Supporting Information

Mechanistic Origins of Chemo- and Regioselectivity of Ru(II)-Catalyzed Reactions Involving *ortho*-Alkenylarylacetylene, Alkyne, and Methanol: the Crucial Role of a Chameleon-like Intermediate

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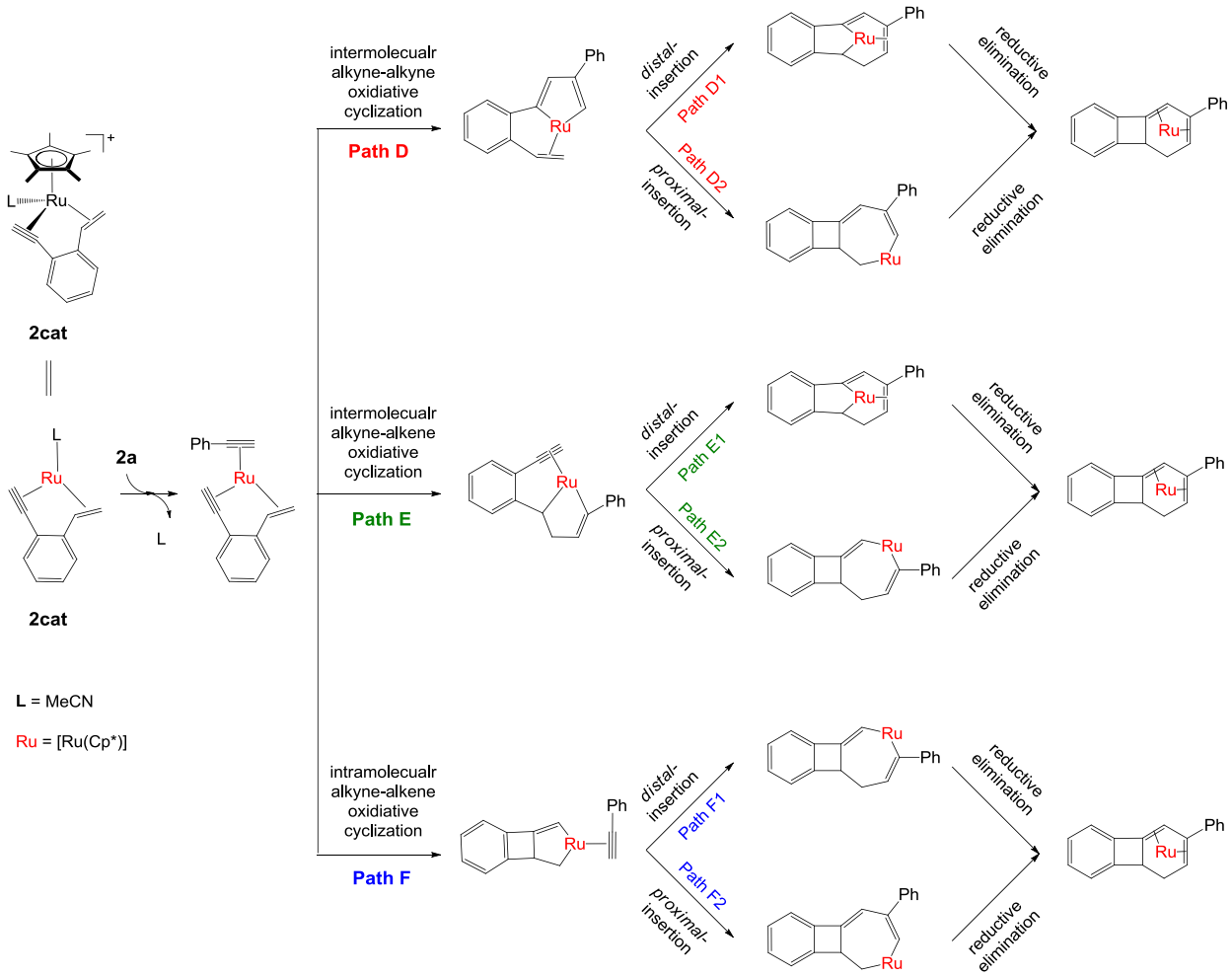
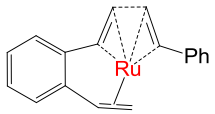
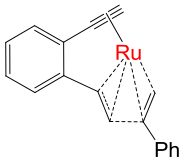
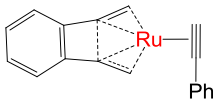
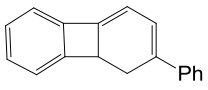
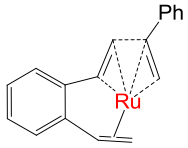
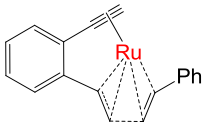
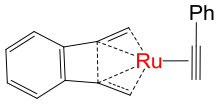
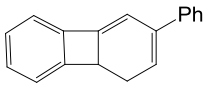
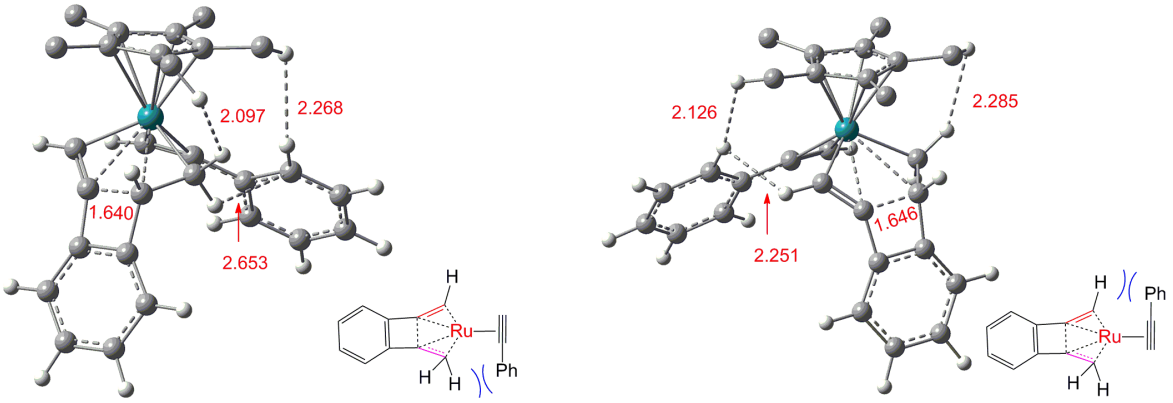
Gaussian 09, Revision **A.1,** Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Scheme S1. Possible Pathways for **2cat**-Catalyzed [2+2+2] Cocyclization of **1a** and **2a** Leading to Product **2b**-r



Scheme S2. Key TSs for the Three Coupling Modes Leading to **2b** (**TS1**/**TS6**/**TS7**) and **2b-r** (**TS1-r**/**TS6-r**/**TS7-r**), where Ru = [Ru(Cp*)]

intermolecualr alkyne-alkyne oxidiative cyclization	intermolecualr alkyne-alkene oxidiative cyclization	intramolecualr alkyne-alkene oxidiative cyclization	product
 **TS1** $\Delta G^{\ddagger}$ = 16.1 kcal/mol	 **TS6** $\Delta G^{\ddagger}$ = 19.6 kcal/mol	 **TS7** $\Delta G^{\ddagger}$ = 44.6 kcal/mol	 **2b**
 **TS1-r** $\Delta G^{\ddagger}$ = 21.7 kcal/mol	 **TS6-r** $\Delta G^{\ddagger}$ = 20.2 kcal/mol	 **TS7-r** $\Delta G^{\ddagger}$ = 44.8 kcal/mol	 **2b-r**



TS7 $\Delta G^{\ddagger}$ = 44.6 **TS7-r** $\Delta G^{\ddagger}$ = 44.8

Figure S1. Optimized geometries and activation energies for the oxidative coupling TSs **TS7** (leading to **1b**) and **TS7-r** (leading to **1b-r**), with selected bond distances given in Å. H atoms in the Cp* ligand are omitted for clarity expect those in question.

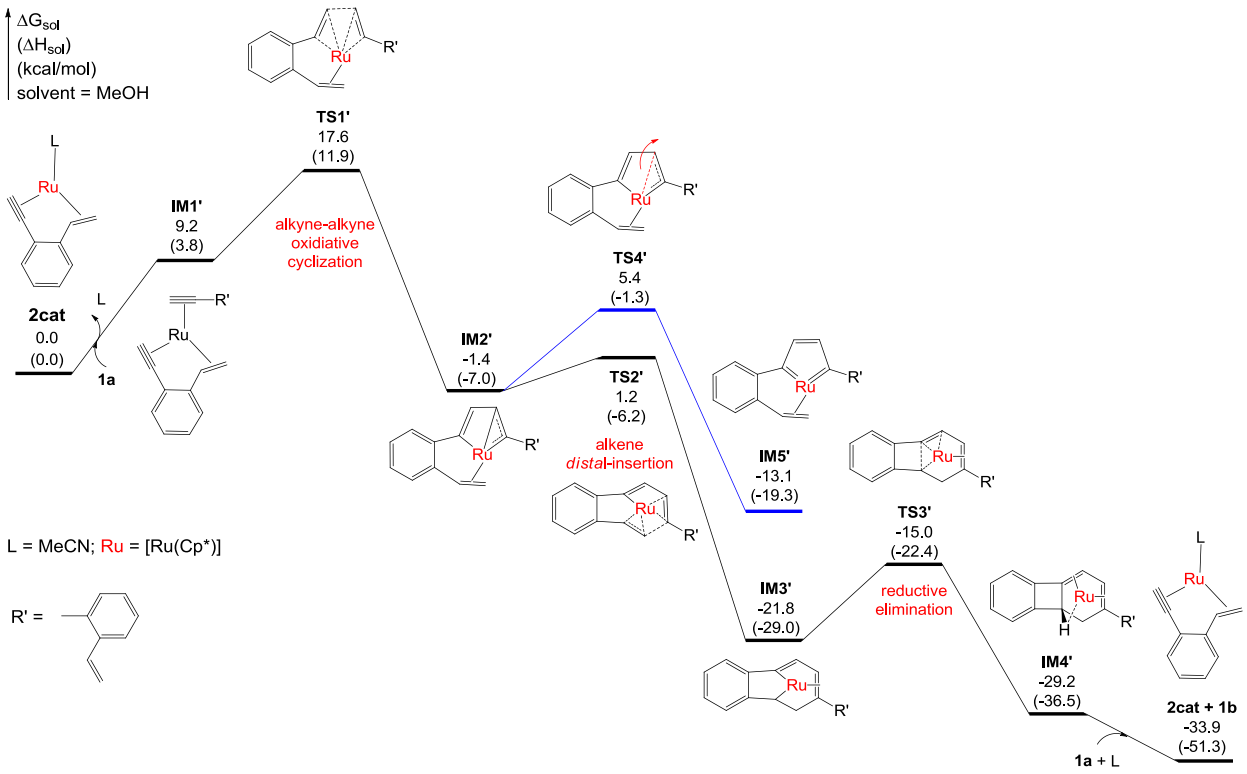


Figure S2. Free energy profile for **2cat**-catalyzed [2+2+2] dimerization of **1a** to produce **1b**. Energies are relative to **2cat** + **1a** and are mass balanced.

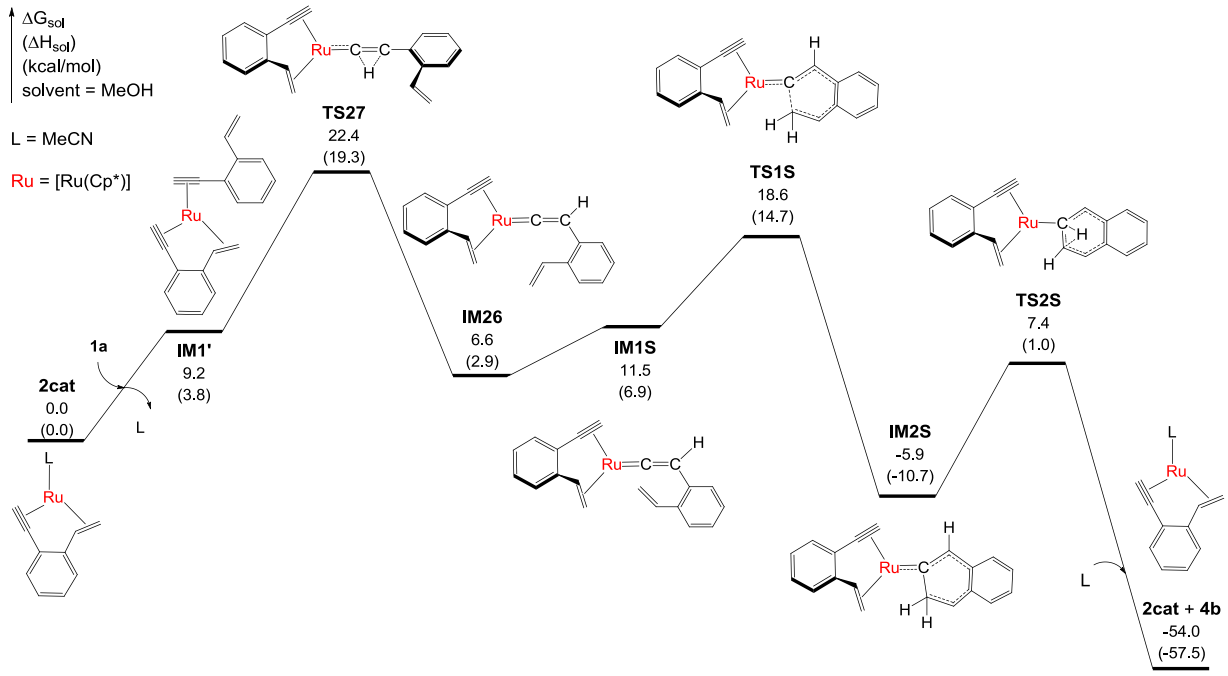


Figure S3. Free energy profile for **2cat**-catalyzed aromatization of **1a** leading to **4b**. Energies are relative to **2cat** +**1a** and are mass balanced.

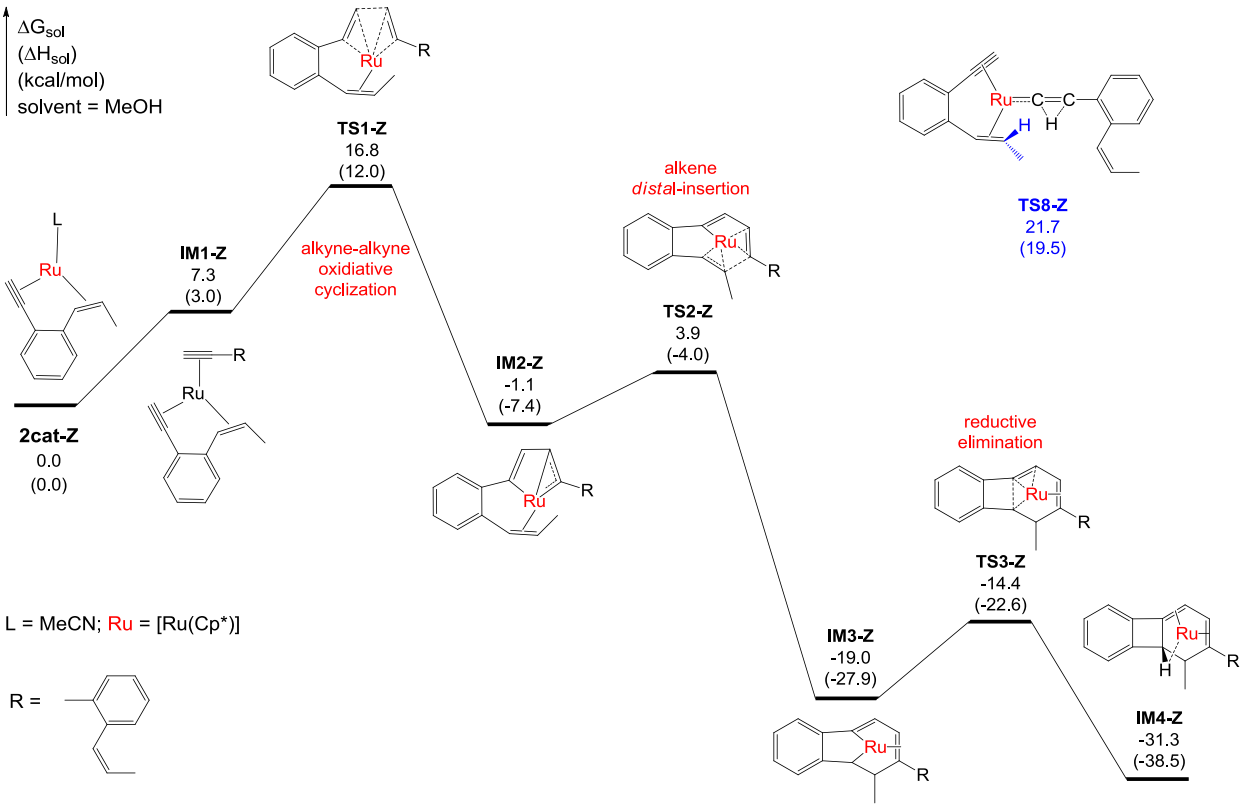


Figure S4. Free energy profile for **2cat-Z**-catalyzed [2+2+2] dimerization of (*Z*)-**3a** to produce **5b**. Energies are relative to **2cat-Z** and are mass balanced.

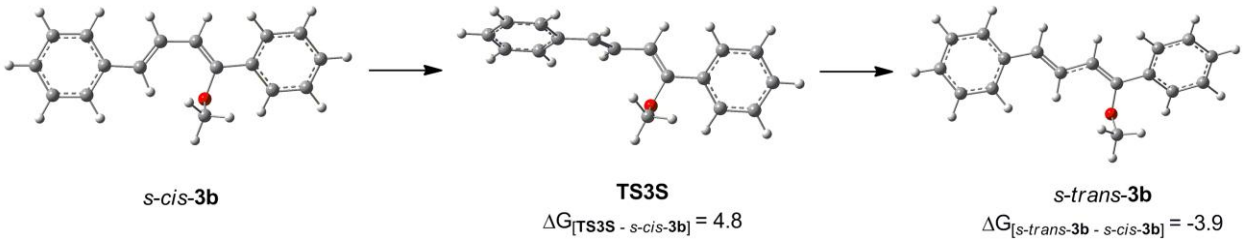


Figure S5. Isomerization from the s-*cis*-**3b** to the thermodynamically more stable s-*trans*-**3b**.

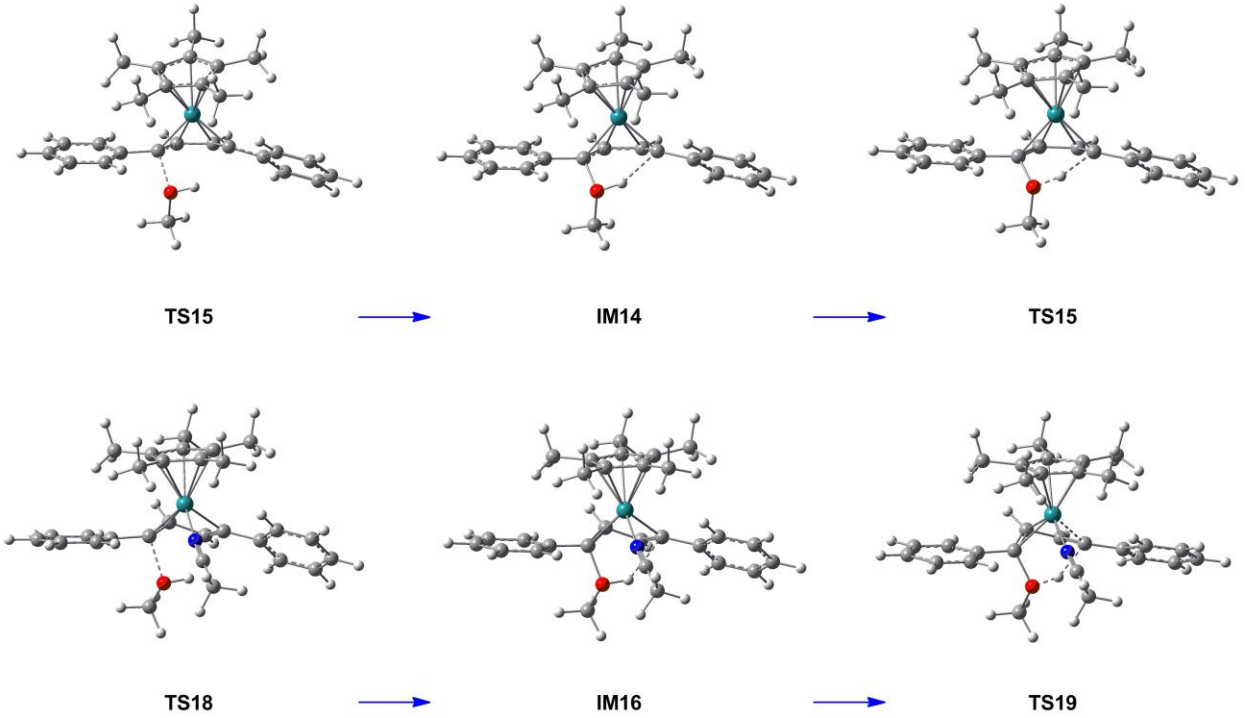
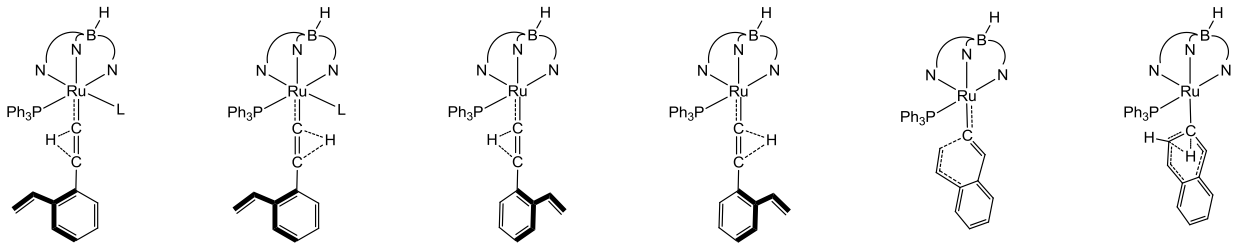


Figure S6. Key structures for the pathways leading to (1*Z*,3*E*) *s-trans*-**3b** (see Figures 6 and 7 in the main text).

