Supporting Information

DFT Mechanistic Insights into the Formation of Metal-dioxygen Complex $[Co(12\text{-}TMC)O_2]^+$ using H_2O_2 as $[O_2]$ unit source

Ruihua Zhao[a,b], Zhi-Xiang Wang*[d], Mian Guo*[c] and Jia Li*[a,b]

[a]Guangzhou HKUST Fok Ying Tung Research Institute, Science and Technology Building, Nansha Information Technology Park, No.2 Huan Shi Avenue South, Nansha District, Guangzhou, 511462, China.

[b]Guangdong-Hong Kong Joint Laboratory for Carbon Neutrality, Jiangmen Laboratory of Carbon Science and Technology, Jiangmen 529199, Guangdong Province, China.

[c]College of Chemistry and Molecular Sciences, Wuhan University, Wuhan, Hubei 430072, P. R. China.

[d]School of Chemical Sciences, University of Chinese Academy of Sciences. Jia #19, Yuquan Road, Beijing, 100039, China.

Corresponding Author: *E-mail: Captureready@gmail.com ; *E-mail: whguomian@whu.edu.cn ; *E-mail: zxwang@ucas.ac.cn

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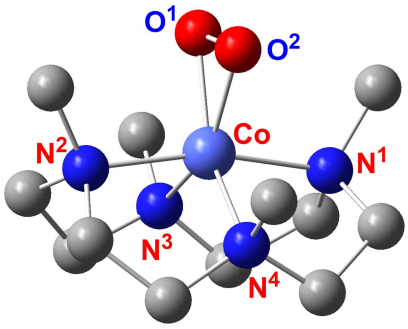
Table S1: Geometric and energetic results at M06(SMD, Solvent=CH_3CN)/6-311++G**//B3LYP(SMD, Solvent=CH_3CN)/6-31G** and energetic results at B3LYP-D3(SMD, Solvent=CH_3CN)/6-311++G**//B3LYP(SMD, Solvent=CH_3CN)/6-31G**.



$Co(12\text{-}TMC)O_2^+$

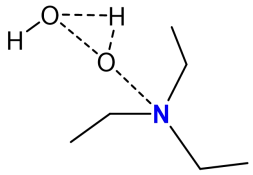
	O^1-O^2	Co-O^1 Co-O^2	Co-N^1 Co-N^2	Co-N^3 Co-N^4	∠O-Co-O	Mulliken Spin	ΔG	ΔG[a]
Exptl. (S=0)	1.439	1.874 1.858	2.016 2.025	2.000 1.997	45.36			
Closed shell singlet	1.435	1.842 1.841	2.046 2.046	2.030 2.031	45.86		0.0	0.0
Triplet	1.416	1.856 1.856	2.232 2.232	2.094 2.094	44.85	Co:2.19 O:-0.18	-0.5	-0.8
Quintet	1.346	2.065 2.062	2.201 2.204	2.150 2.153	38.08	Co:2.69 O:0.57	-8.7	-4.0

[a]At B3LYP-D3/6-311++G**//B3LYP/6-31G** level.

These two DFT levels failed to predict the closed shell singlet to be the ground state of the complex. Therefore, we used BP86/Def2QZVPP//BP86/SVP to perform the study.

SI2: Three possibilities of H_2O_2 reacting with NEt_3 to form N-oxide

Mechanism I



$H_2O_2 + NEt_3 \xrightarrow{TS=21.4\ kcal/mol} H_2O + ONEt_3 \quad \Delta G=-21.5\ kcal/mol$

Mechanism II

$H_2O_2 + NEt_3 \longrightarrow OH^- + NEt_3\text{-}OH^+ \quad \Delta G=16.6\ kcal/mol$ (eq a)

$+$

$OH^- + NEt_3\text{-}OH^+ \longrightarrow H_2O + ONEt_3 \quad \Delta G=-38.1 kcal/mol$

$H_2O_2 + NEt_3 \longrightarrow H_2O + ONEt_3 \quad \Delta G=-21.5\ kcal/mol$

Mechanism III

$H_2O_2 + NEt_3 \longrightarrow \bullet OH + NEt_3\text{-}OH \quad \Delta G=93.1\ kcal/mol$ (eq b)

$+$

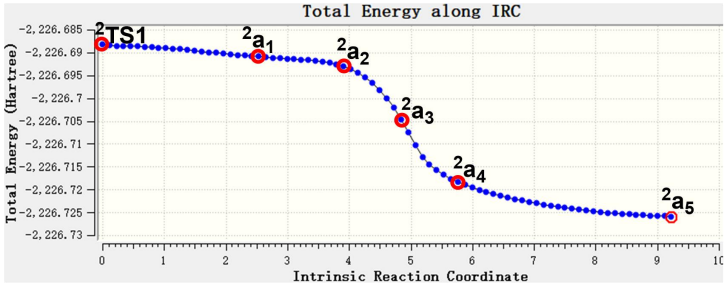
$\bullet OH + NEt_3\text{-}OH \longrightarrow H_2O + ONEt_3 \quad \Delta G=-114.6\ kcal/mol$

$H_2O_2 + NEt_3 \longrightarrow H_2O + ONEt_3 \quad \Delta G=-21.5\ kcal/mol$

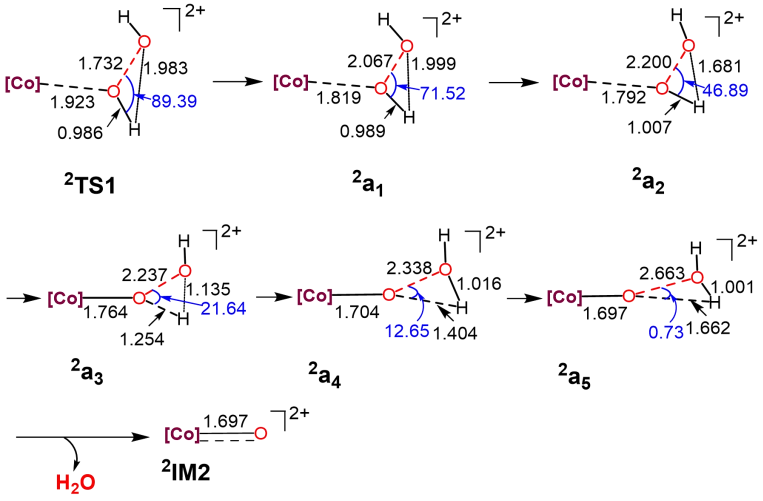
Figure S1

SI3: IRC result from ^{2}TS1 to ^{2}IM2, showing the release of a water molecule

(The IRC calculation was performed at BP86(SMD, solvent=CH_3CN)/SVP level)



^{2}TS1 IRC



^{2}TS1 **^{2}a1** **^{2}a2**

^{2}a3 **^{2}a4** **^{2}a5**

^{2}IM2

Figure S2

SI4: Geometric changes from $^{2}[Co^{II}]^{2+}$ to ^{2,4}IM2

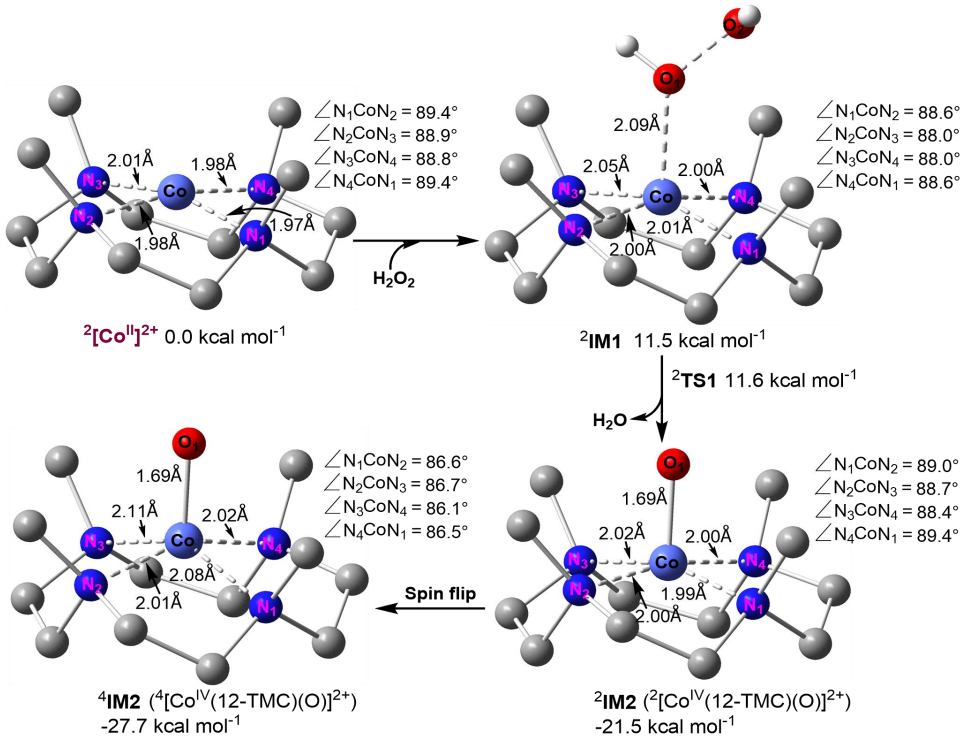
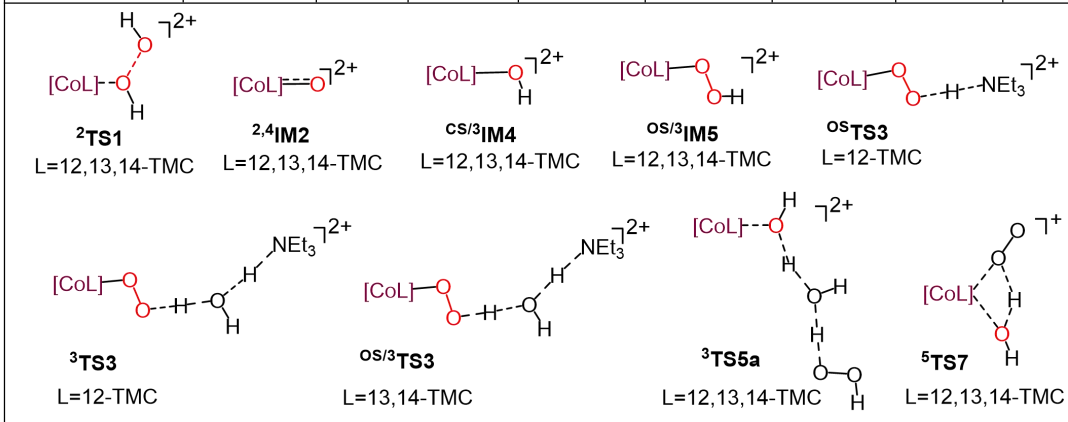


Figure S3

SI5: Mechanism feasibility verification

Table S2: The key intermediates and transition states are used to verify the feasibility of the proposed mechanism, taking $[Co^{III}(13\text{-TMC})(O_2)]^{+}$ and $[Co^{III}(14\text{-TMC})(O_2)]^{+}$ as two examples. Relative free energies are given in kcal mol^{-1}.

L	Key intermediates and transition states in Stage I-III							
	Stage I				Stage II		Stage III	
	$^{2/4}$[Co]$^{2+}$	^{2}TS1	$^{2/4}$IM2	$^{CS/3}$IM4	$^{OS/3}$IM5	$^{OS/3}$TS3	^{3}TS5a	^{5}TS7
L=12-TMC	0.0/ 6.4	11.6	-21.5/ -27.7	-27.4/ -27.2	-10.7/ -12.9	-5.6/ -3.3	19.8	19.6
L=13-TMC	0.0/ 5.5	14.8	-21.9/ -31.3	-24.9/ -29.7	-8.4/ -10.6	-0.1/ -4.6	21.2	20.0
L=14-TMC	0.0/ 7.2	11.1	-22.3/ -29.0	-27.9/ -28.5	-9.7/ -10.1	0.3/ -2.9	20.2	21.3



SI6: Cartesian Coordinates in Å ,SCF Energies and Free Energies (in a.u.) at 298.15 K and 1 atm for the Optimized Structures [BS1=SVP,BS2=Def2QZVPP].

$^{2}[Co]^{2+}$
BP86/BS1 SCF energy in solution: -2075.235429 a.u.
BP86/BS2 SCF energy in solution: -2076.259431 a.u.
BP86/BS2 Free energy in solution: -2075.90018 a.u.

2 2
Co 0.00084500 0.02253000 0.26024900
N 0.02852000 1.97557500 -0.03126500
N 1.97350600 -0.01441300 0.05641800
C 0.04936000 2.75809500 1.22757500
C 2.78867700 -0.53110600 1.18433900
C 2.01043100 -0.92596500 -1.13131800
C -1.20898100 2.23094600 -0.83891800
C 1.26556000 2.18415000 -0.85395900
C 2.41549700 1.38788000 -0.25627400
N -1.97184200 0.04299800 0.05772200
N -0.02891900 -1.96074100 -0.05169700
C -2.80675300 -0.46421600 1.17455000
C -0.06057900 -2.81091600 1.17235400
C 1.25209900 -2.22480500 -0.82386800
C -2.37531100 1.46052300 -0.23931900
C -2.02982600 -0.85233900 -1.13984400
C -1.29972200 -2.17404600 -0.85743400
H 1.04083600 1.83545500 -1.88175900
H 1.52411200 3.26431300 -0.91950600
H 2.74638100 1.84196700 0.69786900
H 3.29389200 1.38126700 -0.93797300
H -0.85009700 2.52674500 1.82800000
H 0.94291900 2.49139600 1.82224800
H 0.07029600 3.84952900 1.01224100
H -1.43726500 3.31879700 -0.88540300
H -1.00452400 1.89435100 -1.87443300
H -2.68457600 1.91413600 0.72241100
H -3.25991400 1.48567700 -0.91267500
H -3.88617400 -0.35471600 0.92905600
H -2.60571500 -1.53150600 1.36954300
H -2.58263600 0.11470500 2.09094000
H -3.08476300 -1.05322600 -1.43719600
H -1.54735500 -0.31500000 -1.98138500
H -1.06594300 -2.67633100 -1.81711300
H -1.95222000 -2.86357200 -0.28734600

H -0.96470800 -2.58591600 1.76752600
H -0.06749500 -3.89041400 0.90467100
H 0.82626200 -2.60289400 1.79899000
H 1.02942600 -2.75904900 -1.76912600
H 1.88035800 -2.90337400 -0.21539600
H 1.53855100 -0.39026300 -1.97992200
H 3.06041400 -1.15525600 -1.42559200
H 2.57581500 0.06594000 2.09181400
H 2.55773600 -1.59000300 1.39353300
H 3.87200600 -0.45422000 0.94372200

$^{4}[Co]^{2+}$
BP86/BS1 SCF energy in solution: -2075.22618 a.u.
BP86/BS2 SCF energy in solution: -2076.245888 a.u.
BP86/BS2 Free energy in solution: -2075.889906 a.u.

2 4
Co -0.00036400 0.00383700 0.70328200
N -0.01435600 2.00268000 -0.11208000
N 2.03903200 0.02438200 0.01298900
C -0.02995900 2.85940000 1.09814900
C 2.99442200 -0.53013700 0.99774000
C 1.95309200 -0.80721000 -1.21724500
C -1.24654600 2.16675000 -0.92513000
C 1.22430800 2.19488700 -0.90895800
C 2.39187200 1.44014300 -0.28123400
N -2.03903400 -0.00283000 0.01215600
N 0.01397500 -2.00168000 -0.13792600
C -2.97927400 -0.55684000 1.01150100
C 0.03361600 -2.88398800 1.06012800
C 1.27067700 -2.15091400 -0.93944600
C -2.41070500 1.40410700 -0.30078100
C -1.94976000 -0.84872900 -1.20849100
C -1.25286000 -2.18033400 -0.91536200
H 1.02552500 1.82549300 -1.93419800
H 1.48109800 3.27505100 -0.99815900
H 2.68167400 1.90802400 0.68130900
H 3.28253000 1.49758000 -0.94849700
H -0.92642900 2.63999500 1.70962200
H 0.86728700 2.66046400 1.71558900
H -0.04118800 3.93841200 0.82110200
H -1.51685100 3.24191000 -1.03412800
H -1.03045300 1.78290100 -1.94189600
H -2.71865800 1.87886400 0.65254200

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H -2.72248700 -1.60319300 1.25875500
H -2.92811700 0.04668900 1.93865200
H -2.96457800 -1.04206800 -1.62894300
H -1.37851700 -0.28325200 -1.97092800
H -1.05140000 -2.70472200 -1.87280100
H -1.92435600 -2.83963200 -0.33080000
H -0.86129700 -2.68942200 1.68236900
H 0.04015300 -3.96051400 0.77395400
H 0.93635300 -2.67410200 1.66588300
H 1.05721800 -2.65292300 -1.90602100
H 1.95678200 -2.81871100 -0.38168800
H 1.37231900 -0.23854400 -1.96983700
H 2.96772600 -0.98501400 -1.64494100
H 2.93463800 0.05196800 1.93806200
H 2.76168600 -1.58692500 1.22282400
H 4.03849300 -0.47807100 0.61192200

$^{6}[Co]^{2+}$
BP86/BS1 SCF energy in solution: -2075.089458 a.u.
BP86/BS2 SCF energy in solution: -2076.113401 a.u.
BP86/BS2 Free energy in solution: -2075.757275 a.u.

2 6
Co -0.01935000 0.00065900 -0.99100400
N 2.06307000 -0.01326600 0.14872500
N 0.03670400 2.02838200 0.04188600
C 2.97580100 -0.05242500 -1.01425300
C -0.56497000 2.99140900 -0.89935000
C -0.73771300 1.83368700 1.29192300
C 2.15798000 -1.23604200 0.98197200
C 2.21736400 1.23515800 0.93404700
C 1.46060300 2.37712600 0.28081500
N 0.00260600 -2.03436900 0.04203100
N -2.06534700 0.02201300 0.16842600
C -0.56978800 -2.98496200 -0.92989700
C -3.05826700 0.06956300 -0.92825900
C -2.11733800 1.25745900 1.01177400
C 1.41544300 -2.38961700 0.33585100
C -0.82072900 -1.85569100 1.26377100
C -2.17725800 -1.25271700 0.93998300
H 1.84982100 1.04671900 1.96049300
H 3.29350900 1.50625700 1.02148200

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H 1.52342600 3.29080200 0.91526100
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H 0.00567200 2.97152600 -1.84851700
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H -0.52516300 4.01911500 -0.47060800

^{2}IM1
BP86/BS1 SCF energy in solution: -2226.688949 a.u.
BP86/BS2 SCF energy in solution: -2227.907675 a.u.
BP86/BS2 Free energy in solution: -2227.52557 a.u.

2 2
Co 0.02232200 0.01299300 0.05501400
N -1.21670200 1.48317400 -0.52537300
N 1.53722600 1.32290000 -0.03074100
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C 2.25536200 0.66470400 -1.16879300
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N 1.39852300 -1.48413800 -0.16183400

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C -2.57742100 -0.52869400 -0.93211700
C -0.64766400 -1.98490700 -1.55015900
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H 2.58769000 -2.96760600 0.85017700
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H 1.83274500 1.91493700 1.98676300
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H 0.46161200 -0.45741500 2.60585600
O -1.40888000 -0.12203100 2.96758200
H -1.52096200 0.78116300 3.35123000

[4]IM1
BP86/BS1 SCF energy in solution: -2226.669437 a.u.
BP86/BS2 SCF energy in solution: -2227.885433 a.u.
BP86/BS2 Free energy in solution: -2227.508721 a.u.

2 4
Co 0.02434100 0.01657800 0.37809700
N -0.70491000 1.76727000 -0.67332200
N 1.94901000 0.91093100 0.11821800
C -1.39292200 2.64496500 0.30161200
C 2.84894700 0.89364900 1.29423100
C 2.46077500 0.06341500 -0.99908800
C -1.64058700 1.29457100 -1.72941100
C 0.50299600 2.43444800 -1.24420400
C 1.70197200 2.31866500 -0.30704100
N -1.63087600 -0.95353500 -0.64664700
N 1.05747200 -1.83544000 -0.11689100
C -2.46346900 -1.84633500 0.18970500
C 1.20679300 -2.59292500 1.15489700
C 2.39819900 -1.42752700 -0.65685400
C -2.47876500 0.12456500 -1.22759400
C -0.89606700 -1.71201600 -1.69625700
C 0.19780600 -2.59062100 -1.08536200
H 0.72340100 1.95849000 -2.21957900
H 0.29763800 3.50879200 -1.44965700
H 1.53194300 2.90908600 0.61535600
H 2.60459300 2.74294400 -0.80363800
H -2.24544400 2.10823500 0.75837100
H -0.69612200 2.94893700 1.10607800
H -1.77420500 3.56145000 -0.20255800
H -2.30909700 2.11909900 -2.06488600
H -1.03656000 0.99393400 -2.60775700
H -3.17238100 0.45883300 -0.43042500
H -3.10682700 -0.27074600 -2.05880800
H -3.25423700 -2.33768600 -0.42221600
H -1.84315400 -2.63333900 0.65736800
H -2.94093900 -1.25222200 0.99079200
H -1.59951600 -2.34532400 -2.28539200
H -0.44322400 -0.98445800 -2.39855400
H 0.81768000 -3.02018700 -1.89973300
H -0.25590300 -3.44529600 -0.54631400
H 0.20834100 -2.80783200 1.58297800
H 1.73774600 -3.55773100 0.98936700
H 1.78614500 -1.99633400 1.88576500
H 2.64299500 -2.01436200 -1.56630600
H 3.16651100 -1.68056000 0.09991500
H 1.82704100 0.26564300 -1.88612200
H 3.50667600 0.34835000 -1.25858400
H 2.40839500 1.51057200 2.10140800

H 2.98079900 -0.13559100 1.67509300
H 3.84976700 1.30687900 1.03262700
O -0.72338900 0.20663100 2.24010000
H -0.29304500 -0.31268400 2.96511700
O -2.14510700 0.23851600 2.72296100
H -2.19720300 1.19063000 2.98988000

^{2}TS1s
BP86/BS1 SCF energy in solution: -2518.89838 a.u.
BP86/BS2 SCF energy in solution: -2520.454885 a.u.
BP86/BS2 Free energy in solution: -2519.887138 a.u.

2 2
Co -1.16688800 -0.05669000 0.07144500
N -2.18865500 -1.03116400 -1.39422200
N -1.03227000 -1.80285600 1.04400700
C -1.40529200 -1.45675700 -2.57826200
C 0.30303100 -2.28918100 1.46259100
C -1.88462700 -1.44588100 2.22199600
C -3.27403000 -0.07273900 -1.78202900
C -2.75453700 -2.22195500 -0.68190200
C -1.67809700 -2.84852900 0.18550700
N -1.92522000 1.66548200 -0.63015700
N -0.97873300 0.87655400 1.89416800
C -1.02573200 2.80426100 -0.93812800
C 0.37029300 1.41191600 2.21055800
C -1.34710100 -0.18849900 2.90398200
C -2.71043600 1.33564500 -1.86328300
C -2.80527200 1.96361000 0.54357900
C -1.97423000 2.01597600 1.82600800
H -3.60564000 -1.87387000 -0.06397100
H -3.15851000 -2.96412200 -1.40627000
H -0.88119700 -3.29106400 -0.44373200
H -2.09525500 -3.66798400 0.81218600
H -1.01895800 -0.56863900 -3.10896000
H -0.54934500 -2.08114000 -2.26055900
H -2.04362800 -2.04491100 -3.27463500
H -3.73490300 -0.36447600 -2.75170200
H -4.07009300 -0.13518200 -1.01434000
H -2.01583300 1.42803400 -2.72096500
H -3.52438400 2.07900100 -2.01842200
H -1.62016400 3.67510900 -1.29431600
H -0.45774900 3.11454900 -0.04409700
H -0.31282400 2.48929800 -1.72097200

H -3.34960400 2.92559000 0.39646300
H -3.56479900 1.15999400 0.61207800
H -2.64781700 1.99603500 2.70655100
H -1.40929300 2.96629000 1.88093300
H 0.67625800 2.13838200 1.43676100
H 0.37777800 1.91515800 3.20328100
H 1.10249400 0.58437800 2.22511300
H -2.09936800 0.19851200 3.62131500
H -0.44075600 -0.42740200 3.49329900
H -2.91615000 -1.27568000 1.85465400
H -1.92488200 -2.29089900 2.94785700
H 0.92290900 -2.45283700 0.56259700
H 0.80906200 -1.55341200 2.11115700
H 0.20907100 -3.24730700 2.02101700
O 0.81581100 0.01575000 -0.70259200
H 1.93410700 0.09231700 -0.35370000
O 0.96162100 0.62753900 -2.04304600
H 1.02294500 -0.17763100 -2.60727600
N 3.31174500 0.14995500 -0.11966600
C 3.61434300 -0.91437600 0.88930000
H 3.02628900 -0.65746500 1.79472300
H 3.19475200 -1.86371700 0.50144900
C 3.64945200 1.50304000 0.42283300
H 3.21473600 1.54888400 1.44242600
H 4.75368600 1.58546400 0.54026300
C 3.98445600 -0.08369400 -1.43670000
H 3.59921500 0.69088300 -2.12627100
H 5.07892800 0.09373000 -1.32557300
C 3.73235200 -1.46412400 -2.03963300
H 4.12665700 -1.48325600 -3.07648400
H 4.23740700 -2.27805700 -1.48125600
H 2.64964900 -1.70374900 -2.08823100
C 5.08556500 -1.11294000 1.26234700
H 5.54759600 -0.19598400 1.68175800
H 5.15324700 -1.90118100 2.04066800
H 5.70020700 -1.44727800 0.40143000
C 3.13213900 2.67505100 -0.40794200
H 3.34189900 3.61922000 0.13604800
H 3.62828900 2.75107200 -1.39666100
H 2.03874000 2.60892000 -0.57337900

^{2}TS1
BP86/BS1 SCF energy in solution: -2226.688249 a.u.
BP86/BS2 SCF energy in solution: -2227.908743 a.u.

BP86/BS2 Free energy in solution: -2227.525305 a.u.

2 2
Co 0.02272600 0.01703200 0.07271200
N -1.45573700 1.22576700 -0.56547700
N 1.25231300 1.60172800 0.01319100
C -2.33715500 1.70974800 0.52659400
C 2.05271400 1.96622000 1.20860400
C 2.10532200 1.08926000 -1.10743900
C -2.20995200 0.38048100 -1.54907800
C -0.74730300 2.35945700 -1.24637900
C 0.43446100 2.79231800 -0.39853200
N -1.09549200 -1.54708100 -0.46330800
N 1.67090500 -1.19361300 -0.12596900
C -1.37263000 -2.57603500 0.57078900
C 2.24698000 -1.79769500 1.11036000
C 2.70298300 -0.26984700 -0.74959400
C -2.40342900 -1.00947600 -0.97147200
C -0.22039100 -2.05944900 -1.56558200
C 1.19720100 -2.30524300 -1.04714800
H -0.41859100 2.00323500 -2.24236800
H -1.44243900 3.21056700 -1.41562900
H 0.09085800 3.28317800 0.53243900
H 1.06898100 3.52575400 -0.94256600
H -2.70580900 0.85381400 1.12107300
H -1.76487500 2.37350100 1.20049500
H -3.19360000 2.27615800 0.10133200
H -3.18950600 0.84573200 -1.79506000
H -1.61857400 0.34472100 -2.48535700
H -3.09776500 -0.98119800 -0.10936900
H -2.83741900 -1.70235500 -1.72464200
H -2.02900900 -3.36656500 0.14633600
H -0.44130300 -3.05412800 0.92209700
H -1.87732800 -2.09197500 1.42768400
H -0.64001200 -2.99913400 -1.99095100
H -0.21936900 -1.30314500 -2.37487800
H 1.89340600 -2.41352800 -1.90239700
H 1.23914200 -3.25257800 -0.47742100
H 1.50098300 -2.45173200 1.60123800
H 3.13545700 -2.41660500 0.85900400
H 2.56313700 -1.00515400 1.81400900
H 3.13617000 -0.73657700 -1.65651800
H 3.52918300 -0.14876900 -0.02419200
H 1.46018900 1.00129800 -2.00535300

H 2.91322700 1.81657400 -1.34787400
H 1.36814900 2.22931700 2.03539100
H 2.69645300 1.13020900 1.53225300
H 2.69845000 2.84031400 0.97320700
O -0.21502200 0.00232800 1.98039700
H 0.24714600 -0.77449300 2.37311200
O -1.57043500 -0.30550300 3.01299800
H -1.69198700 0.64305000 3.24874200

^{2}IM2
BP86/BS1 SCF energy in solution: -2150.345452 a.u.
BP86/BS2 SCF energy in solution: -2151.464093 a.u.
BP86/BS2 Free energy in solution: -2151.103429 a.u.

2 2
Co 0.00343600 0.01661800 0.19954000
N 0.45560700 1.92720300 -0.14032900
N 1.94159600 -0.44391800 -0.02614400
C 0.66694700 2.74809400 1.07994600
C 2.63944800 -1.12934200 1.08645400
C 1.74515500 -1.30933600 -1.23062100
C -0.71503400 2.41748100 -0.94441500
C 1.69818300 1.82490500 -0.98095400
C 2.65743000 0.83718500 -0.34355300
N -1.93919100 0.45581300 -0.03009000
N -0.45194000 -1.91811300 -0.15489300
C -2.87313800 0.13514900 1.07537300
C -0.66558500 -2.75808800 1.05773000
C 0.75015800 -2.43069300 -0.93135600
C -2.00741300 1.93015000 -0.31215600
C -2.14820800 -0.39310600 -1.24637500
C -1.73984300 -1.84118200 -0.96310600
H 1.39036900 1.48332000 -1.98874400
H 2.16727700 2.82542400 -1.09485500
H 3.05667600 1.22992800 0.61059200
H 3.52318200 0.63792300 -1.01090600
H -0.25492000 2.75700200 1.68824200
H 1.48259200 2.32041300 1.68879800
H 0.92623000 3.78565500 0.78089500
H -0.70031400 3.52676500 -1.00405100
H -0.60073300 2.03232700 -1.97642500
H -2.18144300 2.43296600 0.65835200
H -2.87734300 2.15569400 -0.96553700
H -3.88638900 0.51390000 0.82197900

H -2.93882000 -0.95353000 1.24445800
H -2.50460800 0.61511400 1.99955000
H -3.20852800 -0.34685900 -1.57937100
H -1.52657300 0.03062800 -2.06133500
H -1.61452900 -2.38298900 -1.92038100
H -2.52644600 -2.36722900 -0.39056200
H -1.49199700 -2.34328200 1.66061600
H -0.91740000 -3.79555600 0.75093700
H 0.25085200 -2.77223300 1.67369200
H 0.41833200 -2.89511100 -1.88031300
H 1.22620800 -3.22547600 -0.32671800
H 1.36332100 -0.66228700 -2.04876700
H 2.71558400 -1.73368400 -1.57110000
H 2.54676100 -0.50982600 1.99626200
H 2.19756300 -2.12013300 1.28836200
H 3.70972800 -1.26611700 0.82120500
O 0.00893500 0.03054600 1.89074200

^{4}IM2
BP86/BS1 SCF energy in solution: -2150.355666 a.u.
BP86/BS2 SCF energy in solution: -2151.474122 a.u.
BP86/BS2 Free energy in solution: -2151.11343 a.u.

2 4
Co 0.01578000 -0.00275200 0.39452100
N 1.96108300 0.39835200 -0.21286500
N 0.40696000 -1.92875200 -0.03091500
C 2.82599100 0.57040100 0.98646900
C 0.05246800 -2.91753300 1.01827800
C -0.42808000 -2.07156700 -1.27726300
C 1.88429400 1.65940400 -1.01190200
C 2.38318300 -0.78720000 -1.01870400
C 1.87627300 -2.04579300 -0.33767200
N -0.38279600 1.93218600 -0.02608200
N -1.96391700 -0.39454800 -0.22514500
C -1.09911600 2.69948900 1.02407000
C -2.88054700 -0.57833900 0.93482200
C -1.87632900 -1.68152400 -1.01409400
C 0.92384800 2.61564400 -0.32778400
C -1.20818500 1.75512000 -1.27433900
C -2.38379100 0.81821000 -1.02395700
H 1.96050900 -0.67583500 -2.03625900
H 3.48990500 -0.81893000 -1.12042400
H 2.39282200 -2.20817000 0.62768800

H 2.05145000 -2.94518000 -0.96619100
H 2.46314400 1.41206400 1.60236600
H 2.81041100 -0.34568300 1.60345600
H 3.86818800 0.77632000 0.65994400
H 2.88995600 2.12304200 -1.10929700
H 1.54092900 1.39942700 -2.03198600
H 1.33251800 2.96667900 0.63910800
H 0.73410900 3.51283100 -0.95553300
H -1.24999800 3.74296500 0.67303500
H -2.08455300 2.25395500 1.24310700
H -0.49087700 2.70269100 1.94643200
H -1.55708800 2.74931800 -1.63000200
H -0.54361600 1.33221000 -2.05336100
H -2.81775200 0.50700600 -1.99514100
H -3.18507900 1.33382600 -0.46136100
H -2.88917600 0.33160600 1.56177100
H -3.91234700 -0.77803200 0.57131900
H -2.54425700 -1.43154300 1.55095600
H -2.41188600 -1.57898200 -1.97901100
H -2.39509100 -2.46982000 -0.43669200
H 0.01363200 -1.41530400 -2.05275300
H -0.35948900 -3.11877400 -1.64604600
H 0.64054000 -2.70010100 1.92833300
H -1.02171500 -2.87407100 1.26617700
H 0.29541400 -3.93884400 0.65399400
O -0.00200400 -0.00486700 2.08647600

^{2}IM3
BP86/BS1 SCF energy in solution: -2301.801665 a.u.
BP86/BS2 SCF energy in solution: -2303.121528 a.u.
BP86/BS2 Free energy in solution: -2302.737745 a.u.

2 2
Co -0.24958100 0.00963400 0.00845300
N -2.03573700 -0.44273500 -0.81990500
N -0.05930100 -1.93083900 0.52114500
C -1.98389400 -0.68585300 -2.28465300
C 1.13440100 -2.67350500 0.04765400
C -0.07006100 -1.71536700 2.00718400
C -2.89370000 0.74050900 -0.47874600
C -2.45801200 -1.66701500 -0.05975700
C -1.29464600 -2.63659600 0.03364500
N -0.76217700 1.94421600 -0.05170800
N 1.08197300 0.46726700 1.48525500

C 0.15333800 2.90390000 -0.71401000
C 2.48822200 0.71259600 1.06024300
C 1.03833400 -0.74273800 2.40277300
C -2.10984300 2.01848300 -0.71349800
C -0.83342600 2.12109300 1.43528200
C 0.49409700 1.73176900 2.09219000
H -2.78747300 -1.33629100 0.94519700
H -3.33024700 -2.14251600 -0.55751000
H -1.05334400 -3.06263000 -0.95860400
H -1.53819700 -3.48376200 0.70978400
H -1.60800100 0.21231500 -2.80541200
H -1.30425400 -1.52716000 -2.50606500
H -3.00560700 -0.92737200 -2.64662500
H -3.82011300 0.72922800 -1.09154900
H -3.19737700 0.63931700 0.58172800
H -1.92664000 2.17813100 -1.79327400
H -2.66766700 2.90213500 -0.33543900
H -0.29843700 3.91828600 -0.68445000
H 1.13197000 2.94060900 -0.20642100
H 0.30438700 2.58789200 -1.76189400
H -1.10144400 3.17034100 1.68803800
H -1.65113200 1.47006500 1.80821300
H 0.33244100 1.58559800 3.17792100
H 1.24281800 2.53789500 1.97664100
H 2.53033800 1.57023600 0.36600700
H 3.10867500 0.93598000 1.95412500
H 2.88520400 -0.18093300 0.54645700
H 0.89613100 -0.41522200 3.45117800
H 2.02579400 -1.23582500 2.34405100
H -1.06541900 -1.31355300 2.28348800
H 0.05552400 -2.68606000 2.53543600
H 1.11986200 -2.70755600 -1.05612700
H 2.07274800 -2.19895400 0.37943600
H 1.09833400 -3.71018000 0.44652600
O 0.73552100 0.01894700 -1.37660400
O 3.18873200 -0.75679100 -1.85812900
H 2.23600700 -0.46662000 -1.62978300
O 3.83805900 0.51609800 -2.13681200
H 4.39313600 0.62141700 -1.33032600

[4]IM3
BP86/BS1 SCF energy in solution: -2301.808608 a.u.
BP86/BS2 SCF energy in solution: -2303.128086 a.u.
BP86/BS2 Free energy in solution: -2302.745736 a.u.

