Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2021

Electronic Supplementary Information

Theoretical Mechanistic Study of 4CzIPN/Ni^0-Metallaphotoredox Catalyzed Enantioselective Desymmetrization of Cyclic meso-Anhydrides

Yujie Liang,[a,b] Yujiao Dong,[b] Guangyan Sun,*[a] Zhongmin Su,*[a,b] and Wei Guan*[b]

[a]*Department of Chemistry, Faculty of Science, Yanbian University, Yanji, Jilin 133002, P. R. China*

[b]*Faculty of Chemistry, Institute of Functional Material Chemistry, Northeast Normal University, Changchun 130024, P. R. China*

E-mail: guanw580@nenu.edu.cn

Table of Contents

COMPUTATIONAL DETAILS

1. Correction of Translational Entropy in Solution

We evaluated the electronic energy (E_{sol}) with zero-point energy correction in solution. For each species, the E_{sol} is defined through equation (S1):

$$E_{\mathrm{sol}} = E_{sol}^{pot} + E_{gas}^{v_0} \tag{S1}$$

the E_{sol}^{pot} is the potential energy including non-electrostatic energy in solution and $E_{gas}^{v_0}$ delegates the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the Ni(I) complex capture the benzyl radical, the entropy change which can decreases considerably must be taken into consideration. In such case, Gibbs energy (G_{sol}^{o}) need be computed as follows:

$$\begin{aligned} G_{sol}^{o} &= H_0 - T(S_{\mathrm{r}}^{o} + S_{\mathrm{v}}^{o} + S_{\mathrm{t}}^{o}) \\ &= E^{T} + P\Delta V - T(S_{\mathrm{r}}^{o} + S_{\mathrm{v}}^{o} + S_{\mathrm{t}}^{o}) \\ &= E_{sol} + E_{therm} - T(S_{\mathrm{r}}^{o} + S_{\mathrm{v}}^{o} + S_{\mathrm{t}}^{o}) \end{aligned} \tag{S2}$$

where ΔV is 0 in solution, E_{therm} is the thermal correction by translational, vibrational, and rotational movements, and S_{r}^{o}, S_{v}^{o}, and S_{t}^{o} are rotational, vibrational, and translational entropies, respectively. In general, the Sackur-Tetrode equation is used to evaluate translational entropy S_{t}^{o}. In solution, however, the usual Sackur-Tetrode equation cannot be directly applied to the evaluation of S_{t}^{o}, because the translation movement is suppressed very much in solution.[S1] In this context, the translational entropy was corrected with the method developed by Whitesides et al., where the rotational entropy was evaluated in a normal manner. Thermal correction and entropy contributions of vibration movements to the Gibbs energy were evaluated with the frequencies calculated at 298.15 K and 1 atm.

2. Redox potential

We calculated the standard redox potential ($E_{1/2}^{red}$) according to the equation (S3):[S2]

$$E_{1/2}^{red} = -\frac{\Delta G_r}{nF} - E_{SCE} \quad \text{(S3)}$$

where, F is the Faraday constant and n is the number of electrons transferred, E_{SCE} = 4.51V, and ΔG_r is the free energy change of the reaction.

Table S1 The experimental and calculated redox potential of 4CzIPN (PC) complexes

Redox Potential	$E_{1/2}^{red}$ [*PC/PC$^-$]	$E_{1/2}^{red}$ [PC/PC$^-$]
Cal.^{dioxane}	1.53 V	–1.79 V
Cal.^{MeCN}	1.21 V	–1.24 V
Exp. ^{MeCN}	1.35 V	–1.21 V
$\lvert\Delta\rvert$	0.14 V	0.03 V

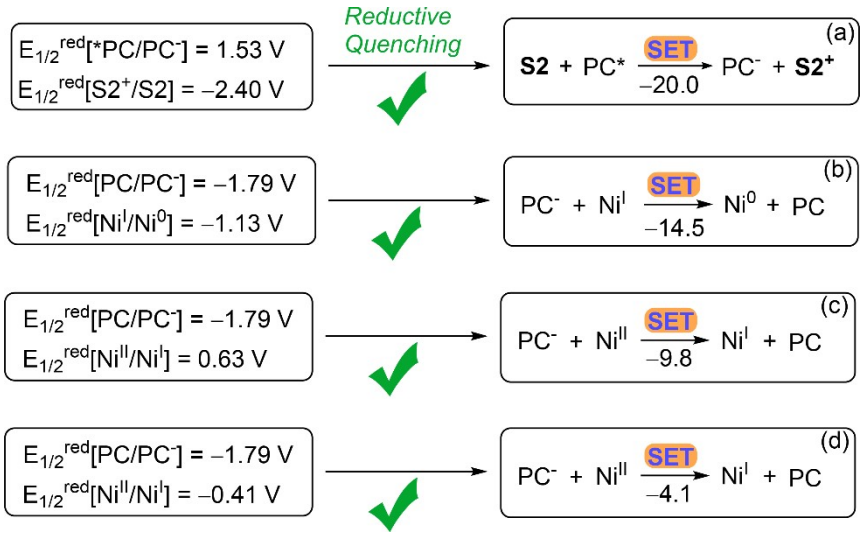
Table S2 The calculated redox potential of Ni complexes and substrate **S2**

Redox Potential	$E_{1/2}^{red}$ [S2$^+$/S2]	$E_{1/2}^{red}$ [Ni^I/Ni^0]
Cal. ^{dioxane}	–2.40 V	–0.94 V

Table S3 The calculated redox potential of Ni complexes

Redox Potential	$E_{1/2}^{red}$ [Ni^{II}(NiCl$_2$)/Ni^I]	$E_{1/2}^{red}$ [Ni^{II}(M1)/Ni^I]
Cal. ^{dioxane}	0.63 V	–0.41 V

Scheme S1 Single electron transfer processes, $\Delta G°$ values of SET processes are given in kcal mol^{-1}.



3. Activation barrier of single electron transfer step

According to the Marcus equation, the reorganization energy λ is normally decomposed into internal energy (λ_i) and external energy (λ_o). The internal reorganization energy λ_i can be estimated according to the equation (S4):

$$\lambda_i = [E^D(Q_R) + E^A(Q_R)] - [E^D(Q_P) + E^A(Q_P)] \quad \text{(S4)}$$

where Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively. In addition, the external reorganization energy λ_o may be calculated from equation (S5−S7)

$$\lambda_o = (332\ \text{kcal/mol})(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R})(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon}) \quad \text{(S5)}$$

$$\lambda = \lambda_o + \lambda_i \quad \text{(S6)}$$

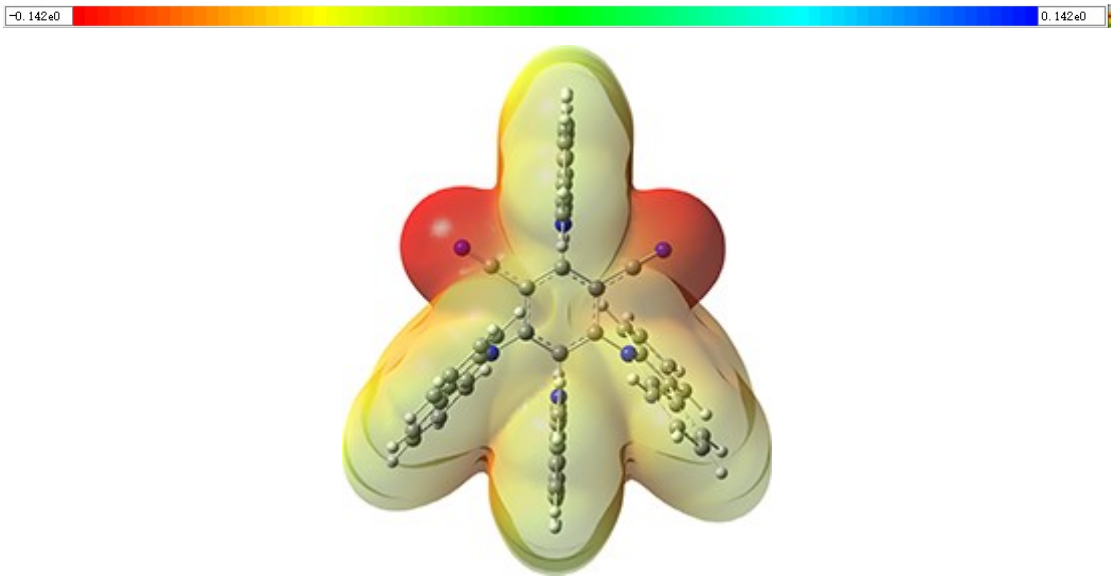
$$\Delta G^{\circ\neq} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \quad \text{(S7)}$$

where a_1 is the radii of the oxidant, a_2 is the radii of the reductant, R = a_1 + a_2, ε_{op} is the optical dielectric constant (ε_{op} = 2.25), ε is the static dielectric constant for the dioxane solvent (ε = 2.2099), and ΔG_r is the free energy change of the reaction.

Table S4 Estimation of the activation barriers for SET step

SET step	a_1 (Å)	a_2 (Å)	R (Å)	λ (kcal mol^{-1})	ΔG_r (kcal mol^{-1})	ΔG_{SET} (kcal mol^{-1})
(a)	4.81	2.87	7.68	12.7	–20.0	1.0
(b)	4.99	4.83	9.82	26.0	–14.5	1.3
(c)	4.99	3.91	8.90	16.2	–9.8	0.6
(d)	4.99	4.51	9.50	17.0	–4.1	2.4

Scheme S2 Electrostatic potential map of PC^-.



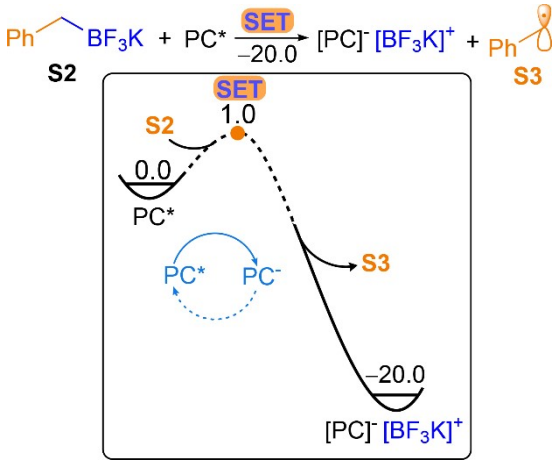
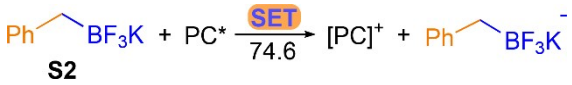


Fig. S1 Gibbs energy profile ($\Delta G°_{298.15}$) of the single-electron reduction of *PC by substrate **S2**.

Scheme S3 Single electron transfer processes. The *PC oxidation by substrate **S2** to deliver benzyl trifluoroborates anion and oxidized PC^+ complex.



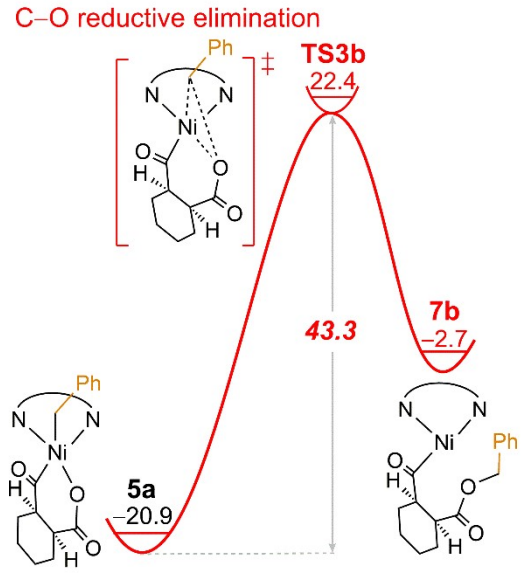


Fig. S2 Gibbs energy profile ($\Delta G°_{298.15}$) of intramolecular O–benzyl reductive elimination from Ni^{III} species **5a**.

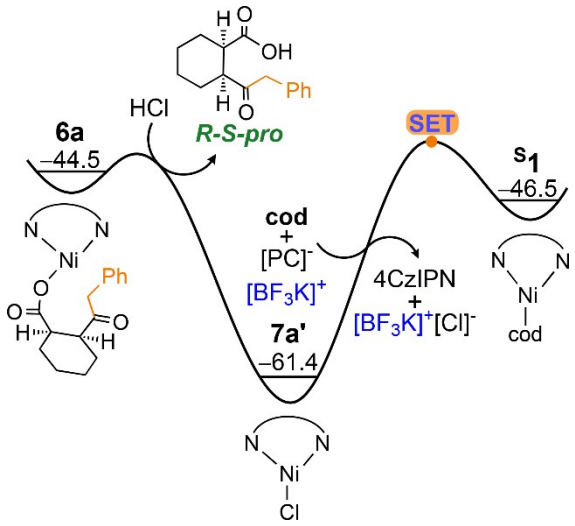
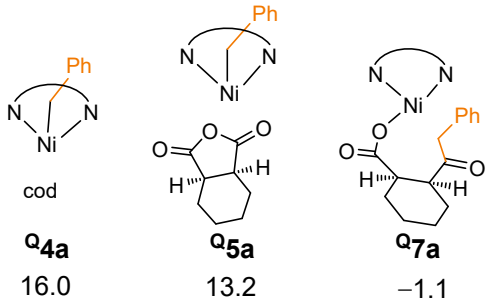


Fig. S3 Gibbs energy profile ($\Delta G°_{298.15}$) of the ion exchange followed by SET from nickel(I) carboxylic intermediate **6a**.

Scheme S4 The quartet structures corresponding to **4a**, **5a** and **7a**.



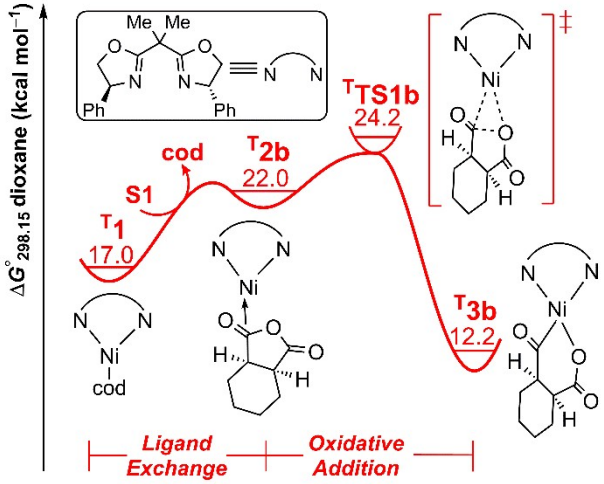


Fig. S4 Gibbs energy profile ($\Delta G°_{298.15}$) of the C–O oxidative addition of substrate **S1** to triplet nickel(0) center in ^{T}**2b**.

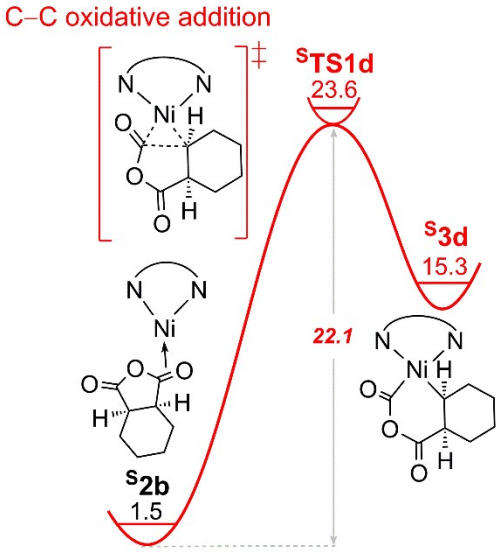


Fig. S5 Gibbs energy profile ($\Delta G°_{298.15}$) of the C(=O)–C oxidative addition of **S1** to nickel(0) center in ^{S}**2b**.

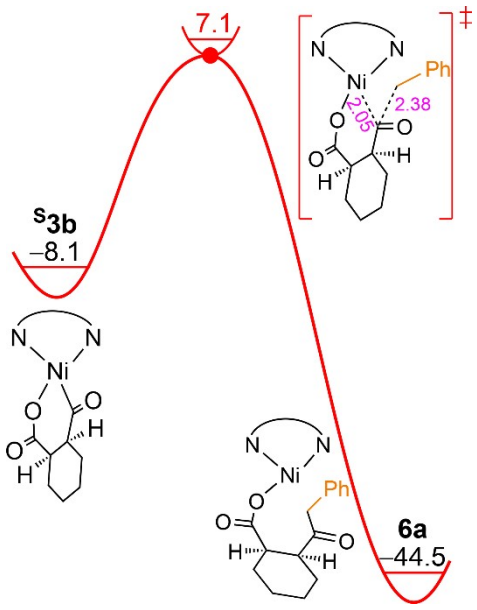


Fig. S6 Gibbs energy profile ($\Delta G°_{298.15}$) of the outer-sphere benzyl radical **S3** directly attack the ^{S}**3b** formation C(=O)–C. The approximate transition state was located by constraint optimization.

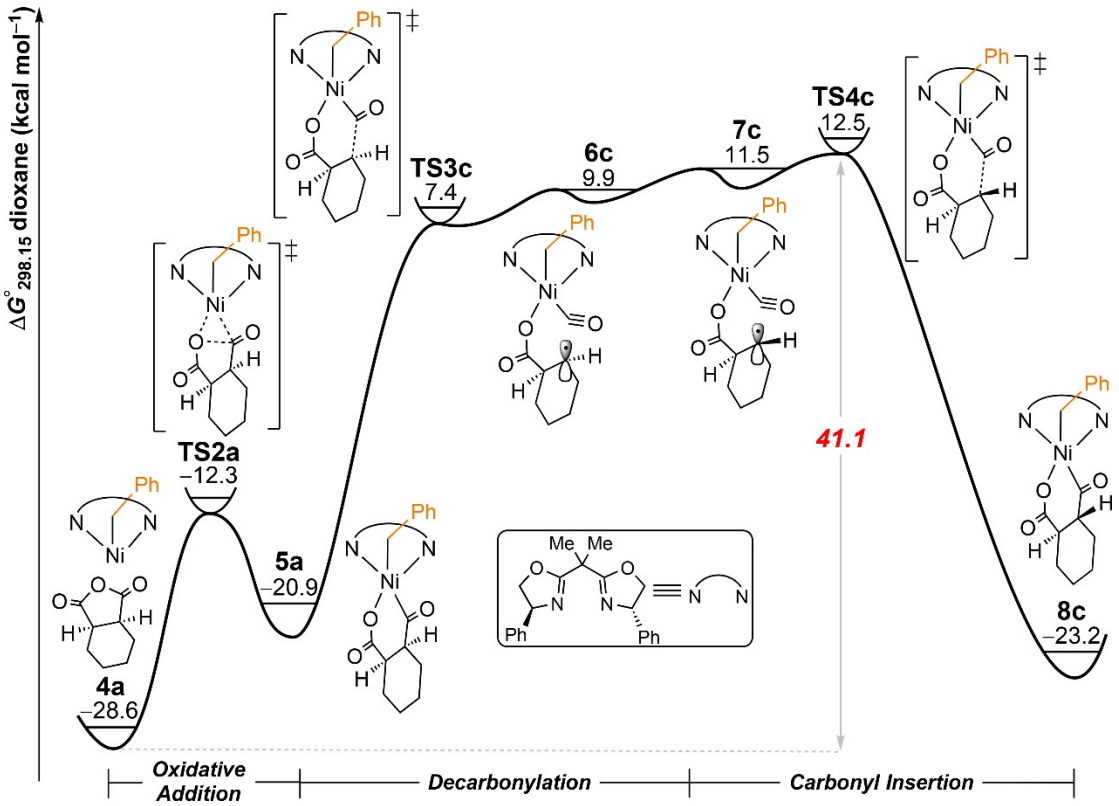


Fig. S7 Energy profile ($\Delta G°_{298.15}$) of the successive decarbonylation from **5a** and carbonyl recombination towards the ***trans-pro*** product.

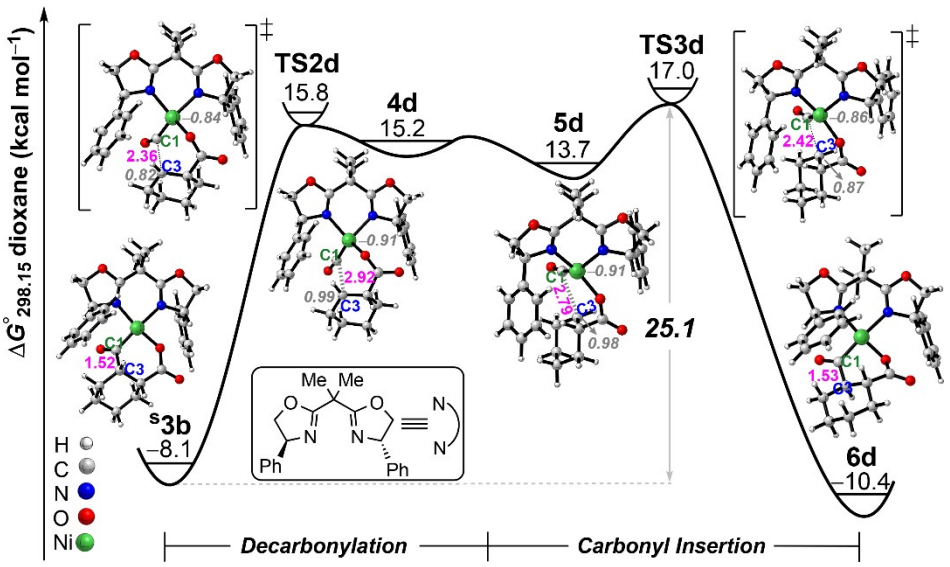


Fig. S8 Gibbs energy profile ($\Delta G°_{298.15}$) of the decarbonylation and carbonyl insertion processes toward ***trans-pro***.

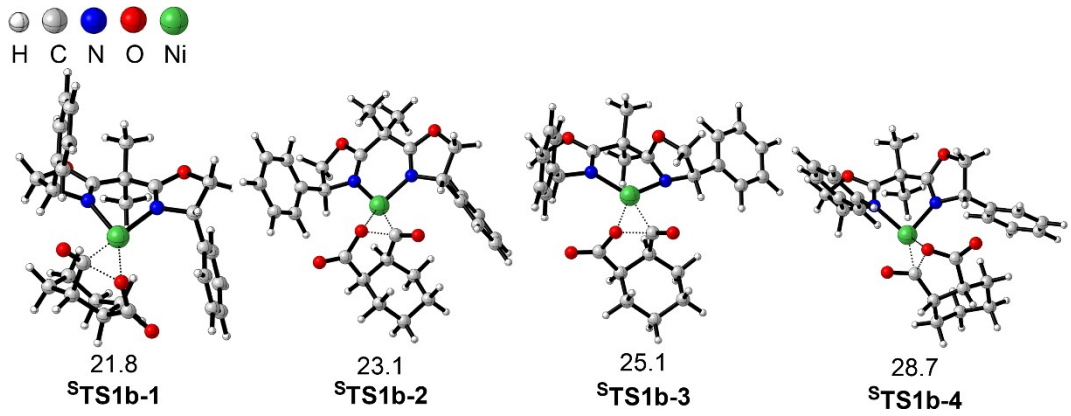


Fig. S9 Optimized structures for selected important stationary points leading to ***R-S-pro***.

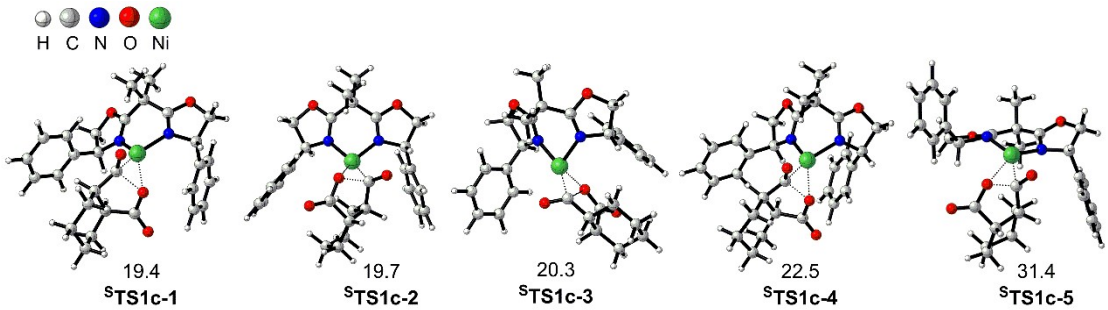


Fig. S10 Optimized structures for selected important stationary points leading to ***S-R-pro***.

4. Fragment Molecular Orbital (FMO) Analysis

Generally, MOs of a total system AB can be represented by a linear combination of MOs of fragments A and B;[S3] see eqn (S8):

$$\varphi_i^{AB} = \sum_m C_{im}^A \varphi_m^A + \sum_{mn} C_{in}^B \varphi_n^B \tag{S8}$$

where φ_i^{AB} represents the *i*th MO of complex AB and φ_m^A and φ_n^B are the *m*th and *n*th MOs of fragments A and B, respectively. C_{im}^A and C_{in}^B are expansion coefficients of φ_m^A and φ_n^B, respectively. Electron populations of φ_m^A and φ_n^B can be obtained from these coefficients.

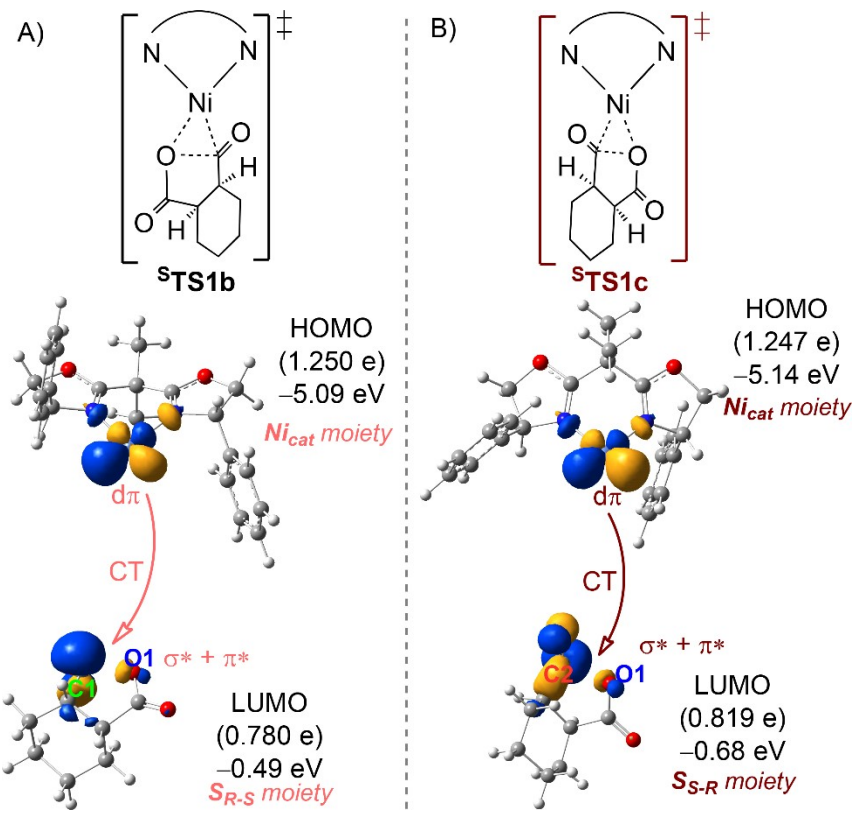


Fig. S11 Important Kohn-Sham orbitals and their electron populations of Ni_{cat} and S moieties in ^{S}**TS1b** and ^{S}**TS1c**.

As shown in Fig. S9A, ^{S}**TS1b** is divided into two fragments as nickel catalyst (Ni_{cat}) and product ($S_{R\text{-}S}$) moieties. Specifically, the electron population of the lowest

unoccupied molecular orbital (LUMO) of the $S_{R\text{-}S}$ moiety highly increases to 0.780 e in **^{S}TS1b**. Consistent with this increase in population, the population of the highest occupied molecular orbital (HOMO) of the Ni_{cat} moiety decreases to 1.250 e. The substantial CT occurs from the d_{π} orbital (HOMO of Ni_{cat} moiety) to the $S_{R\text{-}S}$ $\sigma^* + \pi^*$ orbital (LUMO), indicating that the C1–O1 bond cleavage is under progress. These CT contribute to the change of the Ni^0 to the Ni^{II} and the C1–O1 bond cleavage. As shown in Fig. S9B, **^{S}TS1c** is divided into Ni_{cat} and $S_{S\text{-}R}$ moieties in the same way. The LUMO populations of the $S_{S\text{-}R}$ moiety increase to 0.819 e, and the populations of the HOMO of the Ni_{cat} moiety correspondingly decreases to 1.247 e. This means that a CT similar to that in **^{S}TS1b** from d_{π} to $\sigma^* + \pi^*$ and C2–O1 bond cleavage in **^{S}TS1c**.

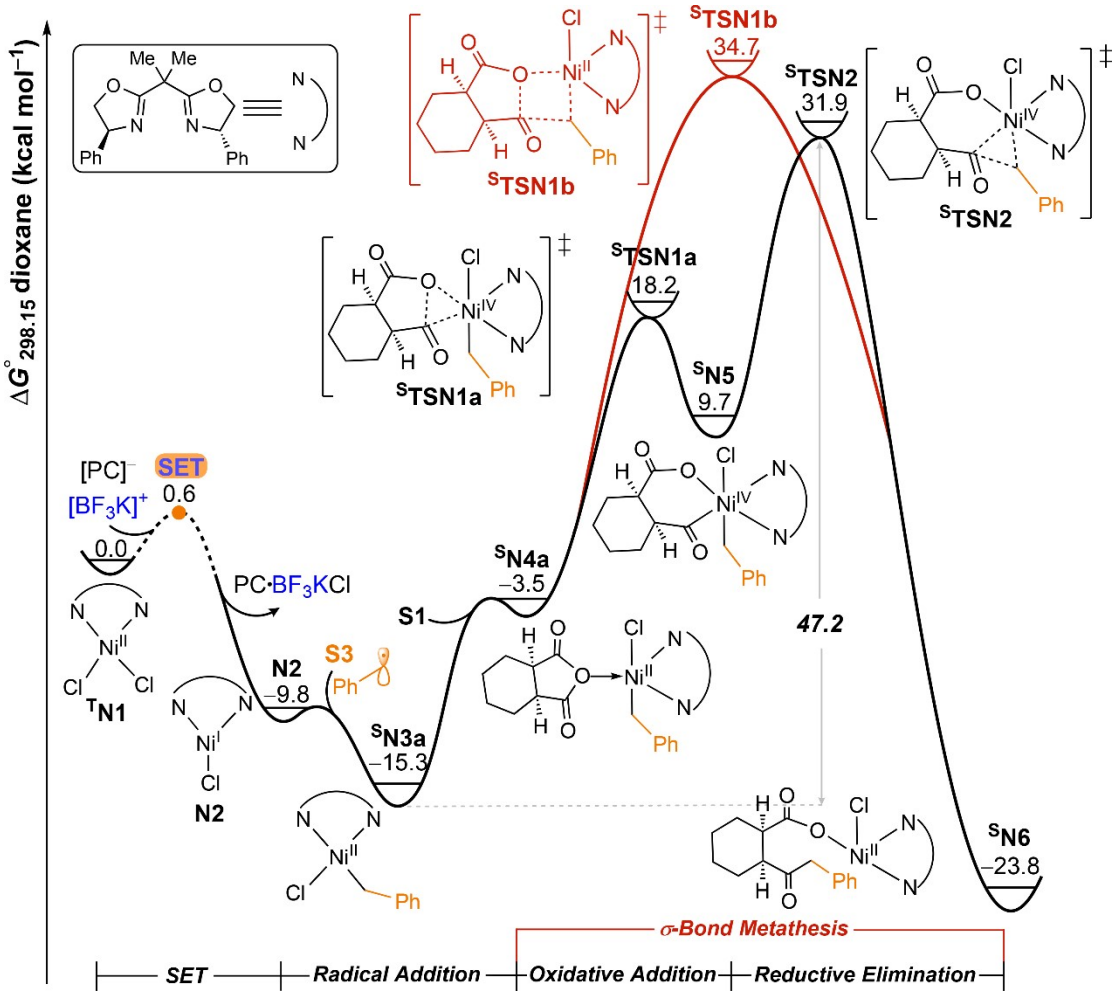


Fig. S12 Energy profiles ($\Delta G°_{298.15}$) of 4CzIPN/Ni^{II} ($NiCl_2$ as the starting catalyst) metallaphotoredox catalytic cycle.

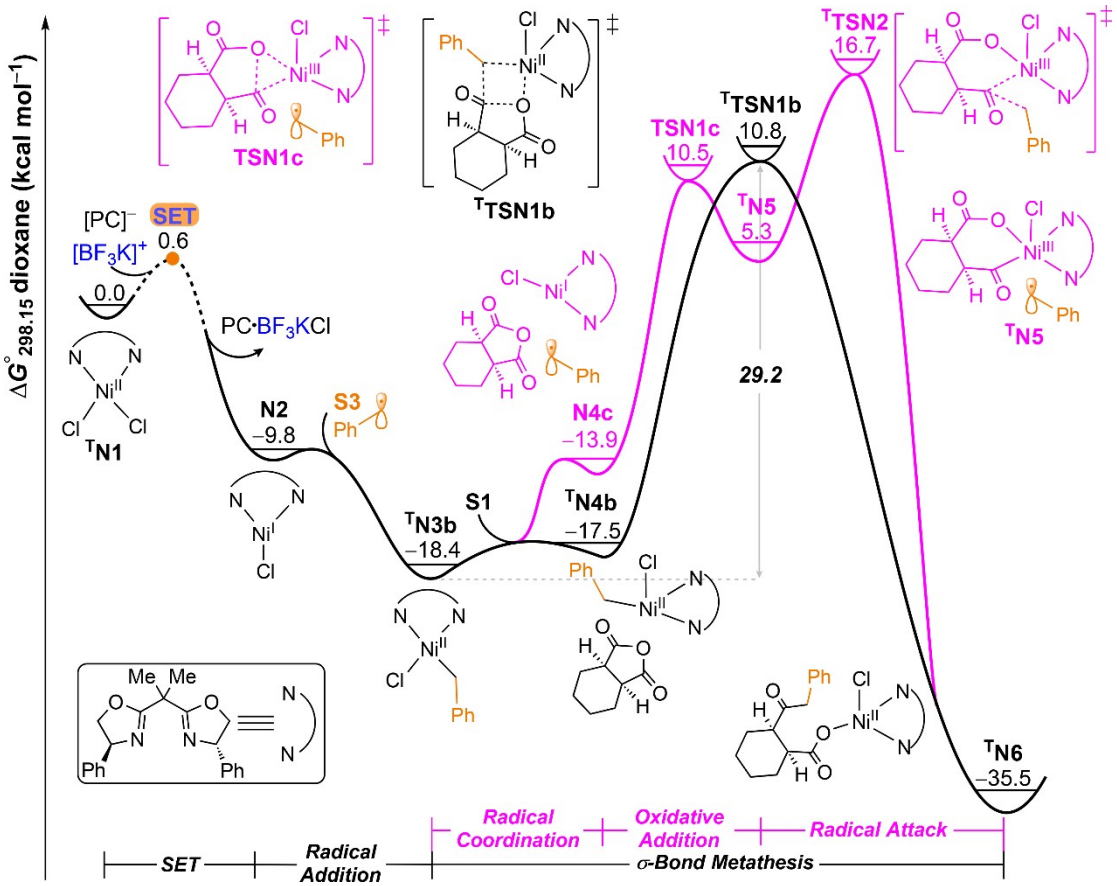


Fig. S13 Energy profiles ($\Delta G°_{298.15}$) of 4CzIPN/Ni^{II} ($NiCl_2$ as the starting catalyst) metallaphotoredox catalytic cycle.

REFERENCES

S1. (a) S. Sakaki, Y. Y. Ohnishi and H. Sato, Theoretical and Computational Studies of Organometallic Reactions: Successful or Not? *Chem. Rec.*, 2010, **10**, 29–45; (b) A. Ishikawa, Y. Nakao, H. Sato and S. Sakaki, Oxygen Atom Transfer Reactions of Iridium and Osmium Complexes: Theoretical Study of Characteristic Features and Significantly Large Differences Between These Two Complexes, *Inorg. Chem.*, 2009, **48**, 8154–8163; (c) A. Ishikawa, Y. Nakao, H. Sato and S. Sakaki, Pd(ii)-promoted Direct Cross-Coupling Reaction of Arenes via Highly Regioselective Aromatic C–H Activation: a Theoretical Study, *Dalton Trans.*, 2010, **39**, 3279–3289.

S2. A. V. Marenich, J. Ho, M. L. Coote, C. J. Cramer and D. G. Truhlar, Computational Electrochemistry: Prediction of Liquid-Phase Reduction Potentials, *Phys. Chem. Chem. Phys.*,

2014, **16**, 15068–15106.

S3. (a) H. Baba, S. Suzuki and T. Takemura, Configuration Analysis in the LCAO Molecular Orbital Theory, *J. Chem. Phys.*, 1969, **50**, 2078–2086; (b) S. Kato, S. Yamabe and K. Fukui, Molecular Orbital Calculations of the Electronic Structure of Borazane, *J. Chem. Phys.*, 1974, **60**, 572–578; (c) S. Dapprich and G. Frenking, Rotational Analysis of n=4–7 Rydberg States of CO Observed by Ion-dip Spectroscopy, *J. Phys. Chem.*, 1995, **99**, 9352–9362.

Cartesian Coordinates of Optimized Structures

^{S}1

(U)M06/BSII SCF energy in solution: -1555.847957 a.u.
(U)M06/BSI SCF energy: -1553.833998 a.u.
(U)M06/BSI SCF Gibbs energy: -1553.321341 a.u.

C	-2.58231200	1.92109600	-2.17391900
O	-1.91842500	2.83741000	-1.29184900
C	-2.28555800	0.53564200	-1.56881400
C	-1.07766100	2.08228700	-0.54335900
N	-1.16256800	0.81088800	-0.65821600
C	-0.23901100	2.85031000	0.44695000
C	3.27106800	2.26766900	1.18190600
O	2.07538900	3.05059500	1.07339400
C	2.80912000	0.81714200	0.93197400
C	1.11423500	2.21049100	0.62007900
N	1.41257300	0.97435200	0.49326900
H	3.97978400	2.61549900	0.41817900
H	-3.64707400	2.17461000	-2.19590500
H	-2.15490300	2.04582500	-3.17776300
H	3.70464600	2.43313700	2.17333500
C	-0.95816400	2.76651100	1.81129900
H	-1.95238300	3.22806800	1.73403100
H	-1.06889900	1.71912600	2.12149600
H	-0.38316800	3.30848000	2.57300900

C	-0.09712500	4.31533200	0.02865400
H	0.41815100	4.41218600	-0.93463400
H	-1.08698400	4.77182000	-0.06984700
H	0.47444200	4.86617200	0.78162000
Ni	0.08208800	-0.55722500	0.18068900
H	2.78865300	0.24004700	1.87021900
H	-1.94999200	-0.17251700	-2.33795400
C	3.66392100	0.08563900	-0.06651200
C	4.47987800	-0.96782200	0.33573600
C	3.65805000	0.46681600	-1.40904000
C	5.26829100	-1.64524300	-0.59006600
H	4.48420100	-1.27300800	1.38331200
C	4.44137400	-0.20772800	-2.33552400
H	3.00825700	1.28202600	-1.73036200
C	5.24721800	-1.26892700	-1.92768900
H	5.89316300	-2.47545500	-0.26524700
H	4.41926700	0.08885900	-3.38287500
H	5.85568800	-1.80301400	-2.65533500
C	-3.46483000	-0.05504600	-0.83484900
C	-4.18006400	-1.11241800	-1.39271300
C	-3.89114100	0.47873800	0.38193800
C	-5.28809500	-1.64488000	-0.74065700
H	-3.85529500	-1.53249100	-2.34596800
C	-4.99628500	-0.05027600	1.03683500
H	-3.33887800	1.30467100	0.83215300
C	-5.69617900	-1.11690000	0.47893300
H	-5.82847700	-2.47855100	-1.18575000
H	-5.31178300	0.36893100	1.99090200
H	-6.55803600	-1.53552900	0.99557600
C	0.14071000	-1.39579400	2.07300400

C	-1.10935500	-1.62445300	1.50860400
C	1.19371800	-2.18823000	-0.44742200
C	-1.53546600	-2.93378300	0.87760100
C	-0.05056700	-2.18210700	-1.07033300
H	0.23105100	-0.56605400	2.78350900
H	-1.06254100	-3.77059400	1.41466600
H	-1.91819000	-0.94491000	1.79191500
H	2.04379300	-1.79093600	-1.00680800
H	-2.61872000	-3.06900700	1.01960700
H	-0.09959300	-1.80320500	-2.09708200
C	1.28723800	-2.37738300	2.08834500
H	2.19992900	-1.81868800	2.35696800
H	1.16559000	-3.13536200	2.88501300
C	1.51944500	-3.07509600	0.73576200
H	0.91780700	-3.99552000	0.68620300
H	2.56833600	-3.40440700	0.67805000
C	-1.21776800	-3.03234600	-0.63050900
H	-2.10496200	-2.71102500	-1.19370200
H	-1.06523500	-4.09305900	-0.90482800

2a

(U)M06/BSII SCF energy in solution: -1514.750467 a.u.
(U)M06/BSI SCF energy: -1512.742765 a.u.
(U)M06/BSI SCF Gibbs energy: -1512.296036 a.u.

C	-1.99412500	2.97763400	-1.40186300
O	-1.22152400	3.24243900	-0.21601300
C	-1.91275000	1.44900100	-1.58646500
C	-0.60826300	2.08865000	0.10310700
N	-0.89643800	1.05713800	-0.59460300
C	0.25280900	2.13744300	1.33975400
C	3.21583500	0.17575600	2.06593300

O	2.38715100	1.35690400	2.13965700
C	2.78855100	-0.50938500	0.76330000
C	1.39189000	1.15509100	1.25381400
N	1.48808200	0.13896400	0.48811900
H	4.26337800	0.48987800	2.09492600
H	-3.01203600	3.34474900	-1.23455900
H	-1.53783200	3.53465600	-2.22802100
H	2.99103100	-0.43783200	2.94717400
C	-0.64935000	1.71843500	2.52218900
H	-1.46368000	2.44704000	2.63370900
H	-1.07996900	0.71987400	2.35773300
H	-0.06408800	1.70930600	3.44973000
C	0.80094900	3.54882600	1.57105300
H	1.44502800	3.87058800	0.74322600
H	-0.02423800	4.26234000	1.65844300
H	1.38874000	3.57110500	2.49359200
Ni	-0.11526700	-0.76609900	-0.26477400
H	2.59564000	-1.58152000	0.90455900
H	-1.53297300	1.19006000	-2.58380200
C	3.69673300	-0.32593300	-0.42590300
C	3.76969300	-1.33819900	-1.38160500
C	4.40426700	0.85942800	-0.62871100
C	4.55573300	-1.17509000	-2.51715900
H	3.18598700	-2.24843100	-1.22322200
C	5.19059700	1.02246700	-1.76348100
H	4.33420200	1.66792300	0.10155800
C	5.27000000	0.00350100	-2.70828900
H	4.61200700	-1.97305100	-3.25578500
H	5.74270700	1.94928200	-1.91175900
H	5.88826000	0.13016000	-3.59549700

C	-3.20869000	0.71696600	-1.35359400
C	-3.69118400	-0.17448200	-2.30765300
C	-3.93120000	0.90836700	-0.17441200
C	-4.88545900	-0.85742500	-2.09826500
H	-3.12002400	-0.34103800	-3.22170600
C	-5.12441300	0.23005000	0.03729900
H	-3.55407300	1.58563900	0.59450400
C	-5.60517800	-0.65331900	-0.92622400
H	-5.25177100	-1.55331600	-2.85073600
H	-5.67727300	0.38341800	0.96239500
H	-6.53904200	-1.18663500	-0.75847100
C	-2.23994800	-2.09942400	0.58403200
C	-1.10545900	-2.54331400	-0.14345600
C	0.08987000	-3.01223300	0.56952900
C	0.06094900	-2.78362500	2.00570200
C	-1.04460300	-2.30336500	2.65112800
C	-2.23341100	-1.95031400	1.95563000
H	-3.14082400	-1.85995300	0.01640400
H	-1.24716800	-2.88064600	-1.17510500
H	0.93855600	-3.08981900	2.58162100
H	-1.01352000	-2.19908200	3.73781800
H	-3.11010200	-1.58694800	2.48925800
C	1.17350400	-3.58060800	-0.06166400
H	2.02311100	-3.95437500	0.51083200
H	1.15684500	-3.78944400	-1.13125000

TS1a

(U)M06/BSII SCF energy in solution: -1514.745327 a.u.

(U)M06/BSI SCF energy: -1512.737624 a.u.

