-1.735926000	4.183695000	N	-2.627320000	-0.944712000	-1.804401000
C	-3.537601000	-0.236674000	3.565113000	C	-3.103880000	-2.205470000	-3.656976000
H	-1.998916000	0.485349000	2.224692000	H	-5.159099000	-1.374413000	-3.907070000
H	-1.601123000	0.699396000	3.931503000	C	-2.120630000	-1.906274000	-2.685121000
				H	-2.981653000	-2.914386000	-4.466731000

C	-0.835996000	-0.819960000	3.460298000	H	5.251771000	-3.517902000	-0.887455000
H	-0.670622000	-0.944765000	4.538886000	H	4.096490000	-2.695754000	0.163149000
C	-0.818849000	-2.450484000	-2.718419000	C	2.777334000	2.559115000	-0.942340000
H	-0.611777000	-3.141185000	-3.533096000	C	3.362882000	2.754428000	-2.348341000
C	0.353208000	2.475245000	-0.592887000	C	3.708872000	3.119315000	0.141332000
H	0.484859000	1.401431000	-0.470234000	H	2.635665000	1.487278000	-0.764773000
N	0.169320000	-0.696607000	2.665899000	C	4.756302000	2.113135000	-2.444307000
N	1.442539000	3.166430000	-0.841636000	H	3.435926000	3.830898000	-2.558196000
N	0.173162000	-2.194904000	-1.906089000	H	2.681937000	2.319676000	-3.089750000
H	0.019061000	-1.550290000	-1.099208000	C	5.096628000	2.468130000	0.041017000
H	0.002440000	-0.575862000	1.070432000	H	3.798879000	4.206641000	0.007932000
H	1.386146000	4.175276000	-0.956316000	H	3.265006000	2.943290000	1.127453000
C	1.532678000	-0.702023000	3.178818000	C	5.700160000	2.652535000	-1.359212000
C	2.275171000	-1.932455000	2.625212000	H	5.175615000	2.290080000	-3.442113000
C	2.243296000	0.591472000	2.733746000	H	4.657431000	1.024489000	-2.328978000
H	1.535585000	-0.749948000	4.281314000	H	5.759214000	2.889987000	0.806504000
C	3.759003000	-1.935009000	3.018188000	H	5.003889000	1.394601000	0.257841000
H	2.188556000	-1.913840000	1.530763000	H	6.673502000	2.150025000	-1.421280000
H	1.776268000	-2.846091000	2.972442000	H	5.879992000	3.722927000	-1.536328000
C	3.727592000	0.592075000	3.127868000	O	-0.233405000	-0.444865000	0.082482000
H	2.152975000	0.673462000	1.640983000				
H	1.725282000	1.458798000	3.162407000	${}^6\text{P}_{3\text{NHi-OH}}$			
C	4.452821000	-0.640899000	2.569565000	Fe	1.826514000	-0.000450000	0.019190000
H	4.256094000	-2.809456000	2.579667000	N	4.123645000	0.004303000	0.041328000
H	3.847196000	-2.033429000	4.109919000	C	4.529036000	0.796663000	-1.137439000
H	4.206416000	1.511417000	2.770023000	H	5.570136000	1.134796000	-1.060721000
H	3.812231000	0.594495000	4.224317000	H	4.459729000	0.141758000	-2.012749000
H	5.503967000	-0.640855000	2.884799000	C	4.491331000	0.634940000	1.327827000
H	4.449452000	-0.594015000	1.470336000	H	5.533273000	0.419945000	1.597766000
C	1.534698000	-2.726475000	-2.023360000	H	4.404084000	1.718577000	1.191446000
C	2.535707000	-1.565248000	-1.872233000	C	4.528546000	-1.413569000	-0.047338000
C	1.773817000	-3.813909000	-0.961386000	H	5.573634000	-1.517590000	-0.365239000
H	1.639136000	-3.168114000	-3.021129000	H	4.445662000	-1.840366000	0.958034000
C	3.984364000	-2.071301000	-1.901132000	C	3.540048000	0.156146000	2.381305000
H	2.345693000	-1.059993000	-0.915474000	C	3.732353000	-0.046263000	3.745618000
H	2.362896000	-0.827070000	-2.664959000	N	2.250585000	-0.145961000	2.018511000
C	3.228389000	-4.307833000	-0.988303000	C	2.496310000	-0.498725000	4.252735000
H	1.543014000	-3.394619000	0.026489000	H	4.655211000	0.110207000	4.289600000
H	1.076419000	-4.642821000	-1.132668000	C	1.597971000	-0.557970000	3.177764000
C	4.221033000	-3.146074000	-0.831118000	H	2.264986000	-0.773521000	5.275024000
H	4.669191000	-1.227248000	-1.753078000	C	3.598952000	-2.121344000	-0.984332000