2 4
Co 0.18916700 -0.00219800 -0.12187200
N 2.06890800 0.49964100 -0.81267200
N 0.06111800 1.89538300 0.57089400
C 2.02106300 0.78154300 -2.27287400
C -1.15604700 2.65653800 0.19015800
C 0.13487200 1.62312700 2.05076200
C 2.93908000 -0.67997800 -0.50725800
C 2.46577900 1.71085200 -0.02749500
C 1.27527400 2.64305400 0.08449600
N 0.82073700 -1.91393400 -0.12006700
N -1.00830800 -0.54857300 1.53870700
C -0.07220200 -2.90470000 -0.77390500
C -2.42326200 -0.79897400 1.14512600
C -0.94187600 0.63447600 2.47565800
C 2.16489700 -1.94991300 -0.79744500
C 0.93874500 -2.12526700 1.36472300
C -0.37907300 -1.81935000 2.06809600
H 2.80695600 1.36607800 0.96794500
H 3.32202200 2.22510200 -0.51496700
H 1.01336700 3.07704900 -0.89913500
H 1.48853400 3.48758200 0.77434400
H 1.70301600 -0.11992600 -2.82650600
H 1.30518200 1.59531100 -2.48381200
H 3.03467100 1.08265300 -2.61507100
H 3.87136700 -0.64203200 -1.11075200
H 3.23131900 -0.61621300 0.55900500
H 1.97491300 -2.06187700 -1.88217000
H 2.72272700 -2.85035900 -0.46182400
H 0.39447000 -3.91067000 -0.70608500
H -1.05955900 -2.93955000 -0.28378800
H -0.20304600 -2.62752300 -1.83546000
H 1.26270500 -3.17068600 1.56291500
H 1.73618300 -1.44997200 1.73288500
H -0.20058400 -1.73209300 3.15824000
H -1.10473100 -2.64189200 1.92209100
H -2.47451200 -1.63210200 0.42160700
H -3.02224300 -1.05889600 2.04485400
H -2.84446000 0.10439200 0.66880100
H -0.74561700 0.29166600 3.51117500
H -1.93687100 1.11733000 2.47594700
H 1.14315500 1.21893600 2.26798300
H 0.03168900 2.58237400 2.60458900

H -1.17714900 2.77131100 -0.90844100
H -2.07578000 2.14583900 0.52143800
H -1.11407000 3.66103000 0.66365600
O -0.89798900 0.03607000 -1.44008300
O -3.37461100 0.78082900 -1.74175600
H -2.40546800 0.47130600 -1.68260900
O -4.05562000 -0.47389100 -1.99760300
H -4.56061100 -0.58494900 -1.15907000

^{2}TS2
BP86/BS1 SCF energy in solution: -2301.80125 a.u.
BP86/BS2 SCF energy in solution: -2303.117271 a.u.
BP86/BS2 Free energy in solution: -2302.738761 a.u.

2 2
Co 0.20149300 0.01138600 -0.01555700
N -0.61755700 1.53961500 1.03091100
N -0.92779600 -1.26279300 1.06032800
C -1.71344400 2.22982200 0.30030000
C -1.76347400 -2.27227500 0.36430300
C 0.20495900 -1.88522400 1.82649500
C 0.54103800 2.46054500 1.28096000
C -1.11844100 0.89050300 2.28764500
C -1.80885900 -0.41467900 1.93409900
N 1.67068500 1.27113900 -0.58608000
N 1.52807800 -1.52254100 -0.28982400
C 1.92419600 1.41858500 -2.03917500
C 1.35710700 -2.24973100 -1.58199600
C 1.25418500 -2.45902100 0.87460200
C 1.34178400 2.61682000 -0.00075600
C 2.79784900 0.60537300 0.14495400
C 2.89593400 -0.86289700 -0.25620600
H -0.24973200 0.72472800 2.95441500
H -1.81759100 1.57209500 2.81725000
H -2.73738200 -0.22407000 1.36285500
H -2.08704900 -0.97960000 2.84992500
H -1.31626900 2.69884200 -0.61723700
H -2.49788400 1.50922100 0.00563700
H -2.14655700 3.01280100 0.95842300
H 0.17473400 3.44694800 1.63814300
H 1.15573000 2.02139100 2.09116100
H 0.76161100 3.17082500 -0.76336500
H 2.27706300 3.18775400 0.18448800
H 2.73671400 2.15985900 -2.19766600

H 2.22619700 0.46009600 -2.49562300
H 0.99729800 1.76709200 -2.52841400
H 3.75452000 1.13422000 -0.06169300
H 2.59334800 0.69791800 1.23089100
H 3.55814900 -1.40069600 0.45017700
H 3.34174600 -0.96420200 -1.26351300
H 1.48540700 -1.54708700 -2.42466300
H 2.11815400 -3.05607600 -1.65347800
H 0.34871800 -2.69679200 -1.63764500
H 2.19114100 -2.64622400 1.43415700
H 0.92365900 -3.42802300 0.45590900
H 0.65569600 -1.09511800 2.45956900
H -0.18101100 -2.67726900 2.50554600
H -2.44324400 -1.76393200 -0.34390600
H -1.13739500 -2.98413200 -0.20035400
H -2.35124300 -2.84117600 1.11626100
O -0.70090300 0.08778900 -1.49826700
O -2.87376900 -0.53153000 -2.26224200
H -1.81733200 -0.28738900 -1.75054600
O -3.78931400 0.33984000 -1.62697400
H -4.09647300 0.90691000 -2.37550000

^{2}TS2a
BP86/BS1 SCF energy in solution: -2301.800768 a.u.
BP86/BS2 SCF energy in solution: -2303.117074 a.u.
BP86/BS2 Free energy in solution: -2302.739614 a.u.

2 2
Co 0.22958800 0.06970300 0.07509900
N 1.69035700 1.21851700 -0.69414700
N -0.45735500 1.66830300 1.05392100
C 1.40812400 1.75665900 -2.04969000
C -1.86462600 2.08592500 0.84487600
C -0.19782300 1.11428400 2.42463300
C 2.87845400 0.30060500 -0.69325200
C 1.82563200 2.31307800 0.32581500
C 0.44563900 2.81801700 0.70599900
N 1.23860500 -1.55925000 -0.53636600
N -0.75212700 -1.12192200 1.40713800
C 0.56184300 -2.55518500 -1.39616100
C -2.07000500 -1.67531700 0.98740100
C -0.94129500 -0.20852800 2.60515700
C 2.46653900 -1.05537900 -1.23867000

C 1.52663300 -2.06663600 0.84138000
C 0.23167600 -2.25835400 1.63505900
H 2.35608800 1.89346200 1.20374100
H 2.45065500 3.13801500 -0.07807000
H -0.02458400 3.34706500 -0.14471100
H 0.49948800 3.53119300 1.55612500
H 1.27637700 0.92465800 -2.76382500
H 0.47832800 2.35191600 -2.03411100
H 2.25849800 2.39432300 -2.37177900
H 3.69989900 0.73646500 -1.30157300
H 3.24547800 0.22432800 0.34935700
H 2.21312900 -0.98145300 -2.31371500
H 3.29289000 -1.79176500 -1.13831800
H 1.28655500 -3.34875700 -1.67827800
H -0.28466600 -3.02709700 -0.86947600
H 0.18244300 -2.04783200 -2.30096600
H 2.09870000 -3.01991500 0.79749000
H 2.17545000 -1.31758100 1.34055100
H 0.47538400 -2.33434300 2.71266000
H -0.27127500 -3.20000800 1.34561500
H -1.94141200 -2.32725700 0.10548400
H -2.49866000 -2.27203800 1.82074300
H -2.76057500 -0.85574200 0.72061200
H -0.59062700 -0.71400700 3.52635900
H -2.02650600 -0.03148100 2.72261200
H 0.89724700 0.96191500 2.52303100
H -0.50623700 1.84536300 3.20427100
H -2.00562600 2.33829900 -0.22129500
H -2.57152800 1.28628200 1.12119700
H -2.08033400 2.98008500 1.46819400
O -0.84519500 0.11345300 -1.28616300
O -3.22365700 0.15045300 -1.41541100
H -2.07425800 0.19208600 -1.34482500
O -3.54264000 -0.89534700 -2.30948900
H -3.98628800 -1.54879100 -1.71601200

^{2}TS4
BP86/BS1 SCF energy in solution: -2301.792412 a.u.
BP86/BS2 SCF energy in solution: -2303.111837 a.u.
BP86/BS2 Free energy in solution: -2302.735559 a.u.

2 4
Co 0.04930300 -0.06667200 0.49346000
N 0.22978400 -2.06055000 -0.31170900

N -1.96075300 -0.24796400 -0.05808200
C 0.33250500 -2.99279400 0.83880200
C -2.90325000 0.17376000 1.00782800
C -2.00234600 0.65084200 -1.25309000
C 1.46133300 -2.08036600 -1.15306000
C -1.00800700 -2.29473200 -1.11042600
C -2.20936500 -1.68126500 -0.41032100
N 2.05313400 0.13817000 -0.18077000
N -0.15022900 1.98433300 -0.18441000
C 2.96350800 0.76853300 0.80572800
C -0.17480700 2.90076900 0.98796800
C -1.46067200 2.04087600 -0.92317600
C 2.55196700 -1.22787100 -0.52047400
C 1.83681800 0.99040100 -1.38841100
C 1.06149700 2.25953800 -1.03695400
H -0.85665800 -1.84311300 -2.10995900
H -1.17302600 -3.38418500 -1.26308700
H -2.42812700 -2.21175300 0.53677600
H -3.11586000 -1.76185100 -1.05000600
H 1.24140600 -2.77290900 1.42758200
H -0.54689000 -2.88846800 1.50044900
H 0.38605500 -4.04006500 0.46764800
H 1.82496700 -3.12295800 -1.28593900
H 1.19170600 -1.69931400 -2.15725500
H 2.90983800 -1.68402400 0.42334600
H 3.42704900 -1.15447600 -1.20384800
H 3.98695400 0.84955800 0.37691600
H 2.61573000 1.78130800 1.07589300
H 2.99268500 0.14942700 1.72072100
H 2.81545700 1.25862900 -1.84734900
H 1.27631600 0.38926900 -2.13140300
H 0.75985200 2.77148900 -1.97333300
H 1.71070100 2.96233900 -0.48122600
H 0.76380500 2.79611300 1.56251200
H -0.27785100 3.95475000 0.64700200
H -1.02711900 2.65008000 1.64584300
H -1.34580900 2.61750100 -1.86367400
H -2.18206600 2.59438900 -0.29199200
H -1.39612700 0.18162700 -2.05260700
H -3.04769600 0.72797500 -1.62805800
H -2.78924800 -0.49724200 1.87869100
H -2.70210600 1.21076900 1.32902800
H -3.94742800 0.11103200 0.62984900
O 0.13179600 -0.03013300 2.23063600

H 0.78677000 -0.42312100 2.97692600
O 1.79204300 -0.79150900 3.89327900
O 1.81713100 0.04057500 4.97307300
H 0.86514400 0.15517600 5.24425000

^{2}TS4a
BP86/BS1 SCF energy in solution: -2301.804365 a.u.
BP86/BS2 SCF energy in solution: -2303.120684 a.u.
BP86/BS2 Free energy in solution: -2302.744235 a.u.

2 4
Co 0.16648700 -0.00089400 -0.09409200
N 1.88086200 0.93198700 -0.74063300
N -0.31758800 1.75527700 0.78529900
C 1.72631900 1.35993800 -2.15738600
C -1.66645900 2.30175200 0.49059200
C -0.16847600 1.35161300 2.22782900
C 2.98424700 -0.06852500 -0.58201900
C 2.06013300 2.10577000 0.17220100
C 0.71704900 2.77419400 0.38653500
N 1.16679900 -1.74018600 -0.31700100
N -0.86411700 -0.93082500 1.46928800
C 0.48315800 -2.82072000 -1.07275200
C -2.21057400 -1.41347000 1.05113200
C -1.02366300 0.13133700 2.53326600
C 2.47533800 -1.43505900 -0.99514000
C 1.35137700 -2.07593100 1.13544600
C 0.01138800 -2.10247900 1.86538300
H 2.47992600 1.72971800 1.12522800
H 2.79348500 2.82215200 -0.25737400
H 0.35812600 3.25341500 -0.54411000
H 0.77937100 3.56398900 1.16599300
H 1.56726900 0.48011300 -2.80551700
H 0.85557800 2.03155800 -2.25987000
H 2.64652400 1.89391000 -2.47803500
H 3.86350600 0.22471400 -1.19531400
H 3.30351200 -0.05609700 0.47848900
H 2.28758900 -1.47555900 -2.08539400
H 3.21271800 -2.23115400 -0.75458700
H 1.15877000 -3.70063800 -1.13651200
H -0.45201200 -3.13202000 -0.57742700
H 0.25078700 -2.45735500 -2.09009100
H 1.87017000 -3.05581800 1.22902700
H 2.01364100 -1.30484200 1.57467600

H 0.18849800 -2.09319800 2.95905200
H -0.54510600 -3.02997400 1.63222900
H -2.11489000 -2.18457600 0.26609400
H -2.73905600 -1.85185600 1.92535400
H -2.80090900 -0.57245900 0.64364700
H -0.75216300 -0.27908500 3.52631200
H -2.09449800 0.40541200 2.57573000
H 0.90184200 1.13156200 2.40748400
H -0.44961300 2.20575800 2.88286300
H -1.74168000 2.51832300 -0.59016100
H -2.45930600 1.58929700 0.77355900
H -1.81026700 3.24348800 1.06322800
O -0.93566100 -0.11771800 -1.46616300
O -3.23478100 0.57313200 -1.53844200
H -2.01693400 0.25020100 -1.53624600
O -3.85420300 -0.41998700 -2.30290900
H -4.35359200 -0.94255600 -1.62691100

^{CS}IM4
BP86/BS1 SCF energy in solution: -2150.996422 a.u.
BP86/BS2 SCF energy in solution: -2152.117454 a.u.
BP86/BS2 Free energy in solution: -2151.745571 a.u.

2 1
Co 0.01688600 -0.00141700 0.15108900
N 1.96298600 -0.32412800 -0.14344200
N -0.31679100 -1.95529000 -0.05146600
C 2.80738700 -0.45182800 1.06766400
C -0.96099900 -2.69899300 1.05829600
C -1.19722300 -1.83265500 -1.25412400
C 2.35482000 0.86338600 -0.97438600
C 1.96642000 -1.58193400 -0.96195800
C 1.01272000 -2.59172300 -0.34640200
N 0.33028200 1.95733000 -0.05165300
N -1.95230900 0.32320900 -0.15365100
C -0.03472200 2.86583200 1.06254700
C -2.83492100 0.45717900 1.03992500
C -2.37624200 -0.89759800 -0.95766200
C 1.79178700 2.12714600 -0.34962000
C -0.54576900 2.11722600 -1.25378500
C -1.96431100 1.62244700 -0.94483500
H 1.65296100 -1.31408500 -1.99013200
H 2.99337800 -2.00094700 -1.03080200
H 1.40830900 -2.96576100 0.61706100

H 0.87748900 -3.46927600 -1.01455700
H 2.74089200 0.46925100 1.67272500
H 2.45434200 -1.29454800 1.68701800
H 3.86230200 -0.62441800 0.76535600
H 3.46066000 0.92727000 -1.06759000
H 1.94908300 0.70882200 -1.99392100
H 2.29272800 2.34269800 0.61347200
H 1.95156900 3.00525300 -1.01188600
H 0.29818800 3.89865700 0.82425200
H -1.12550400 2.88499100 1.22857300
H 0.45725300 2.50781300 1.98509400
H -0.57199300 3.17828800 -1.58841900
H -0.09760400 1.52355900 -2.07722700
H -2.52328400 1.48469200 -1.89099900
H -2.51699600 2.37399600 -0.35019500
H -2.50068100 1.29874200 1.67470300
H -3.88181300 0.64787900 0.72113500
H -2.81718800 -0.47413700 1.63725200
H -2.84379500 -0.58222400 -1.91073300
H -3.15278800 -1.42778500 -0.37436600
H -0.58057900 -1.43026700 -2.08532600
H -1.57000500 -2.83054800 -1.57614700
H -0.37199800 -2.54257200 1.97992500
H -1.99306100 -2.34718200 1.22881400
H -0.99883300 -3.78094100 0.80812500
O 0.14691600 -0.02016700 1.97474800
H -0.76715000 0.03361700 2.32894400

^{3}IM4
BP86/BS1 SCF energy in solution: -2150.996368 a.u.
BP86/BS2 SCF energy in solution: -2152.117888 a.u.
BP86/BS2 Free energy in solution: -2151.745337 a.u.

2 3
Co 0.00430100 -0.01341100 0.32572200
N -0.08343000 -1.98354500 -0.23221400
N -1.97884600 0.06898800 -0.03049300
C -0.12624300 -2.85521100 0.97327600
C -2.86789200 0.62958600 1.01673900
C -1.95213900 0.92109200 -1.27003700
C 1.15879900 -2.21735200 -1.03048400
C -1.33357800 -2.10878100 -1.04141800
C -2.44152100 -1.32577800 -0.35834900
N 1.98271500 -0.08983500 -0.03038300

N 0.08103300 1.97912300 -0.25502600
C 2.89386700 0.39718300 1.03315800
C 0.12243900 2.88747300 0.92897200
C -1.19232600 2.22228700 -1.03327100
C 2.32400600 -1.52152900 -0.34597800
C 2.03588600 0.76242600 -1.26858200
C 1.36274500 2.11640200 -1.04851300
H -1.12066000 -1.71197900 -2.05365800
H -1.62331000 -3.17618300 -1.15620600
H -2.73285500 -1.80491400 0.59604100
H -3.35118700 -1.28008900 -0.99570600
H 0.78117100 -2.70436800 1.58351800
H -1.00396800 -2.60616600 1.59576200
H -0.18718300 -3.91799800 0.65377500
H 1.36093500 -3.30596100 -1.13233200
H 0.98611800 -1.81701300 -2.04862600
H 2.56855200 -2.01467500 0.61468200
H 3.23839600 -1.56094200 -0.97720100
H 3.94867500 0.24344700 0.71830800
H 2.73850100 1.47242100 1.22749800
H 2.69669400 -0.16751900 1.96228200
H 3.09338400 0.89748400 -1.58685800
H 1.51632400 0.20891400 -2.07502200
H 1.15541800 2.58566800 -2.03058400
H 2.03139300 2.80416400 -0.49541800
H 1.02263900 2.68125900 1.53445600
H 0.14379600 3.94539100 0.58792600
H -0.76960400 2.72562700 1.56001800
H -0.96192600 2.70114400 -2.00584600
H -1.80900200 2.93885300 -0.45824400
H -1.45573400 0.33170800 -2.06571800
H -2.99231300 1.12722100 -1.60672400
H -2.81680300 -0.00818300 1.91992800
H -2.58331600 1.66340900 1.27970600
H -3.91799400 0.63447100 0.65260500
O 0.10037600 0.01872400 2.16619300
H -0.78983600 0.05721800 2.58132100

[5]IM4
BP86/BS1 SCF energy in solution: -2150.981269 a.u.
BP86/BS2 SCF energy in solution: -2152.102504 a.u.
BP86/BS2 Free energy in solution: -2151.734534 a.u.

2 5

Co -0.00235600 -0.00872200 0.55748700
N 0.20825400 -2.02628600 -0.23704300
N -2.03103300 -0.20661700 -0.13265200
C 0.28796800 -2.93411000 0.93282400
C -3.02516400 0.25167400 0.86578500
C -2.01552400 0.63978600 -1.35842600
C 1.45865700 -2.04699000 -1.04605700
C -1.00608100 -2.28325200 -1.06196800
C -2.24022800 -1.65170000 -0.43035700
N 2.03688600 0.19350600 -0.11452400
N -0.19878200 2.01247700 -0.26918400
C 2.91323500 0.84491300 0.88666300
C -0.29032300 2.92774700 0.90039600
C -1.47134700 2.04022800 -1.06697800
C 2.53665400 -1.17921000 -0.40842400
C 1.86294900 1.01792600 -1.34419100
C 1.05150400 2.28387200 -1.05904100
H -0.82258000 -1.86745800 -2.07155600
H -1.16655700 -3.37736500 -1.18349200
H -2.48443100 -2.14707000 0.53014600
H -3.11772800 -1.78695800 -1.10182100
H 1.15444000 -2.66915800 1.56658800
H -0.63123500 -2.85560400 1.54163600
H 0.40214700 -3.98466900 0.58445800
H 1.83318500 -3.08871900 -1.15511600
H 1.21100300 -1.68292600 -2.06223000
H 2.87300400 -1.61562500 0.55276200
H 3.42538400 -1.13244700 -1.07701600
H 3.94429900 0.95390800 0.48181400
H 2.53336600 1.84723100 1.15442300
H 2.94748200 0.22484800 1.80183100
H 2.85512700 1.29770800 -1.76600700
H 1.34555500 0.39578200 -2.10092800
H 0.79455300 2.77288100 -2.02067600
H 1.66202100 3.00575800 -0.48344000
H 0.61890400 2.83883600 1.52458000
H -0.38453300 3.98285700 0.55915100
H -1.17811500 2.67682300 1.51208400
H -1.30627700 2.57012600 -2.02701300
H -2.21505200 2.63080700 -0.49787200
H -1.37843700 0.13722800 -2.11261300
H -3.04036500 0.71918700 -1.78739100
H -2.91218700 -0.34096900 1.79273400
H -2.87576800 1.31934700 1.10795800

H -4.05706000 0.12041100 0.47004300
O -0.02276300 -0.08891400 2.34774700
H -0.26549100 0.72516000 2.84530000

^{OS}IM5
BP86/BS1 SCF energy in solution: -2226.089858 a.u.
BP86/BS2 SCF energy in solution: -2227.304251 a.u.
BP86/BS2 Free energy in solution: -2226.928102 a.u.

2 1
Co 0.01526000 0.01922000 0.09174700
N -1.46012600 1.30655300 -0.38286600
N 1.32755200 1.52245100 -0.07214400
C -2.24241600 1.88114200 0.73855900
C 2.21825100 1.85154300 1.06752000
C 2.07173700 0.94228900 -1.23715700
C -2.33044900 0.49122700 -1.29707700
C -0.73790900 2.37950400 -1.14996800
C 0.54068300 2.75200900 -0.42453100
N -1.23195300 -1.50451800 -0.30985500
N 1.57830000 -1.28003200 -0.17180800
C -1.49145600 -2.58224300 0.67642300
C 2.15278700 -1.90126900 1.05028900
C 2.62528200 -0.43353500 -0.86708400
C -2.54331600 -0.89114400 -0.70769700
C -0.45161100 -2.01164500 -1.48572000
C 0.97962300 -2.35205300 -1.06494400
H -0.52323100 1.98965900 -2.16417100
H -1.39055000 3.27023900 -1.27452500
H 0.31123200 3.26775600 0.52792400
H 1.15981800 3.44334700 -1.03648400
H -2.78036200 1.07808100 1.27444100
H -1.57096600 2.41170900 1.44023900
H -2.98838400 2.60382200 0.34407300
H -3.30319200 1.00208800 -1.46412700
H -1.82093300 0.43069900 -2.27809100
H -3.16576500 -0.83840700 0.20646800
H -3.07158800 -1.55106500 -1.42991200
H -2.20651700 -3.31402600 0.24169600
H -0.56317600 -3.11828400 0.93939800
H -1.92003700 -2.13579000 1.59031300
H -0.94827700 -2.90574700 -1.92499500
H -0.45549700 -1.22357500 -2.26614400
H 1.60582000 -2.48731200 -1.96872400

H 1.00441800 -3.30793700 -0.50890500
H 1.37248900 -2.47168700 1.58475300
H 2.98383800 -2.58591800 0.77448900
H 2.53582900 -1.11854100 1.72862800
H 2.99081300 -0.94640700 -1.77901800
H 3.48939200 -0.33340100 -0.18367900
H 1.36657600 0.86363200 -2.08955300
H 2.89529000 1.62144400 -1.55281100
H 1.59762600 2.10764800 1.94520000
H 2.87130400 1.00329800 1.33109000
H 2.85832400 2.71913900 0.79811700
O 0.10949200 0.07153700 1.92314100
O -1.05325100 -0.27906900 2.65140700
H -1.43987700 0.60071000 2.88579400

^{3}IM5
BP86/BS1 SCF energy in solution: -2226.088112 a.u.
BP86/BS2 SCF energy in solution: -2227.30248 a.u.
BP86/BS2 Free energy in solution: -2226.931693 a.u.

2 3
Co 0.01899900 0.00759000 0.17978800
N -0.48569100 1.88756200 -0.45363300
N 1.94752500 0.54260000 -0.04087900
C -0.84134600 2.76290100 0.69451600
C 2.87881100 0.30906000 1.09130800
C 2.27650200 -0.31279600 -1.23037500
C -1.65059300 1.69430000 -1.37146100
C 0.72796800 2.39393700 -1.16797700
C 1.96683600 2.00723400 -0.38072700
N -1.84594800 -0.55869200 -0.34535900
N 0.61368100 -1.92549300 -0.25862200
C -2.68694100 -1.32246300 0.60987600
C 0.75493100 -2.77839000 0.95565300
C 1.95875000 -1.77655900 -0.94011500
C -2.59599400 0.67586300 -0.76223000
C -1.47285300 -1.39269400 -1.53905300
C -0.47863900 -2.47971000 -1.14817900
H 0.73751600 1.94513200 -2.18023900
H 0.67585800 3.49692000 -1.29827400
H 2.00911900 2.55782100 0.57902800
H 2.89285500 2.25225800 -0.94504000
H -1.64253300 2.30029100 1.29893100
H 0.03828100 2.90691700 1.34656800

H -1.18386200 3.74949100 0.31465200
H -2.17491300 2.65868400 -1.54861800
H -1.25787400 1.34905600 -2.34728800
H -3.08161900 1.08019800 0.14659000
H -3.40443900 0.40463200 -1.47559800
H -3.65370100 -1.58076700 0.12535400
H -2.18800300 -2.25674200 0.91977500
H -2.87094300 -0.70323900 1.50465000
H -2.38743500 -1.84019300 -1.98854800
H -1.02512200 -0.72050100 -2.29695000
H -0.03941100 -2.92828500 -2.06137900
H -0.98360500 -3.29659900 -0.59840600
H -0.20704500 -2.82735400 1.49799300
H 1.05917800 -3.80730800 0.66411000
H 1.52007600 -2.35336400 1.62960100
H 1.97643300 -2.35587300 -1.88446200
H 2.72507800 -2.21911500 -0.27601600
H 1.67434200 0.05169200 -2.08587100
H 3.34906000 -0.19137300 -1.50179300
H 2.50893100 0.85284300 1.97952500
H 2.95423100 -0.76504900 1.33392200
H 3.89055600 0.68288100 0.82251500
O 0.07832700 0.15482000 2.02392000
O -1.11633800 0.18759600 2.79893900
H -0.75145300 0.30675900 3.71016400

^{5}IM5
BP86/BS1 SCF energy in solution: -2226.065202 a.u.
BP86/BS2 SCF energy in solution: -2227.278573 a.u.
BP86/BS2 Free energy in solution: -2226.909307 a.u.

2 5
Co 0.00808200 0.00806600 0.43434900
N -0.62798400 1.86896400 -0.52646600
N 1.95117300 0.75088600 -0.06635100
C -1.03541700 2.70811300 0.62622500
C 2.91930600 0.59435600 1.04477300
C 2.28916900 -0.10731900 -1.23815300
C -1.76871800 1.58859000 -1.43802000
C 0.55090400 2.43584400 -1.23723700
C 1.82745100 2.18651700 -0.44574300
N -1.82576800 -0.71341300 -0.48402300
N 0.79868000 -1.90862700 -0.29144000
C -2.62563200 -1.59354800 0.39807400

C 0.98579100 -2.81722800 0.87057100
C 2.12394400 -1.59209200 -0.92205900
C -2.63784700 0.47061700 -0.87605400
C -1.26633300 -1.43515800 -1.66040500
C -0.22211400 -2.46845700 -1.23986500
H 0.60327600 1.95992400 -2.23546700
H 0.41556700 3.52791800 -1.40284900
H 1.83155000 2.77532600 0.49240100
H 2.71154200 2.51065200 -1.03946100
H -1.89401800 2.24874700 1.14953600
H -0.19956400 2.81249000 1.34360900
H -1.33013200 3.72149500 0.27186700
H -2.38296300 2.50444900 -1.58504400
H -1.35432100 1.31392500 -2.42728800
H -3.17418000 0.81055700 0.03193400
H -3.41050700 0.18202800 -1.62411200
H -3.53712800 -1.94701600 -0.13425300
H -2.03990000 -2.47373900 0.71748700
H -2.93156400 -1.02834700 1.29869700
H -2.08111600 -1.94046600 -2.22825800
H -0.80953800 -0.68603900 -2.33641600
H 0.27806100 -2.86648000 -2.14651200
H -0.71323200 -3.32577100 -0.74053100
H 0.01960700 -2.98719900 1.38067900
H 1.39003000 -3.79746600 0.53144400
H 1.70141000 -2.37246100 1.58788400
H 2.25277900 -2.17711800 -1.85622800
H 2.91673000 -1.92180800 -0.22395400
H 1.62381100 0.17965600 -2.07589900
H 3.33632400 0.08706000 -1.56482800
H 2.60063400 1.22244600 1.89819900
H 2.96571800 -0.45833200 1.38013700
H 3.93657400 0.91064500 0.72155800
O -0.22296500 -0.33298600 2.23661300
O -1.16441300 0.42579800 2.95286100
H -0.76039200 0.44855200 3.85777100

^{OS}IM6
BP86/BS1 SCF energy in solution: -2518.297243 a.u.
BP86/BS2 SCF energy in solution: -2519.849676 a.u.
BP86/BS2 Free energy in solution: -2519.292452 a.u.

2 1
Co 1.28810400 -0.00240500 0.01531800

N 1.14410700 0.65085100 1.91579700
N 1.48237800 -1.87264100 0.72057300
C -0.24488200 0.87761900 2.38528400
C 0.58234600 -2.94047400 0.22390900
C 2.90076300 -2.08284300 0.28575700
C 1.93695500 1.92365800 1.92383200
C 1.81930800 -0.42740800 2.70954900
C 1.35756100 -1.78771000 2.21462300
N 1.72822100 1.86900000 -0.54879300
N 2.30686200 -0.64172800 -1.67966100
C 0.97215700 2.51693000 -1.64989300
C 1.44596900 -0.95071100 -2.85215800
C 3.03072500 -1.88826100 -1.22327100
C 1.61872400 2.72872200 0.67610600
C 3.15541900 1.61372700 -0.94146300
C 3.22593100 0.51584300 -2.00475500
H 2.91274700 -0.31191600 2.57425200
H 1.60528600 -0.30936000 3.79405800
H 0.29125500 -1.95498700 2.46133400
H 1.93964000 -2.60308700 2.69725500
H -0.76437600 1.57461200 1.70394900
H -0.80452700 -0.07462600 2.38214200
H -0.23047100 1.29145300 3.41661500
H 1.71743500 2.51572200 2.83901300
H 3.01102700 1.65452900 1.96031400
H 0.58041800 3.11147600 0.70860700
H 2.29244900 3.60946000 0.58977400
H 1.32362900 3.56398200 -1.77772500
H 1.12535800 1.98079100 -2.60275400
H -0.10382600 2.49648700 -1.40058200
H 3.62846400 2.55020800 -1.31404100
H 3.70649700 1.30595500 -0.02990100
H 4.27257300 0.16290300 -2.09951700
H 2.93140900 0.91564600 -2.99365900
H 0.86945200 -0.05332100 -3.14099700
H 2.06678700 -1.27723100 -3.71546700
H 0.73411900 -1.75597900 -2.59424100
H 4.10330100 -1.83744400 -1.49989400
H 2.60055100 -2.75234800 -1.76487000
H 3.52928400 -1.34374300 0.82345800
H 3.25278000 -3.09724700 0.58143300
H -0.46305000 -2.66553800 0.45253600
H 0.68353400 -3.07343000 -0.86696500
H 0.83035100 -3.90281500 0.72260000

O -0.47399100 -0.26742000 -0.52818000
O -1.33044100 0.83633600 -0.56442100
H -2.35714400 0.45031300 -0.32645600
N -3.77307700 0.09317500 -0.26068100
C -3.92554100 -0.90149800 -1.36340400
H -3.58043800 -0.39320800 -2.28823500
H -3.20369500 -1.72111100 -1.17088800
C -4.51616500 1.35243200 -0.55912200
H -4.28826400 1.60646800 -1.61555500
H -5.61359000 1.16623700 -0.50145200
C -4.11164200 -0.44355700 1.08649900
H -3.87902200 0.35759800 1.81625100
H -5.21047400 -0.62399700 1.15620700
C -3.33955200 -1.70523100 1.46560300
H -3.50951100 -1.93200000 2.53810100
H -3.65672400 -2.59577100 0.88554300
H -2.24924200 -1.56413800 1.31292600
C -5.32639900 -1.48289300 -1.57564900
H -6.07399400 -0.70481700 -1.83429200
H -5.29617000 -2.20535800 -2.41774500
H -5.69397700 -2.03228400 -0.68436300
C -4.14900200 2.53490100 0.33808000
H -4.66818000 3.44291000 -0.03242300
H -4.46181200 2.38995700 1.39227200
H -3.05870200 2.74256200 0.32280100

^{3}IM6
BP86/BS1 SCF energy in solution: -2594.685261 a.u.
BP86/BS2 SCF energy in solution: -2596.341357 a.u.
BP86/BS2 Free energy in solution: -2595.763993 a.u.

2 3
Co 1.84937600 -0.01055900 0.00129100
N 2.38954100 1.97054100 -0.10499300
N 2.23723000 0.07779200 1.97446700
C 1.20529000 2.86677500 -0.12267900
C 1.19013400 -0.39353500 2.91369700
C 3.45949500 -0.79274700 2.01365100
C 3.17404700 2.08504000 -1.37148600
C 3.22630500 2.19282800 1.11317400
C 2.57241400 1.50709500 2.30123200
N 2.19886100 -0.11825100 -1.97914500
N 2.39568100 -1.99887500 0.08961900
C 1.18679700 -0.72368200 -2.88113500

C 1.20843900 -2.90352800 0.11074000
C 3.17044700 -2.14969700 1.38083200
C 2.48646400 1.27609500 -2.45740600
C 3.45202300 -0.94459900 -1.92863000
C 3.21072900 -2.24304500 -1.16193400
H 4.23127500 1.77174500 0.91108500
H 3.35707000 3.27948400 1.31254800
H 1.62399000 2.01048000 2.57300600
H 3.23192500 1.54793100 3.19552100
H 0.51235400 2.57103500 -0.93121900
H 0.65704100 2.78849100 0.83294800
H 1.53423200 3.91818700 -0.27150800
H 3.27284400 3.14827800 -1.68282100
H 4.19567400 1.70454600 -1.17444200
H 1.51433400 1.73057600 -2.73170700
H 3.10502400 1.24144200 -3.38140000
H 1.54555400 -0.67006500 -3.93214100
H 1.01167600 -1.78349600 -2.62566300
H 0.23817700 -0.16980900 -2.77202100
H 3.81084200 -1.15797400 -2.96035600
H 4.23317300 -0.34352300 -1.42376700
H 4.18248300 -2.70815000 -0.90226300
H 2.66093900 -2.97123000 -1.78821100
H 0.60222500 -2.75144700 -0.80078800
H 1.53567500 -3.96530700 0.15660100
H 0.58280800 -2.67652200 0.99300400
H 4.12039800 -2.69103600 1.19922700
H 2.56891500 -2.77675700 2.06611200
H 4.26142400 -0.27095300 1.45392600
H 3.80967900 -0.91509700 3.06314500
H 0.26688200 0.18857900 2.74182100
H 0.97159400 -1.46473600 2.76058800
H 1.53295900 -0.24794900 3.96111200
O 0.00742000 0.10333800 0.23093800
O -0.83303100 0.40240000 -0.85049600
H -1.69599700 0.77782800 -0.37485800
N -5.15380000 0.00354400 -0.05332500
C -4.76405800 -1.15032600 -0.90667700
H -4.35844400 -0.72017300 -1.84738700
H -3.91163800 -1.65976800 -0.41092000
C -6.11649600 0.90354800 -0.74119300
H -5.78376700 0.97358200 -1.79873000
H -7.13691300 0.44942600 -0.75700400
C -5.62399200 -0.38098300 1.30158500

H -5.85153400 0.56012000 1.84293600
H -6.58835900 -0.94236900 1.23734300
C -4.60184000 -1.18053700 2.11073700
H -4.95671300 -1.28450500 3.15689000
H -4.44449500 -2.20426100 1.71366000
H -3.61840500 -0.66537300 2.13484100
C -5.85890500 -2.17221600 -1.23648800
H -6.71247900 -1.71566600 -1.77963900
H -5.43795700 -2.96481200 -1.89013500
H -6.25724700 -2.67223400 -0.32939500
C -6.18629600 2.31344800 -0.14904900
H -6.82144300 2.95515400 -0.79465200
H -6.63133700 2.33375700 0.86703800
H -5.17579400 2.76928700 -0.09558200
O -2.91480400 1.40998300 0.21067000
H -3.80230100 0.84487300 0.13050900
H -2.81475100 1.58486400 1.16879900

^{OS}TS3
BP86/BS1 SCF energy in solution: -2518.297251 a.u.
BP86/BS2 SCF energy in solution: -2519.849548 a.u.
BP86/BS2 Free energy in solution: -2519.291246 a.u.