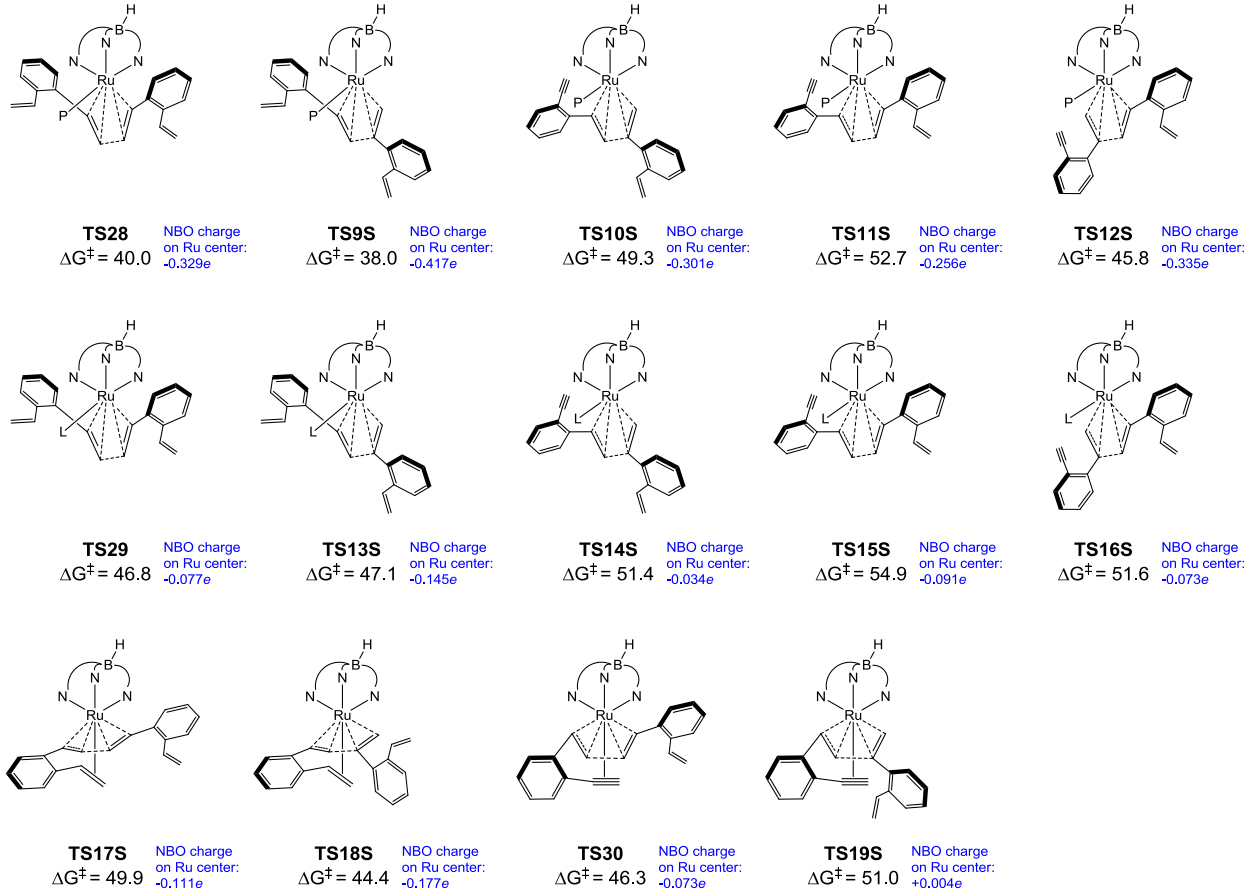
In **TS15** and **TS18**, methanol attacks the coupling unit from the bottom and the methanol moiety lies below the unit afterwards. To obtain (1*E*,3*E*) *s-trans*-**3b**, methanol should attack the unit from the side with Cp* ligand, which is unlikely because of streic hindrance. Furthermore, (*1E*,*3E*) *s-trans*-**3b** is 1.9 kcal/mol less stable than (*1Z*,*3E*) *s-trans*-**3b** (see eq 3 and Figure S5). Therefore, we considered the product of the reaction could be (1*Z*,3*E*) *s-trans*-**3b**, rather than (1*E*,3*E*) *s-trans*-**3b.**

Scheme S3. Selected TSs for **3cat**-Mediated Aromatization of **1a**



TS24 $\Delta G^{\ddagger} = 24.3$ | **TS4S** $\Delta G^{\ddagger} = 27.4$ | **TS5S** $\Delta G^{\ddagger} = 42.5$ | **TS6S** $\Delta G^{\ddagger} = 40.4$ | **TS7S** $\Delta G^{\ddagger} = 33.8$ | **TS8S** $\Delta G^{\ddagger} = 27.5$

Scheme S4. Possible oxidative coupling modes for **1a** with **3cat**, where P = PPh_3 and L = MeCN



TS28 $\Delta G^{\ddagger} = 40.0$ NBO charge on Ru center: -0.329*e*

TS9S $\Delta G^{\ddagger} = 38.0$ NBO charge on Ru center: -0.417*e*

TS10S $\Delta G^{\ddagger} = 49.3$ NBO charge on Ru center: -0.301*e*

TS11S $\Delta G^{\ddagger} = 52.7$ NBO charge on Ru center: -0.256*e*

TS12S $\Delta G^{\ddagger} = 45.8$ NBO charge on Ru center: -0.335*e*

TS29 $\Delta G^{\ddagger} = 46.8$ NBO charge on Ru center: -0.077*e*

TS13S $\Delta G^{\ddagger} = 47.1$ NBO charge on Ru center: -0.145*e*

TS14S $\Delta G^{\ddagger} = 51.4$ NBO charge on Ru center: -0.034*e*

TS15S $\Delta G^{\ddagger} = 54.9$ NBO charge on Ru center: -0.091*e*

TS16S $\Delta G^{\ddagger} = 51.6$ NBO charge on Ru center: -0.073*e*

TS17S $\Delta G^{\ddagger} = 49.9$ NBO charge on Ru center: -0.111*e*

TS18S $\Delta G^{\ddagger} = 44.4$ NBO charge on Ru center: -0.177*e*

TS30 $\Delta G^{\ddagger} = 46.3$ NBO charge on Ru center: -0.073*e*

TS19S $\Delta G^{\ddagger} = 51.0$ NBO charge on Ru center: +0.004*e*

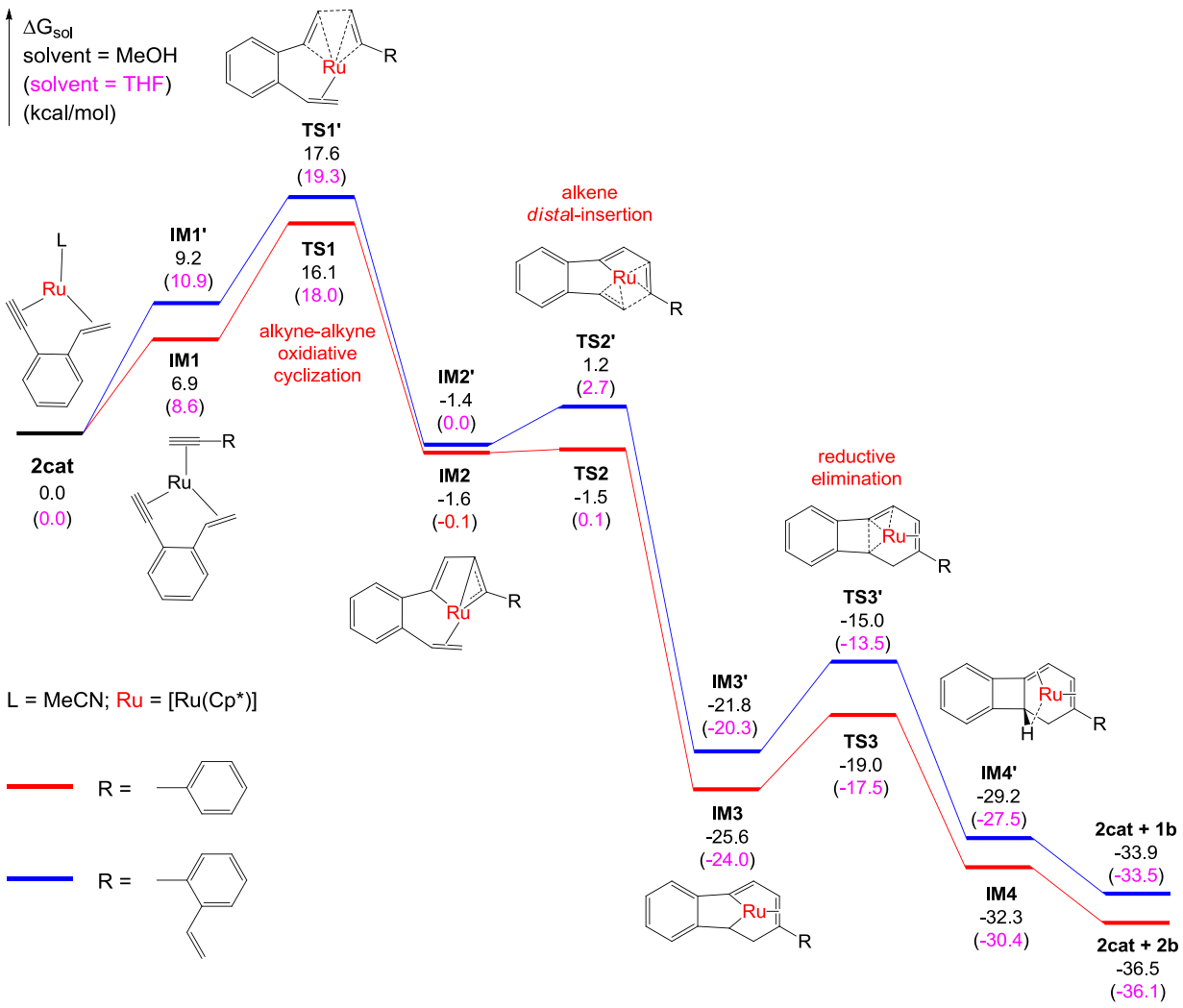
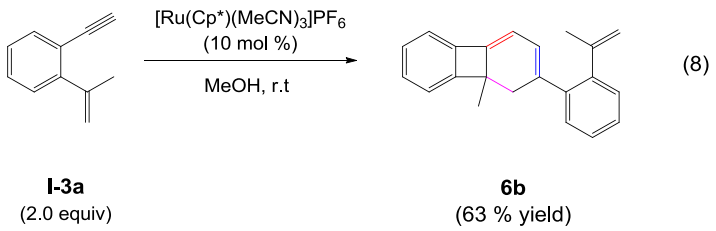


Figure S7. Free energy profiles for **2cat**-catalyzed [2+2+2] dimerization of **1a** (blue) and [2+2+2] cocyclization of **1a** with **2a** (red) in MeOH and THF. Energies are relative to **2cat** and are mass balanced.

The rate-determining barriers in THF are about 2.0 kcal/mol higher than those in methanol solvent (e.g. 18.0 in THF vs 16.1 kcal/mol in methanol for **TS1** and 19.3 in THF vs 17.6 kcal/mol in methnaol for **TS1'**), which qualitatively explains the experimental observation of lower yield in THF than in methanol, and indicates that the polarity of solvent might improve the efficiency of the cationic $(RuCp^*)^+$-catalyzed [2+2+2] reaction. Furthermore, as proposed by the experimentalists, the MeOH molecules could play an important role in the precatalyst activation (from **1cat** to **2cat**) and the regeneration of the active catalyst from complex like **IM4**. Thus, the [2+2+2] reaction proceeds more effectively in MeOH than in THF solvent.



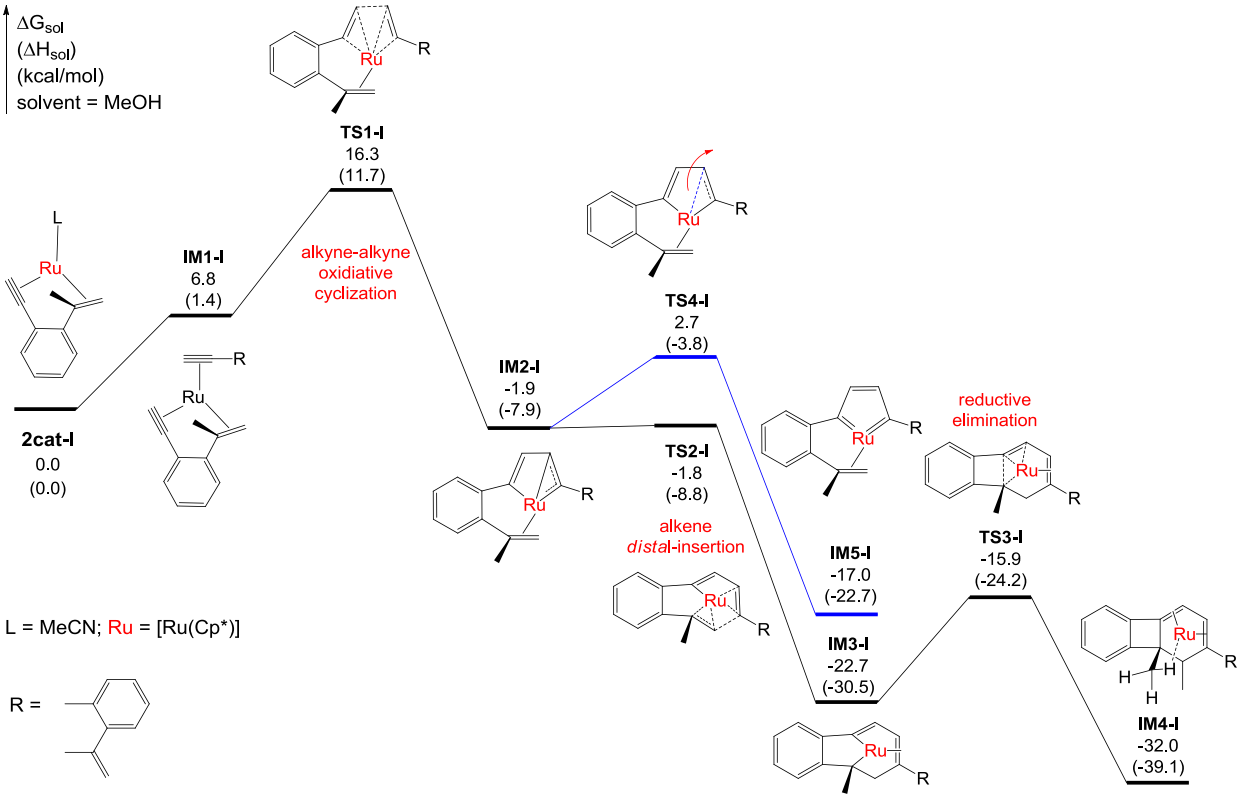
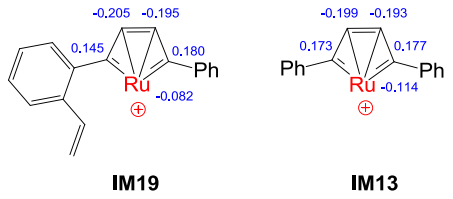


Figure S8. Free energy profile for **2cat-I**-catalyzed [2+2+2] dimerization of **I-3a** to produce **6b**. Energies are relative to **2cat-I** and are mass balanced.

Scheme S5. NBO Charges in **IM19** and **IM13**



IM19 **IM13**

Cartesian Coordinates (Å), SCF Energies, and Free Energies at 298.15 K and 1 atm for the Optimized Structures

1cat

M06/BS1 SCF energy in gas pahse: -882.55628 a.u.

M06/BS2 SCF energy in MeOH: -882.8397352 a.u.

M06/BS2 Free energy in MeOH: -882.5307182 a.u.

Ru	0.00295900	-0.00345700	0.00458900
C	-1.78074700	-0.54762400	-1.10685100
C	-1.80009600	0.85438300	-0.84627900
C	-1.79380900	1.04852500	0.59060200
C	-1.75938300	-1.24596400	0.16295500
C	-1.79862500	-0.25119500	1.19791300
C	-1.89185100	2.36013800	1.29323700
H	-1.35373700	3.14848400	0.75208700
H	-2.93807300	2.68424800	1.39058000
H	-1.46594300	2.31028300	2.30246700
C	-1.86155100	1.94419200	-1.86011600
H	-1.42617000	1.63433900	-2.81758900
H	-2.90252900	2.24273300	-2.04846600
H	-1.32073200	2.83675700	-1.52303600
C	-1.81164400	-1.19779900	-2.44710200
H	-1.26987200	-2.15115800	-2.44407300
H	-2.84601700	-1.40982400	-2.75210400
H	-1.36083300	-0.56143600	-3.21798400
C	-1.81598500	-2.72468200	0.34578800
H	-1.37661600	-3.03036200	1.30298100
H	-2.85216000	-3.09179400	0.32442900
H	-1.26562600	-3.24832300	-0.44595400
C	-1.83347300	-0.52428000	2.66164800
H	-2.87256600	-0.59784600	3.01143600
H	-1.33416500	-1.46848700	2.91046300
H	-1.34830200	0.27409100	3.23591900
C	1.86892000	2.54737300	-0.84156900
C	1.95383600	-1.95902700	-1.74917600
C	1.94254900	-0.49466400	2.58794300
N	1.29577200	-0.31633700	1.64327500
N	1.30185700	-1.24768400	-1.10752900
N	1.25465800	1.61708500	-0.52542600
C	2.63129300	3.71400500	-1.24098000
H	2.42914700	3.95987600	-2.28965500
H	2.36145600	4.57696300	-0.62177500
H	3.70455000	3.52526000	-1.12730400
C	2.76568700	-2.84981600	-2.55458600
H	2.53600500	-3.89482100	-2.31800000
H	2.57294000	-2.68219400	-3.62026300
H	3.82975700	-2.67409200	-2.36078200
C	2.74241400	-0.71846800	3.77593000
H	2.56743800	0.07667000	4.50931600
H	2.48257700	-1.67900200	4.23487000
H	3.80807200	-0.73031100	3.52212700

2cat

M06/BS1 SCF energy in gas pahse: -1002.710266 a.u.

M06/BS2 SCF energy in MeOH: -1003.022206 a.u.

M06/BS2 Free energy in MeOH: -1002.661999 a.u.

Ru	-0.46183200	0.08735400	0.02390800
C	-1.24028100	-1.56790800	-1.28719400
C	-0.74214200	-2.12531500	-0.07433500
C	-1.53797300	-1.59489300	1.01432100
C	-2.29351000	-0.64487000	-0.96157900
C	-2.49656200	-0.69603700	0.46980400
C	-1.45526600	-2.02043900	2.44016100
H	-0.42224000	-2.10917000	2.79970100
H	-1.92064900	-3.00823700	2.56493300
H	-1.98233800	-1.32623300	3.10458000
C	0.27553000	-3.21394700	0.00819300
H	1.17646500	-2.97610900	-0.57282500
H	-0.13535100	-4.15235700	-0.39046100
H	0.58463500	-3.41298700	1.04053200
C	-0.75704300	-1.94327200	-2.64343900
H	-0.97974900	-1.18296200	-3.39966600
H	-1.24185000	-2.87650700	-2.96395200
H	0.32576300	-2.11718700	-2.65211000
C	-3.14949900	0.10749600	-1.92497600
H	-3.33848900	1.13361500	-1.58434400
H	-4.12545100	-0.38215700	-2.04840300
H	-2.69212300	0.16861500	-2.91909400
C	-3.55405000	0.02894100	1.23003400
H	-4.40266100	-0.63498000	1.44603800
H	-3.94266000	0.88291100	0.66361500
H	-3.17710100	0.40835800	2.18835400
C	2.63160800	0.56105000	-0.60166000
C	3.81811600	0.93244500	-1.24334300
C	5.03217100	0.61939400	-0.64950100
C	5.06340300	-0.06062800	0.56882900
C	3.88257000	-0.41859100	1.21158800
C	2.65746700	-0.09221000	0.63505600
H	3.77795100	1.43956100	-2.20544200
H	5.96216200	0.89168900	-1.14356900
H	6.02001800	-0.31106400	1.02278600
H	3.91221900	-0.93829600	2.16888200
C	1.33100800	0.75248400	-1.16874100
C	0.33078000	0.96374800	-1.87650900
H	-0.28929500	1.27045800	-2.70039900
C	1.36172400	-0.36840600	1.30497600
C	0.60486100	0.64363600	1.90077800
H	-0.06254700	0.42454900	2.73589400
H	0.94770600	1.67665800	1.83240600
H	1.25066900	-1.38170000	1.69889500
C	-1.43940000	3.16943900	0.34562500

C	-1.88711200	4.54199600	0.46975800
H	-1.84827200	4.86233200	1.51667300
H	-2.91691800	4.64241100	0.10969300
H	-1.24386300	5.20143100	-0.12333700
N	-1.07626100	2.07415800	0.25022900

IM1

M06/BS1 SCF energy in gas pahse: -1178.186985 a.u.

M06/BS2 SCF energy in MeOH: -1178.543962 a.u.

M06/BS2 Free energy in MeOH: -1178.121289 a.u.

Ru	0.09509300	0.35367000	0.38441200
C	-1.09722200	1.72538300	-1.00526400
C	-0.14516100	2.50534600	-0.26757000
C	1.16319100	2.08275700	-0.66794200
C	-0.38395100	0.76759200	-1.79187500
C	1.02759400	0.99861300	-1.58455300
C	2.44687200	2.71754400	-0.26927200
H	2.37968200	3.21633200	0.70354100
H	2.71948100	3.48086100	-1.01233900
H	3.27219400	1.99705800	-0.22450100
C	-0.47028700	3.66685700	0.60782400
H	-1.43677400	3.53639800	1.10845200
H	-0.52975000	4.59310900	0.01898900
H	0.28999700	3.82408500	1.38246500
C	-2.56078000	1.98931700	-1.02417100
H	-3.13724600	1.15538800	-1.43646500
H	-2.75573700	2.87585600	-1.64475900
H	-2.95159900	2.20287100	-0.02172800
C	-0.95496200	-0.09967100	-2.86109400
H	-0.46356900	-1.07929600	-2.91863300
H	-0.81526600	0.38098000	-3.84053500
H	-2.02902900	-0.26740300	-2.72937100
C	2.13485600	0.40575000	-2.38544500
H	2.34146700	1.04594600	-3.25567000
H	1.88665800	-0.59098700	-2.76756800
H	3.06673600	0.32037900	-1.81255500
C	-1.95808100	-0.05495500	1.18292900
C	-1.33854400	0.64585000	2.02059200
C	2.06057600	0.10175900	1.55594500
C	1.35877300	0.90758000	2.18640200
H	-1.22445200	1.15185100	2.96559300
H	1.07797000	1.59739500	2.96222700
C	-3.09371000	-0.77005500	0.65680200
C	-4.33125600	-0.59364400	1.29577400
C	-3.01789600	-1.60855500	-0.46176100
C	-5.46181400	-1.24135000	0.81937100
H	-4.39163700	0.05743700	2.16679300
C	-4.15267200	-2.25573300	-0.93332800
H	-2.06032700	-1.74656000	-0.96256400
C	-5.37634900	-2.07220000	-0.29583700
H	-6.41685400	-1.09683300	1.32019200
H	-4.08269200	-2.90789900	-1.80163000
H	-6.26520500	-2.57791100	-0.66695100
C	2.97375000	-0.81347100	0.94206200
C	2.41509000	-1.68967800	-0.00327100
C	4.34762400	-0.81251300	1.19238800
C	3.24892800	-2.53753000	-0.72257900
C	5.16862000	-1.67213100	0.46989500
H	4.76497700	-0.12653400	1.92727700
C	4.62232500	-2.52589900	-0.48551800
H	2.82454900	-3.21329700	-1.46520900
H	6.24193100	-1.66677900	0.64511300
H	5.27177000	-3.18760900	-1.05467400
C	0.94523300	-1.68998000	-0.15382900
C	0.10313500	-1.80911600	0.95442500
H	0.55994900	-2.00789100	-1.12691500
H	-0.88426500	-2.24876000	0.84054600
H	0.51965600	-1.88686900	1.96012800

TS1

M06/BS1 SCF energy in gas pahse: -1178.175622 a.u.

M06/BS2 SCF energy in MeOH: -1178.530488 a.u.

M06/BS2 Free energy in MeOH: -1178.106376 a.u.

Ru	0.12088800	0.38743300	0.23244300
C	-0.93455300	2.31663700	-0.36711500
C	0.02646200	2.58696300	0.66724800
C	1.33693700	2.29085000	0.15904200
C	-0.23310200	1.78462100	-1.48725900
C	1.18555600	1.79824100	-1.16706200
C	2.63581000	2.52048900	0.84974600
H	2.52938200	2.52878200	1.94030800
H	3.05891000	3.49130900	0.55479300
H	3.37207000	1.74948800	0.59058200
C	-0.27780300	3.21273600	1.98448500
H	-1.29675500	2.98530000	2.31884800
H	-0.19589200	4.30644400	1.91339700
H	0.42039100	2.88803000	2.76587500
C	-2.39333200	2.59369700	-0.25721000
H	-2.96165200	2.15007000	-1.08128500
H	-2.57461200	3.67744300	-0.27036200
H	-2.81379200	2.20224400	0.67852400
C	-0.79986600	1.47583600	-2.83232200
H	-0.48492200	0.49405300	-3.21117500
H	-0.47168400	2.22363700	-3.56794400
H	-1.89513400	1.48947600	-2.82401400
C	2.30763300	1.56697500	-2.12180200
H	2.75479300	2.53129700	-2.40217600
H	1.97122800	1.08799100	-3.04850500
H	3.10743500	0.95096700	-1.69007400
C	-1.76873800	-0.43817200	0.93351500
C	-1.16914900	-0.02240000	1.98404900
C	1.55079200	-0.76342300	1.40955500
C	0.83950100	-0.20459100	2.29582300
H	-1.34400700	0.44723400	2.94211000
H	0.83303500	0.29596600	3.25287000
C	-2.95963400	-1.04470000	0.39507800

C	-3.71693300	-1.87616800	1.23680600
C	-3.40325000	-0.81792600	-0.91592700
C	-4.89083600	-2.45471500	0.77676700
H	-3.36690900	-2.06366700	2.25079500
C	-4.58271200	-1.39265100	-1.36709400
H	-2.81813200	-0.17845800	-1.57727700
C	-5.32778400	-2.21336700	-0.52348200
H	-5.46960300	-3.09810600	1.43612200
H	-4.92248200	-1.20390600	-2.38341700
H	-6.24919200	-2.66740800	-0.88189300
C	2.55103300	-1.51710100	0.72407900
C	2.35665800	-1.59164800	-0.66366500
C	3.67327600	-2.10043700	1.32054300
C	3.32828100	-2.17777200	-1.46844700
C	4.62429300	-2.70666200	0.50986900
H	3.80712500	-2.04731000	2.39909500
C	4.46012200	-2.73241200	-0.87602000
H	3.18970900	-2.22373400	-2.54856100
H	5.51279400	-3.14644100	0.95744600
H	5.22100100	-3.19665100	-1.49981600
C	1.05401900	-1.11802900	-1.16785800
C	-0.15669800	-1.63140000	-0.67148400
H	1.04807300	-0.73924300	-2.19261900
H	-1.03139900	-1.64817500	-1.31866000
H	-0.14476200	-2.39453500	0.11038600

IM2

M06/BS1 SCF energy in gas pahse: -1178.215746 a.u.

M06/BS2 SCF energy in MeOH: -1178.564037 a.u.

M06/BS2 Free energy in MeOH: -1178.134849 a.u.

Ru	-0.04170000	0.20612900	-0.11061400
C	1.02991400	2.27452300	-0.11827500
C	0.17419800	2.10488000	-1.27768800
C	-1.18717300	2.03453800	-0.83881800
C	0.21065600	2.22312100	1.02672500
C	-1.17255900	2.07841500	0.58147500
C	-2.39890700	1.97964300	-1.70444400
H	-2.19789000	1.46498000	-2.65190500
H	-2.75249000	2.99223700	-1.94567700
H	-3.22147500	1.44938300	-1.20865700
C	0.61597700	2.19354600	-2.69801800
H	1.67014600	1.91699100	-2.82055400
H	0.50828400	3.22571900	-3.06235100
H	0.01354500	1.55400100	-3.35565700
C	2.49743000	2.52973000	-0.18994300
H	2.97904300	2.45376500	0.79134800
H	2.69182600	3.54148800	-0.57302700
H	3.00876000	1.82681200	-0.86130300
C	0.62055000	2.40423300	2.44897700
H	0.21821900	1.61652600	3.10251500
H	0.25299800	3.36228600	2.84329800
H	1.71047900	2.40430500	2.56312700
C	-2.38280500	2.23111800	1.43895100
H	-2.80029700	3.23996600	1.31065600
H	-2.15580000	2.11288200	2.50528400
H	-3.17498800	1.51829200	1.17467300
C	1.51440600	-0.90197100	-0.51557500
C	0.85193500	-1.01451100	-1.74873800
C	-1.23265600	-1.20670100	-1.01659100
C	-0.45181600	-1.67901500	-1.99058900
H	1.39547900	-0.56852500	-2.59619700
H	-0.62673700	-2.39876100	-2.79280700
C	2.84428300	-1.16097100	-0.08601300
C	3.68178400	-2.00254700	-0.84970000
C	3.33631800	-0.60229700	1.11228200
C	4.97557000	-2.26154600	-0.43125800
H	3.29306900	-2.44208300	-1.76744100
C	4.62771700	-0.86734900	1.52762600
H	2.67568200	0.04232800	1.69209000
C	5.44528400	-1.69609500	0.75484200
H	5.62187000	-2.90687700	-1.02157300
H	5.00793400	-0.43833900	2.45191900
H	6.46100900	-1.90653500	1.08421000
C	-2.51973800	-1.49914900	-0.41208500
C	-2.54973300	-1.20126300	0.96083200
C	-3.65144000	-2.01435800	-1.04015500
C	-3.71637700	-1.38741800	1.69256200
C	-4.81618000	-2.20735200	-0.29997200
H	-3.62703500	-2.23734900	-2.10624100
C	-4.85048900	-1.89258100	1.05596000
H	-3.74150000	-1.14797200	2.75597500
H	-5.70896200	-2.59236500	-0.78841500
H	-5.76844300	-2.03532400	1.62214700
C	-1.29105300	-0.69267000	1.55945500
C	-0.07024900	-1.37716000	1.52999200
H	-1.40231500	0.05949200	2.34444500
H	0.70291200	-1.13784300	2.25987200
H	-0.00762100	-2.37191800	1.08634700

TS2

M06/BS1 SCF energy in gas pahse: -1178.214175 a.u.