(U)M06/BSI SCF Gibbs energy: -1512.290549 a.u.

C	-2.36992800	3.13194700	-1.10786500

O	-1.59393900	3.24012700	0.10002900
C	-2.08538200	1.71201600	-1.61414700
C	-0.75168400	2.18835000	0.10972700
N	-0.89176400	1.33170400	-0.82973700
C	0.15609800	2.14641100	1.31033500
C	2.91653800	-0.06814500	2.07080900
O	2.15542600	1.15563500	2.17675800
C	2.55290200	-0.62019600	0.69096100
C	1.21323600	1.07866100	1.21864100
N	1.30964900	0.11745900	0.38614500
H	3.97463500	0.17460400	2.20483500
H	-3.41960500	3.31543800	-0.85923200
H	-2.01909500	3.90570100	-1.80099100
H	2.57586000	-0.73588700	2.87248000
C	-0.73461100	1.80334500	2.52313400
H	-1.50122700	2.57546400	2.65815700
H	-1.21355800	0.82532700	2.37603800
H	-0.11843700	1.75061200	3.42816400
C	0.82671600	3.51348100	1.50484500
H	1.47539600	3.76342500	0.65524400
H	0.06535800	4.29359200	1.60244100
H	1.43760200	3.50218200	2.41257000
Ni	-0.05975900	-0.44145000	-0.92236900
H	2.29021800	-1.68435700	0.75639500
H	-1.81639200	1.70969200	-2.67839800
C	3.54423000	-0.39632100	-0.41885200
C	3.64465200	-1.33993300	-1.43970800
C	4.30900000	0.76866500	-0.48875900
C	4.51214200	-1.13236600	-2.50665100
H	3.02334000	-2.23606200	-1.39694600

C	5.17821000	0.97692800	-1.55303500
H	4.21548400	1.52702600	0.29137800
C	5.28375000	0.02346700	-2.56213800
H	4.58660300	-1.87751600	-3.29670900
H	5.77541500	1.88646600	-1.59546400
H	5.96783800	0.18439000	-3.39365000
C	-3.16760500	0.69248300	-1.36577400
C	-3.41091500	-0.30771600	-2.30416600
C	-3.87215000	0.68507400	-0.16015200
C	-4.36044500	-1.29370800	-2.05214300
H	-2.83928100	-0.32086400	-3.23342700
C	-4.82437500	-0.29436400	0.09088300
H	-3.65945400	1.44089300	0.59902100
C	-5.07193900	-1.28391000	-0.85779300
H	-4.53868000	-2.07338900	-2.79011600
H	-5.36751600	-0.29411900	1.03429700
H	-5.81359200	-2.05523500	-0.65938200
C	-1.71670800	-1.72476400	2.23682100
C	-1.68200200	-2.11689700	0.91178400
C	-0.56575200	-2.80996400	0.35234800
C	0.45819100	-3.14710400	1.28265700
C	0.41610200	-2.73973400	2.60905300
C	-0.65493000	-1.99673700	3.10987300
H	-2.60206500	-1.19696400	2.60216600
H	-2.52555400	-1.88450100	0.25705800
H	1.29894900	-3.75077900	0.92857000
H	1.23100500	-3.03133900	3.27655400
H	-0.69107200	-1.69147400	4.15439500
C	-0.48341900	-3.12134100	-1.03948500
H	0.31590400	-3.77903500	-1.38276000

H	-1.41145500	-3.15870400	-1.61272700

3a

(U)M06/BSII SCF energy in solution: -1514.779579 a.u.
(U)M06/BSI SCF energy: -1512.772729 a.u.
(U)M06/BSI SCF Gibbs energy: -1512.325922 a.u.

C	-3.70024100	2.25644600	-0.93405000
O	-2.90382100	2.80763300	0.13041400
C	-2.94087500	0.99244400	-1.35990200
C	-1.73027600	2.13962700	0.11315200
N	-1.62372100	1.16959600	-0.70959600
C	-0.72447200	2.65946500	1.10176100
C	2.47321400	1.28020900	2.09626000
O	1.43470800	2.27937200	2.04026900
C	2.17110800	0.36010400	0.89769400
C	0.51685300	1.81077200	1.17203500
N	0.80261100	0.74594200	0.53160700
H	3.44051700	1.78790800	2.02997900
H	-4.70444200	2.06103600	-0.54500300
H	-3.76160500	3.00602300	-1.73205200
H	2.38897200	0.76681800	3.06187600
C	-1.37902000	2.68786200	2.49469700
H	-2.25740900	3.34141700	2.48485600
H	-1.69627600	1.68112700	2.79723900
H	-0.66285400	3.06375700	3.23260900
C	-0.31881900	4.08343500	0.67900500
H	0.16427100	4.07511700	-0.30704600
H	-1.20543200	4.72509400	0.62906000
H	0.38362100	4.50528300	1.40545300
Ni	-0.24647900	-0.26901000	-0.89460500
H	2.16980900	-0.69946000	1.19033000

H	-2.78336200	0.96134600	-2.44591400
C	3.13234600	0.55196200	-0.24968200
C	4.33229700	-0.16040200	-0.24616200
C	2.89064700	1.46917100	-1.27059600
C	5.27891400	0.04459800	-1.24276100
H	4.51026000	-0.89727500	0.53903100
C	3.83574900	1.67204100	-2.27119900
H	1.94376800	2.00882000	-1.29745200
C	5.03225700	0.96403300	-2.25814300
H	6.20824100	-0.52256800	-1.23228500
H	3.63297000	2.38568500	-3.06828200
H	5.77032300	1.12204600	-3.04279800
C	-3.53349000	-0.31660200	-0.90423000
C	-3.45788400	-1.43807100	-1.72708500
C	-4.07322200	-0.44594900	0.37611000
C	-3.92155900	-2.67180300	-1.28308700
H	-3.00928200	-1.34524400	-2.71724200
C	-4.54138600	-1.67610400	0.82076300
H	-4.11409800	0.42155700	1.03858000
C	-4.46685400	-2.79153100	-0.00967700
H	-3.85042100	-3.54231300	-1.93225500
H	-4.96155200	-1.76764600	1.82087800
H	-4.82973600	-3.75598900	0.34078600
C	0.55634600	-3.53672800	2.04650800
C	0.06961900	-3.01851900	0.85647400
C	0.92226500	-2.69607200	-0.22094300
C	2.29262000	-2.95885100	-0.03137900
C	2.78292600	-3.47381100	1.16561200
C	1.92393400	-3.76039600	2.22249800
H	-0.13915100	-3.76862100	2.85411400

H	-1.00186500	-2.83269400	0.73779200
H	2.98071900	-2.74500100	-0.85206000
H	3.85340800	-3.66236200	1.26798800
H	2.30611100	-4.16525900	3.15844300
C	0.40902000	-2.05710900	-1.44014500
H	1.14716100	-2.05241900	-2.25348600
H	-0.51271000	-2.55003000	-1.79490600

4a

(U)M06/BSII SCF energy in solution: -2051.220632 a.u.
(U)M06/BSI SCF energy: -2049.063856 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.453594 a.u.

C	2.73474000	-2.76948900	1.84175900
O	2.40394600	-1.71469500	2.76616600
C	2.29182800	-2.23472500	0.47470000
C	1.63869500	-0.84108200	2.08878700
N	1.46241300	-1.06493700	0.84280900
C	1.20793700	0.34341900	2.90940800
C	-0.73385700	3.24829000	1.97089300
O	-0.07879400	2.35214200	2.89172200
C	-0.99870200	2.38539800	0.73298200
C	0.31045000	1.28948100	2.15870500
N	-0.09814900	1.23181800	0.95010500
H	-1.63673500	3.63444200	2.45391700
H	3.80844900	-2.96864800	1.92160700
H	2.16857100	-3.66033700	2.13798500
H	-0.04467500	4.07496300	1.75815400
C	2.49063700	1.11845300	3.27678900
H	3.17170100	0.47182900	3.84046000
H	3.00195100	1.46652200	2.36757400
H	2.23744000	1.98900100	3.89097500

C	0.48318800	-0.13417200	4.17865600
H	-0.41532000	-0.70949700	3.92179300
H	1.14840700	-0.77291200	4.76900600
H	0.19593300	0.72938900	4.78794800
Ni	0.74517600	0.15851400	-0.56285100
H	-0.68363400	2.89775200	-0.18448000
H	1.66391900	-2.97015100	-0.03961400
C	-2.41814800	1.90468000	0.57750000
C	-3.00475600	1.87494000	-0.68665000
C	-3.14774800	1.45190900	1.67989900
C	-4.31231100	1.42256200	-0.84419200
H	-2.42232000	2.21450600	-1.54482400
C	-4.45420100	1.00275500	1.52508500
H	-2.68418300	1.44084800	2.66810400
C	-5.04141800	0.99375200	0.26131100
H	-4.76541200	1.40939400	-1.83495800
H	-5.01477400	0.65698600	2.39194200
H	-6.06615300	0.64549400	0.13822000
C	3.36790800	-1.77456000	-0.47308300
C	3.26706400	-2.09734700	-1.82495200
C	4.40235000	-0.94161300	-0.04312800
C	4.19047700	-1.59728500	-2.73786100
H	2.44290600	-2.72973800	-2.15979900
C	5.32367100	-0.44019800	-0.95376400
H	4.48525500	-0.67226200	1.01225700
C	5.21697100	-0.76614700	-2.30394600
H	4.10095200	-1.85096200	-3.79251500
H	6.12751400	0.20934700	-0.61128600
H	5.93627900	-0.36877700	-3.01786600
C	1.81365200	4.41988500	-1.17696100

C	1.83937200	3.06203300	-1.45503800
C	0.81272500	2.43286700	-2.19242900
C	-0.21668600	3.27014100	-2.66409900
C	-0.24931000	4.63229400	-2.37768500
C	0.75876800	5.22169400	-1.62155700
H	2.62829200	4.86552500	-0.60465900
H	2.66084400	2.44143100	-1.08582300
H	-1.00446900	2.82811500	-3.27945400
H	-1.06975400	5.24075900	-2.75949000
H	0.73900300	6.28744600	-1.39992000
C	0.78682000	0.97587200	-2.37660900
H	0.02299300	0.66116500	-3.10402900
H	1.76756400	0.58980900	-2.70916400
O	-0.72627200	-3.03089700	0.46767000
C	-2.58747200	-1.69272200	-0.00511400
C	-1.73962900	-1.81780300	-1.26659400
C	-3.64467700	-2.92252400	-2.49644200
C	-2.47431500	-1.95162300	-2.58712000
C	-3.80770000	-2.63082100	-0.01215300
C	-4.56090300	-2.55567900	-1.33372100
H	-4.20241100	-2.92969700	-3.44245100
H	-1.75895000	-2.25433700	-3.36346400
H	-3.47416400	-3.67198200	0.14149900
H	-4.94769600	-1.53246400	-1.47981800
H	-2.84667000	-0.95334700	-2.86723800
H	-4.45066600	-2.37974800	0.84254800
H	-5.43365800	-3.22203800	-1.30061700
H	-3.26236600	-3.94751800	-2.35078700
C	-1.63637200	-2.16520600	1.05615300
C	-0.80598400	-2.93828700	-0.91755400

O	-1.61593100	-1.94932600	2.23245600
O	-0.13257100	-3.63777400	-1.61805800
H	-2.90206800	-0.66512400	0.20009000
H	-1.05808600	-0.93221500	-1.31388200

TS2a

(U)M06/BSII SCF energy in solution: -2051.196189 a.u.
(U)M06/BSI SCF energy: -2049.041269 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.429487 a.u.

C	2.78472600	-2.08819400	2.39101600
O	2.37769600	-0.90197400	3.10190400
C	2.38199400	-1.81987500	0.93113300
C	1.64734700	-0.17156500	2.24341000
N	1.58189900	-0.58525500	1.03733600
C	1.00867700	1.03186600	2.88700900
C	-0.70452000	3.84699600	1.35513800
O	0.01291200	3.14804400	2.39057100
C	-0.83630900	2.81949100	0.21106400
C	0.31777000	1.93490400	1.90207100
N	-0.07744600	1.66765000	0.71916700
H	-1.66962000	4.16286500	1.76674000
H	3.86267600	-2.21686100	2.53553000
H	2.25143400	-2.93709500	2.83247500
H	-0.11858000	4.73031900	1.08009600
C	2.09116600	1.81956100	3.64128000
H	2.56113100	1.17769200	4.39218400
H	2.86933500	2.18507100	2.95797300
H	1.64132600	2.68101300	4.14405000
C	-0.07415300	0.53754600	3.87195000
H	-0.85185500	-0.04757000	3.35990800
H	0.38948400	-0.08966000	4.64163900

H	-0.53925000	1.40185600	4.36121000
Ni	0.03875600	-0.16297400	-0.24936100
H	-0.34912500	3.17344400	-0.70860900
H	1.71344800	-2.60254100	0.54786900
C	-2.25440400	2.41594900	-0.10160300
C	-2.83264600	2.73543200	-1.32862700
C	-3.00598900	1.72057900	0.84800900
C	-4.14852300	2.37255500	-1.60218000
H	-2.23899900	3.26571900	-2.07401800
C	-4.31833800	1.35296600	0.57518900
H	-2.56278700	1.44537200	1.80694000
C	-4.89252900	1.68082700	-0.65122600
H	-4.59208500	2.62888000	-2.56290700
H	-4.87858800	0.79633400	1.32495300
H	-5.92106400	1.39545300	-0.86625500
C	3.52752800	-1.62544900	-0.02710200
C	3.58333500	-2.36627400	-1.20522500
C	4.52371900	-0.68169200	0.23211400
C	4.61779200	-2.16749000	-2.11521200
H	2.79305300	-3.08972600	-1.41142200
C	5.55924000	-0.48381100	-0.67283600
H	4.48676400	-0.08611100	1.14727400
C	5.60631400	-1.22642700	-1.85050600
H	4.64706900	-2.74767800	-3.03569900
H	6.33065800	0.25537300	-0.46293900
H	6.41389200	-1.06816100	-2.56302200
C	2.51589100	2.90985300	-2.34385200
C	2.22111200	1.57715400	-2.09076200
C	0.98386300	1.02125900	-2.46611800
C	0.06871900	1.86491100	-3.12012600

C	0.36852100	3.19626200	-3.38242800
C	1.59235200	3.73344500	-2.98776200
H	3.48449800	3.31092400	-2.04582200
H	2.95501200	0.93707500	-1.59517700
H	-0.89510000	1.44962200	-3.42440200
H	-0.35652000	3.81999600	-3.90710900
H	1.83163800	4.77504700	-3.19588100
C	0.62657900	-0.36188700	-2.12771200
H	-0.15487600	-0.77087000	-2.78092700
H	1.47635200	-1.05212900	-2.07583600
O	-1.09152100	-1.48536900	1.25058400
C	-3.14242400	-1.94694800	0.22420900
C	-2.21264000	-1.67715600	-0.96219100
C	-2.83239400	-3.94680100	-1.94251400
C	-2.54059100	-2.47644300	-2.22038500
C	-3.42509200	-3.44025200	0.43027200
C	-3.89388000	-4.09717700	-0.85986900
H	-3.15358500	-4.43734800	-2.87211300
H	-1.72210500	-2.37716600	-2.94770700
H	-2.50380900	-3.93981500	0.77158100
H	-4.83473700	-3.62607100	-1.19436100
H	-3.43008100	-2.01557700	-2.68151000
H	-4.16183800	-3.54838100	1.23809000
H	-4.11912500	-5.15820500	-0.68387200
H	-1.90705700	-4.44478200	-1.61771100
C	-2.39711200	-1.42403700	1.43570600
C	-0.80194000	-1.95398700	-0.41819500
O	-2.92275800	-1.04216800	2.46598400
O	-0.15980000	-2.97380400	-0.53943800
H	-4.09367800	-1.40586300	0.10754200

H	-2.28081900	-0.59830200	-1.19785100

5a

(U)M06/BSII SCF energy in solution: -2051.214576 a.u.
(U)M06/BSI SCF energy: -2049.054677 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.438465 a.u.

C	2.41617700	-2.56408000	2.24171200
O	2.24106200	-1.33122400	2.96609500
C	2.07812100	-2.19794700	0.79160000
C	1.55507100	-0.50902200	2.15080700
N	1.37259500	-0.90970000	0.95154800
C	1.16231300	0.78530400	2.81441500
C	-0.29295000	3.80976200	1.43404600
O	0.33736100	2.98629800	2.43098200
C	-0.52017700	2.86615400	0.23596400
C	0.53083400	1.77749100	1.87361400
N	0.13404100	1.62109100	0.67274000
H	-1.22359100	4.20430900	1.85710600
H	3.44702300	-2.90129800	2.38703800
H	1.72365800	-3.30058700	2.66588900
H	0.38480200	4.63980400	1.20684500
C	2.44720100	1.40958100	3.39169100
H	2.89254400	0.73195000	4.12657900
H	3.18423000	1.59828400	2.59795100
H	2.21387800	2.35954500	3.88181000
C	0.15029300	0.49405700	3.94248100
H	-0.77472700	0.06973600	3.52825600
H	0.58721100	-0.21453500	4.65494500
H	-0.07790700	1.42464900	4.47445900
Ni	-0.21952400	-0.23977800	-0.19570600
H	-0.00381800	3.22897100	-0.66332000

H	1.37923700	-2.91444400	0.34251700
C	-1.96782900	2.60082600	-0.09637100
C	-2.47903700	2.91399900	-1.35497900
C	-2.80493100	2.00710400	0.85142200
C	-3.80728700	2.63379800	-1.66636600
H	-1.82526800	3.37760200	-2.09442500
C	-4.12842100	1.71928800	0.54117100
H	-2.41497000	1.72094300	1.82946000
C	-4.63111100	2.03172500	-0.72041000
H	-4.19703400	2.88450900	-2.65172200
H	-4.74753400	1.21908100	1.28372200
H	-5.66742600	1.80381800	-0.96565800
C	3.26969900	-2.01369700	-0.11482200
C	3.27184500	-2.56202400	-1.39523000
C	4.35955800	-1.24180600	0.29596700
C	4.33774300	-2.33088900	-2.25977200
H	2.41954800	-3.16101800	-1.71830000
C	5.42758300	-1.01532400	-0.56297500
H	4.36802100	-0.80361200	1.29636000
C	5.41503200	-1.55551100	-1.84681900
H	4.32294400	-2.75643800	-3.26145000
H	6.27113300	-0.41094100	-0.23351300
H	6.24677900	-1.37137500	-2.52425000
C	2.97788000	2.75356100	-1.80493300
C	2.41490900	1.49518500	-1.64745100
C	1.18307600	1.17382900	-2.24094000
C	0.56099200	2.15921500	-3.01977600
C	1.12485300	3.42082500	-3.18225500
C	2.33401200	3.72977500	-2.56617600
H	3.93718700	2.97512100	-1.33742400

H	2.92604300	0.73605400	-1.05161300
H	-0.38370600	1.91673900	-3.51073700
H	0.61932800	4.16390200	-3.79912200
H	2.78191400	4.71420600	-2.69243300
C	0.55655400	-0.14684700	-2.04527700
H	-0.20765100	-0.34340900	-2.81239900
H	1.28326500	-0.96800100	-2.04224900
O	-1.37744600	-0.69174400	1.38880000
C	-3.23322800	-1.68880300	0.19803000
C	-2.45934500	-1.44585400	-1.11083200
C	-3.30764800	-3.69063700	-1.98676200
C	-3.07839800	-2.21337900	-2.28649500
C	-3.43153400	-3.18132100	0.47205600
C	-4.10816700	-3.87516300	-0.70281000
H	-3.82611200	-4.15920900	-2.83541000
H	-2.45340800	-2.09026800	-3.18355000
H	-2.45316900	-3.65149000	0.66722700
H	-5.11760100	-3.44863600	-0.83688900
H	-4.04516200	-1.73053200	-2.50795700
H	-4.02164500	-3.27879700	1.39243200
H	-4.24717200	-4.94424200	-0.48923900
H	-2.33457700	-4.19385100	-1.89051700
C	-2.62383900	-1.02038300	1.43819800
C	-0.99231600	-1.79558900	-0.90347600
O	-3.33745700	-0.87012000	2.42571100
O	-0.47256000	-2.86656500	-1.04436100
H	-4.23348700	-1.24220700	0.06073700
H	-2.50541900	-0.36266600	-1.32871000

TS3a

(U)M06/BSII SCF energy in solution: -2051.203955 a.u.
(U)M06/BSI SCF energy: -2049.045819 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.430717 a.u.

C	3.50769200	0.33854300	-2.59270700
O	2.92923500	-0.96150400	-2.80827200
C	2.82241600	0.86048300	-1.31464400
C	1.94760300	-1.10875700	-1.90354400
N	1.81242300	-0.17610400	-1.04117600
C	1.14850600	-2.37164900	-2.10405600
C	-1.24725100	-4.03258100	0.05719200
O	-0.33422200	-3.90812700	-1.04694400
C	-1.28795400	-2.62435600	0.68690100
C	0.19072000	-2.67139800	-0.97941200
N	-0.22522000	-1.91065600	-0.04327400
H	-2.21540600	-4.35875500	-0.33751200
H	4.59088800	0.21378700	-2.48617100
H	3.29527600	0.94890900	-3.47671100
H	-0.85243300	-4.79845100	0.73471600
C	2.12210600	-3.54942300	-2.27292400
H	2.79181800	-3.35950600	-3.11662600
H	2.73258500	-3.69843400	-1.37193300
H	1.56353300	-4.46952500	-2.46705300
C	0.30297100	-2.19135900	-3.38844500
H	-0.37305000	-1.32947500	-3.28618300
H	0.97209500	-2.03097500	-4.24178000
H	-0.27883600	-3.10274100	-3.56977100
Ni	0.04066300	0.16684700	-0.09087600
H	-1.01475100	-2.65704400	1.75132000
H	2.28428600	1.80060200	-1.49628100
C	-2.61900800	-1.92601700	0.54211800
C	-3.42568500	-1.71887600	1.66079400

C	-3.06439700	-1.49221800	-0.70863200
C	-4.65434200	-1.07778600	1.53633100
H	-3.07533200	-2.05211100	2.63843900
C	-4.28602600	-0.83932200	-0.83381100
H	-2.43578200	-1.61106800	-1.59149200
C	-5.08219600	-0.63087000	0.28976800
H	-5.27467600	-0.91977000	2.41730300
H	-4.58663600	-0.46645700	-1.81154100
H	-6.03780900	-0.11782300	0.19269400
C	3.74580900	1.04135100	-0.13760100
C	3.87570000	2.28788600	0.47045400
C	4.46136900	-0.04457100	0.37120700
C	4.70890800	2.44815700	1.57409300
H	3.28795000	3.12510100	0.09389000
C	5.28860100	0.11243000	1.47609200
H	4.35824600	-1.02631900	-0.09670800
C	5.41302100	1.36148800	2.08018500
H	4.80021900	3.42538200	2.04498100
H	5.83791300	-0.74145800	1.86922700
H	6.05900000	1.48479200	2.94754200
C	0.87500100	-1.96739500	3.72432900
C	1.15209800	-0.95425000	2.81788700
C	0.25325700	0.10620600	2.62327000
C	-0.93134600	0.11002200	3.36838900
C	-1.20895400	-0.90529300	4.27801900
C	-0.31061000	-1.95176100	4.46022200
H	1.59668700	-2.77024100	3.87106200
H	2.08587600	-0.95992400	2.25167000
H	-1.64182100	0.92916100	3.23998800
H	-2.13248800	-0.87133400	4.85571400

H	-0.52079300	-2.73946000	5.18170400
C	0.59664400	1.22350700	1.69829700
H	0.27747800	2.16806800	2.15976500
H	1.67351300	1.30358800	1.51137200
O	-0.86469100	0.33897300	-1.86143000
C	-2.32479700	2.16467300	-1.20085100
C	-1.70209200	2.10172400	0.20337700
C	-1.95416600	4.63113200	0.37987900
C	-2.18338300	3.28643500	1.05891100
C	-2.10874600	3.52164200	-1.87502200
C	-2.60812600	4.66282300	-0.99762500
H	-2.35252500	5.43430500	1.01629800
H	-1.70586800	3.26284700	2.05130700
H	-1.03741600	3.65860600	-2.08681100
H	-3.70240300	4.57450900	-0.87910700
H	-3.26339800	3.14170300	1.23190200
H	-2.63147700	3.50298500	-2.83990600
H	-2.42476500	5.63063300	-1.48545600
H	-0.87296600	4.80790800	0.27821100
C	-1.91199200	1.03167900	-2.15647200
C	-0.17865300	2.03922000	0.14330500
O	-2.59683200	0.85417500	-3.16008300
O	0.55489800	2.89650000	-0.29876000
H	-3.41407500	2.04522300	-1.05708800
H	-2.05493100	1.16909500	0.68699500

6a

(U)M06/BSII SCF energy in solution: -2051.253038 a.u.

(U)M06/BSI SCF energy: -2049.100594 a.u.

(U)M06/BSI SCF Gibbs energy: -2048.48341 a.u.

C	-2.41455200	-2.74623800	-2.40182600

O	-3.58718600	-2.11292500	-1.83675500
C	-1.23390100	-2.15018700	-1.61737500
C	-3.12431600	-1.11354500	-1.06358900
N	-1.86440900	-1.02130700	-0.90607700
C	-4.18029200	-0.28251600	-0.37030200
C	-3.64769500	3.32162200	-0.08179900
O	-4.42717800	2.13751100	-0.34800200
C	-2.38215600	2.80367500	0.62578600
C	-3.63224200	1.09139900	-0.06671300
N	-2.49827800	1.34147700	0.46992900
H	-3.42332000	3.80054600	-1.04376900
H	-2.52586100	-3.82881700	-2.28400500
H	-2.38891000	-2.49580500	-3.46864600
H	-4.25686500	3.99705700	0.52543100
C	-4.47728000	-0.98233600	0.97227200
H	-4.86737900	-1.99099000	0.78364200
H	-3.56650500	-1.06101800	1.57931800
H	-5.23455100	-0.41879000	1.53277500
C	-5.45619400	-0.20078000	-1.20670700
H	-5.27615800	0.27011600	-2.17971800
H	-5.84904100	-1.20713700	-1.38019000
H	-6.21464300	0.38719800	-0.67908700
Ni	-0.80605100	0.29004500	0.21383200
H	-2.41051900	3.03159600	1.70334000
H	-0.46147000	-1.72049300	-2.26694700
C	-1.07251400	3.28438600	0.05806300
C	-0.19057100	4.03167300	0.83461100
C	-0.69439000	2.90574000	-1.23312800
C	1.05658900	4.39277100	0.33504800
H	-0.47842800	4.32102400	1.84649800

C	0.54992100	3.26541000	-1.73531700
H	-1.35748700	2.28817000	-1.84130000
C	1.42812000	4.00538400	-0.94842700
H	1.74051300	4.97284800	0.95258800
H	0.84532100	2.92459100	-2.72578500
H	2.41023500	4.27476300	-1.33552500
C	-0.59995800	-3.07690000	-0.61215700
C	0.78542900	-3.13902500	-0.49374900
C	-1.39468900	-3.83990200	0.24736000
C	1.37385000	-3.96835500	0.45665300
H	1.41088000	-2.51753100	-1.13446900
C	-0.81100600	-4.66665100	1.19923900
H	-2.48337400	-3.78287000	0.16847000
C	0.57778800	-4.73491700	1.30108800
H	2.45823600	-3.97508100	0.54827100
H	-1.43821200	-5.26397900	1.85975500
H	1.03652600	-5.38439600	2.04530100
C	-0.28220200	-0.93355100	2.81973800
C	1.07351800	-1.15074700	2.61158300
C	1.97955500	-0.09054600	2.66463300
C	1.51271200	1.18424800	2.97825000
C	0.16003000	1.40282200	3.21522700
C	-0.74543300	0.34935500	3.11967500
H	-0.97822700	-1.77001600	2.74805400
H	1.42836500	-2.14773100	2.34783000
H	2.21378600	2.01983600	3.01706200
H	-0.19059200	2.40233600	3.47195900
H	-1.80794100	0.52234000	3.29149900
C	3.42090900	-0.32978300	2.30143100
H	4.03460800	0.53143100	2.60464000

H	3.80275100	-1.22849800	2.80352900
O	1.09477800	0.18645100	-0.13937000
C	3.05044000	0.55938800	-1.43418600
C	3.72670000	0.66502500	-0.06500100
C	5.92386200	-0.01320100	-1.16785200
C	5.23245100	0.95790100	-0.21796500
C	3.77313100	-0.36255100	-2.41697400
C	5.24818800	-0.00358600	-2.53406800
H	6.98754300	0.25105000	-1.25701500
H	5.72725300	0.95877600	0.76667300
H	3.67736300	-1.40289500	-2.07428100
H	5.34790400	1.00409900	-2.97630000
H	5.33545100	1.98229900	-0.61424500
H	3.26528000	-0.29372100	-3.38694700
H	5.75829500	-0.69565600	-3.21931800
H	5.88347900	-1.03142900	-0.75056600
C	1.55898800	0.22235100	-1.33386000
C	3.55432000	-0.56712100	0.79782500
O	0.92733300	0.02728900	-2.38011400
O	3.58198300	-1.70231900	0.36114400
H	3.08918800	1.57722800	-1.87166300
H	3.26423900	1.50476600	0.47873500

7a

(U)M06/BSII SCF energy in solution: -2363.131932 a.u.

(U)M06/BSI SCF energy: -2360.891681 a.u.

(U)M06/BSI SCF Gibbs energy: -2360.099876 a.u.

C	3.33607300	0.81365700	3.02659800
O	3.48641400	1.91513400	2.10416400
C	2.66631000	-0.28022400	2.19361900
C	2.63118200	1.65041200	1.09369500

N	2.07578500	0.50382100	1.08432700
C	2.49267400	2.75763800	0.08886600
C	0.45490000	2.90029900	-2.90807900
O	1.48071300	3.33651100	-1.99194800
C	-0.42812000	1.97830300	-2.06440200
C	1.44019400	2.48130700	-0.95482100
N	0.47171800	1.64366600	-0.93040200
H	-0.05724300	3.78718700	-3.29229300
H	4.32491500	0.55130200	3.41292500
H	2.69889000	1.15829400	3.85200800
H	0.94982000	2.35890500	-3.72571100
C	3.86225700	2.94930700	-0.58128500
H	4.61488700	3.20266700	0.17311900
H	4.17217400	2.02732300	-1.09024000
H	3.81041000	3.75559900	-1.31993900
C	2.06052100	4.04697000	0.81350300
H	1.08546200	3.90981800	1.30223700
H	2.79931400	4.31487900	1.57616500
H	1.98135800	4.87027100	0.09398800
Ni	0.31484300	0.04092700	0.18086200
H	-0.66841600	1.05556100	-2.61007700
H	1.84506500	-0.76910000	2.73280300
C	-1.69463900	2.61109400	-1.54297200
C	-2.91159800	1.94400400	-1.66439900
C	-1.66057300	3.86168500	-0.91904700
C	-4.07834100	2.51517100	-1.16180700
H	-2.93810300	0.97558200	-2.16711600
C	-2.82472000	4.43249600	-0.41975700
H	-0.71290200	4.39529700	-0.82010100
C	-4.03810100	3.75692300	-0.53787900

H	-5.02414400	1.98358600	-1.26314300
H	-2.78650300	5.40742400	0.06360900
H	-4.95140500	4.20315100	-0.14703700
C	3.58191800	-1.32987700	1.61451200
C	3.06455000	-2.59530600	1.34342700
C	4.90123900	-1.03495700	1.26094100
C	3.85944500	-3.55833700	0.73018200
H	2.01652600	-2.81725100	1.55538500
C	5.69849800	-2.00406900	0.66092400
H	5.31261600	-0.03968000	1.44088800
C	5.17793700	-3.26815400	0.39480600
H	3.42960400	-4.53401000	0.50851700
H	6.72837000	-1.76956500	0.39558100
H	5.80165100	-4.02339100	-0.08076500
C	2.86538300	-0.90487400	-2.03732000
C	1.72196300	-1.67334800	-1.82309100
C	0.68035200	-1.66900400	-2.75294800
C	0.79552800	-0.87612500	-3.89902200
C	1.93510200	-0.10642400	-4.10994700
C	2.97260300	-0.11538300	-3.17669100
H	3.67306600	-0.94024600	-1.30505600
H	1.64575800	-2.31276700	-0.94126600
H	-0.01455300	-0.87426000	-4.62739300
H	2.02651000	0.48403300	-5.02213700
H	3.87362500	0.47040200	-3.35920900
C	-0.54375300	-2.51760700	-2.50591700
H	-0.81467400	-3.05652000	-3.42730400
H	-0.32787200	-3.26143400	-1.73407900
O	-0.25905300	-1.55193600	1.08966700
C	-2.06133500	-2.80386900	0.17715600

C	-2.48653500	-1.72131500	-0.82970200
C	-4.41693900	-3.19450300	-1.53509200
C	-4.00067500	-1.79995200	-1.08077000
C	-2.49527100	-4.19868600	-0.26115600
C	-3.99690200	-4.24940100	-0.51789600
H	-5.50198100	-3.22798700	-1.70695300
H	-4.29333800	-1.04326600	-1.82038200
H	-1.95859900	-4.49711100	-1.17653800
H	-4.53507500	-4.06663600	0.42903200
H	-4.51978000	-1.55249100	-0.14052100
H	-2.19509900	-4.92645100	0.50328600
H	-4.29599900	-5.25153200	-0.85639600
H	-3.94342900	-3.41547500	-2.50864700
C	-0.59357900	-2.69998500	0.61166900
C	-1.76045400	-1.66221600	-2.17593500
O	0.14766100	-3.68210100	0.52634000
O	-2.15768700	-0.87879200	-3.02435200
H	-2.62217400	-2.54745700	1.09466700
H	-2.27667400	-0.73568800	-0.36668300
C	-3.88713300	-0.63154000	2.61999000
C	-3.06699200	-1.04794000	3.58911700
C	-1.96421000	1.94961300	2.30020400
C	-2.15553100	-0.26155800	4.49165700
C	-0.93528000	1.23639300	2.77040600
H	-4.44483200	-1.42045500	2.10270100
H	-2.65857600	0.61162200	4.92514700
H	-3.02263600	-2.13035500	3.73763600
H	-1.72769700	2.63871000	1.48272000
H	-1.89206000	-0.89851700	5.34747700
H	0.03052700	1.43458000	2.29285400

C	-4.18985200	0.73679600	2.09489600
H	-4.02222200	0.72447200	1.00125000
H	-5.27188000	0.92180300	2.21224700
C	-3.41882800	1.91775300	2.68626400
H	-3.55931600	1.94152300	3.77438100
H	-3.88698000	2.83903700	2.30942900
C	-0.85398600	0.16862500	3.81424600
H	-0.40392300	-0.71362500	3.32534600
H	-0.13663800	0.49060400	4.59054000

^{S}2b

(U)M06/BSII SCF energy in solution: -1780.396187 a.u.
(U)M06/BSI SCF energy: -1778.316657 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.809622 a.u.

C	4.28220200	0.52415100	-1.75079800
O	4.22805200	-0.85995900	-1.33880600
C	2.99136900	1.14655600	-1.19470300
C	2.97666500	-1.05699400	-0.88158400
N	2.21152500	-0.04331900	-0.81061900
C	2.59614900	-2.48066900	-0.58291200
C	0.06390300	-3.70131100	1.69611100
O	1.36772200	-3.67922600	1.08950400
C	-0.45143500	-2.26620600	1.53127900
C	1.41301500	-2.55456800	0.35266900
N	0.43372500	-1.73430400	0.47242800
H	-0.55659400	-4.41816400	1.13988300
H	5.20332100	0.96216600	-1.35489000
H	4.31963000	0.54117300	-2.84604300
H	0.16910800	-4.03427100	2.73204700
C	3.79627200	-3.23807500	-0.00758100
H	4.63285700	-3.18397100	-0.71098000

H	4.12249800	-2.81120200	0.94854100
H	3.53636100	-4.28781100	0.15714100
C	2.15276900	-3.12975800	-1.91202800
H	1.29225000	-2.59531400	-2.33398400
H	2.97897300	-3.10494400	-2.63333600
H	1.87488200	-4.17679800	-1.73716300
Ni	0.27163300	-0.03347600	-0.43392700
H	-0.25398800	-1.66867200	2.43582600
H	2.42991100	1.67181700	-1.97788500
C	-1.91905800	-2.21271800	1.22342800
C	-2.82596600	-2.00257700	2.26157900
C	-2.39435600	-2.42465500	-0.06960100
C	-4.19419100	-1.99315500	2.01033000
H	-2.45358000	-1.83132500	3.27304800
C	-3.76027800	-2.40368600	-0.32468900
H	-1.68763000	-2.55045900	-0.89004900
C	-4.66150600	-2.18594500	0.71416600
H	-4.89498100	-1.82073000	2.82548400
H	-4.11984700	-2.50975700	-1.34555000
H	-5.72950900	-2.15451300	0.50675400
C	3.12817100	2.04983400	0.00569600
C	2.16153400	3.03218900	0.22012900
C	4.13428000	1.86333700	0.95291800
C	2.21427600	3.83257800	1.35535600
H	1.34589000	3.13539800	-0.49672600
C	4.18979300	2.66627900	2.08712200
H	4.87937800	1.07713900	0.81618400
C	3.23187900	3.65540700	2.28799200
H	1.45082600	4.59384000	1.51084700
H	4.98211200	2.51670700	2.81888300

H	3.27527100	4.28399600	3.17588600
O	-2.23519300	0.15881900	-1.70113600
C	-3.60340800	1.58515000	-0.45585500
C	-2.34509800	1.29545400	0.36732100
C	-1.86540300	3.79501600	0.50493900
C	-1.82380200	2.44680300	1.21496100
C	-3.58932600	2.97521800	-1.10707500
C	-3.24457800	4.05481800	-0.09104400
H	-1.59336100	4.59423100	1.21050300
H	-0.79998200	2.21238600	1.54698500
H	-2.83497200	2.99264500	-1.91127400
H	-4.00081200	4.06109900	0.71360700
H	-2.44277300	2.51129100	2.12546900
H	-4.56117700	3.15457700	-1.58685900
H	-3.28187900	5.04593700	-0.56487300
H	-1.11865200	3.80683100	-0.30357500
C	-3.51837800	0.54136500	-1.54884000
C	-1.38313800	0.78978400	-0.69958300
O	-4.41783700	0.11209300	-2.22800600
O	-0.40492600	1.49956500	-1.17524400
H	-4.53212600	1.45213200	0.11640700
H	-2.57055700	0.44318500	1.02827000

^{S}TS1b

(U)M06/BSII SCF energy in solution: -1780.369587 a.u.

(U)M06/BSI SCF energy: -1778.288281 a.u.

(U)M06/BSI SCF Gibbs energy: -1777.785945 a.u.

C	-3.81304900	-0.13523500	1.89574000
O	-3.31468400	-1.48639100	1.76611700
C	-2.91296000	0.70751500	0.98046100
C	-2.16756700	-1.40174600	1.07656900

N	-1.84710400	-0.25047900	0.62544300
C	-1.35779900	-2.67018000	1.00670400
C	0.85764700	-3.75145500	-1.66971700
O	-0.07476000	-3.92271700	-0.58713500
C	0.96962200	-2.22296900	-1.85186400
C	-0.45806100	-2.69500300	-0.20395800
N	0.04062000	-1.70016600	-0.83451900
H	1.80554000	-4.21717700	-1.37743800
H	-4.86860400	-0.13557200	1.60589900
H	-3.72720900	0.14428000	2.95127200
H	0.45399800	-4.27010600	-2.54533400
C	-2.27880700	-3.89389600	1.01254300
H	-2.90899500	-3.87744600	1.90659000
H	-2.93238100	-3.91521100	0.13145600
H	-1.68029600	-4.80948500	1.01937800
C	-0.43802700	-2.69238700	2.25188600
H	0.20683100	-1.80261900	2.29767000
H	-1.05828400	-2.72061700	3.15654900
H	0.18357000	-3.59678000	2.23181900
Ni	-0.13570300	0.16577000	-0.09064300
H	0.60121400	-1.91244000	-2.83991600
H	-2.43315200	1.53176600	1.52427500
C	2.35822500	-1.67766500	-1.65317500
C	3.00869500	-0.99948500	-2.68202400
C	2.99985100	-1.83486900	-0.42315500
C	4.29492900	-0.50227100	-2.49291800
H	2.50394700	-0.86179300	-3.63930100
C	4.28185800	-1.33645300	-0.23000000
H	2.48402100	-2.32074400	0.40772100
C	4.93449300	-0.67853600	-1.26989100

H	4.79757900	0.02274800	-3.30350100
H	4.74164800	-1.42449400	0.75152800
H	5.93799800	-0.28411200	-1.11907600
C	-3.54843600	1.24423200	-0.27608400
C	-3.20625800	2.51722500	-0.73034900
C	-4.42192700	0.46097700	-1.03118100
C	-3.74499300	3.00508200	-1.91704700
H	-2.50275400	3.11334200	-0.14793500
C	-4.96028600	0.94745700	-2.21620400
H	-4.68069700	-0.54533600	-0.69503900
C	-4.62329200	2.22345100	-2.65980500
H	-3.47664200	4.00240200	-2.26177400
H	-5.64335500	0.32951600	-2.79687000
H	-5.04555100	2.60732000	-3.58708500
O	0.85014400	0.52909600	2.12315900
C	2.60764100	1.49359500	0.91608200
C	1.42449500	1.73503800	-0.02056400
C	1.92209500	4.20304000	-0.10492300
C	1.51056700	2.97299100	-0.90656800
C	2.99023200	2.77916000	1.65493200
C	3.19751500	3.93717100	0.68775100
H	2.05440000	5.05655800	-0.78446200
H	0.54388400	3.13380800	-1.40763700
H	2.18907500	3.03899300	2.36516700
H	4.02000200	3.69384800	-0.00762400
H	2.25563500	2.78288600	-1.69818100
H	3.89061700	2.57999900	2.25215700
H	3.50380100	4.83973500	1.23481500
H	1.11059200	4.46501100	0.59028100
C	2.13564200	0.44803100	1.92476600

C	0.16473400	1.71026300	0.83793600
O	2.89933100	-0.33722100	2.46889000
O	-0.50131800	2.59949500	1.31837800
H	3.48094900	1.11753000	0.36180000
H	1.40729000	0.83058300	-0.72659700

^{S}3b

(U)M06/BSII SCF energy in solution: -1780.410873 a.u.
(U)M06/BSI SCF energy: -1778.327872 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.8215 a.u.

C	-3.82504100	-1.01536500	1.81707700
O	-3.44517900	-2.20928500	1.09343900
C	-2.85691600	0.06277500	1.31186300
C	-2.24089500	-1.93858400	0.55911700
N	-1.79339300	-0.75402300	0.67731100
C	-1.61360200	-3.09290500	-0.16186000
C	1.59654300	-3.42281600	-1.79388400
O	0.35437700	-3.86182300	-1.21713700
C	1.75691000	-1.98279100	-1.28909000
C	-0.23850500	-2.77939800	-0.68920300
N	0.42603600	-1.68154100	-0.71463600
H	2.38707100	-4.09833300	-1.45207900
H	-4.87579200	-0.80593800	1.59635500
H	-3.70864900	-1.22928700	2.88653500
H	1.50099400	-3.49119300	-2.88386500
C	-2.51617200	-3.44058500	-1.36222600
H	-3.51889000	-3.70228500	-1.00726800
H	-2.59794400	-2.58574100	-2.04603500
H	-2.10077100	-4.29346100	-1.90949000
C	-1.51700900	-4.29460500	0.79295400
H	-0.86242900	-4.06889700	1.64516500

H	-2.51261800	-4.53687000	1.17836800
H	-1.11490300	-5.16554200	0.26651400
Ni	0.00559100	0.03920000	0.11099300
H	1.92750500	-1.28117200	-2.11166300
H	-2.39972900	0.63423400	2.12405200
C	2.84278300	-1.81151000	-0.25812800
C	4.04177400	-1.20072100	-0.61781900
C	2.68175000	-2.27755500	1.04768500
C	5.06621600	-1.05159800	0.31203800
H	4.15723800	-0.80923000	-1.62928500
C	3.70142800	-2.12551900	1.97908700
H	1.74024000	-2.74130600	1.34710700
C	4.89610500	-1.51053900	1.61287200
H	5.99231500	-0.55841000	0.02119100
H	3.56115200	-2.48240300	2.99783300
H	5.69073300	-1.38462200	2.34594000
C	-3.45427300	1.01788400	0.30720400
C	-3.25429800	2.39115200	0.43960800
C	-4.20925100	0.53352100	-0.76352600
C	-3.81103800	3.26583500	-0.48883200
H	-2.63484500	2.77146200	1.25414200
C	-4.76326000	1.40851100	-1.68976600
H	-4.37303300	-0.54127000	-0.87368200
C	-4.56439900	2.77952900	-1.55192400
H	-3.64772600	4.33655400	-0.37860800
H	-5.35220300	1.02109600	-2.51979600
H	-4.99653300	3.46839700	-2.27621400
O	-0.40783500	1.44224900	1.23179300
C	1.38758300	3.02401900	0.80808600
C	2.25294300	1.85500400	0.31444900

C	3.33200000	3.44615700	-1.37568200
C	3.55162900	2.37457300	-0.31291700
C	1.15100400	4.05926000	-0.29578600
C	2.46896900	4.58445900	-0.84730400
H	4.30409200	3.82925200	-1.71950500
H	4.12177200	1.53386800	-0.73336500
H	0.55971100	3.60144500	-1.10849900
H	3.00722500	5.10977000	-0.03878800
H	4.16580700	2.79446800	0.50225900
H	0.54118400	4.86962700	0.12380100
H	2.28776300	5.32859600	-1.63598900
H	2.84278100	2.98920000	-2.24740200
C	0.05083500	2.63598600	1.42620200
C	1.44214200	0.96501900	-0.61875400
O	-0.56037900	3.47828400	2.07608700
O	1.65226200	0.89240700	-1.81268800
H	1.94593200	3.53330800	1.61199400
H	2.49581100	1.21622700	1.18254200

4b

(U)M06/BSII SCF energy in solution: -2051.183744 a.u.
(U)M06/BSI SCF energy: -2049.025904 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.410411 a.u.