2 1
Co 1.28147000 -0.00073100 0.01164800
N 1.19759000 0.65632500 1.91611300
N 1.48580600 -1.87137000 0.71802700
C -0.17678500 0.89466000 2.42162700
C 0.56570400 -2.93269000 0.24576600
C 2.89204100 -2.09358200 0.24967200
C 1.99606100 1.92548300 1.90290300
C 1.88569300 -0.42476000 2.69432900
C 1.40167400 -1.78292900 2.21430600
N 1.72971400 1.86397900 -0.56294900
N 2.26792200 -0.64974300 -1.70290600
C 0.95586700 2.51455300 -1.65020500
C 1.38194000 -0.95022200 -2.85868500
C 2.98689200 -1.90376700 -1.26210600
C 1.64945900 2.72738900 0.66116800
C 3.14788800 1.59777100 -0.97970500
C 3.19220800 0.49870000 -2.04338900
H 2.97619600 -0.31658500 2.53170800
H 1.70009500 -0.30406200 3.78390500
H 0.34163100 -1.94348500 2.49049600

H 1.99147700 -2.60116500 2.68268000
H -0.71181700 1.58656300 1.74707300
H -0.74187800 -0.05420500 2.44484100
H -0.13215200 1.31838800 3.44816200
H 1.80026700 2.52066800 2.82139700
H 3.06977500 1.65251300 1.91358200
H 0.61193000 3.10957100 0.71733700
H 2.32106300 3.60769900 0.55592400
H 1.30298900 3.56273500 -1.78073500
H 1.09411900 1.98181100 -2.60721800
H -0.11610800 2.49032800 -1.38261300
H 3.62165100 2.53062600 -1.36060900
H 3.71196500 1.28508800 -0.07798100
H 4.23408300 0.13619300 -2.15350500
H 2.88673500 0.90041000 -3.02817200
H 0.81039000 -0.04686800 -3.13865600
H 1.98201200 -1.28509300 -3.73354900
H 0.66583800 -1.74688100 -2.58567200
H 4.05280300 -1.86777600 -1.56570800
H 2.53148600 -2.76311400 -1.79047700
H 3.54030600 -1.35959800 0.77019200
H 3.24191600 -3.11071600 0.53886200
H -0.47089800 -2.65046000 0.50382200
H 0.63514000 -3.06339400 -0.84797200
H 0.82033900 -3.89795400 0.73558300
O -0.50275700 -0.24508000 -0.47719000
O -1.35137600 0.86124300 -0.49218300
H -2.41516700 0.46152200 -0.29779400
N -3.77412800 0.09563600 -0.25500800
C -3.89936800 -0.93603200 -1.32961900
H -3.56337100 -0.44521000 -2.26694300
H -3.15872100 -1.73154900 -1.11080200
C -4.53984400 1.33183700 -0.59991400
H -4.29642800 1.56284600 -1.65790000
H -5.63222300 1.11873600 -0.55719600
C -4.11169000 -0.40522800 1.10838900
H -3.88939600 0.42074400 1.81309100
H -5.20832000 -0.59469900 1.17687400
C -3.32540800 -1.64575700 1.52507800
H -3.49841000 -1.84505600 2.60245000
H -3.62854300 -2.55507300 0.96739400
H -2.23661200 -1.49368400 1.37369300
C -5.28538800 -1.55532000 -1.52624800
H -6.05175700 -0.80268200 -1.80396300

H -5.23671000 -2.29690900 -2.35057400
H -5.63931800 -2.09218200 -0.62194600
C -4.21719500 2.54387600 0.27356200
H -4.74762800 3.42982800 -0.13257000
H -4.55036600 2.41959600 1.32402700
H -3.13180700 2.77530500 0.27543600

^{3}TS3
BP86/BS1 SCF energy in solution: -2594.682453 a.u.
BP86/BS2 SCF energy in solution: -2596.338002 a.u.
BP86/BS2 Free energy in solution: -2595.762321 a.u.

2 3
Co 1.82141100 -0.01999000 0.01660800
N 2.37332900 1.95057400 -0.16702500
N 2.64232800 0.01251400 1.85505700
C 1.23324600 2.86634700 0.08757800
C 1.82487200 -0.47102700 2.99273500
C 3.82412900 -0.87279600 1.58797000
C 2.86418300 2.07526100 -1.57129700
C 3.45955800 2.13432700 0.84200300
C 3.06720000 1.42672700 2.12960500
N 1.71589000 -0.08996300 -1.99176300
N 2.31795700 -2.02978900 -0.04926600
C 0.50238000 -0.64336500 -2.64080200
C 1.15834900 -2.91858500 0.24408500
C 3.37941600 -2.21335900 1.01043200
C 1.93222200 1.30835100 -2.49421500
C 2.92038000 -0.95511100 -2.23241300
C 2.80121200 -2.26678000 -1.46132200
H 4.39179200 1.71104800 0.41814600
H 3.64716700 3.21391600 1.03552700
H 2.20409200 1.93321700 2.60393500
H 3.90220700 1.43978100 2.86432300
H 0.36294100 2.57402700 -0.52883000
H 0.92454600 2.79956100 1.14649500
H 1.53006100 3.91360800 -0.14097400
H 2.92352500 3.14291300 -1.87904700
H 3.89275700 1.66642200 -1.61120200
H 0.93746500 1.79319000 -2.53332800
H 2.32992300 1.28292200 -3.53279700
H 0.57725400 -0.52617100 -3.74404800
H 0.38870600 -1.71764600 -2.41300100
H -0.37900000 -0.10166800 -2.25066000

H 3.04167700 -1.15066000 -3.32207000
H 3.81271200 -0.39248500 -1.89330100
H 3.78220100 -2.78295500 -1.45353100
H 2.08487300 -2.94920600 -1.95799500
H 0.34235900 -2.73026600 -0.47704300
H 1.46102300 -3.98720100 0.17830400
H 0.77881800 -2.71510500 1.26187600
H 4.25694900 -2.74731800 0.59328400
H 2.95935900 -2.85909800 1.80536000
H 4.48393800 -0.34451500 0.87196500
H 4.40786500 -1.02670200 2.52399000
H 0.90645600 0.14105400 3.05788900
H 1.53575100 -1.52773800 2.85424700
H 2.40006500 -0.38137000 3.94021700
O 0.05554500 0.10591700 0.61910600
O -0.95393400 0.55738900 -0.21160400
H -1.88667800 0.71067100 0.51689700
N -4.94066300 0.05036700 0.04207400
C -4.47587500 -1.23604000 -0.56667900
H -3.56733400 -0.98419900 -1.15198800
H -4.13681800 -1.88349100 0.26726700
C -5.19608400 1.09764700 -0.99843600
H -4.33648700 1.05092200 -1.69892500
H -6.10592700 0.82845700 -1.57889500
C -6.09777100 -0.09988800 0.97816300
H -6.28437400 0.90349400 1.40916400
H -7.00512300 -0.37138200 0.39345900
C -5.86727200 -1.09862000 2.10895400
H -6.72416900 -1.04862800 2.81178800
H -5.79593600 -2.14630400 1.75288500
H -4.95028500 -0.86394000 2.68940600
C -5.48454700 -1.98128800 -1.43937200
H -5.80676300 -1.38554000 -2.31789800
H -5.01005600 -2.90738200 -1.82513100
H -6.39030400 -2.28646100 -0.87563900
C -5.32040200 2.51214700 -0.43198600
H -5.32642000 3.23920600 -1.26984100
H -6.25787800 2.66477900 0.14025300
H -4.46260500 2.75359800 0.22890600
O -2.88665200 0.89956300 1.24053700
H -3.90749500 0.46681600 0.70315000
H -2.74365800 0.38499200 2.06111600

[5]TS3

BP86/BS1 SCF energy in solution: -2594.666556 a.u.
BP86/BS2 SCF energy in solution: -2596.320929 a.u.
BP86/BS2 Free energy in solution: -2595.750454 a.u.

2 5
Co -1.65476900 0.00296500 -0.11478600
N -2.50919800 1.88838100 0.52027600
N -2.90984000 0.31891400 -1.83038600
C -1.39119800 2.84473800 0.33658700
C -2.24747700 0.02815500 -3.12142100
C -4.01344100 -0.63800000 -1.53263900
C -2.91356200 1.78816900 1.94759600
C -3.65614900 2.20014200 -0.37663000
C -3.37464800 1.73394400 -1.80098200
N -1.71729800 -0.39465600 2.02886500
N -2.36931800 -2.05293100 -0.24142100
C -0.49236700 -1.03410600 2.55440500
C -1.25547300 -2.90895100 -0.72888800
C -3.48610300 -2.04349900 -1.24574900
C -1.94218900 0.90247500 2.71943000
C -2.90452000 -1.28440400 2.10064100
C -2.78062900 -2.46909500 1.14117300
H -4.55000200 1.69213300 0.03502600
H -3.87253500 3.29200500 -0.37398300
H -2.57601200 2.34760900 -2.26270900
H -4.28647300 1.86305600 -2.42744700
H -0.52917100 2.54923300 0.96246100
H -1.06231300 2.85421100 -0.71977500
H -1.71326900 3.87190000 0.62179600
H -2.95617800 2.79693300 2.41569500
H -3.93933600 1.37243300 1.97834700
H -0.95497800 1.39734000 2.81311600
H -2.32229200 0.73845200 3.75393900
H -0.57787900 -1.20959000 3.65099300
H -0.31141700 -2.00420600 2.05698400
H 0.37433500 -0.37488000 2.35721400
H -3.05256800 -1.66090300 3.13979600
H -3.79846500 -0.68385800 1.83906700
H -3.74920000 -3.00934900 1.10733200
H -2.02712300 -3.18770200 1.51806900
H -0.41130200 -2.87251300 -0.01550400
H -1.59108100 -3.96494900 -0.83713700
H -0.90540900 -2.54792700 -1.71469800
H -4.32536200 -2.67864400 -0.89334500

H -3.10709100 -2.50623600 -2.17750000
H -4.56714900 -0.25894900 -0.65113000
H -4.73222800 -0.67703000 -2.38362400
H -1.40737800 0.73368100 -3.26788400
H -1.84627000 -1.00207600 -3.13257000
H -2.96418400 0.13921300 -3.96685600
O 0.14755400 -0.16312300 -0.47732800
O 1.07462700 0.72737100 0.00606100
H 1.94815600 0.61000700 -0.70479800
N 5.08437800 0.10792000 -0.06710800
C 4.73402400 -1.18057700 0.59811800
H 3.74428700 -1.02273300 1.07686000
H 4.57279000 -1.93135600 -0.20304300
C 5.10779500 1.24304500 0.89967000
H 4.23134400 1.10949600 1.56852100
H 6.01594600 1.17974800 1.54395700
C 6.33458800 0.04750300 -0.87209300
H 6.47796000 1.05286500 -1.31622900
H 7.20834300 -0.12659300 -0.20033600
C 6.31226400 -0.99080500 -1.99298700
H 7.23787400 -0.89403300 -2.59698100
H 6.27428700 -2.03377700 -1.61685400
H 5.45046000 -0.83422800 -2.67545900
C 5.73208500 -1.72373500 1.62438200
H 5.89042800 -1.02253400 2.46949200
H 5.33960600 -2.67107600 2.04947500
H 6.72082000 -1.95089000 1.17437300
C 5.03411500 2.62303600 0.24266600
H 4.94500500 3.39855800 1.03146800
H 5.94006000 2.86582200 -0.34995400
H 4.15166700 2.71250800 -0.42417600
O 2.98812400 0.50316800 -1.52615300
H 3.90952200 0.33757100 -0.94428100
H 2.86634600 -0.30973900 -2.06038700

^{OS}IM7
BP86/BS1 SCF energy in solution: -2518.298448 a.u.
BP86/BS2 SCF energy in solution: -2519.851006 a.u.
BP86/BS2 Free energy in solution: -2519.290381 a.u.

2 1
Co 1.28687900 0.00630900 0.00530400
N 1.27071400 0.66688500 1.91728000
N 1.53661700 -1.86216600 0.71564700

C -0.09145100 0.89521400 2.45998500
C 0.60289400 -2.92252300 0.27213100
C 2.92908000 -2.08735500 0.21055700
C 2.05240800 1.94263800 1.86934200
C 1.99005800 -0.40489100 2.67641300
C 1.50065100 -1.76862700 2.21239400
N 1.72139200 1.86157600 -0.58715800
N 2.26427400 -0.64641800 -1.73012400
C 0.90699100 2.48611000 -1.65884300
C 1.35491700 -0.95143300 -2.86532900
C 2.98964500 -1.89776500 -1.30326500
C 1.65428400 2.72944900 0.63267100
C 3.13358200 1.61009800 -1.02679100
C 3.17599400 0.50388600 -2.08502200
H 3.07472000 -0.28804400 2.48238900
H 1.83760900 -0.28833500 3.77231000
H 0.45026700 -1.93251000 2.52186600
H 2.10733400 -2.58259700 2.66747600
H -0.69105200 1.48551800 1.74131000
H -0.60835500 -0.07153100 2.60207900
H -0.02901300 1.41686800 3.44003200
H 1.88205100 2.54603200 2.78817200
H 3.12906100 1.68194600 1.84498500
H 0.60896100 3.08513800 0.71639700
H 2.30029400 3.62643300 0.50557000
H 1.18344400 3.55711600 -1.77343900
H 1.07609700 1.98016800 -2.62587400
H -0.16065200 2.37778400 -1.38106000
H 3.59118500 2.54571100 -1.42221000
H 3.71625600 1.30895000 -0.13344800
H 4.22037600 0.14956900 -2.20216800
H 2.86118500 0.89892700 -3.07003500
H 0.77803000 -0.04978600 -3.14041600
H 1.93141600 -1.29434700 -3.75371600
H 0.64206300 -1.74364000 -2.57031000
H 4.04896600 -1.86762300 -1.63134600
H 2.52011700 -2.75826900 -1.81791100
H 3.59230200 -1.35615500 0.71508300
H 3.28430100 -3.10611400 0.48949200
H -0.42689400 -2.63046900 0.54900600
H 0.64759100 -3.05607600 -0.82311100
H 0.85895800 -3.88965900 0.75846400
O -0.53485700 -0.20254100 -0.39420200
O -1.36414400 0.89053800 -0.38860500

H -2.74312100 0.40981700 -0.25929500
N -3.83371600 0.08323600 -0.25481100
C -3.91142600 -0.99672600 -1.30636200
H -3.59653500 -0.51186300 -2.25233700
H -3.13359400 -1.74208700 -1.05176800
C -4.63945600 1.29523700 -0.64865900
H -4.36947700 1.50509300 -1.70312700
H -5.71315800 1.01806500 -0.62482800
C -4.15209000 -0.38639400 1.13910000
H -3.95809400 0.47813900 1.80264800
H -5.23912500 -0.60622600 1.19073600
C -3.31472100 -1.57872900 1.58788400
H -3.48739200 -1.74934200 2.66986900
H -3.58139000 -2.51448500 1.05693500
H -2.23268900 -1.38443600 1.43803100
C -5.27032400 -1.66961900 -1.46502200
H -6.06708100 -0.95815100 -1.76200600
H -5.19287100 -2.43143600 -2.26773900
H -5.59315200 -2.19464900 -0.54300900
C -4.38018300 2.52667600 0.21313700
H -4.91478700 3.38746200 -0.23814700
H -4.75599700 2.41644700 1.25005700
H -3.30193900 2.78506000 0.25187700

^{3}IM7
BP86/BS1 SCF energy in solution: -2594.685911 a.u.
BP86/BS2 SCF energy in solution: -2596.343646 a.u.
BP86/BS2 Free energy in solution: -2595.764082 a.u.

2 3
Co 1.88294400 -0.02165400 0.02035800
N 2.32592500 1.90756100 -0.57261300
N 2.81473300 0.39414800 1.75386400
C 1.17449300 2.82577900 -0.39750200
C 2.08646800 0.11795700 3.01336000
C 4.01301300 -0.49133300 1.58558200
C 2.69571100 1.76884200 -2.00974900
C 3.47434200 2.30110700 0.29283700
C 3.20218300 1.84340600 1.71951300
N 1.65415800 -0.49021100 -1.91092800
N 2.48710600 -2.00366500 0.29936200
C 0.42704700 -1.21219900 -2.32418600
C 1.39076800 -2.87137000 0.80857300
C 3.59442000 -1.93469200 1.31929300

C 1.73999400 0.79354500 -2.68098600
C 2.88614600 -1.32817200 -2.08695900
C 2.91889000 -2.46931500 -1.06898900
H 4.38610800 1.81947500 -0.11275200
H 3.64521800 3.40117700 0.26736900
H 2.35620900 2.41183000 2.15274100
H 4.08619500 2.02287800 2.37077600
H 0.25972500 2.38113600 -0.83339900
H 0.97735700 2.98240900 0.67883500
H 1.39259500 3.80916900 -0.87101600
H 2.66919400 2.75253200 -2.53058700
H 3.73972800 1.40091300 -2.05971500
H 0.71606400 1.21503100 -2.71229400
H 2.04794400 0.59252000 -3.73143400
H 0.37513200 -1.28202100 -3.43298700
H 0.42010300 -2.23732800 -1.91212100
H -0.44287600 -0.65716600 -1.91884700
H 2.93657800 -1.72911900 -3.12512000
H 3.76584900 -0.67082200 -1.94141100
H 3.94285500 -2.89323300 -1.02901300
H 2.24650200 -3.29204900 -1.38169300
H 0.54419200 -2.86678700 0.09750500
H 1.74470100 -3.91874700 0.94036200
H 1.02982300 -2.48960900 1.78160100
H 4.47465200 -2.52085700 0.98350400
H 3.23177600 -2.41116900 2.25075900
H 4.59617300 -0.10412700 0.72650400
H 4.66817400 -0.43454500 2.48528200
H 1.14073900 0.69106100 3.01038500
H 1.84550600 -0.95629000 3.10072200
H 2.70032200 0.41657100 3.89176300
O 0.14038800 0.15602600 0.68453900
O -0.91270400 0.43236700 -0.13261300
H -2.08949600 0.70028800 0.77766600
N -5.08725400 0.04625000 0.04710900
C -4.72488400 -1.34171100 -0.42983300
H -3.77872600 -1.22045000 -0.99413900
H -4.48471200 -1.93080100 0.47687000
C -5.17479700 1.03214300 -1.09554800
H -4.29673000 0.82145600 -1.73792600
H -6.08731300 0.79704900 -1.67907800
C -6.30417800 0.09877600 0.93662700
H -6.40509700 1.15441300 1.25311100
H -7.18696200 -0.14560000 0.31129400

C -6.21787900 -0.80486600 2.16062300
H -7.09761000 -0.60326000 2.80508900
H -6.23541000 -1.88275700 1.90367000
H -5.30996500 -0.59826800 2.76414600
C -5.78165400 -2.04249400 -1.27308300
H -6.01529300 -1.49215100 -2.20689000
H -5.38951700 -3.03790000 -1.56597400
H -6.72599200 -2.21093400 -0.71685500
C -5.15920200 2.48904600 -0.64309300
H -5.03838100 3.13425000 -1.53686300
H -6.09846300 2.79575100 -0.14110000
H -4.30892600 2.68709400 0.04115600
O -2.92981500 0.88770500 1.37686000
H -4.22233700 0.36397800 0.64469500
H -2.75600200 0.38557500 2.19899300

^{5}IM7
BP86/BS1 SCF energy in solution: -2594.676973 a.u.
BP86/BS2 SCF energy in solution: -2596.333084 a.u.
BP86/BS2 Free energy in solution: -2595.757829 a.u.

2 5
Co -1.66767400 -0.01044400 -0.12201600
N -2.50599300 1.93398500 0.39243100
N -2.92236900 0.22648400 -1.85849000
C -1.37795000 2.86955300 0.16966000
C -2.28193200 -0.15486600 -3.13575300
C -4.04242400 -0.68556800 -1.49474500
C -2.92302400 1.90254600 1.81783700
C -3.64055100 2.21229800 -0.52805400
C -3.36310700 1.64679500 -1.91793600
N -1.74636300 -0.28715000 2.04898000
N -2.41970700 -2.06203300 -0.13851300
C -0.52557700 -0.89619500 2.61279300
C -1.32534000 -2.96247500 -0.58290100
C -3.54479200 -2.08559900 -1.12984400
C -1.96666300 1.05295400 2.65047100
C -2.93635100 -1.16681300 2.17051600
C -2.82485300 -2.39743900 1.26693700
H -4.54966800 1.75420100 -0.09113800
H -3.83723000 3.30610300 -0.60338700
H -2.55228800 2.21720900 -2.41390800
H -4.27052400 1.75486900 -2.55632800

H -0.47957300 2.52764000 0.71971100
H -1.11609300 2.89691600 -0.90535400
H -1.64937300 3.89882600 0.49882900
H -2.97164800 2.93140700 2.24213300
H -3.94996500 1.48882800 1.85879200
H -0.97567900 1.54465500 2.72090500
H -2.35634400 0.96449700 3.69157900
H -0.58794200 -0.96929800 3.72332700
H -0.37267800 -1.91178300 2.20307100
H 0.34822000 -0.27600700 2.33106800
H -3.08118500 -1.49823300 3.22653300
H -3.82958000 -0.57391100 1.89046400
H -3.79473500 -2.93806300 1.27214600
H -2.07160100 -3.09760400 1.67857400
H -0.46846500 -2.87890200 0.11147600
H -1.66414400 -4.02323200 -0.61275900
H -0.98741500 -2.67254500 -1.59609200
H -4.39729000 -2.68005600 -0.73811100
H -3.18645100 -2.60882800 -2.03827700
H -4.57511600 -0.24251700 -0.63037900
H -4.77506500 -0.75884000 -2.33278700
H -1.43892000 0.53307600 -3.33986300
H -1.88466700 -1.18557100 -3.08486200
H -3.00619800 -0.09586300 -3.98106400
O 0.15770200 -0.14293700 -0.43705600
O 1.06210000 0.67165000 0.12901900
H 2.26391600 0.90842400 -0.89956900
N 5.13435800 0.06257700 -0.06468700
C 4.58372000 -1.27235500 0.38721100
H 3.60538600 -1.04008900 0.85274800
H 4.37292100 -1.84865000 -0.53465600
C 5.23926800 1.04972400 1.07747600
H 4.30110900 0.93761300 1.65645400
H 6.08072200 0.72963900 1.72377200
C 6.41658200 -0.02725700 -0.85674700
H 6.64457800 1.00563000 -1.18223200
H 7.21716500 -0.34049300 -0.15618100
C 6.33624500 -0.94991400 -2.06652500
H 7.27634000 -0.84542500 -2.64548600
H 6.23624500 -2.01829000 -1.78924300
H 5.49790200 -0.67704000 -2.74044100
C 5.47623900 -2.06148100 1.33448500
H 5.68483500 -1.51474300 2.27611200
H 4.95085500 -2.99961600 1.60654000

H 6.44173100 -2.34631300 0.86922300
C 5.40569100 2.49330100 0.61513600
H 5.30205900 3.15925900 1.49570400
H 6.40018600 2.69142200 0.16796500
H 4.62203300 2.77262200 -0.11872400
O 3.07625400 1.06663600 -1.50351000
H 4.35980800 0.45408600 -0.71872600
H 2.87202700 0.56388600 -2.31891000

^{OS}IM8
BP86/BS1 SCF energy in solution: -2225.614238 a.u.
BP86/BS2 SCF energy in solution: -2226.828328 a.u.
BP86/BS2 Free energy in solution: -2226.467948 a.u.

1 1
Co -0.00890400 0.02084300 0.20257800
N -1.59470700 1.14126700 -0.47802900
N 1.14973300 1.66502800 -0.00747600
C -2.45020500 1.62741600 0.62913600
C 1.96375800 2.08660000 1.15281100
C 1.99021900 1.20733900 -1.15771000
C -2.33490900 0.20068600 -1.36338800
C -0.95162100 2.26571200 -1.21422300
C 0.23942800 2.78373200 -0.41144100
N -1.02375500 -1.63572700 -0.30921200
N 1.75520900 -1.10935100 -0.20867100
C -1.15344100 -2.71434100 0.69590000
C 2.37438600 -1.67038600 1.01777400
C 2.68481300 -0.12243400 -0.85234300
C -2.38988600 -1.17424400 -0.70954800
C -0.19915100 -2.04500300 -1.49104100
C 1.27601300 -2.21475400 -1.10694500
H -0.62733600 1.88452800 -2.20352000
H -1.67131000 3.09477800 -1.40416900
H -0.10707500 3.27120600 0.52167900
H 0.79732900 3.55381100 -0.99102900
H -2.63749500 0.80917700 1.35282000
H -1.92736900 2.42975500 1.18158100
H -3.40877000 2.03257800 0.23317800
H -3.36693500 0.56569100 -1.57082800
H -1.80525600 0.15416800 -2.33601600
H -2.99588400 -1.13389600 0.21731200
H -2.87111100 -1.91528000 -1.38760100
H -1.89174200 -3.47714100 0.36293300

H -0.18184600 -3.21739800 0.85040900
H -1.46747200 -2.23618100 1.65006600
H -0.59305700 -2.98766800 -1.93700800
H -0.29619100 -1.25071700 -2.25802100
H 1.88680700 -2.26284900 -2.03278100
H 1.42672000 -3.17768100 -0.57937400
H 1.65948700 -2.34007200 1.53100500
H 3.29723000 -2.24861500 0.78011200
H 2.63523300 -0.85298200 1.71543500
H 3.11234700 -0.53358900 -1.79129700
H 3.53809000 0.04365900 -0.16563200
H 1.32118100 1.09539400 -2.03436700
H 2.74741400 1.98274800 -1.42056600
H 1.29645900 2.20530900 2.02775000
H 2.72285400 1.32061300 1.39510200
H 2.48726300 3.04667700 0.94589100
O -1.22509600 -0.40825000 2.66825700
O -0.16752100 0.12959400 2.05263700

^{3}IM8
BP86/BS1 SCF energy in solution: -2225.619388 a.u.
BP86/BS2 SCF energy in solution: -2226.833383 a.u.
BP86/BS2 Free energy in solution: -2226.473537 a.u.

1 3
Co 0.01248000 0.00643200 0.22700000
N -1.26769300 1.51041200 -0.50571900
N 1.53400600 1.32670400 -0.00081500
C -1.98250900 2.18638900 0.59995300
C 2.43496900 1.54107900 1.15134300
C 2.22847300 0.67960700 -1.15885600
C -2.20427800 0.77115500 -1.38646500
C -0.35254000 2.43466700 -1.22184900
C 0.91986400 2.63379300 -0.39967000
N -1.39880300 -1.33447800 -0.30405400
N 1.42343900 -1.50734700 -0.22475700
C -1.81333700 -2.35046700 0.68886100
C 1.87002500 -2.18569900 1.01805000
C 2.57037900 -0.78532300 -0.87136300
C -2.59982800 -0.54255500 -0.71864500
C -0.70332500 -1.93600700 -1.48614400
C 0.68550600 -2.46627400 -1.11291400
H -0.12087900 1.98855100 -2.20969300
H -0.83037500 3.42316300 -1.41623100

H 0.68695400 3.17745900 0.53753400
H 1.65488800 3.25352400 -0.96176800
H -2.39481200 1.43824200 1.30533200
H -1.27640400 2.81237900 1.17667100
H -2.79673000 2.83539000 0.20300800
H -3.12028000 1.36780300 -1.60597000
H -1.69665100 0.58968200 -2.35521600
H -3.18071200 -0.34161400 0.20373100
H -3.24902200 -1.14703100 -1.39222600
H -2.71597400 -2.90033400 0.34080600
H -1.00357700 -3.08464900 0.85434900
H -2.01312200 -1.81727600 1.64315500
H -1.32181700 -2.74974500 -1.93120200
H -0.60092900 -1.14310500 -2.25336100
H 1.25904300 -2.66068200 -2.04312600
H 0.60314800 -3.43715300 -0.58483200
H 1.00101000 -2.63081900 1.53759900
H 2.60761400 -2.99162100 0.79739400
H 2.33499000 -1.45071500 1.70056300
H 2.86352500 -1.28138700 -1.82031700
H 3.44677100 -0.85114800 -0.19667500
H 1.54401200 0.73786300 -2.02924300
H 3.15088800 1.24601800 -1.42623100
H 1.82578400 1.82652200 2.03003400
H 2.98710400 0.61548000 1.39678100
H 3.17509400 2.34349700 0.93382000
O -1.26683800 -0.13569000 2.71178400
O -0.17235300 0.23679000 2.04695200

^{OS}TS4
BP86/BS1 SCF energy in solution: -2225.607643 a.u.
BP86/BS2 SCF energy in solution: -2226.821542 a.u.
BP86/BS2 Free energy in solution: -2226.461859 a.u.

1 1
Co -0.00354800 0.03872100 0.40015200
N -1.33906500 -1.55767000 -0.37135700
N -1.52973900 1.32021500 -0.14420500
C -1.96386400 -2.33391000 0.71567200
C -1.89513000 2.33399200 0.86869000
C -0.96205900 1.93700000 -1.37849300
C -0.46247600 -2.41438100 -1.20489600
C -2.35152600 -0.81530900 -1.15556200
C -2.72692800 0.48403300 -0.44979100

N 1.55112500 -1.29586600 -0.22568700
N 1.30277200 1.55268300 -0.35972200
C 2.64434700 -1.51738100 0.74056200
C 1.91017900 2.24414700 0.80789900
C 0.43741700 2.50303000 -1.13387800
C 0.90214700 -2.59635500 -0.54692600
C 2.02526900 -0.59382500 -1.45310200
C 2.36868100 0.86913700 -1.16626700
H -1.92591300 -0.60494200 -2.15675500
H -3.27294800 -1.42151200 -1.32144100
H -3.22458800 0.26564000 0.51667600
H -3.45512200 1.05938900 -1.06689300
H -1.18800700 -2.80930900 1.34493900
H -2.55894300 -1.66907000 1.36877800
H -2.63010200 -3.12728400 0.30229700
H -0.92070900 -3.41573900 -1.38225600
H -0.35527800 -1.93723600 -2.19949600
H 0.79371600 -3.14784400 0.40887700
H 1.55956300 -3.21390000 -1.20337800
H 3.36520000 -2.27997900 0.36381500
H 3.19411600 -0.57615700 0.92290400
H 2.20939300 -1.84791900 1.70305500
H 2.91372600 -1.11181700 -1.88744500
H 1.21702400 -0.64368900 -2.20886100
H 2.53591200 1.40153500 -2.12628400
H 3.31916600 0.93364200 -0.60019200
H 2.49018500 1.52076800 1.40977800
H 2.58349700 3.06971100 0.48031700
H 1.11520400 2.66506500 1.45192700
H 0.90411100 2.75072300 -2.11028300
H 0.37446300 3.45230700 -0.56569000
H -0.91690300 1.15197400 -2.15817100
H -1.63620500 2.74044600 -1.75877900
H -2.15016900 1.81941800 1.81473500
H -1.04989600 3.01929500 1.06388400
H -2.76671700 2.93944800 0.53081900
O 0.60233300 -0.18282500 2.68365800
O -0.58733100 -0.16280400 2.07913900

^{3}TS4
BP86/BS1 SCF energy in solution: -2225.615056 a.u.
BP86/BS2 SCF energy in solution: -2226.828753 a.u.
BP86/BS2 Free energy in solution: -2226.470763 a.u.

1 3
Co 0.04907400 -0.02811300 0.42655200
N 0.27279400 2.02430800 -0.40253600
N 2.01594400 -0.28156400 -0.14573600
C 0.33618900 3.02234300 0.68300000
C 2.88480400 -0.94182300 0.85243600
C 1.85828200 -1.10708300 -1.38060800
C -0.91707600 2.23960500 -1.25893000
C 1.54303700 1.96472200 -1.16145500
C 2.55833400 1.07573300 -0.44651700
N -2.02821300 0.23434800 -0.24652100
N -0.24205900 -2.02639000 -0.35351400
C -3.08511500 -0.14781000 0.70736400
C -0.36044500 -2.89361200 0.84664300
C 0.99844100 -2.34947000 -1.12764200
C -2.17661900 1.66777900 -0.60959900
C -2.02483900 -0.63740700 -1.45340600
C -1.51263700 -2.04685100 -1.14352100
H 1.32279000 1.57178800 -2.17424100
H 1.98644800 2.97789900 -1.30482000
H 2.84440500 1.52776800 0.52476700
H 3.48884200 0.99487300 -1.05445400
H -0.56562000 2.95563400 1.32073400
H 1.21376200 2.83091400 1.32759600
H 0.40864000 4.05519800 0.26752800
H -1.07591200 3.32351700 -1.47010400
H -0.72621400 1.75221300 -2.23578000
H -2.40774600 2.21813000 0.32518600
H -3.04665300 1.81754500 -1.29249200
H -4.09998300 0.05658300 0.29113100
H -3.01825100 -1.22483800 0.94977000
H -2.94377300 0.42108200 1.64620000
H -3.04616100 -0.69952000 -1.90048000
H -1.36744000 -0.16936900 -2.21274300
H -1.37396800 -2.60046400 -2.09648400
H -2.27082300 -2.60775300 -0.56113100
H -1.21474000 -2.55888800 1.46497200
H -0.50856900 -3.96237100 0.56657300
H 0.55578300 -2.81178300 1.46249300
H 0.74374300 -2.81465200 -2.10321600
H 1.57582800 -3.10609300 -0.55933500
H 1.37628800 -0.47326700 -2.15024800
H 2.85666700 -1.40673100 -1.77705900
H 2.85044200 -0.36814500 1.79797800

H 2.53593000 -1.97125000 1.05470700
H 3.93715400 -0.99118500 0.49161000
O -0.68459100 0.02037300 2.75234100
O 0.42218400 0.39094700 2.10715800

$^{CS}[Co]O_2^+$
BP86/BS1 SCF energy in solution: -2225.64189 a.u.
BP86/BS2 SCF energy in solution: -2226.85683 a.u.
BP86/BS2 Free energy in solution: -2226.492891 a.u.

1 1
Co 0.00001200 -0.00000100 0.42964500
O 0.00543400 -0.71245500 2.17625500
N 0.05443000 1.69714500 -0.70146200
O -0.00497500 0.71245300 2.17627900
N -0.05453700 -1.69716700 -0.70143900
N 2.03855900 -0.04742200 0.17431800
N -2.03859300 0.04741700 0.17444200
C -2.41617400 -1.09274800 -0.74230600
H -2.77007100 -1.92425000 -0.10411500
H -3.27050800 -0.79753100 -1.38806900
C 1.24300600 -1.79189900 -1.42157500
H 1.20282700 -1.13019700 -2.30729600
H 1.42512800 -2.82647600 -1.79142600
C 0.22015800 2.87735100 0.19164600
H 1.10965000 2.75847400 0.83381900
H -0.65503300 2.97658300 0.85699800
H 0.32415500 3.80227300 -0.41886400
C -1.24318500 1.79191700 -1.42151900
H -1.20303100 1.13028800 -2.30729600
H -1.42531000 2.82652700 -1.79126300
C -1.23525300 -1.55554700 -1.58933300
H -1.48465900 -2.51880600 -2.09238000
H -0.98061500 -0.82523200 -2.38041000
C 1.23508100 1.55554900 -1.58941700
H 1.48449300 2.51881300 -2.09244200
H 0.98042900 0.82523900 -2.38050100
C 2.34412900 -1.37479900 -0.45819200
H 2.43572100 -2.11404800 0.36115100
H 3.32918300 -1.33643400 -0.97263900
C -0.22020700 -2.87738600 0.19163700
H -0.32427000 -3.80227800 -0.41889500
H -1.10963600 -2.75851900 0.83389400
H 0.65504400 -2.97664500 0.85690700

C -2.34423000 1.37479700 -0.45804600
H -2.43575000 2.11406100 0.36129700
H -3.32935000 1.33641100 -0.97237100
C 2.41605800 1.09275900 -0.74248100
H 3.27032900 0.79754400 -1.38832400
H 2.76998200 1.92425200 -0.10429600
C -2.79224400 -0.06085900 1.44815100
H -2.43240800 0.73460700 2.12665800
H -2.57005400 -1.03566100 1.91766600
H -3.88574700 0.03837300 1.26916500
C 2.79244800 0.06088500 1.44789700
H 2.43278900 -0.73461500 2.12645100
H 2.57026400 1.03565600 1.91746400
H 3.88591100 -0.03829800 1.26866000

$^{3}[Co]O_{2}^{+}$
BP86/BS1 SCF energy in solution: -2225.633266 a.u.
BP86/BS2 SCF energy in solution: -2226.84707 a.u.
BP86/BS2 Free energy in solution: -2226.489037 a.u.

1 3
Co -0.00164700 -0.02288500 0.55157700
O 0.00462300 -0.74775900 2.21757400
N 0.03740800 1.68712700 -0.66906400
O -0.00354800 0.60920200 2.37669200
N -0.03683800 -1.67681500 -0.69506100
N 2.22308100 -0.01436100 0.11740800
N -2.22402600 0.04561300 0.11744200
C -2.46403200 -1.10924200 -0.79263700
H -2.80938200 -1.95734700 -0.16933600
H -3.28944600 -0.88735900 -1.50803200
C 1.24583300 -1.72062000 -1.45138900
H 1.15771200 -1.03940600 -2.31796300
H 1.42316200 -2.74136400 -1.86081400
C 0.16625500 2.85933500 0.23709100
H 1.06452300 2.76328900 0.87262000
H -0.71372800 2.92347400 0.90198500
H 0.24067800 3.79874000 -0.35678300
C -1.24245200 1.77116300 -1.42430000
H -1.16345800 1.11640600 -2.31219400
H -1.40646500 2.80633300 -1.80266400
C -1.22029600 -1.53388900 -1.58361800
H -1.43529400 -2.49347200 -2.10929700
H -0.96363500 -0.79211600 -2.36249400

C 1.22185300 1.58948400 -1.56042400
H 1.42789800 2.56955000 -2.05134200
H 0.97535200 0.87285400 -2.36625000
C 2.42147200 -1.32291200 -0.55749200
H 2.55873000 -2.08470900 0.23628300
H 3.35698700 -1.32139000 -1.16567400
C -0.16657000 -2.89203600 0.15092900
H -0.24513400 -3.80023800 -0.48857900
H -1.06291000 -2.82369800 0.79324800
H 0.71579200 -2.99060000 0.80926900
C -2.42184800 1.36209300 -0.54073000
H -2.56336000 2.11143300 0.26375400
H -3.35582400 1.36768900 -1.15124600
C 2.46627100 1.15145700 -0.77759800
H 3.29145500 0.93648900 -1.49522800
H 2.81449500 1.98940100 -0.14230700
C -3.06316700 -0.04889600 1.32710700
H -2.78070500 0.75780500 2.03100600
H -2.88564700 -1.01984300 1.82809100
H -4.15040600 0.03920400 1.09223100
C 3.06101400 0.07063500 1.32845400
H 2.82531500 -0.77955400 1.99725400
H 2.83543900 1.00832600 1.87204300
H 4.15035300 0.04605800 1.08827700

^{5}[Co]O_2^+
BP86/BS1 SCF energy in solution: -2225.618833 a.u.
BP86/BS2 SCF energy in solution: -2226.831612 a.u.
BP86/BS2 Free energy in solution: -2226.476296 a.u.