M06/BS2 SCF energy in MeOH: -1178.562779 a.u.

M06/BS2 Free energy in MeOH: -1178.134642 a.u.

Ru	-0.06572800	0.21189000	-0.15687500
C	0.97932300	2.24046000	-0.35137100
C	0.44474100	2.20339200	0.95566800
C	-0.99282700	2.05371000	0.83625000
C	-0.12748300	2.11247300	-1.29040900
C	-1.34405100	2.05062500	-0.54534600
C	-1.96561000	2.12216500	1.96291600
H	-1.49897100	1.89363800	2.92859900
H	-2.37622800	3.13936600	2.03683800
H	-2.81452100	1.44070000	1.81955800
C	1.16518100	2.37792900	2.24956100
H	2.25136900	2.41716400	2.10955700
H	0.86765500	3.31702100	2.73727700

H	0.94628600	1.56752500	2.96068600
C	2.40034400	2.45236000	-0.75075200
H	2.69066100	1.80916400	-1.59214300
H	2.55884000	3.49144100	-1.07185200
H	3.09685000	2.24838500	0.07003200
C	-0.02152000	2.18436900	-2.77553900
H	-0.77897500	1.56175400	-3.26710200
H	-0.17002500	3.21760400	-3.12118600
H	0.96283100	1.86112000	-3.13401900
C	-2.72888900	2.01438900	-1.09507400
H	-3.14413900	3.03013800	-1.15860300
H	-2.75410200	1.58246700	-2.10258300
H	-3.40424500	1.42032300	-0.46517900
C	-1.09869200	-0.85581900	1.41045600
C	0.09779300	-1.61202500	1.13139700
H	-0.01410800	-2.56476100	0.60446900
H	0.88702400	-1.59058300	1.88223000
C	1.44268300	-1.02654900	-0.44331500
C	0.85428800	-1.16658400	-1.71197200
H	-1.07222400	-0.30157400	2.35383700
C	-2.44757500	-1.25309600	0.93455500
C	-2.57373000	-1.40998800	-0.45833400
C	-3.54041700	-1.46352800	1.76508600
C	-3.78301900	-1.81450100	-1.01377000
C	-4.75957200	-1.84556100	1.20168200
H	-3.44547200	-1.33707800	2.84400300
C	-4.87740200	-2.02358900	-0.17423400
H	-3.87871200	-1.93421800	-2.09204300
H	-5.62368300	-2.00298200	1.84355800
H	-5.83497400	-2.31553600	-0.60041600
C	-1.30850900	-1.11778700	-1.10721500
C	-0.50266500	-1.65275300	-2.03115400
H	-0.69909700	-2.35493100	-2.84477200
C	2.81354400	-1.18555100	-0.03781700
C	3.31776400	-0.53528200	1.10299400
C	3.66961000	-2.01282600	-0.78782700
C	4.64418500	-0.68878800	1.46862600
H	2.64871400	0.08893200	1.69598800
C	5.00025700	-2.15434900	-0.42532900
H	3.27446800	-2.54050100	-1.65504100
C	5.48725400	-1.49373400	0.70089000
H	5.02913300	-0.18545000	2.35283300
H	5.65883100	-2.78842000	-1.01455800
H	6.52978600	-1.61290600	0.98876600
H	1.52903900	-0.87833600	-2.52997800

IM3

M06/BS1 SCF energy in gas pahse: -1178.257594 a.u.

M06/BS2 SCF energy in MeOH: -1178.607095 a.u.

M06/BS2 Free energy in MeOH: -1178.173094 a.u.

Ru	0.18922100	0.47023700	0.32371700
C	-1.37118200	1.86593400	-0.72177800
C	-0.64506500	2.58227200	0.26557900
C	0.75659700	2.56503000	-0.10019700
C	-0.42963000	1.33864500	-1.66164800
C	0.89694900	1.79579700	-1.29476100
C	1.84569200	3.28148500	0.62369800
H	1.67054700	3.30347600	1.70669400
H	1.91069800	4.32466900	0.28328300
H	2.82401100	2.81671500	0.45331000
C	-1.21615800	3.26826400	1.46060700
H	-2.15037500	2.79582800	1.78873800
H	-1.43869000	4.32227500	1.24244200
H	-0.52101300	3.25380300	2.30982100
C	-2.84590100	1.67627600	-0.79351900
H	-3.11504100	0.64373800	-1.05634800
H	-3.27448700	2.33413000	-1.56314800
H	-3.33929200	1.91671800	0.15509000
C	-0.80824100	0.62478800	-2.91249800
H	0.03869200	0.10261300	-3.37187500
H	-1.18194900	1.34473900	-3.65490600
H	-1.61195100	-0.10253800	-2.73717500
C	2.14512600	1.61155300	-2.08769900
H	2.26928700	2.42515800	-2.81595800
H	2.13883000	0.66857900	-2.64807100
H	3.03586100	1.60045500	-1.44700300
C	-0.99145200	-1.37082400	0.87727700
C	-0.66384700	-0.62801600	2.04602300
C	1.59733700	-0.34065600	1.33510000
C	0.66540700	-0.19365800	2.37766700
H	-1.46499200	-0.20285400	2.65179600
H	0.82999300	0.38018500	3.29308000
C	-2.40883000	-1.51552900	0.46884600
C	-3.47937000	-1.20726200	1.32083100
C	-2.71576000	-1.96059600	-0.82697500
C	-4.79514700	-1.33014000	0.89234900
H	-3.29966900	-0.89657600	2.34860900
C	-4.03166900	-2.07507400	-1.25917900
H	-1.91476800	-2.20857700	-1.52291900
C	-5.07964700	-1.75690100	-0.40135500
H	-5.60532500	-1.09904800	1.58108500
H	-4.23717800	-2.41951300	-2.27093200
H	-6.11083600	-1.85116500	-0.73443500
C	2.75071600	-0.96050400	0.78083600
C	2.36733600	-1.42729900	-0.50291500
C	4.03639000	-1.17926700	1.28895200
C	3.32071900	-2.01704100	-1.32498500
C	4.97203100	-1.76781600	0.45160800
H	4.30771300	-0.84535000	2.28834200
C	4.61975200	-2.16731200	-0.84402300
H	3.05143000	-2.37533000	-2.31835700
H	5.99294900	-1.91081400	0.79804000
H	5.37476400	-2.62438600	-1.48081700
C	0.90035300	-1.33328600	-0.70803800
C	0.05085800	-2.25319700	0.18906700
H	0.57635900	-1.34895700	-1.75549000
H	-0.42507700	-3.07606200	-0.35928500

H	0.68359800	-2.71631700	0.95966100

TS3

M06/BS1 SCF energy in gas pahse: -1178.244271 a.u.

M06/BS2 SCF energy in MeOH: -1178.594498 a.u.

M06/BS2 Free energy in MeOH: -1178.16251 a.u.

Ru	-0.13518800	0.57590400	-0.26305100
C	1.51457200	1.90222200	0.56235700
C	0.63316700	1.47300500	1.60792000
C	-0.69089500	1.98924100	1.32463000
C	0.73969300	2.61124000	-0.40200000
C	-0.62042200	2.69349500	0.08526500
C	-1.88335200	1.86774200	2.21083600
H	-1.89823700	0.91162300	2.74853300
H	-1.89083000	2.66591800	2.96644200
H	-2.82030800	1.93978500	1.64562200
C	1.05641300	0.76966800	2.85227000
H	1.86187800	0.05072000	2.65604700
H	1.43749400	1.49129800	3.58911900
H	0.22742900	0.23418800	3.33115300
C	2.97579800	1.62816600	0.50187700
H	3.36816200	1.72592400	-0.51722200
H	3.52274700	2.34005900	1.13641300
H	3.21808400	0.61738800	0.85578900
C	1.24563900	3.22396300	-1.66378300
H	0.49021200	3.20043600	-2.45919500
H	1.52295700	4.27597800	-1.50766700
H	2.13474600	2.70182200	-2.03794500
C	-1.73630900	3.41873500	-0.58598900
H	-1.73952300	4.47834700	-0.29332100
H	-1.64473900	3.38289700	-1.67837600
H	-2.71377000	2.99921800	-0.31933500
C	-1.09473100	-1.39574300	0.54468800
C	-0.11043500	-2.34271500	-0.11374700
H	-0.59902400	-2.94413700	-0.89533300
H	0.33998600	-3.04968100	0.59217600
C	0.94622500	-1.44656900	-0.77104700
C	0.56651200	-0.71384400	-1.91772300
H	-0.74891200	-1.08430000	1.53861600
C	-2.58171100	-1.59961000	0.44924300
C	-2.97439800	-0.85041300	-0.65902000
C	-3.49338800	-2.37705200	1.14518900
C	-4.27817600	-0.84538100	-1.13850000
C	-4.81696400	-2.34858500	0.70121500
H	-3.20346800	-2.97967900	2.00436100
C	-5.20086400	-1.59835400	-0.41560700
H	-4.57746900	-0.27597300	-2.01564800
H	-5.57133900	-2.92378800	1.23419100
H	-6.24305100	-1.60837200	-0.72735400
C	-1.65840200	-0.37836000	-1.04323200
C	-0.80037400	-0.36382200	-2.16039000
H	-1.10620500	0.06187300	-3.11857500
H	1.31662500	-0.33358900	-2.61150200
C	2.36528700	-1.64546000	-0.42044700
C	2.71235100	-2.04249700	0.88077200
C	3.40200300	-1.43517800	-1.34090200
C	4.04044600	-2.20924600	1.25240100
H	1.93249300	-2.20388500	1.62593600
C	4.72958500	-1.61340200	-0.97278400
H	3.17723900	-1.16172600	-2.37065400
C	5.05631600	-1.99504200	0.32547300
H	4.28197100	-2.51213900	2.26937500
H	5.51464000	-1.46288500	-1.71114900
H	6.09695900	-2.13433800	0.60998400

IM4

M06/BS1 SCF energy in gas pahse: -1178.263548 a.u.

M06/BS2 SCF energy in MeOH: -1178.616856 a.u.

M06/BS2 Free energy in MeOH: -1178.183666 a.u.

Ru	-0.08403200	0.53413800	-0.11213800
C	1.47978300	2.00503900	0.38613300
C	0.68457700	1.74041300	1.54136800
C	-0.68421100	2.14009100	1.24701600
C	0.60759800	2.51710000	-0.64036900
C	-0.72216400	2.63802900	-0.08639500
C	-1.83096200	2.06163400	2.19612500
H	-1.73222800	1.21104200	2.88244200
H	-1.89375700	2.96981400	2.81234700
H	-2.78725500	1.95060800	1.67017800
C	1.17821200	1.23501000	2.85404800
H	2.06927600	0.60729200	2.73608300
H	1.44756500	2.07112700	3.51513200
H	0.41716200	0.64081200	3.37490000
C	2.94264300	1.76256300	0.25679400
H	3.23151800	1.54477800	-0.77882900
H	3.51209100	2.64476100	0.58163700
H	3.26570100	0.91001300	0.86781000
C	1.02108400	2.96813700	-1.99930800
H	0.23238300	2.79942600	-2.74315300
H	1.24397400	4.04445700	-1.99935900
H	1.92407400	2.45077600	-2.34416200
C	-1.91397200	3.17158200	-0.80293600
H	-1.96618900	4.26576000	-0.71215100
H	-1.88143800	2.93403400	-1.87362100
H	-2.84789500	2.76235100	-0.39930700
C	-1.18985800	-1.55896300	0.20305600
C	-0.00730300	-2.45405000	-0.09072500
H	-0.24433700	-3.25132900	-0.81259700
H	0.37757500	-2.93611300	0.81401200
C	1.03424300	-1.49539300	-0.68936700
C	0.64301600	-0.71172000	-1.78709800
H	-0.84853400	-0.88084100	1.07308400
C	-2.68960000	-1.82926600	0.37398000
C	-3.04848700	-0.97761000	-0.68046400
C	-3.61904600	-2.51265600	1.12583900
C	-4.36562800	-0.73770800	-1.02924400

C	-4.95861300	-2.27294400	0.78169600
H	-3.35981400	-3.19301100	1.93391400
C	-5.31932200	-1.41058600	-0.25705900
H	-4.66095100	-0.09228600	-1.85363400
H	-5.74572700	-2.77272600	1.34299100
H	-6.37563900	-1.26812200	-0.47599000
C	-1.63451000	-0.74775500	-1.01276900
C	-0.74759000	-0.42863000	-2.03546900
H	-1.05927800	0.10351000	-2.93307400
H	1.38699900	-0.24453200	-2.43218800
C	2.45674800	-1.66409600	-0.34139800
C	2.82812000	-1.92972500	0.98548900
C	3.47088400	-1.53205400	-1.29947600
C	4.16465100	-2.03602800	1.34624000
H	2.05972100	-2.02536500	1.75418300
C	4.80848900	-1.64785900	-0.93999600
H	3.21451900	-1.37111400	-2.34612300
C	5.16115200	-1.89293400	0.38367200
H	4.42992700	-2.23617200	2.38259300
H	5.57963100	-1.55585400	-1.70226000
H	6.20870800	-1.98291700	0.66289700

TS4

M06/BS1 SCF energy in gas pahse: -1178.208558 a.u.

M06/BS2 SCF energy in MeOH: -1178.555987 a.u.

M06/BS2 Free energy in MeOH: -1178.128592 a.u.

Ru	-0.03925100	0.14682000	-0.01739500
C	1.03632100	2.04534800	-0.69772700
C	-0.06237800	1.72147800	-1.60483400
C	-1.29023100	1.87618900	-0.88788800
C	0.47588000	2.35731400	0.56129900
C	-0.96448500	2.23094900	0.44819100
C	-2.66076400	1.74187700	-1.45866800
H	-2.67850900	1.05390100	-2.31308900
H	-3.02967000	2.71498500	-1.81305900
H	-3.38020800	1.36638000	-0.71954700
C	0.04266800	1.42960000	-3.06050500
H	1.06918200	1.18586700	-3.35678800
H	-0.28001800	2.29679300	-3.65471700
H	-0.59931500	0.58446600	-3.34688500
C	2.46643000	2.15541900	-1.10654100
H	3.14454600	2.10667200	-0.24649100
H	2.64700900	3.10865200	-1.62249800
H	2.75954700	1.34992200	-1.79217700
C	1.17902600	2.81855100	1.79252000
H	0.89605700	2.22353300	2.67370000
H	0.92761100	3.86451500	2.02036200
H	2.26833900	2.76292100	1.68784500
C	-1.94170600	2.64831200	1.49208500
H	-2.23368800	3.69541000	1.32456700
H	-1.51900800	2.59451800	2.50279800
H	-2.86237600	2.05114700	1.46778000
C	1.47968500	-1.07779200	-0.38241100
C	0.92412700	-1.66839800	-1.54223000
C	-1.20407000	-1.31174500	-0.76406800
C	-0.45740500	-2.02327900	-1.65907700
H	1.59112700	-1.77507100	-2.41107100
H	-0.78120500	-2.83154800	-2.31873700
C	2.84891100	-1.15994000	0.03474200
C	3.75191800	-2.06782500	-0.55907200
C	3.30985800	-0.34443900	1.08885600
C	5.06925500	-2.12436900	-0.13872800
H	3.40714400	-2.72948800	-1.35265900
C	4.62730300	-0.40348200	1.50868300
H	2.59701400	0.32631100	1.56992300
C	5.50901800	-1.29126900	0.89142600
H	5.76011700	-2.82336000	-0.60469300
H	4.97211200	0.22843500	2.32429600
H	6.54382300	-1.34427900	1.22392900
C	-2.53416300	-1.46231100	-0.22029000
C	-2.61789200	-0.98900800	1.10525900
C	-3.66134800	-1.98776600	-0.85237800
C	-3.83428700	-1.00898600	1.77388600
C	-4.87656700	-2.00897400	-0.17382900
H	-3.59157100	-2.34525300	-1.87940500
C	-4.96284300	-1.51802500	1.12736100
H	-3.90632200	-0.63926900	2.79682800
H	-5.76612100	-2.39650700	-0.66572700
H	-5.91916900	-1.52964300	1.64620100
C	-1.36063200	-0.47983800	1.70642400
C	-0.17542700	-1.21991100	1.78746600
H	-1.46160100	0.35707300	2.40205300
H	0.59589300	-0.92236900	2.49847900
H	-0.14090800	-2.26085500	1.46443000

IM5

M06/BS1 SCF energy in gas pahse: -1178.238096 a.u.

M06/BS2 SCF energy in MeOH: -1178.585825 a.u.

M06/BS2 Free energy in MeOH: -1178.157847 a.u.

Ru	-0.04273100	0.10916700	0.24322600
C	1.27311900	1.78723400	-0.66680200
C	0.64495100	1.00136300	-1.69806500
C	-0.77460500	1.23002900	-1.62171300
C	0.24216000	2.41032400	0.09303200
C	-1.02414400	2.10148700	-0.52799900
C	-1.77518900	0.70522700	-2.59261500
H	-1.57574500	-0.34377200	-2.85424500
H	-1.74218400	1.28186900	-3.52777600
H	-2.79851000	0.76067300	-2.20267700
C	1.33308500	0.27922400	-2.80610500
H	2.33494200	-0.05763700	-2.51433800
H	1.44851600	0.93409000	-3.68177100
H	0.76167500	-0.60052000	-3.12894700
C	2.73292000	2.06782100	-0.55595800
H	3.03893100	2.29932100	0.47091700
H	2.98053600	2.94310400	-1.17531100

H	3.35070700	1.23457200	-0.90864700
C	0.45239300	3.34092000	1.24052400
H	-0.40248300	3.35178200	1.92780500
H	0.59784300	4.37381900	0.89204400
H	1.34043600	3.06611400	1.82424800
C	-2.34036800	2.71437400	-0.19062300
H	-2.52153200	3.58586200	-0.83568900
H	-2.38248900	3.07282800	0.84483400
H	-3.17585000	2.01925900	-0.34146800
C	1.29141300	-1.37696200	0.12724400
C	0.80598400	-2.62184500	-0.37701400
C	-1.17117200	-1.41715100	-0.24479000
C	-0.54294800	-2.63179000	-0.63927900
H	1.43850700	-3.50608300	-0.48025300
H	-1.08931900	-3.53070600	-0.93228000
C	2.71255100	-1.17577700	0.31260100
C	3.66832800	-1.73366500	-0.56274900
C	3.16739700	-0.41297000	1.40627900
C	5.01963300	-1.49808200	-0.37128200
H	3.33370200	-2.32652300	-1.41428400
C	4.52341400	-0.20905200	1.61606500
H	2.43145000	-0.01349200	2.10547600
C	5.44889400	-0.74027000	0.72114800
H	5.74799000	-1.91343900	-1.06459200
H	4.86256900	0.36170200	2.47810900
H	6.51293700	-0.57659300	0.88015600
C	-2.57794100	-1.30342900	0.03517200
C	-2.86180900	-0.39687000	1.08554700
C	-3.62513000	-1.96756700	-0.62319300
C	-4.18586200	-0.09951000	1.40214300
C	-4.93616900	-1.67588700	-0.28694900
H	-3.40447200	-2.66496700	-1.43109600
C	-5.21303400	-0.73936300	0.71661700
H	-4.41133200	0.61197900	2.19620600
H	-5.75521200	-2.16171600	-0.81248000
H	-6.24756800	-0.51523100	0.96916700
C	-1.71408800	0.19974100	1.78593000
C	-0.62720200	-0.51880500	2.30417600
H	-1.84935800	1.22352700	2.14528700
H	0.01143100	-0.01760100	3.03389800
H	-0.63547000	-1.60805200	2.34772400

TS5

M06/BS1 SCF energy in gas pahse: -1178.150255 a.u.

M06/BS2 SCF energy in MeOH: -1178.499822 a.u.

M06/BS2 Free energy in MeOH: -1178.072446 a.u.

Ru	-0.06663100	0.28348400	0.13413300
C	1.27157800	2.17157000	0.43596500
C	1.46940800	1.63436600	-0.87753300
C	0.21905900	1.67204500	-1.58936000
C	-0.10335100	2.52121800	0.55015300
C	-0.76611600	2.20958400	-0.70376800
C	0.02252600	1.26793500	-3.01070500
H	0.58637500	0.35689800	-3.25062500
H	0.36183200	2.05684900	-3.69701600
H	-1.03241400	1.06606300	-3.23033500
C	2.77895100	1.31310100	-1.50835000
H	3.52342800	0.95536800	-0.78893200
H	3.17956800	2.22292400	-1.97854400
H	2.68097500	0.55628400	-2.29586800
C	2.31652800	2.45028800	1.46201600
H	1.95836200	2.23010400	2.47665900
H	2.59970700	3.51276200	1.44253100
H	3.22777100	1.86524900	1.29402200
C	-0.72028600	3.17586800	1.73994900
H	-1.81152000	3.07166400	1.75718800
H	-0.49810700	4.25273800	1.74108500
H	-0.32545600	2.76617400	2.67904400
C	-2.19025600	2.49646500	-1.04742800
H	-2.28859000	3.48396700	-1.51947000
H	-2.83918200	2.49105700	-0.16256900
H	-2.59312900	1.75362400	-1.74701700
C	1.10357700	-1.30889800	-0.25517100
C	0.44924900	-2.44162900	-0.80243200
C	-1.51611600	-1.12219500	-0.46798600
C	-0.91581900	-2.34975100	-0.88889800
H	0.97271300	-3.38404300	-0.97751600
H	-1.53550100	-3.16778500	-1.26329300
C	2.52761600	-1.41297200	0.02312400
C	3.38614300	-2.07418600	-0.87517100
C	3.07563600	-0.86115500	1.19408400
C	4.74905700	-2.14382400	-0.62819400
H	2.97940900	-2.49831700	-1.79326900
C	4.43335800	-0.96560400	1.45756900
H	2.40968500	-0.36599100	1.89984600
C	5.27445400	-1.59478800	0.54040600
H	5.40610100	-2.63391200	-1.34339400
H	4.84125500	-0.55526000	2.37959100
H	6.34187900	-1.66314000	0.74028200
C	-3.01203700	-1.03385900	-0.43675700
C	-3.08112700	-1.02833100	0.95005400
C	-4.14134300	-1.12913400	-1.22288700
C	-4.25708400	-1.14713900	1.65575800
C	-5.35939600	-1.21398200	-0.52929700
H	-4.10864500	-1.16041700	-2.31053400
C	-5.41349500	-1.23584100	0.86315100
H	-4.30746300	-1.17878200	2.74149000
H	-6.28763200	-1.28271200	-1.09290700
H	-6.38228600	-1.32039200	1.35149900
C	-1.59212500	-0.76868600	1.19904000
C	-0.38707000	-1.04034800	1.94381000
H	-1.65525000	0.39855600	1.21379200
H	-0.22964200	-0.49477100	2.87568200
H	0.02840600	-2.04877600	1.92986100

IM6

M06/BS1 SCF energy in gas pahse: -1178.153338 a.u.

M06/BS2 SCF energy in MeOH: -1178.508841 a.u.

M06/BS2 Free energy in MeOH: -1178.083067 a.u.

Ru	-0.08346300	0.35189600	0.06886300
C	1.27924300	2.00402200	0.62146300
C	1.53567500	1.72461500	-0.76609700
C	0.33096200	1.93678600	-1.50355100
C	-0.09586400	2.41479800	0.72802800
C	-0.69166500	2.35839800	-0.58973400
C	0.18444900	1.73318100	-2.96944400
H	0.65005100	0.79098600	-3.28895300
H	0.67856000	2.54314100	-3.52548400
H	-0.86683400	1.71200200	-3.27648700
C	2.85733000	1.42944500	-1.38215400
H	3.58012100	1.02468000	-0.66561000
H	3.27446900	2.36197800	-1.78956900
H	2.77258100	0.71856900	-2.21311000
C	2.27986000	2.08760200	1.71926500
H	1.84769200	1.79415300	2.68427100
H	2.63881500	3.12237400	1.82127800
H	3.14988900	1.44954900	1.53392200
C	-0.74035500	2.88337700	1.98733200
H	-1.83455200	2.85201900	1.93190600
H	-0.45009000	3.92196400	2.20165200
H	-0.42775800	2.27455400	2.84531200
C	-2.08576200	2.74391800	-0.96158700
H	-2.11710400	3.76144300	-1.37469700
H	-2.76034500	2.72017500	-0.09713900
H	-2.50165800	2.06611900	-1.71807400
C	1.22591400	-1.21287700	-0.41697900
C	0.57822500	-2.07869400	-1.24189800
C	-1.73535200	-1.40958700	-0.59199100
C	-0.84562400	-1.97930300	-1.45652700
H	1.08326400	-2.95927700	-1.65214500
H	-1.26877300	-2.46063100	-2.34321500
C	2.61672700	-1.40398800	-0.02870200
C	3.56103100	-1.88828300	-0.95022800
C	3.03991800	-1.13415900	1.28227800
C	4.88292500	-2.08307400	-0.57557200
H	3.25150500	-2.08565100	-1.97662600
C	4.35943600	-1.34487500	1.65983500
H	2.31344900	-0.76408500	2.00552100
C	5.28642700	-1.81051600	0.72978300
H	5.60390800	-2.44780400	-1.30448200
H	4.66865900	-1.14403300	2.68406900
H	6.32317200	-1.96292300	1.02277100
C	-3.20350600	-1.35413400	-0.46925300
C	-3.16059600	-1.03406400	0.89471600
C	-4.40103000	-1.56939200	-1.12762300
C	-4.28207600	-0.91470600	1.68372000
C	-5.55361000	-1.44377500	-0.34284000
H	-4.46349900	-1.83896100	-2.17981700
C	-5.49812200	-1.13172100	1.01824400
H	-4.25302400	-0.67907700	2.74508600
H	-6.52707300	-1.60217200	-0.80284400
H	-6.42825500	-1.05501600	1.57761500
C	-1.63373400	-0.92311300	0.87598100
C	-0.45628000	-1.12479200	1.68626500
H	-1.68343000	0.34140500	0.77207400
H	-0.47395500	-0.72807800	2.70394700
H	0.08528900	-2.06134100	1.57248100

TS6

M06/BS1 SCF energy in gas pahse: -1178.170293 a.u.