C	3.26781200	1.62252500	-2.56094000
O	3.32339300	0.18383800	-2.63419400
C	2.18856400	1.90523400	-1.51482900
C	2.21811200	-0.27257600	-2.02485900
N	1.48728800	0.59397400	-1.41989300
C	2.01327800	-1.75665000	-2.20672700
C	0.02100400	-3.93743800	-0.10081400
O	1.19697500	-3.58985100	-0.86613500

C	-0.59792400	-2.58671600	0.26553000
C	1.02092700	-2.30581800	-1.21990200
N	0.01888700	-1.68752400	-0.73705600
H	-0.63557000	-4.53963800	-0.74453600
H	4.26159000	1.98687900	-2.28418200
H	3.00459000	1.99446100	-3.55835700
H	0.33900600	-4.52795700	0.76277600
C	3.36223800	-2.47348600	-2.06898800
H	4.05919500	-2.11155900	-2.83035200
H	3.81175800	-2.29925700	-1.08156600
H	3.22332300	-3.55125400	-2.19518600
C	1.43595600	-1.98556300	-3.61852800
H	0.46767400	-1.48194100	-3.72979100
H	2.13162300	-1.60406600	-4.37540000
H	1.29439400	-3.06112200	-3.78313400
Ni	-0.38762600	0.31258700	-0.97263400
H	-0.20821800	-2.25115700	1.23771300
H	1.45845500	2.63943600	-1.87041000
C	-2.09474200	-2.56608400	0.33561500
C	-2.70835300	-2.20487100	1.53187600
C	-2.88330000	-2.88831400	-0.76754300
C	-4.09663900	-2.17062000	1.63016100
H	-2.08731900	-1.94297800	2.39142700
C	-4.26594700	-2.84666500	-0.67457200
H	-2.40857700	-3.11603000	-1.72294900
C	-4.87528800	-2.49405000	0.52658000
H	-4.56823400	-1.88394300	2.56893200
H	-4.87388100	-3.06006600	-1.55077400
H	-5.96052400	-2.44687300	0.59118600
C	2.71582700	2.32042900	-0.16429200

C	2.16202200	3.40904700	0.50908000
C	3.75692500	1.60867800	0.43748600
C	2.63472600	3.77187000	1.76776800
H	1.34250400	3.95936900	0.04656100
C	4.22546000	1.96595000	1.69543800
H	4.20513100	0.75856200	-0.08292600
C	3.66168600	3.04939100	2.36470600
H	2.19021700	4.62125300	2.28421600
H	5.03029300	1.39655900	2.15697000
H	4.02576700	3.32964400	3.35136500
C	2.58147600	-2.64623700	1.98919300
C	2.16891200	-1.33659800	1.82708300
C	1.22199200	-0.75012700	2.71249500
C	0.72573400	-1.56376400	3.76796300
C	1.14531900	-2.87215400	3.92094500
C	2.07621300	-3.42570700	3.03593200
H	3.29857200	-3.07979900	1.29181000
H	2.54694700	-0.72634400	1.00536400
H	-0.00011600	-1.13483400	4.45969000
H	0.74958400	-3.47411600	4.73741900
H	2.40845400	-4.45468100	3.16207400
C	0.77513200	0.56736700	2.53508400
H	0.04867800	1.00678200	3.21838500
H	1.16635500	1.19784600	1.73787300
O	-2.19425900	-0.03249900	-1.23532400
C	-3.17697800	1.78595100	0.04861800
C	-1.75452700	2.06001300	0.55873100
C	-2.33959200	4.54209700	0.78140200
C	-1.67065800	3.32692500	1.41432300
C	-3.80018500	3.02815000	-0.58996800

C	-3.76764000	4.21888100	0.35826400
H	-2.32695500	5.38164700	1.49201900
H	-0.61577300	3.54033700	1.65435300
H	-3.25230800	3.27899800	-1.51348900
H	-4.36979100	3.98391500	1.25397200
H	-2.16758600	3.10540600	2.37520900
H	-4.82375800	2.77411500	-0.89026500
H	-4.23579500	5.09617100	-0.11050200
H	-1.75990500	4.85531900	-0.09822400
C	-3.28151700	0.59676900	-0.91757800
C	-0.83172600	2.06822700	-0.65621500
O	-4.38800500	0.29577700	-1.34314500
O	-0.51552700	3.07335100	-1.25783200
H	-3.79606100	1.51876400	0.92332300
H	-1.44985200	1.19523000	1.17374100

TS2b

(U)M06/BSII SCF energy in solution: -2051.178163 a.u.
(U)M06/BSI SCF energy: -2049.020139 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.407156 a.u.

C	3.14575300	1.38005100	-2.74746000
O	3.06139900	-0.05261600	-2.86340700
C	2.34944300	1.69770300	-1.48005400
C	2.06983800	-0.44224300	-2.04216800
N	1.56346800	0.45057900	-1.27304100
C	1.72751700	-1.89994500	-2.21588200
C	-0.36560300	-4.04495100	-0.18730200
O	0.76830400	-3.74322400	-1.02554000
C	-0.81787400	-2.68171700	0.35347200
C	0.76669000	-2.40782400	-1.18002800
N	-0.08094600	-1.73293500	-0.51495100

H	-1.12694300	-4.53105900	-0.81172500
H	4.20318300	1.65522100	-2.68834100
H	2.70228000	1.81352700	-3.65233700
H	-0.03742700	-4.74025200	0.59039700
C	3.02583200	-2.71868100	-2.17571900
H	3.71606100	-2.36870200	-2.94878000
H	3.52066400	-2.62896300	-1.19849700
H	2.80418000	-3.77614800	-2.34726300
C	1.02916300	-2.06365800	-3.58199000
H	0.10439100	-1.47216700	-3.61470500
H	1.69478800	-1.73818600	-4.38932200
H	0.77611800	-3.11925800	-3.73835000
Ni	-0.31744700	0.31651100	-0.51416400
H	-0.43043100	-2.53076800	1.36975000
H	1.63711200	2.51359700	-1.63061800
C	-2.30247400	-2.45632500	0.37314800
C	-2.90828500	-1.98546200	1.53406100
C	-3.07672900	-2.64790800	-0.77003700
C	-4.27238900	-1.70706400	1.55418700
H	-2.30080700	-1.83022100	2.42755100
C	-4.43415700	-2.36791000	-0.75565900
H	-2.59896500	-2.95843700	-1.70105700
C	-5.03565400	-1.89828300	0.40886200
H	-4.73699800	-1.33727800	2.46729800
H	-5.01993000	-2.47623800	-1.66537400
H	-6.09804300	-1.66198300	0.41382400
C	3.19981500	1.99233800	-0.27020500
C	2.97846600	3.14351200	0.48363800
C	4.19861200	1.09928800	0.12648800
C	3.73525200	3.39084000	1.62558400

H	2.18400100	3.82696300	0.18686600
C	4.94874800	1.34143100	1.26999500
H	4.38409000	0.19620700	-0.46005100
C	4.71498400	2.48872800	2.02416300
H	3.54863600	4.28895200	2.21164500
H	5.71653300	0.63314500	1.57660700
H	5.29882000	2.67842800	2.92299900
C	2.32011000	-2.82407300	2.36696900
C	2.09997100	-1.53399300	1.91831900
C	1.06130500	-0.73736500	2.46214200
C	0.27184600	-1.30819000	3.49084400
C	0.50472600	-2.59694900	3.94291800
C	1.52475000	-3.36800200	3.38099300
H	3.12201800	-3.41924700	1.93035600
H	2.71533200	-1.10650400	1.12497900
H	-0.52630100	-0.70678900	3.92893100
H	-0.11258100	-3.00963600	4.73958400
H	1.70657500	-4.38039100	3.73722200
C	0.82069300	0.57618200	1.99198100
H	0.07629900	1.19206300	2.49514800
H	1.58058200	1.09528600	1.41524700
O	-2.10434700	0.08977000	-1.03929100
C	-3.16774600	2.06894200	-0.12748800
C	-1.92266700	2.20312600	0.76010500
C	-2.29338500	4.73993400	0.81279800
C	-1.95359200	3.48098900	1.60522300
C	-3.44664400	3.34207200	-0.92459400
C	-3.56338200	4.55185100	-0.00843400
H	-2.40267400	5.58770800	1.50492400
H	-0.98932800	3.60658300	2.12254000

H	-2.63274900	3.50393900	-1.65214600
H	-4.42061800	4.40482600	0.67224100
H	-2.71601100	3.33548400	2.38953800
H	-4.36203300	3.18048300	-1.50635400
H	-3.78043800	5.45864300	-0.59077200
H	-1.45652000	4.97984700	0.14210500
C	-3.14911900	0.85332900	-1.05927000
C	-0.68425700	2.10366000	-0.12929500
O	-4.12771400	0.64813500	-1.76528800
O	-0.08464200	3.07586700	-0.53309100
H	-4.02780500	1.90851200	0.54751400
H	-1.90553500	1.32294400	1.42205400

L1

(U)M06/BSII SCF energy in solution: -1072.963162 a.u.
(U)M06/BSI SCF energy: -1072.67275 a.u.
(U)M06/BSI SCF Gibbs energy: -1072.331619 a.u.

C	-1.37582800	-3.11676000	0.71814800
O	-2.28324400	-2.02111700	0.91277500
C	-0.49799900	-2.67887700	-0.47616000
C	-2.08583100	-1.19695500	-0.13910400
N	-1.18596000	-1.48449900	-0.99021900
C	-2.93866900	0.04986200	-0.19995100
C	-1.26659300	3.28041800	-0.04295300
O	-2.19665700	2.33302100	-0.59029000
C	-0.34955600	2.42455100	0.85951100
C	-2.00948800	1.19655900	0.11880700
N	-1.08510900	1.16121900	0.99156500
H	-0.74020600	3.76472100	-0.87219000
H	-0.81198000	-3.26538200	1.64530200
H	-1.96924600	-4.01545700	0.50769300

H	-1.83681000	4.03321400	0.51679100
C	-4.06029900	0.04259000	0.84116100
H	-4.75279200	-0.78734900	0.65450800
H	-3.65703900	-0.06161200	1.85385000
H	-4.62182400	0.98365800	0.77750200
C	-3.51512900	0.17945100	-1.61074100
H	-2.71636900	0.21754500	-2.35870500
H	-4.14948100	-0.68884500	-1.82852600
H	-4.12303900	1.08701400	-1.69517400
H	-0.22990800	2.89186800	1.84721500
H	-0.48896700	-3.45237600	-1.25756700
C	1.01888000	2.18899500	0.26206300
C	2.13700600	2.83425400	0.78568300
C	1.17598900	1.34712800	-0.84206200
C	3.39347200	2.65434700	0.21401300
H	2.02193700	3.48513300	1.65398400
C	2.42975400	1.16257900	-1.41009600
H	0.32201100	0.79302400	-1.23512100
C	3.54109500	1.81858900	-0.88734900
H	4.25880800	3.16390900	0.63547400
H	2.54232000	0.47726500	-2.24901200
H	4.52419600	1.66623200	-1.33029700
C	0.92849700	-2.35687500	-0.09940600
C	1.99249200	-2.98433400	-0.74202900
C	1.19665800	-1.41786600	0.90045400
C	3.30733400	-2.68817500	-0.39243300
H	1.78879800	-3.71415000	-1.52703900
C	2.50771700	-1.12353000	1.25196100
H	0.37475500	-0.88110200	1.37962900
C	3.56641100	-1.75829400	0.60767600

H	4.12969400	-3.18691700	-0.90349600
H	2.70265300	-0.36896900	2.01310900
H	4.59369000	-1.51964400	0.87960700

Cod

(U)M06/BSII SCF energy in solution: -311.865847 a.u.
(U)M06/BSI SCF energy: -311.771653 a.u.
(U)M06/BSI SCF Gibbs energy: -311.623021 a.u.

C	1.17468400	1.25213500	-0.49269800
C	-0.05233300	1.69017800	-0.19980400
C	0.05233100	-1.69018800	-0.19981200
C	-1.10740500	1.06335300	0.67112500
C	-1.17470200	-1.25214500	-0.49266900
H	1.76103900	1.88155200	-1.16801500
H	-0.68684000	0.66877600	1.60318600
H	-0.35740400	2.62180000	-0.68324300
H	0.35738500	-2.62181100	-0.68325800
H	-1.81279700	1.84720900	0.98126600
H	-1.76109800	-1.88158500	-1.16793100
C	1.90964200	0.02552600	-0.04482500
H	2.38524200	-0.42235400	-0.93371900
H	2.75243400	0.33332100	0.59783600
C	1.10741700	-1.06335700	0.67110100
H	0.68685200	-0.66879700	1.60317000
H	1.81282000	-1.84720800	0.98123200
C	-1.90963400	-0.02550600	-0.04483900
H	-2.38516100	0.42239100	-0.93376600
H	-2.75247800	-0.33327000	0.59776600

S1

(U)M06/BSII SCF energy in solution: -536.413555 a.u.

(U)M06/BSI SCF energy: -536.253263 a.u.
(U)M06/BSI SCF Gibbs energy: -536.113237 a.u.

O	1.77037500	0.70040500	-0.39266800
C	0.31233800	-0.84043000	0.61268900
C	-0.20670100	0.57473200	0.86997200
C	-2.34250500	0.06252000	-0.38350100
C	-1.70998900	0.79273700	0.79355200
C	-0.44343300	-1.55128000	-0.52621600
C	-1.95083900	-1.41034300	-0.37656000
H	-3.43352600	0.17819000	-0.34887400
H	-1.90468500	1.87195900	0.74114100
H	-0.14796800	-1.10519600	-1.49151600
H	-2.28001800	-1.87758800	0.56687600
H	-2.16124600	0.42895100	1.72914500
H	-0.12299200	-2.60016300	-0.56182500
H	-2.45475300	-1.95123000	-1.18842400
H	-2.00761600	0.52422500	-1.32733600
C	1.71729900	-0.58494600	0.12830800
C	0.59547600	1.38076900	-0.12728300
O	2.65654200	-1.31773300	0.08902000
O	0.34780800	2.43629100	-0.62502100
H	0.32491300	-1.47205500	1.50881900
H	0.16020900	0.90865200	1.85558700

S2

(U)M06/BSII SCF energy in solution: -1195.375644 a.u.
(U)M06/BSI SCF energy: -1195.159391 a.u.
(U)M06/BSI SCF Gibbs energy: -1195.064594 a.u.

C	-2.40084500	-0.32670100	-1.20209900
C	-1.12452700	-0.88428500	-1.19787900
C	-0.45124600	-1.17291200	0.00042500

C	-1.12458600	-0.88322900	1.19842800
C	-2.40097400	-0.32579400	1.20206600
C	-3.04677200	-0.03296200	-0.00016700
H	-2.89920600	-0.12796200	-2.15085500
H	-0.62055300	-1.09639700	-2.14150300
H	-0.62080600	-1.09474700	2.14229500
H	-2.89946400	-0.12630300	2.15060100
H	-4.05089000	0.38812600	-0.00035500
C	0.97091500	-1.60120700	0.00053300
H	1.19664600	-2.20793900	0.88839700
H	1.19664200	-2.20862900	-0.88685200
B	1.96043300	-0.29676300	0.00006600
F	1.65005900	0.53046400	1.13978800
F	3.28631800	-0.62305600	-0.00007400
F	1.64982800	0.52982200	-1.14010200
K	-0.15327200	1.86237500	-0.00033700

S3

(U)M06/BSII SCF energy in solution: -270.766697 a.u.
(U)M06/BSI SCF energy: -270.690932 a.u.
(U)M06/BSI SCF Gibbs energy: -270.606525 a.u.

C	-1.12924700	-1.20863500	-0.00016700
C	0.25184800	-1.21448900	0.00020700
C	0.99004700	0.00000900	0.00015800
C	0.25183900	1.21449800	0.00020500
C	-1.12925600	1.20862700	-0.00016900
C	-1.83236200	-0.00000700	-0.00018500
H	-1.67374800	-2.15177100	0.00000000
H	0.79927400	-2.15723700	0.00103400
H	0.79925300	2.15725300	0.00102300
H	-1.67377100	2.15175500	0.00000000

H	-2.92067700	-0.00000500	0.00006600
C	2.39072800	0.00000000	0.00005700
H	2.95405900	0.93083000	-0.00135000
H	2.95402800	-0.93084900	-0.00140600

^{S}2c

(U)M06/BSII SCF energy in solution: -1780.395977 a.u.
(U)M06/BSI SCF energy: -1778.315349 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.809201 a.u.

C	4.06026200	-0.26458700	-2.17497800
O	3.99138900	-1.41573700	-1.30384900
C	3.03830900	0.70287300	-1.58373200
C	2.80575900	-1.30532000	-0.66809000
N	2.15497300	-0.22339900	-0.83610100
C	2.46995600	-2.44867000	0.24447300
C	-0.50458400	-3.09039900	2.20249600
O	0.74026300	-3.41869200	1.56218600
C	-1.00185900	-1.86975400	1.41275300
C	1.09110100	-2.33552200	0.84260200
N	0.22764300	-1.38983500	0.76208300
H	-1.16410300	-3.96081300	2.14046000
H	5.09088900	0.09947200	-2.18094100
H	3.78363400	-0.59498600	-3.18421600
H	-0.29131500	-2.85850500	3.25389000
C	3.49954800	-2.41571500	1.39255200
H	4.50849000	-2.55767200	0.98962500
H	3.46451600	-1.45010300	1.91447600
H	3.28902000	-3.21669900	2.10963600
C	2.56833100	-3.77744800	-0.52091600
H	1.82391100	-3.82517500	-1.32662900
H	3.56457700	-3.87594300	-0.96419200

H	2.39519400	-4.61796200	0.15831000
Ni	0.33048000	0.24353900	-0.24383900
H	-1.37133700	-1.08420800	2.08614500
H	2.44091200	1.19966100	-2.35767800
C	-2.07235000	-2.21406700	0.40267900
C	-3.39912500	-2.28277800	0.83169700
C	-1.77379200	-2.50871600	-0.92663300
C	-4.41425500	-2.62408400	-0.05360600
H	-3.64023900	-2.04866600	1.87093400
C	-2.78956100	-2.85398200	-1.81336600
H	-0.74562600	-2.43296700	-1.27999300
C	-4.11033200	-2.90746300	-1.38194400
H	-5.44560500	-2.66013200	0.29279300
H	-2.54625900	-3.07120500	-2.85200000
H	-4.90371400	-3.16701500	-2.08034600
C	3.57356300	1.72594300	-0.60871600
C	2.78603900	2.83862500	-0.30598500
C	4.78422300	1.54308200	0.06148000
C	3.21866100	3.76550700	0.63471000
H	1.81039700	2.94774300	-0.78144200
C	5.21762200	2.47557400	0.99878900
H	5.40059200	0.66505000	-0.13764000
C	4.43744400	3.59093000	1.28328400
H	2.59335000	4.62529800	0.86752900
H	6.16891900	2.32768700	1.50775800
H	4.77720900	4.32089200	2.01620400
O	-1.19353300	2.29762800	0.93574500
C	-2.54394000	1.21071000	-0.67101600
C	-3.25859200	1.24636400	0.67660000
C	-5.11480200	2.66384600	-0.28049100

C	-4.75140100	1.52754700	0.66645900
C	-3.01939700	2.33334900	-1.60076100
C	-4.53791800	2.41038900	-1.66841200
H	-6.20645200	2.78332600	-0.32304100
H	-5.07560700	1.75217100	1.69179600
H	-2.62876200	3.29502300	-1.22669900
H	-4.94119500	1.46052100	-2.06305300
H	-5.27884300	0.61280400	0.34787900
H	-2.56926400	2.18919800	-2.59183200
H	-4.84901100	3.19882100	-2.36838800
H	-4.70902000	3.60961600	0.11607300
C	-1.10082200	1.44922300	-0.25874700
C	-2.42977400	2.25130800	1.45572200
O	-0.17234700	1.79805700	-1.08748900
O	-2.77912700	2.89745800	2.41255900
H	-2.66047200	0.23630500	-1.16924100
H	-3.07960400	0.28172100	1.18281600

^{S}TS1c

(U)M06/BSII SCF energy in solution: -1780.366863 a.u.
(U)M06/BSI SCF energy: -1778.284865 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.780502 a.u.

C	-0.04266700	2.77643200	2.42160700
O	-1.15133800	3.16948200	1.59528500
C	0.64058900	1.64503200	1.62659300
C	-1.26213700	2.23917000	0.63376100
N	-0.34544500	1.34284300	0.57436600
C	-2.42383300	2.45026700	-0.31521300
C	-4.46908700	-0.24060900	-1.66391500
O	-4.27793300	1.04381200	-1.02508700
C	-3.20577000	-1.02175200	-1.30981800

C	-2.95558900	1.12358400	-0.79181400
N	-2.25743000	0.08311300	-1.02398000
H	-5.40067900	-0.67276700	-1.29041200
H	0.59714200	3.65096400	2.57502400
H	-0.44579900	2.44229700	3.38491300
H	-4.55692200	-0.06073000	-2.74284400
C	-1.88619400	3.21527200	-1.54271600
H	-1.46961900	4.18036200	-1.22471300
H	-1.11018000	2.63639400	-2.05882000
H	-2.70763700	3.40778900	-2.24467600
C	-3.53395100	3.26500600	0.35122200
H	-3.93942400	2.75507800	1.23261300
H	-3.14823300	4.23948300	0.66504400
H	-4.35062300	3.42063000	-0.36027800
Ni	-0.28668100	-0.00674900	-0.85492700
H	-2.82537800	-1.59092200	-2.16695600
H	0.76377400	0.74964000	2.25086400
C	-3.27569000	-1.91113200	-0.08963700
C	-2.24943000	-2.83532700	0.10926900
C	-4.25851600	-1.76214200	0.89015400
C	-2.19881500	-3.59726800	1.27013700
H	-1.44613100	-2.92822100	-0.62202100
C	-4.22279700	-2.54330300	2.04138800
H	-5.05766600	-1.02870600	0.77260700
C	-3.19335600	-3.45938600	2.23391500
H	-1.35988200	-4.27548000	1.41410500
H	-5.00052500	-2.42727700	2.79510600
H	-3.16376700	-4.06094600	3.14121000
C	1.98171800	2.04680900	1.06852700
C	3.14104800	1.71220500	1.76675100

C	2.08504800	2.79871100	-0.10153800
C	4.38921600	2.10763000	1.29718400
H	3.06693600	1.11520900	2.67744400
C	3.33152600	3.19589000	-0.57229200
H	1.18607300	3.05102500	-0.66441700
C	4.48610100	2.84947000	0.12425500
H	5.28708100	1.82668500	1.84501500
H	3.40176300	3.77112300	-1.49364000
H	5.46133400	3.15523900	-0.24991500
O	0.62525100	-2.16215500	-0.77232700
C	2.73137900	-0.76307300	-0.81255800
C	2.50113700	-1.51169200	0.50095100
C	4.53429800	-2.93923200	0.05147300
C	3.75491900	-2.14110900	1.08901100
C	3.56692200	-1.57238600	-1.80967500
C	4.85022700	-2.07578400	-1.16396600
H	5.45723100	-3.33780500	0.49600200
H	3.45950600	-2.77916100	1.93138800
H	2.96646000	-2.42878600	-2.15478400
H	5.46562600	-1.21382500	-0.84801500
H	4.40804400	-1.34475800	1.48705900
H	3.77092600	-0.95690600	-2.69635400
H	5.44709900	-2.63622900	-1.89734500
H	3.93303200	-3.80904200	-0.26015500
C	1.36622400	-0.49994400	-1.36949700
C	1.36118000	-2.51331700	0.24211600
O	0.98011400	-0.33404500	-2.52343200
O	1.19639500	-3.50199600	0.94122800
H	3.22419500	0.20491600	-0.62317900
H	2.09132500	-0.79690900	1.23600400

^{S}3c

(U)M06/BSII SCF energy in solution: -1780.409036 a.u.

(U)M06/BSI SCF energy: -1778.325733 a.u.

(U)M06/BSI SCF Gibbs energy: -1777.821193 a.u.

C	-0.21574600	-3.68120800	1.70812700
O	0.98383600	-3.77432700	0.91142000
C	-0.65486600	-2.22179600	1.55531100
C	0.98966800	-2.68972700	0.12480800
N	0.07401900	-1.81843400	0.33261100
C	2.05807800	-2.62036900	-0.93650800
C	4.06685100	0.32587000	-1.70481600
O	3.80517200	-1.09649700	-1.61966100
C	2.92343900	0.98937000	-0.91185800
C	2.62573200	-1.22034000	-0.99319000
N	2.06264000	-0.15832300	-0.57027200
H	5.06146400	0.50986200	-1.28525200
H	-0.95057500	-4.38555600	1.29523100
H	0.03230600	-3.97318000	2.73131500
H	4.06967200	0.59455600	-2.76640300
C	1.37997500	-2.91443400	-2.29222500
H	1.00759500	-3.94697800	-2.29693600
H	0.53493500	-2.23658000	-2.46906800
H	2.11152500	-2.80727300	-3.10226500
C	3.17288700	-3.63409600	-0.67464100
H	3.66813500	-3.45559600	0.28725300
H	2.76478200	-4.64993300	-0.66457800
H	3.92364800	-3.56335200	-1.46761400
Ni	0.02598600	-0.08283100	-0.48036400
H	2.31665200	1.65498200	-1.53725700
H	-0.24104900	-1.60813100	2.37191500

C	3.32947300	1.73275500	0.33455500
C	2.72388500	2.95016000	0.64424600
C	4.27172100	1.19022900	1.20967600
C	3.08124400	3.62506000	1.80825700
H	1.95422700	3.35959100	-0.01387400
C	4.62711300	1.86534600	2.37073100
H	4.73136100	0.22497400	0.98340200
C	4.03387300	3.08947400	2.66839600
H	2.60559500	4.57620300	2.04079600
H	5.36761300	1.43747900	3.04493500
H	4.31331500	3.62394400	3.57511100
C	-2.13833800	-1.99348400	1.50266100
C	-2.72965400	-1.10950900	2.40394400
C	-2.93675500	-2.63694500	0.55610800
C	-4.09956200	-0.86950300	2.36585800
H	-2.10693200	-0.59662800	3.13821900
C	-4.30343100	-2.39668000	0.51234100
H	-2.47965900	-3.29535000	-0.18295800
C	-4.88785100	-1.51514900	1.41917900
H	-4.54779200	-0.17331800	3.07236700
H	-4.91384500	-2.88984600	-0.24134200
H	-5.95928500	-1.32694600	1.38171900
O	0.06242300	1.69212600	-1.02608200
C	-2.65898100	0.96697500	-0.72528100
C	-2.00440400	2.01735100	0.17370900
C	-3.63498700	3.73942700	-0.70398700
C	-2.99873800	3.11734100	0.53414300
C	-3.28869100	1.59467300	-1.97091300
C	-4.28693100	2.67884000	-1.58319200
H	-4.37317100	4.49849000	-0.40793700

H	-2.49012700	3.88689100	1.12696200
H	-2.48765300	2.02852400	-2.59330800
H	-5.12499100	2.21336100	-1.03438500
H	-3.78835700	2.67572500	1.16819200
H	-3.76026500	0.80550700	-2.57062500
H	-4.71993900	3.13494500	-2.48520400
H	-2.85097800	4.26305600	-1.27153600
C	-1.70118500	-0.14368000	-1.11033200
C	-0.71443500	2.56961100	-0.45782900
O	-1.95721200	-0.98699400	-1.94128100
O	-0.44213500	3.76197100	-0.40289100
H	-3.46149900	0.46461800	-0.15072300
H	-1.68390700	1.50894600	1.10195800

TS2d

(U)M06/BSII SCF energy in solution: -1780.358626 a.u.
(U)M06/BSI SCF energy: -1778.27192 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.779753 a.u.

C	3.82045100	0.36604200	-1.77083400
O	3.93399200	-0.92694600	-1.12851500
C	2.51582100	0.95527700	-1.21671900
C	2.72363900	-1.17263500	-0.59075200
N	1.86307500	-0.23722400	-0.63228300
C	2.60546800	-2.52676100	0.05925200
C	-0.38332700	-4.31244500	1.10190300
O	1.00786600	-4.15707100	0.76469900
C	-0.92719500	-2.87262300	1.16767900
C	1.19610100	-2.85684100	0.48019300
N	0.20414000	-2.07226000	0.66764500
H	-0.85980000	-4.90342300	0.30937900
H	4.71302200	0.94664500	-1.51910400

H	3.78538100	0.19310200	-2.85294900
H	-0.44455200	-4.85850200	2.04760000
C	3.45576800	-2.49287400	1.34694100
H	4.50115000	-2.28058600	1.09500100
H	3.09126400	-1.71401300	2.02950500
H	3.40441100	-3.46378700	1.85367100
C	3.13686600	-3.60594800	-0.89313900
H	2.53850800	-3.65423100	-1.81163300
H	4.16981100	-3.37410600	-1.16931400
H	3.10862200	-4.58733400	-0.41020900
Ni	-0.10635600	-0.19314700	-0.06713000
H	-1.11478000	-2.56170800	2.20676000
H	1.85464300	1.34852300	-2.00064300
C	-2.17679300	-2.63669200	0.36012400
C	-3.39634600	-2.42070000	0.99778600
C	-2.12175300	-2.61297600	-1.03497700
C	-4.54883800	-2.18683500	0.25419900
H	-3.43765900	-2.40821900	2.08759400
C	-3.26918400	-2.36773600	-1.77876200
H	-1.16606800	-2.75245200	-1.54268200
C	-4.48564900	-2.15563100	-1.13479800
H	-5.49544000	-2.01257700	0.76277900
H	-3.20950400	-2.32786600	-2.86440600
H	-5.38319400	-1.95643900	-1.71736300
C	2.70578500	1.99838800	-0.14177300
C	1.99704000	3.19668500	-0.19897200
C	3.57518300	1.76637700	0.92779300
C	2.15623600	4.14893800	0.80522300
H	1.31424900	3.37099200	-1.03371500
C	3.73550900	2.71880200	1.92590900

H	4.14180700	0.83354100	0.97804700
C	3.02260400	3.91415100	1.86614800
H	1.59492800	5.08114400	0.75296700
H	4.41938400	2.53029900	2.75224600
H	3.14733200	4.66220900	2.64767500
O	-0.48557200	0.77540700	-1.76689500
C	-2.05579700	2.48873100	-1.08528800
C	-2.85991900	1.44122800	-0.39272700
C	-3.61906900	3.07201400	1.36840600
C	-3.99248200	1.89173300	0.47159000
C	-1.70101000	3.64870200	-0.14763200
C	-2.93486500	4.17637700	0.57153500
H	-4.51613100	3.45473200	1.87545700
H	-4.38652800	1.05516100	1.06886600
H	-0.96116700	3.29645200	0.59447900
H	-3.64146600	4.58002300	-0.17500600
H	-4.82710600	2.20362800	-0.19018800
H	-1.20702900	4.43084200	-0.73874800
H	-2.66773100	5.01360100	1.23236800
H	-2.93639900	2.71963600	2.15696100
C	-0.80888300	2.00950900	-1.85546100
C	-1.41051900	0.37808800	1.13638200
O	-0.20125400	2.86159000	-2.51210000
O	-1.88894200	0.39671600	2.19229800
H	-2.70844000	2.92472500	-1.87316000
H	-2.97182300	0.48484700	-0.91140300

4d

(U)M06/BSII SCF energy in solution: -1780.362391 a.u.
(U)M06/BSI SCF energy: -1778.274906 a.u.

(U)M06/BSI SCF Gibbs energy: -1777.779967 a.u.

C	-3.43516800	1.59815100	1.81838200
O	-3.98537000	0.38852100	1.24492700
C	-2.03171300	1.71337100	1.20476800
C	-2.94846300	-0.24595400	0.66516400
N	-1.83347300	0.36331700	0.63033100
C	-3.30992800	-1.58041100	0.06551600
C	-1.09468700	-4.24584400	-1.03788200
O	-2.34466300	-3.65659400	-0.63190500
C	-0.13759200	-3.04948500	-1.19937300
C	-2.10612300	-2.35299900	-0.40925400
N	-0.93663600	-1.92123700	-0.68960000
H	-0.77392100	-4.93654400	-0.24808100
H	-4.10208500	2.42697500	1.56197800
H	-3.41451100	1.46667100	2.90640300
H	-1.26899000	-4.80693300	-1.96033100
C	-4.17648300	-1.30006100	-1.18055500
H	-5.08792000	-0.76812600	-0.88488000
H	-3.62469200	-0.68205400	-1.90121600
H	-4.45934900	-2.24376600	-1.66184900
C	-4.10267600	-2.41236700	1.08142700
H	-3.49957200	-2.63621900	1.97016600
H	-4.98910400	-1.85577700	1.39964000
H	-4.41839800	-3.35851400	0.63127000
Ni	0.01597600	-0.20337500	-0.06906200
H	0.07661200	-2.84933700	-2.26097700
H	-1.24923400	1.88044700	1.95961700
C	1.16764600	-3.17252600	-0.45811200
C	2.37629900	-3.19604400	-1.15027300
C	1.17751600	-3.22473200	0.93711600

C	3.58124900	-3.28087300	-0.45979600
H	2.37396500	-3.13232500	-2.23912300
C	2.37927800	-3.30179900	1.62845700
H	0.23693300	-3.17153200	1.48828300
C	3.58369700	-3.33268300	0.92978200
H	4.52043800	-3.29577900	-1.01008300
H	2.37675400	-3.32068400	2.71617900
H	4.52634000	-3.38437200	1.47149500
C	-1.90188800	2.73758000	0.10329400
C	-0.81874400	3.61451800	0.08684600
C	-2.84215500	2.79050100	-0.92902700
C	-0.67965100	4.53051300	-0.95301700
H	-0.08791200	3.56720900	0.89684000
C	-2.70569400	3.70879500	-1.96193700
H	-3.69589700	2.10845600	-0.92117000
C	-1.61900800	4.58061600	-1.97661200
H	0.17333500	5.20818800	-0.95839000
H	-3.44745000	3.74645100	-2.75849700
H	-1.50865100	5.30032200	-2.78631100
O	0.76688000	0.41243700	1.67016700
C	2.81071800	1.64047900	1.26384400
C	3.31013400	0.42311200	0.56767400
C	4.58950800	1.77129300	-1.12103800
C	4.54319500	0.50334200	-0.26571800
C	2.88878100	2.87831100	0.35746000
C	4.26125600	3.00510500	-0.28888000
H	5.57669400	1.87150600	-1.59506100
H	4.63823600	-0.39451000	-0.89751300
H	2.12062200	2.79322600	-0.43340600
H	5.02320400	3.12638200	0.50150900

H	5.43786900	0.49936100	0.39338100
H	2.63473800	3.76661100	0.95054200
H	4.31045700	3.91007500	-0.91192300
H	3.85378500	1.68120500	-1.93592100
C	1.39925800	1.50997000	1.86622300
C	1.21306800	0.07471200	-1.42778700
O	0.96194800	2.47733400	2.50054600
O	1.85121300	0.18621700	-2.37760000
H	3.47304400	1.85972700	2.13006600
H	2.98824100	-0.54728000	0.94678000

5d

(U)M06/BSII SCF energy in solution: -1780.363388 a.u.
(U)M06/BSI SCF energy: -1778.272726 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.779051 a.u.

C	-3.70629400	1.52902000	1.85281300
O	-4.21356700	0.33953200	1.20211200
C	-2.24571600	1.63828000	1.38353600
C	-3.14090800	-0.27180900	0.66593400
N	-2.02137200	0.32489400	0.74526200
C	-3.45126000	-1.55642300	-0.06099500
C	-1.05432200	-4.23114800	-0.68329700
O	-2.36709000	-3.67360600	-0.46408600
C	-0.16660100	-3.01232600	-0.98816700
C	-2.20019800	-2.34488000	-0.35780000
N	-1.03556100	-1.88609900	-0.61136400
H	-0.74951400	-4.74856200	0.23592500
H	-4.33399200	2.37326600	1.55076100
H	-3.79968200	1.37595500	2.93416600
H	-1.12566000	-4.95434600	-1.49982400
C	-4.06064400	-1.15911500	-1.42269600

H	-4.99627000	-0.61057300	-1.26059500
H	-3.36590200	-0.52116000	-1.98479500
H	-4.27965100	-2.05836400	-2.01235500
C	-4.45113700	-2.39663400	0.73770700
H	-4.02614600	-2.72758100	1.69309100
H	-5.34570200	-1.80284400	0.94752700
H	-4.74130200	-3.28453900	0.16721900
Ni	-0.18923200	-0.07412400	-0.14456600
H	0.03224700	-2.92492600	-2.06868600
H	-1.53472100	1.72430400	2.21147300
C	1.14470400	-2.96137900	-0.24936300
C	2.35113700	-3.00602700	-0.94469000
C	1.16170900	-2.82274500	1.14034600
C	3.56053900	-2.92680400	-0.26109800
H	2.34236100	-3.08822800	-2.03254800
C	2.36782600	-2.73466800	1.82359700
H	0.22099900	-2.75111400	1.68880800
C	3.56987900	-2.78994700	1.12307600
H	4.49817700	-2.95569300	-0.81401200
H	2.36927200	-2.60431700	2.90380400
H	4.51620900	-2.70792300	1.65564100
C	-1.96987000	2.72817200	0.37696300
C	-0.82838300	3.52099300	0.49558900
C	-2.81945700	2.90097800	-0.71729100
C	-0.55275400	4.48330800	-0.47172800
H	-0.13805600	3.36166100	1.32703800
C	-2.54158300	3.86236700	-1.68167000
H	-3.70737200	2.27105100	-0.81938500
C	-1.40412700	4.65603900	-1.55857800
H	0.34081900	5.09778400	-0.37315500

H	-3.21198400	3.99265800	-2.52992300
H	-1.18356900	5.41009800	-2.31269100
O	0.57494300	0.91912800	1.37808600
C	2.86201900	0.95189600	0.65986100
C	2.85620500	1.60240000	-0.68551300
C	5.30091100	1.40468700	-0.97026600
C	3.92948800	1.18294100	-1.62767000
C	4.23666000	1.16607400	1.31085600
C	5.36327300	0.71221300	0.38818700
H	6.10590600	1.04584700	-1.62928600
H	3.86253900	1.71104600	-2.58866300
H	4.33432400	2.23574800	1.54848700
H	5.28948200	-0.37955700	0.23289900
H	3.82200600	0.10265700	-1.84788800
H	4.27787200	0.62749400	2.27087600
H	6.33970600	0.89279800	0.86140600
H	5.45836300	2.48696200	-0.83278800
C	1.70860400	1.51890500	1.49108300
C	0.68016800	0.21611400	-1.73804800
O	1.89466000	2.53233800	2.16418000
O	1.02473300	0.23211100	-2.83599700
H	2.71343900	-0.13816800	0.52670200
H	2.40418200	2.59356100	-0.77708800

TS3d

(U)M06/BSII SCF energy in solution: -1780.360717 a.u.
(U)M06/BSI SCF energy: -1778.271329 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.77505 a.u.

C	3.86698100	-1.56018400	1.70262300
O	4.30309100	-0.35313200	1.03510900
C	2.36903100	-1.66156900	1.37680000

C	3.17648000	0.28280600	0.65590200
N	2.07003200	-0.31181800	0.85332900
C	3.41578600	1.60132900	-0.03334000
C	0.94431700	4.15183200	-0.82362300
O	2.26885700	3.63973300	-0.57542200
C	0.08169400	2.89570600	-1.02769500
C	2.13169400	2.31895700	-0.36351400
N	0.97326000	1.81815900	-0.56601600
H	0.63506800	4.73026500	0.05723600
H	4.46128000	-2.39369000	1.31579700
H	4.06495600	-1.43386200	2.77359700
H	0.99202700	4.81292600	-1.69292200
C	4.09937600	1.29370400	-1.38319400
H	5.06088500	0.79823600	-1.20753400
H	3.46614000	0.63628000	-1.99393000
H	4.27900600	2.22592600	-1.93239300
C	4.32459700	2.48417500	0.82931100
H	3.83873900	2.75277300	1.77552400
H	5.24967500	1.94591500	1.05754500
H	4.57486300	3.40769100	0.29796700
Ni	0.18833300	0.05465000	0.06135000
H	-0.11717700	2.71831700	-2.09670400
H	1.75026400	-1.82401100	2.26503700
C	-1.22648300	2.88892200	-0.28299800
C	-2.43441600	2.89653600	-0.97656500
C	-1.24015300	2.84165400	1.11288400
C	-3.64265400	2.86870200	-0.28658200
H	-2.42775800	2.90676600	-2.06756700
C	-2.44508800	2.80209900	1.80284400
H	-0.29846400	2.80638500	1.66310600

C	-3.64906300	2.81854400	1.10340000
H	-4.58138600	2.86837100	-0.83881300
H	-2.44417000	2.74318900	2.88920700
H	-4.59395700	2.77828200	1.64302100
C	2.00393400	-2.67851900	0.32324600
C	0.87241700	-3.47601200	0.48479300
C	2.74641800	-2.76411500	-0.85640200
C	0.49361600	-4.35318800	-0.52717600
H	0.25688100	-3.37892100	1.38052700
C	2.36440300	-3.63817600	-1.86668000
H	3.62985100	-2.13436900	-0.99012000
C	1.23353900	-4.43440400	-1.70243500
H	-0.39608000	-4.96655800	-0.39200800
H	2.94836800	-3.69818400	-2.78390700
H	0.93096700	-5.11826900	-2.49407800
O	-0.55332800	-0.98983300	1.56635200
C	-2.79081900	-0.98620000	0.70512300
C	-2.70456700	-1.47672200	-0.70324200
C	-5.13522800	-1.33078500	-1.08512600
C	-3.74734600	-0.98144000	-1.64729300
C	-4.18941400	-1.31531200	1.25350900
C	-5.28919800	-0.79622700	0.33429100
H	-5.92243100	-0.93469400	-1.74390500
H	-3.61160300	-1.39667900	-2.65510800
H	-4.25823100	-2.40749800	1.36414700
H	-5.25576600	0.30761600	0.30675000
H	-3.67429500	0.11851700	-1.73719100
H	-4.29208500	-0.89262300	2.26460000
H	-6.27700900	-1.06708400	0.73487300
H	-5.25006300	-2.42701700	-1.07403100

C	-1.66850700	-1.62809500	1.53340400
C	-0.75207900	-0.37849100	-1.50330700
O	-1.87380400	-2.72190400	2.06023000
O	-0.84066500	-0.36055000	-2.65805400
H	-2.66672600	0.11289400	0.70348700
H	-2.33694300	-2.49913800	-0.84065700

6d

(U)M06/BSII SCF energy in solution: -1780.411048 a.u.
(U)M06/BSI SCF energy: -1778.32873 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.825941 a.u.