1 5
Co -0.00003100 0.04003800 0.48157900
O 0.00318600 0.25888900 2.34306900
N 0.00209400 1.57851500 -1.00689300
O 0.00788900 1.56166500 2.61054000
N -0.00369300 -1.91051800 -0.35728300
N 2.18538500 -0.04220800 0.07519800
N -2.18595500 -0.03606100 0.07740400
C -2.44629700 -1.40262600 -0.46042600
H -2.72957600 -2.04122900 0.39965100
H -3.31790700 -1.39926200 -1.15481200
C 1.23259200 -2.02356500 -1.17631500
H 1.04213200 -1.51217200 -2.13960000
H 1.45472900 -3.08958600 -1.41686100

C 0.00492300 2.91969700 -0.38205400
H 0.89649400 3.03713700 0.26042800
H -0.88709300 3.04143900 0.25904400
H 0.00730300 3.71542100 -1.16254000
C -1.23480700 1.35397100 -1.80347500
H -1.04334200 0.50723400 -2.48964200
H -1.46250600 2.24095200 -2.43950400
C -1.24011100 -2.01957500 -1.17636000
H -1.46563300 -3.08493900 -1.41674200
H -1.04750800 -1.50916300 -2.13964300
C 1.23672300 1.34992800 -1.80569400
H 1.46640900 2.23650700 -2.44157200
H 1.04104900 0.50432200 -2.49206700
C 2.44069600 -1.41058800 -0.46038000
H 2.72063600 -2.04897600 0.40097000
H 3.31291000 -1.41175000 -1.15401500
C -0.00566100 -2.87719200 0.76437600
H -0.00680500 -3.92495200 0.38463800
H -0.90039500 -2.72838500 1.39794100
H 0.88865300 -2.73056400 1.39898200
C -2.43413700 1.06119200 -0.90053900
H -2.68198600 1.96989800 -0.31633200
H -3.32400200 0.83587100 -1.53276100
C 2.43652000 1.05274000 -0.90465300
H 3.32414500 0.82264000 -1.53828600
H 2.68954000 1.96101600 -0.32202700
C -2.98549000 0.19520300 1.30101700
H -2.68140100 1.15368700 1.76442400
H -2.79522800 -0.61605800 2.02940000
H -4.07892200 0.22731700 1.08237100
C 2.98626400 0.18847100 1.29802300
H 2.79512100 -0.62210200 2.02693600
H 2.68373200 1.14752300 1.76135000
H 4.07959500 0.21866100 1.07866600

^{OS}TS5a
BP86/BS1 SCF energy in solution: -2378.818918 a.u.
BP86/BS2 SCF energy in solution: -2380.236674 a.u.
BP86/BS2 Free energy in solution: -2379.827924 a.u.

2 1
Co 0.54063800 0.01924800 -0.01145100
N -0.49327700 1.48349700 -0.92329100
N 1.96219700 1.35415200 0.45351500

C -1.55520200 2.14544800 -0.12998100
C 2.33096700 1.54513100 1.87783400
C 3.07405700 0.73734100 -0.34264300
C -1.05040300 0.80168000 -2.13973900
C 0.59248700 2.45092000 -1.29805700
C 1.51040200 2.67199800 -0.10933400
N -0.60241000 -1.33113900 -0.94550900
N 1.94287500 -1.44049300 0.25152500
C -1.32153300 -2.37838600 -0.17584700
C 1.94521600 -2.15394200 1.55985400
C 3.26968500 -0.72190200 0.07154800
C -1.60502700 -0.55880300 -1.75510500
C 0.51068500 -1.90116600 -1.77365800
C 1.62697200 -2.42033800 -0.86533400
H 1.14729100 2.02091200 -2.15533600
H 0.15344000 3.41327400 -1.64012400
H 0.97533600 3.20330800 0.70106200
H 2.38809200 3.29299600 -0.39151100
H -2.36170400 1.43121800 0.12422700
H -1.13288700 2.54426300 0.80983900
H -1.99423600 2.97897900 -0.71990800
H -1.83984800 1.42616000 -2.61127500
H -0.22859400 0.70244400 -2.87498900
H -2.51245600 -0.44981900 -1.12936500
H -1.89349500 -1.13835700 -2.65938600
H -1.93761900 -2.98956600 -0.87048400
H -0.61719000 -3.05301700 0.34022900
H -1.97349000 -1.90225300 0.57924300
H 0.13542700 -2.71685700 -2.43242700
H 0.88983100 -1.09141700 -2.43176400
H 2.53566400 -2.61606100 -1.46803200
H 1.33532600 -3.38083000 -0.39992400
H 0.95907600 -2.61757500 1.74713800
H 2.72058000 -2.95018700 1.56283500
H 2.17412800 -1.44495100 2.37843800
H 3.88628000 -1.24502800 -0.68593400
H 3.81733700 -0.78247800 1.03090700
H 2.79675800 0.80586100 -1.41434500
H 4.01815500 1.31041800 -0.20406700
H 1.43838000 1.87640500 2.43891000
H 2.70889900 0.61042300 2.32830900
H 3.12566000 2.31830400 1.95706900
O -0.36504200 0.11713500 1.72564600
O -4.41668500 0.62788600 0.91622500

H -1.46019800 -0.16585400 1.92157000
O -4.76630700 -0.35911300 -0.03148900
H -5.50883400 0.07801700 -0.51390500
O -2.67395500 -0.51615500 2.19524000
H -2.85240400 -0.38642600 3.14937200
H -3.49792800 0.02505600 1.61191600
H 0.14836700 -0.35510700 2.41501700

^{3}TS5a
BP86/BS1 SCF energy in solution: -2378.82212 a.u.
BP86/BS2 SCF energy in solution: -2380.240114 a.u.
BP86/BS2 Free energy in solution: -2379.832401 a.u.

2 3
Co 0.48698300 0.01435300 0.06528400
N -0.37476400 1.53881100 -0.97432900
N 1.94534800 1.31440700 0.57952800
C -1.46506200 2.17577000 -0.19491000
C 2.28417100 1.46172500 2.01712200
C 3.07675800 0.70344200 -0.20021100
C -0.89876200 0.90597700 -2.22706100
C 0.74328800 2.49871300 -1.24211700
C 1.56944400 2.66100000 0.02213300
N -0.58920200 -1.26686000 -1.05951600
N 1.91342000 -1.47873700 0.21281100
C -1.36152300 -2.35806700 -0.41358400
C 1.81376100 -2.26523400 1.47492200
C 3.24760000 -0.76373800 0.17070900
C -1.52896200 -0.43299300 -1.88442500
C 0.54973200 -1.80640800 -1.87569000
C 1.64564400 -2.37736200 -0.97724100
H 1.35117500 2.08806300 -2.07193600
H 0.34305500 3.48049900 -1.57705600
H 0.98722900 3.18531400 0.80455300
H 2.48369700 3.26330700 -0.16981900
H -2.24791700 1.44179900 0.08009900
H -1.06274300 2.61732600 0.73497800
H -1.93093700 2.98037800 -0.80468100
H -1.63929600 1.57221900 -2.72006100
H -0.04814600 0.78389200 -2.92550900
H -2.44822600 -0.29151700 -1.28285600
H -1.81560600 -0.98508300 -2.80632600
H -1.90239600 -2.93866000 -1.19242200
H -0.69082100 -3.04694800 0.12800900

H -2.08627600 -1.93538200 0.30685000
H 0.17933800 -2.58458000 -2.58039900
H 0.95344500 -0.97356900 -2.48528000
H 2.57213100 -2.51229500 -1.56963300
H 1.35962500 -3.37472300 -0.59138900
H 0.82479900 -2.75275200 1.54378100
H 2.60541200 -3.04570000 1.49462800
H 1.94114100 -1.59576900 2.34497600
H 3.92648900 -1.25829600 -0.55250600
H 3.71342800 -0.86007600 1.16987100
H 2.83317900 0.80365300 -1.27657400
H 4.01685300 1.26905600 -0.01333400
H 1.43291100 1.92609500 2.55060500
H 2.51439300 0.48533800 2.47909200
H 3.16789900 2.12706600 2.12887900
O -0.49145000 -0.09442800 1.77448400
O -4.27755500 0.70531600 0.98849500
H -1.58824500 -0.44189800 1.97295300
O -4.83837400 -0.14668100 0.00718700
H -5.36282600 0.49245500 -0.53160800
O -2.77396100 -0.84401200 2.12873400
H -2.99718100 -0.93753000 3.07715000
H -3.52013000 -0.11072200 1.63151400
H -0.28344600 0.60966000 2.42224200

^{5}TS5a
BP86/BS1 SCF energy in solution: -2378.806711 a.u.
BP86/BS2 SCF energy in solution: -2380.222355 a.u.
BP86/BS2 Free energy in solution: -2379.817886 a.u.

2 5
Co -0.35280800 -0.01940400 -0.18995900
N 0.52834300 0.23930600 1.77691500
N -0.83950600 2.08849600 0.03229400
C 1.99724600 0.23653300 1.57923400
C -0.56359400 2.91593500 -1.16060700
C -2.29233100 1.97969200 0.33315600
C 0.07308400 -0.90517200 2.61378900
C 0.04944100 1.54649900 2.30486100
C -0.05158700 2.58647400 1.19321500
N -0.76027400 -1.99746600 0.53360600
N -2.33556200 -0.12674700 -1.06808600
C -0.42783000 -3.06527600 -0.43512600
C -2.22011400 -0.28050500 -2.54322600

C -3.03297400 1.15971900 -0.72812200
C 0.00894700 -2.18994400 1.79491400
C -2.22703800 -1.87444300 0.76957900
C -2.96310800 -1.35468400 -0.47054700
H -0.93890100 1.37916500 2.77583500
H 0.72800400 1.92198800 3.10358400
H 0.95725900 2.84638100 0.81538300
H -0.49742100 3.52342000 1.59955300
H 2.32106400 -0.71263200 1.11262500
H 2.28850800 1.06892300 0.91177700
H 2.52100400 0.35560100 2.55460800
H 0.74680900 -1.05038700 3.48793700
H -0.92753600 -0.64947600 3.01507300
H 1.02865600 -2.51459800 1.50705800
H -0.43348500 -3.00799400 2.40785500
H -0.72692700 -4.06373900 -0.04231000
H -0.94266600 -2.89534500 -1.39840900
H 0.66352800 -3.06368100 -0.61900200
H -2.65842300 -2.85909900 1.06442300
H -2.37736400 -1.18122400 1.62149200
H -4.02089300 -1.15302700 -0.20100500
H -2.97776300 -2.13826000 -1.25277900
H -1.60079600 -1.16579900 -2.78326900
H -3.22356300 -0.40520600 -3.00913600
H -1.74219600 0.61783200 -2.97835300
H -4.06433500 0.95697400 -0.37203700
H -3.12945600 1.74951300 -1.66019100
H -2.39913000 1.50135400 1.32674800
H -2.75622900 2.99119800 0.40525500
H 0.52330900 2.90250800 -1.37104400
H -1.09824200 2.52542800 -2.04644000
H -0.88131200 3.97067600 -0.99480000
O 0.91779700 -0.06175200 -1.59744600
O 4.91278100 0.36160300 -1.36588200
H 2.00943900 -0.65003700 -1.61806700
O 5.25626700 0.25329200 -0.03294200
H 6.03116800 0.86646500 0.04684400
O 3.03703300 -1.22738100 -1.56274100
H 3.15558500 -1.73476400 -2.39453500
H 3.89131700 -0.51154900 -1.48163500
H 0.81390100 0.54312100 -2.36185500

^{5}TS5
BP86/BS1 SCF energy in solution: -2519.578074 a.u.

BP86/BS2 SCF energy in solution: -2521.13927a.u.
BP86/BS2 Free energy in solution: -2520.567862 a.u.

2 5
Co 1.35621900 -0.07821900 -0.02001100
N 2.37027000 -0.21032400 -1.94459000
N 1.45240400 2.05363400 -0.40400900
C 1.38006400 -0.69899800 -2.93454300
C 0.17988000 2.75724500 -0.13609500
C 2.53356500 2.46234700 0.53483100
C 3.50133700 -1.16636400 -1.78692200
C 2.84506800 1.16344800 -2.27168000
C 1.83441400 2.21689700 -1.83323500
N 2.58844100 -1.79583400 0.45035200
N 1.88531500 0.52583500 2.01973600
C 1.87412000 -2.88450000 1.15237600
C 0.69240100 0.32664300 2.88488100
C 2.24254500 1.98245200 1.95740200
C 3.12915700 -2.30250400 -0.84105200
C 3.63054300 -1.15703200 1.29846900
C 3.01239300 -0.36685600 2.45656500
H 3.81333600 1.31676300 -1.75566500
H 3.04074500 1.26453700 -3.36303900
H 0.90421800 2.13396800 -2.42999500
H 2.24888700 3.23465400 -2.01626900
H 1.01199600 -1.69900100 -2.63919900
H 0.51388600 -0.01342900 -2.97913000
H 1.84580300 -0.76583700 -3.94346100
H 3.80342100 -1.58579200 -2.77256900
H 4.37123700 -0.60186300 -1.39769000
H 2.34158500 -2.93879000 -1.29210100
H 4.01709000 -2.95245200 -0.66705500
H 2.57040900 -3.72234000 1.38364000
H 1.43259400 -2.52417000 2.09861000
H 1.05788600 -3.26129400 0.50783000
H 4.33287500 -1.92248400 1.70318000
H 4.22102300 -0.47648200 0.65356900
H 3.80896600 0.23139300 2.94521900
H 2.62077000 -1.06133100 3.22519600
H 0.42250600 -0.74524400 2.91336000
H 0.89627300 0.66975100 3.92424600
H -0.16795400 0.89112500 2.47898600
H 3.12355200 2.19128200 2.59958100
H 1.39653000 2.55584200 2.38271000

H 3.48584900 2.02530200 0.17353300
H 2.65599300 3.57049000 0.53328800
H -0.60827100 2.34537400 -0.79340900
H -0.13301900 2.62041800 0.91487700
H 0.28611300 3.84817800 -0.33421100
O -0.29415900 -0.59323800 -0.16174400
H -1.22577700 -0.35358400 0.41941000
N -4.58935000 -0.33147300 0.01146300
C -5.53563500 0.11275300 1.07975200
H -5.36187600 -0.56139900 1.94512200
H -5.21464700 1.12385100 1.40294300
C -4.76516500 -1.77945200 -0.30944500
H -4.85465300 -2.30414000 0.66488800
H -5.72767900 -1.93174200 -0.84916200
C -4.61967300 0.51778000 -1.21491700
H -3.82326100 0.13495300 -1.88450300
H -5.58516500 0.36668100 -1.75112100
C -4.37881300 2.00317400 -0.95039200
H -4.26217400 2.53098000 -1.91920500
H -5.21836200 2.48709600 -0.41110400
H -3.45118500 2.16497800 -0.36329500
C -7.02240600 0.12602300 0.71753000
H -7.39827200 -0.87779200 0.43134100
H -7.60668200 0.45769000 1.60096400
H -7.24893600 0.82967400 -0.10996100
C -3.61257200 -2.38620600 -1.11027700
H -3.74465100 -3.48657600 -1.16037400
H -3.57081900 -2.01444300 -2.15432300
H -2.63445800 -2.18021100 -0.62873100
O -2.31039100 -0.06479700 1.12354400
H -2.32105800 -0.69582300 1.87335200
H -3.32304400 -0.19653400 0.59546200

^{OS}IM9
BP86/BS1 SCF energy in solution: -2150.477516 a.u.
BP86/BS2 SCF energy in solution: -2151.600379 a.u.
BP86/BS2 Free energy in solution: -2151.242617 a.u.

1 1
Co -0.03077700 0.00192100 0.34945500
N -2.02770100 0.13223600 -0.24981700
N 0.13588600 1.98033200 0.00244300
C -2.92733600 0.19159100 0.92369800
C 0.71194700 2.79755300 1.09242600

C 0.98785700 1.94062200 -1.22877000
C -2.23867800 -1.10944500 -1.03469200
C -2.07267000 1.39187100 -1.03368500
C -1.24482800 2.46483200 -0.32152800
N -0.12904300 -1.98197500 0.00285600
N 2.03951300 -0.13445400 -0.26164700
C 0.33549500 -2.86698700 1.09225100
C 2.90659500 -0.18676300 0.93921900
C 2.27655500 1.12480500 -1.03352100
C -1.56029400 -2.28235000 -0.32276800
C 0.72278600 -2.04788300 -1.22911300
C 2.10967400 -1.41788300 -1.02595100
H -1.66901600 1.17986900 -2.04458900
H -3.11716300 1.75719500 -1.16997200
H -1.72331200 2.73995600 0.63912400
H -1.19821600 3.39049800 -0.93934300
H -2.79132000 -0.70683700 1.55141500
H -2.67773900 1.06728500 1.54929600
H -3.98953600 0.25954800 0.59272400
H -3.32227800 -1.33291200 -1.17204900
H -1.80974500 -0.95293600 -2.04491300
H -2.07147500 -2.49342000 0.63730600
H -1.63389100 -3.20657000 -0.94012700
H 0.03886700 -3.92321200 0.90789300
H 1.43659100 -2.82418000 1.17766200
H -0.09582200 -2.48033700 2.03689900
H 0.82493500 -3.10339300 -1.57312700
H 0.18486500 -1.49610300 -2.02653800
H 2.57685800 -1.26300800 -2.02186300
H 2.77067600 -2.11570800 -0.47336800
H 2.63281700 -1.05885500 1.56046500
H 3.98356900 -0.25765000 0.65904900
H 2.74806400 0.71790100 1.55391100
H 2.70837200 0.90050100 -2.03198200
H 3.03259000 1.72737800 -0.49066300
H 0.37924500 1.47492900 -2.03047000
H 1.23379500 2.97513100 -1.56334300
H 0.23520300 2.47039700 2.03748800
H 1.79894400 2.61242200 1.17651700
H 0.55469900 3.88313300 0.90749900
O -0.04785000 0.00429500 2.09219500

^{3}IM9
BP86/BS1 SCF energy in solution: -2150.485428 a.u.

BP86/BS2 SCF energy in solution: -2151.607706 a.u.
BP86/BS2 Free energy in solution: -2151.252073 a.u.

1 3
Co -0.00515700 0.00027100 0.35004000
N -2.04751200 -0.00445000 -0.26444900
N 0.00790300 1.99316300 0.00414400
C -2.96432800 -0.00370000 0.89210600
C 0.51057600 2.84025900 1.10699400
C 0.87368500 2.02211400 -1.21705800
C -2.14873900 -1.25904500 -1.04530100
C -2.15141000 1.24748400 -1.04927900
C -1.40120400 2.37392400 -0.33045700
N 0.01654700 -1.99281600 0.00419100
N 2.03416400 0.00419900 -0.25469500
C 0.52643500 -2.83855000 1.10481900
C 2.89377600 0.00006700 0.95651400
C 2.20637300 1.28410400 -1.01498500
C -1.39190700 -2.38024600 -0.32542100
C 0.87778700 -2.01674900 -1.22002800
C 2.20719300 -1.26966500 -1.02548500
H -1.71826600 1.06006700 -2.05297100
H -3.21193100 1.55560800 -1.20695200
H -1.90482100 2.61689500 0.62608100
H -1.41618000 3.30098800 -0.94797300
H -2.77821700 -0.89034800 1.52409400
H -2.77854900 0.88387300 1.52287600
H -4.02558600 -0.00422100 0.54939000
H -3.20851900 -1.57170400 -1.19876200
H -1.71967300 -1.07290400 -2.05092400
H -1.89172300 -2.62247100 0.63332000
H -1.40481600 -3.30921300 -0.94015300
H 0.29573800 -3.91259500 0.92935900
H 1.62285200 -2.72907400 1.19653900
H 0.06317200 -2.47010700 2.04222800
H 1.07011100 -3.06718800 -1.53890600
H 0.30151400 -1.53239600 -2.03363600
H 2.65192300 -1.06961900 -2.02280000
H 2.93015800 -1.90866600 -0.47957000
H 2.67645300 -0.89438500 1.56785500
H 3.97382100 0.00150400 0.68110800
H 2.67540900 0.88995800 1.57412300
H 2.66447700 1.09493000 -2.00840500
H 2.91800300 1.92451900 -0.45611600

H 0.30405500 1.53377600 -2.03301600
H 1.06060400 3.07370900 -1.53538500
H 0.04323700 2.47166400 2.04221500
H 1.60657400 2.73202100 1.20484300
H 0.27924700 3.91390100 0.92975000
O -0.15587100 -0.00081100 2.07648300

^{5}IM9
BP86/BS1 SCF energy in solution: -2150.518879 a.u.
BP86/BS2 SCF energy in solution: -2151.641118 a.u.
BP86/BS2 Free energy in solution: -2151.283836 a.u.

1 5
Co -0.00015200 0.01049800 0.61989200
N 0.08519700 2.04986900 -0.21653000
N 2.05140100 -0.07456400 -0.10886900
C 0.12668600 2.97989800 0.93271100
C 2.98911800 -0.67209200 0.86142800
C 1.89089000 -0.90609300 -1.32859900
C -1.14517600 2.23979600 -1.02720300
C 1.32275700 2.13154900 -1.03487500
C 2.45714400 1.32194000 -0.41061200
N -2.05046200 0.09443000 -0.11060400
N -0.08513200 -2.04943300 -0.23007900
C -3.03717800 -0.43222400 0.85285300
C -0.13395400 -3.01912900 0.89108300
C 1.17119500 -2.22585100 -1.02472800
C -2.33894800 1.52261100 -0.40001700
C -1.95229200 -0.73888900 -1.33686400
C -1.34120900 -2.11613300 -1.04284000
H 1.08711500 1.74458000 -2.04672500
H 1.65270600 3.18835000 -1.16608400
H 2.77149900 1.78208000 0.54820100
H 3.34543900 1.34492200 -1.08524800
H -0.77241600 2.84205600 1.56197000
H 1.00963300 2.76372600 1.56264700
H 0.17260900 4.03883600 0.58594900
H -1.38645100 3.32147100 -1.14677900
H -0.94722500 1.84460300 -2.04331200
H -2.60281100 1.99940100 0.56584000
H -3.22873600 1.62674300 -1.06528900
H -4.07452300 -0.36239200 0.44901500
H -2.82690700 -1.49111100 1.09040800
H -2.97267300 0.14898300 1.79238700

H -2.95393000 -0.87675400 -1.81092400
H -1.31867400 -0.19483000 -2.06585800
H -1.15496100 -2.63593800 -2.00737200
H -2.07221200 -2.73793000 -0.48930500
H -1.02625300 -2.82462500 1.51504300
H -0.17213100 -4.07101600 0.52311000
H 0.75978300 -2.89411100 1.53061000
H 0.95786300 -2.74721800 -1.98314400
H 1.84481100 -2.89209900 -0.45065600
H 1.30654400 -0.31871100 -2.06497000
H 2.88063600 -1.12723000 -1.79621900
H 2.97728700 -0.07400700 1.79222600
H 2.68684900 -1.70469700 1.11491300
H 4.02817400 -0.69870100 0.45663500
O -0.00352200 0.00846900 2.30805000

^{5}TS6
BP86/BS1 SCF energy in solution: -2378.344415 a.u.
BP86/BS2 SCF energy in solution: -2379.77067 a.u.
BP86/BS2 Free energy in solution: -2379.3785 a.u.

1 5
Co 0.34136200 -0.00138600 -0.27704500
N -0.60968300 -0.83769900 1.49911700
N 1.28933000 -1.94956400 -0.35349000
C -2.02960900 -1.05886100 1.13590800
C 1.32985000 -2.54224600 -1.70587500
C 2.64284000 -1.61176400 0.16103800
C -0.47323600 0.17109700 2.58211900
C 0.08194600 -2.11182700 1.82855900
C 0.52716100 -2.83897100 0.56263100
N 0.28508100 1.82518600 0.87566100
N 2.36504700 0.70622900 -0.81540600
C -0.19799200 2.98205600 0.09327700
C 2.35929600 1.14813300 -2.23294800
C 3.28201800 -0.46554700 -0.63107700
C -0.61827900 1.58698300 2.03346000
C 1.70692600 1.95222100 1.28628300
C 2.65523100 1.86819500 0.08729500
H 0.95544100 -1.86987200 2.46538100
H -0.57628600 -2.78124400 2.42817500
H -0.35597700 -3.20054600 -0.00240000
H 1.12784100 -3.73734200 0.83682300
H -2.48777100 -0.11558600 0.78757600

H -2.09911900 -1.78618000 0.30654200
H -2.60080100 -1.44904600 2.00958000
H -1.22929000 0.00269700 3.38320000
H 0.52329600 0.03421200 3.04743200
H -1.65341200 1.75607800 1.67651000
H -0.42797400 2.32685900 2.84535200
H -0.19333000 3.91182600 0.70850700
H 0.43695600 3.14674500 -0.79698900
H -1.22952900 2.76389800 -0.24553800
H 1.87947800 2.91438500 1.82472700
H 1.93011400 1.13419500 2.00065100
H 3.70133000 1.82052500 0.45834600
H 2.57744200 2.79352400 -0.51649000
H 1.60933600 1.94951300 -2.37077600
H 3.35939500 1.53133900 -2.54038400
H 2.08647000 0.30233100 -2.89141800
H 4.21448700 -0.15233800 -0.11533100
H 3.58317800 -0.82353700 -1.63497800
H 2.53857500 -1.32046500 1.22570100
H 3.31462400 -2.50218700 0.12775000
H 0.29485700 -2.71093500 -2.05914800
H 1.83193600 -1.86495500 -2.42038400
H 1.87340400 -3.51547200 -1.69990200
O -0.81438400 0.18253900 -1.60867800
O -5.05548100 0.12604900 -1.40571000
H -1.73327000 0.66960800 -1.42567600
O -4.95030700 -0.90474700 -0.42472500
H -5.89027300 -1.18249200 -0.33981700
O -2.98872600 1.39731800 -1.09209200
H -3.06184600 2.12113500 -1.74669800
H -3.95020500 0.77557500 -1.24167500

^{4}IM10
BP86/BS1 SCF energy in solution: -2151.138413 a.u.
BP86/BS2 SCF energy in solution: -2152.263685 a.u.
BP86/BS2 Free energy in solution: -2151.899163 a.u.

1 4
Co -0.00183500 -0.01525400 0.64155100
N -1.10371600 -1.69886400 -0.31630000
N -1.65803700 1.15362300 -0.19701000
C -1.67412500 -2.54285500 0.75214200
C -2.18818600 2.17137900 0.72837000
C -1.04531000 1.75482400 -1.40390600

C -0.10850700 -2.45031200 -1.12052400
C -2.16890400 -1.09789900 -1.15479800
C -2.72254600 0.17386900 -0.51884600
N 1.73199600 -1.13857900 -0.06359300
N 1.17694600 1.71121600 -0.20798300
C 2.78593900 -1.22881200 0.96528300
C 1.61674600 2.50492200 0.96400000
C 0.25393400 2.50091000 -1.07588100
C 1.25086800 -2.49513400 -0.42633900
C 2.16811100 -0.35894700 -1.24924200
C 2.35039900 1.12560900 -0.91973300
H -1.73354500 -0.87008400 -2.14802100
H -3.00398200 -1.81575800 -1.33183400
H -3.23519900 -0.06948100 0.43483700
H -3.49314100 0.62103300 -1.19272200
H -0.88337300 -2.85455700 1.46024400
H -2.43039400 -1.97434800 1.32690900
H -2.16437500 -3.45133400 0.32738600
H -0.45197900 -3.49204100 -1.32429300
H -0.01881600 -1.94797900 -2.10444500
H 1.17862000 -3.07956200 0.51357200
H 1.98716700 -3.02301100 -1.07839500
H 3.67966200 -1.78272500 0.59072300
H 3.10941100 -0.21986900 1.28344800
H 2.38652100 -1.75715400 1.85316200
H 3.12443700 -0.76365300 -1.66270100
H 1.39750300 -0.47520500 -2.03706800
H 2.56147200 1.67920300 -1.86104200
H 3.24330500 1.25668000 -0.27614300
H 2.22307600 1.87053800 1.63961800
H 2.22773300 3.39036800 0.66716100
H 0.73504900 2.85888000 1.53204900
H 0.75354300 2.77932900 -2.02927000
H 0.02192000 3.45404100 -0.55937900
H -0.82879800 0.93692000 -2.11895900
H -1.75251000 2.45628500 -1.91155800
H -2.49005800 1.68170700 1.67390300
H -1.41288800 2.92184600 0.97008700
H -3.06686000 2.70490600 0.29367500
O -0.53356800 -0.11011000 2.42841900
H -1.48624900 -0.27933700 2.57085800

[5]IM11
BP86/BS1 SCF energy in solution: -2301.97829 a.u.

BP86/BS2 SCF energy in solution: -2303.293707 a.u.
BP86/BS2 Free energy in solution: -2302.92056 a.u.

1 5
Co -0.00414700 0.00514900 -0.32177800
N -0.64129500 -1.40502300 1.23647400
N 1.81186800 -1.29925800 -0.28791100
C -1.71394600 -2.22355600 0.62736900
C 2.39241500 -1.66372500 -1.59419400
C 2.73162900 -0.43879000 0.49409900
C -1.15884700 -0.59383400 2.36996400
C 0.51875500 -2.23975500 1.63527900
C 1.42895000 -2.53086200 0.44576100
N -1.01984100 1.44688700 0.93811100
N 1.54090800 1.58161200 -0.40117500
C -1.86327500 2.39584700 0.18100900
C 1.49109700 2.13289800 -1.77856900
C 2.86787500 0.94932800 -0.13143500
C -1.86558100 0.66675400 1.87890500
C 0.12032200 2.11953700 1.61120900
C 1.14828400 2.62750400 0.59701400
H 1.07486500 -1.69568500 2.42390400
H 0.18681400 -3.20261300 2.08836200
H 0.91154600 -3.19343800 -0.27822700
H 2.33062700 -3.08638000 0.79912400
H -2.50176800 -1.56820800 0.20523000
H -1.30390200 -2.82367600 -0.20694400
H -2.16093700 -2.91396400 1.38048800
H -1.85814200 -1.18704700 3.00398600
H -0.29731100 -0.32346200 3.01215100
H -2.79033600 0.39965400 1.32902300
H -2.17126000 1.28830600 2.75357100
H -2.33958800 3.14369200 0.85846400
H -1.26514500 2.94123500 -0.57348300
H -2.65205100 1.82497000 -0.34749600
H -0.23492100 2.97242400 2.23841800
H 0.59758100 1.38724400 2.29281900
H 2.04001600 3.00377200 1.14272500
H 0.73262500 3.49177400 0.04231200
H 0.47796100 2.52854000 -1.98681800
H 2.22882200 2.95655500 -1.92059900
H 1.70744500 1.33180600 -2.51065800
H 3.47896300 1.59095700 0.53881800
H 3.42101600 0.88119800 -1.08908300

H 2.32625500 -0.34066100 1.52036000
H 3.74192500 -0.90810100 0.58107700
H 1.67985000 -2.29683100 -2.15844000
H 2.60842500 -0.76287400 -2.19833100
H 3.34064900 -2.23857700 -1.46951500
O -0.68839700 -0.71051700 -1.99939900
H -0.42014900 -1.62361600 -2.22681500
H -1.94306100 -0.59700600 -2.26473400
O -3.65260600 -0.16968200 -1.33923900
O -3.06679500 -0.44437400 -2.49994100

^{5}TS7
BP86/BS1 SCF energy in solution: -2301.963235 a.u.
BP86/BS2 SCF energy in solution: -2303.277748 a.u.
BP86/BS2 Free energy in solution: -2302.90033 a.u.

1 5
Co 0.03970400 -0.00580100 0.38878800
N -1.33709700 -1.69962100 -0.17217200
N -1.85522100 1.12819300 0.22352400
C -1.43423700 -2.62837000 0.97397700
C -2.05014900 2.16075400 1.26079700
C -1.74191300 1.72209500 -1.12946200
C -0.72491100 -2.37804800 -1.34276700
C -2.66590700 -1.12222500 -0.50305500
C -2.94728400 0.12894700 0.32020200
N 1.36847500 -1.06511700 -1.01631200
N 0.75413000 1.75581200 -0.81716200
C 2.77872800 -1.19465100 -0.58308300
C 1.57721100 2.57063200 0.11119100
C -0.44424300 2.51797500 -1.28404500
C 0.79298500 -2.41799800 -1.23021300
C 1.27005200 -0.22829100 -2.24035300
C 1.59597300 1.22793300 -1.92851000
H -2.67596500 -0.88143100 -1.58392500
H -3.48205800 -1.86315700 -0.34003200
H -3.05555700 -0.13238100 1.39316800
H -3.92160000 0.57041900 -0.00019100
H -0.42696700 -2.90115700 1.34444200
H -1.99754200 -2.15867000 1.80353600
H -1.97341300 -3.56156600 0.68682000
H -1.11513100 -3.41655200 -1.45468100
H -1.02919400 -1.82616600 -2.25382500
H 1.10002400 -3.04343100 -0.36770200

H 1.22272800 -2.89414400 -2.14340100
H 3.41827800 -1.55357800 -1.42376300
H 3.17187300 -0.23324100 -0.20309300
H 2.83210900 -1.90770300 0.25819900
H 1.96009100 -0.60974600 -3.03100400
H 0.23864000 -0.30446600 -2.63741400
H 1.47095900 1.84253700 -2.84679400
H 2.65841600 1.31911300 -1.62860500
H 2.37897900 1.94221500 0.54787300
H 2.03598000 3.44775700 -0.40259200
H 0.94635200 2.94206500 0.94213500
H -0.32948400 2.81170000 -2.34948500
H -0.50163300 3.46135800 -0.70518700
H -1.75790200 0.89905100 -1.87021800
H -2.61345900 2.38444700 -1.35298400
H -2.02879200 1.68341800 2.25803200
H -1.24074700 2.91336400 1.22599100
H -3.02360100 2.68877200 1.12541800
O -0.26631700 -0.13794100 2.45224300
H -0.84438700 -0.83064800 2.83330300
H 0.74313100 -0.36967300 2.68938500
O 2.96361700 0.35071900 2.39894300
O 2.07995500 -0.61893400 2.26332800

^{2}TS3a
BP86/BS1 SCF energy in solution: -2378.20267 a.u.
BP86/BS2 SCF energy in solution: -2379.615531 a.u.
BP86/BS2 Free energy in solution: -2379.218479 a.u.

2 2
Co 0.51443600 0.00843800 -0.04644900
N -0.45210500 1.44369400 -1.04250800
N 1.91172900 1.34543200 0.47527200
C -1.56020000 2.11464800 -0.32112100
C 2.18850400 1.56989500 1.91579800
C 3.05891500 0.68836600 -0.22685400
C -0.93963300 0.72809400 -2.26990700
C 0.65008200 2.40820700 -1.38057300
C 1.50673600 2.65134200 -0.14992400
N -0.60840700 -1.35679300 -0.97049400
N 1.86600500 -1.45737600 0.37563100
C -1.37913300 -2.34548200 -0.18035000
C 1.78335000 -2.12902800 1.70251400
C 3.20991900 -0.75829300 0.24805600

C -1.54807100 -0.60434300 -1.86958800
C 0.53765500 -1.98152900 -1.71005000
C 1.59838400 -2.47510600 -0.72331800
H 1.24687200 1.96139500 -2.20037400
H 0.22646700 3.36237400 -1.76125100
H 0.93581100 3.20974800 0.61660700
H 2.40626800 3.25380700 -0.40066400
H -2.34151400 1.38113800 -0.04633900
H -1.17526300 2.58887700 0.59943400
H -2.01123900 2.89128200 -0.97518100
H -1.68037100 1.35176100 -2.81507500
H -0.07033500 0.58677600 -2.94241900
H -2.48606400 -0.44645500 -1.29979900
H -1.79733000 -1.21463300 -2.76446000
H -1.88581300 -3.05682800 -0.86762700
H -0.72497800 -2.91779300 0.49863400
H -2.14139800 -1.81859900 0.41795600
H 0.18230400 -2.81952100 -2.35088200
H 0.95984400 -1.20806700 -2.38480700
H 2.53541400 -2.69695500 -1.27095200
H 1.27464300 -3.41675700 -0.24139400
H 0.78911700 -2.59505100 1.83668800
H 2.55780500 -2.92218900 1.77818000
H 1.95831900 -1.39537500 2.51310500
H 3.86075800 -1.31402600 -0.45519400
H 3.70104600 -0.79251800 1.23819400
H 2.85154600 0.72156700 -1.31643500
H 4.00173700 1.25345100 -0.05205900
H 1.26243300 1.91159300 2.41126900
H 2.53556400 0.64533600 2.40975000
H 2.97904500 2.34344100 2.02473800
O -0.45062400 0.13636400 1.58069400
O -4.68311400 -0.39373200 1.01144000
H -1.73700300 0.15350000 1.92258000
O -4.50620400 0.18009100 -0.15004700
O -2.75651700 0.21517900 2.36485300
H -2.87450400 1.14921000 2.64355800
H -3.71070900 -0.09507000 1.69691400
H -0.00618500 -0.41178600 2.26250600

^{4}TS3a
BP86/BS1 SCF energy in solution: -2378.203694 a.u.
BP86/BS2 SCF energy in solution: -2379.617951 a.u.
BP86/BS2 Free energy in solution: -2379.220509 a.u.