M06/BS2 SCF energy in MeOH: -1178.52546 a.u.

M06/BS2 Free energy in MeOH: -1178.101035 a.u.

Ru	0.39432900	-0.57789900	-0.23304300
C	0.42958600	-2.81908600	0.08188300
C	0.62432900	-2.17090500	1.34284300
C	1.86094000	-1.43557200	1.27124700
C	1.47962700	-2.40438100	-0.80337600
C	2.36914200	-1.53709400	-0.06031100
C	2.57323000	-0.79085900	2.40961600
H	1.91739000	-0.61647000	3.27014000
H	3.38139000	-1.45339300	2.75088600
H	3.03510000	0.16407900	2.12845500
C	-0.22678900	-2.34588200	2.55322000
H	-1.25875000	-2.59950200	2.28264500
H	0.15359000	-3.15529900	3.19263500
H	-0.25869300	-1.43674200	3.16735600
C	-0.65154700	-3.79869300	-0.21811400
H	-0.74675800	-3.99341800	-1.29194400
H	-0.42959600	-4.75813100	0.26949100
H	-1.62797100	-3.46159200	0.15228800
C	1.70982300	-2.90061400	-2.19082900
H	2.31900400	-2.20212800	-2.77568700
H	2.24361700	-3.86098600	-2.17194400
H	0.77037200	-3.06172600	-2.73515500
C	3.66008400	-0.97555800	-0.54624300
H	4.47031200	-1.70713700	-0.41672700
H	3.61729200	-0.71505900	-1.60991700
H	3.93751500	-0.06956300	0.00544800
C	0.45254600	1.07461600	1.09237800
C	-0.95548700	1.06444900	0.67229600
H	-1.23843400	1.94126300	0.08235900
H	-1.65163400	0.84822900	1.48514900
C	-1.97274600	-0.08707200	-0.55961400
C	-1.34638400	-0.94806200	-1.27476600
H	0.59419800	0.77387700	2.13406700
C	1.32783700	2.18653100	0.65680300
C	1.57668300	2.28434000	-0.72177200
C	1.86147800	3.14085100	1.51768100
C	2.29020300	3.36348000	-1.24783400
C	2.59794000	4.20239100	0.99628400
H	1.68904600	3.06278500	2.59128400
C	2.79920300	4.32116200	-0.37838100
H	2.46689000	3.43029900	-2.31946700

H	3.01546800	4.94826200	1.66952400
H	3.37331400	5.15671500	-0.77222500
C	1.10056600	1.17432300	-1.48847500
C	0.74659800	0.28701900	-2.28291400
H	0.54667500	-0.23262100	-3.20341700
C	-3.32606900	0.39023600	-0.28092300
C	-4.16887100	-0.35950500	0.54621600
C	-3.78658500	1.58532900	-0.84218900
C	-5.46321800	0.07827100	0.79873600
H	-3.80341300	-1.29069100	0.98009900
C	-5.08323400	2.01538300	-0.58983500
H	-3.12929900	2.16409300	-1.49146900
C	-5.91989300	1.26518000	0.23239400
H	-6.11825700	-0.51084300	1.43734100
H	-5.44331300	2.93954300	-1.03703000
H	-6.93378600	1.60617200	0.43123200
H	-1.59570500	-1.64413400	-2.06763700

IM7

M06/BS1 SCF energy in gas pahse: -1178.174839 a.u.

M06/BS2 SCF energy in MeOH: -1178.52912 a.u.

M06/BS2 Free energy in MeOH: -1178.102397 a.u.

Ru	0.23742900	-0.55974800	-0.28161400
C	-0.07951600	-2.73783700	0.12745100
C	0.02517800	-2.05871400	1.38900500
C	1.34903700	-1.50303400	1.49156100
C	1.14967800	-2.53060600	-0.57900800
C	2.03744200	-1.75615100	0.27131900
C	1.93100000	-0.85020800	2.69697500
H	1.15915400	-0.49858500	3.39152700
H	2.55125600	-1.57347800	3.24489400
H	2.57630300	-0.00020200	2.44005600
C	-1.01225900	-2.01534700	2.45673700
H	-2.01400200	-2.21327900	2.05968700
H	-0.80836700	-2.76844800	3.23141700
H	-1.04223800	-1.03746200	2.95438000
C	-1.23060700	-3.56752300	-0.32903300
H	-1.27950600	-3.63622500	-1.42211300
H	-1.14222600	-4.59214400	0.05799300
H	-2.19045500	-3.17060400	0.02370200
C	1.52036300	-3.12526700	-1.89419300
H	2.28012500	-2.52906600	-2.41214200
H	1.93910800	-4.13141900	-1.74979000
H	0.65543700	-3.22307200	-2.56187100
C	3.45911500	-1.41984900	-0.02049200
H	4.11686200	-2.25497700	0.25974800
H	3.62226900	-1.21752700	-1.08592400
H	3.78817900	-0.53550900	0.53889100
C	0.46042900	1.25252700	0.77614000
C	-0.75962200	1.77173100	0.00759200
H	-0.43418200	2.43500900	-0.80502100
H	-1.36875300	2.36206400	0.70390100
C	-1.77525800	0.73601400	-0.62326800
C	-1.43308600	-0.35818500	-1.32928100
H	0.25139200	1.11702300	1.84432800
C	1.73923400	1.93911400	0.50174500
C	2.22419100	1.78573900	-0.81040500
C	2.45480700	2.71642000	1.40646300
C	3.37124100	2.45086100	-1.23925000
C	3.61900200	3.35977000	0.98731500
H	2.09807900	2.82890700	2.43052100
C	4.06754800	3.23863700	-0.32688300
H	3.72823100	2.32779800	-2.25989700
H	4.18172600	3.96690600	1.69339600
H	4.97575500	3.74946200	-0.63843600
C	1.47255900	0.85020200	-1.59244600
C	0.87169900	0.10251500	-2.38133700
H	0.55265200	-0.39073300	-3.28102300
C	-3.20215100	0.98731900	-0.29131300
C	-3.70661300	2.29379400	-0.30547600
C	-4.07294500	-0.06813600	-0.00023100
C	-5.04914300	2.53267500	-0.04288100
H	-3.05474400	3.13092700	-0.55539100
C	-5.41451100	0.17352800	0.27081400
H	-3.68722300	-1.08732000	0.03288000
C	-5.90553500	1.47452100	0.25045000
H	-5.43018900	3.55144600	-0.07208100
H	-6.07649100	-0.65744600	0.50644600
H	-6.95492000	1.66584000	0.46483600
H	-2.10776600	-1.03602500	-1.85233100

TS7

M06/BS1 SCF energy in gas pahse: -1178.129005 a.u.

M06/BS2 SCF energy in MeOH: -1178.482946 a.u.

M06/BS2 Free energy in MeOH: -1178.06112 a.u.

Ru	-0.75555000	0.23735300	0.26912700
C	-2.84662700	0.71047800	0.86180200
C	-2.55509600	1.69135500	-0.15289400
C	-2.28801000	1.00939400	-1.36717800
C	-2.77040100	-0.59407300	0.25052500
C	-2.41057000	-0.40358800	-1.12686400
C	-2.04155200	1.64046400	-2.69239400
H	-1.86396300	2.71840100	-2.60726100
H	-2.91748600	1.50264900	-3.34230200
H	-1.18838000	1.19369100	-3.22131100
C	-2.55567200	3.16966300	0.02202000
H	-2.57763500	3.45763500	1.07885200
H	-3.43870800	3.61334100	-0.45815000
H	-1.66758200	3.63277900	-0.42830000
C	-3.29534400	0.99503200	2.25475300
H	-3.07192600	0.16492900	2.93434700
H	-4.38330300	1.15116800	2.27884100
H	-2.82844000	1.89748600	2.66650300
C	-3.13994700	-1.89100200	0.88173200
H	-2.51768400	-2.71575800	0.51436000
H	-4.18751100	-2.13397900	0.65390100

H	-3.03297800	-1.86194500	1.97100500
C	-2.39164100	-1.46207400	-2.17555400
H	-3.37117500	-1.50415800	-2.67485200
H	-2.20086400	-2.45583200	-1.75445100
H	-1.64378900	-1.27421100	-2.95584700
C	2.36495500	2.34769200	0.46087500
C	3.41608600	2.80314700	1.24878400
C	4.67365200	2.72833000	0.65715600
C	4.86386900	2.19030400	-0.62626700
C	3.80471100	1.70730500	-1.39680000
C	2.55101200	1.83591600	-0.82566000
H	3.28494500	3.19628900	2.25420500
H	5.54238300	3.08655600	1.20597700
H	5.87403700	2.15251200	-1.02973100
H	3.97167400	1.28010100	-2.38345000
C	0.93727100	2.03638800	0.47622100
C	-0.04345800	1.77570800	1.33464100
H	-0.18579700	2.08962500	2.36776900
C	1.09150900	1.51741800	-1.07191300
C	0.67374000	0.10746300	-1.33973400
H	0.21215700	-0.07544600	-2.31356600
H	1.44971200	-0.63362400	-1.12476100
H	0.56972000	2.23611800	-1.71870300
C	-0.10476100	-0.78293700	1.98691500
C	0.25480500	-1.51518000	1.01549500
H	-0.16223500	-0.52840300	3.03609600
C	0.91167300	-2.69035600	0.49315000
C	0.70148400	-3.15920600	-0.81003900
C	1.76801400	-3.40642800	1.34551700
C	1.32431100	-4.32045300	-1.24857000
H	0.04588800	-2.60317000	-1.47907700
C	2.39119500	-4.56254800	0.90085000
H	1.93532500	-3.04117500	2.35770000
C	2.17036500	-5.02313900	-0.39572900
H	1.15092000	-4.67858000	-2.26141300
H	3.05313700	-5.11003300	1.56859900
H	2.66029700	-5.93096100	-0.74162200

IM8

M06/BS1 SCF energy in gas pahse: -1178.144619 a.u.

M06/BS2 SCF energy in MeOH: -1178.497572 a.u.

M06/BS2 Free energy in MeOH: -1178.071966 a.u.

Ru	-0.22304500	0.35839900	0.40345600
C	-0.71659100	2.42478100	0.75706200
C	0.36736300	2.54433200	-0.18328500
C	-0.07767300	2.01388200	-1.41926800
C	-1.84993200	1.84238200	0.05358500
C	-1.42753300	1.54300300	-1.27074700
C	0.64726100	2.07168700	-2.71581600
H	1.64129000	2.51953700	-2.61469600
H	0.07477000	2.69374700	-3.41880300
H	0.75968200	1.08909300	-3.19283600
C	1.65489400	3.25048900	0.06456800
H	1.91635400	3.25691500	1.12715700
H	1.57573000	4.29532400	-0.26910800
H	2.49301600	2.79216700	-0.47176200
C	-0.74162600	2.98255200	2.13873000
H	-1.46344800	2.45813500	2.77496100
H	-1.02943500	4.04402900	2.11460000
H	0.23964800	2.91258900	2.62055700
C	-3.22649500	1.69638700	0.60388100
H	-3.79565500	0.91232000	0.09052400
H	-3.77561000	2.64095900	0.48223500
H	-3.21929500	1.45815500	1.67462700
C	-2.26552300	1.03661600	-2.39340300
H	-2.63112500	1.87622000	-3.00281700
H	-3.14053700	0.47910800	-2.04105400
H	-1.69408100	0.38102100	-3.06373700
C	3.90184600	-0.72610700	0.61844400
C	4.98883800	-1.19614100	1.33936400
C	5.83909300	-2.06071200	0.64749800
C	5.59805800	-2.43512900	-0.68012400
C	4.49790300	-1.95643200	-1.40114700
C	3.67371200	-1.08284400	-0.71955700
H	5.18426300	-0.92331400	2.37417000
H	6.71539700	-2.46285100	1.15263400
H	6.29489100	-3.11667400	-1.16483900
H	4.33159500	-2.25633100	-2.43401000
C	2.61980400	-0.00015800	0.66564700
C	1.57554400	0.27874600	1.46060600
H	1.63116400	0.25601200	2.55240700
C	2.43108600	-0.18654100	-0.82902500
C	1.02342900	-0.66934300	-1.02660800
H	0.58726000	-0.59252600	-2.02848900
H	0.88528000	-1.68838200	-0.63726800
H	2.63410700	0.72213800	-1.41515400
C	-0.66018700	-0.92829100	1.82213000
C	-1.54518800	-1.08968400	0.87773400
H	-0.21287400	-1.33223900	2.72408700
C	-2.75728700	-1.69674400	0.40895400
C	-2.93895600	-1.98446600	-0.95278300
C	-3.77818600	-2.00011900	1.32607800
C	-4.12024300	-2.56662300	-1.38782200
H	-2.13323400	-1.76668000	-1.65388300
C	-4.96672000	-2.55770700	0.87967200
H	-3.62715800	-1.78247700	2.38286900
C	-5.13756300	-2.84148900	-0.47465000
H	-4.25350300	-2.80687400	-2.44047600
H	-5.76082500	-2.78077400	1.58872700
H	-6.06845500	-3.28584800	-0.82098900

TS1-r

M06/BS1 SCF energy in gas pahse: -1178.169679 a.u.

M06/BS2 SCF energy in MeOH: -1178.521452 a.u.

M06/BS2 Free energy in MeOH: -1178.097676 a.u.

Ru	0.25987900	-0.47869900	0.30117700

C	-0.55597200	-2.55118500	-0.13385500
C	-0.66551900	-1.73254500	-1.30894000
C	0.66271900	-1.36878100	-1.72965600
C	0.82150400	-2.63980400	0.21643500
C	1.58259300	-1.93941000	-0.80758300
C	1.02531600	-0.59537500	-2.94974800
H	0.25462500	0.13825300	-3.21451600
H	1.15228100	-1.26388700	-3.81298300
H	1.96740300	-0.05103200	-2.80947900
C	-1.91562700	-1.42310700	-2.05731700
H	-2.79795600	-1.40614200	-1.40743400
H	-2.09108000	-2.18186500	-2.83307900
H	-1.85693200	-0.45090100	-2.56178400
C	-1.67653200	-3.23035200	0.57293200
H	-1.49504200	-3.31028800	1.65109700
H	-1.80239300	-4.25112600	0.18515900
H	-2.63130600	-2.71178200	0.43068500
C	1.38208900	-3.46217900	1.32683400
H	2.34597600	-3.08052600	1.68530500
H	1.54854300	-4.49913800	1.00234100
H	0.70203700	-3.49343800	2.18709000
C	3.06111600	-1.96942300	-0.99706800
H	3.30756700	-2.63130200	-1.83916000
H	3.58865700	-2.36046300	-0.11980300
H	3.47277000	-0.97878900	-1.23061600
C	-1.21285100	-0.17134700	1.76537400
C	-1.82243100	0.59094200	0.94021600
C	0.68385000	1.57899400	-0.19884700
C	-0.56240300	1.49357000	-0.44290400
H	-1.33574300	1.73579200	-1.15985800
C	2.02528300	2.04532500	-0.07385400
C	2.87610100	1.14461500	0.59019700
C	2.52236300	3.24859500	-0.58882300
C	4.24227200	1.40401700	0.65566500
C	3.88210600	3.50796100	-0.49377300
H	1.85154600	3.94563600	-1.08705900
C	4.73864100	2.58438000	0.11067800
H	4.91002300	0.69838300	1.14976800
H	4.28666800	4.42738500	-0.91112800
H	5.80505200	2.79382800	0.16187600
C	2.23026500	-0.00164900	1.25371900
C	1.20087300	0.16440500	2.20339600
H	2.84340800	-0.89893600	1.35362400
H	1.07532700	-0.59382400	2.97641900
H	0.87653900	1.17000100	2.48009200
H	-1.32457900	-0.56952000	2.76592500
C	-3.12226700	1.04959800	0.48196800
C	-3.37751300	2.39647100	0.18766400
C	-4.17849600	0.12656100	0.42639400
C	-4.65523500	2.80343500	-0.16996900
H	-2.57489300	3.12724800	0.27391300
C	-5.45375700	0.53847400	0.06539700
H	-3.98901300	-0.91377800	0.68969300
C	-5.69185300	1.87568000	-0.24038600
H	-4.84722600	3.85255600	-0.38467800
H	-6.26528400	-0.18504800	0.02592300
H	-6.69149300	2.19826600	-0.52401000

TS6-r

M06/BS1 SCF energy in gas pahse: -1178.170188 a.u.

M06/BS2 SCF energy in MeOH: -1178.526188 a.u.

M06/BS2 Free energy in MeOH: -1178.100114 a.u.

Ru	0.14058000	0.18912500	-0.21161500
C	-1.19027900	1.94466400	0.29147500
C	-0.03100900	2.40753400	-0.40827000
C	1.11785500	2.14773900	0.42738700
C	-0.75395700	1.30162100	1.49957400
C	0.68139900	1.41423000	1.56700600
C	2.49408000	2.69078100	0.25519500
H	2.66414200	3.10356400	-0.74537800
H	2.64002400	3.51253600	0.97068200
H	3.27116600	1.94358500	0.46154400
C	-0.04090400	3.16508100	-1.69286100
H	-0.82907900	2.79874500	-2.36257600
H	-0.22355100	4.23565900	-1.52293800
H	0.91293800	3.07967700	-2.22826700
C	-2.59225900	2.18626400	-0.14719100
H	-3.31054100	1.53087300	0.35654900
H	-2.87047400	3.22675900	0.07281700
H	-2.70906400	2.03856900	-1.22828400
C	-1.59525200	0.84810300	2.64352500
H	-1.25085000	-0.11021000	3.05295100
H	-1.53040700	1.58468900	3.45748800
H	-2.65071700	0.75052900	2.37212500
C	1.52487900	0.98688300	2.71755400
H	1.51838300	1.75581600	3.50386700
H	1.15265700	0.05726000	3.16371700
H	2.56806400	0.82201000	2.42322700
C	2.01259100	0.13156800	-1.32560800
C	1.07029900	-0.47647300	-2.22073700
H	1.16239200	-1.55379700	-2.37593500
H	0.85368300	0.09432200	-3.12348000
C	-0.96844500	-0.74227800	-1.99897400
C	-1.64865300	-0.76230200	-0.92095200
C	-2.99936500	-1.04920500	-0.46170900
C	-3.32417500	-1.39064700	0.85570200
C	-4.03391100	-0.98003000	-1.40996600
C	-4.63928400	-1.66141700	1.21541300
H	-2.55055400	-1.43688000	1.61771800
C	-5.34631800	-1.24443900	-1.04759500
H	-3.79352800	-0.70450700	-2.43637500
C	-5.65401400	-1.58678800	0.26726400
H	-4.87142300	-1.93113500	2.24385000
H	-6.13430100	-1.18018200	-1.79516400
H	-6.68349100	-1.79464900	0.55093800
H	-1.01947500	-0.96686200	-3.05336000
H	2.33597800	1.12730100	-1.63417000

C	3.06385900	-0.67480100	-0.66801700
C	2.64143000	-1.68537500	0.20713200
C	4.42233600	-0.51125600	-0.92148900
C	3.55855900	-2.57342200	0.77276000
C	5.34099600	-1.38099900	-0.33766100
H	4.76010900	0.28252000	-1.58824400
C	4.91098800	-2.41388400	0.49394200
H	3.21355600	-3.35825400	1.44290300
H	6.40313400	-1.25447500	-0.53674200
H	5.63697000	-3.08934500	0.94068400
C	1.24108900	-1.68289100	0.49853300
C	0.06514300	-1.83928300	0.85710700
H	-0.81729800	-2.29950200	1.25967400

TS7-r

M06/BS1 SCF energy in gas pahse: -1178.130594 a.u.

M06/BS2 SCF energy in MeOH: -1178.483167 a.u.

M06/BS2 Free energy in MeOH: -1178.060803 a.u.

Ru	-0.73552700	-0.22416600	0.21730100
C	-2.34964700	0.37947200	-1.22606200
C	-2.33395800	-1.06081100	-1.26513800
C	-2.70824100	-1.53749600	0.02076900
C	-2.67283100	0.78956400	0.11221500
C	-2.86569100	-0.41052000	0.89123600
C	-2.97145600	-2.95786200	0.37649600
H	-2.20863900	-3.64424100	-0.01354700
H	-3.93083700	-3.27171200	-0.05866800
H	-3.04673200	-3.10667500	1.45934900
C	-2.07207900	-1.87842800	-2.48095000
H	-1.08946100	-1.64482600	-2.91773800
H	-2.82588800	-1.68460900	-3.25660300
H	-2.09386900	-2.95194800	-2.26286600
C	-2.24520700	1.25763800	-2.42544000
H	-2.01471000	2.29662800	-2.16454800
H	-3.20989800	1.26827200	-2.95390200
H	-1.49092900	0.90475000	-3.13897000
C	-2.92801500	2.17957600	0.58229300
H	-2.59472500	2.32599700	1.61562000
H	-4.00433500	2.39947900	0.54437400
H	-2.41284000	2.92336600	-0.03571700
C	-3.28873200	-0.46058300	2.32090900
H	-4.37496400	-0.61192200	2.39754700
H	-3.05043400	0.47180700	2.84418500
H	-2.80157100	-1.27903300	2.86584000
C	2.60874900	-1.57791200	-0.76761000
C	3.93605400	-1.28079400	-1.05621600
C	4.87455700	-2.09757600	-0.43148100
C	4.50173700	-3.11785700	0.45839200
C	3.16650800	-3.38627700	0.76594900
C	2.23748300	-2.60665100	0.10006800
H	4.23799700	-0.47420100	-1.72012900
H	5.93302000	-1.93795100	-0.62787400
H	5.28419300	-3.71720100	0.92006600
H	2.89632400	-4.17237400	1.46811200
C	1.23622500	-1.10869500	-0.95528300
C	0.57196800	-0.00843800	-1.29281600
H	0.86832200	0.83299400	-1.91762000
C	0.74866400	-2.35700100	-0.00037600
C	-0.01041900	-1.98312700	1.23104700
H	-0.80621700	-2.66601800	1.53209800
H	0.63933200	-1.73977100	2.07698100
H	0.20211300	-3.06686300	-0.63608400
C	0.33710800	1.45477300	1.03219600
C	0.07555500	0.63589700	1.96395600
H	0.10814200	0.29683900	2.98908100
C	0.97338100	2.64829700	0.53419000
C	1.95117100	3.26109000	1.33594500
C	0.64361300	3.22881200	-0.69709900
C	2.57738300	4.42230900	0.91007600
H	2.21029500	2.80961100	2.29236600
C	1.26819900	4.39644800	-1.11603300
H	-0.12040000	2.76460500	-1.31937800
C	2.23754400	4.99305100	-0.31534700
H	3.33452000	4.88788900	1.53749900
H	0.99818000	4.84333900	-2.07069900
H	2.72948300	5.90567500	-0.64531400

IM1'

M06/BS1 SCF energy in gas pahse: -1255.521828 a.u.

M06/BS2 SCF energy in MeOH: -1255.900409 a.u.

M06/BS2 Free energy in MeOH: -1255.444647 a.u.