C	3.42608600	-0.36621400	-2.22388300
O	3.36687900	-1.64599900	-1.54648300
C	2.58857100	0.57234400	-1.34215400
C	2.34608300	-1.54090200	-0.68271500
N	1.80229000	-0.39770500	-0.54037100
C	2.03128300	-2.77534500	0.11944700
C	-1.29097100	-3.89356900	1.08357100
O	0.05919300	-4.04337500	0.60357900
C	-1.55315700	-2.38025800	1.01861200
C	0.56978000	-2.81204300	0.48706000
N	-0.21150300	-1.82807200	0.74591900
H	-1.94678500	-4.48268700	0.43444800
H	4.47740600	-0.07786700	-2.30748200
H	2.99983800	-0.50935600	-3.22461200
H	-1.32712700	-4.29495400	2.10262000
C	2.82974100	-2.67415200	1.43730500
H	3.90440600	-2.66519800	1.21518200
H	2.56955800	-1.75909800	1.98311300
H	2.61234800	-3.54511200	2.06849100
C	2.43744200	-4.03988700	-0.63909500

H	1.87527500	-4.14997600	-1.57406800
H	3.50217200	-3.99198800	-0.88581100
H	2.25672900	-4.92577900	-0.02354900
Ni	0.09719800	0.07054800	0.49288800
H	-1.88324900	-1.98620400	1.98557200
H	1.89621300	1.18559800	-1.92853900
C	-2.53184100	-1.96383000	-0.05009100
C	-3.84419900	-1.65512400	0.30044000
C	-2.15710600	-1.90626100	-1.39436600
C	-4.76878500	-1.28495000	-0.67209500
H	-4.13378400	-1.67559000	1.35213800
C	-3.07726200	-1.53299700	-2.36673900
H	-1.12750600	-2.12760400	-1.68056400
C	-4.38544400	-1.21929500	-2.00708400
H	-5.78693000	-1.03051400	-0.38171500
H	-2.77006100	-1.47865900	-3.40950700
H	-5.10293900	-0.91632400	-2.76736500
C	3.41874200	1.47203300	-0.45717400
C	3.14285800	2.83704700	-0.38750800
C	4.48622100	0.95088400	0.27656900
C	3.93420900	3.66600700	0.40026600
H	2.28230500	3.23349200	-0.92726300
C	5.27177400	1.77946100	1.06926900
H	4.72017300	-0.11472400	0.22168800
C	4.99654200	3.14218000	1.12990800
H	3.71206100	4.73071100	0.44863100
H	6.10240700	1.36139500	1.63594500
H	5.61112800	3.79491500	1.74806400
O	0.39644800	1.81149700	-0.02039000
C	-1.94657800	2.16975200	-0.42336500

C	-2.12233300	1.88740000	1.07008600
C	-4.42102700	2.94866400	1.00038000
C	-3.58949200	1.77155000	1.48760900
C	-2.83635400	3.31487500	-0.89712500
C	-4.29218800	3.10355900	-0.50926600
H	-5.47221500	2.81318600	1.29411600
H	-3.64435900	1.65901000	2.57803600
H	-2.46985500	4.25280000	-0.44695300
H	-4.67720800	2.19045100	-0.99871000
H	-4.00224200	0.84398000	1.05659700
H	-2.71637900	3.43904700	-1.98002200
H	-4.90923400	3.93906500	-0.86947500
H	-4.07550900	3.87568900	1.48942500
C	-0.47613900	2.45299500	-0.73796100
C	-1.34625700	0.65186000	1.52851200
O	-0.15277500	3.26595400	-1.59686600
O	-1.60383600	0.10984600	2.58350000
H	-2.23706800	1.25136000	-0.97273400
H	-1.66508800	2.72794000	1.62741700

TS3c

(U)M06/BSII SCF energy in solution: -2051.164927 a.u.
(U)M06/BSI SCF energy: -2049.006205 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.394306 a.u.

C	2.85566300	-1.88547500	2.53642900
O	2.37569200	-0.65670300	3.10755900
C	2.41090600	-1.82583200	1.06032000
C	1.69110900	-0.01992100	2.14016100
N	1.66420100	-0.56127400	0.98672800
C	1.11203900	1.29546800	2.58257700
C	-0.83300400	3.78215300	0.80281600

O	-0.01089400	3.25341100	1.85424900
C	-1.04920100	2.59463600	-0.15235700
C	0.28072400	1.98035400	1.52633700
N	-0.21143100	1.53624000	0.43636800
H	-1.76147100	4.15639800	1.24938900
H	3.94440600	-1.91705200	2.65905600
H	2.40345800	-2.71316700	3.09190800
H	-0.28986700	4.60944800	0.33190600
C	2.29629900	2.20776600	2.95226200
H	2.91072800	1.72438800	3.71876000
H	2.92444700	2.41093000	2.07285700
H	1.93006800	3.16188100	3.34269100
C	0.20110200	1.06704200	3.80646100
H	-0.63177300	0.40097400	3.54411100
H	0.78131700	0.61688000	4.61928100
H	-0.19336500	2.02903400	4.15304300
Ni	-0.10458500	-0.43347600	-0.23004200
H	-0.65590400	2.82623400	-1.14928200
H	1.71120500	-2.64244100	0.82857000
C	-2.47654300	2.13432300	-0.28480500
C	-3.11034400	2.16045400	-1.52620200
C	-3.16994300	1.65475200	0.82803700
C	-4.42475500	1.71772500	-1.65471200
H	-2.56342000	2.52827300	-2.39591600
C	-4.47639100	1.20074000	0.70042900
H	-2.67544200	1.59279500	1.79872800
C	-5.10715300	1.23463400	-0.54228900
H	-4.91369100	1.74553800	-2.62734300
H	-4.98033200	0.78811000	1.57291300
H	-6.13092900	0.87760500	-0.64370600

C	3.53027700	-1.83921400	0.05204200
C	3.53362800	-2.75917200	-0.99350200
C	4.55118500	-0.88981900	0.12846600
C	4.54644800	-2.73457700	-1.94850500
H	2.72033900	-3.48187000	-1.07397400
C	5.56044000	-0.86137400	-0.82458900
H	4.54467800	-0.15416000	0.93685300
C	5.55985700	-1.78697400	-1.86571900
H	4.53689600	-3.45464300	-2.76472800
H	6.34859700	-0.11334600	-0.75852400
H	6.34888000	-1.76369000	-2.61521500
C	2.40854000	3.36814700	-1.59753100
C	2.15330200	2.01580400	-1.42241300
C	1.17316400	1.35722600	-2.18250000
C	0.49321500	2.10742000	-3.15308400
C	0.75769200	3.46088200	-3.34270200
C	1.70821600	4.10344600	-2.55558900
H	3.16896500	3.85699000	-0.98842000
H	2.69772200	1.44409900	-0.66839800
H	-0.25769500	1.60756100	-3.76840600
H	0.21800900	4.01495700	-4.11015200
H	1.91740500	5.16242300	-2.69809100
C	0.85966200	-0.06712700	-1.97812500
H	0.27855900	-0.46273400	-2.82324200
H	1.76122800	-0.68088400	-1.85046800
O	-1.05345500	-0.79401400	1.49031700
C	-2.97238800	-1.88082700	0.46967300
C	-2.51010700	-1.53898900	-0.91280300
C	-3.09166500	-3.86893400	-1.73642000
C	-3.04411900	-2.37415600	-2.04230500

C	-2.98058200	-3.39017700	0.72798000
C	-3.72231500	-4.13487300	-0.37423000
H	-3.64651400	-4.38778500	-2.53039000
H	-2.48613300	-2.17261000	-2.96929000
H	-1.94101800	-3.75557400	0.79158000
H	-4.77503100	-3.80264200	-0.38469800
H	-4.07522900	-2.01132600	-2.23065700
H	-3.43729000	-3.56460400	1.71085000
H	-3.73802700	-5.21389700	-0.16663700
H	-2.07047500	-4.27646300	-1.74913200
C	-2.27642800	-1.15985900	1.64117300
C	-0.39796400	-2.01927700	-0.96207900
O	-2.91867800	-1.01889100	2.67954200
O	-0.00343400	-3.04706400	-1.35427200
H	-4.02672800	-1.54014200	0.52119300
H	-2.49481200	-0.46518600	-1.13287700

6c

(U)M06/BSII SCF energy in solution: -2051.158859 a.u.
(U)M06/BSI SCF energy: -2049.001811 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.392005 a.u.

C	2.50910000	-2.53887400	1.70738200
O	2.02335600	-1.51032100	2.58439000
C	2.59485900	-1.85202000	0.32541400
C	1.67079900	-0.48604500	1.78959300
N	1.93856700	-0.55847800	0.54582200
C	1.12863300	0.71344100	2.51196300
C	-0.76871700	3.52749300	1.24063200
O	0.03122800	2.78636100	2.17570800
C	-1.17164800	2.49049700	0.18161200
C	0.26996300	1.58381400	1.63004600

N	-0.30000900	1.34452700	0.50705500
H	-1.61778200	3.95721200	1.78216600
H	3.47662100	-2.88647600	2.08694900
H	1.78664100	-3.36253600	1.72808700
H	-0.14409300	4.32771700	0.82419000
C	2.36088900	1.51529100	2.97494500
H	2.99892100	0.86597700	3.58759200
H	2.94686100	1.87341600	2.11717200
H	2.05884600	2.37661500	3.57927700
C	0.27744000	0.30321200	3.72563500
H	-0.57976800	-0.31471100	3.42154600
H	0.89572300	-0.27423200	4.42170200
H	-0.07862300	1.20244200	4.24236400
Ni	-0.24773600	-0.32704800	-0.56653500
H	-0.91287300	2.85133600	-0.82036800
H	2.01794900	-2.42022700	-0.42085800
C	-2.62211400	2.08658700	0.20061300
C	-3.42412300	2.31077600	-0.91739500
C	-3.17294200	1.47071400	1.32529400
C	-4.76258200	1.92683900	-0.91413000
H	-2.98951100	2.78472200	-1.79944500
C	-4.50547600	1.07772300	1.32729200
H	-2.55034700	1.25405200	2.19482500
C	-5.30317300	1.30644700	0.20799200
H	-5.38075700	2.10723300	-1.79208900
H	-4.90649000	0.56561300	2.20035100
H	-6.34690900	0.99646400	0.20988500
C	3.99411700	-1.65454800	-0.19977500
C	4.41381800	-2.27961500	-1.37060500
C	4.88990400	-0.83346000	0.48879700

C	5.70938400	-2.09714700	-1.84653400
H	3.71529200	-2.91494300	-1.91731400
C	6.18312100	-0.64987800	0.01767800
H	4.56139500	-0.32994200	1.40018600
C	6.59635100	-1.28304800	-1.15220800
H	6.02358700	-2.59025900	-2.76488400
H	6.87258400	-0.00706400	0.56266800
H	7.60894300	-1.13669900	-1.52409700
C	2.30836700	3.68157900	-1.17724300
C	2.03597500	2.32459000	-1.27645800
C	1.00494100	1.85478100	-2.10507900
C	0.29005500	2.79566700	-2.85932500
C	0.56688300	4.15660600	-2.76781400
C	1.57000800	4.60804200	-1.91495700
H	3.11103300	4.02337200	-0.52390800
H	2.60825600	1.59543200	-0.70127000
H	-0.50123600	2.44273800	-3.52437800
H	-0.00222800	4.86650000	-3.36681400
H	1.79051000	5.67169100	-1.84013300
C	0.67684000	0.41951700	-2.18516300
H	0.10362400	0.19892900	-3.09485700
H	1.57774700	-0.20906500	-2.16010500
O	-0.84921400	-1.28455200	1.06513600
C	-3.04717000	-2.03999300	0.39369500
C	-2.96784600	-1.40494400	-0.95212900
C	-3.58600600	-3.57504400	-2.10092100
C	-3.67224300	-2.04860600	-2.10027400
C	-2.90875200	-3.56714900	0.31280100
C	-3.86600300	-4.14987900	-0.71774900
H	-4.28569700	-3.98441400	-2.84278300

H	-3.31289800	-1.63583200	-3.05597000
H	-1.86943500	-3.81869400	0.04000000
H	-4.90307700	-3.91404700	-0.42195200
H	-4.74091700	-1.75223500	-2.03963300
H	-3.08687300	-3.98919900	1.31143600
H	-3.78850600	-5.24594700	-0.73900800
H	-2.57809600	-3.88301500	-2.41746700
C	-2.06319700	-1.50797400	1.44382600
C	-0.49233900	-1.71696900	-1.61062200
O	-2.44951500	-1.40553100	2.60664100
O	-0.43986000	-2.62295000	-2.31832400
H	-4.05735200	-1.83518500	0.80337300
H	-2.88502900	-0.31632200	-0.98297000

7c

(U)M06/BSII SCF energy in solution: -2051.157081 a.u.

(U)M06/BSI SCF energy: -2049.001302 a.u.

(U)M06/BSI SCF Gibbs energy: -2048.390741 a.u.

C	2.72894900	-1.99068100	2.47717400
O	1.95611300	-0.92654600	3.05387400
C	2.54574500	-1.80535700	0.95918200
C	1.61562700	-0.12227200	2.03199400
N	1.94559800	-0.47063800	0.85147000
C	0.99461500	1.17986500	2.45194800
C	-0.85832500	3.61252000	0.50470200
O	-0.13622200	3.10366600	1.63950600
C	-1.19440600	2.36400100	-0.31891600
C	0.17560700	1.82766200	1.36451500
N	-0.30466500	1.34865300	0.27782200
H	-1.73523000	4.15506000	0.87170600
H	3.77471100	-1.86633100	2.79251900

H	2.34473500	-2.93933500	2.86154300
H	-0.19076100	4.29450500	-0.03894900
C	2.16781600	2.10601500	2.82738600
H	2.78101500	1.61333800	3.59143200
H	2.79943900	2.32165600	1.95383500
H	1.79547500	3.05234600	3.23286300
C	0.06491900	0.97970000	3.66253600
H	-0.74810600	0.27779600	3.42754300
H	0.64330100	0.58119600	4.50286300
H	-0.35772700	1.94604700	3.96207200
Ni	-0.00969500	-0.43309400	-0.51761900
H	-0.89529800	2.51316700	-1.36133400
H	1.81235000	-2.53476900	0.57676800
C	-2.63480800	1.92717900	-0.29312800
C	-3.30482100	1.70866900	-1.49667900
C	-3.31197700	1.72550500	0.91034700
C	-4.63987900	1.31617200	-1.50348500
H	-2.76877800	1.84903600	-2.43760700
C	-4.64399400	1.33071200	0.90656700
H	-2.79581600	1.84826300	1.86369800
C	-5.31242600	1.13253800	-0.29916000
H	-5.15299100	1.15059900	-2.44969700
H	-5.15406700	1.15949100	1.85282700
H	-6.35605800	0.82084900	-0.29848900
C	3.80766200	-1.91172100	0.14772000
C	3.98113000	-2.94602100	-0.76826000
C	4.81806300	-0.95846500	0.29328400
C	5.14810600	-3.03581300	-1.52205500
H	3.19062800	-3.68685600	-0.89602600
C	5.98255800	-1.04408600	-0.45791100

H	4.67592000	-0.13448500	0.99618900
C	6.15045100	-2.08557300	-1.36780400
H	5.26990700	-3.84757500	-2.23711000
H	6.76123300	-0.29245400	-0.33865400
H	7.06160000	-2.15027000	-1.95997300
C	2.69898000	3.49896900	-1.10621200
C	2.37935000	2.14929900	-1.14876000
C	1.42850400	1.65740100	-2.05719800
C	0.84527000	2.57133300	-2.94545600
C	1.16757600	3.92507300	-2.91005900
C	2.08947700	4.39871400	-1.98140300
H	3.43739400	3.85682400	-0.38859400
H	2.84884200	1.44276600	-0.46327400
H	0.12152600	2.20276500	-3.67640600
H	0.70128200	4.61126000	-3.61597500
H	2.34713000	5.45615300	-1.95168800
C	1.05707400	0.22838000	-2.09157800
H	0.54638900	-0.02304700	-3.03009500
H	1.93767500	-0.41805600	-1.96986400
O	-0.74063500	-1.19121500	1.16937900
C	-2.91549500	-1.69035000	0.30036200
C	-2.30061900	-2.68750300	-0.61753500
C	-4.46207500	-3.56225600	-1.38665000
C	-3.09399800	-3.01392900	-1.83409000
C	-4.27190200	-2.24399700	0.76717000
C	-5.15074100	-2.59217000	-0.42981100
H	-5.09425400	-3.76657400	-2.26299000
H	-2.57676200	-3.73174500	-2.48527100
H	-4.09692100	-3.14083200	1.38426100
H	-5.39501600	-1.66307800	-0.97447200

H	-3.26138200	-2.09191300	-2.42170500
H	-4.75470800	-1.50766700	1.42267200
H	-6.10685700	-3.01566100	-0.08961500
H	-4.30480600	-4.52685500	-0.87650700
C	-2.00129800	-1.25310700	1.44514100
C	-0.04983900	-1.91405400	-1.48311300
O	-2.48243200	-0.97164800	2.54093600
O	0.19229700	-2.79750700	-2.18092200
H	-3.12957700	-0.77674900	-0.28661500
H	-1.70871100	-3.48645300	-0.16033500

TS4c

(U)M06/BSII SCF energy in solution: -2051.157037 a.u.
(U)M06/BSI SCF energy: -2049.001294 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.389259 a.u.

C	2.74276600	-1.97520500	2.48145300
O	1.97359600	-0.90815400	3.05771800
C	2.55378400	-1.79585600	0.96313500
C	1.61946100	-0.11262700	2.03366900
N	1.94098700	-0.46709000	0.85261300
C	0.99401700	1.18806900	2.45156200
C	-0.86826400	3.61045400	0.50000800
O	-0.14050600	3.10811500	1.63414100
C	-1.20229900	2.35788900	-0.31869200
C	0.17183800	1.83108700	1.36377700
N	-0.31121600	1.34604400	0.28128900
H	-1.74616500	4.15065300	0.86820200
H	3.78971900	-1.85141000	2.79259600
H	2.35863100	-2.92200700	2.87057600
H	-0.20541800	4.29344400	-0.04803500
C	2.16407500	2.11907500	2.82446800

H	2.78124900	1.62958000	3.58729400
H	2.79264900	2.33689700	1.94911600
H	1.78881200	3.06416300	3.23010400
C	0.06503000	0.98523400	3.66232300
H	-0.74440200	0.27918500	3.42709800
H	0.64480600	0.59033900	4.50339900
H	-0.36222500	1.94999800	3.96048900
Ni	-0.01307800	-0.44406300	-0.50343700
H	-0.90384900	2.50331200	-1.36187100
H	1.82680900	-2.53312000	0.58369200
C	-2.64215100	1.91919900	-0.29048900
C	-3.31378800	1.69892200	-1.49276700
C	-3.31708400	1.71748800	0.91427700
C	-4.64835100	1.30456600	-1.49699700
H	-2.77940900	1.83941200	-2.43461900
C	-4.64839000	1.32028700	0.91309800
H	-2.79941300	1.84165800	1.86662000
C	-5.31855900	1.12043200	-0.29143500
H	-5.16294000	1.13779000	-2.44221400
H	-5.15647000	1.14862100	1.86034700
H	-6.36172000	0.80716100	-0.28893800
C	3.81504900	-1.89123000	0.14898700
C	3.99333900	-2.92046000	-0.77167300
C	4.81939100	-0.93179700	0.29607300
C	5.15880400	-2.99893800	-1.52907200
H	3.20762800	-3.66616200	-0.90029900
C	5.98239700	-1.00617500	-0.45856200
H	4.67390600	-0.11160300	1.00279200
C	6.15495600	-2.04246500	-1.37353000
H	5.28415300	-3.80678000	-2.24794800

H	6.75635600	-0.24988000	-0.33804200
H	7.06482200	-2.09821600	-1.96858100
C	2.67335800	3.49126200	-1.13130400
C	2.36014500	2.13979000	-1.16299600
C	1.41141500	1.63587200	-2.06718200
C	0.82419200	2.54004300	-2.96295200
C	1.14057700	3.89543300	-2.93891100
C	2.05996400	4.38104200	-2.01399600
H	3.40992300	3.85820600	-0.41634200
H	2.83339700	1.44133500	-0.47190300
H	0.10155300	2.16246700	-3.69038500
H	0.67114600	4.57368000	-3.65041800
H	2.31275000	5.43987800	-1.99284400
C	1.04435500	0.20547000	-2.08884700
H	0.53102800	-0.05508000	-3.02337400
H	1.92653600	-0.43839900	-1.96486800
O	-0.73577300	-1.19177100	1.19456700
C	-2.90106200	-1.68828600	0.30340300
C	-2.27429200	-2.67565400	-0.61718200
C	-4.42466300	-3.55862000	-1.40524700
C	-3.05826500	-2.99656800	-1.84166500
C	-4.25614100	-2.25597000	0.75812300
C	-5.12649400	-2.60136700	-0.44546300
H	-5.04920400	-3.76151300	-2.28729200
H	-2.53390700	-3.70640000	-2.49569400
H	-4.07835700	-3.15584500	1.36997100
H	-5.37542800	-1.67022300	-0.98425700
H	-3.22856200	-2.07074300	-2.42189000
H	-4.74629600	-1.52691700	1.41622500
H	-6.08074200	-3.03527500	-0.11336300

H	-4.26276400	-4.52587200	-0.90161100
C	-1.99811800	-1.25490800	1.45934300
C	-0.06347600	-1.93386700	-1.45930200
O	-2.49065900	-0.97640800	2.55075900
O	0.20191900	-2.81376700	-2.15515300
H	-3.11813600	-0.77223500	-0.27806400
H	-1.69637600	-3.48287000	-0.15560700

8c

(U)M06/BSII SCF energy in solution: -2048.440262 a.u.
(U)M06/BSI SCF energy: -2049.056693 a.u.
(U)M06/BSI SCF Gibbs energy: -2051.218356 a.u.

C	3.28760100	-1.46757700	2.62484800
O	2.89116500	-0.13522600	3.00280300
C	2.73672200	-1.63162100	1.20504100
C	1.95074900	0.24209400	2.11799600
N	1.74571900	-0.53682500	1.12582400
C	1.32381300	1.56954500	2.44938100
C	-0.53475300	3.81722100	0.29628800
O	0.22664600	3.43436300	1.45412000
C	-0.88097500	2.48588800	-0.39281000
C	0.48663900	2.12069300	1.32581100
N	-0.04048400	1.51663600	0.33314800
H	-1.41183200	4.37922700	0.63340200
H	4.37818300	-1.52945000	2.69018000
H	2.83455800	-2.16514100	3.33911300
H	0.10076500	4.46040100	-0.32515300
C	2.45767600	2.56082000	2.76553000
H	3.04851600	2.19469900	3.60998400
H	3.12562300	2.69036600	1.90260400
H	2.03520400	3.53621300	3.02258300

C	0.40569600	1.40494800	3.68009000
H	-0.39644000	0.68591800	3.46721000
H	0.99827100	1.04695100	4.53025200
H	-0.02508100	2.37907400	3.94210900
Ni	-0.06045300	-0.57179700	0.07771100
H	-0.57038600	2.50200900	-1.44355900
H	2.20918500	-2.58315700	1.08022300
C	-2.33665200	2.10610500	-0.31704700
C	-3.10458400	2.03654700	-1.47838900
C	-2.93305500	1.83661600	0.91603600
C	-4.45643900	1.71171900	-1.40793000
H	-2.63363800	2.23912400	-2.44133100
C	-4.27981900	1.50366500	0.98801600
H	-2.33102300	1.85251100	1.82641700
C	-5.04376900	1.44432900	-0.17534400
H	-5.05065500	1.66238400	-2.31918000
H	-4.71652600	1.25317700	1.95283100
H	-6.09783400	1.17540400	-0.12080700
C	3.75357200	-1.47534200	0.10192900
C	3.78046700	-2.38254900	-0.95510000
C	4.64419900	-0.39884400	0.09836800
C	4.67744700	-2.21413500	-2.00580500
H	3.07200000	-3.21160300	-0.95862400
C	5.54477000	-0.23316900	-0.94657600
H	4.63169300	0.32045100	0.92044300
C	5.55964300	-1.13979500	-2.00379900
H	4.68324900	-2.92403800	-2.83085500
H	6.23528700	0.60857600	-0.93917300
H	6.26125100	-1.00684600	-2.82526200
C	2.00141200	2.46986300	-2.89079400

C	1.85475700	1.24104300	-2.26148400
C	0.72881400	0.43664700	-2.49958800
C	-0.23078600	0.90677000	-3.40724300
C	-0.08164300	2.13393600	-4.04550000
C	1.03205200	2.92814000	-3.78375000
H	2.88637500	3.07429700	-2.69317800
H	2.61679600	0.87896600	-1.56692200
H	-1.10947700	0.28836000	-3.60603100
H	-0.83872200	2.47213400	-4.75313000
H	1.15315500	3.88868500	-4.28192500
C	0.55796100	-0.85590000	-1.81656900
H	-0.09843000	-1.52591300	-2.38556800
H	1.50702300	-1.36821400	-1.62315800
O	-0.98523200	-0.78549800	1.84351000
C	-2.77237300	-1.61127300	0.50206000
C	-1.89169100	-2.74528400	-0.02271600
C	-3.80990500	-3.63900500	-1.37191400
C	-2.35140800	-3.19752200	-1.41386800
C	-4.22423500	-2.06608200	0.55293200
C	-4.70579000	-2.53880400	-0.81314100
H	-4.13933700	-3.93809600	-2.37694900
H	-1.69986500	-4.00533300	-1.77670500
H	-4.31259200	-2.87967000	1.29196200
H	-4.70566700	-1.68305700	-1.51136600
H	-2.24525800	-2.35182700	-2.11644700
H	-4.84880500	-1.24684200	0.93004300
H	-5.74549300	-2.89021500	-0.75287200
H	-3.89293300	-4.53514100	-0.73437600
C	-2.25074400	-1.06339900	1.84000900
C	-0.40226300	-2.43781000	-0.06095100

O	-3.00331200	-0.89336800	2.79039800
O	0.44186300	-3.29098700	-0.08480900
H	-2.70258600	-0.76906500	-0.22080500
H	-1.97617100	-3.60883800	0.66299100

TS3b

(U)M06/BSII SCF energy in solution: -2051.140653 a.u.
(U)M06/BSI SCF energy: -2048.988308 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.376826 a.u.

C	2.60982100	-1.07665200	-3.02817800
O	2.20292600	-2.32223000	-2.42830700
C	2.34241100	-0.03284200	-1.93462800
C	1.44562600	-1.98187700	-1.36442000
N	1.40222200	-0.74720100	-1.04013000
C	0.84511300	-3.15624500	-0.63940700
C	-1.91668600	-3.21352500	1.70327600
O	-0.90338300	-3.79925200	0.86055100
C	-2.11949600	-1.81007100	1.11458100
C	-0.33355400	-2.76677700	0.20896500
N	-0.88577800	-1.62261100	0.33862600
H	-2.80549900	-3.85017400	1.66283800
H	3.66226600	-1.16173300	-3.31380200
H	1.99613800	-0.92245800	-3.92459700
H	-1.52073600	-3.18873200	2.72722100
C	1.95081100	-3.73063500	0.26533200
H	2.81367900	-4.02518300	-0.34516000
H	2.27042500	-2.97749300	0.99727900
H	1.57974900	-4.61272800	0.79914800
C	0.37689500	-4.22335700	-1.64151700
H	-0.37727000	-3.81942700	-2.32955300
H	1.22469700	-4.57833800	-2.23541100

H	-0.06072800	-5.07065000	-1.10424400
Ni	-0.23308700	0.17703400	-0.17760200
H	-2.16533100	-1.03271800	1.88776300
H	1.83495700	0.85375700	-2.33462800
C	-3.34781800	-1.69178800	0.24346400
C	-4.53810700	-1.24495500	0.81725900
C	-3.34200900	-2.05781100	-1.10090900
C	-5.70427700	-1.17645500	0.06611500
H	-4.53810400	-0.92184200	1.85845200
C	-4.50778500	-1.98646900	-1.85711000
H	-2.41045300	-2.37940000	-1.56722800
C	-5.69246500	-1.54848300	-1.27539200
H	-6.62372400	-0.81711100	0.52525900
H	-4.48797600	-2.27072900	-2.90806200
H	-6.60383200	-1.48992900	-1.86793800
C	3.58497100	0.39671100	-1.19452000
C	3.85778700	1.74958200	-1.00335500
C	4.48368700	-0.55729000	-0.70911800
C	5.01994600	2.14182800	-0.34244300
H	3.13917900	2.50077800	-1.33929800
C	5.64192000	-0.16568300	-0.04945100
H	4.27690500	-1.62087800	-0.84704100
C	5.91362500	1.18871800	0.13363600
H	5.22182900	3.20214500	-0.19743300
H	6.33556400	-0.91763500	0.32359000
H	6.82117200	1.49810500	0.64932100
C	2.57574700	-0.98274100	2.84386600
C	2.66716300	0.24552100	2.20770200
C	1.58023500	1.13794900	2.20855400
C	0.39621800	0.75193300	2.86885700

C	0.31019500	-0.47750600	3.50199000
C	1.39497800	-1.35755200	3.48882200
H	3.43701300	-1.65229200	2.84343700
H	3.58790600	0.53455200	1.70118100
H	-0.46920800	1.41522700	2.84619700
H	-0.61109900	-0.75375400	4.01581400
H	1.32664900	-2.32258200	3.99066800
C	1.63511800	2.36997300	1.45979800
H	1.00996900	3.19596900	1.80214900
H	2.59947300	2.68148600	1.06269500
O	0.70901500	1.98239100	-0.03079600
C	-1.09688700	3.37078600	-0.93764300
C	-2.08198100	2.19210300	-1.02369600
C	-3.90056900	3.68386100	-0.00080100
C	-3.53339900	2.68056600	-1.08892200
C	-1.48177800	4.31761100	0.21402100
C	-2.90417000	4.83341500	0.04461000
H	-4.91694500	4.06689600	-0.17510400
H	-4.19828800	1.80425700	-1.03990900
H	-1.39907600	3.76933500	1.16845100
H	-2.96092800	5.41404800	-0.89292100
H	-3.69332100	3.14560100	-2.07760900
H	-0.76208400	5.14753900	0.24587900
H	-3.15280900	5.52966900	0.85834000
H	-3.90873400	3.16803400	0.96873400
C	0.38699800	3.07013700	-0.74647800
C	-1.80395200	1.20211700	0.12220100
O	1.22532600	3.89027800	-1.07741200
O	-2.46231400	1.24107100	1.15374400
H	-1.15979500	3.95078300	-1.87300000

H	-1.85886400	1.63668700	-1.95066900

7b

(U)M06/BSII SCF energy in solution: -2051.18663 a.u.
(U)M06/BSI SCF energy: -2049.03993 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.42239 a.u.

C	2.30622500	-1.63825300	-2.94046900
O	1.84184100	-2.76141100	-2.16424100
C	2.24017300	-0.46517900	-1.95548400
C	1.17004100	-2.22814700	-1.12428400
N	1.26163000	-0.96196200	-0.95711500
C	0.48252900	-3.24301600	-0.24861000
C	-2.16630600	-2.64402800	2.16147200
O	-1.13171300	-3.42356400	1.52080800
C	-2.42220600	-1.48090200	1.19442700
C	-0.63107400	-2.62772700	0.55314700
N	-1.21299300	-1.51378900	0.34044500
H	-3.03151600	-3.29420000	2.32274400
H	3.31384500	-1.86554800	-3.29948400
H	1.62415300	-1.51796600	-3.79182200
H	-1.77366500	-2.30938300	3.13075800
C	1.54964600	-3.86251800	0.67036600
H	2.34558700	-4.31139800	0.06272700
H	1.98952100	-3.10663700	1.33572600
H	1.09670300	-4.64806700	1.28512000
C	-0.15972800	-4.34089000	-1.11471800
H	-0.90072100	-3.91321600	-1.80239000
H	0.60490200	-4.85935700	-1.70192900
H	-0.66198400	-5.06926000	-0.46810600
Ni	-0.21551400	0.19990500	-0.22797800
H	-2.45073300	-0.50395800	1.69516900

H	1.83389500	0.44548300	-2.41258100
C	-3.64670600	-1.63329800	0.32299300
C	-4.44608300	-0.52746900	0.03370200
C	-3.96976200	-2.86996600	-0.24108000
C	-5.54991100	-0.65996100	-0.80359500
H	-4.18209700	0.44207900	0.45740600
C	-5.07273900	-3.00225000	-1.07535600
H	-3.35278800	-3.74485800	-0.02545600
C	-5.86619800	-1.89432800	-1.35991300
H	-6.16503600	0.21172700	-1.02340200
H	-5.31398700	-3.97320800	-1.50559300
H	-6.73034200	-1.99496700	-2.01464700
C	3.57836000	-0.15539200	-1.32660300
C	4.12222900	1.12328700	-1.42783000
C	4.31529900	-1.15612200	-0.68669100
C	5.38011600	1.39954600	-0.89572300
H	3.53811900	1.91039600	-1.90337100
C	5.56950200	-0.88282200	-0.15638300
H	3.90437500	-2.16314800	-0.59787300
C	6.10630700	0.39889300	-0.25993100
H	5.79294400	2.40359600	-0.98147100
H	6.13126100	-1.67263300	0.34014000
H	7.09010900	0.61370700	0.15390600
C	2.68189600	-0.81284100	2.59554200
C	2.91216500	0.41054400	1.97610900
C	1.89795000	1.36179700	1.88581100
C	0.64545000	1.07729900	2.43320000
C	0.41979200	-0.14389100	3.06219200
C	1.43059600	-1.09607500	3.13919200
H	3.48653500	-1.54709200	2.65003500

H	3.89190300	0.62303400	1.54484900
H	-0.15887800	1.80532800	2.36161300
H	-0.56290700	-0.34286400	3.49123400
H	1.24593100	-2.05636300	3.62308200
C	2.19462800	2.68714000	1.23820500
H	2.65230500	3.37910800	1.95787700
H	2.88605800	2.55823800	0.39621300
O	1.00733500	3.34506400	0.80086800
C	-0.72988200	3.78602200	-0.75497200
C	-1.69495800	2.60888900	-1.06889300
C	-3.63497900	4.08997900	-0.27067700
C	-3.11535900	3.11652500	-1.32283500
C	-1.28110800	4.69324800	0.34112200
C	-2.65097700	5.23155800	-0.05193000
H	-4.61512400	4.48353700	-0.57859200
H	-3.78655700	2.24629800	-1.40100300
H	-1.36932700	4.12481200	1.27797400
H	-2.55901800	5.82563700	-0.97908400
H	-3.13325500	3.61435700	-2.30874800
H	-0.57590500	5.51439200	0.53418000
H	-3.02163100	5.91912300	0.72154500
H	-3.77642000	3.54737700	0.67339000
C	0.64598100	3.22090800	-0.48997500
C	-1.55159900	1.54959700	0.04893100
O	1.34954200	2.71637100	-1.34202700
O	-2.31954100	1.63784000	1.01877000
H	-0.63119700	4.36991600	-1.68690200
H	-1.31668400	2.13354900	-1.98934600

^{T}1

(U)M06/BSII SCF energy in solution: -1555.817193 a.u.
(U)M06/BSI SCF energy: -1553.800473 a.u.
(U)M06/BSI SCF Gibbs energy: -1553.291438 a.u.

C	1.32430600	2.45593000	1.40317800
O	0.90745100	2.99302700	0.14823400
C	1.57515000	0.95747100	1.12401400
C	0.65786600	1.92128000	-0.66313200
N	0.89070600	0.73831900	-0.14598100
C	-0.12623800	2.13689800	-1.92306900
C	-3.62621800	1.87541200	-0.95231400
O	-2.45389800	2.60833100	-1.29301300
C	-3.09819500	0.50498900	-0.49233200
C	-1.49648000	1.66262000	-1.53427000
N	-1.77801500	0.44140200	-1.13180200
H	-4.17187400	2.42490100	-0.17772200
H	2.22047600	2.99369900	1.73366000
H	0.52114200	2.61109600	2.13928400
H	-4.25754500	1.78466800	-1.84907700
C	0.43554300	1.26976900	-3.05507100
H	1.48556200	1.53712500	-3.24171600
H	0.38892100	0.20072200	-2.80728100
H	-0.14344300	1.43809000	-3.97270500
C	-0.12626500	3.59831100	-2.35264300
H	-0.50937100	4.25600500	-1.56761400
H	0.89718100	3.90966000	-2.59646000
H	-0.75399000	3.72198400	-3.24357600
Ni	-0.28046000	-0.90247100	-0.65083900
H	-3.75047200	-0.29602700	-0.87615000
H	1.10756900	0.34709100	1.91391300
C	-3.02162700	0.38147500	1.01199100
C	-3.86188200	-0.49508900	1.69776700

C	-2.12853900	1.16808700	1.74620500
C	-3.79544700	-0.61143100	3.08506800
H	-4.57228200	-1.10336200	1.13436900
C	-2.06960500	1.06404000	3.12901300
H	-1.47609700	1.86641800	1.21884300
C	-2.89685800	0.16519700	3.80435300
H	-4.45080300	-1.31113100	3.60162100
H	-1.37421300	1.68785000	3.69056800
H	-2.84199900	0.07932800	4.88820900
C	3.04793000	0.61823000	1.06698800
C	3.70569100	0.18690200	2.21963700
C	3.78150300	0.77211000	-0.11007800
C	5.06962100	-0.08390100	2.20089400
H	3.13572500	0.05605600	3.14163900
C	5.14500600	0.50168900	-0.13142000
H	3.26580100	1.09313400	-1.01602500
C	5.79364400	0.07352600	1.02349500
H	5.56733400	-0.42568300	3.10727600
H	5.70507400	0.62309200	-1.05749900
H	6.86048000	-0.14267700	1.00434500
C	-1.65878300	-2.56711400	-0.19214400
C	-1.42364700	-2.71250700	-1.52921700
C	1.23985500	-2.33983000	0.10266300
C	-0.42818200	-3.65075700	-2.15608600
C	1.42688300	-2.14243500	-1.24011200
H	-2.53354500	-1.98575800	0.09793700
H	-0.32883400	-4.55570000	-1.54409200
H	-2.07902400	-2.16717700	-2.21170400
H	1.80729200	-1.68948400	0.77208800
H	-0.81440000	-3.99259200	-3.12646600

H	2.11932100	-1.34578500	-1.52221300
C	-0.97001400	-3.25894000	0.95264900
H	-1.10665400	-2.61708100	1.83832100
H	-1.47218600	-4.21315300	1.19166300
C	0.53342400	-3.50497300	0.74963000
H	0.69882900	-4.42169900	0.16873100
H	0.98836200	-3.69605200	1.73108400
C	0.94507100	-3.00084700	-2.37747100
H	0.89152000	-2.36295600	-3.27321300
H	1.69069100	-3.78100200	-2.61293800

^{T}2b

(U)M06/BSII SCF energy in solution: -1780.355069 a.u.
(U)M06/BSI SCF energy: -1778.272326 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.773765 a.u.

C	3.66598800	0.35723900	-2.06981200
O	3.26361000	-1.03001100	-2.12392200
C	2.81097800	0.97446300	-0.94791700
C	2.28812600	-1.18116500	-1.21350800
N	1.98027100	-0.16202600	-0.51375400
C	1.60248400	-2.52188000	-1.24026700
C	-0.45888900	-4.12561500	1.28840300
O	0.39211700	-4.06177500	0.12924600
C	-0.60659600	-2.65866600	1.74455000
C	0.77313600	-2.78243100	-0.00824300
N	0.31435800	-1.94415500	0.84530000
H	-1.40846200	-4.57954100	0.98531000
H	4.74384400	0.38925300	-1.87695700
H	3.46720600	0.79666200	-3.05234400
H	0.03191700	-4.76577800	2.02927600
C	2.62845800	-3.64281900	-1.43743200

H	3.20951000	-3.45292600	-2.34485100
H	3.32320400	-3.70528600	-0.59035900
H	2.12012500	-4.60634200	-1.53889700
C	0.61446000	-2.48537600	-2.43286200
H	-0.10636400	-1.66072600	-2.33326000
H	1.17586500	-2.34787600	-3.36451600
H	0.07214000	-3.43690900	-2.49067300
Ni	0.27822700	0.01990700	0.49453700
H	-0.25503600	-2.52721300	2.77698500
H	2.10744900	1.72386100	-1.33375900
C	-2.00860100	-2.11625900	1.63036400
C	-2.72846800	-1.77993000	2.77418500
C	-2.61065600	-1.97275600	0.37759300
C	-4.03828200	-1.31856700	2.67270600
H	-2.25943100	-1.88093800	3.75382300
C	-3.91652500	-1.51026000	0.27269400
H	-2.05196600	-2.19818100	-0.53301800
C	-4.63356100	-1.18636900	1.42326000
H	-4.59157200	-1.05791200	3.57330500
H	-4.35376500	-1.37883200	-0.71614400
H	-5.65545100	-0.81953200	1.34199000
C	3.54877200	1.55491100	0.23045800
C	3.03628400	2.69066000	0.85663500
C	4.68319900	0.93637000	0.75566000
C	3.67022000	3.21633900	1.97777400
H	2.11935300	3.13598700	0.46838100
C	5.31680200	1.46155900	1.87565900
H	5.07197700	0.02639000	0.29347300
C	4.81359400	2.60775300	2.48482000
H	3.26641900	4.10605800	2.45812000

H	6.20504700	0.97504300	2.27567800
H	5.31133900	3.02291200	3.35972200
O	-1.20387600	0.53984800	-1.55967400
C	-3.18301100	1.63880300	-1.02667300
C	-2.29508300	1.73206000	0.21761200
C	-2.38862600	4.27093500	0.09270800
C	-2.38043600	3.03954000	0.99054700
C	-3.17811900	2.92715700	-1.86050400
C	-3.45372900	4.14551400	-0.98992300
H	-2.55962700	5.17225600	0.69889600
H	-1.54476700	3.08625000	1.70505800
H	-2.18994500	3.04663300	-2.33388700
H	-4.44933200	4.04798300	-0.52181200
H	-3.30734500	3.02839500	1.58842800
H	-3.90968400	2.82991100	-2.67482800
H	-3.48553600	5.05256000	-1.61015600
H	-1.40118700	4.37863400	-0.38023200
C	-2.51310900	0.53587600	-1.82007400
C	-0.89176100	1.42766300	-0.33863100
O	-3.03685400	-0.24240900	-2.58823700
O	-0.00896600	2.30904800	-0.55258500
H	-4.21845900	1.35773300	-0.78360200
H	-2.58076800	0.90125500	0.88566500

^{T}TS1b

(U)M06/BSII SCF energy in solution: -1780.352949 a.u.
(U)M06/BSI SCF energy: -1778.270252 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.770323 a.u.

C	3.55646700	0.20800900	-2.08899400
O	3.02722800	-1.13098300	-2.19841700
C	2.81642300	0.82786900	-0.88979600

C	2.11779700	-1.26804400	-1.22168300
N	1.95133400	-0.27620800	-0.43771100
C	1.36016100	-2.56777200	-1.25624300
C	-0.79421600	-4.08755200	1.24413600
O	0.06587500	-4.05174300	0.09070700
C	-0.85866300	-2.62396500	1.72698200
C	0.51522400	-2.79406500	-0.02861200
N	0.10426900	-1.94780900	0.84115000
H	-1.76694100	-4.47831200	0.92696500
H	4.64071600	0.13199400	-1.94981700
H	3.35357800	0.72211600	-3.03331300
H	-0.34720500	-4.77075500	1.97423000
C	2.33782100	-3.73499900	-1.44456000
H	2.92237600	-3.57980900	-2.35631100
H	3.03180300	-3.82006400	-0.59851000
H	1.78642100	-4.67558200	-1.53527600
C	0.38208300	-2.49394200	-2.45506500
H	-0.30270200	-1.63716300	-2.37001900
H	0.95771900	-2.39227400	-3.38231700
H	-0.20000000	-3.42192600	-2.50657400
Ni	0.28510200	0.02063800	0.60261400
H	-0.50370000	-2.53059600	2.76252700
H	2.13878200	1.63350900	-1.20499500
C	-2.22294600	-1.99473500	1.61237500
C	-2.92021600	-1.60018600	2.75189200
C	-2.80355300	-1.80971100	0.35606200
C	-4.18931700	-1.03875500	2.64033100
H	-2.46526500	-1.73275900	3.73446400
C	-4.06604600	-1.24197800	0.24095000
H	-2.25922300	-2.07393900	-0.55272900

C	-4.76314700	-0.86041100	1.38563800
H	-4.72744100	-0.73524800	3.53672600
H	-4.47435400	-1.07459300	-0.75475600
H	-5.75194300	-0.41320600	1.29685200
C	3.67127300	1.32663400	0.24576600
C	3.31871600	2.50955400	0.89368500
C	4.76447000	0.59327600	0.70835600
C	4.06684600	2.96580400	1.97455100
H	2.43690700	3.05369500	0.55402500
C	5.51206900	1.04844100	1.78756700
H	5.03077400	-0.35041700	0.22744200
C	5.16657100	2.24014800	2.41940200
H	3.78648800	3.89237600	2.47272200
H	6.36647300	0.47141100	2.13771700
H	5.75340400	2.59848700	3.26358000
O	-0.92896900	0.54053800	-1.48749800
C	-2.89802900	1.72172900	-1.10207400
C	-2.17306400	1.88084600	0.23600200
C	-2.32330100	4.41713000	0.00547400
C	-2.42415700	3.21343300	0.93506400
C	-2.76747000	2.96842200	-1.98301300
C	-3.19069000	4.22384400	-1.23345000
H	-2.61719200	5.32759600	0.54752800
H	-1.73127800	3.31920200	1.78315900
H	-1.71550000	3.07178300	-2.29391600
H	-4.25020000	4.13502500	-0.93472100
H	-3.44019600	3.17635000	1.36315400
H	-3.35829100	2.82150000	-2.89812600
H	-3.12412800	5.10152700	-1.89197600
H	-1.27579600	4.54859200	-0.30318700

C	-2.20297100	0.55162200	-1.78204200
C	-0.69032000	1.62978800	-0.06885800
O	-2.76183200	-0.25402300	-2.51305800
O	0.15043100	2.50258000	-0.30677900
H	-3.96435900	1.49334100	-0.94664000
H	-2.51054300	1.06483800	0.89615800

^{T}3b

(U)M06/BSII SCF energy in solution: -1780.370893 a.u.
(U)M06/BSI SCF energy: -1778.282687 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.783911 a.u.