2 4
Co 0.45178800 0.00832400 0.05714900
N -0.28710200 1.60865600 -0.97795000
N 1.84650700 1.27028000 0.80005300
C -1.44545200 2.21985600 -0.27498200
C 2.03044400 1.33697400 2.27033800
C 3.04664800 0.68969200 0.10641700
C -0.69777800 1.05894400 -2.30837400
C 0.86232000 2.56210000 -1.07657100
C 1.54748300 2.64936000 0.27555500
N -0.50694900 -1.18347100 -1.24981000
N 1.84461400 -1.49978300 0.23958800
C -1.34245100 -2.30669600 -0.75693700
C 1.59513300 -2.35424000 1.43733500
C 3.17616400 -0.79845400 0.39793800
C -1.36570600 -0.28859500 -2.09959100
C 0.70395200 -1.67984100 -1.99199000
C 1.70342300 -2.31820300 -1.02847800
H 1.55137200 2.18518000 -1.85763400
H 0.50935000 3.56471800 -1.40274900
H 0.89415100 3.14912200 1.01626000
H 2.48625700 3.24067300 0.21038300
H -2.26706300 1.48647600 -0.17354700
H -1.15179600 2.55218500 0.73640200
H -1.80450000 3.09334000 -0.86097000
H -1.38776700 1.76090700 -2.82447600
H 0.21066300 0.96961500 -2.93521000
H -2.32743500 -0.17224800 -1.55966500
H -1.58290500 -0.78400000 -3.07098200
H -1.78981400 -2.83945800 -1.62385100
H -0.74158000 -3.02845600 -0.17761000
H -2.14785800 -1.91863000 -0.10940600
H 0.39647500 -2.40634900 -2.77668300
H 1.16845900 -0.81421200 -2.50401000
H 2.68621500 -2.41428500 -1.53013200
H 1.38532200 -3.33847600 -0.74107700
H 0.60636400 -2.84055800 1.36163600
H 2.38008800 -3.13819700 1.50815600
H 1.61553800 -1.73435700 2.35198000
H 3.93207800 -1.24999900 -0.27529500
H 3.52469200 -0.96624300 1.43431800
H 2.91564800 0.85648200 -0.98133200
H 3.96528400 1.23371000 0.42057300

H 1.12111600 1.76176200 2.73672200
H 2.22819000 0.33689100 2.69457200
H 2.88781700 2.00261700 2.51044900
O -0.73668400 -0.13661800 1.54887600
O -4.79807000 0.16182100 1.14738000
H -1.96137900 -0.70683300 1.79381400
O -4.44637500 0.58157900 -0.04109800
O -2.93101700 -1.18166700 1.95445600
H -3.01336200 -1.37145000 2.91341500
H -3.89177100 -0.47347700 1.57428600
H -0.46353400 0.38272800 2.33458900

[Co(12-TMC)]$^{0+}$
BP86/BS1 SCF energy in solution: -2075.348926 a.u.
BP86/BS2 SCF energy in solution: -2076.39396 a.u.
BP86/BS2 Free energy in solution: -2076.046977 a.u.
0 2
Co 0.03750200 0.00016500 0.44897800
N 2.15007800 0.00069900 -0.08903600
N -0.00238900 -1.99433500 0.10299700
C 3.06787500 0.00209200 1.04901500
C -0.55155000 -2.95629700 1.08058400
C -0.84905500 -1.93198900 -1.12145000
C 2.19986900 1.24333600 -0.87558200
C 2.20218900 -1.24302700 -0.87367600
C 1.40452600 -2.37242200 -0.20666000
N -0.00386500 1.99427900 0.10280900
N -2.14768200 -0.00082500 -0.11133800
C -0.55181400 2.95505000 1.08234200
C -3.01846800 -0.00290000 1.06981300
C -2.22105000 -1.26228800 -0.87825800
C 1.40248100 2.37303800 -0.20884400
C -0.85247400 1.93304500 -1.12031500
C -2.22355200 1.26225200 -0.87538600
H 1.79361700 -1.03060800 -1.88290600
H 3.25124300 -1.60760700 -1.03089600
H 1.88131300 -2.64494400 0.75712800
H 1.45067700 -3.28555400 -0.85540000
H 2.88172400 0.89221500 1.68394900
H 2.88161000 -0.88656700 1.68604900
H 4.14610500 0.00163000 0.73297500
H 3.24835700 1.60849000 -1.03541800
H 1.78932400 1.02897800 -1.88361800
H 1.88028800 2.64674800 0.75408400

H 1.44736100 3.28556200 -0.85849100
H -0.52490500 4.00996700 0.69992000
H -1.60048800 2.70451100 1.32841400
H 0.04022900 2.88856800 2.01743800
H -1.02984900 2.95958600 -1.54107600
H -0.29355600 1.36398900 -1.89101100
H -2.70851100 1.11071500 -1.86838800
H -2.88026700 1.96399100 -0.31962700
H -2.80040100 0.88519800 1.69657100
H -4.11231100 -0.00350400 0.81922800
H -2.79884400 -0.89194600 1.69464900
H -2.70329200 -1.10869900 -1.87225300
H -2.87909200 -1.96560700 -0.32597400
H -0.28909600 -1.36163900 -1.89042500
H -1.02508400 -2.95811200 -1.54387100
H 0.03811500 -2.88964200 2.01719700
H -1.60117600 -2.70731200 1.32420600
H -0.52248700 -4.01093500 0.69762500

[Co(12-TMC)]$^{1+}$
BP86/BS1 SCF energy in solution: -2075.327858 a.u.
BP86/BS2 SCF energy in solution: -2076.361546 a.u.
BP86/BS2 Free energy in solution: -2076.004269 a.u.
1 1
Co 0.00155400 -0.02247600 0.25242500
N 0.13950400 -1.95845800 -0.03354300
N -1.95656500 -0.14854400 0.06838500
C 0.21392800 -2.78997400 1.19297700
C -2.82659600 0.31077000 1.17937900
C -2.09418500 0.73514000 -1.12526000
C 1.37906800 -2.09120700 -0.85908000
C -1.07859000 -2.27978200 -0.83801200
C -2.28312800 -1.58008500 -0.22587200
N 1.96023600 0.12845100 0.06812700
N -0.14038500 1.93776900 -0.05646700
C 2.75604800 0.68829100 1.18885600
C -0.22338600 2.79197000 1.16560800
C -1.41313100 2.08878400 -0.86224700
C 2.48246800 -1.23815200 -0.25041100
C 1.97442700 1.04248500 -1.11154100
C 1.11669600 2.28401700 -0.82369800
H 0.31100400 -3.87344500 0.93985000
H 1.08359600 -2.48489500 1.80464700
H -0.69725000 -2.64467000 1.80263600

H -3.90352900 0.15782700 0.93157400
H -2.57822000 -0.25917600 2.09551600
H -2.67300300 1.38456400 1.38468000
H -3.17330400 0.90150500 -1.37663500
H -1.62821000 0.22083700 -1.98788600
H 1.13997700 -1.74728300 -1.88488100
H 1.70599200 -3.15612100 -0.93452400
H -1.25285900 -3.38107100 -0.89095600
H -2.55026700 -2.05572800 0.73862400
H 3.84395200 0.69178300 0.94139600
H 2.45324700 1.72702100 1.41057200
H 2.59147400 0.07464200 2.09561000
H -0.29481600 3.87384200 0.90253700
H -1.11034600 2.51400600 1.76449700
H 0.67146300 2.63768300 1.79605100
H -2.09830700 2.75984900 -0.30452300
H -1.20395900 2.58975100 -1.82954400
H 3.36856300 -1.18683300 -0.92391700
H 2.82756900 -1.68487400 0.70307200
H 3.02002500 1.35957400 -1.35967800
H 1.69534700 3.01424700 -0.22232600
H 0.86756000 2.79225700 -1.77811200
H 1.58151100 0.48507900 -1.98368000
H -0.90398000 -1.92599600 -1.87317400
H -3.17643000 -1.66559700 -0.88662100

[Co(12-TMC)]$^{3+}$
BP86/BS1 SCF energy in solution: -2075.040172 a.u.
BP86/BS2 SCF energy in solution: -2076.062635 a.u.
BP86/BS2 Free energy in solution: -2075.701327 a.u.
3 3
Co -0.01740300 -0.00207900 0.48332500
N 0.00804700 -1.81482500 -0.41469900
N 0.03163800 1.81070400 -0.41257900
N -2.02707300 0.01217000 0.32189600
N 2.00654200 -0.00947000 0.33375100
C 2.41781500 1.19186800 -0.49922900
H 2.81394700 1.95540200 0.19555700
H 3.24452800 0.90894900 -1.18049400
C -1.26072200 1.85613400 -1.18317600
H -1.13311900 1.23651700 -2.09114800
H -1.45847600 2.89936000 -1.51074100
C -0.09421900 -2.89852300 0.59556500
H -0.98097000 -2.75384200 1.23777300

H 0.81193500 -2.91333800 1.22633900
H -0.18524800 -3.87119700 0.06564100
C 1.30496900 -1.86242800 -1.16759700
H 1.19455100 -1.23819000 -2.07476700
H 1.51362900 -2.90488300 -1.49057700
C 1.23894800 1.72752600 -1.29480400
H 1.46615900 2.73174700 -1.71499400
H 0.98250300 1.05756600 -2.13744400
C -1.19753800 -1.71512300 -1.30274200
H -1.41488900 -2.71317500 -1.74299600
H -0.93566100 -1.03407400 -2.13543000
C -2.39251400 1.33848700 -0.31179200
H -2.61460400 2.04244500 0.51169700
H -3.32163700 1.22316600 -0.90649300
C 0.11176300 2.88966700 0.60463100
H 0.09504500 3.87181000 0.08502300
H 1.04549600 2.80710700 1.18747000
H -0.74937000 2.83017500 1.29452800
C 2.40528600 -1.33966500 -0.26333200
H 2.59047800 -2.03282700 0.57853800
H 3.35925200 -1.23080000 -0.81814600
C -2.39460300 -1.20203300 -0.51426100
H -3.22273900 -0.94311600 -1.20370900
H -2.77459000 -1.97392100 0.18014500
C 2.53946600 0.11091000 1.71761600
H 2.17444100 -0.73622400 2.32946900
H 2.20441500 1.06899700 2.15946000
H 3.65120300 0.09072000 1.69883600
C -2.62567600 -0.09041500 1.67854700
H -2.30266700 0.77089000 2.29273500
H -2.30034400 -1.03526000 2.15481400
H -3.73532100 -0.08636500 1.60398600

[Co(12-TMC)]O_2^{0+}
BP86/BS1 SCF energy in solution: -2225.720838 a.u.
BP86/BS2 SCF energy in solution: -2226.945059 a.u.
BP86/BS2 Free energy in solution: -2226.592505 a.u.
0 2
Co -0.00002200 -0.00007200 0.55482200
O 0.01876700 -0.72180600 2.31909900
N 0.01821900 1.68499500 -0.67628800
O -0.01902700 0.72192500 2.31891000
N -0.01817200 -1.68501700 -0.67626700
N 2.26372700 -0.01121900 0.08244300

N -2.26369300 0.01127800 0.08236900
C -2.47248600 -1.19836300 -0.73276400
H -2.76201100 -2.01769500 -0.04358400
H -3.32486600 -1.07956600 -1.44896300
C 1.22919600 -1.69772600 -1.47842400
H 1.08950800 -1.00738700 -2.33174200
H 1.42291900 -2.70930600 -1.91523400
C 0.06679000 2.87041100 0.20810200
H 0.96047600 2.82506300 0.85626900
H -0.81242800 2.87664500 0.87740900
H 0.08748500 3.81875900 -0.38348600
C -1.22910400 1.69774800 -1.47848900
H -1.08940100 1.00742800 -2.33182300
H -1.42278600 2.70934500 -1.91528900
C -1.22940900 -1.63065100 -1.52978100
H -1.43854500 -2.62184700 -2.00560900
H -1.02647300 -0.92219700 -2.35565400
C 1.22948700 1.63070000 -1.52975700
H 1.43862100 2.62192200 -2.00552600
H 1.02659200 0.92228500 -2.35567500
C 2.44647300 -1.28157500 -0.63952300
H 2.64890300 -2.06623700 0.11807600
H 3.34410000 -1.25558200 -1.30948700
C -0.06680100 -2.87051300 0.20801900
H -0.08769600 -3.81880600 -0.38365700
H -0.96039000 -2.82509400 0.85631700
H 0.81251700 -2.87695600 0.87719000
C -2.44643400 1.28160900 -0.63965100
H -2.64891800 2.06629000 0.11791100
H -3.34401500 1.25557200 -1.30966700
C 2.47255800 1.19838700 -0.73272800
H 3.32492400 1.07953500 -1.44893700
H 2.76212800 2.01773200 -0.04358100
C -3.01736500 -0.01443300 1.33826300
H -2.65909800 0.81637400 1.97935700
H -2.78076600 -0.94923200 1.88321400
H -4.12640300 0.06055900 1.19970000
C 3.01735000 0.01450600 1.33836700
H 2.65900700 -0.81624400 1.97949200
H 2.78082100 0.94935800 1.88325600
H 4.12639000 -0.06057600 1.19985300

[Co(12-TMC)]O_2^{2+}
BP86/BS1 SCF energy in solution: -2225.485997 a.u.

BP86/BS2 SCF energy in solution: -2226.697872 a.u.
BP86/BS2 Free energy in solution: -2226.328876 a.u.
2 2
Co -0.00007900 -0.00042300 0.42466000
O -0.01155700 -0.66284800 2.21945900
N 0.06858200 1.66941100 -0.69174600
O 0.01046600 0.64774300 2.23225400
N -0.06838500 -1.66729400 -0.69485400
N 2.04657400 -0.06444100 0.16986900
N -2.04641700 0.06578000 0.16965100
C -2.42030100 -1.03719800 -0.80733100
H -2.82918800 -1.87626500 -0.21513500
H -3.23445500 -0.68163200 -1.47142800
C 1.24547100 -1.81826000 -1.39226000
H 1.24106700 -1.17742400 -2.29334600
H 1.38216000 -2.86748100 -1.73075800
C 0.29368700 2.84271700 0.21076200
H 1.20574300 2.71086900 0.81789800
H -0.56470800 2.97803400 0.89175200
H 0.40601300 3.75491000 -0.41296000
C -1.24501500 1.82266100 -1.38903000
H -1.24078300 1.18394500 -2.29162500
H -1.38142500 2.87270600 -1.72514400
C -1.22178600 -1.49635300 -1.62220100
H -1.45117100 -2.45467100 -2.13833000
H -0.92598000 -0.76327400 -2.39497100
C 1.22211200 1.50116100 -1.61922200
H 1.45159100 2.46065800 -2.13316500
H 0.92665000 0.76968100 -2.39368800
C 2.33457000 -1.42210100 -0.41533700
H 2.38907100 -2.13825200 0.42718600
H 3.33178500 -1.41311300 -0.90312400
C -0.29394700 -2.84377800 0.20337300
H -0.40878900 -3.75311000 -0.42400300
H -1.20473400 -2.71279300 0.81259000
H 0.56530900 -2.98360200 0.88234800
C -2.33425000 1.42456700 -0.41310100
H -2.38875100 2.13891400 0.43090600
H -3.33151100 1.41642700 -0.90082000
C 2.42053600 1.04024400 -0.80524000
H 3.23458100 0.68563100 -1.46997500
H 2.82966000 1.87813100 -0.21156500
C -2.83747800 -0.09932200 1.41780400
H -2.58326900 0.70712700 2.13010900

H -2.61609200 -1.08250400 1.87389900
H -3.92240800 -0.04431800 1.18409300
C 2.83743700 0.09920000 1.41834200
H 2.58565700 -0.70989200 2.12846100
H 2.61368400 1.08053700 1.87722700
H 3.92246000 0.04761300 1.18424300

[Co(12-TMC)]O_2^{3+}
BP86/BS1 SCF energy in solution: -2225.245204 a.u.
BP86/BS2 SCF energy in solution: -2226.459682 a.u.
BP86/BS2 Free energy in solution: -2226.09555 a.u.
3 3
Co -0.00001000 0.00000200 0.30683500
O 0.00832200 0.64157900 2.13399500
N -0.06898200 -1.80957000 -0.62592600
O -0.00852700 -0.64157700 2.13398000
N 0.06904200 1.80957600 -0.62591600
N -2.06588700 0.06621400 0.13570200
N 2.06586600 -0.06622400 0.13589900
C 2.44297100 1.12377800 -0.73432500
H 2.84308900 1.90285400 -0.06058100
H 3.26033500 0.82688000 -1.42168300
C -1.22900700 1.87857300 -1.37962000
H -1.13389200 1.25885300 -2.29002100
H -1.39549700 2.92972000 -1.70036400
C -0.22991000 -2.93343100 0.33757900
H -1.12567300 -2.78197600 0.96501400
H 0.66818800 -3.02891600 0.97260500
H -0.35597200 -3.86443800 -0.25472900
C 1.22914000 -1.87858600 -1.37950100
H 1.13412500 -1.25887200 -2.28991700
H 1.39565100 -2.92973800 -1.70021700
C 1.25759300 1.64491100 -1.52478100
H 1.49677000 2.63106300 -1.98132400
H 0.96261000 0.96134500 -2.34321400
C -1.25745100 -1.64490400 -1.52490000
H -1.49657600 -2.63105400 -1.98147400
H -0.96239800 -0.96132400 -2.34329500
C -2.36061000 1.41591500 -0.48629500
H -2.51094900 2.12634400 0.34896800
H -3.31110400 1.35883600 -1.05514500
C 0.22987100 2.93344900 0.33759000
H 0.35598900 3.86444600 -0.25472200
H 1.12557200 2.78200600 0.96511400

H -0.66829000 3.02894400 0.97252400
C 2.36064800 -1.41593200 -0.48605500
H 2.51088300 -2.12635600 0.34923100
H 3.31120800 -1.35886500 -1.05479600
C -2.44290400 -1.12379300 -0.73454100
H -3.26022000 -0.82691600 -1.42196600
H -2.84305800 -1.90287800 -0.06082700
C 2.80528700 0.02991300 1.42421100
H 2.54472100 -0.82138600 2.08067300
H 2.58181300 0.98989200 1.92681300
H 3.89530600 -0.01210300 1.21005500
C -2.80541300 -0.02990300 1.42395500
H -2.54488600 0.82139900 2.08042900
H -2.58199100 -0.98988100 1.92658600
H -3.89541600 0.01212400 1.20971500

$[CoTp^{tBu,Me}]^{0+}$
BP86/BS1 SCF energy in solution: -2674.038482 a.u.
BP86/BS2 SCF energy in solution: -2675.761149 a.u.
BP86/BS2 Free energy in solution: -2675.230072 a.u.
0 3
Co 0.00071200 0.00003400 -0.85758600
B -0.00217900 -0.00118400 2.03513300
N 1.19841500 -1.17412700 0.15213500
N 1.06978200 -1.01045400 1.50515500
N 0.41875700 1.62442800 0.15248100
N 0.33707600 1.43179500 1.50526300
N -1.61628000 -0.45108200 0.14943500
N -1.41151800 -0.42387700 1.50256900
C 2.19471000 -2.05854400 -0.06930100
C 2.72367600 -2.47625300 1.18000000
C 1.98854400 -1.79139400 2.15836100
C 2.12011600 -1.83763900 3.65079100
C 2.52380500 -2.50863200 -1.48820500
C 1.54944700 -3.64930800 -1.88594800
C 3.97720900 -3.02544400 -1.55946300
C 2.35203000 -1.32718500 -2.47076000
C 0.68673000 2.92952000 -0.06867300
C 0.77933800 3.59706700 1.18069300
C 0.55106600 2.61828100 2.15868400
C 0.52056300 2.75559200 3.65094800
C 0.91573500 3.43907600 -1.48712700
C 2.39038500 3.16110900 -1.88300700
C -0.02246400 2.70241800 -2.47089700

C 0.64154600 4.95703300 -1.55815500
C -2.88033100 -0.87094300 -0.07393200
C -3.50758300 -1.12262400 1.17428400
C -2.54766500 -0.83052400 2.15398800
C -2.65465900 -0.92413300 3.64614100
C -3.43384600 -0.92763200 -1.49321400
C -2.32426600 -1.36703400 -2.47632300
C -3.93454900 0.48742700 -1.88771600
C -4.60813400 -1.92757100 -1.56693000
H -0.00404800 -0.00178000 3.25370300
H 0.98386700 4.65757700 1.36442500
H 0.73287700 3.80415200 3.93642100
H -0.46859600 2.48108500 4.07506100
H 1.27543600 2.10810600 4.14513100
H 0.17799500 3.01090400 -3.51853800
H 0.13228400 1.59116200 -2.41602100
H -1.08918700 2.90458400 -2.24284400
H 1.33125400 5.52495400 -0.89966600
H 0.78877900 5.33017400 -2.59350700
H -0.39768100 5.19522900 -1.25017200
H 3.09069900 3.67472600 -1.19243600
H 2.60777900 2.07395400 -1.83680000
H 2.59856400 3.51550400 -2.91572900
H -2.47212700 0.05379000 4.13973000
H -3.66974200 -1.26368300 3.92969100
H -1.92366300 -1.64332600 4.07289000
H -4.52887700 -1.47503500 1.35601000
H -5.44564600 -1.61815600 -0.90767400
H -5.00493400 -1.98562500 -2.60238900
H -4.29175100 -2.94649500 -1.26143000
H -3.10477600 1.22242100 -1.83693300
H -4.34186500 0.49161400 -2.92193300
H -4.73337200 0.83247000 -1.19925100
H -1.44138900 -0.67488500 -2.41973200
H -1.96304900 -2.39118400 -2.24944700
H -2.69068300 -1.34739000 -3.52429200
H 2.37920500 -0.84560700 4.07792600
H 1.18025500 -2.16623000 4.14265000
H 2.91949800 -2.54885800 3.93582600
H 3.53921800 -3.18440600 1.36351900
H 4.70059600 -2.24199600 -1.25205900
H 4.12714600 -3.90611400 -0.90086200
H 4.22758000 -3.33904800 -2.59484700
H 1.75259700 -4.00422000 -2.91948400

H 1.64770100 -4.51368100 -1.19720000
H 0.49800100 -3.29789200 -1.83826300
H 3.05751400 -0.50226400 -2.24125300
H 2.52126500 -1.65347000 -3.51853900
H 1.31089700 -0.90881400 -2.41723000

$[CoTp^{tBu,Me}]^{1+}$
BP86/BS1 SCF energy in solution: -2673.84486 a.u.
BP86/BS2 SCF energy in solution: -2675.59791 a.u.
BP86/BS2 Free energy in solution: -2675.068659 a.u.
1 4
Co -0.05937900 0.00696800 -0.88850300
B 0.12095400 0.01253400 2.09089500
N 1.67280900 0.00241900 0.12379900
N 1.55244600 0.00825300 1.48250200
N -0.80278400 1.43482200 0.22076800
N -0.63656200 1.28277500 1.56903600
N -0.81139300 -1.42096700 0.21868200
N -0.63935600 -1.25789400 1.56771300
C 2.98360700 0.03314300 -0.19497300
C 3.73415900 0.05262000 1.00623500
C 2.79897100 0.03745700 2.05215400
C 3.02838200 0.05446900 3.53196500
C 3.43448500 0.00142900 -1.64848900
C 3.87315300 -1.44065600 -2.01546900
C 4.61988500 0.97505900 -1.85369800
C 2.26839700 0.43968400 -2.56143600
C -1.53040500 2.55693400 -0.00814400
C -1.83079900 3.14707300 1.23721200
C -1.25564500 2.31369700 2.21784000
C -1.28024000 2.45615600 3.70705300
C -1.84120600 3.00866700 -1.42754700
C -0.82141900 4.10236200 -1.84391300
C -1.74286800 1.80978200 -2.39768200
C -3.27632400 3.58460900 -1.49151000
C -1.45589300 -2.59675000 -0.00006500
C -1.70340100 -3.20129600 1.24855300
C -1.17643700 -2.32816500 2.22267000
C -1.16445500 -2.47883100 3.71123900
C -1.83613000 -3.03681100 -1.40682000
C -0.87033700 -2.40847200 -2.43650400
C -3.28857600 -2.57466700 -1.70045000
C -1.74913900 -4.57718900 -1.51703300
H 0.16223000 0.01067000 3.30327300

H -2.39973700 4.06379200 1.42600800
H -1.82583600 3.37567000 3.98988800
H -1.78404700 1.59584800 4.19423800
H -0.25640200 2.52062900 4.12970600
H -1.94957000 2.12291000 -3.44150100
H -0.70313900 1.38018300 -2.43417600
H -2.46295100 1.00663400 -2.13598000
H -3.38352300 4.46818400 -0.83049800
H -3.51552600 3.91352200 -2.52368000
H -4.03175100 2.83315000 -1.18321500
H -0.88210400 4.97923100 -1.16839100
H 0.22024100 3.72087800 -1.80579100
H -1.02568600 4.45248000 -2.87739900
H -1.68921100 -1.64012900 4.21329500
H -1.66899900 -3.41976000 3.99974400
H -0.13024600 -2.50725400 4.11237500
H -2.20154400 -4.15686000 1.44361200
H -2.46229800 -5.07177000 -0.82706500
H -2.00515200 -4.90519200 -2.54537800
H -0.73013300 -4.94600600 -1.28046000
H -3.38441900 -1.47086800 -1.62993600
H -3.59831500 -2.88498100 -2.72032300
H -4.00121900 -3.01899500 -0.97670200
H -0.92369400 -1.28508100 -2.42542300
H 0.17990600 -2.71900000 -2.25910100
H -1.14507800 -2.69787500 -3.47138100
H 2.57281900 0.94549300 4.01151000
H 2.60169800 -0.84215700 4.02726700
H 4.11393400 0.07390700 3.74363900
H 4.82367900 0.07859100 1.11564000
H 4.34411400 2.01517100 -1.58421900
H 5.49008000 0.68139700 -1.23276800
H 4.95079200 0.96661000 -2.91278600
H 4.21000800 -1.49152800 -3.07213000
H 4.71348400 -1.77405400 -1.37379400
H 3.04136700 -2.16310100 -1.87964200
H 1.93843300 1.47579500 -2.33714900
H 2.55191900 0.39722300 -3.63307800
H 1.39164000 -0.26186300 -2.47774800

$[CoTp^{tBu,Me}]O_2^{0+}$
BP86/BS1 SCF energy in solution: -2824.32695 a.u.
BP86/BS2 SCF energy in solution: -2826.237033 a.u.
BP86/BS2 Free energy in solution: -2825.697804 a.u.

0 3
Co -0.09181900 -0.00019700 -0.86808400
B 0.06443200 0.00120200 2.13094600
O 0.25931600 -0.68366400 -2.55643800
O 0.25575500 0.68458800 -2.55651600
N -0.87330400 1.42882000 0.28063900
N -0.69563000 1.25467800 1.62508600
N -0.86490700 -1.43302000 0.28143500
N -0.68780800 -1.25730100 1.62576000
N 1.73201800 0.00528100 0.21555900
N 1.50746700 0.00543500 1.56893700
C -1.58561800 2.57580200 0.10325100
C -1.85645800 3.13292700 1.37704500
C -1.27809000 2.27426700 2.31903500
C -1.25740300 2.38274700 3.81383300
C -1.99077000 3.14561300 -1.25489100
C -0.73290000 3.68141400 -1.98715500
C -2.97270400 4.32163300 -1.04598200
C -2.70046400 2.06562400 -2.10627400
C -1.56977200 -2.58473500 0.10467800
C -1.83634400 -3.14323100 1.37876100
C -1.26319100 -2.28051400 2.32022800
C -1.24097600 -2.38857100 3.81504000
C -1.97167000 -3.15783600 -1.25310100
C -2.68831200 -2.08295600 -2.10509100
C -0.71061400 -3.68611600 -1.98528200
C -2.94603600 -4.33999100 -1.04326600
C 3.08298000 0.00893000 0.03427500
C 3.71166300 0.01139100 1.30420100
C 2.68709900 0.00911800 2.25519400
C 2.79169100 0.01021700 3.75105100
C 3.79770200 0.00991600 -1.31882600
C 3.42220100 1.28044000 -2.12080100
C 3.42771400 -1.26290300 -2.11969900
C 5.32690800 0.01332400 -1.09063900
H 0.09503700 0.00162500 3.34601600
H -2.38299700 -4.06525300 1.59766000
H -1.77580600 -3.30489900 4.13075600
H -0.20613600 -2.44423400 4.21259800
H -1.73241800 -1.52122900 4.30314600
H -0.98694700 -4.09617000 -2.97993000
H 0.03688400 -2.88634200 -2.14237600
H -0.22974900 -4.49764400 -1.40014300
H -3.86384600 -4.02521200 -0.50422800

H -3.25536500 -4.74832000 -2.02756800
H -2.47571200 -5.16829400 -0.47386100
H -3.58843400 -1.69618500 -1.58384400
H -2.01571100 -1.23397000 -2.33171300
H -3.00982400 -2.51640000 -3.07545800
H 2.31506500 -0.88347000 4.20523400
H 3.85818100 0.01317900 4.04808300
H 2.31036500 0.90188200 4.20425100
H 4.78489300 0.01439100 1.51562500
H 5.66515000 -0.88529900 -0.53373000
H 5.84708600 0.01394200 -2.07076900
H 5.66133400 0.91393800 -0.53464100
H 2.34441500 -1.29920900 -2.34357000
H 3.97670200 -1.27580000 -3.08547000
H 3.70434000 -2.17880800 -1.55635700
H 2.33873000 1.31192400 -2.34457500
H 3.69502300 2.19802200 -1.55832900
H 3.97099800 1.29480100 -3.08666200
H -1.74341700 1.51227100 4.30179700
H -0.22317600 2.44521500 4.21197800
H -1.79840700 3.29559300 4.12911000
H -2.40936400 4.05136000 1.59536000
H -3.88865600 4.00107500 -0.50719000
H -2.50800000 5.15313800 -0.47665800
H -3.28424500 4.72755100 -2.03057500
H -1.01153600 4.08847600 -2.98238200
H -0.25771900 4.49680100 -1.40273000
H 0.02014800 2.88660600 -2.14307400
H -3.59861400 1.67408300 -1.58519000
H -3.02386200 2.49608400 -3.07734600
H -2.02268200 1.22039100 -2.33148300

$[CoTp^{tBu,Me}]O_2^{1+}$
BP86/BS1 SCF energy in solution: -2824.08112 a.u.
BP86/BS2 SCF energy in solution: -2826.01936 a.u.
BP86/BS2 Free energy in solution: -2825.482805 a.u.

1 4
Co 0.00017200 0.02575700 -0.77109000
B 0.00016300 -0.24478500 2.16493400
O 0.00036300 -0.74089300 -2.41554700
O -0.00041400 0.53827800 -2.73172900
N -0.00007400 1.56710500 0.43158700
N 0.00019200 1.24811100 1.76303200

N -1.48214700 -0.85092700 0.20109200
N -1.26936100 -0.90324800 1.55583600
N 1.48241000 -0.85059100 0.20103700
N 1.26968700 -0.90323300 1.55577900
C -0.00060500 2.93482700 0.31977200
C -0.00060400 3.46756800 1.62623900
C -0.00007700 2.38312200 2.51702800
C 0.00011800 2.38860900 4.01322700
C -0.00112900 3.71898500 -0.98942900
C 1.27943700 3.39310100 -1.79947500
C -0.00154400 5.23469400 -0.68130500
C -1.28186900 3.39221400 -1.79886000
C -2.69813300 -1.44416600 -0.06387700
C -3.22746100 -1.89176600 1.15954700
C -2.30604600 -1.54145100 2.16555300
C -2.38486200 -1.79445100 3.63606600
C -3.35197400 -1.56846900 -1.43743300
C -3.37145800 -0.19490300 -2.15181300
C -2.60558000 -2.63053200 -2.28812500
C -4.81588100 -2.03845400 -1.25908200
C 2.69870600 -1.44319800 -0.06407600
C 3.22819800 -1.89083800 1.15924100
C 2.30663500 -1.54110600 2.16534400
C 2.38545100 -1.79453600 3.63577800
C 3.35264900 -1.56681000 -1.43763400
C 3.37125700 -0.19304100 -2.15165200
C 2.60687400 -2.62916500 -2.28850200
C 4.81686100 -2.03588200 -1.25943200
H 0.00017900 -0.36755700 3.36989200
H -4.17893500 -2.40826800 1.31558300
H -3.33207800 -2.31126800 3.87796100
H -1.54764900 -2.43210200 3.98848600
H -2.34664400 -0.85114700 4.21882000
H -3.12175200 -2.75712500 -3.26222500
H -1.55928800 -2.34098200 -2.50108100
H -2.59731400 -3.61441700 -1.77590400
H -5.40322500 -1.33632300 -0.63247000
H -5.30706600 -2.09475200 -2.25117700
H -4.87560700 -3.04904900 -0.80613400
H -3.93202300 0.55625800 -1.55848400
H -2.35682400 0.20342700 -2.34031500
H -3.87005000 -0.29059200 -3.13791500
H 1.54948500 -2.43423000 3.98750700
H 3.33366800 -2.30943800 3.87783800

H 2.34487100 -0.85161500 4.21895900
H 4.17988100 -2.40698200 1.31519400
H 4.87727200 -3.04665800 -0.80698400
H 5.30811800 -2.09132500 -2.25154000
H 5.40369500 -1.33364500 -0.63246000
H 1.56036000 -2.34026200 -2.50123200
H 3.12299900 -2.75522800 -3.26269500
H 2.59929300 -3.61315100 -1.77646700
H 2.35638300 0.20490300 -2.33965100
H 3.93165900 0.55820600 -1.55827500
H 3.86956500 -0.28820700 -3.13794900
H -0.89381500 1.87914100 4.42853600
H 0.89454600 1.87983000 4.42831900
H -0.00023600 3.43099200 4.38272900
H -0.00088300 4.52585500 1.90214600
H -0.90194100 5.54178200 -0.11097900
H 0.89898000 5.54233800 -0.11147700
H -0.00196300 5.80292000 -1.63315600
H 1.27733400 3.95615600 -2.75531000
H 2.18805400 3.68339700 -1.23312200
H 1.36096900 2.31788000 -2.04854000
H -2.19039800 3.68221900 -1.23221900
H -1.28044900 3.95494600 -2.75488400
H -1.36294100 2.31685300 -2.04748100

^{OS}IM3A
BP86/BS1 SCF energy in solution: -2358.293388 a.u.
BP86/BS2 SCF energy in solution: -2359.663943 a.u.
BP86/BS2 Free energy in solution: -2359.258224 a.u.
1 1
N 0.99272000 -2.00499100 -0.43491200
N -1.18044100 -1.11679200 1.27564500
C 2.29332700 -2.43685200 0.14134800
C -1.30793100 -0.58085300 2.65215700
C -2.52069500 -1.13827500 0.62200800
C 1.07447800 -1.91291000 -1.93430700
C -0.08669300 -2.94554400 0.00883300
C -0.63894500 -2.50667800 1.35166300
N 0.20552400 0.39093600 -1.61674600
N -2.45335900 1.25343900 -0.24917700
C 0.51323800 1.82712200 -1.85720700
C -2.96553800 2.58683300 0.05148700
C -3.20832700 0.22113000 0.45358200
C 1.20757300 -0.45726500 -2.35014500

C -1.17977200 0.07461900 -2.10711100
C -2.29728900 1.03443200 -1.68277200
H -0.88615200 -2.94910400 -0.75628300
H 0.30602200 -3.98405500 0.06980800
H 0.16333900 -2.51331400 2.11730100
H -1.42453600 -3.21864500 1.69679100
H 3.07883900 -1.71672900 -0.14408100
H 2.22693000 -2.44915600 1.24675100
H 2.54650000 -3.45885000 -0.21799200
H 1.94084100 -2.49323200 -2.31379000
H 0.16714000 -2.37410200 -2.36877200
H 2.20484500 -0.06812100 -2.07524300
H 1.06297400 -0.34350400 -3.44735200
H 0.27014800 2.09067700 -2.90977900
H -0.07463000 2.45874700 -1.16989900
H 1.58901900 2.00042700 -1.68598000
H -1.14052500 0.09330900 -3.22064900
H -1.41709700 -0.96369100 -1.82392700
H -3.23626500 0.63652500 -2.15533200
H -2.12126400 2.01843800 -2.16104100
H -2.31741400 3.35966000 -0.41155300
H -4.01374900 2.76043600 -0.31356100
H -2.96166800 2.75765200 1.14794700
H -4.19317900 0.00964900 -0.04800700
H -3.46271000 0.62096800 1.45660900
H -2.42628500 -1.65645400 -0.34975200
H -3.20148000 -1.77200800 1.24038000
H -0.33183400 -0.64841500 3.16797800
H -1.60721700 0.48139700 2.62280600
H -2.06231200 -1.16426200 3.22957800
Co 0.53209800 -0.10942100 0.30136700
O 1.41128700 2.25347600 1.37754500
O 0.22857300 1.33675100 1.30774100
N 2.29746900 0.46778400 0.20224000
C 2.45000100 1.59784600 0.81115100
C 3.75612500 2.33707200 0.96112600
H 3.97918800 2.53950100 2.02957700
H 3.71634100 3.31391000 0.43393000
H 4.56997300 1.72821900 0.52411200

^{3}IM3A
BP86/BS1 SCF energy in solution: -2358.299256 a.u.
BP86/BS2 SCF energy in solution: -2359.666506 a.u.
BP86/BS2 Free energy in solution: -2359.262161 a.u.