Ru	0.33581300	0.35480600	0.24928600
C	-0.81143700	1.41196400	-1.43037000
C	0.01014300	2.36352100	-0.73702000
C	1.37645800	1.99508200	-0.95537900
C	0.03705400	0.41254400	-1.99975300
C	1.40287300	0.78174800	-1.70506600
C	2.57936700	2.76856800	-0.54812500
H	2.37257900	3.45985000	0.27566900
H	2.93221200	3.36600700	-1.40103000
H	3.40587300	2.11532600	-0.24137900
C	-0.48626300	3.60275900	-0.07445300
H	-1.43192500	3.42739600	0.45328500
H	-0.66961800	4.39328700	-0.81586400
H	0.23415300	3.99900200	0.65088100
C	-2.27888200	1.56113200	-1.62371800
H	-2.77079000	0.62440400	-1.90486700
H	-2.45601900	2.29175600	-2.42657300
H	-2.77453800	1.94486000	-0.72352900
C	-0.36464300	-0.64035200	-2.97551100
H	0.19027000	-1.57708300	-2.83712800
H	-0.15093500	-0.29505300	-3.99768400
H	-1.43397900	-0.87021600	-2.92404700
C	2.62168800	0.17193000	-2.30681100
H	2.89027300	0.71668800	-3.22384100
H	2.46762500	-0.87687400	-2.58512800

H	3.48714300	0.21500400	-1.63367700
C	-1.76335200	-0.07361800	0.93803300
C	-1.24515900	0.77030200	1.71033800
C	2.20006600	0.41663000	1.59618000
C	1.40271900	1.26152000	2.03228700
H	-1.24114200	1.41133700	2.57740500
H	1.01939300	2.05089000	2.65425200
C	-2.79875700	-0.91187300	0.39050500
C	-4.13822400	-0.70134500	0.80119100
C	-2.51633300	-1.87838500	-0.58262400
C	-5.13839200	-1.47874500	0.20790800
C	-3.52629400	-2.63242600	-1.15967300
H	-1.48343900	-2.01532600	-0.89844500
C	-4.84576800	-2.42590900	-0.76353400
H	-6.16576800	-1.34621200	0.54343000
H	-3.28706600	-3.38277500	-1.91042200
H	-5.64768300	-3.01542900	-1.20293400
C	3.21427400	-0.51625600	1.20934500
C	2.79476000	-1.55724200	0.36413600
C	4.55720900	-0.38223500	1.56806300
C	3.73856600	-2.43843900	-0.14967000
C	5.48894600	-1.27703500	1.05256500
H	4.86527700	0.43115300	2.22255300
C	5.08173300	-2.29563600	0.19408800
H	3.42366000	-3.24206200	-0.81547700
H	6.53978500	-1.17101000	1.31185400
H	5.81712000	-2.98634700	-0.21310200
C	1.34700300	-1.68128600	0.09487500
C	0.41500900	-1.69741300	1.13559500
H	1.07406300	-2.16341000	-0.84846300
H	-0.53317500	-2.21255700	1.00746100
H	0.74041400	-1.59670800	2.17210900
C	-4.47455000	0.30262100	1.81608100
C	-5.59549700	1.02766200	1.81868000
H	-3.74793400	0.44913300	2.61739400
H	-5.80584500	1.74199300	2.61085700
H	-6.34164100	0.94279300	1.02889900

TS1’

M06/BS1 SCF energy in gas pahse: -1255.510098 a.u.

M06/BS2 SCF energy in MeOH: -1255.8861 a.u.

M06/BS2 Free energy in MeOH: -1255.43134 a.u.

Ru	-0.37457300	0.39813800	-0.22045500
C	0.37355100	2.54832600	-0.01402800
C	-0.46892900	2.42596200	-1.17191800
C	-1.79361600	2.08030400	-0.73683900
C	-0.40128500	2.19908200	1.12879600
C	-1.75933700	1.93604100	0.67811900
C	-3.00328000	1.95750700	-1.59622900
H	-2.75542400	1.62401100	-2.61095000
H	-3.51099200	2.92839200	-1.68585300
H	-3.72485700	1.24433600	-1.17922900
C	-0.06864400	2.76802800	-2.56571300
H	1.00647700	2.62578800	-2.72753900
H	-0.29143200	3.82374600	-2.77626600
H	-0.61075500	2.17205300	-3.31040400
C	1.79157300	3.00198300	-0.05551000
H	2.26828800	2.96737100	0.92942500
H	1.84390900	4.03892000	-0.41507400
H	2.39839200	2.38885500	-0.73549300
C	0.01570400	2.29472400	2.55800300
H	-0.23116500	1.39056400	3.13108100
H	-0.49042500	3.13607200	3.05204400
H	1.09376800	2.46236500	2.65682800
C	-2.95834200	1.77794100	1.55059100
H	-3.53986500	2.71074100	1.54927400
H	-2.68772900	1.56962700	2.59207800
H	-3.62578700	0.97698900	1.20686100
C	1.67350100	-0.30596400	-0.50407300
C	1.16734100	-0.23113300	-1.67717700
C	-1.51816900	-1.16542000	-1.22148400
C	-0.75412900	-0.73774300	-2.13649300
H	1.42182700	0.02282300	-2.69734700
H	-0.66834800	-0.48097600	-3.18205700
C	2.83715900	-0.56061000	0.30137000
C	3.88480300	-1.36864800	-0.21002700
C	2.97055500	0.03231900	1.56609900
C	5.02114800	-1.54860500	0.58664900
C	4.11643800	-0.14227300	2.32261000
H	2.15114500	0.64712100	1.93846400
C	5.14649400	-0.94118300	1.82748200
H	5.81132200	-2.20375000	0.22354300
H	4.20601400	0.32816700	3.29942300
H	6.04433600	-1.10447200	2.41988600
C	-2.52354600	-1.85361400	-0.47687800
C	-2.49696500	-1.58398200	0.90075500
C	-3.50611400	-2.68480700	-1.02311600
C	-3.50625500	-2.07641000	1.72181100
C	-4.49351000	-3.19354300	-0.18882400
H	-3.50876800	-2.89867200	-2.09002200
C	-4.50227800	-2.87901600	1.17089000
H	-3.50040400	-1.85528000	2.78913500
H	-5.27593100	-3.82567100	-0.60265500
H	-5.29109700	-3.27089100	1.80950500
C	-1.31134600	-0.86384700	1.40085300
C	-0.00951100	-1.32854700	1.14510500
H	-1.45548100	-0.27613600	2.31003500
H	0.78096600	-1.11125700	1.86072600
H	0.13759600	-2.23822300	0.55762000
C	3.78491000	-2.01516100	-1.52155900
C	4.82138600	-2.25693100	-2.32762200
H	2.78351500	-2.30748200	-1.84504900
H	4.69026800	-2.76370300	-3.28056600
H	5.83600500	-1.94819500	-2.07727900

IM2’

M06/BS1 SCF energy in gas pahse: -1255.550428 a.u.

M06/BS2 SCF energy in MeOH: -1255.919044 a.u.

M06/BS2 Free energy in MeOH: -1255.461508 a.u.

Ru	-0.29575900	0.30051900	-0.08080900
C	0.51159200	2.35525600	-0.76319900
C	-0.29870800	1.73447300	-1.79751300
C	-1.64690600	1.65163300	-1.33001500
C	-0.31773800	2.58187300	0.35575700
C	-1.66273800	2.14403000	0.00412600
C	-2.82569000	1.19306300	-2.11788900
H	-2.55517100	0.40201300	-2.82803700
H	-3.25291100	2.02469400	-2.69641900
H	-3.61803900	0.79881100	-1.47030200
C	0.13972700	1.41653800	-3.18610000
H	1.22895900	1.32351200	-3.26700500
H	-0.16954200	2.21739900	-3.87345000
H	-0.31169000	0.48465000	-3.55107900
C	1.93948100	2.74656200	-0.93926800
H	2.43273800	2.96198100	0.01511400
H	2.01360500	3.65058800	-1.56005200
H	2.52264300	1.96240900	-1.44003600
C	0.04343900	3.25671900	1.63593800
H	-0.28723600	2.68508600	2.51520000
H	-0.42435600	4.24912100	1.70605600
H	1.12605300	3.40357300	1.72591400
C	-2.89664700	2.41320900	0.79746900
H	-3.43475300	3.26676900	0.36123700
H	-2.67008500	2.67528800	1.83775600
H	-3.58954900	1.56097200	0.79940000
C	1.43518000	-0.63083100	-0.04008200
C	0.91268800	-1.18146500	-1.21888400
C	-1.19352500	-1.47627600	-0.59728100
C	-0.25888600	-2.08432200	-1.33167300
H	1.48899800	-0.92882900	-2.12328300
H	-0.25287200	-3.02012800	-1.89545800
C	2.72704900	-0.52914500	0.53333100
C	3.79013100	-1.40094300	0.14426200
C	2.96859900	0.48204600	1.49302800
C	5.04773800	-1.19122900	0.71739000
C	4.22032100	0.66658100	2.03868400
H	2.13216900	1.12099200	1.77663900
C	5.26356800	-0.17588800	1.63914700
H	5.86178100	-1.86632700	0.46061200
H	4.39520400	1.44636900	2.77608100
H	6.25438000	-0.05033800	2.07210100
C	-2.49134200	-1.76991500	-0.01665600
C	-2.69689800	-1.09748600	1.20088300
C	-3.48327600	-2.60061500	-0.53247200
C	-3.90266200	-1.23107700	1.87847300
C	-4.68774000	-2.73682500	0.15507100
H	-3.32302500	-3.11318000	-1.48048000
C	-4.89786800	-2.05443400	1.35034000
H	-4.06533200	-0.70473000	2.81948200
H	-5.47351800	-3.36951300	-0.25242100
H	-5.84611100	-2.15826300	1.87362000
C	-1.57491900	-0.26412100	1.69964900
C	-0.28205500	-0.74532300	1.94101100
H	-1.85557200	0.64786600	2.23246000
H	0.37930200	-0.20118200	2.61466700
H	-0.05749200	-1.80539500	1.81306100
C	3.58927300	-2.50023800	-0.80172900
C	4.51693400	-2.92060600	-1.66713100
H	2.61902900	-2.99861300	-0.78248500
H	4.32734700	-3.75784500	-2.33398600
H	5.48970600	-2.43803600	-1.75732400

TS2'

M06/BS1 SCF energy in gas pahse: -1255.547969 a.u.

M06/BS2 SCF energy in MeOH: -1255.917183 a.u.

M06/BS2 Free energy in MeOH: -1255.457327 a.u.

Ru	-0.31779700	0.31106200	-0.14803500
C	0.45112900	2.33591100	-0.88374800
C	-0.15772700	2.59236600	0.36533800
C	-1.54687400	2.19970000	0.26328100
C	-0.56454700	1.78658500	-1.77326400
C	-1.80575400	1.75350400	-1.06618200
C	-2.58406300	2.43497000	1.30606600
H	-2.16448600	2.43825300	2.31950600
H	-3.04743100	3.42008200	1.14988000
H	-3.38811700	1.68949700	1.26699000
C	0.44529800	3.23252600	1.56983100
H	1.52038200	3.40567500	1.44622600
H	-0.01902500	4.20977800	1.76432200
H	0.30243800	2.62642000	2.47712500
C	1.85881600	2.62977500	-1.27996800
H	2.25693700	1.87225600	-1.96767900
H	1.92205700	3.59812800	-1.79578600
H	2.53248800	2.66651600	-0.41588700
C	-0.38001900	1.45072500	-3.21425400
H	-0.99002400	0.58821600	-3.50975800
H	-0.67562200	2.29878500	-3.84831400
H	0.66427900	1.21543500	-3.45061500
C	-3.13669500	1.35201100	-1.60390300
H	-3.72928600	2.23946400	-1.86684300
H	-3.04157500	0.73649500	-2.50605200
H	-3.71453800	0.77269900	-0.87110200
C	-1.31254500	-0.46018400	1.58802000
C	0.01155000	-1.05922900	1.57951800
H	0.06519000	-2.12834100	1.34553200
H	0.70417400	-0.72172900	2.35070300
C	1.36481000	-0.73060400	0.02830900
C	0.92886500	-1.27100800	-1.19339200
H	-1.44826500	0.31229800	2.35214800
C	-2.54377000	-1.18727200	1.18676500
C	-2.52754200	-1.71828500	-0.11691000
C	-3.66283800	-1.34654200	1.99367600
C	-3.61372700	-2.44263800	-0.59605600

C	-4.76257100	-2.05076900	1.49941000
H	-3.68057100	-0.92937500	3.00094100
C	-4.73530400	-2.59700700	0.21861800
H	-3.59857000	-2.85151300	-1.60537000
H	-5.64865300	-2.16990900	2.11923000
H	-5.60260800	-3.13707600	-0.15547000
C	-1.26417600	-1.40387100	-0.75866000
C	-0.30703000	-2.03229500	-1.45149500
H	-0.32428100	-2.94617600	-2.05072900
C	2.69781800	-0.53600100	0.53432600
C	2.95372700	0.55064900	1.39229000
C	3.76150000	-1.40335100	0.16386100
C	4.22947600	0.82377700	1.84474900
H	2.11517600	1.18334500	1.68367900
C	5.04527300	-1.10214100	0.63380700
C	5.28200000	-0.00549200	1.44961700
H	4.41222600	1.66765000	2.50625100
H	5.86456300	-1.77332700	0.38296100
H	6.29159100	0.19110100	1.80493800
H	1.65421700	-1.11677200	-2.00431000
C	3.54488500	-2.60182400	-0.65304200
C	4.42364700	-3.08367300	-1.53627400
H	2.59851200	-3.12759900	-0.51048600
H	4.22243900	-3.99607500	-2.09204100
H	5.36779800	-2.58278000	-1.74846100

IM3'

M06/BS1 SCF energy in gas pahse: -1255.587603 a.u.

M06/BS2 SCF energy in MeOH: -1255.956651 a.u.

M06/BS2 Free energy in MeOH: -1255.494035 a.u.

Ru	0.40390300	0.47141800	0.26207900
C	-0.35346700	2.59594700	0.42171200
C	-0.94807700	2.07823100	-0.75999600
C	0.10476500	1.66486600	-1.63641500
C	1.08418700	2.56982200	0.25711900
C	1.37516300	1.98921400	-1.01544800
C	-0.07150000	1.17696200	-3.03271000
H	-0.97576400	0.56667600	-3.14659200
H	-0.16565900	2.03038900	-3.71914200
H	0.78553300	0.58606900	-3.37663100
C	-2.41439100	1.96730400	-1.00199500
H	-2.92586100	1.43676900	-0.18470300
H	-2.86530500	2.96596700	-1.08178800
H	-2.63841100	1.42301300	-1.92487300
C	-1.09086400	3.11182100	1.61087500
H	-0.53216200	2.94900700	2.54141800
H	-1.26920400	4.19316000	1.52456100
H	-2.06903200	2.62548200	1.71873000
C	2.07531300	3.10642600	1.23313800
H	3.05281600	2.62096600	1.12838600
H	2.22206500	4.18472000	1.07854500
H	1.74232200	2.96821300	2.26951900
C	2.71855900	1.86658900	-1.64936100
H	2.95211400	2.75689100	-2.25003200
H	3.51175200	1.75480600	-0.89979600
H	2.77734200	0.99607300	-2.31436400
C	1.16466300	-1.22537600	-0.90011500
C	0.15587600	-2.19329800	-0.24804600
H	0.65982000	-2.78857600	0.52743100
H	-0.28006800	-2.90656800	-0.95928000
C	-0.93754000	-1.35210900	0.41926600
C	-0.73119200	-0.75476700	1.69394700
H	0.99184100	-1.09443700	-1.97535600
C	2.58157000	-1.44509400	-0.52245100
C	2.80981500	-1.17159300	0.85147200
C	3.60256500	-1.99839600	-1.28705500
C	3.99933600	-1.54903400	1.48644400
C	4.81114100	-2.30633600	-0.66732500
H	3.44991400	-2.21100200	-2.34493900
C	5.00455800	-2.09787000	0.70494600
H	4.15017600	-1.36448600	2.54814500
H	5.61827300	-2.73935200	-1.25514800
H	5.95842400	-2.35940200	1.15722600
C	1.62418400	-0.55097900	1.33029500
C	0.56477900	-0.45325400	2.24781800
H	0.62757100	0.01370500	3.23425800
C	-2.28666600	-1.38165400	-0.20333500
C	-2.33981600	-1.44946200	-1.60497500
C	-3.50882100	-1.32038400	0.50824100
C	-3.53558800	-1.40848500	-2.30426800
H	-1.40774100	-1.50598000	-2.16661000
C	-4.70841800	-1.28310700	-0.21725100
C	-4.73361400	-1.31056200	-1.60308600
H	-3.53217900	-1.46167300	-3.39136900
H	-5.64299600	-1.27703500	0.34142400
H	-5.68434200	-1.28811500	-2.13142900
H	-1.58615100	-0.32597700	2.21734300
C	-3.60265200	-1.37364000	1.97799700
C	-4.43735000	-0.62941100	2.70745500
H	-2.96212000	-2.10080400	2.48436600
H	-4.51122000	-0.74748700	3.78591900
H	-5.08256200	0.12240100	2.25193900

TS3'

M06/BS1 SCF energy in gas pahse: -1255.574985 a.u.

M06/BS2 SCF energy in MeOH: -1255.944565 a.u.

M06/BS2 Free energy in MeOH: -1255.483068 a.u.

Ru	-0.34441100	0.58569000	-0.18747500
C	1.17284500	2.05493600	0.63742400
C	0.23427000	1.68174400	1.65478900
C	-1.08475200	2.10228300	1.22710200
C	0.44382700	2.63634100	-0.44226300
C	-0.95210800	2.69482800	-0.06436600
C	-2.33233100	1.99980600	2.03620800
H	-2.36250700	1.07553900	2.62668200
H	-2.40778100	2.83825400	2.74318500

H	-3.22964800	2.01803600	1.40672300
C	0.57279900	1.12591800	2.99606500
H	1.48040000	0.51055500	2.96756100
H	0.75120800	1.93924900	3.71396600
H	-0.23986900	0.51295200	3.40662500
C	2.64731700	1.85758100	0.69480100
H	3.08162100	1.70194800	-0.30109700
H	3.13101900	2.74479700	1.12814900
H	2.92375100	0.99565000	1.31403000
C	1.02293500	3.13779600	-1.72149400
H	0.30793700	3.05164200	-2.54929600
H	1.30618900	4.19662400	-1.64112300
H	1.92259400	2.57554100	-2.00203000
C	-2.04996700	3.28432900	-0.88194900
H	-2.16065300	4.35707100	-0.67006900
H	-1.85564600	3.18166400	-1.95654600
H	-3.01250500	2.80234200	-0.67241500
C	-1.31818400	-1.36480800	0.66332300
C	-0.24443600	-2.31215600	0.16105300
H	-0.63626200	-2.96519100	-0.63355800
H	0.14826100	-2.97177300	0.94323500
C	0.85793300	-1.42242600	-0.43465400
C	0.58043700	-0.77065200	-1.65875600
H	-1.09416200	-0.98823700	1.66962300
C	-2.77886600	-1.62757900	0.42275200
C	-3.07248000	-0.97535300	-0.77461000
C	-3.73845600	-2.38488500	1.07560400
C	-4.31638700	-1.05588200	-1.38844100
C	-5.00697800	-2.43774800	0.49474300
H	-3.52449600	-2.91293100	2.00343800
C	-5.28960100	-1.78677300	-0.71133800
H	-4.53568300	-0.56379900	-2.33345400
H	-5.79736100	-2.99953500	0.98846300
H	-6.29092500	-1.85938600	-1.13045800
C	-1.74216600	-0.47529300	-1.05559600
C	-0.76474300	-0.49336200	-2.06946300
H	-0.97107000	-0.12756700	-3.07802000
H	1.38826900	-0.38917000	-2.28263600
C	2.22059700	-1.53267400	0.13413100
C	2.31852400	-1.69944200	1.52611000
C	3.41960500	-1.42811300	-0.61164300
C	3.53802200	-1.72258400	2.18503800
C	4.64255900	-1.45892400	0.07251600
C	4.71317000	-1.59047700	1.45134000
H	3.57029000	-1.85052500	3.26528600
H	5.55818400	-1.42061200	-0.51562300
H	5.68113100	-1.61910200	1.94710500
C	3.46299600	-1.36501500	-2.08299100
C	4.27084100	-0.56028700	-2.77769500
H	2.81236000	-2.05688900	-2.62442500
H	4.31113200	-0.59269000	-3.86387000
H	4.92860300	0.15646200	-2.28440600
H	1.40637100	-1.77805800	2.11742100

IM4'

M06/BS1 SCF energy in gas pahse: -1255.595693 a.u.

M06/BS2 SCF energy in MeOH: -1255.968709 a.u.

M06/BS2 Free energy in MeOH: -1255.505724 a.u.

Ru	-0.31485800	0.57846200	-0.03846700
C	1.14150900	2.17813000	0.34757100
C	0.32268100	1.99191500	1.50299700
C	-1.05275200	2.27792500	1.12732800
C	0.27913500	2.52932400	-0.75236100
C	-1.07409400	2.62842200	-0.25298000
C	-2.22812000	2.22056500	2.04214200
H	-2.09078600	1.46934200	2.83004000
H	-2.38739800	3.18820200	2.53890600
H	-3.14948700	1.96867500	1.50217400
C	0.80326200	1.67449000	2.87782500
H	1.75501200	1.13043300	2.85548700
H	0.96371000	2.59633900	3.45528000
H	0.08067100	1.06375200	3.43362300
C	2.61976400	2.00768200	0.29001100
H	2.96672400	1.79725900	-0.72932400
H	3.12664800	2.92195900	0.63003100
H	2.95683500	1.18135300	0.92961800
C	0.72000500	2.85096500	-2.13947800
H	-0.06677400	2.64649900	-2.87599800
H	0.97865500	3.91576400	-2.22590100
H	1.60817400	2.27619800	-2.43003400
C	-2.26973600	3.01301100	-1.05413100
H	-2.36722800	4.10635000	-1.11077500
H	-2.20488900	2.63693700	-2.08300300
H	-3.19517200	2.62113800	-0.61554100
C	-1.36221900	-1.54143700	0.36993300
C	-0.12917600	-2.40870600	0.25518500
H	-0.27831800	-3.25776600	-0.43035600
H	0.18207300	-2.82132600	1.22004000
C	0.94073000	-1.45966200	-0.31422900
C	0.62886000	-0.78020300	-1.50317800
H	-1.13146200	-0.77806000	1.20310700
C	-2.85971100	-1.86945300	0.41705100
C	-3.14337800	-1.13155800	-0.74105300
C	-3.83247500	-2.53664400	1.12805600
C	-4.42494600	-0.99529500	-1.24413400
C	-5.13658800	-2.40067700	0.62805300
H	-3.62926200	-3.13247700	2.01508800
C	-5.42365000	-1.65128300	-0.51625100
H	-4.65996300	-0.43852700	-2.14879200
H	-5.95540400	-2.89370200	1.14866400
H	-6.45587900	-1.58760900	-0.85445100
C	-1.71446100	-0.85983000	-0.95174700
C	-0.74224200	-0.59199700	-1.90833500
H	-0.98235400	-0.16081400	-2.87896000
H	1.41271600	-0.32780600	-2.10874700
C	2.30909600	-1.51503700	0.24234500
C	2.43504600	-1.55085900	1.64115300

C	3.48614500	-1.46501100	-0.54119600
C	3.66981800	-1.50144000	2.26834500
H	1.53382500	-1.57253200	2.25551500
C	4.72572800	-1.42671700	0.11243500
C	4.82628800	-1.43202700	1.49549700
H	3.73101300	-1.52425900	3.35451000
H	5.62855800	-1.43327700	-0.49637100
H	5.80532500	-1.40629000	1.96934500
C	3.47282700	-1.51587300	-2.01234900
C	4.28677500	-0.80856600	-2.80002900
H	2.75846900	-2.20297200	-2.47312700
H	4.27222000	-0.92222900	-3.88135900
H	5.00276900	-0.09383200	-2.39299800

TS4'

M06/BS1 SCF energy in gas pahse: -1255.541943 a.u.

M06/BS2 SCF energy in MeOH: -1255.908826 a.u.

M06/BS2 Free energy in MeOH: -1255.450671 a.u.

Ru	0.30455000	0.30284300	-0.02376300
C	-0.51987800	2.07787000	1.17730700
C	0.53582500	1.38475700	1.91520000
C	1.76295800	1.57595200	1.20813400
C	0.06073400	2.65950100	0.02935900
C	1.46575400	2.31999900	0.03077600
C	3.11481000	1.12736200	1.64987500
H	3.05004200	0.29916300	2.36597500
H	3.65528200	1.94760600	2.14325500
H	3.73091400	0.78325500	0.80784200
C	0.40777800	0.72908300	3.24533300
H	-0.63831800	0.53981300	3.51171500
H	0.84485700	1.35747000	4.03445000
H	0.93531000	-0.23531800	3.26932500
C	-1.91926900	2.25454200	1.66125200
H	-2.63143400	2.38129600	0.83685700
H	-1.99161800	3.14293000	2.30414400
H	-2.25817100	1.39620500	2.25447100
C	-0.58537600	3.55067800	-0.97687000
H	-0.38491800	3.22260700	-2.00766600
H	-0.20165100	4.57782700	-0.89097600
H	-1.67250200	3.59947000	-0.84473800
C	2.47091900	2.88354100	-0.91173500
H	2.77595800	3.88298900	-0.56769800
H	2.07154400	3.00769800	-1.92640700
H	3.37986000	2.27145100	-0.96457700
C	-1.40991600	-0.72957600	-0.01687200
C	-1.04432900	-1.62030900	1.02199500
C	1.15924900	-1.45651500	0.41844800
C	0.25311200	-2.20877200	1.11556400
H	-1.79377500	-1.79383300	1.80945800
H	0.40762200	-3.17054100	1.61005400
C	-2.72700600	-0.49836000	-0.52208200
C	-3.82615500	-1.37774900	-0.27784900
C	-2.94922300	0.67712600	-1.27482600
C	-5.09403600	-0.98420800	-0.71389800
C	-4.21148000	1.04405100	-1.69408400
H	-2.08196300	1.29568500	-1.50501300
C	-5.29192100	0.21096600	-1.39355900
H	-5.93341600	-1.65874700	-0.55489400
H	-4.36220000	1.95791800	-2.26447000
H	-6.29287900	0.47729800	-1.72762200
C	2.49006300	-1.71355300	-0.08167100
C	2.77051500	-0.96872600	-1.24540700
C	3.45557800	-2.56293000	0.46054200
C	4.02803700	-1.04237700	-1.82933000
C	4.71141600	-2.63663700	-0.13396900
H	3.23286700	-3.13252600	1.36252700
C	4.99676800	-1.87561300	-1.26642400
H	4.25468200	-0.46237100	-2.72403600
H	5.47819800	-3.27839200	0.29444800
H	5.98508600	-1.93179200	-1.71823400
C	1.67140400	-0.12067400	-1.76705000
C	0.39590300	-0.59847700	-2.09476500
H	1.97054500	0.82358300	-2.22768300
H	-0.24582800	-0.00894000	-2.75071700
H	0.16794900	-1.66397000	-2.04701900
C	-3.66475400	-2.68577700	0.36432100
C	-4.54680500	-3.21658200	1.21766700
H	-2.77633800	-3.26096000	0.09523500
H	-4.40332400	-4.20893800	1.63797100
H	-5.43661500	-2.67460100	1.53731600

IM5'

M06/BS1 SCF energy in gas pahse: -1255.570237 a.u.