C	-3.50821600	-0.25053600	2.15642700
O	-3.08305900	-1.61667800	1.93054200
C	-2.78344400	0.55486500	1.07201100
C	-2.00457100	-1.53550800	1.13417000
N	-1.69770600	-0.38304200	0.68139800
C	-1.31206800	-2.85380300	0.91925000
C	1.11817200	-3.83774200	-1.58111800
O	0.19532000	-4.03505300	-0.49475000
C	1.41054400	-2.32925500	-1.54345000
C	-0.26797300	-2.81548400	-0.16766500
N	0.28330700	-1.81247500	-0.74015900
H	1.99809100	-4.46083600	-1.39797900
H	-4.59843800	-0.22166500	2.07619500
H	-3.20287300	0.02360100	3.17385200
H	0.62028700	-4.15789900	-2.50507200
C	-2.36488200	-3.92197100	0.58316500
H	-3.09945700	-3.98634200	1.39113700
H	-2.89558400	-3.67556000	-0.34565700
H	-1.88465200	-4.89725600	0.45993100
C	-0.58850600	-3.22217600	2.23098700

H	0.14248100	-2.44790900	2.50053400
H	-1.32086800	-3.30651500	3.04167100
H	-0.06964700	-4.18127500	2.12100700
Ni	-0.05426400	0.16983200	-0.35243800
H	1.36464900	-1.88489100	-2.54569900
H	-2.33513900	1.47827600	1.45969500
C	2.74282100	-1.99670500	-0.91697500
C	3.81179800	-1.63410200	-1.73092400
C	2.93012500	-2.06411100	0.46264100
C	5.04670700	-1.31927300	-1.17714600
H	3.66287400	-1.55711800	-2.80834300
C	4.16271100	-1.74563600	1.02082100
H	2.09664700	-2.33269500	1.11252200
C	5.22281700	-1.36842900	0.20164600
H	5.86929700	-1.01804700	-1.82296600
H	4.29467400	-1.78643000	2.10081700
H	6.18542900	-1.11023100	0.63949400
C	-3.65074200	0.89462100	-0.11697100
C	-3.75238400	2.21808500	-0.54257500
C	-4.38102100	-0.09624100	-0.77699600
C	-4.58303800	2.54284300	-1.61006300
H	-3.15338700	2.97547000	-0.03632300
C	-5.20587100	0.22901000	-1.84713300
H	-4.31580700	-1.13645000	-0.44871200
C	-5.30866500	1.55300500	-2.26443400
H	-4.65670800	3.57866600	-1.93734900
H	-5.77123200	-0.55145800	-2.35449000
H	-5.95414000	1.81161600	-3.10259500
O	-0.61295300	2.09209300	-0.39194100
C	1.08921400	3.25164100	0.84612500

C	1.98156200	2.01410900	1.10253000
C	3.96566000	3.27917400	0.09907600
C	3.46245700	2.38790300	1.22870600
C	1.62609900	4.09354700	-0.31238400
C	3.07479700	4.50269200	-0.07760600
H	5.00210500	3.58301600	0.30735000
H	4.06538600	1.46826900	1.28804400
H	1.54151300	3.51870500	-1.24683200
H	3.13067300	5.13113400	0.82862700
H	3.58907300	2.91381000	2.19024100
H	0.98466500	4.97938400	-0.42807200
H	3.43644500	5.12296400	-0.91005300
H	3.98362300	2.70050200	-0.83565900
C	-0.38115300	2.87969800	0.60122400
C	1.71022200	1.00669700	0.00415400
O	-1.24761600	3.37384700	1.32952700
O	2.29487700	0.95204400	-1.05790000
H	1.11720600	3.86042800	1.76408300
H	1.64141200	1.54851000	2.04140200

^{S}TS1d

(U)M06/BSII SCF energy in solution: -1780.358553 a.u.
(U)M06/BSI SCF energy: -1778.278389 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.773872 a.u.

C	-3.99839200	0.12045400	-1.84825000
O	-3.65047500	1.47236500	-1.46298500
C	-2.97798000	-0.76043400	-1.12179400
C	-2.41398000	1.39147600	-0.94117600
N	-1.92548800	0.22410200	-0.78523700
C	-1.71041200	2.69328800	-0.67545300
C	0.56149100	3.44528100	2.05986100

O	-0.38798300	3.73801100	1.02084700
C	0.91371800	1.95833500	1.84602700
C	-0.70667500	2.56446900	0.44846700
N	-0.07800900	1.52238900	0.84546600
H	1.41766200	4.11645700	1.93834300
H	-5.03890300	-0.05764800	-1.56304500
H	-3.90323400	0.05702400	-2.93872100
H	0.07561700	3.64227400	3.02269800
C	-2.72509500	3.79719600	-0.36367400
H	-3.43378600	3.89363600	-1.19170800
H	-3.29329600	3.57584700	0.54811700
H	-2.20980500	4.75195300	-0.22441000
C	-0.91749800	3.05033100	-1.95282900
H	-0.21081800	2.25122700	-2.21401800
H	-1.61491000	3.18686600	-2.78879700
H	-0.36701700	3.98775900	-1.80270300
Ni	-0.17488600	-0.25530300	-0.19281900
H	0.75329200	1.37926500	2.76602500
H	-2.53265100	-1.51228600	-1.78500200
C	2.33128200	1.74516600	1.37655600
C	3.29273100	1.27121800	2.26784500
C	2.70845000	2.05303900	0.06887100
C	4.61411400	1.11209900	1.86148200
H	3.00084000	1.01529900	3.28755400
C	4.02521700	1.88410000	-0.34359300
H	1.96057500	2.39994000	-0.64590100
C	4.98149100	1.41977100	0.55528500
H	5.35485900	0.73639900	2.56532000
H	4.29364800	2.08356300	-1.37857900
H	6.01105100	1.28176600	0.23055500

C	-3.44434000	-1.42417400	0.15171500
C	-2.84699700	-2.62007100	0.55236700
C	-4.39572700	-0.82382400	0.97733900
C	-3.21186600	-3.21330900	1.75619700
H	-2.07851000	-3.06464800	-0.08244300
C	-4.76215700	-1.42059800	2.17846200
H	-4.85418500	0.12364800	0.68807300
C	-4.17189600	-2.61882400	2.56903400
H	-2.74176600	-4.14758800	2.05924400
H	-5.51130300	-0.94800700	2.81184500
H	-4.46050200	-3.08768300	3.50842500
O	0.99764900	-1.00601400	-2.39348300
C	2.68042100	-1.46004900	-0.79747600
C	1.46444800	-1.48681100	0.13413400
C	2.67259900	-3.27490100	1.36116200
C	1.29618500	-2.77369200	0.92845000
C	3.13613000	-2.88768900	-1.12333500
C	3.54445500	-3.64013000	0.14756100
H	3.16415000	-2.47444000	1.93990000
H	0.78104800	-3.54102500	0.32933000
H	2.30613400	-3.41004900	-1.62196100
H	4.59957600	-3.43203700	0.37851600
H	0.65566900	-2.58287900	1.80213000
H	3.96410600	-2.85720500	-1.84437700
H	3.48252200	-4.71992500	-0.04949800
H	2.58565300	-4.13403400	2.04081200
C	2.28211200	-0.76169300	-2.07567400
C	0.20894900	-1.60622800	-1.30637300
O	3.00614900	-0.09582900	-2.77593300
O	-0.33357500	-2.66187100	-1.56918000

H	3.52576800	-0.90296000	-0.36464700
H	1.60102100	-0.66354300	0.85500700

^{S}3d

(U)M06/BSII SCF energy in solution: -1780.372258 a.u.
(U)M06/BSI SCF energy: -1778.289378 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.784381 a.u.

C	-4.12095300	0.49495200	-1.70895100
O	-3.57602300	1.77790700	-1.31429600
C	-3.15549500	-0.52455100	-1.10783300
C	-2.30964200	1.52594700	-0.94724600
N	-1.94395500	0.30559400	-0.89778700
C	-1.43481700	2.71244000	-0.65446200
C	0.64303900	2.91423200	2.31577500
O	-0.15081000	3.44267200	1.23783400
C	1.05576800	1.52360400	1.81232900
C	-0.50069200	2.38578400	0.48898200
N	0.05282800	1.26071100	0.75909100
H	1.48410700	3.59180500	2.48616300
H	-5.14662700	0.43147600	-1.33556400
H	-4.12862100	0.46675900	-2.80520000
H	0.00636700	2.87690700	3.20903300
C	-2.27940200	3.94769700	-0.33875800
H	-2.92963100	4.17679300	-1.18864800
H	-2.91138100	3.79295300	0.54349300
H	-1.62855400	4.80635300	-0.14931900
C	-0.56155600	2.98333900	-1.89854500
H	0.04577900	2.10730500	-2.16080300
H	-1.20514800	3.23219400	-2.75183600
H	0.09962800	3.83850000	-1.70536100
Ni	-0.18919200	-0.42859500	-0.35369200

H	0.95013700	0.76814500	2.60159500
H	-2.90190000	-1.32486700	-1.80997900
C	2.47091200	1.50333600	1.28397100
C	3.49477400	1.00601300	2.09069500
C	2.79035300	2.02929100	0.03309000
C	4.81498900	1.03384300	1.65611800
H	3.24955000	0.57334900	3.06232000
C	4.10987000	2.05295000	-0.40679200
H	2.00248500	2.39549700	-0.62518200
C	5.12527300	1.55900400	0.40479500
H	5.60205200	0.63336500	2.29273600
H	4.33898200	2.43826300	-1.39807100
H	6.15631900	1.56915500	0.05689900
C	-3.55266700	-1.12207300	0.22266000
C	-3.01067600	-2.35256100	0.59824200
C	-4.37313000	-0.43596300	1.11939100
C	-3.29668400	-2.89105000	1.84816700
H	-2.35075700	-2.86976500	-0.09971000
C	-4.66266300	-0.97882700	2.36678200
H	-4.78923900	0.53686700	0.85264300
C	-4.12514400	-2.20849100	2.73357100
H	-2.86939100	-3.85228200	2.12971600
H	-5.31067500	-0.43769300	3.05458600
H	-4.35208200	-2.63416900	3.70970300
O	0.90668600	-1.62723100	-2.55983700
C	2.50173400	-1.38503900	-0.74055900
C	1.34873300	-1.42830700	0.27249600
C	2.28493500	-3.47345300	1.41254500
C	1.05014500	-2.84537500	0.75156600
C	3.29334000	-2.70703400	-0.78516900

C	3.58138800	-3.15088800	0.64273000
H	2.37407200	-3.10526600	2.44645200
H	0.71877600	-3.47944300	-0.08446600
H	2.71680000	-3.48046000	-1.31681600
H	4.12113400	-2.33076600	1.14494100
H	0.20803000	-2.83593800	1.46068000
H	4.22037500	-2.55840500	-1.35584700
H	4.26188100	-4.01316400	0.64986500
H	2.14562300	-4.56228400	1.48797500
C	2.06957500	-1.03752900	-2.14133900
C	-0.17892100	-1.72914100	-1.66750600
O	2.71927100	-0.38189800	-2.91487400
O	-1.01815200	-2.54630100	-1.96979700
H	3.21132200	-0.59438600	-0.45960600
H	1.66374300	-0.85438500	1.15915200

^{S}TS1b-1

(U)M06/BSII SCF energy in solution: -1780.359112 a.u.
(U)M06/BSI SCF energy: -1778.280917 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.776535 a.u.

C	1.80558700	-3.01440400	-2.10090500
O	0.69766700	-3.63994400	-1.42122800
C	1.92465600	-1.63675400	-1.43646100
C	0.05332400	-2.64963900	-0.77466800
N	0.60785400	-1.49639100	-0.77949700
C	-1.25940900	-3.08217400	-0.17588400
C	-3.22449100	-1.45219400	2.40261400
O	-2.82993600	-2.54909100	1.55576600
C	-2.64949600	-0.22133800	1.70176200
C	-1.84080400	-2.07011900	0.77320400
N	-1.59801800	-0.81835800	0.84080700

H	-4.31452400	-1.45781500	2.48950800
H	2.68648900	-3.64862100	-1.96556700
H	1.55108200	-2.95524200	-3.16650900
H	-2.77855600	-1.61746000	3.39150400
C	-1.07408000	-4.43223600	0.52955000
H	-0.70088000	-5.17590000	-0.18077600
H	-0.35491200	-4.35318100	1.35527500
H	-2.02962500	-4.77529300	0.93762400
C	-2.27314700	-3.22186400	-1.33261700
H	-2.42737300	-2.25404300	-1.82748500
H	-1.89808000	-3.94404400	-2.06689800
H	-3.23432300	-3.57991000	-0.94471300
Ni	-0.12871000	0.15195800	-0.11822800
H	-2.16985700	0.46336300	2.41394200
H	2.02711000	-0.81989300	-2.16095900
C	-3.59779900	0.54547800	0.81622200
C	-3.34272700	1.88843100	0.55347800
C	-4.65170200	-0.08861200	0.15353200
C	-4.11926300	2.59734700	-0.35551000
H	-2.50758000	2.39010300	1.04682900
C	-5.44442000	0.62219400	-0.73931900
H	-4.85425500	-1.14795700	0.32116500
C	-5.17834900	1.96460000	-0.99570500
H	-3.86138100	3.63014700	-0.57593100
H	-6.26867600	0.12202100	-1.24559800
H	-5.79261400	2.51512100	-1.70599800
C	3.04440300	-1.54022800	-0.42939700
C	4.14875900	-0.73197700	-0.69381500
C	3.01075000	-2.27614900	0.75622300
C	5.20543600	-0.66352300	0.20896700

H	4.15887800	-0.12760200	-1.59918700
C	4.06308600	-2.20551700	1.66174300
H	2.14769200	-2.90540700	0.98155500
C	5.16421200	-1.39859200	1.38877800
H	6.05671900	-0.01953000	-0.00614700
H	4.02364100	-2.78162000	2.58488600
H	5.98688300	-1.33976600	2.09944800
O	-0.34569900	2.09554400	-1.26715100
C	0.60758000	3.41454900	0.42027400
C	1.16558600	2.00860700	0.62230400
C	3.52824600	2.89765600	0.63992700
C	2.54020800	1.92005400	1.26457400
C	1.66302500	4.35960600	-0.16970200
C	2.95786200	4.31261600	0.63126000
H	4.47872400	2.86316000	1.19183900
H	2.91032900	0.88707100	1.19772200
H	1.87558000	4.05548700	-1.20711900
H	2.76392400	4.63973500	1.66825400
H	2.43736700	2.15097100	2.33861700
H	1.23970400	5.37189200	-0.21568000
H	3.68594500	5.02039800	0.21084700
H	3.73891300	2.58429300	-0.39340400
C	-0.50955700	3.22860900	-0.58776400
C	1.07869300	1.38879900	-0.78640700
O	-1.40555200	4.02348000	-0.77513700
O	1.95175200	1.32774400	-1.64199200
H	0.20484900	3.84771200	1.34991900
H	0.43098000	1.46901400	1.28463900

^{S}TS1b-2

(U)M06/BSII SCF energy in solution: -1780.359117 a.u.
(U)M06/BSI SCF energy: -1778.280917 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.776538 a.u.

C	-3.22412100	-1.45221600	2.40270500
O	-2.82969900	-2.54907200	1.55574000
C	-2.64933800	-0.22132400	1.70175200
C	-1.84069400	-2.07005300	0.77304700
N	-1.59796200	-0.81827800	0.84062500
C	-1.25936600	-3.08209400	-0.17610800
C	1.80576100	-3.01432900	-2.10092000
O	0.69789400	-3.63994100	-1.42121000
C	1.92484600	-1.63673900	-1.43637400
C	0.05344900	-2.64963000	-0.77476500
N	0.60799600	-1.49638800	-0.77952500
H	2.68668400	-3.64855600	-1.96578100
H	-4.31413500	-1.45789400	2.48983000
H	-2.77796200	-1.61749000	3.39149300
H	1.55110700	-2.95502600	-3.16648200
C	-2.27305800	-3.22158200	-1.33290200
H	-3.23430300	-3.57952700	-0.94507200
H	-2.42715500	-2.25372300	-1.82772900
H	-1.89807800	-3.94379000	-2.06720100
C	-1.07426300	-4.43223000	0.52924500
H	-0.35538800	-4.35328400	1.35523200
H	-2.02994400	-4.77529700	0.93699100
H	-0.70086000	-5.17584700	-0.18101900
Ni	-0.12849000	0.15198200	-0.11829200
H	2.02740700	-0.81987200	-2.16085100
H	-2.16966300	0.46344900	2.41383600
C	3.04450800	-1.54020600	-0.42922100
C	4.14884200	-0.73191200	-0.69359800

C	3.01081400	-2.27610200	0.75640900
C	5.20547700	-0.66341300	0.20922600
H	4.15894200	-0.12750700	-1.59895500
C	4.06309800	-2.20540400	1.66198600
H	2.14772900	-2.90531900	0.98173700
C	5.16422600	-1.39847300	1.38904300
H	6.05676900	-0.01942800	-0.00587600
H	4.02363400	-2.78150000	2.58513200
H	5.98688300	-1.33964300	2.09973000
C	-3.59785900	0.54534100	0.81631100
C	-3.34294100	1.88829200	0.55342600
C	-4.65189800	-0.08886200	0.15395600
C	-4.11967700	2.59707000	-0.35549600
H	-2.50777100	2.39006900	1.04660400
C	-5.44487000	0.62183000	-0.73876400
H	-4.85425300	-1.14823200	0.32166900
C	-5.17889500	1.96421500	-0.99537300
H	-3.86184600	3.62985100	-0.57608400
H	-6.26923300	0.12158100	-1.24479400
H	-5.79333600	2.51463000	-1.70559500
O	-0.34588100	2.09545100	-1.26730800
C	0.60744600	3.41454800	0.42002600
C	1.16556700	2.00867700	0.62218900
C	3.52814100	2.89786500	0.63995400
C	2.54010100	1.92032300	1.26468500
C	1.66284100	4.35961500	-0.17001700
C	2.95768300	4.31279300	0.63095700
H	4.47857100	2.86355000	1.19196000
H	2.91029500	0.88734500	1.19810600
H	1.87540800	4.05545700	-1.20742000

H	2.76372700	4.64013100	1.66787900
H	2.43707200	2.15146800	2.33866100
H	1.23946700	5.37187600	-0.21604000
H	3.68575800	5.02050300	0.21040900
H	3.73893800	2.58429600	-0.39328900
C	-0.50976800	3.22845600	-0.58792200
C	1.07896500	1.38865700	-0.78640800
O	-1.40588400	4.02326300	-0.77510100
O	1.95197400	1.32772600	-1.64200300
H	0.20475600	3.84774500	1.34967500
H	0.43092100	1.46907100	1.28447900

^{S}TS1b-3

(U)M06/BSII SCF energy in solution: -1780.354619 a.u.
(U)M06/BSI SCF energy: -1778.279808 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.7768 a.u.

C	3.30235300	-2.00965300	-2.06553100
O	2.03478800	-2.71514300	-2.10126900
C	3.10022800	-0.85841500	-1.05260500
C	1.19921900	-1.99836900	-1.34752500
N	1.66646500	-0.97170700	-0.74643800
C	-0.26008200	-2.33458100	-1.28610600
C	-1.54464300	-1.41450200	2.00643200
O	-0.82920300	-2.24468100	1.07613400
C	-2.39717300	-0.51260000	1.11156200
C	-0.81911300	-1.54435000	-0.09781200
N	-1.63210000	-0.49671300	-0.16269600
H	-2.11625100	-2.06867500	2.67253000
H	4.07581700	-2.72428000	-1.76676400
H	3.50810900	-1.65821000	-3.08197000
H	-0.81879100	-0.82720800	2.58634900

C	-0.47229400	-3.84014500	-1.12016600
H	-0.04967700	-4.36742300	-1.98382000
H	0.00048100	-4.22108200	-0.20933600
H	-1.54512600	-4.06353800	-1.07140000
C	-0.91415200	-1.85720100	-2.58777600
H	-0.79249500	-0.77606500	-2.72173500
H	-0.46704300	-2.37884400	-3.44334400
H	-1.98917300	-2.07294600	-2.55880500
Ni	0.23899500	0.18400400	0.00045400
H	-2.43987900	0.50385700	1.51942800
H	3.26319800	0.12492700	-1.51444900
C	-3.79101100	-1.01554900	0.83406800
C	-4.86250600	-0.12465100	0.81511200
C	-4.03279900	-2.36454800	0.56036500
C	-6.15020900	-0.56606700	0.52880300
H	-4.68063800	0.92863400	1.03206300
C	-5.31779700	-2.80926400	0.27593900
H	-3.20482000	-3.07497100	0.58572600
C	-6.38068400	-1.91006000	0.25810100
H	-6.97688300	0.14248200	0.52114000
H	-5.49299000	-3.86430800	0.07046600
H	-7.38788900	-2.25895600	0.03667000
C	3.92328400	-0.94814800	0.20560400
C	4.55247500	0.18948200	0.70537600
C	4.02581300	-2.15241600	0.90340000
C	5.29110500	0.11878900	1.88252800
H	4.43915900	1.13407400	0.17272600
C	4.76312200	-2.22345700	2.07819900
H	3.51517500	-3.04268200	0.52949200
C	5.40082700	-1.08611800	2.56741400

H	5.77918900	1.01235400	2.26772000
H	4.83877600	-3.16722000	2.61578100
H	5.97968100	-1.13977200	3.48796600
O	1.23695100	1.83606900	0.38314500
C	0.41340800	3.42561900	-1.11962200
C	-0.85034200	2.65970900	-0.70903900
C	-1.85001900	4.79409300	0.24968800
C	-2.10227800	3.51172800	-0.53071700
C	0.57799600	4.74251500	-0.34084300
C	-0.69568100	5.57490600	-0.36719400
H	-2.76430800	5.40339000	0.26757800
H	-2.88188000	2.90244500	-0.05047800
H	0.82681500	4.50874600	0.70740300
H	-0.94376300	5.84120600	-1.40941800
H	-2.47987900	3.76944100	-1.53366500
H	1.43544000	5.29027500	-0.75459100
H	-0.53418300	6.52040800	0.16835100
H	-1.60972200	4.54445500	1.29413200
C	1.56136200	2.52535400	-0.72589400
C	-0.45198600	1.90894300	0.56380800
O	2.65245900	2.47570000	-1.24767100
O	-0.85930800	2.07215900	1.69185400
H	0.43893800	3.63095100	-2.19911900
H	-1.05383200	1.89626700	-1.47634700

^{S}TS1b-4

(U)M06/BSII SCF energy in solution: -1780.35197 a.u.

(U)M06/BSI SCF energy: -1778.271574 a.u.

(U)M06/BSI SCF Gibbs energy: -1777.765545 a.u.

C	0.52422700	2.41730200	2.20432200
O	-0.19663300	3.12889900	1.17528100

C	1.15120000	1.23596500	1.45307100
C	-0.36199700	2.24454600	0.18211100
N	0.29093100	1.14202400	0.25543500
C	-1.30314000	2.65342400	-0.92764200
C	-4.15446700	0.65406700	-1.96851700
O	-3.48081900	1.90012900	-1.68673100
C	-3.39777300	-0.39083200	-1.13600500
C	-2.31944000	1.55609900	-1.10986200
N	-2.14617500	0.32667800	-0.82046000
H	-5.21008500	0.78630700	-1.72228400
H	1.25109600	3.10199600	2.64978500
H	-0.20726800	2.10068200	2.95874500
H	-4.06073100	0.46690800	-3.04513000
C	-0.50527200	2.77440100	-2.23987000
H	0.23540800	3.57984000	-2.14940400
H	0.01504000	1.83579200	-2.46815500
H	-1.18336000	3.01968500	-3.06678200
C	-1.99587900	3.98031400	-0.61627500
H	-2.60365000	3.92077900	0.29327800
H	-1.24710500	4.76628300	-0.47186000
H	-2.64577900	4.26232200	-1.45078500
Ni	-0.33676000	-0.50487900	-0.65465300
H	-3.12928300	-1.26060500	-1.75205500
H	1.07493000	0.30314000	2.03058700
C	-4.04268600	-0.87838100	0.14814400
C	-3.25514100	-1.62743700	1.03050500
C	-5.37350200	-0.63501300	0.47836400
C	-3.78972500	-2.10358500	2.21978600
H	-2.21054800	-1.83223700	0.79090400
C	-5.90962400	-1.11628100	1.67096600

H	-6.02284900	-0.06791800	-0.18703800
C	-5.11933200	-1.84833900	2.54603900
H	-3.15883000	-2.67973100	2.89410400
H	-6.95192100	-0.91260600	1.91151000
H	-5.53649000	-2.22294900	3.47933700
C	2.59760100	1.49384800	1.10632100
C	3.55881400	1.22926100	2.08393300
C	3.00140000	2.00402700	-0.12529800
C	4.90336400	1.46737800	1.83273800
H	3.24379400	0.78637500	3.02985100
C	4.35122400	2.22921000	-0.38279200
H	2.26136200	2.18362400	-0.90466100
C	5.30412400	1.96372100	0.59470300
H	5.64504500	1.24726900	2.59879000
H	4.65926900	2.61166000	-1.35480100
H	6.35924600	2.13916700	0.39128300
O	0.28852400	-1.93656100	0.85584400
C	2.49672000	-2.65954600	0.34576400
C	1.71702700	-3.00626600	-0.92018700
C	3.51445300	-1.90271200	-2.34749800
C	2.52227100	-3.04985300	-2.22067300
C	3.58079600	-1.60384900	0.12021500
C	4.41801800	-1.85723800	-1.12201300
H	4.09914700	-2.01861400	-3.27088400
H	1.82909000	-3.08032900	-3.07389800
H	3.09623600	-0.62502900	-0.00216700
H	4.96572100	-2.81214400	-1.03410900
H	3.08025100	-3.99973200	-2.23812400
H	4.19344400	-1.52711600	1.02759200
H	5.17318200	-1.06437100	-1.22359100

H	2.97264700	-0.94400700	-2.43031300
C	1.48403000	-2.09890700	1.35809200
C	0.56073600	-2.06025600	-0.96697200
O	1.83291200	-1.75655800	2.48079900
O	-0.53373400	-2.21654200	-1.53222200
H	2.96337500	-3.56437500	0.76379700
H	1.23542000	-3.98972000	-0.78066000

^{S}TS1c-1

(U)M06/BSII SCF energy in solution: -1780.364801 a.u.
(U)M06/BSI SCF energy: -1778.284955 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.780794 a.u.

C	0.11802100	-2.79383500	2.40529400
O	1.20296200	-3.18237000	1.54644300
C	-0.57910400	-1.64540300	1.64546300
C	1.27594500	-2.25462700	0.57812500
N	0.36302400	-1.35318900	0.55191800
C	2.39558100	-2.45317300	-0.42326200
C	4.55312900	0.28526300	-1.49093000
O	4.31417100	-1.02839500	-0.93506400
C	3.25795700	1.05095100	-1.21564400
C	2.97814800	-1.11221700	-0.79647300
N	2.29767500	-0.05869600	-1.02179700
H	5.44540700	0.70193800	-1.01625600
H	-0.52493600	-3.66621200	2.56002800
H	0.54602000	-2.47949000	3.36442000
H	4.73796500	0.15834500	-2.56494200
C	1.77075400	-3.06747800	-1.69430300
H	1.32385600	-4.04171700	-1.45352400
H	0.99898700	-2.40713200	-2.11161800
H	2.55044900	-3.22456300	-2.45074900

C	3.47322900	-3.38545500	0.12781100
H	3.93722900	-2.98197400	1.03478000
H	3.03675400	-4.35957300	0.36970100
H	4.25734400	-3.52641400	-0.62311100
Ni	0.32158700	0.03419800	-0.84695200
H	2.94078400	1.63451200	-2.08914300
H	-0.66075200	-0.75072300	2.27847100
C	3.22627400	1.92284400	0.01754500
C	2.18908700	2.84786500	0.14458300
C	4.12680900	1.75899800	1.07021100
C	2.05485700	3.60318700	1.30340200
H	1.44960700	2.95524000	-0.65036300
C	4.00488500	2.52884500	2.22333600
H	4.92735500	1.02063000	1.00568000
C	2.97063300	3.45175900	2.34080300
H	1.21570300	4.29144700	1.38208800
H	4.72101600	2.40173000	3.03400400
H	2.87551300	4.04899400	3.24642600
C	-1.95024300	-2.02048100	1.14626000
C	-3.07380600	-1.64583700	1.88167800
C	-2.11529200	-2.77963600	-0.01211200
C	-4.34847200	-2.01234000	1.46208000
H	-2.94907800	-1.04158000	2.78207200
C	-3.38824800	-3.14675300	-0.43326300
H	-1.24452100	-3.05494500	-0.60817200
C	-4.50716000	-2.76289100	0.30139100
H	-5.21890700	-1.70283000	2.03820600
H	-3.50778700	-3.72427300	-1.34797700
H	-5.50330900	-3.04470500	-0.03459500
O	-0.65857500	2.04634000	-1.12054200

C	-2.68638100	0.69797500	-0.75937500
C	-2.36824800	1.59558500	0.43468200
C	-4.48739500	2.90805200	0.03364400
C	-3.56596700	2.28117700	1.07208500
C	-3.66362900	1.35056200	-1.74198500
C	-4.89315500	1.88044400	-1.01760100
H	-5.37217500	3.33693000	0.52466800
H	-3.20381700	3.03622800	1.78230700
H	-3.15484900	2.18203200	-2.25618700
H	-5.41951700	1.04231400	-0.52498300
H	-4.13654200	1.53276800	1.64855100
H	-3.92747000	0.62204200	-2.52015500
H	-5.60040700	2.31676200	-1.73703000
H	-3.96267100	3.74433300	-0.45756000
C	-1.34994400	0.47647900	-1.40976000
C	-1.29011500	2.55309800	-0.07591000
O	-1.06714500	0.09371300	-2.54766600
O	-1.04424300	3.63447800	0.42204500
H	-3.09547000	-0.26782300	-0.43079300
H	-1.85736600	0.98548300	1.20120200

^{S}TS1c-2

(U)M06/BSII SCF energy in solution: -1780.363399 a.u.

(U)M06/BSI SCF energy: -1778.282918 a.u.

(U)M06/BSI SCF Gibbs energy: -1777.779786 a.u.

C	-4.45296900	-0.14423400	-0.50944100
O	-4.13000800	1.26231200	-0.57568000
C	-3.09468200	-0.86134500	-0.55847700
C	-2.79638800	1.35274100	-0.45753300
N	-2.14194000	0.25487800	-0.40868400
C	-2.22730600	2.75075200	-0.51774600

C	0.67966900	3.97132900	1.27531500
O	-0.68020700	4.06017400	0.79807700
C	0.91966400	2.46573900	1.40431000
C	-0.94898500	2.84803400	0.27911000
N	-0.08814100	1.92379900	0.47335600
H	1.33796900	4.42030100	0.51725300
H	-4.99474900	-0.31990000	0.42890100
H	-5.10908000	-0.37714200	-1.35254500
H	0.75328100	4.53261600	2.20991600
C	-3.24848700	3.77587200	-0.01893400
H	-4.15654600	3.72167500	-0.62679900
H	-3.52474000	3.59915800	1.02744200
H	-2.82909700	4.78336300	-0.09699200
C	-1.87583300	3.03890100	-1.99377400
H	-1.15130300	2.30844800	-2.37550300
H	-2.78568800	2.99087900	-2.60524300
H	-1.45037900	4.04682700	-2.08089800
Ni	-0.24384300	0.14979300	-0.52861300
H	0.63364600	2.12072800	2.41252700
H	-2.89166400	-1.29836900	-1.54563300
C	2.33151400	2.03596200	1.13671000
C	3.19126100	1.81584900	2.21337900
C	2.80868800	1.88521200	-0.16510200
C	4.51861900	1.46638700	1.99391200
H	2.81286200	1.91856900	3.23188200
C	4.13368700	1.52199900	-0.38552000
H	2.13509300	2.00749100	-1.01448900
C	4.99021700	1.32125500	0.69267900
H	5.18190600	1.29579400	2.84026500
H	4.47369200	1.35322600	-1.40336600

H	6.02520100	1.03353600	0.51654000
C	-2.87267500	-1.91153900	0.49565600
C	-2.49180300	-3.19897400	0.12425800
C	-2.99191100	-1.59992900	1.85174400
C	-2.23719900	-4.16483800	1.09401600
H	-2.36110100	-3.42802900	-0.93343100
C	-2.73896500	-2.56256000	2.82087800
H	-3.26497400	-0.58619500	2.15180500
C	-2.36043400	-3.84866800	2.44224600
H	-1.93405000	-5.16620800	0.79253300
H	-2.83102500	-2.30882400	3.87562900
H	-2.16007600	-4.60282700	3.20134600
O	1.25156200	-0.33964900	-2.08677400
C	0.77252900	-2.35715900	-0.69736200
C	2.04769700	-2.47636500	-1.53391200
C	3.44597400	-2.64958800	0.55871500
C	3.21729700	-3.17030500	-0.85453400
C	1.05917200	-1.91740600	0.74359400
C	2.16631400	-2.74893000	1.37976000
H	4.26219400	-3.20593900	1.04074200
H	4.11303500	-3.02700700	-1.47277400
H	1.38842500	-0.85785000	0.76360100
H	1.84226500	-3.80387100	1.43304900
H	3.01697000	-4.25324300	-0.81035600
H	0.13405100	-1.97317300	1.33730000
H	2.33735200	-2.41856400	2.41435400
H	3.76800300	-1.59432900	0.51257200
C	-0.09236300	-1.36234100	-1.50771900
C	2.35293300	-1.06029700	-2.00377000
O	-0.84747900	-1.72379900	-2.39981200

O	3.45949900	-0.67331000	-2.32632100
H	0.23006800	-3.31587600	-0.67570300
H	1.77828500	-3.01935000	-2.45611300

^{S}TS1c-3

(U)M06/BSII SCF energy in solution: -1780.362773 a.u.
(U)M06/BSI SCF energy: -1778.276688 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.773182 a.u.

C	0.68594700	3.92932300	0.96890200
O	-0.75378600	3.84528100	0.98507500
C	1.15542200	2.48416900	0.71218300
C	-1.05685700	2.54094500	0.98606300
N	-0.08555700	1.70703500	0.91986800
C	-2.53198500	2.19611600	1.02956500
C	-3.96357700	0.25739500	-1.73159800
O	-3.97467600	1.30586200	-0.73251200
C	-2.66821200	-0.53704000	-1.46226300
C	-2.80289600	1.21737700	-0.08913300
N	-2.01788600	0.27009400	-0.41939300
H	-4.87520000	-0.33598300	-1.60749900
H	0.97371300	4.62591800	0.17557300
H	1.00617000	4.32418900	1.94030400
H	-3.97869100	0.74090200	-2.71395000
C	-3.40367100	3.44253100	0.89600000
H	-3.18628000	4.14120900	1.71043100
H	-3.23383900	3.96176600	-0.05355800
H	-4.46011400	3.15954500	0.94718700
C	-2.84111300	1.47328200	2.35502600
H	-2.21099500	0.58184700	2.47018900
H	-2.66551600	2.15063800	3.20020500
H	-3.89573800	1.16794500	2.36893900

Ni	-0.37759600	-0.20506400	0.57104500
H	-2.00541200	-0.54347100	-2.33885700
H	1.89415900	2.17420300	1.46182600
C	-2.84979100	-1.94711000	-0.96845100
C	-2.04414400	-2.96697500	-1.46617700
C	-3.75775300	-2.22424300	0.05420700
C	-2.15850900	-4.25800000	-0.96084900
H	-1.30407700	-2.74141300	-2.23368900
C	-3.87284800	-3.51219500	0.55952100
H	-4.37443600	-1.42183000	0.46717000
C	-3.07343700	-4.53204500	0.04838700
H	-1.52153300	-5.04880700	-1.35215400
H	-4.58446300	-3.72189500	1.35624700
H	-3.16167400	-5.54161000	0.44590500
C	1.70819000	2.24332700	-0.66920300
C	3.06255000	1.98108100	-0.85461300
C	0.86589800	2.29283900	-1.77964100
C	3.56342300	1.72347400	-2.12495500
H	3.73075700	1.94975700	0.00837700
C	1.36703200	2.04983500	-3.05042700
H	-0.19951200	2.48984300	-1.64523200
C	2.71441300	1.75064300	-3.22309200
H	4.61281000	1.46609600	-2.25104400
H	0.69951000	2.07214700	-3.91039700
H	3.10093700	1.52251300	-4.21404000
O	1.27359900	-0.98339000	-0.90651000
C	2.19500300	-1.66406700	1.59883300
C	2.77950700	-2.34834900	0.34337200
C	5.03998500	-1.36344100	0.89804200
C	4.26869100	-2.61880000	0.50947400

C	2.98454200	-0.41955500	1.97838400
C	4.46353300	-0.73289900	2.16038700
H	6.10427100	-1.59866400	1.04133400
H	4.64566200	-3.01318200	-0.44164100
H	2.86462300	0.30817900	1.16212800
H	4.58894400	-1.42821800	3.00916000
H	4.41971700	-3.39347800	1.28123900
H	2.55679600	0.03680500	2.88561100
H	5.01242500	0.18292200	2.42607300
H	4.98097100	-0.64884200	0.06182100
C	0.77449700	-1.36747100	1.26625400
C	2.43616800	-1.51585800	-0.92583700
O	-0.17451200	-2.13746800	1.21984300
O	3.26421000	-1.46419700	-1.83527000
H	2.19612400	-2.38501400	2.43556500
H	2.24793600	-3.30656200	0.21900900

^{S}TS1c-4

(U)M06/BSII SCF energy in solution: -1780.362521 a.u.
(U)M06/BSI SCF energy: -1778.284902 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.778155 a.u.

C	1.19632000	-2.50018900	2.10812600
O	2.21741100	-2.65863800	1.10708000
C	0.18017000	-1.51658500	1.48171600
C	1.92559500	-1.78924600	0.12749100
N	0.84288200	-1.10986900	0.23317500
C	2.92949300	-1.65505100	-1.00594300
C	4.47893300	1.63616400	-0.62393100
O	4.49973700	0.19089900	-0.61449600
C	2.98958200	1.98124800	-0.62529700
C	3.26415600	-0.18019900	-1.00129000

N	2.39452600	0.74028900	-1.17086400
H	5.03016200	1.98909300	0.25273400
H	0.76923900	-3.48702500	2.31743500
H	1.67358200	-2.10924400	3.01428100
H	4.98530400	1.97233600	-1.53721900
C	2.24862400	-2.04461400	-2.32834000
H	1.95060800	-3.10077100	-2.28779000
H	1.35682300	-1.43364100	-2.52711000
H	2.95567900	-1.91940900	-3.15790800
C	4.16435600	-2.51845700	-0.77376300
H	4.66465300	-2.28068500	0.17001600
H	3.88112500	-3.57669200	-0.75621800
H	4.87987000	-2.36374200	-1.58945200
Ni	0.42537200	0.29583200	-1.09416900
H	2.75990600	2.82559100	-1.28588600
H	0.06682700	-0.61883600	2.10927300
C	2.35228700	2.18774400	0.73069800
C	1.16626200	2.91604000	0.81780800
C	2.82718000	1.52383400	1.86489100
C	0.46217700	2.98256900	2.01682300
H	0.75625200	3.40831500	-0.06538600
C	2.13043700	1.59716500	3.06662600
H	3.74068500	0.92886900	1.81472700
C	0.94477300	2.32422700	3.14407100
H	-0.47364200	3.53815000	2.04444700
H	2.51771300	1.08596700	3.94749200
H	0.40026500	2.38060800	4.08560600
C	-1.17063900	-2.13565800	1.23993300
C	-2.25256000	-1.80770400	2.05354700
C	-1.34265300	-3.07688100	0.22326900

C	-3.49325600	-2.40675400	1.85467500
H	-2.12495100	-1.06446100	2.84269700
C	-2.57917000	-3.67810500	0.02448300
H	-0.50581800	-3.31931300	-0.43457400
C	-3.65804600	-3.34334400	0.83956800
H	-4.33465600	-2.13430800	2.48995800
H	-2.70540900	-4.40334100	-0.77724200
H	-4.62875700	-3.80895500	0.67891100
O	-1.07493300	1.89815400	-1.49100100
C	-2.62926900	0.11938500	-0.92101400
C	-2.53064700	1.15342000	0.19705100
C	-4.94487400	1.80640200	-0.14485400
C	-3.84032700	1.53250500	0.86836800
C	-3.79894100	0.40132300	-1.87140100
C	-5.09615700	0.63526500	-1.10978700
H	-5.89144800	2.01007800	0.37511900
H	-3.67030500	2.40785800	1.50982000
H	-3.56273200	1.29674700	-2.46984800
H	-5.36221400	-0.27434100	-0.54209000
H	-4.14931900	0.69921400	1.52252200
H	-3.88570500	-0.42785600	-2.58587200
H	-5.92041400	0.81710600	-1.81387700
H	-4.69540400	2.71760500	-0.71351200
C	-1.32029400	0.27948600	-1.65333700
C	-1.79164700	2.31674700	-0.45004700
O	-0.99025600	-0.12046900	-2.77694400
O	-1.82435600	3.46886400	-0.07124600
H	-2.71327300	-0.90061100	-0.52183100
H	-1.82892800	0.77453500	0.96332500

^{S}TS1c-5

(U)M06/BSII SCF energy in solution: -1780.345715 a.u.
(U)M06/BSI SCF energy: -1778.271824 a.u.
(U)M06/BSI SCF Gibbs energy: -1777.767669 a.u.

C	-2.92660200	-0.90156300	2.28232800
O	-1.79096000	-1.77732200	2.42675100
C	-2.69175700	-0.18737300	0.94284600
C	-1.16912400	-1.78782000	1.23050600
N	-1.61299100	-0.99529100	0.32647400
C	-0.06224800	-2.80971900	1.12968500
C	2.35665200	-3.22584600	-1.55735000
O	1.56442900	-3.65406400	-0.43204100
C	2.23013200	-1.69339400	-1.55630200
C	0.85327000	-2.57192200	-0.04538500
N	1.11210100	-1.46031200	-0.61961100
H	3.37955200	-3.58844000	-1.41234100
H	-3.83445400	-1.51996000	2.27804600
H	-2.95168100	-0.23226900	3.14636100
H	1.93341400	-3.68502000	-2.45850800
C	-0.72069400	-4.19466300	1.03464300
H	-1.37666800	-4.34926500	1.89871200
H	-1.32018000	-4.28007500	0.11938400
H	0.04096100	-4.98110600	1.02429100
C	0.83034000	-2.73042400	2.38251200
H	1.28217900	-1.73309600	2.47324900
H	0.24880300	-2.94120400	3.28597300
H	1.63411500	-3.47259200	2.30030200
Ni	-0.34385600	-0.08860100	-0.91672400
H	1.93155300	-1.30479900	-2.53811800
H	-2.28262800	0.82312400	1.10212400
C	3.44281900	-0.94268200	-1.07104600

C	4.14201700	-1.37914700	0.05630000
C	3.82284900	0.24328000	-1.69409700
C	5.20803600	-0.63973400	0.55339200
H	3.83650100	-2.30033500	0.55751300
C	4.89265400	0.98364300	-1.19878500
H	3.24622400	0.59934900	-2.54849200
C	5.58529600	0.54479200	-0.07531000
H	5.74586500	-0.98535100	1.43464000
H	5.18227900	1.91055000	-1.69170100
H	6.42068100	1.12510400	0.31262000
C	-3.90027200	-0.06992300	0.05814000
C	-4.31951000	1.18483300	-0.37842400
C	-4.60089700	-1.20852300	-0.34400200
C	-5.43766000	1.29877200	-1.19928300
H	-3.75391100	2.07059900	-0.08328100
C	-5.71401700	-1.09417800	-1.16578400
H	-4.26035500	-2.19543200	-0.02342900
C	-6.13662500	0.16295900	-1.59160700
H	-5.75920100	2.28195200	-1.53826500
H	-6.25358600	-1.98702100	-1.47784900
H	-7.00972000	0.25349800	-2.23579700
O	-0.95525700	2.14840000	-0.94653000
C	1.36373000	2.27542200	-0.30809500
C	0.61388400	3.59184000	-0.03973400
C	1.25834800	3.52033800	2.40761200
C	1.03356000	4.39436300	1.18088000
C	1.60280900	1.49567500	0.98770500
C	2.20222600	2.37174700	2.07731100
H	1.64901700	4.12942000	3.23440100
H	0.26800000	5.15711200	1.37812900

H	0.63882900	1.08633700	1.34701200
H	3.17134000	2.77424800	1.73250300
H	1.96805500	4.92790200	0.94568600
H	2.23732800	0.62521900	0.77251500
H	2.41481400	1.76914900	2.97173100
H	0.29221600	3.11060100	2.74688700
C	0.41265400	1.55263800	-1.26851800
C	-0.82838400	3.12902600	-0.04183500
O	0.59549900	1.24353900	-2.46170300
O	-1.74802200	3.54436100	0.62524100
H	2.32399700	2.44797100	-0.81525100
H	0.70441800	4.22007600	-0.94237500

R-S-pro

(U)M06/BSII SCF energy in solution: -807.833451 a.u.
(U)M06/BSI SCF energy: -807.595597 a.u.
(U)M06/BSI SCF Gibbs energy: -807.333854 a.u.