H	4.203544000	-2.490071000	-2.893748000	C	3.836658000	-3.228630000	-1.816927000
H	3.378034000	-5.051184000	-0.195586000	N	2.320090000	-1.680657000	-1.101653000
H	3.418006000	-4.818035000	-1.943784000	C	2.637824000	-3.473881000	-2.487988000

H	4.773898000	-3.760797000	-1.912734000	H	-2.891776000	1.361691000	-0.399515000
C	1.703963000	-2.509826000	-2.041037000	H	-2.904682000	2.602588000	-1.654498000
H	2.435602000	-4.240300000	-3.225940000	C	-3.400300000	3.462580000	2.178306000
C	3.589752000	1.952917000	-1.287423000	H	-1.854165000	1.960339000	1.938598000
C	3.826203000	3.233055000	-1.816047000	H	-1.222146000	3.592040000	2.182491000
N	2.305112000	1.819471000	-0.867291000	C	-4.526270000	2.727097000	1.435898000
C	2.620204000	3.926570000	-1.705823000	H	-5.169072000	2.329121000	-0.606279000
H	4.767453000	3.592032000	-2.210954000	H	-4.532856000	3.954044000	-0.346854000
C	1.683933000	3.045406000	-1.115639000	H	-3.478894000	3.292883000	3.259332000
H	2.414922000	4.949804000	-1.995405000	H	-3.507839000	4.544917000	2.016796000
C	0.248413000	-1.047566000	3.289141000	H	-5.503388000	3.096724000	1.771480000
H	-0.005516000	-1.411428000	4.293823000	H	-4.485847000	1.657966000	1.683818000
C	0.368140000	3.425310000	-0.785268000	C	-1.848624000	-1.439632000	-2.839752000
H	0.109825000	4.464415000	-0.975770000	C	-2.979317000	-1.719155000	-1.838212000
C	0.395883000	-2.402202000	-2.553414000	C	-1.972467000	-0.029471000	-3.442934000
H	0.141221000	-3.084388000	-3.361389000	H	-1.886571000	-2.182771000	-3.644729000
N	-0.629968000	-1.105388000	2.348497000	C	-4.356566000	-1.508223000	-2.484039000
N	-0.544196000	-1.570410000	-2.181746000	H	-2.865653000	-1.041649000	-0.982005000
N	-0.574534000	2.682186000	-0.264622000	H	-2.882258000	-2.741377000	-1.454879000
H	-0.394579000	1.667568000	-0.106336000	C	-3.354480000	0.183801000	-4.079210000
H	-0.362715000	-0.419489000	0.868335000	H	-1.816162000	0.705387000	-2.642580000
H	-0.372795000	-0.935520000	-1.374347000	H	-1.175951000	0.119396000	-4.181918000
C	-1.925177000	-1.720221000	2.619187000	C	-4.486969000	-0.099632000	-3.080838000
C	-3.053585000	-0.724058000	2.304945000	H	-5.141132000	-1.683770000	-1.737695000
C	-2.061862000	-2.989684000	1.756928000	H	-4.500010000	-2.254211000	-3.278976000
H	-1.999238000	-2.009584000	3.681594000	H	-3.427254000	1.209654000	-4.461125000
C	-4.440233000	-1.365843000	2.449713000	H	-3.459351000	-0.486365000	-4.944546000
H	-2.919852000	-0.360290000	1.277321000	H	-5.460992000	0.014566000	-3.572957000
H	-2.961189000	0.147569000	2.964291000	H	-4.449042000	0.640451000	-2.270307000
C	-3.449399000	-3.630737000	1.900417000	O	-0.043127000	0.015070000	0.001390000
H	-1.886883000	-2.711488000	0.709249000				
H	-1.273930000	-3.700621000	2.036808000	⁶ P _{3NH_i-O}			
C	-4.567336000	-2.626432000	1.581482000	Fe	-1.748630000	0.026584000	-0.075448000
H	-5.215209000	-0.636094000	2.182297000	N	-4.105019000	0.107791000	-0.114036000
H	-4.606768000	-1.634553000	3.503116000	C	-4.460262000	0.241883000	-1.538889000
H	-3.522758000	-4.506832000	1.243382000	H	-5.513501000	-0.007798000	-1.725714000
H	-3.575022000	-3.995309000	2.930551000	H	-4.319664000	1.294240000	-1.810402000
H	-5.549864000	-3.092629000	1.729244000	C	-4.535775000	-1.173401000	0.480967000
H	-4.504585000	-2.341714000	0.522214000	H	-5.586694000	-1.146415000	0.798439000
C	-1.884871000	3.181959000	0.164075000	H	-4.448636000	-1.940701000	-0.296002000
C	-3.007436000	2.438959000	-0.575501000	C	-4.495885000	1.274411000	0.696322000
C	-2.014426000	3.017044000	1.688148000	H	-5.505486000	1.627395000	0.446643000