M06/BS2 SCF energy in MeOH: -1255.938814 a.u.

M06/BS2 Free energy in MeOH: -1255.480094 a.u.

Ru	0.28712100	0.26492400	-0.25886700
C	-0.99518800	1.52088200	1.18970000
C	-0.17881600	0.56842400	1.90223400
C	1.19670100	0.95342800	1.71947500
C	-0.12665400	2.44141600	0.53411800
C	1.22249000	2.11307900	0.89244900
C	2.35155900	0.33403900	2.42865700
H	2.21970600	-0.74944500	2.54557100
H	2.44567900	0.75665200	3.43955500
H	3.30549000	0.50015300	1.91320300
C	-0.64126900	-0.50196800	2.83081600
H	-1.69370100	-0.76271700	2.66791000
H	-0.53217400	-0.18309200	3.87754100
H	-0.05215800	-1.42084300	2.70626400
C	-2.47442200	1.66491000	1.30355900
H	-2.95041600	1.92466100	0.35038200
H	-2.70136000	2.47138500	2.01599900
H	-2.95159800	0.75444200	1.68171800
C	-0.54604200	3.60482900	-0.30035300
H	0.14520100	3.77785800	-1.13650500
H	-0.57229500	4.53153900	0.29186900

H	-1.54729200	3.45873400	-0.72353300
C	2.42106900	2.94070400	0.58297700
H	2.56654700	3.68926500	1.37529500
H	2.31356000	3.49597900	-0.35708400
H	3.34131200	2.34607500	0.53145600
C	-1.16622500	-1.05686400	-0.64609200
C	-0.80485100	-2.43192800	-0.57733000
C	1.25430400	-1.44723200	-0.17732000
C	0.51385300	-2.65455000	-0.24775700
H	-1.49428800	-3.23695500	-0.84178500
H	0.97120100	-3.64596600	-0.24922200
C	-2.54005000	-0.63795900	-0.86414700
C	-3.66952700	-1.15417300	-0.16439900
C	-2.74663600	0.35275000	-1.84842600
C	-4.93875400	-0.69657200	-0.52948500
C	-4.01566800	0.79204400	-2.18742300
H	-1.87580500	0.73559700	-2.37929800
C	-5.11773700	0.25623700	-1.52474500
H	-5.81124800	-1.11254700	-0.02889400
H	-4.14915200	1.53076100	-2.97469600
H	-6.12410400	0.57418300	-1.78976000
C	2.68549600	-1.38911500	-0.33228800
C	3.11630200	-0.24911500	-1.05332400
C	3.62748200	-2.30394500	0.16175900
C	4.47909300	0.01113400	-1.18745400
C	4.97893400	-2.04217600	0.00818000
H	3.29401900	-3.18160500	0.71520300
C	5.40108500	-0.88407500	-0.65586600
H	4.81599800	0.89535200	-1.72826500
H	5.71664500	-2.72803100	0.41869300
H	6.46564700	-0.68790100	-0.76709600
C	2.07437500	0.61393500	-1.62901900
C	0.98372700	0.16171400	-2.38353600
H	2.30883500	1.68026900	-1.68768900
H	0.44649600	0.89804600	-2.98386900
H	0.91287100	-0.87233400	-2.72209000
C	-3.52042000	-2.06075900	0.97893800
C	-4.38109900	-2.15689500	1.99781600
H	-2.61502900	-2.66838900	1.01982200
H	-4.21121000	-2.85687300	2.81221200
H	-5.27936000	-1.54409000	2.06694300

TS1-*Z*-3a

M06/BS1 SCF energy in gas pahse: -1334.077042 a.u.

M06/BS2 SCF energy in MeOH: -1334.474769 a.u.

M06/BS2 Free energy in MeOH: -1333.969205 a.u.

Ru	0.58269600	0.48889700	0.21170200
C	0.00696300	2.68916400	-0.03168100
C	0.72351900	2.50177600	1.19946800
C	2.05552000	2.06287000	0.88890300
C	0.86378100	2.29446500	-1.09967300
C	2.14966200	1.93265300	-0.52378600
C	3.16863900	1.83282100	1.85081400
H	2.80164700	1.64142300	2.86545800
H	3.82575200	2.71263300	1.89765700
H	3.78440900	0.97460600	1.55260100
C	0.21443600	2.86436700	2.55224500
H	-0.87500100	2.76240200	2.62023700
H	0.45656100	3.91248500	2.77889600
H	0.66449400	2.25272800	3.34381200
C	-1.37288900	3.24073100	-0.12407700
H	-1.78111700	3.17068300	-1.13766000
H	-1.37552100	4.30086800	0.16554100
H	-2.06675700	2.71646500	0.54644500
C	0.59523400	2.43704100	-2.56000000
H	0.86982100	1.53961400	-3.13113400
H	1.17684900	3.27123000	-2.97728400
H	-0.46154400	2.64609600	-2.76100400
C	3.41718900	1.69096200	-1.27075400
H	4.05721400	2.58250300	-1.20808800
H	3.24340200	1.49587400	-2.33531400
H	3.98835500	0.84864500	-0.85922200
C	-1.51335600	-0.05893800	0.31308900
C	-1.10294000	-0.06918100	1.52813500
C	1.56079900	-1.12283500	1.27111700
C	0.72834800	-0.70554900	2.13365000
H	-1.43710300	0.16043300	2.53111300
H	0.56385800	-0.47852100	3.17691200
C	-2.64314000	-0.22287800	-0.56342300
C	-3.75113700	-0.99864500	-0.12905400
C	-2.67656200	0.39021000	-1.82510000
C	-4.83160400	-1.14341900	-1.00733300
C	-3.77477400	0.25817900	-2.65856400
H	-1.82271000	0.99091600	-2.13929500
C	-4.85381900	-0.52212500	-2.24882600
H	-5.66009400	-1.78384300	-0.71072900
H	-3.78615400	0.74750700	-3.63011400
H	-5.71067500	-0.65743100	-2.90559400
C	2.57902100	-1.86752500	0.59754900
C	2.63514900	-1.62616200	-0.78353900
C	3.48233800	-2.74313700	1.20808900
C	3.64209800	-2.20873500	-1.54591400
C	4.47288400	-3.33337200	0.43338200
H	3.42089600	-2.93166200	2.27817700
C	4.55968800	-3.05869000	-0.93216000
H	3.70064100	-2.01172300	-2.61636900
H	5.19488200	-4.00147900	0.89759000
H	5.34924600	-3.51670100	-1.52421000
C	1.54703100	-0.80221300	-1.34907100
C	0.19653600	-1.20162700	-1.30117700
H	1.82570400	-0.16093100	-2.18788600
H	-0.43990600	-0.75371100	-2.06591900
C	-0.28632700	-2.53819300	-0.80671200
H	0.21011600	-3.33748200	-1.37608200
H	-1.36559600	-2.63894800	-0.96553000
H	-0.08546400	-2.72001400	0.25448300
C	-3.74530600	-1.67739900	1.17132200

C	-4.76759900	-1.77049700	2.03474200
H	-2.80125300	-2.14813000	1.45731400
H	-4.58610000	-2.35368900	2.94003100
C	-6.12014000	-1.15105700	1.93520400
H	-6.88724700	-1.90527600	1.70508200
H	-6.17644400	-0.37081000	1.16764100
H	-6.40922800	-0.70659600	2.89638100

TS1-*E*-3a

M06/BS1 SCF energy in gas pahse: -1334.073299 a.u.

M06/BS2 SCF energy in MeOH: -1334.472805 a.u.

M06/BS2 Free energy in MeOH: -1333.963886 a.u.

Ru	0.60994400	-0.52073400	-0.29047700
C	0.60739500	-2.81929000	-0.39958700
C	1.38356400	-2.26645800	-1.47467400
C	2.51128700	-1.57725300	-0.91472500
C	1.19818100	-2.40247000	0.82434500
C	2.40535200	-1.65638600	0.50035800
C	3.63439700	-0.96226100	-1.67364600
H	3.30742400	-0.57825500	-2.64694500
H	4.42287700	-1.70503700	-1.86143600
H	4.08906300	-0.12996600	-1.12278900
C	1.16168500	-2.53976100	-2.92243000
H	0.10758300	-2.74264000	-3.14455800
H	1.73322500	-3.42773400	-3.22873200
H	1.49709400	-1.71182900	-3.55938600
C	-0.55070300	-3.73444200	-0.59305200
H	-0.99634200	-4.04343500	0.35837500
H	-0.22099500	-4.64817600	-1.10750300
H	-1.33866600	-3.28236800	-1.21048600
C	0.79664800	-2.84098200	2.19128400
H	1.01620700	-2.08078000	2.95124000
H	1.34193800	-3.75086500	2.48083200
H	-0.27559600	-3.06420400	2.25154700
C	3.48801800	-1.26523400	1.44828800
H	4.33500400	-1.95664100	1.33463600
H	3.16972500	-1.32127300	2.49513700
H	3.86809900	-0.25268200	1.25972000
C	-1.58522800	-0.40604600	-0.66345400
C	-0.99151800	-0.27889600	-1.78346900
C	1.19613900	1.42399000	-1.06716100
C	0.66244900	0.86665700	-2.07114300
H	-1.11029600	-0.49625700	-2.83648300
H	0.72387900	0.68995000	-3.13486900
C	-2.82255400	-0.48743300	0.06492600
C	-3.74560400	0.58789600	0.02141800
C	-3.11336000	-1.63769500	0.81294800
C	-4.92967200	0.45009600	0.76023200
C	-4.30628300	-1.75719900	1.50314300
H	-2.37736200	-2.43921600	0.84298600
C	-5.21559500	-0.69952100	1.47951000
H	-5.63353700	1.28010700	0.78391600
H	-4.52462100	-2.65946600	2.07015900
H	-6.14691100	-0.76719100	2.03820200
C	1.91555200	2.32020900	-0.22327600
C	2.01717800	1.87853300	1.10353100
C	2.55046700	3.49591100	-0.63804300
C	2.83204200	2.56527800	1.99951600
C	3.33699900	4.18903600	0.27208400
H	2.45308600	3.83494000	-1.66751500
C	3.49084300	3.71656600	1.57721800
H	2.93326300	2.21381000	3.02648500
H	3.85585100	5.09254400	-0.04022800
H	4.12684200	4.25867000	2.27393600
C	1.15181500	0.74912800	1.49206000
C	-0.25132400	0.82431800	1.39481000
H	1.52145100	0.13634300	2.31986200
H	-0.66355500	1.69576500	0.87598700
C	-1.09335500	0.27305800	2.50709600
H	-0.80410600	-0.74733300	2.78763400
H	-2.16275500	0.27996400	2.28579600
H	-0.94503200	0.91149900	3.39105200
C	-3.45199000	1.80781800	-0.73150800
C	-4.35255600	2.71382700	-1.13502700
H	-2.40503500	1.97736400	-0.99895400
H	-5.41312700	2.54794300	-0.92784000
C	-4.01610100	3.95557800	-1.88118300
H	-4.33175800	4.84962000	-1.32498000
H	-4.53742400	3.99472000	-2.84762100
H	-2.93804200	4.03494100	-2.06851600

TS8-*E*-3a

M06/BS1 SCF energy in gas pahse: -1334.066143 a.u.

M06/BS2 SCF energy in MeOH: -1334.465124 a.u.

M06/BS2 Free energy in MeOH: -1333.964852 a.u.

Ru	-0.85886300	-0.57919200	0.02737000
C	-2.33278700	-2.20692200	0.56776500
C	-2.65861100	-1.73563500	-0.73252700
C	-1.52373000	-1.99429900	-1.59762100
C	-0.99081500	-2.73195400	0.53579700
C	-0.51426100	-2.63084500	-0.82161800
C	-1.50805000	-1.82793600	-3.07845900
H	-2.04229300	-0.92782900	-3.40771900
H	-2.00444600	-2.68390700	-3.55845800
H	-0.48817200	-1.77822900	-3.47705700
C	-3.99707400	-1.22775700	-1.15146400
H	-4.41197000	-0.51920900	-0.42294600
H	-4.70960200	-2.05967600	-1.24377400
H	-3.96270100	-0.72379400	-2.12410100
C	-3.25369700	-2.18535400	1.73742500
H	-2.71725400	-2.17998500	2.69271600
H	-3.89979100	-3.07455800	1.72832900
H	-3.90658700	-1.30365000	1.71896200
C	-0.27979900	-3.41300400	1.65717000
H	0.79541400	-3.19142700	1.64675400
H	-0.39373300	-4.50410800	1.59350900

H	-0.67157600	-3.10252000	2.63281600
C	0.78259500	-3.15409400	-1.34048200
H	0.64378200	-4.14846900	-1.78769600
H	1.52977300	-3.25247400	-0.54431600
H	1.20544200	-2.49917200	-2.11331900
C	-2.44679500	1.87552700	1.20870400
C	-3.15207600	2.70204800	2.08873700
C	-4.08592800	3.59397300	1.57811300
C	-4.31412400	3.65896200	0.20380100
C	-3.59503200	2.85204700	-0.67394600
C	-2.63967800	1.96938700	-0.17771400
H	-2.98524900	2.61877500	3.16098400
H	-4.65444900	4.22892600	2.25388100
H	-5.05873500	4.34909300	-0.18787300
H	-3.76532900	2.91875000	-1.74848500
C	-1.54392100	0.84780800	1.63000400
C	-0.81223800	0.00930200	2.18858500
H	-0.28299800	-0.51978900	2.96323200
C	-1.76728700	1.15878400	-1.05844500
C	-0.37094300	1.32286800	-1.09852700
H	0.06107500	2.02186500	-0.37254200
H	-2.23506500	0.81170700	-1.98553800
C	1.12055400	-0.39934300	0.25971700
C	2.37884200	-0.38668100	0.36119800
C	3.80259000	-0.37821500	0.46419600
C	4.44133500	-1.52394500	0.96800000
C	4.54823600	0.76170000	0.07062100
C	5.81958900	-1.56519700	1.07088000
C	5.94032900	0.68711400	0.19162300
C	6.56432600	-0.45009500	0.68274600
H	6.31537800	-2.45554900	1.44973300
H	6.54634200	1.53102100	-0.13242200
H	7.64983200	-0.47388400	0.75575200
H	1.58605100	0.34069300	1.14250200
C	3.87132900	1.95253600	-0.43444100
C	4.36317600	3.19851800	-0.43220900
H	2.86545000	1.80181700	-0.83634700
H	5.35012100	3.38727600	-0.00153300
H	3.83472500	-2.37635700	1.27136400
C	0.41334800	1.14396200	-2.36527500
H	-0.11592500	0.49486300	-3.07300400
H	1.40765300	0.71241000	-2.19078800
H	0.56141600	2.11711900	-2.85726000
C	3.63844400	4.37960900	-0.97030500
H	4.20493700	4.85580700	-1.78271800
H	3.50089700	5.14932900	-0.19853300
H	2.65049000	4.10237900	-1.36066400

TS1-4a

M06/BS1 SCF energy in gas pahse: -1569.763987 a.u.

M06/BS2 SCF energy in MeOH: -1570.230943 a.u.

M06/BS2 Free energy in MeOH: -1569.559545 a.u.

Ru	0.40504500	-0.69529000	-0.48938200
C	-0.53646900	-1.22642700	-2.52140300
C	0.26920500	-0.04531100	-2.64641500
C	1.63503900	-0.38653100	-2.35564000
C	0.30876500	-2.28300700	-2.08958100
C	1.67093200	-1.76661500	-2.02010700
C	2.81943000	0.51052500	-2.46404200
H	2.55509200	1.56009400	-2.28310100
H	3.26333300	0.45270800	-3.46819600
H	3.59825500	0.23413300	-1.74184800
C	-0.20852300	1.24307400	-3.22201600
H	-1.25539100	1.44712800	-2.96715600
H	-0.14633200	1.19772200	-4.31931500
H	0.39861100	2.09919700	-2.90417700
C	-1.98444000	-1.29558100	-2.86318100
H	-2.42494200	-2.26418100	-2.60481400
H	-2.12506400	-1.14637000	-3.94329500
H	-2.56514500	-0.51915400	-2.34766000
C	-0.07860000	-3.71594400	-1.94911300
H	0.36922200	-4.19538400	-1.06920000
H	0.25053600	-4.28989000	-2.82696100
H	-1.16492300	-3.83612000	-1.86869400
C	2.91856600	-2.57069000	-1.87242400
H	3.39701700	-2.68868500	-2.85519300
H	2.72484400	-3.57890700	-1.48868000
H	3.64879500	-2.08980300	-1.20860400
C	-1.49166500	-0.28128600	0.43447900
C	-1.08663500	0.89939900	0.12804000
C	1.62173800	0.38119100	0.89664800
C	0.94819200	1.37013900	0.45599600
C	-2.61590900	-0.98438200	1.00550600
C	-3.32577800	-0.39370600	2.07996900
C	-3.05131800	-2.20978000	0.48170300
C	-4.46552100	-1.04709800	2.56135700
C	-4.18876500	-2.83293300	0.96930800
H	-2.48652100	-2.66109400	-0.33447100
C	-4.90245800	-2.24424200	2.01179600
H	-4.99591300	-0.61059400	3.40641500
H	-4.51801100	-3.77908400	0.54466200
H	-5.79037400	-2.73076900	2.41013700
C	2.66612800	-0.29320800	1.60924500
C	2.64375300	-1.68581200	1.44910200
C	3.67824600	0.31371100	2.36022400
C	3.67956900	-2.46644500	1.95227600
C	4.69380100	-0.47591800	2.88458100
H	3.68572400	1.39319600	2.49906000
C	4.70443400	-1.85501000	2.66918700
H	3.67038500	-3.54713600	1.80984800
H	5.49838800	-0.01089900	3.45015400
H	5.51506700	-2.45815800	3.07250100
C	1.43149200	-2.23525400	0.82277400
C	0.15185600	-1.96037200	1.33428700
H	1.55431900	-3.17486200	0.28211000
H	-0.64700900	-2.68402300	1.18576200
H	0.04834800	-1.33728100	2.22603100

C	1.15442900	2.78457300	0.04249900
H	0.40076400	3.45088200	0.48397400
H	1.03731000	2.88504900	-1.05015000
C	-1.71417900	2.20231000	-0.23999000
H	-1.15368100	2.71910100	-1.03059500
H	-1.67877500	2.86604700	0.64144100
C	-2.87261500	0.86201800	2.69217200
C	-3.68629200	1.82119600	3.14087100
H	-1.79044600	1.00357100	2.76750800
H	-3.29963700	2.71973900	3.61620600
H	-4.76995700	1.74651600	3.04508700
C	2.54520900	3.26638700	0.44801900
H	2.64241600	3.19764600	1.54403200
H	3.30967300	2.59273700	0.02645500
C	2.81551100	4.69640700	0.00218600
H	2.03315400	5.35989400	0.40340400
H	2.73119900	4.75678600	-1.09536600
C	4.18481100	5.18270500	0.44516300
H	4.37531700	6.21035700	0.11599600
H	4.27581400	5.16258600	1.53956000
H	4.98262300	4.54865900	0.03506300
C	-3.17096700	2.05206800	-0.67137600
H	-3.22477600	1.48831200	-1.61911700
H	-3.72171800	1.45456400	0.07063800
C	-3.85117000	3.40315000	-0.83675000
H	-3.80685600	3.94339600	0.12320000
H	-3.28572400	4.01668700	-1.55736900
C	-5.29550500	3.26765400	-1.28684000
H	-5.88126600	2.68843700	-0.56013800
H	-5.77824900	4.24504000	-1.40028700
H	-5.36328200	2.74925100	-2.25309700

IM9

M06/BS1 SCF energy in gas pahse: -1233.520746 a.u.

M06/BS2 SCF energy in THF: -1233.89302 a.u.

M06/BS2 Free energy in THF: -1233.461897 a.u.

Ru	0.04308600	0.50385900	-0.34391800
C	0.11840300	2.68729800	0.01529300
C	1.42113200	2.15161800	0.22995800
C	1.34897900	1.22724900	1.33389600
C	-0.76205600	2.12715700	1.01668600
C	-0.00354400	1.23085500	1.82088000
C	2.49252300	0.58919800	2.04549400
H	3.38813000	0.50755600	1.42026800
H	2.75794400	1.18917800	2.92869000
H	2.24591200	-0.42022000	2.39721200
C	2.65024100	2.55398200	-0.50710100
H	2.44662500	2.72829800	-1.57071300
H	3.05115000	3.48777900	-0.08815300
H	3.43727100	1.79497700	-0.43653100
C	-0.23648300	3.77504900	-0.93917000
H	-1.29326200	3.73713700	-1.22851700
H	-0.06027700	4.75813200	-0.47933300
H	0.36768300	3.72928200	-1.85389500
C	-2.17374700	2.55639700	1.22084700
H	-2.72917500	1.87776000	1.87672500
H	-2.19452800	3.55611400	1.67764500
H	-2.72161700	2.62135200	0.27242200
C	-0.46280200	0.48182300	3.02453300
H	-0.00068900	0.89812900	3.93119300
H	-1.54861900	0.54034600	3.15930700
H	-0.17897600	-0.57809400	2.97626100
C	-2.09063500	0.35248100	-1.10053500
C	-1.39111300	0.96221100	-1.93951500
C	1.84771500	-0.49697100	-1.31757700
C	1.07665800	-0.01766900	-2.18010300
H	-1.19135600	1.51332100	-2.84389500
H	0.77063000	0.09573900	-3.20856300
C	-3.23975600	-0.33658600	-0.57024200
C	-3.34516300	-0.71957500	0.77356700
C	-4.29114900	-0.63964700	-1.44944100
C	-4.47811100	-1.38276900	1.22804800
H	-2.52275500	-0.50055200	1.45316600
C	-5.41996200	-1.30490000	-0.99007000
H	-4.20990400	-0.34654000	-2.49490300
C	-5.51697200	-1.67836800	0.34821600
H	-4.55326900	-1.66856000	2.27574900
H	-6.22903700	-1.53233000	-1.68105200
H	-6.40360100	-2.19766500	0.70621500
C	3.00193000	-1.11559200	-0.72656400
C	2.90271400	-2.10646700	0.25904600
C	4.27272500	-0.71255000	-1.16788100
C	4.04963100	-2.67411600	0.79620200
C	5.41569500	-1.28001900	-0.62046500
H	4.34946200	0.04631200	-1.94590100
C	5.30722500	-2.25812100	0.36482700
H	3.96390100	-3.44462100	1.56008900
H	6.39574400	-0.95955000	-0.96780100
H	6.20402700	-2.70056800	0.79354800
H	1.91744300	-2.41477400	0.60520400
C	-0.87730100	-2.59316300	-0.00660200
C	-1.50261600	-3.89668500	0.06270600
H	-1.22303500	-4.50124700	-0.80696500
H	-1.20322200	-4.42696900	0.97323600
H	-2.59285400	-3.76640900	0.06996200
N	-0.43150000	-1.52654500	-0.06969800

TS9

M06/BS1 SCF energy in gas pahse: -1233.507073 a.u.

M06/BS2 SCF energy in THF: -1233.877907 a.u.

M06/BS2 Free energy in THF: -1233.445224 a.u.

Ru	-0.03652800	-0.83025700	-0.22935000
C	0.64901600	-2.22338800	1.39207400
C	1.01517000	-2.80526900	0.15038000
C	-0.19531300	-3.01617400	-0.60385700
C	-0.80502700	-2.12970300	1.43504900

C	-1.31935300	-2.65609200	0.22287500
C	-0.28654500	-3.69385600	-1.92868700
H	0.58548300	-3.48606300	-2.56033000
H	-0.33628900	-4.78383700	-1.79593400
H	-1.18624100	-3.39538800	-2.48040500
C	2.39077000	-3.14010300	-0.31060300
H	3.15033300	-2.51973200	0.17926000
H	2.62662800	-4.19135200	-0.09398400
H	2.50442800	-2.99480800	-1.39179000
C	1.54616900	-1.91283600	2.54189600
H	1.31391800	-0.94170700	2.99779500
H	1.43453700	-2.67378800	3.32778700
H	2.60191700	-1.90457000	2.24749900
C	-1.58480600	-1.69990300	2.63080200
H	-2.64244000	-1.53777300	2.39352500
H	-1.54046100	-2.47284000	3.41151400
H	-1.19075900	-0.77466200	3.06993500
C	-2.74878700	-2.81109700	-0.16175100
H	-3.05441500	-3.86485600	-0.10170400
H	-3.41269500	-2.23314000	0.49065300
H	-2.92885300	-2.47578500	-1.19095400
C	1.61539900	0.18244400	-1.18582900
C	0.97281900	-0.40313900	-2.12553000
C	-1.57828600	0.34582400	-1.16927400
C	-1.00848600	-0.29785900	-2.11849900
H	1.09635700	-0.97596300	-3.03584300
H	-1.19696600	-0.85495200	-3.02742700
C	2.57286500	1.13759500	-0.71195300
C	2.89906900	2.23815900	-1.52292000
C	3.17743700	1.01716400	0.54934000
C	3.80441200	3.19102500	-1.07651100
H	2.42794300	2.33385700	-2.49993500
C	4.09110400	1.96643800	0.98335600
H	2.91878100	0.16592800	1.17853700
C	4.40263100	3.05899400	0.17469100
H	4.04962400	4.04053900	-1.71082000
H	4.56634200	1.85514700	1.95636100
H	5.11700100	3.80420000	0.51891100
C	-2.44270800	1.38475800	-0.69160800
C	-3.03076900	1.33554100	0.58257500
C	-2.69874000	2.49188600	-1.51870100
C	-3.86111500	2.36097400	1.01154700
C	-3.51973200	3.52019800	-1.07739300
H	-2.24047700	2.53132200	-2.50561800
C	-4.10333600	3.45817800	0.18613700
H	-4.32673200	2.30469300	1.99383500
H	-3.71147000	4.37284000	-1.72565400
H	-4.75280400	4.26240100	0.52593000
H	-2.83097200	0.47905200	1.22626100
C	0.11552700	1.88001000	1.48632300
N	0.05989900	0.85174100	0.96063400
C	0.18605500	3.19904200	2.07450500
H	-0.69323800	3.78039200	1.76948400
H	0.21337400	3.14192400	3.16775700
H	1.09343100	3.70519500	1.72171000

IM10

M06/BS1 SCF energy in gas pahse: -1233.549365 a.u.