C	-3.80333600	0.76983600	-0.27202300
C	-2.57189400	0.64680100	-0.90693400
C	-1.76932200	-0.47569900	-0.69178800
C	-2.23129900	-1.47881500	0.16165000
C	-3.45997400	-1.35401000	0.80154200
C	-4.24840900	-0.22822300	0.59035400
H	-4.41901700	1.64959600	-0.45443100
H	-2.21397700	1.43785500	-1.56626600
H	-1.62333200	-2.36995600	0.32299000
H	-3.80272200	-2.14299600	1.46895800
H	-5.20998100	-0.13043400	1.09128200
C	-0.43496900	-0.60804400	-1.39143100
H	-0.53724800	-1.24982200	-2.27730300
H	-0.09788500	0.38101800	-1.73236200

O	-0.55604600	1.69677700	1.35340100
C	1.51058300	0.96857000	0.50179200
C	1.22830100	-0.54092500	0.67631900
C	3.65117800	-0.98105600	0.10859500
C	2.52728600	-1.22384500	1.11278700
C	2.58582500	1.21333000	-0.54877100
C	3.87592700	0.50612000	-0.14623300
H	4.57904900	-1.44733600	0.46738700
H	2.35336800	-2.29819500	1.23577500
H	2.23802200	0.84407700	-1.52799600
H	4.26530600	0.97681100	0.77299800
H	2.81645800	-0.82137200	2.09684400
H	2.74708900	2.29175600	-0.67524700
H	4.64460400	0.65164000	-0.91739600
H	3.39983500	-1.48520300	-0.83700700
C	0.28084400	1.81550700	0.30673300
C	0.61989500	-1.27491600	-0.52535100
O	0.04780900	2.53002800	-0.64093300
O	0.91820200	-2.43288300	-0.73868900
H	1.90834000	1.29000200	1.48170400
H	0.47071800	-0.65001900	1.47248800
H	-1.36215300	2.19342500	1.12390300

4CzIPN(PC)

(U)M06/BSII SCF energy in solution: -2480.609591 a.u.

(U)M06/BSI SCF energy: -2479.983795 a.u.

(U)M06/BSI SCF Gibbs energy: -2479.339253 a.u.

C	0.45573800	-0.00696100	0.00556000
C	-0.25601200	-1.14390400	-0.43609400
C	-1.66435300	-1.12606400	-0.44834900
C	-2.37105000	-0.00454100	0.00841400

C	-1.66149500	1.11341000	0.47040800
C	-0.25356200	1.12873900	0.45602000
C	-2.38421400	-2.21998600	-1.02128000
C	-2.37877100	2.20730400	1.04659400
N	-2.97320500	-3.10601200	-1.48854700
N	-2.96548500	3.09318800	1.51700600
C	-5.94180500	-0.49323000	0.49992300
C	-4.60024900	-0.80169900	0.79532100
C	-4.25110600	-1.73533100	1.76266000
C	-5.28340000	-2.38547500	2.42671000
C	-6.62361000	-2.10435700	2.13876200
C	-6.95966800	-1.15802000	1.18171700
C	-5.92891600	0.53393100	-0.51610900
C	-4.57990000	0.81872800	-0.80072100
C	-4.20657300	1.74436000	-1.76676800
C	-5.22185900	2.41192400	-2.43963300
C	-6.56914200	2.15510000	-2.16182500
C	-6.92941300	1.21565800	-1.20666200
H	-3.20959500	-1.94491600	2.00291000
H	-5.04242600	-3.12610400	3.18678700
H	-7.40943700	-2.63147200	2.67585800
H	-8.00363200	-0.93252100	0.96738300
H	-3.15964300	1.93327800	-2.00049300
H	-4.96158000	3.14659300	-3.19913700
H	-7.34129700	2.69517300	-2.70579800
H	-7.97880300	1.00833700	-1.00073300
N	-3.77117600	0.00145500	0.00070400
C	4.01280400	0.57446000	-0.49506800
C	2.66195400	0.86864600	-0.75753800
C	2.28915100	1.84025800	-1.67854900

C	3.29909100	2.56190000	-2.30115300
C	4.64788200	2.30129100	-2.03316500
C	5.01071300	1.30164900	-1.14183100
C	4.03356600	-0.52513000	0.43984000
C	2.69467400	-0.85257100	0.72544900
C	2.36206100	-1.83182200	1.65401700
C	3.40121400	-2.52138600	2.26523500
C	4.73827600	-2.22626300	1.97562600
C	5.06047900	-1.22290200	1.07337100
H	1.24526200	2.04212700	-1.91165400
H	3.02665600	3.34822500	-3.00331500
H	5.41813600	2.88213700	-2.53670400
H	6.06073700	1.08401100	-0.94953600
H	1.32757300	-2.05922100	1.90558800
H	3.16340800	-3.30623000	2.98111000
H	5.53116400	-2.78273700	2.47154300
H	6.10121300	-0.97834800	0.86368100
N	1.85689500	-0.00163300	-0.00910100
C	2.16361200	-3.51980100	-1.70489700
C	1.47045500	-2.30196000	-1.81594300
C	1.81797900	-1.34253800	-2.75652900
C	2.93384800	-1.58883800	-3.54519700
C	3.65860300	-2.77989300	-3.42471100
C	3.26962500	-3.75649800	-2.51858300
C	1.50092400	-4.29337100	-0.68133300
C	0.42629300	-3.52079900	-0.20223400
C	-0.38514700	-3.96128700	0.83554500
C	-0.10594500	-5.20560000	1.38896400
C	0.95362200	-5.98907300	0.92084000
C	1.75993000	-5.53867400	-0.11457600

H	1.25065200	-0.42118400	-2.86890300
H	3.24663800	-0.83569800	-4.26659700
H	4.52787800	-2.94586500	-4.05771600
H	3.81974500	-4.69337100	-2.44040800
H	-1.21310100	-3.36142600	1.20888100
H	-0.73162000	-5.57561900	2.19885900
H	1.14309100	-6.96063500	1.37275400
H	2.59283700	-6.14186900	-0.47353000
N	0.41207100	-2.28968800	-0.89065100
C	1.52857900	4.26279000	0.70450000
C	0.44074500	3.50490600	0.23195900
C	-0.37448200	3.95981100	-0.79663000
C	-0.08094900	5.19988700	-1.35202800
C	0.99444700	5.96696500	-0.89276100
C	1.80104000	5.50497300	0.13721900
C	2.18957300	3.47882600	1.72102500
C	1.48344500	2.26873300	1.83322700
C	1.82687100	1.30260500	2.76830900
C	2.95017700	1.53449800	3.55086300
C	3.68758600	2.71747000	3.42873200
C	3.30389700	3.70072400	2.52755400
H	-1.21619900	3.37458800	-1.16212300
H	-0.70848900	5.58027200	-2.15565000
H	1.19487300	6.93566800	-1.34608500
H	2.64511600	6.09585000	0.49052700
H	1.25110000	0.38638100	2.88045600
H	3.25930600	0.77548400	4.26758100
H	4.56284500	2.87165400	4.05644400
H	3.86419500	4.63141700	2.44792000
N	0.41804500	2.27077500	0.91558000

***PC**

(U)M06/BSII SCF energy in solution: -2480.519534 a.u.

(U)M06/BSI SCF energy: -2479.893121 a.u.

(U)M06/BSI SCF Gibbs energy: -2479.25283 a.u.

C	0.33696600	0.00007400	-0.00005900
C	-0.32350500	1.12619300	0.47498900
C	-1.77198500	1.12639500	0.49169200
C	-2.45288800	0.00028300	0.00004500
C	-1.77220700	-1.12594100	-0.49171600
C	-0.32372300	-1.12589500	-0.47513500
C	-2.46605800	2.23041800	1.03326100
C	-2.46646000	-2.22983600	-1.03327600
N	-2.99957400	3.17404100	1.46934100
N	-3.00012000	-3.17339600	-1.46932800
C	-6.02582300	0.51906200	-0.50192200
C	-4.67796400	0.81986400	-0.78278500
C	-4.31782600	1.77004000	-1.73137400
C	-5.34036000	2.43328500	-2.39592200
C	-6.68552100	2.15414100	-2.12637000
C	-7.03431000	1.19871800	-1.18315100
C	-6.02581300	-0.51862400	0.50195300
C	-4.67794800	-0.81924800	0.78297200
C	-4.31779600	-1.76935100	1.73163000
C	-5.34031700	-2.43272100	2.39607100
C	-6.68548300	-2.15375300	2.12636400
C	-7.03428900	-1.19838900	1.18309000
H	-3.27189700	1.98750700	-1.94230800
H	-5.08894800	3.18644000	-3.14063600
H	-7.46391400	2.69219900	-2.66396300
H	-8.08140600	0.97742400	-0.97865400

H	-3.27186100	-1.98665500	1.94270100
H	-5.08889200	-3.18582300	3.14083400
H	-7.46386800	-2.69189300	2.66388900
H	-8.08139000	-0.97722500	0.97848300
N	-3.86163500	0.00038500	0.00017000
C	3.93215100	-0.47070400	0.55162800
C	2.57561500	-0.72823000	0.85763100
C	2.19849400	-1.58033400	1.89636600
C	3.21195600	-2.21589400	2.60622800
C	4.55341400	-1.98130100	2.30681600
C	4.92359200	-1.10102400	1.28288000
C	3.93245700	0.46969800	-0.55094700
C	2.57608900	0.72770300	-0.85732800
C	2.19959100	1.58001700	-1.89614000
C	3.21349100	2.21523900	-2.60566700
C	4.55478300	1.98016200	-2.30586800
C	4.92434100	1.09971800	-1.28186000
H	1.15268300	-1.74291900	2.13882600
H	2.94773200	-2.90310400	3.40675900
H	5.32756600	-2.48677200	2.87982100
H	5.97564000	-0.92082500	1.06770600
H	1.15392600	1.74308100	-2.13891100
H	2.94975400	2.90261000	-3.40622000
H	5.32927600	2.48540000	-2.87862000
H	5.97625700	0.91914700	-1.06635600
N	1.77308100	-0.00013400	0.00002500
C	2.23767600	3.25917600	1.91573100
C	1.32641300	2.18820200	2.01835000
C	1.38040700	1.27714100	3.06496700
C	2.40748300	1.42061200	3.99257300

C	3.34181600	2.45565100	3.88757400
C	3.25482100	3.38712000	2.85951400
C	1.85207000	4.01842100	0.74894300
C	0.73121200	3.35949100	0.19014900
C	0.09059200	3.83522600	-0.95541900
C	0.60150700	4.98013900	-1.54638600
C	1.72231700	5.63539400	-1.01478700
C	2.34891800	5.16313400	0.13170600
H	0.63221000	0.49237400	3.16012400
H	2.47781900	0.71530000	4.81902300
H	4.13281500	2.54310600	4.62962600
H	3.97181400	4.20463100	2.79146100
H	-0.78921900	3.33180700	-1.35386100
H	0.11747000	5.38349700	-2.43384500
H	2.09640800	6.53409800	-1.50131900
H	3.21321300	5.68328200	0.54299300
N	0.43339300	2.23292700	0.94306300
C	1.85130500	-4.01855200	-0.74936800
C	0.73059200	-3.35943900	-0.19047400
C	0.08990000	-3.83518400	0.95505800
C	0.60056100	-4.98029300	1.54585400
C	1.72122200	-5.63571900	1.01415700
C	2.34791900	-5.16343900	-0.13227900
C	2.23706000	-3.25924800	-1.91606400
C	1.32601300	-2.18807900	-2.01855300
C	1.38020200	-1.27689900	-3.06505500
C	2.40724400	-1.42048400	-3.99268600
C	3.34134600	-2.45574200	-3.88783000
C	3.25415600	-3.38731500	-2.85987800
H	-0.78981000	-3.33165500	1.35358000

H	0.11643700	-5.38366700	2.43325800
H	2.09512900	-6.53456700	1.50056500
H	3.21210600	-5.68371200	-0.54363400
H	0.63216300	-0.49197100	-3.16012000
H	2.47773400	-0.71507400	-4.81903800
H	4.13230900	-2.54328300	-4.62990900
H	3.97096000	-4.20499900	-2.79193500
N	0.43303900	-2.23271700	-0.94322900

4CzIPN-BF_3K^+

(U)M06/BSII SCF energy in solution: -3405.161451 a.u.
(U)M06/BSI SCF energy: -3404.407003 a.u.
(U)M06/BSI SCF Gibbs energy: -3403.755153 a.u.

C	1.18898100	-0.05564800	-0.05990900
C	1.34879000	1.32161100	0.28628600
C	0.18328600	2.12192600	0.48024500
C	-1.07354000	1.63092100	0.19412300
C	-1.22227200	0.30344400	-0.32423300
C	-0.07072400	-0.56979100	-0.31375500
C	0.30757000	3.44783300	1.00228600
C	-2.41769600	-0.10153400	-0.86970200
N	0.39610200	4.53130500	1.41418400
N	-3.45219900	-0.44054700	-1.31740400
C	-4.34367900	3.13556300	-0.09457200
C	-2.99731400	3.05884600	-0.50043000
C	-2.54646000	3.61340100	-1.69071500
C	-3.48355100	4.26601300	-2.47923400
C	-4.82766000	4.36061600	-2.09182200
C	-5.26651100	3.79976500	-0.90304200
C	-4.43950500	2.43018200	1.16275700
C	-3.13891100	1.96322700	1.46470900

C	-2.86431500	1.22796100	2.61555400
C	-3.92481500	0.95078800	3.47554600
C	-5.22566700	1.39765900	3.18880400
C	-5.48636700	2.14216700	2.04023300
H	-1.49936400	3.54400300	-1.98206900
H	-3.16647400	4.71445700	-3.41869500
H	-5.53376200	4.87949900	-2.73641600
H	-6.31317400	3.86869400	-0.60993100
H	-1.84552900	0.91691400	2.84684700
H	-3.73402500	0.40560700	4.39950800
H	-6.03083800	1.19224200	3.89285300
H	-6.49465400	2.49812100	1.83168800
N	-2.25854100	2.36230400	0.46499000
C	4.01772400	-2.24738400	0.60360200
C	2.68047700	-1.86150100	0.82975700
C	1.93881600	-2.37689100	1.88611600
C	2.55986400	-3.29432700	2.72398000
C	3.88568000	-3.69178400	2.51339200
C	4.61787800	-3.17297500	1.45530700
C	4.48831900	-1.49425600	-0.53426600
C	3.41755900	-0.68399400	-0.95825700
C	3.51641500	0.14244000	-2.07183000
C	4.73815600	0.19461400	-2.72911900
C	5.82392200	-0.58017100	-2.30355500
C	5.70229100	-1.43542400	-1.21731600
H	0.91054000	-2.06502400	2.06226800
H	1.99973900	-3.71432900	3.55780500
H	4.34285100	-4.41484300	3.18622800
H	5.65245900	-3.47514400	1.29597500
H	2.67702500	0.75291700	-2.40131100

H	4.84944600	0.86155800	-3.58253000
H	6.77040100	-0.51611600	-2.83706100
H	6.54377000	-2.05006300	-0.89921400
N	2.31817200	-0.90195800	-0.12154000
C	4.81455200	1.99811000	1.14030300
C	3.55225400	1.45559600	1.45269800
C	3.35372200	0.64716500	2.56508400
C	4.46125100	0.33678900	3.34202900
C	5.73092200	0.83658300	3.02702100
C	5.91235300	1.67612800	1.93724300
C	4.63847900	2.81728200	-0.03576800
C	3.27904300	2.73224900	-0.39534900
C	2.76977100	3.38823300	-1.51002700
C	3.65472900	4.13645100	-2.27563600
C	5.00968100	4.23303500	-1.93484600
C	5.50630200	3.57898200	-0.81630400
H	2.36669000	0.26143700	2.81397000
H	4.33723100	-0.31654200	4.20410900
H	6.58188500	0.57170500	3.65186500
H	6.89785600	2.07950200	1.70649200
H	1.71584200	3.31339300	-1.77772200
H	3.28427800	4.66324000	-3.15347500
H	5.67590500	4.83263600	-2.55231300
H	6.56132900	3.65215900	-0.55411800
N	2.61760800	1.88934500	0.50583300
C	-1.39816000	-3.94703200	-0.22284300
C	-1.19731600	-2.66067300	0.32139000
C	-1.79114800	-2.26825900	1.51973600
C	-2.61827700	-3.18621000	2.16480700
C	-2.85426600	-4.45650000	1.62121300

C	-2.24045300	-4.84185700	0.43483800
C	-0.60035900	-4.01540100	-1.42433200
C	0.04488200	-2.76881500	-1.56328100
C	0.87838500	-2.48626300	-2.63861000
C	1.06692700	-3.48975800	-3.57827400
C	0.44337000	-4.73836100	-3.45407200
C	-0.39254800	-5.00792800	-2.38215400
H	-1.58701900	-1.28705400	1.94990000
H	-3.05310700	-2.92356700	3.13221700
H	-3.50049000	-5.15659900	2.14733000
H	-2.41011700	-5.83740800	0.02704300
H	1.36822600	-1.51996700	-2.73948800
H	1.71825700	-3.29914200	-4.42904400
H	0.61667600	-5.50167800	-4.20988000
H	-0.88311800	-5.97615600	-2.28937500
N	-0.32346300	-1.94624500	-0.49309500
B	-4.91147100	-1.00588100	-1.67325100
F	-5.77925900	-0.15524600	-0.98560500
F	-5.09673400	-1.02888900	-3.00188500
F	-4.94961200	-2.26345500	-1.06806600
K	-4.81998500	-1.09648500	1.24774800

^{Q}4a

(U)M06/BSII SCF energy in solution: -1826.600424 a.u.
(U)M06/BSI SCF energy: -1824.501423 a.u.
(U)M06/BSI SCF Gibbs energy: -1823.884009 a.u.

C	-1.87572400	2.62149500	1.98004500
O	-1.21755400	1.70065000	2.86691200
C	-1.75345700	1.97751000	0.58819000
C	-0.65044100	0.75098900	2.10817200
N	-0.86807800	0.83520200	0.84666300

C	0.07076000	-0.34845500	2.83209300
C	2.19691100	-2.92456000	1.77017600
O	1.98301700	-1.82584600	2.64556900
C	1.92862700	-2.35200900	0.37888100
C	1.16639000	-0.91367100	1.95322600
N	0.88549100	-1.38937900	0.69682400
H	3.21338900	-3.30838700	1.92172400
H	-2.90977900	2.74469200	2.32024800
H	-1.35324200	3.58311900	2.04991100
H	1.46883400	-3.72445700	1.99014300
C	-0.99340700	-1.42690100	3.15103700
H	-1.79087900	-1.02897500	3.79570300
H	-1.43540800	-1.81967200	2.22436300
H	-0.49962400	-2.25372200	3.67770200
C	0.67848200	0.18140000	4.13117100
H	1.40877600	0.97462400	3.92085000
H	-0.09163300	0.57771700	4.80274300
H	1.20462800	-0.63605100	4.63426100
Ni	-0.27217300	-0.49173900	-0.51768900
H	1.51731700	-3.12363400	-0.29133800
H	-1.24341100	2.64910000	-0.11729300
C	3.12734800	-1.71702300	-0.29136000
C	3.22298900	-1.72560100	-1.68364300
C	4.13007400	-1.07199500	0.44124800
C	4.29312300	-1.12205100	-2.33655200
H	2.44131600	-2.22228600	-2.26348500
C	5.20682800	-0.47617500	-0.20743500
H	4.06143400	-1.04163000	1.52833300
C	5.29482600	-0.49983100	-1.59723600
H	4.35222300	-1.14992900	-3.42402000

H	5.98466300	0.01294100	0.37779300
H	6.14062800	-0.03476500	-2.10135600
C	-3.04642200	1.49938700	-0.02067600
C	-3.35997800	1.81863100	-1.33974100
C	-3.92060300	0.69096500	0.71014000
C	-4.53615300	1.35175600	-1.92134300
H	-2.66785000	2.43688000	-1.91448500
C	-5.09896700	0.23080900	0.13572800
H	-3.67225200	0.40818300	1.73573600
C	-5.40965900	0.56201800	-1.18193800
H	-4.77072500	1.60817200	-2.95294900
H	-5.77516300	-0.39535800	0.71567700
H	-6.33210200	0.19915600	-1.63158500
C	-3.11682300	-3.55112900	-0.50206000
C	-2.69993500	-2.37479700	-1.10191600
C	-1.46951900	-2.30536500	-1.79348700
C	-0.70062900	-3.48474800	-1.87905300
C	-1.12082800	-4.65832000	-1.27276900
C	-2.32618900	-4.69877700	-0.57300800
H	-4.06906100	-3.57594800	0.02707500
H	-3.32068200	-1.47877600	-1.04784800
H	0.23990500	-3.45966200	-2.43185400
H	-0.50622600	-5.55435900	-1.34813200
H	-2.65394600	-5.62179100	-0.09833500
C	-0.96866500	-1.03238400	-2.28322700
H	-0.15918600	-1.06581700	-3.02159100
H	-1.73079700	-0.27419100	-2.50879600
C	1.40432000	3.49317300	0.89623700
C	2.07534700	2.42761800	0.44790000
C	0.30873500	3.84315100	-2.01087400

C	2.74191200	2.24852100	-0.88642700
C	0.57260100	2.55963000	-2.27958000
H	1.01576800	3.42742600	1.91927900
H	3.23812500	3.17004100	-1.21297800
H	2.13197700	1.55685500	1.11558300
H	-0.66746900	4.22103700	-2.33176500
H	3.53984100	1.49991500	-0.78201400
H	-0.20730000	2.00114800	-2.81062600
C	1.09005200	4.79730000	0.21892400
H	0.06245900	5.08443700	0.50615200
H	1.72638800	5.59539200	0.63818700
C	1.18083000	4.85043800	-1.31163100
H	2.22380000	4.75488400	-1.63179300
H	0.87338900	5.85817900	-1.62583700
C	1.78811300	1.73931400	-1.96944000
H	1.44735600	0.73261100	-1.66115100
H	2.35456300	1.56054200	-2.89984200

^{Q}5a

(U)M06/BSII SCF energy in solution: -2051.151119 a.u.
(U)M06/BSI SCF energy: -2048.990966 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.383651 a.u.

C	2.98975900	-2.82613000	1.23048300
O	2.41919800	-2.15675300	2.37078200
C	2.59337900	-1.95742000	0.02717300
C	1.61219600	-1.19986000	1.90601600
N	1.60329400	-1.04548200	0.62874700
C	0.93127200	-0.34297000	2.93206100
C	-1.24408400	2.36675400	2.73492700
O	-0.92142500	1.13439900	3.36341300
C	-1.37714200	1.99007800	1.26243600

C	-0.30803500	0.33207300	2.37877200
N	-0.32370500	0.98405800	1.16706400
H	-2.15464200	2.77040300	3.19441200
H	4.07036300	-2.90796800	1.38845400
H	2.54413200	-3.82608400	1.18106800
H	-0.41596500	3.08772700	2.86165100
C	1.97391100	0.72403400	3.35024500
H	2.89054000	0.26734700	3.74904400
H	2.23257900	1.36833300	2.49725100
H	1.52755500	1.34877300	4.13330500
C	0.54398900	-1.19459700	4.14449400
H	-0.12973800	-2.00614300	3.84182700
H	1.42854500	-1.62695400	4.62720900
H	0.01988200	-0.56069200	4.86692300
Ni	0.85591000	0.54841600	-0.26641300
H	-1.13732100	2.83822300	0.60422000
H	2.09371200	-2.56572500	-0.73489900
C	-2.74856700	1.45456200	0.89825900
C	-3.29652400	1.73656200	-0.35429700
C	-3.48601100	0.64825200	1.77803200
C	-4.54170700	1.23747300	-0.72728800
H	-2.73260200	2.36908800	-1.04221800
C	-4.72881100	0.14516200	1.40579400
H	-3.07724400	0.41730600	2.76101800
C	-5.26334100	0.43611800	0.15304800
H	-4.95349600	1.48199100	-1.70677300
H	-5.28792300	-0.47614200	2.10462000
H	-6.24144500	0.04961200	-0.13126300
C	3.68308500	-1.15546900	-0.63519400
C	3.81464200	-1.18918000	-2.02214300

C	4.50549500	-0.30662100	0.10975300
C	4.76354400	-0.39335700	-2.65871900
H	3.14784300	-1.82743300	-2.60428800
C	5.44957500	0.49115600	-0.52438100
H	4.40359400	-0.26254500	1.19600200
C	5.58002700	0.44835500	-1.91127000
H	4.85768800	-0.42578300	-3.74261800
H	6.08754900	1.14812500	0.06447200
H	6.31960100	1.07405400	-2.40776400
C	0.88404900	4.78880100	-0.38302600
C	1.44164400	3.56988900	-0.73279000
C	0.79358300	2.70764200	-1.64704300
C	-0.44017000	3.13155700	-2.18417900
C	-0.98367100	4.36211900	-1.84700800
C	-0.32919800	5.19644400	-0.94112700
H	1.40150500	5.43572300	0.32362300
H	2.39561500	3.25270500	-0.30581700
H	-0.95645200	2.47346300	-2.88668200
H	-1.93023600	4.67372800	-2.28737500
H	-0.76001600	6.15908300	-0.67276100
C	1.35031600	1.40738700	-1.96552100
H	0.91100800	0.88144600	-2.82099700
H	2.44456000	1.32488100	-1.92462400
O	-0.15930300	-3.02697200	-0.58291400
C	-2.25931100	-2.01663100	-0.30045400
C	-1.55384300	-1.36570200	-1.49128100
C	-3.31887900	-2.23103400	-3.07582400
C	-2.37263300	-1.08583100	-2.74196500
C	-3.31890700	-3.05911700	-0.71379400
C	-4.18368300	-2.57403700	-1.86860000

H	-3.94229100	-1.96095600	-3.93865100
H	-1.68296600	-0.87632800	-3.57166400
H	-2.81434500	-3.98954000	-1.02897700
H	-4.75237000	-1.68135200	-1.55851500
H	-2.95927700	-0.17141400	-2.56561700
H	-3.92003100	-3.31630000	0.16837700
H	-4.91848800	-3.34953800	-2.12414900
H	-2.73723000	-3.11994300	-3.37689600
C	-1.13846600	-2.75594700	0.37492000
C	-0.36340500	-2.26364300	-1.71104900
O	-1.01737300	-3.15693300	1.49175400
O	0.38959200	-2.32493500	-2.64254800
H	-2.68805900	-1.27758000	0.38790900
H	-1.11672700	-0.41093300	-1.13058300

^{Q}7a

(U)M06/BSII SCF energy in solution: -2051.182274 a.u.
(U)M06/BSI SCF energy: -2049.020957 a.u.
(U)M06/BSI SCF Gibbs energy: -2048.405323 a.u.

C	2.16049300	2.88722700	-2.11861800
O	3.38557400	2.23077500	-1.72386400
C	1.07787800	2.28669400	-1.20098800
C	3.04840600	1.26692600	-0.86366800
N	1.80651600	1.19667200	-0.53266100
C	4.11841300	0.34537000	-0.34040300
C	2.80911300	-2.77767400	-1.65227600
O	3.74612700	-1.70223000	-1.64394400
C	2.38682700	-2.90414100	-0.18184500
C	3.61976800	-1.06841800	-0.42105900
N	2.46594300	-1.50673300	0.24194600
H	1.95912400	-2.50303500	-2.29516500

H	2.29937900	3.96520100	-1.98469900
H	1.99344300	2.66554000	-3.17787300
H	3.29904000	-3.67154300	-2.05592400
C	4.36469200	0.71951300	1.12777700
H	4.75204000	1.74589900	1.19833000
H	3.44461400	0.65035200	1.72000600
H	5.10573900	0.03146000	1.55505900
C	5.41601500	0.49054100	-1.13264000
H	5.27034500	0.26798500	-2.19428100
H	5.81421800	1.50799200	-1.04055000
H	6.15398400	-0.21602800	-0.73383100
Ni	0.93930900	-0.42727400	0.28861600
H	3.17646900	-3.47689100	0.34358900
H	0.27166300	1.84128300	-1.79617400
C	1.06170800	-3.55652300	0.09268000
C	0.95074200	-4.45939100	1.15173500
C	-0.07933700	-3.25954600	-0.65794000
C	-0.26951600	-5.04802500	1.46689400
H	1.83927000	-4.70108100	1.73676600
C	-1.30211200	-3.84523100	-0.34214600
H	-0.02039400	-2.56264000	-1.49551100
C	-1.40211300	-4.73841000	0.71936000
H	-0.33479400	-5.75375400	2.29361600
H	-2.18303000	-3.60769500	-0.93949700
H	-2.35859500	-5.20164100	0.95708600
C	0.50189400	3.24701100	-0.19461600
C	-0.86888700	3.47947100	-0.15638600
C	1.32925200	3.89048900	0.73036900
C	-1.41186700	4.35247000	0.78270900
H	-1.52860300	2.94658200	-0.84143700

C	0.79083000	4.75858100	1.67143800
H	2.40548800	3.70098400	0.71990300
C	-0.58382500	4.99331300	1.69694100
H	-2.48981800	4.50184100	0.80753400
H	1.44297200	5.25479100	2.38860000
H	-1.00541500	5.67437300	2.43456300
C	0.15799100	0.89212900	2.77859700
C	-1.18963000	1.13907500	2.54661600
C	-2.09736600	0.08300300	2.46260700
C	-1.64772300	-1.22253100	2.65761500
C	-0.30135900	-1.48024200	2.88322100
C	0.61032300	-0.42267900	2.93166500
H	0.86089900	1.72418400	2.82601800
H	-1.54006200	2.15801300	2.37929800
H	-2.35932600	-2.04766100	2.60973800
H	0.04523900	-2.50580500	3.00668500
H	1.66502500	-0.62598100	3.11308800
C	-3.50796500	0.36161100	2.01985400
H	-4.15774000	-0.49723200	2.24220200
H	-3.91106300	1.25355900	2.51570800
O	-0.88137000	-0.16930000	-0.21338200
C	-2.73756400	-0.48080300	-1.67530700
C	-3.56175600	-0.56748800	-0.38673100
C	-5.58989600	0.20364300	-1.71779700
C	-5.04488700	-0.81924400	-0.72749100
C	-3.29196200	0.51110500	-2.70014700
C	-4.75834300	0.22079700	-2.99580600
H	-6.64124200	-0.02398900	-1.94355400
H	-5.65339300	-0.83579300	0.19059700
H	-3.19001500	1.53449900	-2.31130300

H	-4.84132400	-0.76271300	-3.49122600
H	-5.12156700	-1.82843600	-1.16623200
H	-2.68205000	0.44223500	-3.60970700
H	-5.15870300	0.95996900	-3.70367500
H	-5.57180100	1.20452400	-1.25986100
C	-1.24056100	-0.28765800	-1.44786800
C	-3.48776100	0.64415800	0.51745700
O	-0.47437700	-0.29785600	-2.41288100
O	-3.45574000	1.79062600	0.11468400
H	-2.81238100	-1.47929800	-2.15052300
H	-3.18672400	-1.42278900	0.19866800

PC•BF_3KCl

(U)M06/BSII SCF energy in solution: -3865.419562 a.u.
(U)M06/BSI SCF energy: -3864.633433 a.u.
(U)M06/BSI SCF Gibbs energy: -3863.985286 a.u.

C	1.42350300	-0.35349800	0.03501900
C	0.06285700	-0.21751000	-0.28630600
C	-0.53456000	1.06070800	-0.30618200
C	0.18166000	2.20447300	0.07245100
C	1.52397200	2.05778100	0.45847700
C	2.15645200	0.79780700	0.41977400
C	-1.85046900	1.18512900	-0.84300500
C	2.21873500	3.17683500	1.01234200
N	-2.92060300	1.24634300	-1.29142400
N	2.77701900	4.08753800	1.46987200
C	-1.89213600	5.15268600	0.53720300
C	-1.57697700	3.81019000	0.81637600
C	-2.30581700	3.05496400	1.72688200
C	-3.39210100	3.66435400	2.34309700
C	-3.73203900	4.99322800	2.06584600

C	-2.98386800	5.74414800	1.17083600
C	-0.91365200	5.63486900	-0.41128700
C	-0.03066700	4.57232400	-0.67605900
C	1.00774700	4.68432900	-1.59165000
C	1.17150600	5.90826200	-2.22690200
C	0.31755800	6.98461900	-1.96227200
C	-0.72917000	6.85393500	-1.06132700
H	-2.03576800	2.02694000	1.96466500
H	-3.98477800	3.09586500	3.05715100
H	-4.58764200	5.44224600	2.56550400
H	-3.24022000	6.78297800	0.96756000
H	1.66703500	3.84573000	-1.81270100
H	1.98008900	6.02932200	-2.94489300
H	0.47459500	7.93193700	-2.47362600
H	-1.40238400	7.68785600	-0.86771600
N	-0.43490800	3.45540000	0.07575600
C	3.66473100	-3.15669700	-0.50469000
C	3.19335700	-1.86879300	-0.81739500
C	3.80404400	-1.07872000	-1.78375300
C	4.95442500	-1.57153100	-2.38696400
C	5.46457100	-2.83095300	-2.05448200
C	4.81618700	-3.63458000	-1.12698600
C	2.75732300	-3.71311400	0.47074000
C	1.77138000	-2.74168100	0.72892500
C	0.77189300	-2.94973800	1.67164800
C	0.76275100	-4.16537300	2.34502400
C	1.72690500	-5.14690200	2.09109000
C	2.72805800	-4.92516800	1.15687100
H	3.41565400	-0.09885000	-2.05727100
H	5.46612900	-0.95774600	-3.12602400

H	6.37027900	-3.18859300	-2.53996900
H	5.19927200	-4.62577900	-0.88771300
H	0.02394300	-2.19149900	1.89589100
H	-0.01407500	-4.35190500	3.08406000
H	1.69003500	-6.08933900	2.63356200
H	3.48849800	-5.68168900	0.96722500
N	2.04559100	-1.60563700	-0.05298300
C	-1.66848900	-3.07061600	-1.75222100
C	-0.57796100	-2.18069800	-1.72590400
C	0.40770600	-2.19482400	-2.70456000
C	0.29998700	-3.15093700	-3.70595300
C	-0.76617300	-4.05714900	-3.73943300
C	-1.75722000	-4.01920700	-2.76992400
C	-2.51698300	-2.74514400	-0.62806700
C	-1.90962300	-1.67046600	0.04963000
C	-2.45352900	-1.13238800	1.21317100
C	-3.65362600	-1.66788000	1.67371500
C	-4.29206900	-2.71187500	0.99191200
C	-3.72516500	-3.25879700	-0.15290000
H	1.23889900	-1.49316200	-2.69205100
H	1.06479600	-3.19310000	-4.47877600
H	-0.81952400	-4.79443300	-4.53757300
H	-2.59425700	-4.71537000	-2.80210500
H	-1.96050200	-0.31971100	1.74765000
H	-4.12382500	-1.25482800	2.56430600
H	-5.26263200	-3.06088700	1.33569700
H	-4.23012400	-4.06900000	-0.67772600
N	-0.72751400	-1.32236900	-0.62259600
C	5.76979300	0.67206900	0.52624000
C	4.57628000	1.27640500	0.09060800

C	4.56230200	2.21589700	-0.93216900
C	5.77874900	2.55667900	-1.51163700
C	6.97612300	1.97440600	-1.08391900
C	6.97803200	1.03076200	-0.06652900
C	5.41961800	-0.28666400	1.54888300
C	4.02366000	-0.23345600	1.70544800
C	3.36182900	-0.97967900	2.67012400
C	4.12000300	-1.85377600	3.43858200
C	5.50487700	-1.95359700	3.26725800
C	6.16396500	-1.16169500	2.33697300
H	3.63737300	2.67664800	-1.27554600
H	5.79586400	3.29743400	-2.30858500
H	7.91294200	2.26646900	-1.55387100
H	7.90819500	0.56807500	0.26081200
H	2.28784400	-0.89454100	2.82238400
H	3.62028000	-2.47023100	4.18358600
H	6.07280800	-2.64704400	3.88407900
H	7.24589800	-1.21869200	2.22570600
N	3.49702800	0.70866100	0.80208600
B	-7.84793300	-1.50061600	-0.09734400
F	-6.86890800	-2.42456100	-0.45123200
F	-9.06406300	-2.02928100	0.09518300
F	-7.81385500	-0.45777000	-1.02032900
K	-5.24249800	-0.22820500	-0.79293700
Cl	-7.19728600	-0.69315700	1.60089800

^{T}N1

(U)M06/BSII SCF energy in solution: -2164.482154 a.u.

(U)M06/BSI SCF energy: -2162.470472 a.u.

(U)M06/BSI SCF Gibbs energy: -2162.133449 a.u.

C	3.00616700	1.28637100	2.10139700

O	2.25101500	2.35438000	1.48152000
C	2.37886300	-0.00969400	1.55733300
C	1.24324600	1.77614700	0.81756600
N	1.20523400	0.50247400	0.82900700
C	0.35969400	2.71753700	0.04430700
C	-3.08027400	2.19074400	-1.01675700
O	-1.89059200	2.96836800	-0.74780500
C	-2.58562100	0.74182200	-1.01744200
C	-0.97299700	2.10322300	-0.29467700
N	-1.29457500	0.86866300	-0.31539000
H	-3.80285200	2.39413500	-0.21551900
H	4.05749000	1.41363000	1.82460400
H	2.89804600	1.39624300	3.18533300
H	-3.49174100	2.52667600	-1.97124800
C	1.07456500	2.95760900	-1.30805800
H	2.06800700	3.38576400	-1.12459400
H	1.17859700	2.01273400	-1.86066200
H	0.49440900	3.66573300	-1.91115900
C	0.17619500	4.03671700	0.79805500
H	-0.31135000	3.88330600	1.76866400
H	1.15103500	4.50183600	0.97416900
H	-0.43970900	4.71971600	0.20527000
Ni	-0.07318300	-0.70880000	-0.11146900
H	-2.32778900	0.41678000	-2.03851500
H	2.01030700	-0.65941900	2.36182200
C	-3.47638900	-0.28936100	-0.38685500
C	-3.69779200	-1.49320800	-1.05244500
C	-4.01652800	-0.10190300	0.88585800
C	-4.46203700	-2.49335600	-0.46187800
H	-3.24814600	-1.65212200	-2.03348000

C	-4.78387100	-1.09774600	1.47429300
H	-3.81059000	0.81727700	1.43669100
C	-5.01032000	-2.29427800	0.79916600
H	-4.62182300	-3.43337200	-0.98625900
H	-5.19545200	-0.94719600	2.47059700
H	-5.60424900	-3.07781000	1.26598100
C	3.23026100	-0.81254700	0.60959900
C	3.25085600	-2.20196200	0.70168100
C	3.92460000	-0.18082500	-0.42367000
C	3.96998700	-2.95275800	-0.22245500
H	2.67764000	-2.69629200	1.48615900
C	4.64339500	-0.92958600	-1.34468200
H	3.88172100	0.90652100	-0.52516500
C	4.66819400	-2.31803700	-1.24295300
H	3.97600500	-4.03835900	-0.14807000
H	5.17515000	-0.43110500	-2.15298000
H	5.22522100	-2.90599400	-1.97011800
Cl	0.45017200	-0.73985400	-2.31351400
Cl	-0.52017000	-2.10377400	1.57882300

N2

(U)M06/BSII SCF energy in solution: -1704.235013 a.u.
(U)M06/BSI SCF energy: -1702.269943 a.u.
(U)M06/BSI SCF Gibbs energy: -1701.933914 a.u.

C	2.75869100	1.59097100	2.08713500
O	1.96603600	2.46653500	1.26184700
C	2.42468800	0.18742100	1.57397400
C	1.05605600	1.68197100	0.64819600
N	1.17381000	0.42029000	0.81433400
C	0.08347100	2.43930100	-0.21582200
C	-2.74541400	1.20163800	-2.11052700

O	-1.93275600	2.22016100	-1.48843200
C	-2.38403900	-0.07575200	-1.33407300
C	-0.98345000	1.55638300	-0.80263000
N	-1.10002900	0.28861100	-0.72801200
H	-3.79384900	1.49935800	-2.01927400
H	3.80985800	1.87273300	1.97712500
H	2.44903400	1.74296400	3.12815500
H	-2.46120800	1.15313800	-3.16956700
C	0.88952800	3.06749600	-1.36906600
H	1.64009500	3.75804800	-0.96842000
H	1.40178300	2.28975500	-1.95119000
H	0.21838600	3.62209100	-2.03397900
C	-0.59972000	3.53536100	0.61851000
H	-1.18776700	3.09713800	1.43575600
H	0.15251800	4.20353100	1.04980300
H	-1.27430600	4.12071800	-0.01445300
Ni	0.16753600	-1.06117500	0.02492900
H	-2.22180400	-0.93198400	-2.00273200
H	2.20114100	-0.50204800	2.39784300
C	-3.41260600	-0.44304300	-0.28764800
C	-4.64816200	-0.92858400	-0.71933400
C	-3.18782500	-0.27872900	1.07651600
C	-5.64725900	-1.23594800	0.19398600
H	-4.82343900	-1.07480500	-1.78719200
C	-4.18841000	-0.58994500	1.99319600
H	-2.21627600	0.07174500	1.42445200
C	-5.41897200	-1.06427300	1.55675800
H	-6.60426800	-1.61758100	-0.15779800
H	-3.99902800	-0.46543000	3.05813100
H	-6.19829300	-1.30798800	2.27660300

C	3.42897700	-0.44525400	0.64535700
C	3.54603200	-1.83340300	0.60887200
C	4.16743500	0.32701500	-0.25295100
C	4.40117100	-2.44322400	-0.30196700
H	2.94141800	-2.44288300	1.28160200
C	5.02955200	-0.28105900	-1.15731400
H	4.06167400	1.41380000	-0.25702200
C	5.14909300	-1.66773300	-1.18085500
H	4.47504300	-3.52822900	-0.32818900
H	5.60746800	0.32932200	-1.84923600
H	5.82185100	-2.14366600	-1.89196600
Cl	-0.22275000	-3.15919800	-0.39470300

^{S}N3a

(U)M06/BSII SCF energy in solution: -1975.034733 a.u.
(U)M06/BSI SCF energy: -1972.999026 a.u.
(U)M06/BSI SCF Gibbs energy: -1972.545315 a.u.