1 3
N 0.08927100 2.20807100 -0.10360200
N -1.47969000 0.26683600 -1.62688800
C 1.24769100 2.70827400 -0.86601700
C -1.37202000 -0.50609200 -2.88216700
C -2.71641100 -0.08965900 -0.89426500
C 0.13329400 2.67929300 1.30012400
C -1.18080700 2.58140200 -0.76037400
C -1.45018700 1.70848000 -1.97044900
N 0.22061700 0.28945300 2.01359600
N -1.45264100 -1.58201200 0.66466000
C 1.04385500 -0.65841900 2.79862800
C -0.97512800 -2.98505000 0.68266800
C -2.60145900 -1.47309400 -0.27543700
C 0.79675700 1.64598100 2.19658100
C -1.21236700 0.22331900 2.39206500
C -1.80462100 -1.13827300 2.05137300
H -1.99656000 2.47296400 -0.01780900
H -1.17430400 3.65351600 -1.07327200
H -0.65695900 1.85236800 -2.73109800
H -2.41064400 2.01444100 -2.44972000
H 2.18346400 2.40003100 -0.36612100
H 1.25696900 2.27729000 -1.88607900
H 1.21644000 3.82107900 -0.94997600
H 0.68401700 3.64344500 1.38644300
H -0.90136300 2.88330400 1.63944200
H 1.87216700 1.55858700 1.94951600
H 0.71127400 1.95725400 3.26378000
H 1.00708100 -0.40258200 3.88251000
H 0.69585000 -1.69885500 2.67289500
H 2.08869100 -0.59618100 2.44205800
H -1.34093300 0.42866800 3.48168800
H -1.75324400 1.01589800 1.84164900
H -2.90765900 -1.09554300 2.17771500
H -1.43999900 -1.90230500 2.76559800
H -0.09915700 -3.08400300 1.35211400
H -1.77360100 -3.67595000 1.04021000
H -0.66305700 -3.28010400 -0.33534300
H -3.55381100 -1.73557900 0.23872700
H -2.45670200 -2.22916500 -1.07177400
H -2.89510000 0.66914500 -0.10693900
H -3.59880200 -0.06212600 -1.57847800
H -0.42254500 -0.25576400 -3.39049000
H -1.36888600 -1.59221900 -2.68513800

H -2.22348100 -0.26295200 -3.56144000
Co 0.26962800 -0.22288800 -0.10676700
O 2.14320700 -1.71336200 -1.52652900
O 0.66848300 -1.53508300 -1.28467700
N 2.12836100 -0.00138300 0.03239200
C 2.76476100 -0.83099000 -0.73563900
C 4.26921700 -0.90727500 -0.84013500
H 4.59959600 -0.73266800 -1.88533800
H 4.63270800 -1.91036100 -0.53349800
H 4.71821500 -0.14024300 -0.18231500

^{5}IM3A
BP86/BS1 SCF energy in solution: -2358.283089 a.u.
BP86/BS2 SCF energy in solution: -2359.648132 a.u.
BP86/BS2 Free energy in solution: -2359.245595 a.u.
1 5
N 0.54267400 2.03874500 0.73969800
N 1.58926600 -0.59222900 1.45515100
C -0.39501400 2.53841400 1.76683500
C 1.38018000 -1.65353700 2.46491400
C 2.59711200 -1.01774500 0.44779200
C 0.53801200 2.92040700 -0.45728400
C 1.90840000 1.88063400 1.29034800
C 2.01522600 0.64194900 2.16451000
N -0.27845900 1.00601400 -1.85265700
N 0.86559400 -1.58029200 -1.27716500
C -1.37638600 0.60477300 -2.75128800
C -0.00166800 -2.72803700 -1.63431800
C 2.03367400 -2.07050900 -0.49627400
C -0.45281300 2.43670900 -1.50716400
C 1.05293900 0.68201600 -2.40727400
C 1.26446100 -0.83120900 -2.51378900
H 2.61366900 1.80978300 0.43789600
H 2.21085200 2.77649200 1.88311400
H 1.36950900 0.74568100 3.05947200
H 3.06204600 0.53638700 2.53544100
H -1.40392600 2.64387200 1.32853200
H -0.47172100 1.82125200 2.60705700
H -0.05429300 3.52302800 2.16585400
H 0.28614700 3.96830200 -0.17762800
H 1.56384300 2.95209800 -0.87392200
H -1.48827600 2.53469800 -1.12476300
H -0.36541300 3.07500600 -2.41918300
H -1.33276700 1.17244500 -3.71080900

H -1.33581700 -0.47437900 -2.98569100
H -2.34184500 0.81230000 -2.25242400
H 1.19692000 1.14114400 -3.41556800
H 1.82135100 1.11869600 -1.74007400
H 2.33187000 -1.02408300 -2.75486000
H 0.67692600 -1.23337600 -3.36244400
H -0.89758300 -2.37191500 -2.17793900
H 0.54199100 -3.45397400 -2.28268400
H -0.33856100 -3.23022300 -0.71011600
H 2.84027800 -2.42403200 -1.17867900
H 1.70174200 -2.95383200 0.08338900
H 2.92452500 -0.13054500 -0.12954600
H 3.50265200 -1.42390200 0.95837400
H 0.59559200 -1.33533400 3.17589500
H 1.04464300 -2.59097100 1.99004700
H 2.32534100 -1.84375800 3.02583900
Co -0.20670600 -0.09364200 0.12582500
O -2.38156300 -1.67973700 1.16833100
O -0.98173200 -1.71132500 0.96058000
N -2.10033900 0.44986000 0.32100600
C -2.88132600 -0.44719200 0.77920400
C -4.37482600 -0.39039800 0.98651800
H -4.63307000 -0.56149900 2.05271100
H -4.88431600 -1.17581100 0.38929400
H -4.75387100 0.60094900 0.67624300

^{3}TS4A
BP86/BS1 SCF energy in solution: -2358.285441 a.u.
BP86/BS2 SCF energy in solution: -2359.656672 a.u.
BP86/BS2 Free energy in solution: -2359.2573 a.u.
1 3
N -0.94087700 1.99467200 -0.58636900
N 1.14687500 1.23209500 1.33749500
C -2.27073900 2.45428200 -0.12980800
C 1.16567900 0.76809600 2.74021200
C 2.50276000 1.18557000 0.74001100
C -0.92568300 1.81291700 -2.07290500
C 0.11895000 2.94551800 -0.13368100
C 0.58814700 2.60841900 1.27011800
N -0.08739400 -0.52070900 -1.71896200
N 2.50160800 -1.24254500 -0.07052300
C -0.41259800 -1.94598700 -1.95618700
C 2.77100800 -2.58908400 0.40978400
C 3.18241300 -0.19246400 0.67662600

C -1.06373700 0.34537900 -2.45096400
C 1.31396800 -0.20863000 -2.10750500
C 2.42699500 -1.10587800 -1.51873200
H 0.96507300 2.88679300 -0.84567600
H -0.25425800 3.99376400 -0.16778200
H -0.26274400 2.65822000 1.97965400
H 1.34134500 3.35739900 1.61166800
H -3.03514000 1.70533600 -0.40342700
H -2.27694900 2.55478800 0.97279600
H -2.51764400 3.43905400 -0.58692700
H -1.75139000 2.38492200 -2.54724500
H 0.01603500 2.23393900 -2.47514600
H -2.07098000 -0.02873300 -2.18546800
H -0.92125300 0.22149500 -3.54909900
H -0.19713000 -2.21481500 -3.01473400
H 0.17585800 -2.58770200 -1.27795600
H -1.48451600 -2.11358200 -1.74978200
H 1.39609300 -0.31760000 -3.21412000
H 1.50465800 0.85498400 -1.87709800
H 3.38225200 -0.68303800 -1.91868900
H 2.33393700 -2.12194400 -1.94859800
H 2.11266400 -3.31677500 -0.10308500
H 3.83286300 -2.89441300 0.22839600
H 2.57562800 -2.65133900 1.49842900
H 4.19932800 -0.00829200 0.24369000
H 3.34782200 -0.57179400 1.70402800
H 2.45303500 1.63278900 -0.27029100
H 3.18324200 1.83814700 1.33941200
H 0.14569300 0.84076000 3.16516200
H 1.48091300 -0.28978300 2.78690800
H 1.85755300 1.38813000 3.35719900
Co -0.45259300 -0.01326700 0.28896400
O 0.16778200 -1.36238900 0.96791800
O -1.98991400 -2.63767300 1.09982900
N -2.19109700 -0.41000400 0.38017100
C -2.63302400 -1.58003700 0.89445800
C -4.13425300 -1.56988500 1.23202500
H -4.27390900 -1.92554000 2.27391200
H -4.65743400 -2.28356300 0.56072800
H -4.58669100 -0.56676700 1.11575600

[5]TS4A
BP86/BS1 SCF energy in solution: -2358.264097 a.u.
BP86/BS2 SCF energy in solution: -2359.631893 a.u.

BP86/BS2 Free energy in solution: -2359.233067 a.u.
1 5
N -0.19695400 2.23659200 0.07348100
N -1.56921900 0.24312700 -1.56103900
C 0.88407200 2.93018100 -0.65266500
C -1.47546500 -0.41393400 -2.88526900
C -2.68957500 -0.32223700 -0.76297000
C -0.16249900 2.56352600 1.52057000
C -1.51652200 2.52491100 -0.52849700
C -1.73454700 1.70459100 -1.78782300
N 0.29599600 0.16234500 2.05194200
N -1.19865400 -1.82372700 0.60037800
C 1.29265900 -0.72186800 2.68709300
C -0.56890800 -3.15681800 0.46201600
C -2.39363900 -1.73841500 -0.28276500
C 0.69127600 1.56981500 2.29447000
C -1.08314400 -0.14687700 2.48972900
C -1.50742900 -1.54382700 2.03880700
H -2.29818200 2.29698300 0.22290200
H -1.62267700 3.60757300 -0.77742500
H -1.00375800 1.99593000 -2.56846400
H -2.74914500 1.91198500 -2.20111000
H 1.86111300 2.66193000 -0.21140100
H 0.90300100 2.61313700 -1.71358100
H 0.73994100 4.03595600 -0.61071500
H 0.23521700 3.59041500 1.68879200
H -1.20103000 2.56948900 1.90584800
H 1.75028800 1.65294400 1.97805000
H 0.64447700 1.80677400 3.38421000
H 1.28061300 -0.60134200 3.79578500
H 1.10154200 -1.78416300 2.44951500
H 2.29648100 -0.46034700 2.30352600
H -1.17659500 -0.08054900 3.60069500
H -1.76783500 0.61051600 2.06205100
H -2.59492600 -1.66901100 2.22982000
H -0.99248500 -2.30885000 2.65185200
H 0.36020100 -3.19974400 1.06213800
H -1.25927900 -3.95868500 0.81209600
H -0.30137600 -3.32567300 -0.59587600
H -3.29174500 -2.13672000 0.24134200
H -2.21479700 -2.40028900 -1.15195400
H -2.87826900 0.34148600 0.10269000
H -3.62147300 -0.33205700 -1.37588600
H -0.59992100 -0.01537200 -3.42956100

H -1.33991500 -1.50306800 -2.77699400
H -2.39828700 -0.20906800 -3.47577200
Co 0.18229600 -0.12067200 -0.19478700
O 2.41950900 -1.47847600 -1.72250400
O 0.66283000 -1.33887200 -1.38525800
N 2.12386900 0.22350900 -0.18065200
C 2.87827900 -0.53291800 -0.92315100
C 4.39354000 -0.39805900 -0.93018500
H 4.75864200 -0.21333700 -1.96219000
H 4.86026000 -1.33914600 -0.56989100
H 4.70535800 0.43789800 -0.27407800

^{OS}IM4A
BP86/BS1 SCF energy in solution: -2358.288612 a.u.
BP86/BS2 SCF energy in solution: -2359.658299 a.u.
BP86/BS2 Free energy in solution: -2359.256207 a.u.
1 1
N 1.10724300 1.48041300 1.10068600
N -1.11874200 1.66899800 -0.75987400
C 2.45354300 1.97898700 0.73564500
C -1.24894300 1.78035100 -2.23073000
C -2.44921500 1.49491600 -0.11595000
C 1.16165800 0.72508700 2.39388100
C 0.13626100 2.61406700 1.15445100
C -0.43706500 2.88239400 -0.22368300
N 0.03646400 -1.16847900 1.21924200
N -2.72297500 -1.06478700 -0.27256200
C 0.22473800 -2.59354200 0.83493000
C -3.27389700 -2.09435500 -1.14229500
C -3.27616900 0.26509200 -0.51884300
C 1.15823700 -0.77114700 2.13197000
C -1.29335000 -0.94650300 1.86121700
C -2.52412300 -1.48613700 1.11225500
H -0.67282800 2.34948000 1.86255800
H 0.62367300 3.53159600 1.55330600
H 0.37188300 3.15143000 -0.93210100
H -1.14407400 3.74332100 -0.18999000
H 3.17173100 1.14087200 0.70630300
H 2.42996300 2.44807500 -0.26592200
H 2.79642000 2.73048600 1.48214600
H 2.07301200 0.99365800 2.96922500
H 0.29752200 1.02168600 3.01903800
H 2.09228800 -1.09399700 1.62692800
H 1.06708300 -1.33368800 3.08885300

H 0.08554900 -3.23655900 1.73207500
H -0.49955700 -2.86755800 0.04950300
H 1.25476200 -2.70752300 0.44200800
H -1.28256400 -1.46740300 2.84637600
H -1.39979800 0.13043900 2.07709600
H -3.40703400 -1.19184800 1.73268200
H -2.49608200 -2.59239500 1.11770800
H -2.71241200 -3.04018500 -1.01506000
H -4.35082000 -2.29325800 -0.91498500
H -3.19741400 -1.77521000 -2.20002900
H -4.24819000 0.37022100 0.02681200
H -3.52044600 0.32144800 -1.59748200
H -2.30909000 1.53439500 0.97950400
H -3.07963000 2.37781300 -0.37869400
H -0.24685200 1.93846900 -2.67384200
H -1.66279400 0.84389800 -2.64358900
H -1.90600900 2.63888600 -2.50015500
Co 0.30969800 0.04042900 -0.39165100
O -0.66390200 -0.92858700 -1.34226300
O 3.18646900 -2.01134300 -0.24279200
N 1.92403700 -0.27053300 -1.04138500
C 2.99230300 -1.05960700 -1.05875300
C 4.02133700 -0.74209800 -2.14134300
H 4.13580500 -1.62818800 -2.80158300
H 5.00574000 -0.54815100 -1.66497600
H 3.73371900 0.13333000 -2.75795000

^{3}IM4A
BP86/BS1 SCF energy in solution: -2358.294348 a.u.
BP86/BS2 SCF energy in solution: -2359.665134 a.u.
BP86/BS2 Free energy in solution: -2359.266534 a.u.
1 3
N 1.04005800 1.82869400 0.81839300
N -0.91313500 1.30385600 -1.29573600
C 2.44136900 2.23157800 0.55528900
C -0.83476900 0.90374500 -2.72088300
C -2.33214000 1.36141100 -0.84285000
C 0.84373700 1.53447000 2.27623000
C 0.09802900 2.88218200 0.32950600
C -0.26313600 2.63652600 -1.12243900
N -0.20222800 -0.63517600 1.61475100
N -2.67814400 -1.08966700 -0.18723100
C -0.02591600 -2.10595000 1.72222400
C -3.19759600 -2.34795100 -0.70616000

C -3.15142800 0.06712300 -0.93749500
C 0.79176300 0.03541100 2.51691100
C -1.59513000 -0.21768300 1.95651300
C -2.73195200 -0.99064200 1.26762200
H -0.80832000 2.86161100 0.96476800
H 0.54678000 3.89333700 0.44555800
H 0.64934700 2.64788700 -1.75171400
H -0.93257900 3.44410300 -1.49825900
H 3.12863000 1.42322200 0.86182600
H 2.59014600 2.41038100 -0.52670200
H 2.68020200 3.16287600 1.11554700
H 1.66650700 1.97286400 2.87889700
H -0.09094900 2.02077400 2.61632400
H 1.77586200 -0.42779200 2.30919200
H 0.52788700 -0.17588500 3.57811200
H -0.26239000 -2.43532200 2.75868100
H -0.69084200 -2.61673700 1.00472800
H 1.02214700 -2.36084400 1.46821800
H -1.73143900 -0.36053000 3.05419400
H -1.68163500 0.86688900 1.76910700
H -3.68196700 -0.50224700 1.60945100
H -2.76004000 -2.02072300 1.67345200
H -2.70431700 -3.20335700 -0.20168400
H -4.30431700 -2.45683300 -0.56124300
H -2.99082700 -2.42558200 -1.79262100
H -4.19085800 0.35169600 -0.62100500
H -3.23233300 -0.23644200 -2.00052100
H -2.35198600 1.76337700 0.18651900
H -2.86136400 2.11252600 -1.47637800
H 0.22266300 0.91510900 -3.04703000
H -1.22687300 -0.12050800 -2.85113900
H -1.41757600 1.61012200 -3.35545800
Co 0.49296300 -0.03675300 -0.25339700
O -0.14083200 -1.34416400 -1.04739300
O 2.91122200 -2.47755700 0.11425200
N 2.18844500 -0.41492300 -0.48919100
C 2.88862100 -1.53927100 -0.72196500
C 3.70974900 -1.56846900 -1.99991200
H 3.29535500 -2.35207300 -2.67002100
H 4.75881800 -1.84323100 -1.76292500
H 3.69097000 -0.59694800 -2.53347100

[5]IM4A
BP86/BS1 SCF energy in solution: -2358.292294 a.u.

BP86/BS2 SCF energy in solution: -2359.664603 a.u.
BP86/BS2 Free energy in solution: -2359.26572 a.u.
1 5
N -1.72682400 -1.92885300 0.17078400
N 0.37428300 -0.66405600 -1.86947900
C -3.15039900 -1.70793200 -0.01488100
C 0.39331900 0.21958100 -3.06146100
C 1.69041200 -1.33411300 -1.68239200
C -1.32689400 -2.24920200 1.53419200
C -1.05495200 -2.59770100 -0.93155400
C -0.71551400 -1.66178500 -2.09123500
N 0.33211200 -0.31911700 1.89008400
N 2.44730200 0.30010300 0.08726900
C 0.57504900 0.78500100 2.85727100
C 3.20952300 1.56905100 0.16492500
C 2.77009200 -0.37239900 -1.20647300
C -0.90404600 -1.02413900 2.34581600
C 1.49032900 -1.24858700 1.80976100
C 2.73481200 -0.54169800 1.29182200
H -0.14560500 -3.10106600 -0.54677500
H -1.69541900 -3.40931500 -1.36170200
H -1.62163500 -1.09110300 -2.37749800
H -0.43456100 -2.27993500 -2.97716600
H -3.53890400 -1.00304100 0.74612900
H -3.35520600 -1.27035600 -1.01243500
H -3.73182200 -2.66313900 0.06449100
H -2.17368900 -2.71619400 2.09120300
H -0.52544300 -3.01556800 1.51790000
H -1.71766400 -0.27238600 2.32063700
H -0.75355800 -1.33360700 3.40681800
H 0.78121500 0.37440100 3.87168600
H 1.42702300 1.41784900 2.55027300
H -0.32787600 1.42294700 2.90457000
H 1.70329200 -1.69235900 2.81086100
H 1.21449600 -2.07809800 1.13381900
H 3.51905400 -1.29414200 1.06016700
H 3.15234500 0.12032900 2.07412500
H 2.97098500 2.10157600 1.10526900
H 4.30435200 1.36860700 0.13718300
H 2.92717300 2.21502500 -0.68654000
H 3.73454500 -0.92090800 -1.11885700
H 2.92313300 0.42533700 -1.95898400
H 1.56684600 -2.16143700 -0.95884000
H 2.01824000 -1.79390000 -2.64432500

H -0.57183000 0.75469700 -3.13421400
H 1.19497400 0.97326400 -2.97823600
H 0.54396700 -0.38696200 -3.98375700
Co 0.25822800 0.68145200 -0.05294400
O -1.60771100 3.31293300 0.20928300
O 0.63603900 2.04864700 -0.92702400
N -1.48696400 1.03142200 0.16776900
C -2.14008100 2.20191800 -0.01889300
C -3.60826100 2.09969200 -0.41430100
H -3.89934300 3.01540100 -0.96770200
H -4.23874900 2.03530700 0.49828400
H -3.80881100 1.20433700 -1.03553500

^{OS}TS5A
BP86/BS1 SCF energy in solution: -2358.269592 a.u.
BP86/BS2 SCF energy in solution: -2359.638717 a.u.
BP86/BS2 Free energy in solution: -2359.237073 a.u.
1 1
N 0.94801800 0.49685300 1.70817800
N -0.72959300 1.93808500 -0.05003500
C 2.43111800 0.58680400 1.61808600
C -0.73333400 2.65415200 -1.34527200
C -2.10429100 1.77297800 0.52606400
C 0.58856500 -0.61977000 2.62838600
C 0.40692200 1.81884500 2.14299600
C 0.15177800 2.66631600 0.91019600
N -0.31509600 -1.82733200 0.66716300
N -2.43784600 -0.33539600 -0.77612400
C -0.05325100 -2.96888300 -0.24032000
C -2.65033700 -0.58303400 -2.20759700
C -3.04179500 0.93822500 -0.34013800
C 0.60122500 -1.91941800 1.84530000
C -1.73845900 -1.78543800 1.13800500
C -2.74984800 -1.53176200 0.02785500
H -0.52027000 1.65263300 2.72312900
H 1.12089700 2.33471400 2.82091900
H 1.10229600 2.87517600 0.37970800
H -0.30646200 3.64407300 1.18158700
H 2.85025900 -0.36049200 1.23588400
H 2.72404700 1.40131400 0.93295700
H 2.84388300 0.78977700 2.63113400
H 1.30281100 -0.67603400 3.47914700
H -0.40978800 -0.41473500 3.06021400
H 1.61454400 -2.13236400 1.45140000

H 0.30167800 -2.77600700 2.49039900
H -0.19476500 -3.92712300 0.30777400
H -0.73718400 -2.93608300 -1.10607400
H 0.98649100 -2.87886800 -0.60909200
H -1.97187200 -2.75013200 1.64576900
H -1.82074500 -0.98799400 1.89937300
H -3.76012100 -1.45835000 0.49462300
H -2.78522200 -2.40325500 -0.65487100
H -2.06603000 -1.46610700 -2.52816000
H -3.72873200 -0.76161200 -2.44040800
H -2.30350900 0.28314000 -2.80254000
H -3.97854400 0.76755200 0.23953100
H -3.33556600 1.50883500 -1.24349900
H -1.99654100 1.29130300 1.51528400
H -2.54579500 2.78255000 0.69637200
H 0.29963000 2.66433700 -1.74173800
H -1.38565900 2.14517200 -2.07528400
H -1.09066800 3.69857900 -1.20509500
Co 0.07494400 0.01322400 -0.24149600
O 0.14463900 -0.56202900 -1.84741600
O 2.84836200 -1.48733700 -0.96867700
N 1.68563900 0.53421300 -1.19366500
C 2.75615400 -0.29086000 -1.33930400
C 3.95877400 0.39978500 -1.99064900
H 4.26578500 -0.17992800 -2.88755700
H 4.81389100 0.39044400 -1.28158900
H 3.74656500 1.44476100 -2.29042500

^{3}TS5A
BP86/BS1 SCF energy in solution: -2358.276781 a.u.
BP86/BS2 SCF energy in solution: -2359.646319 a.u.
BP86/BS2 Free energy in solution: -2359.245764 a.u.
1 3
N 1.09621100 0.86944200 1.50755500
N -0.74799500 1.91692600 -0.40113600
C 2.55068900 1.07798000 1.26681300
C -0.75986600 2.37807200 -1.80589500
C -2.12997800 1.79451700 0.16884000
C 0.92268800 -0.09827400 2.63815900
C 0.43227800 2.18580000 1.76091300
C 0.07602200 2.83960600 0.43521700
N -0.19686400 -1.59507500 1.01189000
N -2.62331400 -0.59194200 -0.61266600
C -0.09239100 -2.90045700 0.31820000

C -3.12402900 -1.26177000 -1.81426200
C -3.06957500 0.80273100 -0.52679300
C 0.84787900 -1.50933800 2.07885200
C -1.56359200 -1.35656400 1.58130800
C -2.73315100 -1.42723200 0.58924500
H -0.47333600 2.00431800 2.37113700
H 1.09581800 2.85352000 2.35316500
H 0.99216300 3.07643700 -0.14166500
H -0.46609000 3.79774200 0.60569300
H 3.04734300 0.10792900 1.08560100
H 2.70803700 1.72436800 0.38562900
H 3.00555000 1.55414600 2.16369200
H 1.76443700 -0.01712900 3.35919000
H 0.00255400 0.16329100 3.19454300
H 1.80594300 -1.79918700 1.60261400
H 0.62853600 -2.24234300 2.88860100
H -0.21877900 -3.72970500 1.04968100
H -0.86822000 -2.97606200 -0.46347800
H 0.90221700 -2.94221800 -0.16672600
H -1.74615300 -2.11660200 2.37656800
H -1.55572400 -0.36933500 2.07995300
H -3.65236800 -1.17317900 1.17362300
H -2.86318200 -2.47481800 0.25506900
H -2.65259300 -2.25828800 -1.92109200
H -4.23412600 -1.40360000 -1.78723800
H -2.87488200 -0.66655300 -2.71416900
H -4.04849100 0.87498500 0.01178700
H -3.26275000 1.14848800 -1.56133800
H -2.03536300 1.53366400 1.23982000
H -2.61355100 2.79850700 0.12604500
H 0.27904000 2.38204800 -2.18639300
H -1.35418900 1.68815600 -2.43029100
H -1.18710500 3.40367700 -1.87685600
Co 0.15071300 0.01713000 -0.20229900
O -0.19640000 -0.71106000 -1.65331200
O 2.64912800 -1.88890400 -0.98383600
N 1.72366900 0.21582600 -1.43666400
C 2.69860600 -0.70852800 -1.42026000
C 4.00828500 -0.17107000 -2.01939000
H 4.29163700 -0.81061600 -2.88272300
H 4.81233200 -0.25389700 -1.25808100
H 3.93509000 0.88037200 -2.36165000

^{5}TS5A

BP86/BS1 SCF energy in solution: -2358.278811 a.u.
BP86/BS2 SCF energy in solution: -2359.648161 a.u.
BP86/BS2 Free energy in solution: -2359.24917 a.u.
1 5
N 1.07669300 0.75069800 -1.63241300
N -0.25472100 -1.75180900 -0.96226500
C 2.53217700 0.88983900 -1.43351700
C -0.05120000 -3.01649000 -0.21733600
C -1.63592600 -1.61718800 -1.49756200
C 0.47365800 2.07312300 -1.92106800
C 0.80378100 -0.26981200 -2.67099800
C 0.75517900 -1.65892900 -2.04975700
N -0.77309600 1.99056000 0.23505400
N -2.35850700 -0.45765500 0.61755700
C -0.83360000 2.57976800 1.58995400
C -2.68789100 -0.94315000 1.97351900
C -2.68080400 -1.50382700 -0.39348000
C 0.12968900 2.79718800 -0.62541900
C -2.12038900 1.84464200 -0.38178000
C -3.00770600 0.86209200 0.37427600
H -0.15538300 -0.02398500 -3.16701300
H 1.58248500 -0.25285600 -3.46774600
H 1.73609500 -1.91771100 -1.60261400
H 0.54019400 -2.41945900 -2.83662300
H 2.74443400 1.57562400 -0.59297700
H 2.98701400 -0.09236900 -1.20793600
H 3.00844600 1.29565300 -2.35664800
H 1.16523200 2.70756800 -2.52181000
H -0.43127100 1.92232200 -2.54128700
H 1.05037500 2.99195000 -0.03969700
H -0.33297800 3.78585800 -0.85292600
H -1.25898700 3.60915300 1.55655100
H -1.45305500 1.95742700 2.26151200
H 0.19064400 2.62185000 2.00660600
H -2.63011700 2.83574000 -0.43205700
H -1.98490900 1.49242100 -1.42250800
H -3.95537700 0.73066500 -0.19370800
H -3.28673800 1.28741300 1.35780000
H -2.39296500 -0.18904200 2.72630300
H -3.78149700 -1.14020500 2.06661900
H -2.13505400 -1.87795200 2.18329100
H -3.67045100 -1.30291000 -0.86026700
H -2.77356900 -2.47050500 0.13807700
H -1.66881400 -0.71144600 -2.13328500

H -1.88084900 -2.48883900 -2.14911100
H 0.94783800 -2.97995500 0.25843800
H -0.80614100 -3.12420700 0.58222900
H -0.12748300 -3.88985100 -0.90495500
Co -0.01726000 -0.05708800 0.39342800
O 2.64371300 -1.75239100 1.27876400
O 0.03125900 -0.78351800 1.94686000
N 1.61991300 0.36855900 1.29651900
C 2.65444900 -0.51130200 1.40040600
C 3.96300600 0.21910800 1.74073200
H 4.73869200 -0.06882900 1.00154300
H 4.29894100 -0.12938700 2.74114400
H 3.86297200 1.32165900 1.76652700

$^{2}[CoL]^{2+}$, L=13-TMC
BP86/BS1 SCF energy in solution: -2114.50922666 a.u.
BP86/BS2 SCF energy in solution: -2115.57782275 a.u.
BP86/BS2 Free energy in solution: -2115.19204575 a.u.
2 2

Co	-0.11372800	-0.06802900	0.47638100
N	0.26408700	1.81458900	-0.28136300
N	-2.06833400	0.35886200	0.37681900
N	-0.49578900	-1.69440300	-0.63796400
C	1.95513500	-1.83986500	-0.42128100
H	2.05245300	-2.78778900	0.14324000
H	2.90102500	-1.70425700	-0.98346800
C	1.31907800	1.71756200	-1.32865500
H	1.43354100	2.71411900	-1.81585900
H	0.91590700	1.03273200	-2.09968500
C	-1.61356400	-1.22747500	-1.50891900
H	-2.04572500	-2.07491700	-2.08902200
H	-1.19001100	-0.50631800	-2.23408500
C	-1.03973600	2.18749600	-0.92137300
H	-1.11225700	1.64914700	-1.88634800
H	-1.06328300	3.27743300	-1.14766900
C	-2.68687100	-0.57288800	-0.64483300
H	-3.41054700	-0.02250200	-1.28041900
H	-3.26289900	-1.34140700	-0.09454400
C	0.77666000	-1.90027300	-1.39009800
H	0.84548500	-1.09682300	-2.14850000
H	0.76601500	-2.87330100	-1.93238000
C	0.61136100	2.82107800	0.75661400
H	1.55882400	2.56214600	1.25969500
H	-0.18158400	2.86818700	1.52627900

H	0.72003100	3.82708800	0.29210600
C	-0.88259100	-2.90964300	0.12502600
H	-1.19333400	-3.71499600	-0.57678000
H	-1.72103700	-2.68650000	0.80991900
H	-0.03084100	-3.27574200	0.72576700
C	-2.67051100	0.13035600	1.71584700
H	-3.75844100	0.36606700	1.71268100
H	-2.16747900	0.77481700	2.46239100
H	-2.53742400	-0.92946900	2.00623100
C	-2.18484100	1.80416900	-0.00247300
H	-2.15001400	2.39957900	0.93105500
H	-3.16623200	2.00731000	-0.48263500
C	2.78517500	0.37096000	0.41250100
H	3.80084500	-0.08223600	0.47106300
H	2.68679100	1.01411300	1.30808400
C	2.70350500	1.22036400	-0.86125200
H	3.15113300	0.67100400	-1.71556000
H	3.37768500	2.08293200	-0.67810700
C	1.89027500	-1.23271300	1.97208500
H	2.90380100	-1.65449500	2.15500800
H	1.13825000	-2.02573500	2.14421700
H	1.71437500	-0.40391400	2.68537300
N	1.77391400	-0.71394300	0.57829600

^{4}[CoL]$^{2+}$, L=13-TMC

BP86/BS1 SCF energy in solution: -2114.50190395 a.u.

BP86/BS2 SCF energy in solution: -2115.5666991 a.u.

BP86/BS2 Free energy in solution: -2115.1832251 a.u.

2 4

Co	-0.07050400	-0.08036700	0.60455400
N	0.00181400	1.88160800	-0.29335400
N	-2.21039500	0.11549700	0.40133500
N	-0.30743300	-1.75809100	-0.67815100
C	2.18973200	-1.58742600	-0.51580300
H	2.41548800	-2.55313200	-0.02237900
H	3.07857300	-1.33436900	-1.13104900
C	1.07243200	1.85088200	-1.32898300
H	1.06487400	2.81329700	-1.89311100
H	0.76427600	1.06753800	-2.04892700
C	-1.50085600	-1.41060100	-1.48943500
H	-1.84876000	-2.28274900	-2.09043600
H	-1.20215100	-0.61763900	-2.20195100
C	-1.32939900	2.03260100	-0.94989200
H	-1.29974000	1.47110800	-1.90429800

H	-1.51822700	3.09967400	-1.20903900
C	-2.64272300	-0.92936800	-0.58554600
H	-3.47878000	-0.55174900	-1.21385400
H	-3.04194400	-1.78540900	-0.00742200
C	0.96861100	-1.74437200	-1.44369100
H	0.91513300	-0.90264000	-2.16139000
H	1.08497300	-2.67658800	-2.04288800
C	0.22320100	2.94558900	0.71032300
H	1.18973400	2.80045700	1.22728400
H	-0.58110800	2.92784500	1.47058600
H	0.22948900	3.94772900	0.22312700
C	-0.48935600	-3.01931700	0.07128900
H	-0.57904200	-3.88122200	-0.62863000
H	-1.40391900	-2.97190800	0.69179300
H	0.37115500	-3.19917200	0.74251500
C	-2.85204300	-0.11282800	1.71931500
H	-3.95925600	-0.00077500	1.66232100
H	-2.46124800	0.61837900	2.45432800
H	-2.61875900	-1.13463500	2.07671800
C	-2.45191400	1.51500800	-0.05548400
H	-2.53210000	2.14857800	0.84994000
H	-3.42436500	1.59437500	-0.59152500
C	2.77518400	0.69959000	0.38668000
H	3.86310600	0.45194000	0.40591500
H	2.57869800	1.29142400	1.30325900
C	2.51406200	1.57245200	-0.85237400
H	3.04647000	1.15181200	-1.73145700
H	3.02908400	2.53149900	-0.63212400
C	2.31116700	-1.11911000	1.89945300
H	3.38756400	-1.39877400	1.97099700
H	1.69678100	-2.01902500	2.09329000
H	2.09236800	-0.36406300	2.68008300
N	1.98982100	-0.55765800	0.56163500

^{2}[CoL]$^{2+}$, L=14-TMC

BP86/BS1 SCF energy in solution: -2153.80071714 a.u.

BP86/BS2 SCF energy in solution: -2154.91451191 a.u.

BP86/BS2 Free energy in solution: -2154.50129891 a.u.