H	-1.928690000	4.247385000	-0.090009000	H	-4.516722000	0.954489000	1.744210000
C	-4.388620000	2.896144000	-0.083891000	C	-3.629979000	-1.502703000	1.631546000

C	-3.913852000	-2.178249000	2.834558000	H	4.480255000	-1.023206000	3.793714000
N	-2.333114000	-1.113632000	1.581810000	H	3.583279000	2.651843000	3.353707000
C	-2.722838000	-2.192817000	3.562653000	H	3.561866000	1.332415000	4.524356000
H	-4.874541000	-2.584707000	3.123296000	H	5.536130000	1.092491000	3.042079000
C	-1.750618000	-1.527992000	2.777090000	H	4.502779000	1.131996000	1.612671000
H	-2.550247000	-2.611547000	4.546686000	C	1.772672000	-2.818044000	-1.792419000
C	-3.483346000	2.368721000	0.537192000	C	2.984343000	-1.878274000	-1.864017000
C	-3.651585000	3.757180000	0.716348000	C	1.794230000	-3.655040000	-0.501463000
N	-2.200137000	2.060303000	0.234932000	H	1.792127000	-3.493230000	-2.656101000
C	-2.397097000	4.328190000	0.514795000	C	4.299662000	-2.660417000	-1.740742000
H	-4.580431000	4.257161000	0.958504000	H	2.915592000	-1.158720000	-1.042004000
C	-1.503767000	3.269602000	0.213653000	H	2.952548000	-1.306913000	-2.799402000
H	-2.129386000	5.376919000	0.557805000	C	3.115273000	-4.428152000	-0.365953000
C	-3.545924000	-0.625680000	-2.352068000	H	1.668529000	-2.979475000	0.354672000
C	-3.797315000	-1.308755000	-3.558097000	H	0.939554000	-4.342231000	-0.502105000
N	-2.281856000	-0.842281000	-1.916251000	C	4.331011000	-3.492532000	-0.450553000
C	-2.620058000	-1.989188000	-3.870103000	H	5.144377000	-1.960594000	-1.766464000
H	-4.729830000	-1.304843000	-4.107502000	H	4.410226000	-3.327330000	-2.608071000
C	-1.688480000	-1.695933000	-2.844238000	H	3.121831000	-4.981022000	0.581548000
H	-2.432389000	-2.638031000	-4.716903000	H	3.178508000	-5.174853000	-1.170658000
C	-0.430851000	-1.271038000	3.200291000	H	5.259621000	-4.074556000	-0.396502000
H	-0.179247000	-1.581950000	4.212148000	H	4.326680000	-2.815171000	0.414236000
C	-0.407516000	-2.275647000	-2.763530000	C	2.136782000	2.870725000	-0.779668000
H	-0.166127000	-3.005303000	-3.533542000	C	2.898811000	1.556812000	-0.968259000
C	-0.148233000	3.464604000	-0.103882000	C	2.209471000	3.724996000	-2.057894000
H	0.194625000	4.496736000	-0.099970000	H	2.586255000	3.432592000	0.050432000
N	0.521028000	-0.686391000	2.517574000	C	4.356475000	1.804150000	-1.371040000
N	0.743188000	2.553294000	-0.412339000	H	2.395377000	0.976160000	-1.751460000
N	0.520044000	-2.056740000	-1.864344000	H	2.850137000	0.966328000	-0.049516000
H	0.360950000	-1.319506000	-1.130916000	C	3.670089000	3.983969000	-2.458116000
H	0.347264000	-0.410691000	1.515909000	H	1.691674000	3.184805000	-2.862543000
H	0.476767000	1.538821000	-0.353642000	H	1.681245000	4.674273000	-1.910840000
C	1.841928000	-0.353199000	3.058655000	C	4.444768000	2.669572000	-2.636170000
C	2.934556000	-1.105569000	2.283879000	H	4.860147000	0.841350000	-1.524412000
C	2.046916000	1.170841000	2.989373000	H	4.879477000	2.309104000	-0.546167000
H	1.860518000	-0.670971000	4.107731000	H	3.698992000	4.575627000	-3.381202000
C	4.338514000	-0.698165000	2.752918000	H	4.155626000	4.587258000	-1.677532000
H	2.822565000	-0.881268000	1.216724000	H	5.493150000	2.876773000	-2.884738000
H	2.783922000	-2.185401000	2.400178000	H	4.018140000	2.112323000	-3.482865000
C	3.455713000	1.566973000	3.455366000	O	0.026855000	-0.051574000	-0.078448000
H	1.893679000	1.498506000	1.953329000				
H	1.280989000	1.665083000	3.599318000				
C	4.541704000	0.821369000	2.665828000				
H	5.090865000	-1.222471000	2.150639000				