C	3.08504100	-3.01799900	-0.13264300
O	1.86623200	-3.52864700	0.45498800
C	2.70612900	-1.63280300	-0.69799100
C	0.92183500	-2.61251200	0.20343800
N	1.25861600	-1.56302300	-0.43158200
C	-0.47763000	-2.93874900	0.64370400
C	-2.39228000	-0.43228000	2.43106400
O	-1.98607900	-1.77841000	2.11193400
C	-2.16681200	0.31483200	1.11722600
C	-1.17218500	-1.66247300	1.05539300
N	-1.12719500	-0.51511000	0.47435900
H	-3.43326000	-0.45689800	2.76338300
H	3.84325900	-2.97101900	0.65669700
H	3.40496700	-3.72981700	-0.90066700

H	-1.74317300	-0.07704100	3.24253000
C	-0.47634500	-3.96433300	1.77669900
H	0.03029800	-4.87606200	1.44544000
H	0.04056500	-3.58991700	2.66750300
H	-1.50386700	-4.21531300	2.05741400
C	-1.22849900	-3.51133400	-0.57707600
H	-1.19554500	-2.81348100	-1.42276000
H	-0.75989900	-4.45539300	-0.88230800
H	-2.27464300	-3.71270600	-0.31081400
Ni	0.05214600	-0.05279600	-1.01685400
H	-1.76192200	1.32001900	1.29302400
H	2.83642800	-1.58480400	-1.78531600
C	-3.44285800	0.40156100	0.30901100
C	-4.40045300	1.33857200	0.70466700
C	-3.72505900	-0.44508300	-0.75928800
C	-5.61991400	1.42685900	0.04612300
H	-4.18119600	2.00832900	1.53913200
C	-4.94542100	-0.35479400	-1.42236800
H	-2.96968800	-1.15107300	-1.10053000
C	-5.89560000	0.57702000	-1.02107800
H	-6.35450700	2.16518900	0.36275700
H	-5.14976600	-1.01406800	-2.26409000
H	-6.84782300	0.64757900	-1.54353400
C	3.43630900	-0.47497900	-0.06763500
C	4.16827800	0.40566700	-0.86014200
C	3.39209100	-0.27356100	1.31284800
C	4.86405900	1.46209700	-0.27959200
H	4.17256400	0.27058900	-1.94113900
C	4.07926600	0.78446200	1.89423000
H	2.80892500	-0.95133700	1.94043700

C	4.82329700	1.65070100	1.09767400
H	5.43604800	2.14232400	-0.90838300
H	4.03470900	0.93470400	2.97151000
H	5.36548400	2.47824000	1.55295100
Cl	1.15876700	0.07203900	-2.93707600
C	-0.80998300	1.63856100	-1.39840700
H	-0.57808900	1.84410700	-2.44656900
H	-1.89788700	1.59220800	-1.26655500
C	-0.16928800	2.59843000	-0.46795500
C	-0.93370200	3.38905700	0.40666500
C	1.22837800	2.74771300	-0.41653300
C	-0.33854300	4.27563700	1.29858200
H	-2.02337200	3.32836000	0.34819700
C	1.82248100	3.62947400	0.47605700
H	1.84590000	2.14843500	-1.08793500
C	1.04601300	4.39561800	1.34328100
H	-0.96202100	4.88431400	1.95345000
H	2.90913800	3.71254700	0.49670500
H	1.51643500	5.08682000	2.04112400

^{S}N4a

(U)M06/BSII SCF energy in solution: -2511.441746 a.u.
(U)M06/BSI SCF energy: -2509.260586 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.645448 a.u.

C	-2.34215400	1.42337800	2.98052500
O	-2.53745300	-0.00224500	2.96502000
C	-1.91964800	1.76850700	1.54115100
C	-2.09234300	-0.42553200	1.76325500
N	-1.74044300	0.45027900	0.91182500
C	-2.18325000	-1.91918900	1.57070000
C	-0.21897600	-4.20565700	-0.45607000

O	-1.22213500	-3.81299900	0.49460300
C	0.56797800	-2.91598900	-0.74433700
C	-1.16302700	-2.47325100	0.60783700
N	-0.24912800	-1.89381400	-0.07125400
H	0.38867700	-4.99663000	-0.00375000
H	-3.28083400	1.89453900	3.29400100
H	-1.55512500	1.64064800	3.71078600
H	-0.73306500	-4.59832900	-1.34177800
C	-3.59288300	-2.20738900	1.01724000
H	-4.33953900	-1.82340800	1.72452900
H	-3.74081300	-1.71550800	0.04635700
H	-3.74591500	-3.28627700	0.89924700
C	-1.98031700	-2.64035000	2.91335700
H	-0.98860700	-2.42069500	3.32975000
H	-2.73186700	-2.30083700	3.63213100
H	-2.08053100	-3.72156100	2.77733400
Ni	0.18162700	-0.03256000	-0.20667200
H	0.57370900	-2.69266800	-1.81960500
H	-0.94812300	2.27884600	1.53496000
C	1.98808300	-2.88575300	-0.24432900
C	3.02519500	-2.57346200	-1.11865700
C	2.27670800	-3.13374100	1.09816100
C	4.33875100	-2.51357000	-0.66167900
H	2.80114300	-2.35056600	-2.16219300
C	3.58489800	-3.07392100	1.55706100
H	1.46655600	-3.34238300	1.79904600
C	4.61978500	-2.76301100	0.67730100
H	5.14139900	-2.27434000	-1.35833500
H	3.79718600	-3.25539200	2.60892200
H	5.64621200	-2.71501100	1.03828200

C	-2.90847000	2.57649300	0.74274500
C	-2.47157600	3.66355700	-0.01080900
C	-4.25304300	2.20383700	0.68750900
C	-3.36878100	4.37773300	-0.80094100
H	-1.41561400	3.93507800	0.01935000
C	-5.15046900	2.91840900	-0.09609900
H	-4.59514400	1.32936500	1.24681600
C	-4.70861600	4.00854100	-0.84281300
H	-3.01867300	5.22560900	-1.38759200
H	-6.19763500	2.62084900	-0.13132700
H	-5.41030900	4.56743600	-1.45976200
C	-4.28398100	-0.43647400	-2.22143000
C	-3.04501500	0.15107900	-2.00156300
C	-1.85108700	-0.54220000	-2.25533500
C	-1.96407100	-1.84434700	-2.76699700
C	-3.20122600	-2.44246200	-2.97644700
C	-4.37236000	-1.74211500	-2.70112600
H	-5.19021900	0.13366700	-2.01632100
H	-2.98989100	1.17371500	-1.62790000
H	-1.05694600	-2.38964300	-3.03537000
H	-3.25180000	-3.45474500	-3.37710200
H	-5.34391100	-2.20346000	-2.87125000
C	-0.54651600	0.08520300	-1.99527800
H	0.26456800	-0.29888700	-2.63174600
H	-0.59476300	1.18303600	-2.06091400
O	1.58483600	1.56379500	-0.76946700
C	3.29379700	2.42389500	0.61121800
C	3.76847600	1.11423900	-0.02368300
C	5.74187700	2.30739400	-1.07778500
C	5.23052800	1.02774500	-0.43008200

C	3.92493500	3.66911700	-0.03979700
C	5.42937300	3.51606800	-0.20381900
H	6.82153500	2.22657500	-1.26117300
H	5.35639900	0.16586500	-1.09899800
H	3.48105000	3.82109500	-1.03988600
H	5.90171700	3.39009400	0.78503900
H	5.82329000	0.81449200	0.47286200
H	3.65504900	4.55318500	0.55183000
H	5.84956900	4.43238800	-0.63959500
H	5.26620100	2.43970100	-2.06442200
C	1.82727100	2.45884700	0.28981600
C	2.78672600	0.92531200	-1.14128700
O	0.97142300	3.19838000	0.66786800
O	2.88425100	0.35801300	-2.18570300
H	3.42963100	2.43892500	1.69900200
H	3.51114200	0.29129800	0.67027600
Cl	1.21817300	0.03383500	1.91692200

^{S}TSN1a

(U)M06/BSII SCF energy in solution: -2511.411734 a.u.
(U)M06/BSI SCF energy: -2509.229882 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.610215 a.u.

C	-2.66562100	0.92534700	2.89876600
O	-2.50648900	-0.50837700	2.87333300
C	-2.23552100	1.38659500	1.49504100
C	-1.88408100	-0.79061500	1.71755500
N	-1.71601500	0.14966000	0.87835200
C	-1.52317000	-2.24343400	1.55889500
C	0.89074900	-3.91407900	-0.57582700
O	-0.17895900	-3.79741600	0.37451400
C	1.38034100	-2.46716500	-0.78609600

C	-0.41377700	-2.49361400	0.56696500
N	0.36834200	-1.68823200	-0.05581400
H	1.65750400	-4.56742400	-0.14709400
H	-3.71116600	1.14726900	3.13963300
H	-2.01155200	1.31379500	3.68607200
H	0.48186100	-4.37332900	-1.48403100
C	-2.79776200	-2.97961300	1.10540500
H	-3.58697400	-2.80217800	1.84611800
H	-3.14534100	-2.61566000	0.12958700
H	-2.61772700	-4.05800400	1.03913600
C	-1.03777800	-2.80786100	2.90788100
H	-0.17687000	-2.23511700	3.27376500
H	-1.84111500	-2.73057000	3.64645400
H	-0.76059900	-3.86111700	2.79588500
Ni	0.25031500	0.20739200	-0.11793200
H	1.33078600	-2.18817600	-1.84877200
H	-1.40306300	2.10020700	1.56050600
C	2.78869400	-2.24313700	-0.29480600
C	3.84166700	-2.30159200	-1.20865900
C	3.06781200	-2.07747700	1.06201600
C	5.15993400	-2.21070500	-0.77363400
H	3.62493600	-2.41445600	-2.27205700
C	4.38537200	-1.96669000	1.49345300
H	2.25432200	-1.97488100	1.77973800
C	5.43317700	-2.04274000	0.58030300
H	5.97297600	-2.26044900	-1.49591500
H	4.59017200	-1.81508000	2.55172000
H	6.46334900	-1.96200900	0.92297600
C	-3.32589700	1.97379200	0.63875700
C	-3.06786700	3.10984400	-0.12624100

C	-4.57087300	1.34923500	0.54095500
C	-4.04568700	3.61347000	-0.98085200
H	-2.08910900	3.58640500	-0.04494000
C	-5.54904700	1.85526900	-0.30592200
H	-4.76474600	0.43838200	1.11353400
C	-5.28538300	2.98904100	-1.07212200
H	-3.83581900	4.49946400	-1.57789800
H	-6.51850100	1.36292100	-0.37479400
H	-6.04851000	3.38478900	-1.74038700
C	-4.09472200	-1.23969000	-2.08559100
C	-3.00564800	-0.39647100	-1.91610100
C	-1.69586600	-0.84827400	-2.13341900
C	-1.52959500	-2.17401900	-2.56471700
C	-2.61471800	-3.02442900	-2.73161900
C	-3.90548400	-2.56187500	-2.48442300
H	-5.09787300	-0.85403500	-1.90505800
H	-3.15975900	0.63680600	-1.60848600
H	-0.52592200	-2.52867500	-2.80520400
H	-2.45618100	-4.04764300	-3.07056400
H	-4.75914300	-3.22451200	-2.61690700
C	-0.55363500	0.05099700	-1.96414500
H	0.31858500	-0.21808200	-2.56478300
H	-0.80739300	1.10936500	-2.07184300
O	0.48096100	2.07990500	-0.49936700
C	2.45745400	2.89731800	0.51778700
C	2.96972000	1.52093000	0.07026400
C	4.79783200	2.65366200	-1.31711200
C	4.42313500	1.49330000	-0.40788200
C	2.93681300	4.03785400	-0.39759000
C	4.43302200	3.97897500	-0.66163700

H	5.87232400	2.61231600	-1.54361000
H	4.63177800	0.52233600	-0.87979600
H	2.40532900	3.97168400	-1.36304000
H	4.98176900	4.08302400	0.28993100
H	5.04815500	1.53208200	0.49950200
H	2.63585100	4.99075900	0.05740700
H	4.73502500	4.82484800	-1.29426100
H	4.26994900	2.56117000	-2.27969200
C	0.94615300	2.91294800	0.44000700
C	2.01772300	1.05299800	-1.00559500
O	0.24315300	3.71039700	1.01851000
O	2.18370400	0.88153300	-2.16446300
H	2.76763800	3.09164600	1.55382800
H	2.85347600	0.83263300	0.91616000
Cl	0.95898400	0.35621300	2.24181900

^{S}N5

(U)M06/BSII SCF energy in solution: -2511.423656 a.u.
(U)M06/BSI SCF energy: -2509.238127 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.62011 a.u.

C	-2.73448200	0.45947800	2.94390400
O	-2.47757300	-0.95275400	2.77794500
C	-2.34696800	1.08197000	1.59394200
C	-1.77992800	-1.06460800	1.64193400
N	-1.66308900	-0.03544500	0.90107200
C	-1.26866900	-2.45114700	1.37643000
C	1.29042500	-3.66688400	-0.87473700
O	0.24055900	-3.74620600	0.10162900
C	1.71010200	-2.18965800	-0.85505100
C	-0.12038600	-2.49435500	0.40242000
N	0.59201100	-1.56052600	-0.12072800

H	2.09121700	-4.34787200	-0.57191600
H	-3.79023100	0.58308500	3.20575000
H	-2.09779300	0.80944600	3.76309100
H	0.87205700	-3.98869000	-1.83705100
C	-2.44870900	-3.27302800	0.82505500
H	-3.27481900	-3.22767000	1.54479600
H	-2.80050900	-2.87359300	-0.13554100
H	-2.15793600	-4.32040000	0.69066700
C	-0.75793000	-3.07216100	2.69121100
H	0.01610400	-2.43699200	3.13931400
H	-1.58840800	-3.15158100	3.39917100
H	-0.35352200	-4.07218500	2.50395800
Ni	0.24121900	0.34308900	-0.02523800
H	1.74064600	-1.77146400	-1.87008200
H	-1.61213300	1.88290100	1.72836800
C	3.05834900	-1.97389300	-0.20919500
C	4.18646800	-1.91597800	-1.03000100
C	3.21567800	-1.90519300	1.17395500
C	5.45644800	-1.79543300	-0.47976000
H	4.06277000	-1.94552100	-2.11360100
C	4.48688900	-1.76525400	1.72357900
H	2.34352600	-1.89244800	1.82626000
C	5.60790900	-1.71672900	0.90236500
H	6.32762500	-1.74896200	-1.13088700
H	4.59473300	-1.68503900	2.80359800
H	6.59970800	-1.60705200	1.33773400
C	-3.50068000	1.59598300	0.77210800
C	-3.40187600	2.83175900	0.13384700
C	-4.65635800	0.82880000	0.60718400
C	-4.44672600	3.28818300	-0.66588800

H	-2.49555100	3.42458500	0.26765000
C	-5.70108400	1.28762500	-0.18631200
H	-4.73065300	-0.14984800	1.08911700
C	-5.59421000	2.51915100	-0.82897400
H	-4.36260900	4.25404900	-1.16148700
H	-6.59979700	0.68389000	-0.30663300
H	-6.41008200	2.87965600	-1.45356900
C	-3.82331700	-1.55119300	-2.27943700
C	-2.90062100	-0.55999600	-1.97578900
C	-1.52974700	-0.75459500	-2.20598200
C	-1.12570700	-1.97282100	-2.77713200
C	-2.04385400	-2.97081100	-3.07179400
C	-3.39911900	-2.76440000	-2.81895300
H	-4.88277700	-1.37377700	-2.09863500
H	-3.23294200	0.39029200	-1.56010400
H	-0.07146300	-2.11744600	-3.01962200
H	-1.70672700	-3.90622200	-3.51699700
H	-4.12348300	-3.54219900	-3.05469900
C	-0.57257600	0.30824700	-1.92793300
H	0.34079900	0.26416000	-2.52254900
H	-1.00976100	1.30641400	-1.86733600
O	-0.17497600	2.15278900	-0.04151700
C	1.99068900	3.20418100	0.29532900
C	2.71424200	1.85330200	0.19289200
C	4.40373100	2.90337800	-1.42256700
C	4.18549300	2.00761700	-0.21067600
C	2.23479400	4.07141900	-0.94888900
C	3.71923800	4.25062900	-1.23252600
H	5.48159000	3.03734100	-1.59174300
H	4.62823300	1.01218300	-0.36349200

H	1.74520900	3.59780700	-1.81898600
H	4.18511300	4.78301600	-0.38567500
H	4.69780100	2.44783700	0.66082800
H	1.73803400	5.03838000	-0.79513000
H	3.86226800	4.88555100	-2.11787700
H	4.00395000	2.41063900	-2.32149800
C	0.48307400	3.14506200	0.49638100
C	1.98009400	0.93826400	-0.76040300
O	-0.09637400	4.09372100	1.00041100
O	2.34467800	0.58394100	-1.83684600
H	2.40721900	3.72885700	1.16873100
H	2.64563700	1.36868700	1.17512300
Cl	0.91445900	0.32836000	2.38111900

^{S}TSN2

(U)M06/BSII SCF energy in solution: -2511.388927 a.u.
(U)M06/BSI SCF energy: -2509.202441a.u.
(U)M06/BSI SCF Gibbs energy: -2508.583808 a.u.

C	2.70184000	-1.48907000	-2.69208100
O	1.94682800	-2.60277400	-2.17312600
C	2.61579600	-0.41644600	-1.58863700
C	1.36342300	-2.14914600	-1.05173300
N	1.65104900	-0.98899900	-0.62499500
C	0.49701700	-3.15236200	-0.35612100
C	-2.13285200	-2.74077300	2.07455000
O	-1.17667900	-3.43956400	1.26498100
C	-2.36843000	-1.44865900	1.29506500
C	-0.59988200	-2.53097000	0.46942700
N	-1.12634700	-1.35276300	0.48840700
H	-3.02622800	-3.36337800	2.17145000
H	3.72182400	-1.83447000	-2.89372100

H	2.22457100	-1.17633500	-3.62704300
H	-1.67869400	-2.58104700	3.06258000
C	1.43873900	-3.95547800	0.56069000
H	2.26247100	-4.35317400	-0.04524000
H	1.86068100	-3.30333400	1.33806800
H	0.91346000	-4.79227300	1.03246000
C	-0.18764000	-4.07869200	-1.37689100
H	-0.75134600	-3.49429200	-2.11460000
H	0.57507300	-4.65295200	-1.91227400
H	-0.86174700	-4.77664100	-0.86904900
Ni	-0.36691100	0.29653000	-0.23959500
H	-2.43769300	-0.58649800	1.96512000
H	2.17703100	0.50927300	-1.97493200
C	-3.62420900	-1.52335500	0.45869800
C	-4.83349500	-1.18977700	1.07171400
C	-3.63293700	-2.01098300	-0.84415600
C	-6.03532600	-1.34695800	0.39611800
H	-4.82613900	-0.78710000	2.08608600
C	-4.83835800	-2.16111500	-1.52512200
H	-2.69417800	-2.22633600	-1.35088600
C	-6.03973400	-1.83661600	-0.90762600
H	-6.97064900	-1.07682400	0.88345400
H	-4.83143600	-2.52752400	-2.55000200
H	-6.98032000	-1.95455000	-1.44297800
C	3.93187200	-0.09347800	-0.93080400
C	4.36369400	1.22930300	-0.85084200
C	4.73272800	-1.10795300	-0.40236500
C	5.59055000	1.53021300	-0.26393800
H	3.71193000	2.02748500	-1.21401900
C	5.95543900	-0.80884800	0.18588800

H	4.38923600	-2.14486100	-0.44332200
C	6.39016300	0.51365500	0.24989200
H	5.92022200	2.56640800	-0.20674400
H	6.57412400	-1.60746500	0.59307300
H	7.35142300	0.74958100	0.70420400
C	3.16385700	0.47019600	2.23312700
C	2.05872900	1.17909400	1.78306800
C	0.76705300	0.73493500	2.08115900
C	0.61868400	-0.40302300	2.88248400
C	1.72322900	-1.12178800	3.31909600
C	3.00395100	-0.69184600	2.98157400
H	4.16277100	0.81714400	1.97077000
H	2.19975300	2.06929500	1.16982500
H	-0.38459000	-0.71441800	3.17744500
H	1.58351800	-2.00787600	3.93839800
H	3.87813200	-1.25100500	3.31235700
C	-0.45739100	1.49908100	1.66073700
H	-1.23164000	1.34397400	2.41659200
H	-0.21470400	2.56389200	1.59020500
O	0.72706500	1.62024600	-0.87249100
C	-0.59570300	3.65470800	-0.81548700
C	-1.82298500	2.75579200	-0.71888000
C	-3.05505500	4.65179500	0.43059300
C	-3.10843000	3.59104200	-0.66071100
C	-0.56261300	4.80428200	0.19968100
C	-1.86962900	5.58390400	0.21152400
H	-3.99650600	5.21754800	0.45182800
H	-3.97245100	2.92916500	-0.53844300
H	-0.36807400	4.42311000	1.21626800
H	-1.99509200	6.10159900	-0.75461000

H	-3.21782400	4.08741100	-1.63834400
H	0.29366300	5.44340100	-0.04688400
H	-1.83616200	6.36522600	0.98318400
H	-2.96499900	4.16313500	1.41704700
C	0.72962700	2.91696600	-0.86384000
C	-1.85392300	1.67715300	0.36671200
O	1.77726000	3.54936100	-0.92578300
O	-2.88543400	1.27565900	0.82277700
H	-0.66987700	4.13517700	-1.80770300
H	-1.85258700	2.13704400	-1.63269900
Cl	-0.98326300	-0.28118500	-2.35637500

^{S}N6

(U)M06/BSII SCF energy in solution: -2511.477288 a.u.
(U)M06/BSI SCF energy: -2509.283842a.u.
(U)M06/BSI SCF Gibbs energy: -2508.665486a.u.

C	4.16878300	0.33719500	-2.18385400
O	4.14132700	-1.04357700	-1.74075100
C	2.93667300	0.98034400	-1.53196100
C	2.94473600	-1.23083600	-1.18286900
N	2.18947500	-0.20611500	-1.04238200
C	2.61480800	-2.65786700	-0.83018200
C	0.34890100	-3.32677000	1.95472600
O	1.55063900	-3.51090000	1.16966200
C	-0.47383700	-2.26460500	1.19834500
C	1.47368400	-2.66279700	0.14871800
N	0.41568700	-1.95113600	0.05113000
H	-0.15709400	-4.29550300	2.02036800
H	5.11751500	0.77311900	-1.85752600
H	4.12545300	0.32672800	-3.27839600
H	0.65401600	-2.99942500	2.95391900

C	3.84910100	-3.35792800	-0.26112900
H	4.65297100	-3.34621900	-1.00321800
H	4.21010800	-2.86611100	0.65043100
H	3.60885600	-4.39730400	-0.01558400
C	2.13201600	-3.37436500	-2.10911100
H	1.23330100	-2.89593700	-2.51925500
H	2.92743700	-3.36284900	-2.86382700
H	1.89454600	-4.41943200	-1.87129100
Ni	0.21512900	-0.43785800	-1.10512700
H	-0.55871600	-1.34732100	1.79758000
H	2.29106300	1.48568500	-2.25731300
C	-1.84420900	-2.73499500	0.80271700
C	-2.96628900	-2.02822000	1.22113900
C	-2.00379300	-3.88220100	0.02583200
C	-4.23952800	-2.45327000	0.85456100
H	-2.83951600	-1.12555700	1.82284400
C	-3.27087900	-4.30884200	-0.34022400
H	-1.12279300	-4.42319300	-0.32887600
C	-4.39206200	-3.59095100	0.07212700
H	-5.11187900	-1.88541500	1.17402200
H	-3.38768600	-5.19495500	-0.96122800
H	-5.38676600	-3.92074700	-0.22225700
C	3.24363100	1.92072000	-0.39677500
C	2.59772800	3.15413500	-0.32460100
C	4.14441100	1.55282500	0.60689300
C	2.85283300	4.00744700	0.74681700
H	1.86514400	3.42678300	-1.08970200
C	4.39534100	2.40510100	1.67445000
H	4.64906100	0.58444800	0.55751900
C	3.74660800	3.63639900	1.74529200

H	2.34016400	4.96648900	0.80092900
H	5.09545000	2.10979300	2.45422300
H	3.93963700	4.30519400	2.58217000
C	1.30873400	-0.04853400	3.15247600
C	0.94648100	0.92262700	2.22458600
C	-0.30495200	1.53986200	2.28438200
C	-1.20284800	1.13726400	3.27785200
C	-0.84828800	0.15464700	4.19841100
C	0.41353800	-0.43429500	4.14736300
H	2.30148600	-0.49946400	3.09484700
H	1.65078300	1.22578700	1.45110400
H	-2.18223400	1.61390400	3.34039100
H	-1.55709200	-0.14120500	4.97036100
H	0.69828600	-1.18374600	4.88563800
C	-0.64191700	2.65237000	1.32145300
H	-0.49185000	3.62566700	1.81008100
H	0.03507900	2.60811600	0.45892200
O	0.16759300	1.23179400	-1.87021600
C	-2.14173100	1.97704300	-1.59913300
C	-2.47932400	1.55469300	-0.14383800
C	-4.90212800	2.24739100	-0.61043600
C	-3.96003700	1.17304000	-0.06953600
C	-3.02663300	3.13800800	-2.03696900
C	-4.49019000	2.71350600	-2.00194800
H	-5.92911900	1.85401900	-0.63041300
H	-4.22433800	0.93298000	0.97319700
H	-2.85950800	4.00940400	-1.38520300
H	-4.63696200	1.89248000	-2.72495900
H	-4.07850600	0.24508900	-0.65364500
H	-2.73398500	3.45496900	-3.04672800

H	-5.13754600	3.53882700	-2.33113700
H	-4.89964800	3.10378400	0.07639000
C	-0.66520500	2.24162900	-1.83252200
C	-2.09545700	2.60238800	0.88486000
O	-0.24955500	3.38462900	-1.99224400
O	-2.90579600	3.33526200	1.41922400
H	-2.39409000	1.09436600	-2.20548400
H	-1.87373400	0.65662000	0.08242900
Cl	-1.56664000	-1.26468800	-2.07305200

^{S}TSN1b

(U)M06/BSII SCF energy in solution: -2511.378444 a.u.
(U)M06/BSI SCF energy: -2509.189573a.u.
(U)M06/BSI SCF Gibbs energy: -2508.576911a.u.

C	-3.12355800	0.68719500	-2.26873400
O	-2.76441200	2.06813800	-2.05205900
C	-2.81455300	0.00622400	-0.92503100
C	-2.00379800	2.05612500	-0.94457200
N	-1.93878400	0.98999200	-0.24966600
C	-1.40373200	3.38423400	-0.55932800
C	1.76656400	3.99802800	1.08790800
O	0.39198600	4.27502400	0.74506700
C	1.84948100	2.47904900	1.01145200
C	-0.05212100	3.20457600	0.07478800
N	0.74327800	2.19607600	0.06845200
H	2.40924900	4.47572000	0.33459700
H	-4.17701400	0.65019000	-2.56345600
H	-2.48751000	0.31225200	-3.08002400
H	1.96488100	4.42189300	2.07474300
C	-2.36337100	4.00308000	0.47572400
H	-3.35546500	4.09830700	0.01632000

H	-2.45424700	3.36379800	1.36200000
H	-2.02429900	4.99937600	0.77865400
C	-1.25110000	4.33455000	-1.75468200
H	-0.60526700	3.89528500	-2.52204300
H	-2.23448400	4.52925400	-2.19507900
H	-0.82418300	5.28537500	-1.41487400
Ni	0.64176900	0.49328300	-0.71418000
H	1.55825600	2.02414800	1.97478800
H	-2.24770800	-0.92239700	-1.07445500
C	3.18185700	1.92491700	0.59887600
C	4.03485600	1.41798400	1.58053900
C	3.58189400	1.90985300	-0.73843200
C	5.28030600	0.90843200	1.23242000
H	3.71099600	1.41034900	2.62298000
C	4.82136700	1.38436300	-1.08479200
H	2.90307900	2.26097400	-1.51666400
C	5.67298400	0.88992200	-0.10287900
H	5.94106400	0.51543700	2.00334200
H	5.11069600	1.34572800	-2.13242000
H	6.64102600	0.47640500	-0.37995300
C	-4.01726400	-0.27678200	-0.05850600
C	-4.14189300	-1.49958400	0.59792300
C	-5.00274900	0.69640100	0.12468800
C	-5.24023600	-1.75008600	1.41617000
H	-3.36533500	-2.25188700	0.46413400
C	-6.09950000	0.44693400	0.93931600
H	-4.91099000	1.65969300	-0.38130600
C	-6.22134000	-0.78007900	1.58677000
H	-5.32983300	-2.71148700	1.91988300
H	-6.86391700	1.21157600	1.07020100

H	-7.08227900	-0.97836900	2.22324400
C	-0.49263600	-1.09843200	4.57896000
C	-0.49122800	-0.93592100	3.20080600
C	0.71063900	-0.98579300	2.47933700
C	1.90731500	-1.19758400	3.17768100
C	1.90225500	-1.35787500	4.55767800
C	0.70299300	-1.30889200	5.26324500
H	-1.43338900	-1.05907200	5.12589500
H	-1.42468600	-0.77449800	2.65760500
H	2.84598200	-1.23194400	2.62002300
H	2.84034700	-1.52152600	5.08636500
H	0.69947300	-1.43268800	6.34477500
C	0.69025700	-0.87840900	1.01869700
H	1.68798000	-0.68170800	0.58732100
H	-0.20294500	-0.29129600	0.70489500
O	0.53578300	-1.28437700	-1.53121700
C	1.65514700	-3.28668200	-1.76194000
C	1.22356600	-3.46364500	-0.29446100
C	-0.09277600	-5.54613800	-0.96627800
C	0.83446100	-4.90072900	0.05649300
C	0.69022700	-3.96136800	-2.73742400
C	0.47777900	-5.42482800	-2.37365800
H	-0.25057300	-6.60114200	-0.70191100
H	0.38826400	-4.92673600	1.06048800
H	-0.27658200	-3.43615400	-2.71817900
H	1.44025700	-5.96241600	-2.43091900
H	1.76812700	-5.48440100	0.11203700
H	1.08420000	-3.85926700	-3.75814400
H	-0.19119200	-5.90217700	-3.10273800
H	-1.07580800	-5.05571200	-0.92682500

C	1.70583700	-1.77662800	-1.92062500
C	0.09120100	-2.47649000	-0.03422400
O	2.69343700	-1.13905200	-2.21098100
O	-1.08342800	-2.69940600	-0.01401600
H	2.66874600	-3.68976600	-1.89986600
H	2.06255600	-3.15318300	0.34843500
Cl	0.55822300	1.42114900	-2.71330200

N3

(U)M06/BSII SCF energy in solution: -2240.662196 a.u.
(U)M06/BSI SCF energy: -2238.547797a.u.
(U)M06/BSI SCF Gibbs energy: -2238.045763a.u.

C	-4.01935600	0.73687400	1.76829800
O	-4.21881100	-0.54426900	1.12339500
C	-2.74005100	1.27785300	1.11985500
C	-3.02451600	-0.86065600	0.58589800
N	-2.11555500	0.03643000	0.61178200
C	-2.94284800	-2.25659600	0.02260900
C	-0.27684500	-3.71781000	-1.95837900
O	-1.65864300	-3.49485600	-1.60286900
C	0.45235900	-2.46223400	-1.45677600
C	-1.64749200	-2.48716900	-0.71191000
N	-0.53332100	-1.89287300	-0.52346400
H	0.06148300	-4.62507100	-1.43797100
H	-4.90688500	1.34809100	1.58354500
H	-3.90653900	0.55168400	2.84360000
H	-0.22428100	-3.87347900	-3.03874400
C	-4.13347700	-2.47500200	-0.92124400
H	-5.07132900	-2.34860000	-0.37123900
H	-4.11753300	-1.75739200	-1.75173500
H	-4.10021000	-3.48604000	-1.33916200

C	-2.99414900	-3.26544700	1.18620800
H	-2.15012200	-3.10882300	1.87100400
H	-3.92935100	-3.14204100	1.74419700
H	-2.95084300	-4.28910100	0.79440700
Ni	-0.22845300	-0.59859500	0.91538900
H	0.59559300	-1.72406000	-2.26047200
H	-2.05584300	1.73039200	1.85033800
C	1.77773600	-2.72048100	-0.79660900
C	2.96285100	-2.43424700	-1.47111800
C	1.83712000	-3.23284900	0.50044500
C	4.19227600	-2.66332100	-0.86106300
H	2.91742600	-2.00445500	-2.47224200
C	3.06396200	-3.44166500	1.11865900
H	0.91383500	-3.43299000	1.04667500
C	4.24429600	-3.15988600	0.43741600
H	5.11263100	-2.43381400	-1.39668600
H	3.09562100	-3.81043100	2.14181800
H	5.20584500	-3.32096600	0.92189000
C	-2.98872500	2.23549300	-0.02171000
C	-2.22476500	3.39248600	-0.14679000
C	-3.97841300	1.96465000	-0.97094100
C	-2.45392000	4.27254900	-1.20040100
H	-1.43290500	3.58766100	0.57597200
C	-4.20619500	2.84284900	-2.02224100
H	-4.58125700	1.05792800	-0.88689000
C	-3.44434700	4.00280500	-2.13719400
H	-1.85135500	5.17520600	-1.28680500
H	-4.98226000	2.62382300	-2.75405300
H	-3.62372300	4.69405100	-2.95910700
O	0.78791000	1.89017300	-0.28137900

C	2.77610200	2.33405300	0.89187800
C	2.97508800	1.08032700	0.03989400
C	4.81467600	2.23500400	-1.27526300
C	4.30675600	0.92836800	-0.68203300
C	3.41122000	3.59397200	0.27231400
C	4.82623200	3.33338900	-0.21912600
H	5.81729300	2.08771400	-1.69922200
H	4.19834500	0.15291800	-1.45278100
H	2.80373600	3.92003600	-0.59046600
H	5.46661100	3.02767300	0.62536000
H	5.04561500	0.54898900	0.04092800
H	3.36520000	4.40950900	1.00530400
H	5.25606200	4.26018600	-0.62282600
H	4.16407900	2.54303900	-2.11195600
C	1.28744700	2.54189500	0.84184900
C	1.76335000	1.10193500	-0.85838500
O	0.59158200	3.24865100	1.50773200
O	1.57802400	0.53724200	-1.89947800
H	3.10067800	2.20160700	1.93001800
H	2.80513900	0.20387300	0.69117700
Cl	0.97407800	-0.01704300	2.66429100

TSN1

(U)M06/BSII SCF energy in solution: -2240.629714 a.u.
(U)M06/BSI SCF energy: -2238.512623a.u.
(U)M06/BSI SCF Gibbs energy: -2238.011382a.u.

C	-3.70009400	-0.54876500	1.85639600
O	-3.22598900	-1.88607100	1.57806100
C	-2.97778000	0.34323500	0.82755500
C	-2.25452400	-1.75676500	0.66733900
N	-2.04498800	-0.59946600	0.17427800

C	-1.55024400	-3.04641600	0.34006200
C	1.41408000	-3.67258600	-1.65266700
O	0.12176300	-3.96782500	-1.09017200
C	1.58922900	-2.15385200	-1.44878200
C	-0.30851200	-2.85046500	-0.49096800
N	0.42618000	-1.80999500	-0.61930100
H	2.16187100	-4.25406300	-1.09928600
H	-4.79000900	-0.54874400	1.74983800
H	-3.42593200	-0.31423800	2.89009200
H	1.40856900	-3.98762000	-2.70016000
C	-2.54649100	-3.95498300	-0.39752600
H	-3.43846100	-4.09286800	0.22284100
H	-2.85282100	-3.51444500	-1.35516600
H	-2.09856400	-4.93478000	-0.59125700
C	-1.08272600	-3.71197900	1.65096100
H	-0.43130700	-3.02991700	2.21389100
H	-1.95215100	-3.95771100	2.26951200
H	-0.53977700	-4.63642900	1.42135100
Ni	-0.04815000	0.01697600	0.03579100
H	1.49657800	-1.60546800	-2.39836900
H	-2.37447800	1.10890100	1.33489100
C	2.90828200	-1.79971200	-0.81453800
C	3.99954300	-1.52261900	-1.63811000
C	3.07711800	-1.80888600	0.57001600
C	5.25221400	-1.27331200	-1.08903200
H	3.86130200	-1.49234100	-2.71998800
C	4.32727700	-1.53729800	1.11878200
H	2.22184600	-1.97978000	1.22510900
C	5.41753300	-1.27993300	0.29350400
H	6.09745100	-1.05953200	-1.74095300

H	4.44363000	-1.52562600	2.20109800
H	6.39466900	-1.07464500	0.72748000
C	-3.87035900	1.01228800	-0.18305900
C	-3.79182200	2.38990800	-0.37590900
C	-4.77337800	0.26236500	-0.93887800
C	-4.61872700	3.01040800	-1.30789900
H	-3.06620400	2.96621600	0.20118400
C	-5.59582100	0.88167800	-1.87100000
H	-4.82916000	-0.82031300	-0.79986900
C	-5.52071700	2.26034500	-2.05429000
H	-4.55362800	4.08750500	-1.45270200
H	-6.29638600	0.28911100	-2.45749100
H	-6.16601900	2.74804500	-2.78326200
O	-0.30462700	1.96475200	-0.14331200
C	1.44453400	3.09709600	0.96796200
C	2.23336700	1.84676100	0.54162900
C	3.84339800	3.31412500	-0.79532100
C	3.67962800	2.10133400	0.10842300
C	1.72059300	4.30664400	0.05974000
C	3.20670100	4.54250300	-0.15924600
H	4.91096400	3.48387400	-0.99261900
H	4.08701800	1.19319000	-0.35939600
H	1.24179400	4.13226900	-0.91912500
H	3.69721600	4.75374100	0.80632600
H	4.26126200	2.25935800	1.03128800
H	1.22528300	5.18343100	0.49779500
H	3.35647600	5.42980200	-0.78937900
H	3.37060000	3.12003500	-1.77151900
C	-0.04265900	2.81249200	0.84386400
C	1.42149000	1.18639600	-0.54260800

O	-0.89689600	3.40102900	1.47067200
O	1.57839300	0.99069200	-1.70711000
H	1.68620000	3.35268200	2.00892200
H	2.22161100	1.14174000	1.38489800
Cl	0.33896900	-0.27947800	2.32197100

N4

(U)M06/BSII SCF energy in solution: -2240.637249 a.u.
(U)M06/BSI SCF energy: -2238.516282a.u.
(U)M06/BSI SCF Gibbs energy: -2238.011746a.u.

C	-3.61149600	-0.85058100	1.88534300
O	-3.04866400	-2.13473700	1.52829300
C	-2.97087600	0.14425000	0.90031900
C	-2.08646000	-1.88347000	0.63506800
N	-1.95855100	-0.68719200	0.21299500
C	-1.29792400	-3.09737500	0.23083400
C	1.60769000	-3.39596600	-1.92237900
O	0.45378600	-3.84183500	-1.18753100
C	1.76033400	-1.91130800	-1.53626700
C	-0.08231400	-2.76869600	-0.59629100
N	0.54010500	-1.65779000	-0.74990100
H	2.46221600	-4.00869000	-1.61758500
H	-4.69994000	-0.92371100	1.79230200
H	-3.33799300	-0.65523700	2.92748100
H	1.40524100	-3.55337000	-2.98761400
C	-2.23676700	-4.01770200	-0.56838000
H	-3.11798400	-4.25205900	0.03833500
H	-2.57128200	-3.53397700	-1.49539500
H	-1.72856000	-4.95253100	-0.82482500
C	-0.79130500	-3.81743200	1.49694700
H	-0.18899800	-3.13325400	2.10860300

H	-1.64642300	-4.15484800	2.09171200
H	-0.18978700	-4.68934300	1.21547500
Ni	-0.04684300	0.11518000	-0.01452800
H	1.73554400	-1.26569800	-2.42425200
H	-2.43399400	0.93964800	1.43261800
C	3.02651300	-1.62806100	-0.76602900
C	4.15962600	-1.19794200	-1.45856400
C	3.10573800	-1.84486100	0.60868200
C	5.36237400	-1.00027100	-0.78976900
H	4.09195000	-1.00498300	-2.53037600
C	4.30407100	-1.62534900	1.28128300
H	2.21765400	-2.13097400	1.17129400
C	5.43501400	-1.21248900	0.58460700
H	6.24043200	-0.66725200	-1.34048400
H	4.34671000	-1.77319200	2.35871200
H	6.37218900	-1.04547300	1.11276200
C	-3.92321600	0.76938200	-0.08483700
C	-3.97454700	2.15579000	-0.21719300
C	-4.75854300	-0.02696300	-0.87045800
C	-4.86306000	2.73556500	-1.11759600
H	-3.29853800	2.77277200	0.37702600
C	-5.64180200	0.55253400	-1.77247500
H	-4.71536500	-1.11536100	-0.77841000
C	-5.69679300	1.93863800	-1.89459600
H	-4.89966600	3.81935200	-1.21471000
H	-6.28863700	-0.07703900	-2.38189500
H	-6.38993900	2.39536400	-2.59943700
O	-0.72500400	1.88599700	0.07741100
C	1.16841200	3.18229400	0.83785100
C	2.10112300	1.97813200	0.58101900

C	3.63832100	3.47738400	-0.80847400
C	3.54121800	2.38249500	0.24417500
C	1.33978100	4.27941100	-0.22250100
C	2.79528300	4.68115100	-0.41025100
H	4.69051800	3.76479300	-0.94283300
H	4.11290100	1.48974400	-0.05063400
H	0.93068200	3.92160200	-1.18294500
H	3.18252200	5.10408600	0.53256500
H	3.98922300	2.74250400	1.18485700
H	0.72142100	5.13538500	0.07873300
H	2.87371800	5.47517700	-1.16559900
H	3.29108100	3.08964600	-1.77901400
C	-0.32273800	2.84353000	0.86965100
C	1.48264100	1.16322500	-0.51499300
O	-1.08808600	3.55404600	1.49901200
O	1.67986800	1.11328500	-1.68647500
H	1.43756000	3.59773700	1.82049200
H	2.08579100	1.33989000	1.47445300
Cl	0.40961800	-0.35922500	2.25233500

^{S}N5

(U)M06/BSII SCF energy in solution: -2511.423656 a.u.
(U)M06/BSI SCF energy: -2509.238127 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.62011 a.u.

C	-2.73448200	0.45947800	2.94390400
O	-2.47757300	-0.95275400	2.77794500
C	-2.34696800	1.08197000	1.59394200
C	-1.77992800	-1.06460800	1.64193400
N	-1.66308900	-0.03544500	0.90107200
C	-1.26866900	-2.45114700	1.37643000
C	1.29042500	-3.66688400	-0.87473700

O	0.24055900	-3.74620600	0.10162900
C	1.71010200	-2.18965800	-0.85505100
C	-0.12038600	-2.49435500	0.40242000
N	0.59201100	-1.56052600	-0.12072800
H	2.09121700	-4.34787200	-0.57191600
H	-3.79023100	0.58308500	3.20575000
H	-2.09779300	0.80944600	3.76309100
H	0.87205700	-3.98869000	-1.83705100
C	-2.44870900	-3.27302800	0.82505500
H	-3.27481900	-3.22767000	1.54479600
H	-2.80050900	-2.87359300	-0.13554100
H	-2.15793600	-4.32040000	0.69066700
C	-0.75793000	-3.07216100	2.69121100
H	0.01610400	-2.43699200	3.13931400
H	-1.58840800	-3.15158100	3.39917100
H	-0.35352200	-4.07218500	2.50395800
Ni	0.24121900	0.34308900	-0.02523800
H	1.74064600	-1.77146400	-1.87008200
H	-1.61213300	1.88290100	1.72836800
C	3.05834900	-1.97389300	-0.20919500
C	4.18646800	-1.91597800	-1.03000100
C	3.21567800	-1.90519300	1.17395500
C	5.45644800	-1.79543300	-0.47976000
H	4.06277000	-1.94552100	-2.11360100
C	4.48688900	-1.76525400	1.72357900
H	2.34352600	-1.89244800	1.82626000
C	5.60790900	-1.71672900	0.90236500
H	6.32762500	-1.74896200	-1.13088700
H	4.59473300	-1.68503900	2.80359800
H	6.59970800	-1.60705200	1.33773400

C	-3.50068000	1.59598300	0.77210800
C	-3.40187600	2.83175900	0.13384700
C	-4.65635800	0.82880000	0.60718400
C	-4.44672600	3.28818300	-0.66588800
H	-2.49555100	3.42458500	0.26765000
C	-5.70108400	1.28762500	-0.18631200
H	-4.73065300	-0.14984800	1.08911700
C	-5.59421000	2.51915100	-0.82897400
H	-4.36260900	4.25404900	-1.16148700
H	-6.59979700	0.68389000	-0.30663300
H	-6.41008200	2.87965600	-1.45356900
C	-3.82331700	-1.55119300	-2.27943700
C	-2.90062100	-0.55999600	-1.97578900
C	-1.52974700	-0.75459500	-2.20598200
C	-1.12570700	-1.97282100	-2.77713200
C	-2.04385400	-2.97081100	-3.07179400
C	-3.39911900	-2.76440000	-2.81895300
H	-4.88277700	-1.37377700	-2.09863500
H	-3.23294200	0.39029200	-1.56010400
H	-0.07146300	-2.11744600	-3.01962200
H	-1.70672700	-3.90622200	-3.51699700
H	-4.12348300	-3.54219900	-3.05469900
C	-0.57257600	0.30824700	-1.92793300
H	0.34079900	0.26416000	-2.52254900
H	-1.00976100	1.30641400	-1.86733600
O	-0.17497600	2.15278900	-0.04151700
C	1.99068900	3.20418100	0.29532900
C	2.71424200	1.85330200	0.19289200
C	4.40373100	2.90337800	-1.42256700
C	4.18549300	2.00761700	-0.21067600

C	2.23479400	4.07141900	-0.94888900
C	3.71923800	4.25062900	-1.23252600
H	5.48159000	3.03734100	-1.59174300
H	4.62823300	1.01218300	-0.36349200
H	1.74520900	3.59780700	-1.81898600
H	4.18511300	4.78301600	-0.38567500
H	4.69780100	2.44783700	0.66082800
H	1.73803400	5.03838000	-0.79513000
H	3.86226800	4.88555100	-2.11787700
H	4.00395000	2.41063900	-2.32149800
C	0.48307400	3.14506200	0.49638100
C	1.98009400	0.93826400	-0.76040300
O	-0.09637400	4.09372100	1.00041100
O	2.34467800	0.58394100	-1.83684600
H	2.40721900	3.72885700	1.16873100
H	2.64563700	1.36868700	1.17512300
Cl	0.91445900	0.32836000	2.38111900

^{S}TSN2

(U)M06/BSII SCF energy in solution: -2511.388927 a.u.
(U)M06/BSI SCF energy: -2509.202441 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.583808 a.u.