2 2

Co	-0.00002300	0.00000900	0.27508500
N	1.14424800	-1.66158500	-0.20587300
N	-1.14424500	1.66167700	-0.20585900
N	-1.60974400	-1.29155600	0.33144500
N	1.60976200	1.29149500	0.33147500

C	2.58948700	1.07732700	-0.78610800
H	3.41028900	1.81827800	-0.65306900
H	2.06648300	1.33454800	-1.72940600
C	-1.04843800	-2.67777800	0.17337700
H	-1.82965800	-3.36578400	-0.21509400
H	-0.76038100	-3.05196100	1.17425100
C	3.18492700	-0.31948200	-0.91366700
H	3.79250800	-0.58812000	-0.02455400
H	3.90970800	-0.27717500	-1.75392700
C	-2.17649400	1.40930200	-1.25604400
H	-1.63087400	1.13551600	-2.18248000
H	-2.70708500	2.36960400	-1.45347700
C	1.04846100	2.67773100	0.17362600
H	1.82969500	3.36582600	-0.21467000
H	0.76035500	3.05171400	1.17455800
C	-3.18484000	0.31958200	-0.91363800
H	-3.79228400	0.58827100	-0.02444700
H	-3.90974200	0.27731000	-1.75379500
C	-0.14570800	2.63103100	-0.74960600
H	-0.60935700	3.63795800	-0.85525800
H	0.14327300	2.28856200	-1.76320900
C	1.77076600	-2.23907900	1.01920200
H	1.04144800	-2.29307300	1.84768000
H	2.62117800	-1.62284700	1.35466600
H	2.14579400	-3.26343800	0.79972700
C	-2.58949200	-1.07726700	-0.78610800
H	-3.41033900	-1.81817400	-0.65310000
H	-2.06651000	-1.33448300	-1.72942000
C	0.14577700	-2.63091700	-0.74978300
H	0.60949200	-3.63780800	-0.85551700
H	-0.14314200	-2.28835700	-1.76337400
C	2.17662500	-1.40928200	-1.25595300
H	1.63108600	-1.13564000	-2.18247800
H	2.70726300	-2.36959100	-1.45322500
C	-1.77105500	2.23912000	1.01909800
H	-1.04205800	2.29276900	1.84787300
H	-2.62180600	1.62305800	1.35399100
H	-2.14574000	3.26362100	0.79968900
C	-2.28009100	-1.21335200	1.65619500
H	-3.05564700	-2.00669800	1.74338800
H	-2.77065300	-0.23595500	1.79886400
H	-1.53087500	-1.35424700	2.45874000
C	2.28017000	1.21306500	1.65617400
H	3.05577600	2.00635500	1.74345200

H	2.77069700	0.23561900	1.79862100
H	1.53101700	1.35386400	2.45879300

$^{4}[CoL]^{2+}$, L=14-TMC
BP86/BS1 SCF energy in solution: -2153.78910512 a.u.
BP86/BS2 SCF energy in solution: -2154.90015423 a.u.
BP86/BS2 Free energy in solution: -2154.48977623 a.u.
2 4

Co	0.00002600	-0.00000600	0.32412100
N	-0.88806000	1.86626200	-0.22033000
N	0.88804700	-1.86627100	-0.22033600
N	1.88247300	1.11850600	0.34325100
N	-1.88247300	-1.11849700	0.34326200
C	-2.73987200	-0.70223600	-0.80930400
H	-3.68176100	-1.30053700	-0.77166400
H	-2.21192000	-0.99741400	-1.73975200
C	1.47401900	2.54132300	0.14815500
H	2.31466300	3.13576200	-0.27682900
H	1.25379700	2.97409500	1.14345100
C	-3.09776000	0.78354500	-0.89844400
H	-3.63745100	1.12313700	0.01010400
H	-3.84074400	0.87343500	-1.71945900
C	1.95412000	-1.73617500	-1.25350700
H	1.45671400	-1.38885800	-2.18337500
H	2.36791900	-2.75051400	-1.46525200
C	-1.47403300	-2.54131500	0.14816300
H	-2.31468500	-3.13574600	-0.27681700
H	-1.25380800	-2.97410200	1.14345100
C	3.09775200	-0.78355000	-0.89844000
H	3.63745000	-1.12315100	0.01010200
H	3.84072800	-0.87345900	-1.71945800
C	-0.25501500	-2.65500300	-0.75785600
H	0.03221900	-3.72592900	-0.87234200
H	-0.47981400	-2.26624400	-1.77192900
C	-1.40855100	2.48010400	1.02522800
H	-0.64114500	2.46132000	1.82200900
H	-2.29163000	1.92842700	1.39052400
H	-1.70318100	3.53870500	0.84110500
C	2.73987300	0.70223700	-0.80931200
H	3.68176400	1.30053300	-0.77167500
H	2.21192200	0.99740100	-1.73976400
C	0.25499700	2.65500000	-0.75785200
H	-0.03224900	3.72592300	-0.87234500
H	0.47979500	2.26625100	-1.77193000

C	-1.95412800	1.73617000	-1.25351000
H	-1.45672300	1.38883800	-2.18337300
H	-2.36791000	2.75051400	-1.46526500
C	1.40854000	-2.48009300	1.02523900
H	0.64119700	-2.46113800	1.82207500
H	2.29171600	-1.92850200	1.39043000
H	1.70301700	-3.53874600	0.84117500
C	2.61310300	0.99272900	1.62386200
H	3.50044500	1.66773400	1.65126000
H	2.96625600	-0.04392700	1.77323000
H	1.94084000	1.25690400	2.46396500
C	-2.61311800	-0.99271500	1.62386100
H	-3.50044600	-1.66773700	1.65126400
H	-2.96629000	0.04393800	1.77320900
H	-1.94086300	-1.25685600	2.46398400

^{2}TS1, L=13-TMC
BP86/BS1 SCF energy in solution: -2265.95807021 a.u.
BP86/BS2 SCF energy in solution: -2267.22302748 a.u.
BP86/BS2 Free energy in solution: -2266.81207448 a.u.
2 2

N	-0.14655600	1.87595100	0.56367800
N	2.12018000	0.09604600	0.01382900
N	0.22254600	-1.63880300	1.03485100
C	-2.19108500	-1.66901500	0.62016800
H	-2.27825800	-2.64496000	0.10684900
H	-3.18177500	-1.45457500	1.07007300
C	-1.22814000	1.77839400	1.57421400
H	-1.30174300	2.74100500	2.13299000
H	-0.89602800	1.01787200	2.30664000
C	1.30885900	-1.25554900	1.97947800
H	1.58131900	-2.11259500	2.63543300
H	0.91269300	-0.45105600	2.62774200
C	1.17685200	2.06171600	1.22808400
H	1.16420700	1.52129000	2.19361700
H	1.34726200	3.13634300	1.46342500
C	2.51864700	-0.79657800	1.17677000
H	3.24437500	-0.26652500	1.82767700
H	3.04719200	-1.67097900	0.75292500
C	-1.11361800	-1.73254400	1.69188500
H	-1.19597000	-0.89243000	2.40631600
H	-1.19932400	-2.67625700	2.27506400
C	-0.38839300	3.01288700	-0.35859500
H	-1.34611800	2.89850500	-0.89760500

H	0.42994500	3.08918300	-1.09869300
H	-0.43278200	3.96469000	0.21845700
C	0.55609400	-2.90089200	0.31174500
H	0.64247700	-3.73357600	1.04366900
H	1.51348800	-2.79837100	-0.22956300
H	-0.23101000	-3.14964000	-0.42245400
C	2.97512900	-0.23686700	-1.15736600
H	4.04788600	-0.10469700	-0.89669900
H	2.73279100	0.43990400	-1.99603000
H	2.80598400	-1.28759900	-1.45947600
C	2.29061800	1.55116000	0.33287100
H	2.29189300	2.10022700	-0.62923100
H	3.28192400	1.71595700	0.80859700
C	-2.70713900	0.60802000	-0.28914100
H	-3.77027300	0.30740900	-0.42926000
H	-2.46211400	1.24854300	-1.15961400
C	-2.61708200	1.40989900	1.01479900
H	-3.16384200	0.88112700	1.82331600
H	-3.20404700	2.33128300	0.81681300
C	-2.17679700	-1.21412200	-1.77349500
H	-3.23694300	-1.54681800	-1.80369400
H	-1.51833500	-2.08138900	-1.96275700
H	-2.02734600	-0.46583800	-2.57271600
N	-1.86770300	-0.62603700	-0.43699900
Co	0.12352100	-0.17020800	-0.32711800
O	0.27897000	0.66806200	-2.00183300
H	-0.54390100	1.06464800	-2.37576400
O	0.41910100	-0.42808600	-3.30932700
H	1.30379800	-0.09401600	-3.59060300

^{2}TS1, L=14-TMC
BP86/BS1 SCF energy in solution: -2305.25199297 a.u.
BP86/BS2 SCF energy in solution: -2306.56421462 a.u.
BP86/BS2 Free energy in solution: -2306.12733862 a.u.
2 2

N	-1.11352400	1.79154100	-0.15948300
N	1.08636300	-1.62407800	-0.61409200
N	1.68407300	1.28071500	0.15841400
N	-1.70658100	-1.23030600	-0.05556600
C	-2.57790800	-0.85768700	-1.21544500
H	-3.41785200	-1.58751900	-1.25126600
H	-1.98560400	-0.99383300	-2.14289400
C	1.13785900	2.67359700	0.29318200
H	1.91458300	3.41251400	0.00025900

H	0.91416800	2.84856500	1.36427900
C	-3.12483600	0.56425200	-1.17813600
H	-3.76820000	0.73964400	-0.29181300
H	-3.79714800	0.67055500	-2.05516100
C	2.04395400	-1.27917700	-1.71475500
H	1.42783000	-0.95967300	-2.58007200
H	2.56305000	-2.21863700	-2.01220600
C	-1.14528800	-2.60108900	-0.29248500
H	-1.93239100	-3.25874000	-0.72093300
H	-0.86217200	-3.02783900	0.68840200
C	3.06409200	-0.19268500	-1.40625300
H	3.76942300	-0.49713200	-0.60598800
H	3.68843000	-0.08148500	-2.31742500
C	0.04344500	-2.51757200	-1.21169300
H	0.47428800	-3.52602400	-1.39859800
H	-0.24274700	-2.09771100	-2.19576800
C	-1.83434300	2.25203100	1.05895300
H	-1.11068900	2.54374800	1.84196300
H	-2.48292900	1.45889400	1.46520000
H	-2.45610200	3.13740700	0.80440100
C	2.45175400	1.17582100	-1.12771900
H	3.25472400	1.94646900	-1.09524600
H	1.76423100	1.45055700	-1.95353400
C	-0.10062900	2.82904900	-0.55030700
H	-0.53782800	3.84395800	-0.43122000
H	0.12989200	2.69797500	-1.62500300
C	-2.05333600	1.63513000	-1.32107800
H	-1.42685300	1.41034000	-2.20994900
H	-2.52552100	2.62876300	-1.49310700
C	1.76948200	-2.33743700	0.49903800
H	1.08040500	-2.45977200	1.35538200
H	2.64677500	-1.76436500	0.84493200
H	2.12017500	-3.33214700	0.14859700
C	2.60159400	1.06246100	1.31175600
H	3.43539800	1.79547400	1.25440400
H	3.02931100	0.04723400	1.31192400
H	2.07688700	1.22882200	2.27057800
C	-2.52268100	-1.30757200	1.18720300
H	-3.31006600	-2.08067300	1.04884300
H	-3.01732900	-0.34541700	1.40176800
H	-1.87404000	-1.57809900	2.03755000
Co	-0.01020200	0.04254100	0.01919400
O	-0.14763200	-0.09739200	1.87107400
H	0.27149300	0.64814900	2.35928100

O	0.27911100	-1.23848900	3.29080500
H	1.23875900	-1.28141300	3.07064200

^{2}IM2, L=13-TMC
BP86/BS1 SCF energy in solution: -2189.6230483 a.u.
BP86/BS2 SCF energy in solution: -2190.78708194 a.u.
BP86/BS2 Free energy in solution: -2190.39599394 a.u.
2 2

Co	-0.10709400	-0.10241200	0.54483500
N	0.08706500	1.80928000	-0.47636800
N	-2.14182800	0.09542000	0.29632900
N	-0.29885700	-1.68838300	-0.76382400
C	2.13150300	-1.70194200	-0.46083500
H	2.23436700	-2.64766700	0.10251300
H	3.10048800	-1.52071800	-0.96851100
C	1.11623200	1.67633500	-1.54025200
H	1.13815600	2.62543000	-2.12306500
H	0.74596100	0.89516400	-2.23155500
C	-1.44238800	-1.35130700	-1.65400400
H	-1.75662500	-2.23746900	-2.24908800
H	-1.09229900	-0.57820900	-2.36367700
C	-1.27626100	1.99290400	-1.06430900
H	-1.32581300	1.42704000	-2.01328200
H	-1.43234700	3.06481500	-1.31431400
C	-2.60205200	-0.85782200	-0.79495700
H	-3.36872300	-0.35813700	-1.42143100
H	-3.09834800	-1.70970300	-0.29423300
C	1.00323600	-1.81115900	-1.47850700
H	1.05128400	-1.00660000	-2.23602400
H	1.06568600	-2.78124600	-2.01929600
C	0.39606100	2.94605400	0.43215000
H	1.34539300	2.78459000	0.96871900
H	-0.40806000	3.07301700	1.17702100
H	0.48106400	3.87055200	-0.18062000
C	-0.58408400	-2.90764200	0.04353800
H	-0.71051300	-3.77810200	-0.63643800
H	-1.50875900	-2.77924200	0.63280600
H	0.24347200	-3.11921600	0.74351300
C	-2.87932200	-0.19120100	1.55672300
H	-3.97100600	-0.06770800	1.38926100
H	-2.54443500	0.50950700	2.34303900
H	-2.67624600	-1.22910100	1.88131700
C	-2.33796500	1.53213300	-0.08280800
H	-2.29312100	2.13112900	0.84739700

H	-3.35128700	1.66742500	-0.51749000
O	-0.10836200	0.63936300	2.03552000
C	2.70981200	0.62032400	0.29365900
H	3.77568100	0.31339000	0.38471800
H	2.51025100	1.30425800	1.13989700
C	2.53885600	1.34344500	-1.04680800
H	3.03517500	0.77085100	-1.85733300
H	3.12853100	2.27726000	-0.93887500
C	2.20949900	-1.10471300	1.91814800
H	3.26272900	-1.45790500	1.93468000
H	1.53901500	-1.94399200	2.18143800
H	2.08229900	-0.29001100	2.65365600
N	1.87615100	-0.59798000	0.55245300

^{4}IM2, L=13-TMC
BP86/BS1 SCF energy in solution: -2189.6368764 a.u.
BP86/BS2 SCF energy in solution: -2190.80083368 a.u.
BP86/BS2 Free energy in solution: -2190.41100368 a.u.
2 4

Co	-0.10112600	-0.13458300	0.52933400
N	0.04468200	1.92156300	-0.45268800
N	-2.13966800	0.06418100	0.30206900
N	-0.28013200	-1.72904500	-0.76334700
C	2.16501200	-1.67846000	-0.49579700
H	2.29943700	-2.62792400	0.05488300
H	3.11933600	-1.46904700	-1.02035100
C	1.06038800	1.74448200	-1.51836500
H	1.09439000	2.66306200	-2.15019000
H	0.68126100	0.93533000	-2.17210600
C	-1.42557700	-1.36734000	-1.64845200
H	-1.73290900	-2.24200100	-2.26383600
H	-1.07363100	-0.57858700	-2.33999700
C	-1.32885100	2.04166900	-1.01578400
H	-1.36304500	1.49045000	-1.97483000
H	-1.55783500	3.10587300	-1.24615600
C	-2.59185200	-0.88514000	-0.79506200
H	-3.35455700	-0.38548300	-1.42638700
H	-3.08840400	-1.74123700	-0.30127200
C	1.02141100	-1.80267900	-1.49374800
H	1.03612200	-0.98333300	-2.23647300
H	1.09745600	-2.76163000	-2.05201500
C	0.34297800	3.05132500	0.44938500
H	1.31978000	2.92211300	0.94705000
H	-0.43372600	3.13180500	1.23163200

H	0.36484200	3.99854100	-0.13629600
C	-0.54356500	-2.96642300	0.01818400
H	-0.64178500	-3.82765300	-0.67780900
H	-1.47677400	-2.86767700	0.60028600
H	0.28607900	-3.16341300	0.72096200
C	-2.84726500	-0.26409300	1.56991100
H	-3.94411500	-0.16285200	1.42254000
H	-2.51599000	0.42849100	2.36454700
H	-2.61467500	-1.30347500	1.86965300
C	-2.36642800	1.50685000	-0.03983900
H	-2.33318200	2.07680900	0.90906800
H	-3.38694800	1.62515900	-0.46327000
O	-0.07052500	0.54761900	2.03339000
C	2.68345000	0.66403400	0.28876800
H	3.76107800	0.39846800	0.37473400
H	2.45340100	1.32089700	1.14903500
C	2.48728000	1.41514300	-1.03366300
H	2.98924700	0.87150900	-1.86126200
H	3.06700600	2.35317700	-0.90447600
C	2.26068100	-1.10778600	1.88598100
H	3.32825400	-1.41560300	1.89241400
H	1.62826300	-1.98092900	2.13517500
H	2.10161000	-0.31372200	2.63768200
N	1.90064000	-0.59295700	0.53236800

^{2}IM2, L=14-TMC
BP86/BS1 SCF energy in solution: -2228.91585272 a.u.
BP86/BS2 SCF energy in solution: -2230.12384917 a.u.
BP86/BS2 Free energy in solution: -2229.70581217 a.u.
2 2

Co	0.00451300	0.00197600	0.21155700
N	1.05494800	-1.75456300	-0.19850000
N	-1.05683300	1.75255300	-0.19779300
N	-1.74007400	-1.20989800	0.22976400
N	1.73850700	1.21080900	0.22974100
O	-0.00082300	-0.00373900	1.89670200
C	2.51438400	0.95516800	-1.02674100
H	3.35550200	1.68386800	-1.05131800
H	1.85246900	1.18517500	-1.88655200
C	-1.20864000	-2.61112300	0.23602100
H	-2.00604700	-3.30997800	-0.09747800
H	-0.96249700	-2.87180800	1.28308100
C	3.05406100	-0.46468600	-1.17063900
H	3.75117000	-0.72900900	-0.34993000

H	3.67121800	-0.47753100	-2.09323700
C	-1.98059900	1.52299000	-1.35938100
H	-1.33841200	1.24420200	-2.22043500
H	-2.44790700	2.50417700	-1.60199800
C	1.20693100	2.61270500	0.23411300
H	2.00388900	3.31058500	-0.10221000
H	0.96247100	2.87510500	1.28107300
C	-3.05638100	0.46359200	-1.17076600
H	-3.75446700	0.72831000	-0.35096400
H	-3.67260100	0.47646800	-2.09401200
C	-0.00653800	2.72346500	-0.64996900
H	-0.41931700	3.75503100	-0.62815900
H	0.24489600	2.49407700	-1.70351400
C	1.76267000	-2.31609600	0.98296700
H	1.03065700	-2.55953400	1.77304900
H	2.48212100	-1.59453200	1.40061800
H	2.30411700	-3.23838200	0.68160100
C	-2.51636000	-0.95598600	-1.02601500
H	-3.35763100	-1.68467200	-1.05008000
H	-1.85504000	-1.18643800	-1.88614200
C	0.00366400	-2.72444200	-0.64940700
H	0.41506700	-3.75658500	-0.62693900
H	-0.24833500	-2.49563600	-1.70292100
C	1.97831700	-1.52427100	-1.36023900
H	1.33595700	-1.24473500	-2.22097100
H	2.44572500	-2.50512100	-1.60373200
C	-1.76356600	2.31283700	0.98477400
H	-1.03085500	2.55539300	1.77453200
H	-2.48268700	1.59065500	1.40183800
H	-2.30502200	3.23559600	0.68481000
C	-2.60919500	-1.08310400	1.42889400
H	-3.32526000	-1.93272200	1.44499200
H	-3.19367900	-0.14876300	1.41157300
H	-1.97091300	-1.09860000	2.32992500
C	2.60966600	1.08665000	1.42834500
H	3.33992200	1.92427600	1.42769200
H	3.17771800	0.14215400	1.42431900
H	1.97617900	1.12703100	2.33161400

[4]IM2, L=14-TMC
BP86/BS1 SCF energy in solution: -2228.92568485 a.u.
BP86/BS2 SCF energy in solution: -2230.1336822 a.u.
BP86/BS2 Free energy in solution: -2229.7166012 a.u.
2 4

Co	0.00002700	-0.00003600	0.34580300
N	1.22946800	-1.69634100	-0.30002500
N	-1.22942000	1.69632600	-0.30005700
N	-1.60203300	-1.35494700	0.27777300
N	1.60200100	1.35492900	0.27781500
O	-0.00006700	0.00010400	2.01152500
C	2.38540500	1.14798900	-0.99047500
H	3.14668600	1.95935300	-1.01837200
H	1.69453200	1.32051000	-1.83955800
C	-0.94777800	-2.70704000	0.22862000
H	-1.70406700	-3.46251200	-0.07518900
H	-0.62750900	-2.95938600	1.25796600
C	3.07522200	-0.19953000	-1.17690700
H	3.77879700	-0.42333900	-0.34944500
H	3.71124700	-0.09411500	-2.08052800
C	-2.12612700	1.36427400	-1.44145200
H	-1.47725700	1.12412100	-2.30895100
H	-2.70915600	2.27717100	-1.70429500
C	0.94774700	2.70702300	0.22877800
H	1.70407200	3.46250300	-0.07491300
H	0.62739700	2.95927700	1.25811500
C	-3.07525200	0.19967200	-1.17685800
H	-3.77878800	0.42355800	-0.34937600
H	-3.71131900	0.09428200	-2.08045200
C	-0.22611100	2.71438900	-0.72418900
H	-0.69116300	3.72506500	-0.74779000
H	0.08981600	2.48076100	-1.75932700
C	2.00554700	-2.22941700	0.85069700
H	1.32913700	-2.48886400	1.68383600
H	2.73049700	-1.48685000	1.22162400
H	2.56091000	-3.13942200	0.53262700
C	-2.38555800	-1.14790400	-0.99043700
H	-3.14695500	-1.95916300	-1.01825400
H	-1.69481000	-1.32052600	-1.83959500
C	0.22614500	-2.71434100	-0.72426800
H	0.69119400	-3.72501900	-0.74794800
H	-0.08969100	-2.48060500	-1.75940700
C	2.12615300	-1.36420700	-1.44142700
H	1.47724800	-1.12406400	-2.30890200
H	2.70921100	-2.27707000	-1.70432800
C	-2.00555200	2.22925000	0.85071300
H	-1.32921000	2.48836000	1.68400700
H	-2.73068100	1.48670600	1.22133400
H	-2.56073600	3.13941600	0.53279300

C	-2.48616800	-1.32450900	1.47171200
H	-3.21904400	-2.15656800	1.39750900
H	-3.04052800	-0.37396100	1.54139300
H	-1.87174700	-1.45151000	2.38124100
C	2.48629000	1.32442800	1.47164200
H	3.21922700	2.15642800	1.39733900
H	3.04059800	0.37384600	1.54126600
H	1.87201800	1.45151300	2.38125700

^{CS}IM4, L=13-TMC

BP86/BS1 SCF energy in solution: -2190.27170009 a.u.

BP86/BS2 SCF energy in solution: -2191.43808356 a.u.

BP86/BS2 Free energy in solution: -2191.03343056 a.u.

2 1

Co	-0.11561400	-0.10098300	0.52229000
N	0.04381300	1.70380600	-0.53402000
N	-2.14914900	0.05603500	0.28383300
N	-0.24962500	-1.66087300	-0.76037400
C	2.16700100	-1.65422300	-0.42408700
H	2.26232300	-2.58917900	0.15810700
H	3.14617000	-1.48391400	-0.91625000
C	1.07680800	1.61933000	-1.60258400
H	1.05772100	2.57736000	-2.16942400
H	0.73727900	0.84005200	-2.30902300
C	-1.40274300	-1.38011200	-1.65615400
H	-1.68558500	-2.29116200	-2.22933100
H	-1.07973200	-0.61705800	-2.38786600
C	-1.32011800	1.89358200	-1.13302800
H	-1.38582200	1.30125200	-2.06451600
H	-1.45227000	2.95992100	-1.41519200
C	-2.57929700	-0.91386300	-0.80269600
H	-3.35901100	-0.44313100	-1.43624500
H	-3.05425800	-1.77787800	-0.30197300
C	1.05853300	-1.79017900	-1.45896200
H	1.11159200	-1.00742400	-2.23734200
H	1.13410100	-2.77306100	-1.97459400
C	0.32594300	2.87642500	0.35100000
H	1.31328500	2.78847400	0.83174700
H	-0.44180200	2.95843000	1.13777200
H	0.32394300	3.79291700	-0.27780600
C	-0.51734200	-2.87450900	0.06892900
H	-0.63092300	-3.75677900	-0.59728300
H	-1.44248300	-2.75151100	0.65863400
H	0.31293600	-3.06141300	0.77265700

C	-2.89635700	-0.21688600	1.53764600
H	-3.98650600	-0.08012900	1.36844600
H	-2.54592000	0.48051200	2.31904400
H	-2.70917100	-1.25703900	1.86570800
C	-2.37250500	1.47443700	-0.12770100
H	-2.31659500	2.10053100	0.78348900
H	-3.39177600	1.59257400	-0.55441400
O	-0.23098900	0.69158100	2.15779700
C	2.71575100	0.67846200	0.25585500
H	3.78657500	0.38701300	0.34120100
H	2.53083400	1.39737900	1.07670700
C	2.51367000	1.33930600	-1.11278800
H	3.01256100	0.73828800	-1.90089700
H	3.08447800	2.28908200	-1.05921500
C	2.26109100	-1.00938100	1.93030500
H	3.31009900	-1.37590100	1.92551800
H	1.58950200	-1.83446400	2.23522400
H	2.18640700	-0.18450200	2.66258800
N	1.88980800	-0.53009700	0.56545700
H	0.62500500	1.03822500	2.49164300

^{3}IM4, L=13-TMC
BP86/BS1 SCF energy in solution: -2190.27568355 a.u.
BP86/BS2 SCF energy in solution: -2191.44113277 a.u.
BP86/BS2 Free energy in solution: -2191.04106877 a.u.
2 3

Co	-0.10923500	-0.14371400	0.48447900
N	0.05177000	1.89184800	-0.49349000
N	-2.13568200	0.06051300	0.28566500
N	-0.27339900	-1.73850200	-0.75666400
C	2.16079000	-1.68361600	-0.46311100
H	2.27471700	-2.62422500	0.10714900
H	3.12745000	-1.49697900	-0.97400000
C	1.06138300	1.72361500	-1.56658800
H	1.09842400	2.64670700	-2.19153300
H	0.67730200	0.92043900	-2.22504800
C	-1.41567100	-1.38635500	-1.65102400
H	-1.71973400	-2.26891400	-2.25666700
H	-1.05891300	-0.60747700	-2.35137600
C	-1.32497800	2.01911500	-1.05269800
H	-1.36818800	1.45693700	-2.00549200
H	-1.54513500	3.08259000	-1.29568700
C	-2.58631200	-0.88967300	-0.80985000
H	-3.34042700	-0.39196300	-1.45351800

H	-3.09380700	-1.74038700	-0.31747300
C	1.03321500	-1.81950000	-1.47496800
H	1.05348500	-1.00802800	-2.22620800
H	1.11721100	-2.78462500	-2.02151100
C	0.35250600	3.02969000	0.39881600
H	1.36286700	2.93877800	0.83443900
H	-0.37884200	3.06828800	1.22634500
H	0.30581600	3.98059900	-0.17937700
C	-0.54279600	-2.96600400	0.03655000
H	-0.62948900	-3.83759000	-0.64788600
H	-1.48347100	-2.86091400	0.60549500
H	0.27816800	-3.14856700	0.75334500
C	-2.86234200	-0.24951500	1.54492100
H	-3.95402300	-0.10108000	1.39686000
H	-2.49842400	0.41863500	2.34490600
H	-2.67569200	-1.30105800	1.83500300
C	-2.35987800	1.50075500	-0.06626300
H	-2.31490600	2.07803800	0.87756900
H	-3.38307200	1.62439500	-0.48304200
O	-0.20216000	0.60425000	2.12935200
C	2.68570500	0.66559000	0.25717800
H	3.76227400	0.39529700	0.34307600
H	2.47527300	1.35598500	1.09678200
C	2.48837600	1.37954200	-1.08651800
H	2.97214500	0.79979800	-1.90040300
H	3.08847500	2.30897200	-0.99342400
C	2.28241900	-1.07759700	1.89117400
H	3.33577600	-1.43025400	1.86429600
H	1.62550900	-1.91807500	2.18634600
H	2.21898900	-0.27309300	2.64832600
N	1.88867100	-0.57460100	0.54145500
H	0.68283600	0.81297100	2.50247900

^{CS}IM4, L=14-TMC

BP86/BS1 SCF energy in solution: -2229.56359841 a.u.

BP86/BS2 SCF energy in solution: -2230.77431035 a.u.

BP86/BS2 Free energy in solution: -2230.34747235 a.u.

2 1

Co	0.00380100	-0.00315700	0.16267100
N	1.09552400	-1.73444300	-0.20217100
N	-1.10249500	1.73057100	-0.18459300
N	-1.70980800	-1.23385500	0.20458600
N	1.69881700	1.24992800	0.20147500
O	-0.03954000	-0.03927100	1.99550800

C	2.47241000	1.00734300	-1.05999400
H	3.28514900	1.76686100	-1.10727400
H	1.79067500	1.19494600	-1.91520400
C	-1.15626600	-2.62587900	0.21480300
H	-1.93911400	-3.34175600	-0.11771300
H	-0.90525900	-2.87809500	1.26283300
C	3.06081600	-0.39526100	-1.18247800
H	3.76264000	-0.62346100	-0.35484900
H	3.68247000	-0.40131000	-2.10225000
C	-2.03870200	1.49790700	-1.33686300
H	-1.40057500	1.24888100	-2.21033800
H	-2.53520000	2.46916800	-1.56137300
C	1.14460600	2.64497000	0.20423700
H	1.92298100	3.35571700	-0.14855900
H	0.90921900	2.90956400	1.25284400
C	-3.08421800	0.40519600	-1.16479800
H	-3.78620700	0.63462700	-0.33757300
H	-3.70439900	0.41777300	-2.08552000
C	-0.08590600	2.72575900	-0.65684700
H	-0.51883100	3.74945500	-0.63273800
H	0.15460600	2.49917500	-1.71388300
C	1.81451800	-2.30937600	0.96373800
H	1.10214100	-2.51092200	1.78395300
H	2.58991700	-1.61979900	1.33796200
H	2.30710100	-3.25967700	0.66525200
C	-2.50238800	-1.00003100	-1.04383300
H	-3.32127800	-1.75402800	-1.07140200
H	-1.83931000	-1.19966000	-1.91088000
C	0.06084600	-2.71634400	-0.66589200
H	0.48480900	-3.74373100	-0.65497300
H	-0.19291000	-2.47914900	-1.71750400
C	2.02022200	-1.49217000	-1.36104200
H	1.37500300	-1.23785600	-2.22753800
H	2.51811500	-2.45996300	-1.59620100
C	-1.80187500	2.27381400	1.00642700
H	-1.06918100	2.47972300	1.80651600
H	-2.53223900	1.55084900	1.40361600
H	-2.33192700	3.21184400	0.73303800
C	-2.58134600	-1.12773300	1.40565000
H	-3.29725500	-1.97786200	1.40692200
H	-3.16497100	-0.19293200	1.40454900
H	-1.94309700	-1.15693100	2.30546600
C	2.60261000	1.17113400	1.38241600
H	3.40884900	1.92851000	1.27333100

H	3.07589100	0.18041000	1.48213100
H	2.02935700	1.39945400	2.29899500
H	0.87031800	-0.20180000	2.32397500

^{3}IM4, L=14-TMC
BP86/BS1 SCF energy in solution: -2229.56582586 a.u.
BP86/BS2 SCF energy in solution: -2230.77639243 a.u.
BP86/BS2 Free energy in solution: -2230.34850043 a.u.
2 3

Co	-0.01251700	0.00853500	0.30407600
N	1.11723400	-1.73864400	-0.32586000
N	-1.10722100	1.74280000	-0.28384700
N	-1.68812000	-1.24696900	0.24419700
N	1.66484900	1.26525900	0.25736500
O	-0.00368800	-0.20191600	2.12260300
C	2.42402200	1.02662900	-1.02167700
H	3.22059600	1.80296600	-1.06504600
H	1.73042400	1.21890300	-1.86422400
C	-1.11216700	-2.63239500	0.18979900
H	-1.90655200	-3.34590100	-0.11954700
H	-0.80853700	-2.90762500	1.21795000
C	3.04722700	-0.35323800	-1.20464400
H	3.73680300	-0.60953800	-0.37440500
H	3.68899200	-0.28610400	-2.10794300
C	-2.03449300	1.48719000	-1.42564600
H	-1.40417600	1.21418600	-2.29723400
H	-2.54604200	2.44589100	-1.67187800
C	1.10707000	2.66013600	0.22259000
H	1.90461300	3.36945200	-0.08720200
H	0.81153700	2.92916800	1.25546700
C	-3.06711400	0.39420700	-1.17946600
H	-3.75080100	0.65595800	-0.34618700
H	-3.71068400	0.35505900	-2.08315000
C	-0.07562700	2.73541100	-0.71149100
H	-0.50882500	3.75970100	-0.70916500
H	0.21350900	2.50793700	-1.75538300
C	1.85739800	-2.32235600	0.82499800
H	1.16760700	-2.51064900	1.66584800
H	2.64589200	-1.63749500	1.17886000
H	2.33505300	-3.27630300	0.51022300
C	-2.47666300	-1.00174600	-1.01118600
H	-3.29480100	-1.75626900	-1.02998300
H	-1.81305400	-1.21718000	-1.87236700
C	0.06192200	-2.70033600	-0.75819500

H	0.47386000	-3.73361400	-0.78716800
H	-0.23769100	-2.44282000	-1.79268800
C	2.03642800	-1.46406700	-1.46544300
H	1.40424000	-1.19082000	-2.33563600
H	2.56527700	-2.41073700	-1.72290700
C	-1.83955700	2.29280000	0.89087000
H	-1.13708500	2.49627800	1.71828600
H	-2.59987300	1.58380700	1.25408000
H	-2.34532700	3.23897500	0.59825100
C	-2.56944600	-1.19160700	1.44058200
H	-3.30279200	-2.02498800	1.38809900
H	-3.12842500	-0.24197500	1.48637400
H	-1.94694100	-1.28781000	2.34688500
C	2.59164500	1.19531800	1.41896000
H	3.44421700	1.88739900	1.24790100
H	2.99277400	0.17855800	1.56573700
H	2.07210400	1.52949600	2.33717000
H	0.79051100	0.17818800	2.55682700

^{OS}IM5, L=13-TMC

BP86/BS1 SCF energy in solution: -2265.36195531 a.u.

BP86/BS2 SCF energy in solution: -2266.62111604 a.u.

BP86/BS2 Free energy in solution: -2266.21635304 a.u.