M06/BS2 SCF energy in THF: -1233.915784 a.u.

M06/BS2 Free energy in THF: -1233.479368 a.u.

Ru	0.10083900	-0.44384600	-0.07599500
C	0.63023800	-2.26649900	1.19870700
C	1.07830400	-2.49426700	-0.12025900
C	-0.08551800	-2.46046300	-0.99459500
C	-0.82399500	-2.13543000	1.15815700
C	-1.25773400	-2.31694100	-0.17829100
C	-0.11580500	-2.79211200	-2.44853300
H	0.87890000	-2.74424100	-2.90624200
H	-0.49396700	-3.81366100	-2.59798600
H	-0.77772500	-2.11437200	-3.00295600
C	2.47651800	-2.75923200	-0.56684100
H	3.21542900	-2.36977200	0.14328700
H	2.65300000	-3.83863100	-0.67348900
H	2.68796900	-2.30070300	-1.54135100
C	1.43877800	-2.26252400	2.45185500
H	1.18064700	-1.41515900	3.10115000
H	1.26249700	-3.17938900	3.03272300
H	2.51357100	-2.20948400	2.24389400
C	-1.68522000	-2.02407100	2.37090000
H	-2.72452500	-1.78577500	2.11808700
H	-1.69286600	-2.97830800	2.91712300
H	-1.32239600	-1.25980300	3.07050900
C	-2.65777700	-2.38330400	-0.68336100
H	-2.99165300	-3.42941700	-0.73964700
H	-3.36000500	-1.84124900	-0.04019500
H	-2.74287700	-1.95634000	-1.69017900
C	1.52274400	0.58529200	-0.84452200
C	0.74459200	0.35038000	-1.99879700
C	-1.22855100	0.84768400	-1.08260300
C	-0.53899600	1.04936200	-2.22027100
H	1.15952300	-0.31549600	-2.76780400
H	-0.81500900	1.53888500	-3.15833400
C	2.79130400	1.14570400	-0.54870000
C	3.50536600	1.85413400	-1.53841000
C	3.34939300	0.99773500	0.73873900
C	4.74446800	2.39681800	-1.24454600
H	3.06357900	1.96762500	-2.52752200
C	4.58974500	1.53863500	1.02442000
H	2.78073700	0.44303900	1.48559800
C	5.28353800	2.23715100	0.03280100
H	5.29717800	2.94312800	-2.00524900
H	5.02803600	1.42096500	2.01306400
H	6.25976700	2.66211300	0.25903400
C	-2.58135400	1.26765400	-0.72697600
C	-3.16266200	0.90711400	0.49672100
C	-3.34221900	2.05376600	-1.60856000
C	-4.45364600	1.30217400	0.82779600

C	-4.62830200	2.45431800	-1.27761300
H	-2.91509100	2.35666900	-2.56394800
C	-5.19220500	2.07810100	-0.05953600
H	-4.88637200	1.00083500	1.78080000
H	-5.19966600	3.06328600	-1.97584900
H	-6.20360700	2.38915300	0.19428500
H	-2.58312100	0.29850100	1.19019400
C	-0.22079300	1.70868600	2.31929400
N	-0.05749600	0.90429800	1.50306800
C	-0.46571700	2.73120700	3.31468300
H	-1.47781900	3.13391300	3.18902800
H	-0.37009300	2.31776100	4.32450900
H	0.25451300	3.54864400	3.19979400

TS10

M06/BS1 SCF energy in gas pahse: -1233.541734 a.u.

M06/BS2 SCF energy in THF: -1233.90607 a.u.

M06/BS2 Free energy in THF: -1233.470671 a.u.

Ru	-0.06487200	0.22123100	0.00247600
C	-0.68209300	2.27110500	0.85998100
C	-0.93903400	2.23525700	-0.52807700
C	0.33489500	2.00534400	-1.20413900
C	0.75423000	2.11176200	1.05283000
C	1.37779800	2.03360800	-0.20878700
C	0.58238100	2.00214700	-2.67417900
H	-0.33040200	1.79169900	-3.24391300
H	0.97170700	2.97357700	-3.01237800
H	1.32631500	1.23993200	-2.94657000
C	-2.24018700	2.46438500	-1.21871700
H	-3.09899000	2.22722900	-0.58008500
H	-2.33261200	3.51553700	-1.52563100
H	-2.33046200	1.85246600	-2.12551700
C	-1.64657100	2.53205200	1.96633300
H	-1.53754900	1.80452300	2.78345800
H	-1.47896200	3.52765800	2.40263700
H	-2.68638000	2.49827900	1.62157600
C	1.43093000	2.13518100	2.38109000
H	2.40934200	1.63994700	2.34753000
H	1.59447900	3.16859300	2.71845000
H	0.82607400	1.63708800	3.15002500
C	2.83656500	2.03120100	-0.50507200
H	3.16912500	3.05328900	-0.73789500
H	3.43642600	1.67218500	0.33912000
H	3.07998700	1.40454300	-1.37204000
C	-1.46191900	-0.87354200	-0.79394200
C	-0.75198800	-1.25994300	-1.95815800
C	1.25483400	-1.14692100	-0.82577700
C	0.60798500	-1.66944400	-1.91744400
H	-1.25643700	-1.15424100	-2.93067100
H	1.02760700	-2.30191100	-2.70389600
C	-2.87326600	-1.03760900	-0.57476600
C	-3.68329600	-1.76500500	-1.47058700
C	-3.46885000	-0.48812800	0.57813000
C	-5.04160300	-1.90229800	-1.23804700
H	-3.23564400	-2.22281900	-2.35186200
C	-4.82702100	-0.62786200	0.80972100
H	-2.83016300	0.04385500	1.28380700
C	-5.61504500	-1.33097400	-0.10167400
H	-5.66011300	-2.46033400	-1.93753400
H	-5.27811600	-0.19832800	1.70192200
H	-6.68220500	-1.44423300	0.07954100
C	2.67980500	-1.25833600	-0.56379400
C	3.18921600	-1.09136900	0.73583600
C	3.59335800	-1.49226900	-1.60834200
C	4.55093300	-1.17548100	0.98690900
C	4.95690700	-1.55700900	-1.36061500
H	3.22390600	-1.59537000	-2.62820700
C	5.43941700	-1.40092600	-0.06281600
H	4.92767900	-1.05586700	2.00125500
H	5.65035400	-1.72540900	-2.18215000
H	6.50928200	-1.45065000	0.12970300
H	2.49204400	-0.89065400	1.54837600
C	-0.04791600	-1.55742300	2.71675800
N	-0.00624800	-0.91697700	1.75207500
C	-0.09334700	-2.37214200	3.91365700
H	0.62900100	-2.00356900	4.65042300
H	-1.09397900	-2.34308000	4.35886900
H	0.15407700	-3.41144200	3.67029900

IM11

M06/BS1 SCF energy in gas pahse: -1233.570546 a.u.

M06/BS2 SCF energy in THF: -1233.934464 a.u.

M06/BS2 Free energy in THF: -1233.497921 a.u.

Ru	-0.01008900	0.24290600	-0.00974200
C	0.92644800	1.34764300	1.84476900
C	1.05852400	-0.05613400	2.00515800
C	-0.26420300	-0.63310000	1.99495600
C	-0.47783200	1.65493000	1.77255500
C	-1.21652900	0.44989400	1.93444300
C	-0.58783600	-2.06399500	2.26874200
H	0.16223000	-2.73664000	1.83358700
H	-0.62678700	-2.26449400	3.34920900
H	-1.56151000	-2.34075100	1.84537200
C	2.30427700	-0.81240900	2.31261400
H	3.20646000	-0.33937000	1.90726300
H	2.42413400	-0.88150300	3.40363400
H	2.26596700	-1.83837200	1.92797400
C	2.02094600	2.36059800	1.82243500
H	1.86467500	3.11353100	1.03682500
H	2.06707500	2.90389100	2.77751300
H	3.00251000	1.90219900	1.65404500
C	-1.04631200	3.02821000	1.64452900
H	-2.05357800	3.01213100	1.21058300
H	-1.11997300	3.51823000	2.62615400
H	-0.41795000	3.66774100	1.01081700
C	-2.67285200	0.33634400	2.23073900

H	-2.82294300	0.39926700	3.31901700
H	-3.26257200	1.13761700	1.77198700
H	-3.09805300	-0.61808600	1.90055300
C	1.25081200	-0.98106300	-0.93060100
C	0.66364300	-2.01334300	-1.71944200
C	-1.27927600	-0.96018500	-0.93154000
C	-0.70805000	-2.00279800	-1.71830100
H	1.25182600	-2.69546600	-2.33692900
H	-1.31053800	-2.67776200	-2.33008900
C	2.69926000	-0.92500600	-0.81159100
C	3.47555500	-2.09880800	-0.76021200
C	3.36023400	0.31478700	-0.73732300
C	4.85065700	-2.03437400	-0.60018200
H	2.98112500	-3.06914500	-0.80730300
C	4.74022000	0.37945800	-0.60191300
H	2.76911100	1.22845500	-0.80417400
C	5.48617000	-0.79491600	-0.52226100
H	5.43456500	-2.95047600	-0.54014500
H	5.23928200	1.34608500	-0.55960500
H	6.56730700	-0.74524500	-0.40909500
C	-2.72662200	-0.89667500	-0.80349000
C	-3.38926900	0.34190600	-0.87121100
C	-3.49691700	-2.06292200	-0.63139400
C	-4.77136700	0.41295700	-0.76732100
C	-4.87338900	-1.98575700	-0.48647500
H	-2.99657600	-3.03024300	-0.57832100
C	-5.51309300	-0.74772800	-0.55951700
H	-5.27553200	1.37447500	-0.84476800
H	-5.45506200	-2.89138000	-0.32735800
H	-6.59565200	-0.69056500	-0.46517900
H	-2.79673200	1.24417100	-1.02921500
C	0.07262200	2.41014600	-2.44192500
N	0.04585100	1.63940600	-1.57730600
C	0.10419700	3.35689300	-3.53639500
H	-0.11762700	2.84686000	-4.48049100
H	-0.63825400	4.14713200	-3.37954800
H	1.09594500	3.81668700	-3.61160600

TS11

M06/BS1 SCF energy in gas pahse: -1349.183354 a.u.

M06/BS2 SCF energy in THF: -1349.591352 a.u.

M06/BS2 Free energy in THF: -1349.105374 a.u.

Ru	-0.05793300	0.32633300	-0.06522600
C	0.00993800	2.19376100	1.21889200
C	1.37086100	1.82407400	1.11879700
C	1.51384700	0.52557500	1.70054900
C	-0.71699300	1.09950100	1.86127200
C	0.22556400	0.06105700	2.13282700
C	2.80070600	-0.08656500	2.10549200
H	3.63337300	0.17069600	1.44328400
H	3.03888200	0.30338000	3.10837800
H	2.74276300	-1.17637000	2.18646800
C	2.48888400	2.67606700	0.62645600
H	2.13224200	3.47838400	-0.03013000
H	3.00642700	3.15324200	1.47172500
H	3.23565500	2.08758800	0.07775300
C	-0.53878900	3.53279300	0.86182800
H	-1.63277100	3.55645200	0.89788300
H	-0.17327400	4.28702100	1.57282600
H	-0.22306600	3.85096500	-0.14058600
C	-2.12257200	1.16743100	2.34819600
H	-2.57237300	0.17402800	2.44191900
H	-2.15304900	1.64811000	3.33634300
H	-2.76406000	1.74945200	1.67735100
C	0.00697300	-1.18798300	2.91566000
H	0.43445900	-1.08682000	3.92358000
H	-1.05792600	-1.41551600	3.03031400
H	0.48312500	-2.05262700	2.43597800
C	1.47252700	-1.20552300	-0.74920100
C	0.86129400	-2.45470000	-0.71781800
C	-1.19530200	-1.38264200	-0.26055700
C	-0.52111300	-2.55367800	-0.49823400
H	1.44909200	-3.35910100	-0.90344200
H	-1.04688700	-3.50524900	-0.60357300
C	2.94986700	-1.14040400	-0.72346800
C	3.71115300	-2.13649600	-0.08966300
C	3.64768500	-0.11343200	-1.37668300
C	5.09950100	-2.10205700	-0.09808700
H	3.20305500	-2.94267600	0.44145800
C	5.03653900	-0.06386300	-1.37101800
H	3.09354600	0.64991700	-1.91914600
C	5.77000800	-1.05808700	-0.72913000
H	5.66065100	-2.88948000	0.40177200
H	5.55000800	0.74396200	-1.88985100
H	6.85738200	-1.02429800	-0.72902900
C	-2.66723200	-1.46491500	-0.17979000
C	-3.42399200	-1.26468800	-1.34369200
C	-3.33092900	-1.85478000	0.98791500
C	-4.80529700	-1.42081800	-1.32753700
C	-4.71586500	-1.99416400	1.00721200
H	-2.75084800	-2.08237100	1.88324500
C	-5.45855200	-1.77065300	-0.14730100
H	-5.37376000	-1.29140800	-2.24817100
H	-5.21377900	-2.30074700	1.92532000
H	-6.53950400	-1.89368600	-0.13477500
H	-2.90531500	-1.01649100	-2.27168600
O	0.36040000	0.57747300	-2.15041300
C	0.89004800	1.80188900	-2.58294100
H	1.78923700	2.11528300	-2.02668000
H	1.15348100	1.72912300	-3.64745500
H	0.13390500	2.59735800	-2.46815300
H	1.04695200	-0.42832900	-1.72296800
C	-2.70685700	1.70962800	-1.31712600
N	-1.77609100	1.24740700	-0.81258800
C	-3.90191700	2.22924400	-1.94536500
H	-3.71958300	2.41430900	-3.00966500
H	-4.70349800	1.48667200	-1.84239800

H	-4.21597400	3.16552600	-1.47143300

IM12

M06/BS1 SCF energy in gas pahse: -1349.221648 a.u.

M06/BS2 SCF energy in THF: -1349.625664 a.u.

M06/BS2 Free energy in THF: -1349.137452 a.u.

Ru	-0.21925400	-0.52564500	0.15201800
C	-0.14173200	-2.51622500	-0.71477900
C	1.20413200	-2.03629600	-0.81021900
C	1.21866700	-0.92034800	-1.69936100
C	-0.97086100	-1.67047000	-1.56403600
C	-0.11791700	-0.69711400	-2.16336600
C	2.43964900	-0.27373800	-2.24305600
H	3.25140500	-0.22871000	-1.50796000
H	2.80256000	-0.86560000	-3.09767300
H	2.24334200	0.74209500	-2.60427400
C	2.40725800	-2.58574800	-0.13213000
H	2.14770400	-3.33568400	0.62101800
H	3.07412700	-3.05801700	-0.86712600
H	2.97163700	-1.79011300	0.37219900
C	-0.58972600	-3.71251600	0.05012200
H	-1.64342800	-3.63887700	0.34273800
H	-0.47628800	-4.62623600	-0.55017800
H	-0.00126100	-3.83759200	0.96685100
C	-2.40093700	-1.92109200	-1.90178800
H	-3.00382900	-1.00634900	-1.86942100
H	-2.48032100	-2.34062600	-2.91462200
H	-2.85614100	-2.64480000	-1.21652100
C	-0.47996000	0.26876900	-3.23615700
H	0.02181000	-0.01798100	-4.17148000
H	-1.55767100	0.27832600	-3.43184900
H	-0.16742800	1.29248400	-2.99578600
C	1.97945900	1.60448200	0.43234400
C	1.26963400	2.36348100	-0.44261200
C	-1.01122600	1.34137600	-0.22184700
C	-0.16526200	2.38801700	-0.46710800
H	1.78900900	3.05325400	-1.11380000
H	-0.62571300	3.36301300	-0.67196500
C	3.41972200	1.43668300	0.51178800
C	4.31941000	2.02362000	-0.39345500
C	3.93150400	0.61946900	1.53300800
C	5.68245700	1.80085700	-0.27528000
H	3.94930600	2.66079000	-1.19662000
C	5.29630900	0.38796500	1.64240400
H	3.23405800	0.15973300	2.23494600
C	6.17506300	0.98009300	0.73954200
H	6.36972300	2.26697200	-0.97853000
H	5.67749800	-0.24891900	2.43820000
H	7.24581200	0.80714300	0.82689300
C	-2.45342300	1.66489200	-0.11621700
C	-2.92560400	2.19868200	1.09174100
C	-3.36140300	1.49933100	-1.16665000
C	-4.26562600	2.53772300	1.24893000
C	-4.70534200	1.82576100	-1.00749700
H	-3.00480200	1.14379300	-2.13299600
C	-5.16402700	2.34052200	0.20168400
H	-4.60803500	2.96809900	2.18902400
H	-5.39398900	1.69910800	-1.84107300
H	-6.21205700	2.60903000	0.31963900
H	-2.21936600	2.34561100	1.91053100
O	0.73141000	-1.00490300	1.78678400
C	0.14041700	-1.29022600	3.02014300
H	-0.41965600	-2.24176400	3.00146800
H	0.94576400	-1.39801300	3.76145700
H	-0.53937200	-0.49297500	3.36329300
H	1.42155600	1.11738200	1.23316800
C	-3.03590200	-0.96659100	1.59699700
N	-1.97249500	-0.80734900	1.17211500
C	-4.38335000	-1.10859700	2.10323500
H	-4.37129500	-1.32351500	3.17737000
H	-4.92357200	-0.16825400	1.93168700
H	-4.90602700	-1.92034500	1.58523700

TS12

M06/BS1 SCF energy in gas pahse: -1349.157586 a.u.

M06/BS2 SCF energy in THF: -1349.563872 a.u.

M06/BS2 Free energy in THF: -1349.07882 a.u.

Ru	-0.20946600	-0.26229600	0.34287200
C	0.70919000	-2.21608900	1.20376600
C	0.78069500	-2.26908200	-0.22078900
C	-0.54603100	-2.15549000	-0.75739000
C	-0.67052500	-2.06987300	1.55279900
C	-1.46241000	-2.07247900	0.35044400
C	-0.90862200	-2.29501900	-2.19635000
H	-0.17999300	-1.79556500	-2.84760700
H	-0.94451300	-3.35371700	-2.49128000
H	-1.89351600	-1.86106600	-2.40738800
C	1.98250400	-2.58070800	-1.03882400
H	2.92097200	-2.32926400	-0.53364000
H	1.99433000	-3.66100000	-1.24618600
H	1.96858300	-2.06745200	-2.00724800
C	1.83475100	-2.34725700	2.17426400
H	1.75319700	-1.61504100	2.98927700
H	1.84108600	-3.34534200	2.63526500
H	2.80773400	-2.19832000	1.69289000
C	-1.21691400	-1.99817700	2.93722200
H	-2.12929000	-1.39015200	2.97794900
H	-1.47380700	-3.00336400	3.30094200
H	-0.49380500	-1.56663400	3.63943000
C	-2.94202600	-2.23519900	0.28502800
H	-3.19428600	-3.30502000	0.33303000
H	-3.45245600	-1.73912600	1.11849400
H	-3.36773300	-1.83937400	-0.64410800
C	1.30643100	0.83289500	-0.80319900
C	0.68223000	1.42824500	-1.97149000
C	-1.33507400	0.79858900	-0.90193700

C	-0.67524200	1.44100600	-2.00098300
H	1.28391800	1.89257000	-2.75459100
H	-1.22182800	1.99321000	-2.76775000
C	2.70955600	0.46790200	-0.79728300
C	3.44528900	0.29071400	-1.98115800
C	3.36667300	0.29485300	0.43493000
C	4.77990400	-0.08294300	-1.93257400
H	2.95868300	0.41728600	-2.94813200
C	4.70263500	-0.07317300	0.48346300
H	2.80569000	0.46783300	1.35575400
C	5.41024500	-0.26878000	-0.70240700
H	5.33507300	-0.22956900	-2.85656200
H	5.19958000	-0.19695200	1.44383800
H	6.45927100	-0.55575100	-0.66870600
C	-2.78684200	0.83984800	-0.86118000
C	-3.46416900	0.91636200	0.37060300
C	-3.55179700	0.79033200	-2.04409700
C	-4.84962300	0.95036000	0.41718400
C	-4.93679400	0.77723800	-1.99218300
H	-3.04882900	0.71989800	-3.00819300
C	-5.58776600	0.86525700	-0.76172500
H	-5.36030900	1.03337000	1.37459400
H	-5.51491000	0.71058600	-2.91140000
H	-6.67517500	0.87301500	-0.72297800
H	-2.87757300	0.96007100	1.28816700
C	-0.21231900	2.16889500	2.44152700
N	-0.37359100	1.15224700	1.90802000
C	0.05855200	3.47153100	2.99503500
H	0.73896800	3.94964100	2.27335600
H	-0.85912700	4.06451900	3.06869100
H	0.52956200	3.40171400	3.98084800
H	1.00204300	1.40880000	0.15963700
O	1.33439600	2.97318600	0.14484000
C	2.59522100	3.47724700	-0.04198600
H	2.87025000	3.60451900	-1.10975300
H	2.66841100	4.48649300	0.41237200
H	3.39996800	2.87694400	0.43553000

TS13

M06/BS1 SCF energy in gas pahse: -1349.171302 a.u.

M06/BS2 SCF energy in THF: -1349.575594 a.u.

M06/BS2 Free energy in THF: -1349.089704 a.u.

Ru	-0.14087900	0.62321100	0.08995700
C	-0.31649200	2.05616500	1.83607600
C	0.92601000	1.36799900	1.95599500
C	0.62476200	-0.03218300	2.10341600
C	-1.39216300	1.10411000	1.96545100
C	-0.80422100	-0.18365100	2.12987700
C	1.60298900	-1.08887600	2.48106400
H	2.59997000	-0.90294800	2.06499200
H	1.70198000	-1.12183100	3.57669400
H	1.28544400	-2.08420100	2.15009200
C	2.28808100	1.96817900	2.06756100
H	2.34033400	2.96486100	1.61197800
H	2.57594400	2.07511400	3.12327900
H	3.04807600	1.33931300	1.58605800
C	-0.50285700	3.53043900	1.70149900
H	-1.39503000	3.77195600	1.10976300
H	-0.63162600	3.99880500	2.68775200
H	0.35789100	4.01106200	1.21939700
C	-2.83362400	1.47649700	2.06916000
H	-3.48599200	0.59611200	2.06385200
H	-3.02576900	2.02117200	3.00502200
H	-3.15022200	2.13406300	1.24649000
C	-1.49651000	-1.47347700	2.41449900
H	-1.43693300	-1.70369800	3.48807300
H	-2.55587800	-1.45714800	2.13346400
H	-1.02801400	-2.30762000	1.87493800
C	1.50838600	0.05350100	-1.19396000
C	0.92569500	-0.38858500	-2.47411700
C	-0.93963000	-0.77701600	-1.07575600
C	-0.28588900	-0.97771700	-2.34936200
H	1.48073300	-0.34997600	-3.41463200
H	-0.76170500	-1.53106100	-3.16294900
C	2.50852800	-0.94849600	-0.67645300
C	2.14196700	-2.28953300	-0.50225300
C	3.82981600	-0.58284900	-0.39784600
C	3.06074400	-3.22907300	-0.05765500
H	1.11553400	-2.59792900	-0.70363700
C	4.74986000	-1.52926100	0.05086500
H	4.14919900	0.44801100	-0.53346700
C	4.37281800	-2.85419200	0.22444400
H	2.74927900	-4.26427000	0.07067300
H	5.77225400	-1.21971600	0.26049100
H	5.09264800	-3.59101700	0.57422500
C	-2.14764400	-1.55207400	-0.82568400
C	-3.30707600	-0.92465100	-0.34679500
C	-2.18175300	-2.93585500	-1.07019000
C	-4.46344900	-1.65535300	-0.10982600
C	-3.32165400	-3.67346500	-0.78141200
H	-1.29246500	-3.43527000	-1.45685100
C	-4.46606000	-3.03447400	-0.30667400
H	-5.36334800	-1.15193000	0.24003900
H	-3.32538000	-4.74982900	-0.94086400
H	-5.36395600	-3.61261500	-0.09795400
H	-3.28263000	0.15209700	-0.18320400
C	-1.40129000	2.77078500	-1.95677400
N	-0.88729900	1.98774400	-1.27187400
C	-2.05613900	3.74492800	-2.80682700
H	-1.37696900	4.09307600	-3.59331900
H	-2.93956000	3.30156800	-3.27999200
H	-2.37484300	4.61084600	-2.21541900
H	1.24682100	1.69158700	-0.49536000
O	2.19528200	1.40376500	-1.24669300
C	2.46001000	2.02001400	-2.50879700
H	1.54510300	2.10441200	-3.11045400
H	2.86938000	3.01012900	-2.29669900

H	3.20796600	1.42026800	-3.04106000

TS14

M06/BS1 SCF energy in gas pahse: -1233.528253 a.u.

M06/BS2 SCF energy in THF: -1233.894171 a.u.

M06/BS2 Free energy in THF: -1233.458766 a.u.