C	2.70184000	-1.48907000	-2.69208100
O	1.94682800	-2.60277400	-2.17312600
C	2.61579600	-0.41644600	-1.58863700
C	1.36342300	-2.14914600	-1.05173300
N	1.65104900	-0.98899900	-0.62499500
C	0.49701700	-3.15236200	-0.35612100
C	-2.13285200	-2.74077300	2.07455000
O	-1.17667900	-3.43956400	1.26498100
C	-2.36843000	-1.44865900	1.29506500

C	-0.59988200	-2.53097000	0.46942700
N	-1.12634700	-1.35276300	0.48840700
H	-3.02622800	-3.36337800	2.17145000
H	3.72182400	-1.83447000	-2.89372100
H	2.22457100	-1.17633500	-3.62704300
H	-1.67869400	-2.58104700	3.06258000
C	1.43873900	-3.95547800	0.56069000
H	2.26247100	-4.35317400	-0.04524000
H	1.86068100	-3.30333400	1.33806800
H	0.91346000	-4.79227300	1.03246000
C	-0.18764000	-4.07869200	-1.37689100
H	-0.75134600	-3.49429200	-2.11460000
H	0.57507300	-4.65295200	-1.91227400
H	-0.86174700	-4.77664100	-0.86904900
Ni	-0.36691100	0.29653000	-0.23959500
H	-2.43769300	-0.58649800	1.96512000
H	2.17703100	0.50927300	-1.97493200
C	-3.62420900	-1.52335500	0.45869800
C	-4.83349500	-1.18977700	1.07171400
C	-3.63293700	-2.01098300	-0.84415600
C	-6.03532600	-1.34695800	0.39611800
H	-4.82613900	-0.78710000	2.08608600
C	-4.83835800	-2.16111500	-1.52512200
H	-2.69417800	-2.22633600	-1.35088600
C	-6.03973400	-1.83661600	-0.90762600
H	-6.97064900	-1.07682400	0.88345400
H	-4.83143600	-2.52752400	-2.55000200
H	-6.98032000	-1.95455000	-1.44297800
C	3.93187200	-0.09347800	-0.93080400
C	4.36369400	1.22930300	-0.85084200

C	4.73272800	-1.10795300	-0.40236500
C	5.59055000	1.53021300	-0.26393800
H	3.71193000	2.02748500	-1.21401900
C	5.95543900	-0.80884800	0.18588800
H	4.38923600	-2.14486100	-0.44332200
C	6.39016300	0.51365500	0.24989200
H	5.92022200	2.56640800	-0.20674400
H	6.57412400	-1.60746500	0.59307300
H	7.35142300	0.74958100	0.70420400
C	3.16385700	0.47019600	2.23312700
C	2.05872900	1.17909400	1.78306800
C	0.76705300	0.73493500	2.08115900
C	0.61868400	-0.40302300	2.88248400
C	1.72322900	-1.12178800	3.31909600
C	3.00395100	-0.69184600	2.98157400
H	4.16277100	0.81714400	1.97077000
H	2.19975300	2.06929500	1.16982500
H	-0.38459000	-0.71441800	3.17744500
H	1.58351800	-2.00787600	3.93839800
H	3.87813200	-1.25100500	3.31235700
C	-0.45739100	1.49908100	1.66073700
H	-1.23164000	1.34397400	2.41659200
H	-0.21470400	2.56389200	1.59020500
O	0.72706500	1.62024600	-0.87249100
C	-0.59570300	3.65470800	-0.81548700
C	-1.82298500	2.75579200	-0.71888000
C	-3.05505500	4.65179500	0.43059300
C	-3.10843000	3.59104200	-0.66071100
C	-0.56261300	4.80428200	0.19968100
C	-1.86962900	5.58390400	0.21152400

H	-3.99650600	5.21754800	0.45182800
H	-3.97245100	2.92916500	-0.53844300
H	-0.36807400	4.42311000	1.21626800
H	-1.99509200	6.10159900	-0.75461000
H	-3.21782400	4.08741100	-1.63834400
H	0.29366300	5.44340100	-0.04688400
H	-1.83616200	6.36522600	0.98318400
H	-2.96499900	4.16313500	1.41704700
C	0.72962700	2.91696600	-0.86384000
C	-1.85392300	1.67715300	0.36671200
O	1.77726000	3.54936100	-0.92578300
O	-2.88543400	1.27565900	0.82277700
H	-0.66987700	4.13517700	-1.80770300
H	-1.85258700	2.13704400	-1.63269900
Cl	-0.98326300	-0.28118500	-2.35637500

^{S}N6

(U)M06/BSII SCF energy in solution: -2511.477288 a.u.
(U)M06/BSI SCF energy: -2509.283842 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.665486 a.u.

C	4.16878300	0.33719500	-2.18385400
O	4.14132700	-1.04357700	-1.74075100
C	2.93667300	0.98034400	-1.53196100
C	2.94473600	-1.23083600	-1.18286900
N	2.18947500	-0.20611500	-1.04238200
C	2.61480800	-2.65786700	-0.83018200
C	0.34890100	-3.32677000	1.95472600
O	1.55063900	-3.51090000	1.16966200
C	-0.47383700	-2.26460500	1.19834500
C	1.47368400	-2.66279700	0.14871800
N	0.41568700	-1.95113600	0.05113000

H	-0.15709400	-4.29550300	2.02036800
H	5.11751500	0.77311900	-1.85752600
H	4.12545300	0.32672800	-3.27839600
H	0.65401600	-2.99942500	2.95391900
C	3.84910100	-3.35792800	-0.26112900
H	4.65297100	-3.34621900	-1.00321800
H	4.21010800	-2.86611100	0.65043100
H	3.60885600	-4.39730400	-0.01558400
C	2.13201600	-3.37436500	-2.10911100
H	1.23330100	-2.89593700	-2.51925500
H	2.92743700	-3.36284900	-2.86382700
H	1.89454600	-4.41943200	-1.87129100
Ni	0.21512900	-0.43785800	-1.10512700
H	-0.55871600	-1.34732100	1.79758000
H	2.29106300	1.48568500	-2.25731300
C	-1.84420900	-2.73499500	0.80271700
C	-2.96628900	-2.02822000	1.22113900
C	-2.00379300	-3.88220100	0.02583200
C	-4.23952800	-2.45327000	0.85456100
H	-2.83951600	-1.12555700	1.82284400
C	-3.27087900	-4.30884200	-0.34022400
H	-1.12279300	-4.42319300	-0.32887600
C	-4.39206200	-3.59095100	0.07212700
H	-5.11187900	-1.88541500	1.17402200
H	-3.38768600	-5.19495500	-0.96122800
H	-5.38676600	-3.92074700	-0.22225700
C	3.24363100	1.92072000	-0.39677500
C	2.59772800	3.15413500	-0.32460100
C	4.14441100	1.55282500	0.60689300
C	2.85283300	4.00744700	0.74681700

H	1.86514400	3.42678300	-1.08970200
C	4.39534100	2.40510100	1.67445000
H	4.64906100	0.58444800	0.55751900
C	3.74660800	3.63639900	1.74529200
H	2.34016400	4.96648900	0.80092900
H	5.09545000	2.10979300	2.45422300
H	3.93963700	4.30519400	2.58217000
C	1.30873400	-0.04853400	3.15247600
C	0.94648100	0.92262700	2.22458600
C	-0.30495200	1.53986200	2.28438200
C	-1.20284800	1.13726400	3.27785200
C	-0.84828800	0.15464700	4.19841100
C	0.41353800	-0.43429500	4.14736300
H	2.30148600	-0.49946400	3.09484700
H	1.65078300	1.22578700	1.45110400
H	-2.18223400	1.61390400	3.34039100
H	-1.55709200	-0.14120500	4.97036100
H	0.69828600	-1.18374600	4.88563800
C	-0.64191700	2.65237000	1.32145300
H	-0.49185000	3.62566700	1.81008100
H	0.03507900	2.60811600	0.45892200
O	0.16759300	1.23179400	-1.87021600
C	-2.14173100	1.97704300	-1.59913300
C	-2.47932400	1.55469300	-0.14383800
C	-4.90212800	2.24739100	-0.61043600
C	-3.96003700	1.17304000	-0.06953600
C	-3.02663300	3.13800800	-2.03696900
C	-4.49019000	2.71350600	-2.00194800
H	-5.92911900	1.85401900	-0.63041300
H	-4.22433800	0.93298000	0.97319700

H	-2.85950800	4.00940400	-1.38520300
H	-4.63696200	1.89248000	-2.72495900
H	-4.07850600	0.24508900	-0.65364500
H	-2.73398500	3.45496900	-3.04672800
H	-5.13754600	3.53882700	-2.33113700
H	-4.89964800	3.10378400	0.07639000
C	-0.66520500	2.24162900	-1.83252200
C	-2.09545700	2.60238800	0.88486000
O	-0.24955500	3.38462900	-1.99224400
O	-2.90579600	3.33526200	1.41922400
H	-2.39409000	1.09436600	-2.20548400
H	-1.87373400	0.65662000	0.08242900
Cl	-1.56664000	-1.26468800	-2.07305200

^{T}N5

(U)M06/BSII SCF energy in solution: -2511.423739 a.u.
(U)M06/BSI SCF energy: -2509.231536 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.620369 a.u.

C	-2.79811300	0.78877200	2.93699100
O	-2.67944800	-0.64773400	2.81178800
C	-2.28519400	1.33008600	1.59700100
C	-1.89982900	-0.85679100	1.74394700
N	-1.61322200	0.14642800	1.00907700
C	-1.49281500	-2.29139900	1.55604800
C	0.82737200	-3.76307300	-0.81363800
O	-0.26558600	-3.73308600	0.12107200
C	1.37801800	-2.32354000	-0.81132100
C	-0.41525600	-2.46600400	0.51809600
N	0.42169500	-1.61331500	0.05123700
H	1.55463100	-4.50150100	-0.45954600
H	-3.84589900	1.02484500	3.14642200

H	-2.16932600	1.09293000	3.78087100
H	0.42525500	-4.07445500	-1.78459900
C	-2.74589000	-3.08704700	1.15497100
H	-3.52522300	-2.93631900	1.91029400
H	-3.12751300	-2.75857500	0.17924400
H	-2.51453500	-4.15563900	1.09917400
C	-0.91983100	-2.83731800	2.87958600
H	-0.10651500	-2.19496600	3.23838100
H	-1.70868100	-2.86128200	3.63828000
H	-0.54654200	-3.85698500	2.72937100
Ni	0.36988700	0.37208700	0.35221700
H	1.32296200	-1.88118400	-1.81714500
H	-1.52414200	2.10638400	1.74331000
C	2.79752400	-2.22474500	-0.30999600
C	3.84962700	-2.27063000	-1.22560200
C	3.07946400	-2.12112600	1.05111900
C	5.16771800	-2.22175500	-0.78842700
H	3.62884200	-2.32185900	-2.29294500
C	4.39937900	-2.05647000	1.48801700
H	2.26744500	-2.03083800	1.77193400
C	5.44488000	-2.11287000	0.57233200
H	5.98032700	-2.25500200	-1.51213100
H	4.60561500	-1.95198100	2.55162700
H	6.47656500	-2.06310700	0.91624400
C	-3.34410600	1.84142600	0.65475000
C	-3.09233400	2.97184200	-0.12205500
C	-4.55768200	1.16518000	0.51244700
C	-4.04999900	3.41875500	-1.02917800
H	-2.13714000	3.48835800	-0.00836800
C	-5.51511000	1.61615800	-0.38864300

H	-4.74983800	0.26498300	1.10190500
C	-5.26014900	2.74530900	-1.16338800
H	-3.84823800	4.30304000	-1.63135200
H	-6.46059600	1.08486000	-0.49051100
H	-6.00749200	3.10087000	-1.87091200
C	-3.86155100	-1.64320300	-2.06093200
C	-2.99492200	-0.56714400	-2.04640400
C	-1.68240000	-0.67750200	-2.57464100
C	-1.29519000	-1.93489300	-3.11055000
C	-2.16541400	-3.01153900	-3.10573800
C	-3.45481400	-2.87675400	-2.58290100
H	-4.86762400	-1.52475200	-1.65733500
H	-3.31189700	0.39199700	-1.63977900
H	-0.29939500	-2.03344100	-3.54862000
H	-1.84871300	-3.96555000	-3.52695600
H	-4.13838100	-3.72391600	-2.58861500
C	-0.81151700	0.42417100	-2.56195700
H	0.17572200	0.36547600	-3.01615900
H	-1.11415300	1.37661500	-2.12654100
O	0.09479500	2.22503500	-0.02174700
C	2.29560800	3.20422900	0.23539300
C	2.91658500	1.79531200	0.34022500
C	4.64908500	2.44452200	-1.42989900
C	4.38346400	1.74483200	-0.10501400
C	2.61933000	3.88013300	-1.10453400
C	4.11043300	3.86937800	-1.40893600
H	5.72865100	2.44064200	-1.63578500
H	4.72237300	0.69775200	-0.13056800
H	2.07364500	3.36490700	-1.91427800
H	4.64273200	4.45141200	-0.63717200

H	4.96261000	2.24167800	0.69047800
H	2.22405500	4.90363200	-1.06561100
H	4.30367200	4.36999100	-2.36777800
H	4.17190200	1.88236300	-2.24729900
C	0.77494200	3.25692700	0.39690800
C	2.06503300	0.86714900	-0.47766000
O	0.24771500	4.29209500	0.76936900
O	2.19146000	0.47602400	-1.59219100
H	2.73374500	3.80954700	1.04348300
H	2.82752200	1.45904200	1.38055700
Cl	1.03516800	0.33522800	2.62113700

^{T}TSN2

(U)M06/BSII SCF energy in solution: -2511.407451 a.u.
(U)M06/BSI SCF energy: -2509.214051 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.600997 a.u.

C	2.60895500	-1.22001900	-2.84409300
O	2.04603400	-2.42015300	-2.26971900
C	2.49621200	-0.18165700	-1.72368600
C	1.37208100	-2.02202500	-1.18500900
N	1.52281400	-0.81525400	-0.79371600
C	0.61348600	-3.12951100	-0.51664300
C	-1.95519800	-3.05143400	2.01689100
O	-0.99197700	-3.65523300	1.13992400
C	-2.22542200	-1.69071900	1.35961400
C	-0.47435000	-2.65301700	0.40668200
N	-1.02162600	-1.50175400	0.52446300
H	-2.83624500	-3.69759600	2.06387900
H	3.63711800	-1.44152500	-3.14579200
H	2.00352100	-0.96406200	-3.72092600
H	-1.49858500	-2.97511900	3.01415100

C	1.65761800	-3.94151800	0.27196900
H	2.41439600	-4.32821400	-0.42066700
H	2.15615500	-3.30290200	1.01449200
H	1.18190600	-4.78527900	0.78213000
C	-0.07146800	-4.01133000	-1.57829800
H	-0.73146300	-3.40674100	-2.21340600
H	0.68626000	-4.47490500	-2.21767900
H	-0.65763600	-4.79831500	-1.09216600
Ni	-0.14589600	0.33634900	-0.19289500
H	-2.28401200	-0.89372500	2.11264500
H	2.05160800	0.75015400	-2.08315900
C	-3.51562000	-1.70452100	0.57132100
C	-4.70613100	-1.48144300	1.26574300
C	-3.56487800	-2.01337900	-0.78377200
C	-5.92994100	-1.56699500	0.61697500
H	-4.66916900	-1.22172500	2.32582300
C	-4.79259600	-2.09200900	-1.43630500
H	-2.64187000	-2.13550600	-1.34698600
C	-5.97512400	-1.87411000	-0.74068900
H	-6.85055200	-1.38172800	1.16802200
H	-4.81760800	-2.31691700	-2.50104000
H	-6.93279900	-1.93459200	-1.25501600
C	3.80165000	0.11654500	-1.02998900
C	4.18493900	1.43472000	-0.78927400
C	4.64497900	-0.92323400	-0.63110400
C	5.40821600	1.70863700	-0.18261400
H	3.50082300	2.24492300	-1.04257800
C	5.86300300	-0.65187000	-0.01995300
H	4.34450700	-1.95979600	-0.80277900
C	6.25084600	0.66862500	0.19834400

H	5.69793200	2.74244500	-0.00196900
H	6.51513900	-1.47079800	0.28066300
H	7.20965300	0.88436300	0.66763400
C	3.21750600	0.38109600	2.27600700
C	2.10273000	1.11898000	1.91502300
C	0.80528500	0.62163800	2.18114700
C	0.69184200	-0.62409400	2.84347100
C	1.80865900	-1.36372400	3.17831200
C	3.08116000	-0.86639100	2.88012300
H	4.20916600	0.77954700	2.07003300
H	2.21581100	2.08255100	1.41520200
H	-0.30149600	-0.97518200	3.11983700
H	1.69639800	-2.32062900	3.68798200
H	3.96818900	-1.44421500	3.13707100
C	-0.38074200	1.38257000	1.86326500
H	-1.29203400	1.08451900	2.38034200
H	-0.24343200	2.45936800	1.78042100
O	0.89147300	1.96579700	-0.73838300
C	-0.68372100	3.78192700	-0.56309100
C	-1.76391400	2.75366300	-0.90208100
C	-3.51539500	4.33529400	0.05176000
C	-3.13506100	3.41266300	-1.09811800
C	-1.09162300	4.73617700	0.55919700
C	-2.43858200	5.38931000	0.27967400
H	-4.48624300	4.80731900	-0.15387900
H	-3.89781300	2.64199100	-1.26573700
H	-1.16097600	4.19365500	1.51880100
H	-2.35760400	6.02498200	-0.61876100
H	-3.06827000	4.00251000	-2.02689200
H	-0.29322700	5.47651800	0.68713500

H	-2.71797700	6.05493200	1.10827100
H	-3.64909700	3.74046400	0.97041700
C	0.71614400	3.18448200	-0.36773200
C	-1.89080400	1.58821100	0.07055200
O	1.59801100	3.90457900	0.10000600
O	-2.87702700	1.15372800	0.55955200
H	-0.59140500	4.39904200	-1.47592700
H	-1.46634100	2.24577500	-1.83108500
Cl	-1.06391200	-0.14607700	-2.33031900

^{T}N6

(U)M06/BSII SCF energy in solution: -2511.497099 a.u.
(U)M06/BSI SCF energy: -2509.298238 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.678827 a.u.

C	3.67111100	-0.85916700	-2.59870000
O	3.37265700	-2.08739200	-1.88413000
C	2.98824800	0.23194800	-1.77000600
C	2.34315000	-1.79547000	-1.08313800
N	2.01905100	-0.56530000	-0.98481700
C	1.76016700	-2.96688500	-0.34701300
C	-0.94405100	-3.03052700	2.07136700
O	0.18729100	-3.55027600	1.34203600
C	-1.41281600	-1.83006500	1.23298000
C	0.52657800	-2.61730300	0.44835900
N	-0.25955200	-1.61223900	0.33822200
H	-1.68929600	-3.82610500	2.15889900
H	4.75811300	-0.76519200	-2.66714400
H	3.23405500	-0.95672800	-3.59930800
H	-0.58319200	-2.73316400	3.06414800
C	2.85388900	-3.47489100	0.60946400
H	3.74977600	-3.74159700	0.03881500

H	3.11964600	-2.69622700	1.33837100
H	2.50222400	-4.35818900	1.15111700
C	1.35829500	-4.05947600	-1.35488000
H	0.64474100	-3.66484600	-2.08970800
H	2.24581400	-4.41587100	-1.88822000
H	0.90108000	-4.90338100	-0.82617100
Ni	0.12584500	0.03492300	-0.76683700
H	-1.53024700	-0.94414000	1.87328900
H	2.42009600	0.92468300	-2.40056600
C	-2.70596700	-2.07507100	0.49624200
C	-3.90311800	-1.82611900	1.17203800
C	-2.74148300	-2.58708700	-0.79826900
C	-5.12163500	-2.09868400	0.56305000
H	-3.87641500	-1.38460300	2.16905100
C	-3.96404700	-2.83837700	-1.41435600
H	-1.81634500	-2.73730300	-1.35245000
C	-5.15339900	-2.60276900	-0.73467200
H	-6.04937000	-1.89524900	1.09503100
H	-3.98068700	-3.21136900	-2.43665300
H	-6.10815200	-2.79969900	-1.21939800
C	3.88002700	0.99889800	-0.82312200
C	3.61943700	2.34307500	-0.55618600
C	4.92338600	0.35646300	-0.15070400
C	4.40185100	3.03596900	0.36311800
H	2.76987500	2.83140100	-1.03520300
C	5.70584500	1.05140400	0.76462800
H	5.12760900	-0.70053600	-0.33622200
C	5.44584200	2.39486100	1.02184600
H	4.18543100	4.08295100	0.56740400
H	6.51995900	0.54279000	1.27876200

H	6.05680400	2.94039600	1.73900300
C	2.02604600	0.50598500	2.42980600
C	1.10964400	1.43841300	1.94329100
C	-0.17328200	1.52470800	2.48844500
C	-0.52043600	0.66854100	3.54030600
C	0.39467200	-0.25845100	4.02708100
C	1.66994700	-0.34833900	3.46744700
H	3.02453500	0.46313100	1.99249000
H	1.39476900	2.10949700	1.13296200
H	-1.52105500	0.73992900	3.96804200
H	0.11897500	-0.90228300	4.86264200
H	2.38890300	-1.06762400	3.85888100
C	-1.17922500	2.52197100	1.95549800
H	-1.63180500	3.06646500	2.79563900
H	-0.68812100	3.25210400	1.30391800
O	0.52196100	1.86721800	-1.06568100
C	-1.74307500	2.67691100	-1.13648300
C	-2.37769100	1.59343600	-0.24509500
C	-4.64896400	2.58890100	-0.70145100
C	-3.80783900	1.31671800	-0.72313500
C	-2.56657800	3.95905200	-1.06723600
C	-4.00151200	3.70431400	-1.51361500
H	-5.65900400	2.37344800	-1.07699200
H	-4.26334100	0.53728000	-0.10144300
H	-2.55702400	4.35255000	-0.03573300
H	-3.99727800	3.41897600	-2.57934800
H	-3.74148800	0.91695000	-1.74778800
H	-2.08649800	4.73046600	-1.68086500
H	-4.59451300	4.62692400	-1.44078100
H	-4.77174200	2.91806200	0.34367800

C	-0.24111900	2.91301100	-0.96070400
C	-2.33241400	1.79004000	1.27555400
O	0.20395300	4.03638600	-0.75930200
O	-3.17739700	1.26587600	1.97811000
H	-1.82770300	2.26751300	-2.16054000
H	-1.83968300	0.62761300	-0.39230100
Cl	-0.58201400	-0.71083600	-2.81802800

^{T}N3b

(U)M06/BSII SCF energy in solution: -1975.031439 a.u.
(U)M06/BSI SCF energy: -1972.991024 a.u.
(U)M06/BSI SCF Gibbs energy: -1972.545499 a.u.

C	2.88794900	2.30743300	1.34241400
O	2.08120400	2.99310200	0.36622200
C	2.52516000	0.82131400	1.15444300
C	1.19198400	2.09234000	-0.08179800
N	1.34081400	0.87767000	0.27989000
C	0.13204100	2.68577000	-0.96922700
C	-2.84841900	1.22598300	-2.39638400
O	-1.71269300	2.10966000	-2.37122300
C	-2.44228300	0.05881800	-1.48157600
C	-0.93873500	1.69898500	-1.35199200
N	-1.26070800	0.59802200	-0.79004600
H	-3.71222000	1.77547300	-1.99833300
H	3.93874800	2.53621300	1.13685800
H	2.60144300	2.68610500	2.32977200
H	-3.04105400	0.94348400	-3.43490000
C	0.81208100	3.24280700	-2.22962900
H	1.57287300	3.97557000	-1.94160100
H	1.29558800	2.44364600	-2.80691900
H	0.07559500	3.73676200	-2.87095100

C	-0.58122700	3.81492500	-0.19505200
H	-0.98593000	3.42996700	0.75173800
H	0.12912900	4.61856800	0.02508100
H	-1.39402000	4.22201900	-0.80770400
Ni	-0.42391900	-0.17910700	0.88791000
H	-2.10895800	-0.81344900	-2.06691700
H	2.21291900	0.38228100	2.11359600
C	-3.52511900	-0.37106700	-0.52956000
C	-4.33021400	-1.46698500	-0.83751800
C	-3.74068500	0.32619900	0.65965400
C	-5.33384900	-1.87167300	0.03646500
H	-4.15978600	-2.01572100	-1.76599800
C	-4.73328900	-0.08794300	1.53976800
H	-3.09309000	1.15941800	0.93492900
C	-5.53173800	-1.18511200	1.23040500
H	-5.95257600	-2.73268300	-0.21051500
H	-4.86678800	0.44275900	2.48051600
H	-6.30434200	-1.51166300	1.92441100
C	3.61847100	-0.01917300	0.54674700
C	4.22043000	-1.03850700	1.28059700
C	4.05383000	0.22410000	-0.75683600
C	5.23589000	-1.81033300	0.72300800
H	3.88553000	-1.23250300	2.30091500
C	5.06750100	-0.54223100	-1.31665800
H	3.58397100	1.01679900	-1.34163300
C	5.66062100	-1.56372200	-0.57822800
H	5.69471700	-2.60622100	1.30702900
H	5.39546800	-0.34529700	-2.33597000
H	6.45377300	-2.16571800	-1.01803700
Cl	-0.83770600	1.31592700	2.61795600

C	-0.92769700	-1.99499100	1.58463300
H	-0.42359400	-2.03212400	2.55528700
H	-2.01307600	-2.10465600	1.64165700
C	-0.23283700	-2.55246900	0.45299700
C	-0.91006500	-2.94418800	-0.73179700
C	1.18418700	-2.64089900	0.43707400
C	-0.21269200	-3.36515100	-1.85106800
H	-2.00166500	-2.91960800	-0.73544900
C	1.87503400	-3.05221400	-0.68913100
H	1.73101600	-2.36395700	1.34114700
C	1.18360300	-3.41516400	-1.84602600
H	-0.76183800	-3.66889700	-2.74259300
H	2.96498800	-3.08407300	-0.66351700
H	1.72548300	-3.74132700	-2.73186500

^{T}N4b

(U)M06/BSII SCF energy in solution: -2511.46375 a.u.
(U)M06/BSI SCF energy: -2509.271412 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.656538 a.u.

C	0.48765300	-3.34605200	-2.34868200
O	-0.20912200	-3.83737400	-1.18313900
C	0.93992500	-1.94550500	-1.92988200
C	-0.52242300	-2.75662400	-0.46309100
N	0.03306600	-1.64551200	-0.79985100
C	-1.41343500	-3.05037800	0.71508500
C	-3.48290400	-0.74436000	2.59179400
O	-2.82069000	-2.00471500	2.34857600
C	-2.62452900	0.27095400	1.83399800
C	-2.01224400	-1.80072300	1.29994900
N	-1.86759000	-0.59329800	0.90975600
H	-4.50544100	-0.82014900	2.19617400

H	1.30173900	-4.04022700	-2.57583100
H	-0.23995700	-3.31718600	-3.16803800
H	-3.51674400	-0.58391900	3.67173700
C	-0.52012500	-3.73705400	1.77044600
H	-0.13713400	-4.67821000	1.35798600
H	0.31678600	-3.09178200	2.06207300
H	-1.11034200	-3.96014100	2.66620400
C	-2.55560400	-3.99551600	0.30931200
H	-3.18484000	-3.52928600	-0.45756500
H	-2.14285200	-4.92599200	-0.09289300
H	-3.16244500	-4.22985200	1.19030300
Ni	-1.33313400	-0.08151700	-1.01210700
H	-1.89519500	0.73033700	2.51534800
H	0.74708300	-1.21295900	-2.72577400
C	-3.32740400	1.35590200	1.06871000
C	-2.92685500	2.68240600	1.22999300
C	-4.28864300	1.03976200	0.10570400
C	-3.50037400	3.68711800	0.45517500
H	-2.14410700	2.92359300	1.95269100
C	-4.85583500	2.04249400	-0.67149000
H	-4.55807500	-0.00118500	-0.07803400
C	-4.46590200	3.36776000	-0.49423100
H	-3.18199300	4.71989900	0.58723300
H	-5.59092200	1.78355800	-1.43099400
H	-4.90814700	4.15185000	-1.10635200
C	2.37776100	-1.84270600	-1.48331600
C	3.17046000	-0.78223800	-1.91633300
C	2.92914500	-2.78593400	-0.60973900
C	4.49577700	-0.67130300	-1.50516300
H	2.74001200	-0.03016700	-2.57768700

C	4.25058700	-2.67492400	-0.19330800
H	2.32082200	-3.61908500	-0.25233100
C	5.04087800	-1.62049500	-0.64765900
H	5.10201300	0.16074800	-1.86242100
H	4.66893700	-3.41854800	0.48305800
H	6.08004200	-1.54205100	-0.33154900
C	1.12917300	3.97367800	-1.19317500
C	0.02885500	3.13836300	-1.32769900
C	0.00089500	2.11179500	-2.29429500
C	1.15088500	1.95233400	-3.09377000
C	2.25684200	2.77930900	-2.94868300
C	2.25273900	3.80166700	-2.00167900
H	1.11402700	4.75778600	-0.43767300
H	-0.84858900	3.28740300	-0.69227800
H	1.14169400	1.18620100	-3.87273100
H	3.12338700	2.63823000	-3.59582800
H	3.11360600	4.46038800	-1.89701400
C	-1.16264000	1.25218800	-2.46724900
H	-2.12509900	1.75257600	-2.27113800
H	-1.20682200	0.70835300	-3.41590400
O	0.30295400	1.26239800	2.54345600
C	2.13306400	0.04051200	1.72202100
C	2.08860800	1.39982900	1.01820700
C	4.35241900	1.99605100	1.99730100
C	3.41546800	2.11854100	0.80480300
C	3.21392300	-0.05947800	2.82006600
C	4.54140900	0.53450600	2.38035500
H	5.31572100	2.46649700	1.75931400
H	3.20612400	3.16881600	0.56555200
H	2.87426600	0.48960600	3.71607700

H	4.93262800	-0.02629300	1.51533900
H	3.89760600	1.68183000	-0.08349100
H	3.30533700	-1.11139100	3.12147900
H	5.27653300	0.43132100	3.18999400
H	3.93985200	2.55021800	2.85840000
C	0.81293600	-0.01623600	2.43815400
C	1.09303200	2.17093900	1.84861600
O	0.26346800	-0.93870400	2.96867900
O	0.90237800	3.34475600	1.95027500
H	2.22517400	-0.79828600	1.01800200
H	1.58420800	1.28168000	0.03743200
Cl	-2.83720400	-1.43355400	-2.23020300

^{T}TSN1b

(U)M06/BSII SCF energy in solution: -2511.41706 a.u.
(U)M06/BSI SCF energy: -2509.21988 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.60661 a.u.

C	-0.65967600	-3.30661900	-2.47286600
O	-1.85050700	-3.42445100	-1.67029800
C	0.18593700	-2.26611100	-1.72231400
C	-1.87232400	-2.35660300	-0.86440100
N	-0.80897800	-1.64066300	-0.83250000
C	-3.16070800	-2.23990600	-0.08442500
C	-4.38395400	0.54200200	1.91066300
O	-4.35672400	-0.83282000	1.45857900
C	-3.00384900	1.08867200	1.53268500
C	-3.30001600	-0.93159300	0.63602200
N	-2.54356400	0.08448800	0.56196400
H	-5.20741400	1.04976000	1.39198000
H	-0.19434900	-4.29434100	-2.53887100
H	-0.96693000	-2.96220700	-3.46735700

H	-4.58188400	0.53655000	2.98493400
C	-3.15148800	-3.36669700	0.96917500
H	-3.00464400	-4.33529900	0.47805200
H	-2.35041500	-3.20379500	1.70270000
H	-4.11009400	-3.38624200	1.49852700
C	-4.35108000	-2.38987500	-1.04599600
H	-4.31353100	-1.61609000	-1.82405000
H	-4.32839800	-3.37442300	-1.52338500
H	-5.28769900	-2.29076800	-0.48687500
Ni	-0.89053000	0.37991200	-0.54073900
H	-2.31449400	1.02493000	2.38906300
H	0.56162000	-1.50008600	-2.41569700
C	-2.90522500	2.46291500	0.92641000
C	-1.79432800	3.25027200	1.23185800
C	-3.79982000	2.89339400	-0.05401600
C	-1.58608200	4.45807100	0.57353800
H	-1.05430500	2.89446400	1.94945800
C	-3.60001800	4.10575400	-0.70012300
H	-4.63594100	2.26028400	-0.35349400
C	-2.49270600	4.89028900	-0.38737700
H	-0.70115500	5.04771500	0.80796600
H	-4.29776700	4.42852800	-1.47030300
H	-2.33055100	5.83319000	-0.90674900
C	1.33729800	-2.86208300	-0.94853200
C	2.64712500	-2.67518100	-1.38915200
C	1.10887700	-3.64258200	0.18711900
C	3.71522100	-3.24614800	-0.70429600
H	2.83457700	-2.06490800	-2.27328800
C	2.17312300	-4.22785100	0.86313800
H	0.09502600	-3.76769600	0.56917200

C	3.47905000	-4.02802700	0.42176500
H	4.73245600	-3.07883700	-1.05356300
H	1.98118700	-4.83023800	1.74927300
H	4.31170500	-4.47976000	0.95794200
C	4.12668300	3.46476000	-1.57058500
C	2.81224000	3.16035200	-1.24052800
C	2.24061600	1.93094400	-1.60225600
C	3.03784100	1.03960200	-2.33539000
C	4.35494700	1.33810900	-2.66066000
C	4.91229100	2.55333200	-2.27324200
H	4.54327600	4.42765000	-1.27660300
H	2.20710400	3.87200100	-0.68023000
H	2.59531900	0.09674000	-2.66629300
H	4.94692400	0.62268100	-3.23122600
H	5.94214800	2.79520900	-2.53057800
C	0.85476500	1.57281600	-1.23407800
H	0.23655900	2.47661400	-1.10031800
H	0.45607100	1.01446400	-2.10156900
O	0.09287900	0.45193200	1.29207100
C	1.94928200	-0.72083100	2.05753200
C	2.43324300	0.17501700	0.90643000
C	4.20946500	1.14139900	2.46468500
C	3.87141600	0.65667900	1.06076400
C	2.33881300	-0.19093700	3.44625900
C	3.82932400	0.10398500	3.51359700
H	5.28233300	1.37139300	2.52272500
H	4.08641200	1.43444900	0.31788000
H	1.78190400	0.73749300	3.65545800
H	4.39593900	-0.82700500	3.33653600
H	4.51640400	-0.20381700	0.80967200

H	2.02688900	-0.92377100	4.20310000
H	4.09791600	0.44981500	4.52132700
H	3.67317700	2.08094600	2.66576900
C	0.45029700	-0.68883600	1.93772700
C	1.35965200	1.25569200	0.87722800
O	-0.35689900	-1.47481100	2.36647700
O	1.40827700	2.38023700	1.30867500
H	2.31174100	-1.75230100	1.94383700
H	2.34852200	-0.39995100	-0.02559000
Cl	-2.09274000	0.62509500	-2.52335600

N4c

(U)M06/BSII SCF energy in solution: -2511.452701 a.u.
(U)M06/BSI SCF energy: -2509.266282 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.656859 a.u.

C	-3.58290900	1.47410400	2.73314200
O	-3.95945600	0.20818100	2.14722900
C	-2.23770100	1.80885400	2.08361000
C	-2.83038400	-0.28665700	1.60208400
N	-1.82040100	0.48950100	1.56109800
C	-2.89673800	-1.74146600	1.22119400
C	-0.61448100	-3.75826400	-0.74933000
O	-1.88701400	-3.37634900	-0.19905300
C	0.29224000	-2.53435300	-0.50722800
C	-1.70667800	-2.19683600	0.41438300
N	-0.54374900	-1.66943600	0.33092000
H	-0.26759800	-4.65320500	-0.21706100
H	-4.38141900	2.19490300	2.53921600
H	-3.49228100	1.32028300	3.81560200
H	-0.76408000	-3.99668000	-1.80788800
C	-4.19940500	-2.02921500	0.46716300

H	-5.05439800	-1.75883800	1.09526100
H	-4.25286000	-1.45313700	-0.46516000
H	-4.26070300	-3.09391300	0.22118700
C	-2.85948400	-2.55072800	2.53740100
H	-1.93395600	-2.34880300	3.09334300
H	-3.71665200	-2.27739000	3.16331600
H	-2.91362000	-3.62291900	2.31495400
Ni	0.06376200	-0.03333100	1.22118300
H	0.48385500	-1.99068600	-1.44498300
H	-1.49052400	2.11162600	2.82878300
C	1.62399600	-2.88171900	0.10653500
C	2.58651200	-3.48430000	-0.70692800
C	1.91724100	-2.65482100	1.44966600
C	3.81623500	-3.86433400	-0.18528700
H	2.37097100	-3.63691000	-1.76616000
C	3.16163200	-3.00984800	1.96677100
H	1.17962800	-2.17840300	2.09680000
C	4.10972800	-3.62058400	1.15480300
H	4.55593200	-4.33504400	-0.83101900
H	3.38311900	-2.80566800	3.01285700
H	5.07875600	-3.90407900	1.56203600
C	-2.24763400	2.81103800	0.95509000
C	-1.03881800	3.40502500	0.58574400
C	-3.39853700	3.09551400	0.22107700
C	-0.98292200	4.27177200	-0.49932300
H	-0.12763600	3.16542800	1.13854300
C	-3.34764800	3.98005200	-0.85336400
H	-4.34600200	2.61543600	0.47260600
C	-2.13960200	4.56726600	-1.21612700
H	-0.02160800	4.69791200	-0.77848400

H	-4.25501800	4.20283700	-1.41359500
H	-2.09974000	5.25154500	-2.06204300
C	-4.62554600	-0.33738900	-2.75984400
C	-3.55754900	0.41043400	-2.29638900
C	-2.22584200	-0.07668600	-2.38776900
C	-2.04696600	-1.36692000	-2.95640900
C	-3.12311800	-2.11698900	-3.39497600
C	-4.42211600	-1.60924100	-3.30567500
H	-5.63510200	0.06691300	-2.69268800
H	-3.71331900	1.40195400	-1.86985000
H	-1.02879800	-1.74460500	-3.07080000
H	-2.95539200	-3.10314500	-3.82774600
H	-5.26714900	-2.19574700	-3.66135500
C	-1.12708600	0.68869800	-1.95987100
H	-0.10600400	0.34207900	-2.11484300
H	-1.25875700	1.68611700	-1.54241900
O	1.88277800	1.78608200	-1.06411200
C	3.91807900	2.04051900	0.08790700
C	3.65635900	0.55242400	-0.13970100
C	5.78509900	0.35578500	-1.50471200
C	4.84199600	-0.32102800	-0.51882200
C	4.95827400	2.62672400	-0.88477400
C	6.18680400	1.73749700	-1.00256900
H	6.67024200	-0.27411100	-1.66674800
H	4.46401200	-1.27401500	-0.91437200
H	4.50557000	2.72397800	-1.88751500
H	6.67692300	1.64393000	-0.01868100
H	5.39517200	-0.56604800	0.40110000
H	5.20873400	3.64580100	-0.56326900
H	6.91861400	2.20124700	-1.67783700

H	5.29030700	0.45697400	-2.48618600
C	2.59687400	2.67305500	-0.25929200
C	2.52798100	0.57363800	-1.13624300
O	2.20439200	3.78298800	-0.06357600
O	2.15169100	-0.29143900	-1.88093100
H	4.18155400	2.27274200	1.12602600
H	3.17932700	0.15705100	0.77703300
Cl	1.45983200	1.26973800	2.35274800

TSN1c

(U)M06/BSII SCF energy in solution: -2511.414745 a.u.
(U)M06/BSI SCF energy: -2509.226831 a.u.
(U)M06/BSI SCF Gibbs energy: -2508.616424 a.u.

C	-2.60493400	1.09222600	2.91569500
O	-2.58469700	-0.35191900	2.86271600
C	-2.13046800	1.52872700	1.52265700
C	-1.89103000	-0.66853200	1.76065300
N	-1.58599200	0.27342600	0.95489800
C	-1.60195300	-2.13955500	1.62648400
C	0.65016000	-3.90232900	-0.60751900
O	-0.48624400	-3.74037400	0.25997400
C	1.24375700	-2.48316100	-0.74577500
C	-0.54376800	-2.44813400	0.59995700
N	0.35430500	-1.68250500	0.10352100
H	1.34315100	-4.60412500	-0.12894800
H	-3.62384000	1.40769100	3.16096900
H	-1.91418500	1.39917100	3.70832700
H	0.29451500	-4.32973400	-1.55114000
C	-2.91872400	-2.83615200	1.24717900
H	-3.68128200	-2.60013100	1.99831200
H	-3.27273600	-2.49931100	0.26348400

H	-2.77971900	-3.92185900	1.21671800
C	-1.07012600	-2.67856900	2.96944000
H	-0.18702000	-2.10882300	3.28758000
H	-1.84361700	-2.57952400	3.73769600
H	-0.80854000	-3.73799900	2.86649100
Ni	0.42287900	0.29855300	0.31103900
H	1.15173200	-2.10985100	-1.77794500
H	-1.30990500	2.25616300	1.59541500
C	2.68845400	-2.39828400	-0.32454900
C	3.69174900	-2.51494800	-1.28634300
C	3.03933600	-2.25764800	1.01801100
C	5.03114000	-2.50823300	-0.91298700
H	3.41774900	-2.59483400	-2.33935100
C	4.37997700	-2.23275100	1.38932000
H	2.26529500	-2.11237200	1.77202100
C	5.37703900	-2.36710600	0.42827000
H	5.80581300	-2.60228700	-1.67219100
H	4.64205900	-2.10082700	2.43752300
H	6.42518100	-2.35155400	0.72221900
C	-3.20122000	2.07831700	0.61778300
C	-2.92301100	3.17623300	-0.19427900
C	-4.45609300	1.47036900	0.54543200
C	-3.89030200	3.65723600	-1.07315100
H	-1.94084600	3.64779600	-0.12344900
C	-5.42560800	1.95731300	-0.32314800
H	-4.66960000	0.59461800	1.16344000
C	-5.14119100	3.05102200	-1.13812000
H	-3.66615500	4.51486800	-1.70519900
H	-6.40351000	1.47966800	-0.37120800
H	-5.89733400	3.43198800	-1.82264600

C	-4.31464700	-1.47464700	-2.00875300
C	-3.36006800	-0.47623200	-2.04733700
C	-2.03037100	-0.74838600	-2.46280700
C	-1.72400000	-2.08358700	-2.83595700
C	-2.68342200	-3.07950900	-2.78470600
C	-3.98711300	-2.78547900	-2.37323800
H	-5.32925500	-1.23159000	-1.69234600
H	-3.62209400	0.54480900	-1.77245000
H	-0.71434600	-2.30845700	-3.18715700
H	-2.42403400	-4.09723000	-3.07539100
H	-4.74065600	-3.57031600	-2.33925900
C	-1.06524500	0.27221200	-2.49860000
H	-0.06164100	0.09716400	-2.88202500
H	-1.30998500	1.28580600	-2.18288300
O	0.61269700	2.13572800	-0.41526800
C	2.65347200	3.05867100	0.31756600
C	3.11106700	1.59934000	0.15499900
C	4.80469000	2.32325600	-1.61447600
C	4.51065900	1.41066500	-0.43339800
C	3.06629300	3.94787100	-0.86831000
C	4.52937000	3.77490900	-1.24545700
H	5.84769400	2.19025100	-1.93345300
H	4.65241700	0.35269400	-0.69859700
H	2.44503700	3.68740600	-1.74248500
H	5.17075900	4.06880900	-0.39707500
H	5.22808300	1.62612000	0.37487100
H	2.82735200	4.98971100	-0.61576900
H	4.78236700	4.44449500	-2.07886500
H	4.17313900	2.03667200	-2.47109600
C	1.13699600	3.08977700	0.35025400

C	2.05606800	0.91450700	-0.68111000
O	0.47776600	3.95312200	0.88726900
O	2.07791200	0.41924000	-1.76539200
H	3.05276600	3.47638100	1.25199900
H	3.06316400	1.12188400	1.14342000
Cl	1.15130300	0.41575800	2.53447000