2 1

Co	0.11816800	0.03790100	0.43247400
N	-0.12245500	-1.40213400	-1.05938000
N	2.16200800	-0.27644500	0.24373300
N	0.50143500	1.86071500	-0.37919400
C	-1.93771000	2.01167600	-0.26736900
H	-2.06578100	2.79042700	0.50749300
H	-2.85544500	2.02613400	-0.88867900
C	-1.08309400	-0.93446600	-2.09733600
H	-1.08069400	-1.68063500	-2.92343700
H	-0.65854100	-0.00542800	-2.51978100
C	1.69665300	1.69779200	-1.25041900
H	2.09920700	2.69042200	-1.55296100
H	1.37195900	1.17711900	-2.17062500
C	1.24514200	-1.55882800	-1.66055700
H	1.39933500	-0.74853900	-2.39622100
H	1.29500800	-2.51800000	-2.21910800
C	2.75275300	0.92031000	-0.47761900
H	3.56826000	0.58645300	-1.15207900
H	3.21406000	1.57042200	0.28857500
C	-0.71108500	2.30746100	-1.11809300

H	-0.73685400	1.77096200	-2.08383200
H	-0.65359600	3.39445300	-1.34845700
C	-0.55344100	-2.72942500	-0.53388100
H	-1.47443900	-2.64784500	0.06482700
H	0.23929500	-3.16757900	0.09675200
H	-0.74261700	-3.40204000	-1.39737300
C	0.80001900	2.78536300	0.75398000
H	1.21008100	3.73764200	0.35330200
H	1.53823000	2.34061500	1.44668600
H	-0.11767900	3.00890400	1.32474500
C	2.86008700	-0.45510400	1.54346600
H	3.94409000	-0.63233300	1.37187200
H	2.42531700	-1.32008100	2.07546100
H	2.73554100	0.45516000	2.16012500
C	2.28766500	-1.52906800	-0.56235000
H	2.15462400	-2.38455600	0.12797100
H	3.30976200	-1.60743200	-0.99143200
O	0.13407400	-1.14195700	1.82324600
C	-2.74781200	-0.34817600	-0.13662000
H	-3.78956500	0.02660300	-0.02347500
H	-2.66632300	-1.23686500	0.51679600
C	-2.52672300	-0.71973800	-1.60842200
H	-2.97620100	0.04879400	-2.27076700
H	-3.12303700	-1.64089800	-1.77194300
C	-2.22655500	0.88167200	1.87925200
H	-3.23746600	1.34152400	1.91982000
H	-1.50426500	1.55804600	2.37407500
H	-2.24629600	-0.08674600	2.40579200
N	-1.82920400	0.67284000	0.45246300
O	-1.03444200	-1.82014500	2.29858200
H	-0.68144700	-2.73285600	2.43689300

^{3}IM5, L=13-TMC
BP86/BS1 SCF energy in solution: -2265.36315918 a.u.
BP86/BS2 SCF energy in solution: -2266.62140395 a.u.
BP86/BS2 Free energy in solution: -2266.21991595 a.u.
2 3

Co	0.13288900	0.10032400	0.40832800
N	-0.20413700	-1.64397300	-0.96530200
N	2.14741200	-0.31787300	0.26026000
N	0.57534900	1.85071400	-0.49851100
C	-1.86809500	2.06751600	-0.44131300
H	-1.98693500	2.91773900	0.25599300
H	-2.77686100	2.04620200	-1.07559500

C	-1.13392900	-1.17731700	-2.02244600
H	-1.22495300	-1.96262400	-2.80951800
H	-0.64463100	-0.30999000	-2.50700500
C	1.74523000	1.54149200	-1.37615100
H	2.17790200	2.48188300	-1.78423100
H	1.36569100	0.94919300	-2.22937000
C	1.17825300	-1.81974400	-1.50128800
H	1.33946600	-1.07735100	-2.30621800
H	1.28615000	-2.82459800	-1.96820700
C	2.78434000	0.77598100	-0.57461700
H	3.55391800	0.34127000	-1.24534300
H	3.30761300	1.45907600	0.12053500
C	-0.62380700	2.24986800	-1.29309800
H	-0.64895900	1.60870800	-2.19364000
H	-0.52913300	3.30394300	-1.63434500
C	-0.66821500	-2.90529200	-0.34757200
H	-1.66515900	-2.78237100	0.10901700
H	0.03186500	-3.22947100	0.44339200
H	-0.72777700	-3.69998100	-1.12548200
C	0.91763900	2.86296900	0.53723400
H	1.29278000	3.78464900	0.04190600
H	1.69565100	2.47430100	1.21918100
H	0.02649400	3.11984800	1.13712700
C	2.83779600	-0.38089300	1.57527000
H	3.91445000	-0.61374600	1.42512600
H	2.37621900	-1.16844800	2.19707200
H	2.74695700	0.59498000	2.08960200
C	2.21181200	-1.66524000	-0.39658200
H	2.04420700	-2.42042200	0.39584200
H	3.23389400	-1.83185600	-0.80086700
O	0.09103500	-0.91757400	1.91183800
C	-2.71708800	-0.27457800	-0.09641400
H	-3.75745200	0.10940600	0.00428400
H	-2.61903000	-1.10291000	0.63012600
C	-2.54282800	-0.78834000	-1.53151600
H	-2.94405200	-0.04874400	-2.25576700
H	-3.22287500	-1.66356500	-1.59779600
C	-2.20467300	1.15264000	1.79047400
H	-3.21595800	1.61262800	1.77529100
H	-1.48453400	1.87383500	2.22082500
H	-2.23215400	0.24094500	2.41018900
N	-1.79474800	0.79972200	0.39763400
O	-1.08572000	-1.57602900	2.38606000
H	-0.90904600	-1.59696000	3.35940200

^{OS}IM5, L=14-TMC
BP86/BS1 SCF energy in solution: -2304.65475071 a.u.
BP86/BS2 SCF energy in solution: -2305.95891697 a.u.
BP86/BS2 Free energy in solution: -2305.52766697 a.u.
2 1

Co	-0.01578200	0.02251700	0.07591200
N	1.12094700	-1.67893400	-0.40742600
N	-1.15410600	1.73115800	-0.21795000
N	-1.67684500	-1.26583600	0.08782200
N	1.66273300	1.29231900	0.12451800
O	-0.16840500	0.24803100	1.88855900
C	2.41600000	1.17490600	-1.16271900
H	3.24124700	1.92225900	-1.14286800
H	1.73339100	1.46466500	-1.98726200
C	-1.09394600	-2.64752000	0.04812800
H	-1.86953000	-3.37127100	-0.28579600
H	-0.81154300	-2.93143000	1.08068200
C	2.97355000	-0.21710300	-1.44064200
H	3.72320900	-0.52570100	-0.68374200
H	3.53116900	-0.15354800	-2.39837900
C	-2.04711500	1.50011000	-1.40358000
H	-1.37877900	1.27982100	-2.26206200
H	-2.55931400	2.46331100	-1.62626700
C	1.07126800	2.66221800	0.24692400
H	1.82988700	3.42524400	-0.03332100
H	0.81892500	2.82130300	1.31287500
C	-3.07006000	0.38071200	-1.27091300
H	-3.79269000	0.57832900	-0.45326100
H	-3.67339900	0.39503700	-2.20274200
C	-0.15470700	2.77662200	-0.61912200
H	-0.61024500	3.78644900	-0.53341800
H	0.09577500	2.62278100	-1.68606500
C	1.99607600	-2.32746200	0.60317100
H	1.38045600	-2.78113400	1.39961000
H	2.68145800	-1.60536000	1.07437300
H	2.59349000	-3.12628500	0.11232600
C	-2.45798600	-1.01349000	-1.16853800
H	-3.25840400	-1.78530900	-1.22864200
H	-1.77664900	-1.17321400	-2.02873400
C	0.10167900	-2.68573100	-0.86334300
H	0.55179900	-3.70100400	-0.88293200
H	-0.18665500	-2.44267500	-1.90402500
C	1.89991800	-1.27948800	-1.63261300

H	1.15651000	-0.91514500	-2.37342400
H	2.35182500	-2.20642200	-2.05212400
C	-1.91736700	2.23360900	0.95293500
H	-1.22538500	2.44447400	1.78754600
H	-2.65444300	1.49324300	1.30230300
H	-2.45251900	3.16615200	0.67254800
C	-2.59030600	-1.22937200	1.26156600
H	-3.36956000	-2.01205700	1.13455600
H	-3.09213400	-0.25520800	1.36648500
H	-2.03428900	-1.44026400	2.19154700
C	2.59400000	1.13472600	1.27391500
H	3.34422400	1.95456600	1.24334700
H	3.13485300	0.17638200	1.22680300
H	2.02843000	1.18909700	2.21882600
O	0.55559800	-0.66508000	2.68816600
H	-0.11767800	-1.35603000	2.91804700

^{3}IM5, L=14-TMC
BP86/BS1 SCF energy in solution: -2304.65297385 a.u.
BP86/BS2 SCF energy in solution: -2305.95586858 a.u.
BP86/BS2 Free energy in solution: -2305.52826158 a.u.
2 3

Co	0.00143300	-0.01701300	0.18445700
N	1.09878500	-1.81895600	-0.19211400
N	-1.10989700	1.66032800	-0.56409600
N	-1.68636900	-1.27477900	0.23444900
N	1.68610300	1.18924700	-0.04417300
O	-0.17869900	0.11949900	2.02094000
C	2.39606800	0.82936100	-1.32007700
H	3.19652000	1.58811300	-1.46862000
H	1.67780100	0.93894400	-2.15650700
C	-1.13209700	-2.65853000	0.40280000
H	-1.92561400	-3.40375700	0.17570600
H	-0.86319000	-2.78381900	1.46977400
C	3.00051700	-0.56944700	-1.36410600
H	3.74958200	-0.72294600	-0.56065600
H	3.57287600	-0.63512300	-2.31309600
C	-1.98673300	1.26833900	-1.71170200
H	-1.31350700	0.93153400	-2.52685700
H	-2.50663300	2.18601700	-2.07098800
C	1.13052500	2.57952700	-0.15720700
H	1.92549500	3.26292100	-0.52795800
H	0.85824600	2.90992300	0.86322700
C	-3.00782000	0.17600400	-1.41751500

H	-3.74547700	0.49636400	-0.65346000
H	-3.59530000	0.03540800	-2.34890900
C	-0.06532900	2.60150400	-1.07413100
H	-0.48009200	3.63038900	-1.14846900
H	0.21054300	2.28953600	-2.09956000
C	1.87860700	-2.25731600	0.99815800
H	1.19953800	-2.43712100	1.85124400
H	2.61432600	-1.49556600	1.30259800
H	2.41973200	-3.19925600	0.76005700
C	-2.39945900	-1.18225200	-1.08352800
H	-3.19902000	-1.95703900	-1.07514700
H	-1.67863300	-1.46304900	-1.87728700
C	0.06418300	-2.86123500	-0.48911100
H	0.49596000	-3.87527300	-0.34338500
H	-0.21390800	-2.77972700	-1.55710600
C	1.97042800	-1.68907700	-1.40327500
H	1.29066800	-1.52719400	-2.26519700
H	2.47835900	-2.66812600	-1.55993400
C	-1.89030100	2.34491900	0.50094800
H	-1.23670000	2.60125900	1.35416400
H	-2.70327400	1.70220300	0.87686800
H	-2.34161200	3.27366100	0.08858600
C	-2.64009000	-1.06376900	1.35659800
H	-3.43077400	-1.84356800	1.30811600
H	-3.12020500	-0.07392500	1.30130000
H	-2.10010800	-1.14438700	2.31547600
C	2.66905000	1.21261200	1.07654400
H	3.41875500	2.00855000	0.87654800
H	3.20565900	0.25400000	1.16228700
H	2.14545500	1.42842800	2.02296700
O	0.18822800	1.28933400	2.75810200
H	0.03396400	0.98659600	3.68669900

^{OS}TS3, L=13-TMC
BP86/BS1 SCF energy in solution: -2633.95476709 a.u.
BP86/BS2 SCF energy in solution: -2635.6532742 a.u.
BP86/BS2 Free energy in solution: -2635.0489892 a.u.
2 1

N	-2.27723400	0.03828200	1.86354300
N	-1.26105600	-2.07983700	0.16000400
N	-2.99267100	-0.61397400	-1.44157800
C	-3.30912600	1.81177200	-1.58558500
H	-2.94210900	1.98324200	-2.61504900
H	-4.01086100	2.63900100	-1.35401200

C	-3.57203800	0.76792600	1.90635600
H	-3.98875100	0.69067900	2.93678400
H	-4.26653100	0.20909900	1.25288100
C	-3.53482800	-1.89907100	-0.92747500
H	-4.18084000	-2.39027700	-1.69023900
H	-4.17473600	-1.66808600	-0.05520600
C	-2.48846200	-1.40469700	2.20385400
H	-3.46608000	-1.72115100	1.79482400
H	-2.54561300	-1.52885500	3.30742400
C	-2.37419600	-2.81503700	-0.56039500
H	-2.72827800	-3.66551500	0.05954600
H	-1.93687800	-3.25191400	-1.47752800
C	-4.01590100	0.46691600	-1.49683700
H	-4.64014800	0.39281300	-0.58804700
H	-4.69174600	0.32837700	-2.37055800
C	-1.33131700	0.61774700	2.85535500
H	-1.04728000	1.64883200	2.58779600
H	-0.41036800	0.01218800	2.90562800
H	-1.81866200	0.62693200	3.85500200
C	-2.35451200	-0.79945100	-2.77609800
H	-1.52377100	-1.52490300	-2.71602400
H	-1.94703600	0.15862500	-3.14613700
H	-3.10714800	-1.17370400	-3.50491900
C	0.03796200	-2.62867600	-0.30610000
H	0.09037400	-3.71774500	-0.08310800
H	0.88135700	-2.11674000	0.18941300
H	0.13204900	-2.48494800	-1.39886800
C	-1.35650900	-2.24173000	1.64006500
H	-0.38602300	-1.92515200	2.07034300
H	-1.50146100	-3.31357200	1.90047400
C	-2.37825200	2.70009100	0.55918300
H	-2.60078200	3.73967100	0.22761800
H	-1.41405100	2.74632600	1.10000700
C	-3.50684000	2.25048000	1.49235600
H	-4.49287100	2.51030100	1.05366900
H	-3.40610000	2.89069400	2.39340300
C	-0.98815100	2.53173500	-1.39353100
H	-1.30372000	3.54073400	-1.73881900
H	-0.70621100	1.91976100	-2.26970400
H	-0.11476900	2.62481100	-0.72581200
N	-2.11023500	1.87883600	-0.66052600
Co	-1.53223600	-0.02376700	-0.14141000
O	0.08667300	0.47013900	0.55684400
O	0.83671800	0.35039300	-0.63089100

H	1.74789400	-0.23599700	-0.25998800
N	5.04174100	0.19752900	-0.15189600
C	5.13955400	1.20072900	0.95784300
H	4.27740900	1.88701600	0.82461500
H	4.96178900	0.65465700	1.90670000
C	4.99309000	0.86362100	-1.49178900
H	4.24446900	1.67764500	-1.39971300
H	5.97476100	1.34224800	-1.70304900
C	6.07605100	-0.88073500	-0.08606600
H	5.89211700	-1.54545400	-0.95227300
H	7.08477900	-0.43431400	-0.23247300
C	6.02101900	-1.70689200	1.19715200
H	6.71719300	-2.56554100	1.10438100
H	6.32394300	-1.13355500	2.09689200
H	5.00165100	-2.11304800	1.36383500
C	6.44241900	1.99431300	1.04785600
H	6.64103800	2.58965700	0.13328400
H	6.37045300	2.70744900	1.89504600
H	7.32128800	1.34455800	1.23852000
C	4.59962800	-0.06467400	-2.64034700
H	4.43548000	0.54521600	-3.55236900
H	5.38567800	-0.80787900	-2.88309700
H	3.65777500	-0.61094400	-2.42602000
O	2.78298900	-0.85385000	0.26530600
H	3.88257600	-0.35387100	0.04133800
H	2.64671700	-0.75117600	1.22999300

^{3}TS3, L=13-TMC
BP86/BS1 SCF energy in solution: -2633.9610297 a.u.
BP86/BS2 SCF energy in solution: -2635.66020241 a.u.
BP86/BS2 Free energy in solution: -2635.05619141 a.u.
2 3

N	-2.39002300	-0.31227500	1.88944700
N	-1.35813100	-2.06787000	-0.26607700
N	-3.04161300	-0.33807900	-1.59981900
C	-3.32841100	2.08178900	-1.33166700
H	-2.96112200	2.40613400	-2.32359900
H	-4.01567800	2.87501000	-0.97083400
C	-3.66847500	0.42319500	2.00224300
H	-4.13153700	0.23350900	3.00096500
H	-4.35841500	-0.02171200	1.25996000
C	-3.60347800	-1.69188100	-1.33893500
H	-4.24005500	-2.02506400	-2.18924700
H	-4.25375000	-1.61459700	-0.44807400

C	-2.60377700	-1.78236300	1.89126200
H	-3.57636300	-2.00491400	1.41173500
H	-2.67182500	-2.17382900	2.93265800
C	-2.45205100	-2.66687700	-1.12458600
H	-2.81975300	-3.60907300	-0.66725500
H	-1.99732600	-2.94069300	-2.09463900
C	-4.05293600	0.74872300	-1.44814700
H	-4.65185400	0.52577500	-0.54651200
H	-4.74865800	0.75614700	-2.31655800
C	-1.48539300	0.04762900	3.00401000
H	-1.24339300	1.12510200	2.99117100
H	-0.53576100	-0.51203100	2.92976600
H	-1.96938300	-0.19329400	3.97960700
C	-2.40096600	-0.27747700	-2.94391400
H	-1.66481600	-1.09293300	-3.06215300
H	-1.87210200	0.68277700	-3.08195500
H	-3.17722300	-0.37738800	-3.73401600
C	-0.03376400	-2.48348900	-0.79906400
H	0.04964700	-3.59269500	-0.79556300
H	0.77478300	-2.05872700	-0.17759300
H	0.08036400	-2.11807300	-1.83745000
C	-1.46830000	-2.48938100	1.16600300
H	-0.49939600	-2.25423000	1.64850700
H	-1.60634700	-3.59184900	1.21740800
C	-2.39556100	2.51526600	0.95880500
H	-2.56813200	3.61077400	0.85132800
H	-1.44051700	2.40108600	1.50663000
C	-3.56127600	1.94849800	1.78114400
H	-4.52853500	2.29258500	1.35807800
H	-3.47470400	2.46416900	2.76103100
C	-1.00801400	2.76486900	-0.99339800
H	-1.31483900	3.82712000	-1.11467200
H	-0.73001800	2.35563500	-1.98264600
H	-0.13081400	2.71313700	-0.32451000
N	-2.13044000	1.97463900	-0.41582000
Co	-1.57086100	-0.00342800	-0.25891500
O	-0.01028800	0.22500500	0.59114400
O	1.00575700	0.51463200	-0.31638400
H	1.90085000	0.02269600	0.17129200
N	5.23594800	0.01522900	-0.08248700
C	4.95731600	0.89648400	-1.25724100
H	4.34104000	0.29213900	-1.95632200
H	4.30673500	1.72151500	-0.90179300
C	5.92241300	-1.24752300	-0.48974800

H	5.41443600	-1.59477800	-1.41362900
H	6.97981000	-1.02900800	-0.76374300
C	5.95283900	0.70215900	1.03125400
H	6.05063000	-0.03924300	1.84950900
H	6.98916000	0.95795200	0.71067800
C	5.23408200	1.94112100	1.56316200
H	5.74062100	2.28823200	2.48698400
H	5.24178200	2.78610300	0.84513800
H	4.17802000	1.71636600	1.82122300
C	6.17293500	1.46679500	-1.99156300
H	6.82407100	0.67230300	-2.41014800
H	5.82354900	2.08952600	-2.84125000
H	6.79445600	2.11688000	-1.34156200
C	5.86683400	-2.35546400	0.56303300
H	6.27734800	-3.29031300	0.12869300
H	6.46790600	-2.12581900	1.46652900
H	4.82145600	-2.55520800	0.87741300
O	2.90736600	-0.65267000	0.71105000
H	3.96427600	-0.34535100	0.37849700
H	2.87762600	-0.52896000	1.68251900

^{OS}TS3, L=14-TMC
BP86/BS1 SCF energy in solution: -2673.24694183 a.u.
BP86/BS2 SCF energy in solution: -2674.98967881 a.u.
BP86/BS2 Free energy in solution: -2674.35769681 a.u.
2 1

N	-1.67686300	1.09445200	-1.81086400
N	-2.65658800	-1.14883100	1.46714600
N	-1.24677200	-1.68044000	-1.18645800
N	-2.24316100	1.68339800	1.12029400
C	-3.42426800	2.39657900	0.54178200
H	-3.68984900	3.23448500	1.22627400
H	-4.28145900	1.69382400	0.53881000
C	-0.79256200	-1.09180900	-2.48741900
H	-0.77618300	-1.87992700	-3.27322400
H	0.24879800	-0.74326200	-2.34507300
C	-3.21548300	2.92818700	-0.87372000
H	-2.42958700	3.71055000	-0.90975600
H	-4.15456900	3.44510700	-1.16335300
C	-3.65014900	-2.07088600	0.82588300
H	-4.37569300	-1.42678400	0.28654400
H	-4.21202600	-2.58262200	1.64066900
C	-2.60079300	1.10218000	2.45097600
H	-3.14731000	1.85627100	3.06008900

H	-1.65360600	0.87321100	2.97681600
C	-3.08131100	-3.10482100	-0.13848200
H	-2.38052800	-3.79678700	0.37195100
H	-3.93399900	-3.73958200	-0.45941700
C	-3.42708800	-0.14514100	2.26937700
H	-3.71066200	-0.58047600	3.25226800
H	-4.36848400	0.07944700	1.73171300
C	-0.51504100	1.98814000	-2.04623200
H	0.40988000	1.38707700	-2.08175600
H	-0.39810200	2.71939500	-1.23145200
H	-0.64968100	2.52995300	-3.00865700
C	-2.47071500	-2.51603100	-1.40759300
H	-2.19732200	-3.33753000	-2.10855500
H	-3.22956900	-1.89344100	-1.92166300
C	-1.68702400	0.05119500	-2.88714000
H	-1.35853000	0.49295300	-3.85301100
H	-2.73027300	-0.29153400	-3.02993800
C	-2.97360300	1.84468800	-1.91698900
H	-3.78463500	1.08911700	-1.85411300
H	-3.02100200	2.28835600	-2.93807400
C	-1.74696100	-1.88055500	2.38338000
H	-1.04186800	-1.17086300	2.85180200
H	-1.15457500	-2.63577500	1.84276300
H	-2.34105700	-2.38975600	3.17373400
C	-0.13464800	-2.55134900	-0.71688500
H	0.06301200	-3.32392600	-1.49319600
H	-0.39422500	-3.07305000	0.21837100
H	0.78367000	-1.95862100	-0.55739700
C	-1.14083000	2.65191300	1.36252600
H	-1.44575100	3.35709100	2.16655900
H	-0.92529800	3.24359600	0.45783400
H	-0.23029700	2.10507600	1.65694000
Co	-1.75574000	-0.01462200	-0.02575800
O	-0.12929900	-0.05833900	0.86959800
O	0.91757500	0.62116500	0.25376400
H	1.76071800	-0.17032100	0.11664000
N	5.10048800	-0.03441200	0.06692200
C	5.06004500	1.19407900	-0.79757900
H	4.74518500	0.84491000	-1.80235700
H	4.24049300	1.83143100	-0.41039200
C	6.00611300	-1.09192800	-0.50188200
H	5.84513000	-1.07806200	-1.59891900
H	7.05964400	-0.79462900	-0.31522400
C	5.40500600	0.24481700	1.51183000

H	5.32922300	-0.72927700	2.03380700
H	6.46205300	0.57693400	1.59453500
C	4.45485100	1.25000200	2.15710600
H	4.61971200	1.24879900	3.25383000
H	4.61831100	2.28637700	1.79849000
H	3.39562100	0.97880700	1.96957100
C	6.36068100	1.98740800	-0.88753900
H	7.19248800	1.39076900	-1.31456200
H	6.20001700	2.85800700	-1.55620900
H	6.68377700	2.38226400	0.09723600
C	5.72986200	-2.49274900	0.03901600
H	6.37344600	-3.21735800	-0.50049900
H	5.95857300	-2.59283200	1.11954700
H	4.67223800	-2.78171700	-0.12838000
O	2.73862400	-1.00085600	0.04020900
H	3.99376600	-0.47875800	0.04354700
H	2.67396800	-1.50057900	0.87996200

^{3}TS3, L=14-TMC

BP86/BS1 SCF energy in solution: -2673.24983402 a.u.

BP86/BS2 SCF energy in solution: -2674.99248547 a.u.

BP86/BS2 Free energy in solution: -2674.36277047 a.u.

2 3

N	-2.02892600	1.12923000	-1.81395800
N	-2.54696400	-1.01020900	1.70665900
N	-1.77491800	-1.69022900	-1.19961300
N	-1.73474700	1.71715200	1.22826200
C	-2.94045000	2.53967500	0.86916000
H	-3.00435900	3.36742000	1.61184600
H	-3.83565300	1.90285200	1.01292100
C	-1.56758000	-1.15495700	-2.58492200
H	-1.82333000	-1.94325900	-3.32710400
H	-0.48756500	-0.93290900	-2.68442300
C	-2.97580600	3.11942200	-0.54275400
H	-2.10742700	3.78244200	-0.73609600
H	-3.86179000	3.78801900	-0.58004800
C	-3.77076500	-1.77499300	1.32241000
H	-4.51052400	-1.03241400	0.95756700
H	-4.19448700	-2.24067200	2.24263800
C	-1.91066700	1.18308600	2.61741000
H	-2.20086000	2.01092600	3.30199500
H	-0.92443700	0.81025200	2.95738700
C	-3.55738700	-2.84091800	0.25459700
H	-2.86934700	-3.63660500	0.60672700

H	-4.53497300	-3.34698700	0.10877800
C	-2.94378900	0.08085600	2.64596800
H	-3.05411900	-0.31943300	3.67831400
H	-3.93941800	0.45687300	2.34182700
C	-0.80094300	1.81988600	-2.28396600
H	0.04658500	1.11053400	-2.31810400
H	-0.52372100	2.64318200	-1.60470200
H	-0.97363500	2.24788700	-3.29694900
C	-3.14918300	-2.29392100	-1.10994800
H	-3.19347500	-3.10995900	-1.86629900
H	-3.88198800	-1.52253200	-1.41830200
C	-2.39976300	0.08689600	-2.81252800
H	-2.24749500	0.46776000	-3.84710600
H	-3.48086400	-0.12690500	-2.70682000
C	-3.15943700	2.08965700	-1.65405000
H	-4.06828200	1.48669100	-1.44728300
H	-3.32065300	2.61081000	-2.62680500
C	-1.56078400	-1.88300400	2.39771800
H	-0.72413000	-1.27428100	2.78671400
H	-1.13690400	-2.63872400	1.71613100
H	-2.05086700	-2.40524100	3.25004500
C	-0.75196200	-2.74848800	-0.98191500
H	-0.79952900	-3.47926000	-1.81857500
H	-0.93639000	-3.29515400	-0.04224000
H	0.24854000	-2.28118900	-0.95546500
C	-0.51600800	2.56445400	1.23848800
H	-0.63426100	3.37117600	1.99462200
H	-0.33993000	3.02710500	0.25342600
H	0.35885800	1.94229300	1.49539400
Co	-1.65899800	0.00531600	0.00800600
O	0.17170500	0.04720800	0.19549400
O	1.02697800	-0.36917200	-0.81903000
H	1.95548300	-0.80575900	-0.26899100
N	5.15985500	-0.09782300	0.01156400
C	4.81466400	1.06209600	-0.86874000
H	4.40467300	0.62461700	-1.80302000
H	3.97646400	1.60199100	-0.38375000
C	6.10776300	-1.04050600	-0.66092800
H	5.76521000	-1.12840000	-1.71295900
H	7.12526300	-0.58997900	-0.68500900
C	5.63970500	0.29642500	1.37059300
H	5.80943500	-0.64531900	1.92989800
H	6.62978100	0.79840900	1.28267000
C	4.65745100	1.17217600	2.14624100

H	5.01512100	1.28255900	3.19047500
H	4.56072200	2.19187600	1.72115100
H	3.64668700	0.71478900	2.18254500
C	5.95090000	2.03187300	-1.19462600
H	6.79231500	1.53655500	-1.72142900
H	5.56446800	2.82726500	-1.86530100
H	6.35341800	2.53157400	-0.28955900
C	6.15400800	-2.43045300	-0.02636500
H	6.77630900	-3.09682300	-0.65860000
H	6.60447300	-2.42825200	0.98709500
H	5.13710400	-2.86890200	0.04135200
O	2.98033600	-1.36353800	0.25367600
H	4.00406300	-0.75956400	0.16707400
H	2.80633600	-1.49927600	1.20760500

^{3}TS5a, L=13-TMC
BP86/BS1 SCF energy in solution: -2418.0964788 a.u.
BP86/BS2 SCF energy in solution: -2419.56114208 a.u.
BP86/BS2 Free energy in solution: -2419.12558208 a.u.
2 3

N	1.22499400	-0.49614800	1.82853800
N	1.19998900	1.96316600	0.25062100
N	1.53235500	0.03254800	-1.70767100
C	0.45639700	-2.16913200	-1.86144500
H	-0.11898700	-2.02967300	-2.79590400
H	0.62511600	-3.25960700	-1.74876900
C	1.87628100	-1.80090000	1.55816900
H	2.45329800	-2.12468000	2.45693600
H	2.62485300	-1.61563700	0.76322600
C	2.76535500	0.78034300	-1.32822400
H	3.41731900	0.93861500	-2.21587600
H	3.32035100	0.14963900	-0.60932600
C	2.24037000	0.57207700	2.04799800
H	3.13329700	0.34044200	1.43569400
H	2.57673100	0.58669100	3.10944400
C	2.36283500	2.11460600	-0.71607500
H	3.22539500	2.57968700	-0.19594900
H	2.04759700	2.82166400	-1.50559900
C	1.78090700	-1.42307500	-1.93934100
H	2.49118700	-1.76796600	-1.16576700
H	2.26384200	-1.58060900	-2.92918700
C	0.33949400	-0.58630500	3.01336700
H	-0.51959200	-1.25420300	2.82771400
H	-0.05040600	0.41102900	3.29221300

H	0.91454500	-0.97987800	3.88267100
C	0.86098200	0.65545000	-2.88446500
H	1.53967700	0.60671300	-3.76367200
H	0.61770600	1.71250000	-2.67767000
H	-0.07554900	0.12201600	-3.12586100
C	0.27801100	3.11815300	0.06652600
H	0.81669900	4.07242500	0.25388100
H	-0.56947000	3.04609100	0.77112000
H	-0.11041600	3.12340700	-0.96957400
C	1.66520000	1.92792600	1.67611200
H	0.79445400	2.17307700	2.31603100
H	2.41849900	2.72883700	1.84120300
C	-0.41486200	-2.57513300	0.46345900
H	-0.89458500	-3.52609900	0.13772100
H	-1.11061200	-2.10402700	1.18385900
C	0.91349100	-2.93295900	1.14282700
H	1.48963700	-3.63865000	0.50788300
H	0.61576100	-3.51990800	2.03708800
C	-1.80351500	-1.51908000	-1.19778400
H	-2.16837400	-2.49812100	-1.57697700
H	-1.85304700	-0.77685900	-2.01693500
H	-2.45163900	-1.19417800	-0.36604700
N	-0.39827100	-1.65293800	-0.71930100
Co	0.30210000	0.16054500	-0.13299000
O	-1.36867800	0.59001000	0.77010900
O	-5.07810500	0.03871400	-0.35820900
H	-2.24333900	1.10132800	0.14379200
O	-5.77654900	0.43210800	0.78228400
H	-6.56225200	-0.16799000	0.76622400
O	-3.19669600	1.62510300	-0.44937400
H	-2.96498400	1.73005800	-1.39577900
H	-4.06636500	0.91919200	-0.41244000
H	-1.26194500	1.15427400	1.56484300

^{3}TS5a, L=14-TMC

BP86/BS1 SCF energy in solution: -2457.38819232 a.u.

BP86/BS2 SCF energy in solution: -2458.89694043 a.u.

BP86/BS2 Free energy in solution: -2458.43461143 a.u.

2 3

N	-1.31851900	1.91913100	-0.62939300
N	-0.43617600	-1.59876200	1.33348500
N	-1.98183600	-0.80185800	-1.22315400
N	0.92246000	0.94251400	1.24540400
C	0.26508500	1.96902100	2.11875200

H	1.03353300	2.32650400	2.84071600
H	-0.52568000	1.46112400	2.70552100
C	-2.52053600	0.32505800	-2.05704300
H	-3.50096200	0.03209800	-2.49168500
H	-1.82425000	0.48412600	-2.90238700
C	-0.34409000	3.15975500	1.38563300
H	0.41693900	3.71639300	0.80169600
H	-0.68898000	3.86894600	2.16696600
C	-1.81220300	-2.01464100	1.74606400
H	-2.26683800	-1.15102400	2.27460300
H	-1.71057100	-2.84014700	2.48737700
C	1.42113200	-0.18853800	2.09721500
H	1.96859300	0.22042300	2.97461000
H	2.14912000	-0.76256000	1.49067300
C	-2.72620500	-2.44575700	0.60532700
H	-2.33078300	-3.33218600	0.06808700
H	-3.67595100	-2.78457000	1.06968700
C	0.27246200	-1.06092800	2.53560300
H	0.63586200	-1.89881800	3.17002800
H	-0.45862000	-0.49042300	3.14010200
C	-0.49566900	2.60192400	-1.66315700
H	-0.37010800	1.94951200	-2.54575900
H	0.50537300	2.85331000	-1.27772100
H	-1.00170700	3.54165900	-1.97623500
C	-3.09304400	-1.31877700	-0.35165900
H	-3.90821800	-1.65424900	-1.03149600
H	-3.48502800	-0.46559300	0.23656100
C	-2.64875900	1.57461700	-1.22492600
H	-3.02042200	2.42201800	-1.84145300
H	-3.37128000	1.43624300	-0.39800800
C	-1.56598500	2.81619900	0.54337300
H	-2.31714500	2.30582500	1.18095900
H	-2.03804100	3.74959900	0.15984800
C	0.32602500	-2.76504600	0.81105500
H	1.32718700	-2.45509900	0.45907200
H	-0.20793500	-3.23797400	-0.02998200
H	0.43782600	-3.52353400	1.61701700
C	-1.53790800	-1.87227600	-2.15969400
H	-2.42788500	-2.32290000	-2.64999400
H	-0.97676400	-2.66736700	-1.64298100
H	-0.90310000	-1.44649700	-2.95906900
C	2.11531700	1.54270100	0.58532700
H	2.81075100	1.91290400	1.36958000
H	1.83749500	2.39074200	-0.06211200

H	2.63439400	0.79069700	-0.02868200
Co	-0.50054400	0.05551300	-0.01402700
O	0.93212100	-0.31634000	-1.34316900
O	4.83732200	-0.13335500	-1.61384700
H	1.88304100	-0.92073800	-1.16421500
O	5.80994200	-0.31447800	-0.61600600
H	6.57010300	0.19941900	-0.98150300
O	2.98703500	-1.55688500	-0.90701100
H	3.01037100	-2.38144500	-1.43487000
H	3.89445000	-0.90472800	-1.23588500
H	0.64330400	-0.51912500	-2.25567100

[5]TS7, L=13-TMC
BP86/BS1 SCF energy in solution: -2341.24170008 a.u.
BP86/BS2 SCF energy in solution: -2342.59933948 a.u.
BP86/BS2 Free energy in solution: -2342.19523048 a.u.
1 5

N	-1.51759300	1.49639400	-0.37126800
N	1.41995900	1.74430300	0.01576000
N	0.72109100	-0.49374600	1.73089000
C	-0.99842900	-2.26507400	1.33254300
H	-0.29630600	-3.12159200	1.31716200
H	-1.96378900	-2.65801100	1.72208000
C	-2.57260400	1.04425100	0.57599500
H	-3.35777200	1.83415300	0.66234300
H	-2.08170800	0.99605300	1.56688300
C	0.97581500	0.82824900	2.35068600
H	1.47717200	0.72386600	3.34305500
H	-0.00690600	1.30242300	2.53714600
C	-0.88119900	2.73475800	0.16546500
H	-0.90266200	2.68272400	1.27128000
H	-1.47584600	3.63484600	-0.11788500
C	1.85192600	1.71152400	1.44857000
H	1.89273600	2.73989000	1.87490600
H	2.89050100	1.32593000	1.46677900
C	-0.46455100	-1.19117400	2.29189000
H	-1.24207400	-0.42997900	2.49642200
H	-0.22123600	-1.67165100	3.26937500
C	-2.06165300	1.74423900	-1.72175700
H	-2.50099400	0.82081900	-2.14302100
H	-1.25384500	2.07885100	-2.39952800
H	-2.85424100	2.52881000	-1.69179900
C	1.91914600	-1.36056000	1.75690000
H	2.11950600	-1.72357400	2.79229600

H	2.80186700	-0.80060100	1.39932200
H	1.79418200	-2.22732500	1.08064100
C	2.60861700	1.76196100	-0.86745500
H	3.22245900	2.68017000	-0.70955100
H	2.27929100	1.73318500	-1.92364800
H	3.23054800	0.86824300	-0.67520400
C	0.55004600	2.89933300	-0.32714300
H	0.55404000	2.99462400	-1.43177900
H	0.97167000	3.84977900	0.07936400
C	-2.54113400	-1.42483400	-0.46950600
H	-3.18372900	-2.33741300	-0.40742600
H	-2.48412700	-1.16527800	-1.54623200
C	-3.27169900	-0.30146700	0.28342200
H	-3.63333600	-0.67754500	1.26441100
H	-4.19156300	-0.12096800	-0.31279600
C	-0.67821300	-2.83341300	-1.01393100
H	-1.28818700	-3.76289400	-0.92105100
H	0.38448300	-3.07399000	-0.82176300
H	-0.76655700	-2.47234200	-2.05707100
N	-1.14932300	-1.78486800	-0.07871200
Co	0.08959400	-0.00525900	-0.26576100
O	0.45511900	-0.03136900	-2.38276000
H	-0.21795600	-0.52406700	-2.89702900
H	1.26766700	-0.66101800	-2.34724400
O	2.61399800	-2.62707800	-1.40249800
O	2.39117300	-1.34723900	-1.52419800

^{5}TS7, L=14-TMC
BP86/BS1 SCF energy in solution: -2380.53349432 a.u.
BP86/BS2 SCF energy in solution: -2381.93477146 a.u.
BP86/BS2 Free energy in solution: -2381.50059446 a.u.
1 5

N	-1.71773600	0.36450000	-1.12214000
N	2.17072700	-0.81843100	0.05834900
N	0.66297500	2.00012700	-0.36155100
N	-0.48827900	-2.20281300	0.38991300
C	-0.97739800	-2.81950300	-0.87540300
H	-1.25549100	-3.88182600	-0.66625000
H	-0.13000400	-2.85123500	-1.58981400
C	-0.60675000	2.58939400	-0.87405100
H	-0.40137700	3.54651900	-1.41106900
H	-1.24317100	2.82854500	-0.00043100
C	-2.14851300	-2.11477100	-1.56102100
H	-3.04541000	-2.08955600	-0.90758500

H	-2.43695600	-2.75550900	-2.42166900
C	2.83558500	-0.27137200	-1.15571000
H	2.24002900	-0.60021500	-2.03384300
H	3.84566000	-0.74005400	-1.25636300
C	0.82069600	-2.80483800	0.76103500
H	0.77637000	-3.91808200	0.68270500
H	1.00837500	-2.56668000	1.82677100
C	2.98077000	1.25077700	-1.18857500
H	3.51050100	1.62362500	-0.28695000
H	3.65751400	1.48800300	-2.03711900
C	1.96233400	-2.28398100	-0.10603500
H	2.89696800	-2.84350100	0.13429200
H	1.75063200	-2.47954400	-1.17639500
C	-3.01122700	0.56303100	-0.42963800
H	-2.97014000	1.43888900	0.24230200
H	-3.26264500	-0.31496000	0.19325200
H	-3.82788600	0.70992900	-1.17713500
C	1.68979400	2.03312300	-1.44334200
H	1.94318500	3.10158600	-1.65123300
H	1.22123300	1.63381200	-2.36542200
C	-1.33510200	1.63043600	-1.80964000
H	-2.23606400	2.13367000	-2.23175000
H	-0.69052800	1.37027700	-2.67354000
C	-1.84068500	-0.72768600	-2.12947200
H	-0.88592100	-0.76614000	-2.69640300
H	-2.63949700	-0.44664600	-2.85923800
C	3.01309500	-0.57824600	1.24951300
H	2.60602800	-1.11760200	2.12524100
H	3.06643000	0.50054000	1.49309300
H	4.05300600	-0.94500700	1.07776200
C	1.13259500	2.77764500	0.80436200
H	1.32906500	3.84109300	0.52769800
H	2.07271700	2.34886800	1.20148800
H	0.36364200	2.74953900	1.59861900
C	-1.45966500	-2.43978200	1.47819500
H	-1.61218600	-3.53231000	1.65103100
H	-2.43997900	-1.99182500	1.22804200
H	-1.08795700	-1.97605300	2.41034900
Co	0.03313900	-0.03096700	0.20230900
O	0.29771200	-0.03875000	2.33620400
H	1.12388300	0.40395200	2.62343100
H	-0.44036500	0.60161000	2.62037900
O	-2.58263200	2.25728200	2.29045300
O	-1.52525400	1.54438600	2.03210700