Ru	-0.02556100	0.55458400	-0.14533900
C	-0.29944400	2.34811100	1.17845900
C	-0.57765600	2.73125000	-0.15381800
C	0.61662900	2.47648800	-0.93368200
C	1.11075400	1.95487300	1.24851500
C	1.68206300	2.07931900	-0.03268800
C	0.79583800	2.78309800	-2.37938300
H	-0.15789500	2.78306900	-2.91929400
H	1.23943900	3.78213200	-2.50039400
H	1.46479700	2.06489000	-2.86933000
C	-1.86238700	3.26364000	-0.69352500
H	-2.71105900	3.00558400	-0.04924700
H	-1.83085600	4.35885800	-0.77666000
H	-2.07889500	2.86659200	-1.69414400
C	-1.18880300	2.45666500	2.36659500
H	-1.11276000	1.56627200	3.00261800
H	-0.90536900	3.32736400	2.97633000
H	-2.23868800	2.58671200	2.07957600
C	1.80799800	1.58909800	2.51089400
H	2.78315700	1.12664900	2.32162500
H	1.97875500	2.49231200	3.11500700
H	1.20600300	0.89861700	3.11241000
C	3.09614200	1.82098200	-0.42355700
H	3.70328800	2.72999600	-0.31092900
H	3.55384000	1.03191600	0.18838500
H	3.17099300	1.50036800	-1.46984300
C	-1.56172300	-0.32935300	-0.83896500
C	-0.78271000	-0.36763000	-2.03847700
C	1.02546800	-1.09230100	-0.80519900
C	0.41426300	-1.15866300	-2.04853800
H	-1.13140300	0.15480100	-2.93713300
H	0.83700000	-1.53826600	-2.98717300
C	-2.87012300	-0.80909800	-0.55921700
C	-3.58629700	-1.55254600	-1.52362000
C	-3.45841400	-0.56023300	0.70030400
C	-4.85327400	-2.02729900	-1.23482400
H	-3.12687100	-1.74668000	-2.49207600
C	-4.72597900	-1.03762000	0.98125400
H	-2.88491400	-0.00182100	1.43917200
C	-5.42045700	-1.76915800	0.01476200
H	-5.40661000	-2.59767200	-1.97729400
H	-5.18110300	-0.84759900	1.95066100
H	-6.41758000	-2.14395400	0.23846500
C	2.37315600	-1.54423900	-0.49471200
C	2.79477300	-1.57413500	0.84669300
C	3.30052900	-1.90337900	-1.48983400
C	4.09159400	-1.93999300	1.18275500
C	4.59652100	-2.26477800	-1.15476800
H	3.00840000	-1.87850600	-2.53912500
C	4.99696200	-2.28123800	0.18110100
H	4.39813600	-1.96084700	2.22701000
H	5.30462500	-2.52968600	-1.93755300
H	6.01607700	-2.56238600	0.43931800
H	2.07851500	-1.30859200	1.62517400
C	-0.59720000	-1.99958900	2.07030000
N	-0.49750600	-0.91252400	2.47110000
C	-0.70905600	-3.32397900	1.49543100
H	-0.18113300	-3.33085300	0.53078800
H	-0.26308000	-4.07788200	2.15251400
H	-1.76258100	-3.57516000	1.32482100

IM13

M06/BS1 SCF energy in gas pahse: -1100.891328 a.u.

M06/BS2 SCF energy in THF: -1101.215771 a.u.

M06/BS2 Free energy in THF: -1100.82173 a.u.

Ru	-0.00302100	0.42872700	-0.33947000
C	-0.74475100	1.98569300	1.12549300
C	-1.10782800	2.41315300	-0.18762600
C	0.10176200	2.58639500	-0.94332300
C	0.69130100	1.93501300	1.19975400
C	1.21479700	2.32572800	-0.07115500
C	0.18593600	3.04074100	-2.36093600
H	-0.67538600	2.69776000	-2.94695800
H	0.20827600	4.13782500	-2.42215800
H	1.09114100	2.66672800	-2.85453200
C	-2.49354700	2.64907500	-0.68373300
H	-3.22222000	2.00632500	-0.17484600
H	-2.79721800	3.69148000	-0.51168100
H	-2.58015800	2.45774500	-1.76015700
C	-1.64280500	1.85931200	2.30827400
H	-1.32893900	1.04494800	2.97347700
H	-1.61274100	2.78703800	2.89911300
H	-2.68775200	1.69190200	2.02466300
C	1.44989500	1.74582100	2.46954900
H	2.52673800	1.64049000	2.29722900
H	1.31285000	2.62329900	3.11879700
H	1.10150900	0.87127200	3.03415700
C	2.65669800	2.46115000	-0.42595100
H	3.01841100	3.47661200	-0.21120700
H	3.28414500	1.76122100	0.14052800
H	2.83242900	2.27035800	-1.49168500
C	-1.35141600	-0.97121500	-0.50660000
C	-0.72609200	-1.09369600	-1.78112800
C	1.31497800	-0.99491100	-0.51008500
C	0.68510500	-1.10845700	-1.78273500
H	-1.28140900	-0.99250400	-2.71925800
H	1.24117100	-1.01679000	-2.72148600
C	-2.61898200	-1.47395200	-0.08638100
C	-3.35695400	-2.34786400	-0.91381200
C	-3.13559400	-1.13772200	1.17979200

C	-4.58785400	-2.82805000	-0.50200300
H	-2.94984600	-2.64361200	-1.87968600
C	-4.36018200	-1.63148000	1.59392300
H	-2.53602700	-0.50850000	1.83331300
C	-5.09017500	-2.46885300	0.74945600
H	-5.15785600	-3.49293700	-1.14696200
H	-4.74990700	-1.37549100	2.57660300
H	-6.05305900	-2.85704000	1.07587500
C	2.57907900	-1.50392900	-0.08848100
C	3.10930000	-1.14212400	1.16497900
C	3.30193200	-2.40302200	-0.90168600
C	4.33276100	-1.63712600	1.58107200
C	4.53112900	-2.88594000	-0.48749400
H	2.88391000	-2.71605900	-1.85744600
C	5.04704300	-2.50210800	0.75111700
H	4.73346800	-1.36051400	2.55370700
H	5.08963300	-3.57149300	-1.12071300
H	6.00872400	-2.89196700	1.07911100
H	2.51979600	-0.49187800	1.80717300

TS15

M06/BS1 SCF energy in gas pahse: -1216.535004 a.u.

M06/BS2 SCF energy in THF: -1216.900311 a.u.

M06/BS2 Free energy in THF: -1216.455911 a.u.

Ru	0.10010200	0.42215200	-0.26356500
C	1.01350100	2.47761800	-0.09517400
C	0.53449900	2.10071000	1.19336200
C	-0.88822700	1.91274600	1.10126700
C	-0.12087300	2.52523100	-0.98968200
C	-1.29806300	2.21320500	-0.23770200
C	-1.77578000	1.66082700	2.27102400
H	-1.31427000	0.97147100	2.98962500
H	-1.97228800	2.60376600	2.80249600
H	-2.74447500	1.24320900	1.97528100
C	1.30582400	2.05533800	2.46858200
H	2.38702000	2.10945200	2.29906500
H	1.03592400	2.91240300	3.10308300
H	1.09149100	1.14648000	3.04571800
C	2.42436700	2.80686100	-0.44896900
H	2.63238400	2.61607700	-1.50883400
H	2.64048600	3.86756900	-0.25779300
H	3.13954100	2.21243700	0.13496500
C	-0.08071300	2.92191100	-2.42638300
H	-0.90807500	2.47536700	-2.99123600
H	-0.16186500	4.01281100	-2.53398400
H	0.85429800	2.61408500	-2.91036900
C	-2.70138400	2.22222500	-0.74163600
H	-3.14793000	3.22136900	-0.63951400
H	-2.75720400	1.94560300	-1.80271000
H	-3.33598800	1.51803200	-0.18773200
C	-1.17927300	-1.14386500	-0.29888200
C	-0.53160000	-1.19317700	-1.57770300
C	1.57329100	-0.84277600	-0.43072200
C	0.88405600	-1.12399600	-1.64412200
H	-1.11064400	-1.11210600	-2.50077600
H	1.36282200	-1.04983700	-2.62733900
C	-2.62187600	-1.25317100	-0.06400800
C	-3.12195100	-1.28128400	1.24500200
C	-3.52745900	-1.26962700	-1.13376300
C	-4.48964200	-1.31130400	1.47797600
H	-2.42180700	-1.29359300	2.07818800
C	-4.89699700	-1.28151000	-0.89579900
H	-3.16921900	-1.25645600	-2.16199600
C	-5.38200500	-1.30165600	0.40788500
H	-4.86235900	-1.34201700	2.49984900
H	-5.58751300	-1.28589100	-1.73658400
H	-6.45434300	-1.31791200	0.59073200
C	2.96003800	-1.08030200	-0.13284600
C	3.53430300	-0.51573800	1.02160500
C	3.76395500	-1.88138800	-0.96720700
C	4.87318500	-0.71613800	1.31525500
C	5.10419000	-2.07559900	-0.67415500
H	3.32364800	-2.34765700	-1.84830600
C	5.66029900	-1.49113500	0.46394500
H	5.30852800	-0.27733900	2.21063200
H	5.72099400	-2.68971000	-1.32686000
H	6.71160700	-1.65172700	0.69461200
H	2.89543800	0.06910800	1.68253700
H	0.37612800	-2.16519900	0.90299300
O	-0.54681400	-2.48210100	0.80162100
C	-0.61637000	-3.81044000	0.26039500
H	-0.04165200	-3.88488200	-0.67025600
H	-0.24174700	-4.51826200	1.00535000
H	-1.67469300	-4.00592100	0.06776600

IM14

M06/BS1 SCF energy in gas pahse: -1216.538725 a.u.

M06/BS2 SCF energy in THF: -1216.905248 a.u.

M06/BS2 Free energy in THF: -1216.458435 a.u.

Ru	0.11359400	0.39933000	-0.22228600
C	1.02471100	2.44630300	-0.09096100
C	0.53382500	2.10475800	1.20083600
C	-0.88689800	1.89312400	1.09497900
C	-0.10233500	2.46950200	-0.99926700
C	-1.28455800	2.17043600	-0.25621800
C	-1.78939200	1.63731900	2.25342700
H	-1.33323400	0.95043300	2.97833900
H	-2.00530200	2.57633700	2.78416800
H	-2.74958200	1.20854700	1.94341500
C	1.29495000	2.06167300	2.48140100
H	2.37885300	2.06144600	2.32100900
H	1.05612300	2.94450500	3.09262000
H	1.03732500	1.17736600	3.07864700
C	2.43287500	2.77004300	-0.45947300
H	2.68387700	2.39078100	-1.45840100
H	2.59705100	3.85691100	-0.46904500

H	3.15233600	2.33242300	0.24283000
C	-0.03926700	2.83222900	-2.44367100
H	-0.85957200	2.37574000	-3.01103800
H	-0.11395900	3.92085600	-2.57764900
H	0.90276700	2.51026300	-2.90488900
C	-2.68254900	2.18146100	-0.77294700
H	-3.12303700	3.18453600	-0.68223900
H	-2.72813800	1.89991200	-1.83307900
H	-3.32896400	1.48649600	-0.22158300
C	-1.19618000	-1.26340600	-0.25919700
C	-0.53230500	-1.18603800	-1.53436600
C	1.58175600	-0.90875800	-0.38922300
C	0.89074000	-1.14989500	-1.60665900
H	-1.11351700	-1.02242500	-2.44250400
H	1.36182600	-1.06833500	-2.59287300
C	-2.65932300	-1.28748400	-0.07716800
C	-3.19187700	-1.35730000	1.21794600
C	-3.54008900	-1.19589100	-1.16149000
C	-4.56526600	-1.32622200	1.42209300
H	-2.51811400	-1.42329200	2.07137600
C	-4.91361600	-1.15501000	-0.95275700
H	-3.16034400	-1.14970900	-2.18085200
C	-5.43132500	-1.21799600	0.33723200
H	-4.96113200	-1.38318700	2.43412200
H	-5.58351500	-1.08385100	-1.80715800
H	-6.50709000	-1.18903700	0.49616500
C	2.98677300	-1.11002100	-0.12922800
C	3.55918300	-0.56956200	1.03631100
C	3.80481400	-1.84968000	-1.00304900
C	4.90854700	-0.73385400	1.30514900
C	5.15526400	-2.01104500	-0.73412900
H	3.36856100	-2.29947900	-1.89479000
C	5.70895300	-1.45169900	0.41702100
H	5.34133700	-0.31194900	2.20999100
H	5.78139900	-2.58156200	-1.41691800
H	6.76786500	-1.58652600	0.62861500
H	2.91052500	-0.02422600	1.72233500
H	0.36272200	-1.90200100	0.78524400
O	-0.58201000	-2.26376800	0.73204000
C	-0.69489200	-3.67989100	0.38356200
H	-0.20292100	-3.85803800	-0.57703900
H	-0.22695700	-4.24091700	1.19371400
H	-1.76438600	-3.89098200	0.33080100

TS16

M06/BS1 SCF energy in gas pahse: -1216.537837 a.u.

M06/BS2 SCF energy in THF: -1216.903402 a.u.

M06/BS2 Free energy in THF: -1216.458982 a.u.

Ru	0.10790700	0.40201100	-0.19693300
C	1.04944100	2.43439000	-0.09821000
C	0.53266300	2.13389900	1.19116300
C	-0.89059300	1.92662300	1.06951800
C	-0.06184500	2.43257300	-1.02824500
C	-1.26164900	2.16881700	-0.29516700
C	-1.81233400	1.70160500	2.21927700
H	-1.36663600	1.03375600	2.96798200
H	-2.03856800	2.65308600	2.72271900
H	-2.76634600	1.26116700	1.90530600
C	1.27702100	2.10053900	2.48107800
H	2.36255900	2.10433800	2.33343900
H	1.02545400	2.98558600	3.08386600
H	1.01442300	1.21911200	3.08057800
C	2.46931800	2.72042300	-0.45112500
H	2.72783300	2.31265900	-1.43689800
H	2.65805600	3.80279600	-0.48249500
H	3.16721300	2.28141100	0.27200200
C	0.02950900	2.73556700	-2.48435200
H	-0.77206700	2.24289800	-3.04863600
H	-0.05567600	3.81612700	-2.66766600
H	0.98604000	2.40555100	-2.90876100
C	-2.64862600	2.16482600	-0.84023200
H	-3.08852100	3.17081200	-0.78804500
H	-2.67388500	1.85158800	-1.89223100
H	-3.30637400	1.48731800	-0.28087000
C	-1.22208900	-1.28101100	-0.26994400
C	-0.54733600	-1.16116900	-1.53059900
C	1.55618000	-0.97697800	-0.35457000
C	0.87924500	-1.15065500	-1.58829600
H	-1.12233800	-0.95216300	-2.43317300
H	1.36432900	-1.05004800	-2.56504000
C	-2.68119800	-1.30088100	-0.08468700
C	-3.20657000	-1.33896100	1.21464500
C	-3.56496900	-1.23219700	-1.16817200
C	-4.57871300	-1.29548400	1.42358900
H	-2.52713200	-1.38916000	2.06479000
C	-4.93717200	-1.17984300	-0.95453600
H	-3.18701400	-1.21962800	-2.18950900
C	-5.44856000	-1.20809300	0.33954700
H	-4.97098900	-1.32662800	2.43810900
H	-5.61122100	-1.12797800	-1.80703400
H	-6.52346500	-1.16983100	0.50243600
C	2.97000900	-1.15227000	-0.11265200
C	3.53055200	-0.65832000	1.07822800
C	3.80589300	-1.81695900	-1.02766000
C	4.88567900	-0.79518900	1.33455900
C	5.16180300	-1.95179800	-0.77122000
H	3.38035300	-2.23389000	-1.94020200
C	5.70368000	-1.43958600	0.40703000
H	5.30887900	-0.40945300	2.25985100
H	5.80161700	-2.46490200	-1.48609500
H	6.76689000	-1.55417500	0.60859000
H	2.86792000	-0.17043100	1.79391300
H	0.43774300	-1.73235700	0.65751100
O	-0.55445000	-2.18590700	0.72432000
C	-0.66791200	-3.61468500	0.45167700
H	-0.19850500	-3.84058900	-0.51102200
H	-0.16737900	-4.12789400	1.27410700

H	-1.73404900	-3.85138100	0.43909900

IM15

M06/BS1 SCF energy in gas pahse: -1216.608752 a.u.

M06/BS2 SCF energy in THF: -1216.970696 a.u.

M06/BS2 Free energy in THF: -1216.520206 a.u.

Ru	0.04457200	0.15121800	0.04241000
C	1.37454800	1.95107400	0.14565300
C	0.60502900	1.84496300	1.33699700
C	-0.80076700	1.92966200	0.98135400
C	0.45810100	2.01630300	-0.96701000
C	-0.88465800	2.07362600	-0.43783500
C	-1.93126600	1.93837700	1.95184100
H	-1.73445100	1.26462200	2.79592800
H	-2.08686600	2.94500400	2.36547500
H	-2.87224500	1.61803600	1.48774800
C	1.13793500	1.72517900	2.72301000
H	2.13965700	1.27886300	2.73383300
H	1.20995200	2.71298900	3.20066300
H	0.48780200	1.10475600	3.35210300
C	2.85733800	2.00614700	0.06277600
H	3.23732900	1.64487100	-0.89983600
H	3.19401700	3.04612200	0.18071800
H	3.34034700	1.40979800	0.84633200
C	0.83148000	2.13737000	-2.40469700
H	0.11193700	1.61656200	-3.04968600
H	0.85693900	3.18983600	-2.72083300
H	1.82269800	1.71050500	-2.60044000
C	-2.12860100	2.25232900	-1.23534100
H	-2.36659700	3.32069300	-1.33698100
H	-2.02375600	1.84334500	-2.24850600
H	-2.99227000	1.76241900	-0.76773800
C	-1.56170600	-1.31853200	-0.17505200
C	-0.69359500	-1.44826300	-1.28888600
C	1.57892300	-1.49444600	-0.14405600
C	0.73515400	-1.49581900	-1.27247800
H	-1.13882600	-1.25961600	-2.26513100
H	1.18690700	-1.29919600	-2.24672700
C	-3.00837000	-1.07695000	-0.24195400
C	-3.74178500	-0.99970200	0.95028900
C	-3.67881100	-0.89346500	-1.45984600
C	-5.10255000	-0.72281100	0.92471900
H	-3.23408400	-1.14960000	1.90128200
C	-5.03930700	-0.62121000	-1.48000800
H	-3.14495000	-0.96421900	-2.40620600
C	-5.75523700	-0.52758900	-0.28891600
H	-5.65728000	-0.66528600	1.85901100
H	-5.54467000	-0.48527100	-2.43385800
H	-6.82141000	-0.31251600	-0.30834500
C	3.02918600	-1.28765000	-0.20360700
C	3.74449700	-1.33563200	1.00181500
C	3.73263800	-1.01857400	-1.38527800
C	5.11423700	-1.11107800	1.03176500
C	5.10390100	-0.79892100	-1.35628500
H	3.21543400	-0.99032300	-2.34454500
C	5.79877300	-0.83764700	-0.14952600
H	5.65083800	-1.15585500	1.97741100
H	5.63632200	-0.60092300	-2.28459200
H	6.87284100	-0.66595500	-0.13227100
H	3.20720000	-1.54914000	1.92806200
H	1.25441600	-1.96661400	0.78412700
O	-1.05710200	-1.63173100	1.07608900
C	-0.89508900	-3.03349300	1.35472000
H	-0.32024900	-3.53579500	0.56753500
H	-0.37822500	-3.10509900	2.31451300
H	-1.89305900	-3.48222800	1.43119800

TS9-r

M06/BS1 SCF energy in gas pahse: -1233.497231 a.u.

M06/BS2 SCF energy in THF: -1233.865402 a.u.

M06/BS2 Free energy in THF: -1233.435165 a.u.

Ru	-0.04358800	-0.61275300	0.18230800
C	-0.03716000	-2.83389400	0.24572300
C	1.27865500	-2.43503300	-0.10498800
C	1.19560800	-1.68409700	-1.32881800
C	-0.93865000	-2.40174800	-0.81705000
C	-0.16828300	-1.72329600	-1.79792300
C	2.34649600	-1.11745600	-2.09036700
H	3.07991700	-0.62853900	-1.43576700
H	2.87060800	-1.91332100	-2.63847600
H	2.01351900	-0.37886700	-2.82920700
C	2.51710200	-2.76227600	0.65702100
H	2.45212900	-2.44216200	1.70621100
H	2.68898400	-3.84742700	0.65614400
H	3.40086200	-2.29130900	0.21231800
C	-0.41454000	-3.68255900	1.41145200
H	-1.42282900	-3.44935600	1.77432200
H	-0.40357500	-4.74789500	1.13836600
H	0.28219500	-3.54857800	2.24790900
C	-2.38010400	-2.77409800	-0.89588300
H	-2.88983600	-2.26726600	-1.72356000
H	-2.48484100	-3.85593300	-1.06019400
H	-2.91989100	-2.53501600	0.02957600
C	-0.64465300	-1.13364100	-3.08045300
H	-0.17258400	-1.63199800	-3.93804100
H	-1.72960100	-1.23345600	-3.19584400
H	-0.40486600	-0.06317300	-3.14815400
C	0.97519000	0.19791900	1.80452200
C	1.59169300	0.91388600	0.94056800
C	-0.86549000	1.22827500	-0.52064900
C	0.40481000	1.39018800	-0.62247400
H	1.16383200	1.76272600	-1.29932000
C	-2.19950700	1.75305200	-0.54806900
C	-3.30728400	0.93441300	-0.82204100
C	-2.41149700	3.11384500	-0.26546600
C	-4.58927300	1.46532900	-0.82815300

C	-3.69811500	3.63424300	-0.25456500
H	-1.55350100	3.74708100	-0.04544400
C	-4.78882200	2.81449800	-0.53686000
H	-5.43948400	0.82770800	-1.06393600
H	-3.85185800	4.68791800	-0.03041500
H	-5.79516600	3.22844500	-0.53626500
H	-3.14406000	-0.12086700	-1.03850200
C	-2.55316800	-0.22483400	2.15376100
N	-1.62381400	-0.45005400	1.50221300
C	-3.73424600	0.11568700	2.91845500
H	-4.36879400	0.77701100	2.31415400
H	-4.30342200	-0.78279400	3.18019900
H	-3.45558000	0.63727800	3.84054300
C	2.89249000	1.45770900	0.57250200
C	4.03659300	0.69018400	0.84006500
C	3.04814400	2.74449600	0.04032600
C	5.30148400	1.18768900	0.55662600
H	3.91600500	-0.29619700	1.28591800
C	4.31543000	3.23962400	-0.23736400
H	2.17328900	3.37185800	-0.12195300
C	5.44242200	2.46028300	0.01012900
H	6.18059500	0.58301400	0.76997200
H	4.42532700	4.24431400	-0.64027900
H	6.43347800	2.85135700	-0.21072200
H	0.85176900	0.01664500	2.86326500

TS17

M06/BS1 SCF energy in gas pahse: -1100.804328 a.u.

M06/BS2 SCF energy in THF: -1101.134304 a.u.

M06/BS2 Free energy in THF: -1100.745205 a.u.

Ru	0.28840500	-0.81305100	-0.49541400
C	1.19018300	-2.80042200	0.02309200
C	0.29353800	-2.35893300	1.08931400
C	0.85905900	-1.20069900	1.69006600
C	2.29195800	-1.91343900	-0.02364400
C	2.07012800	-0.89939600	0.96557900
C	0.40083200	-0.52625300	2.93714500
H	-0.67844300	-0.63701700	3.09398700
H	0.90013600	-0.96604800	3.81273400
H	0.63476400	0.54486200	2.94036000
C	-0.92176300	-3.10019800	1.53558300
H	-1.50536000	-3.48111600	0.68812400
H	-0.63653400	-3.96720700	2.14913000
H	-1.58773600	-2.47303100	2.13916500
C	0.98444500	-4.01693300	-0.81039600
H	1.49180900	-3.93919100	-1.77841300
H	1.38274100	-4.90431200	-0.29687900
H	-0.07841800	-4.20434900	-1.00407700
C	3.46945400	-1.99740200	-0.93331400
H	3.83024200	-1.00433600	-1.22854600
H	4.30716900	-2.51193900	-0.44210200
H	3.23566900	-2.55217800	-1.84974700
C	3.04968000	0.16469100	1.32327900
H	3.80626800	-0.25020800	2.00483500
H	3.57935300	0.55139200	0.44468100
H	2.57986800	1.01488600	1.82971900
C	1.08105100	1.12731100	-1.07204500
C	0.99162800	0.35933200	-2.11405700
C	-1.50159000	-0.19003800	-0.92015900
C	-0.79602200	-0.38905600	-2.06618800
H	1.39914600	0.18076600	-3.10305800
H	-0.92702400	-0.46747900	-3.14500200
C	1.22922000	2.40280900	-0.45382700
C	0.67358000	2.65534500	0.81145200
C	1.90542100	3.43244600	-1.13481200
C	0.79730800	3.91127700	1.38619400
H	0.11545100	1.85925300	1.30462500
C	2.04362100	4.67629700	-0.54127900
H	2.32322500	3.23920600	-2.12167100
C	1.49004100	4.91757200	0.71660200
H	0.35127500	4.10983600	2.35844000
H	2.57622300	5.46831900	-1.06308300
H	1.59398200	5.89976800	1.17315500
C	-2.82486600	0.13173600	-0.47802300
C	-3.11744700	0.15068800	0.89586400
C	-3.84121500	0.43599700	-1.40246700
C	-4.39415200	0.45604700	1.33722300
C	-5.11856800	0.73752700	-0.95753700
H	-3.61325500	0.43322300	-2.46783800
C	-5.39501200	0.74546400	0.40922500
H	-4.61767300	0.47306000	2.40172400
H	-5.90370300	0.96912800	-1.67384600
H	-6.39876700	0.98473800	0.75480500
H	-2.31332100	-0.06641600	1.59978300

TS18

M06/BS1 SCF energy in gas pahse: -1349.204379 a.u.

M06/BS2 SCF energy in THF: -1349.610301 a.u.

M06/BS2 Free energy in THF: -1349.121966 a.u.

Ru	-0.00296100	0.44991800	-0.05408700
C	-0.87997700	2.34391800	0.83619600
C	-1.36548000	2.19700500	-0.48435700
C	-0.21959600	2.22055300	-1.38143400
C	0.56699600	2.49782900	0.75927600
C	0.95645200	2.47665200	-0.60359300
C	-0.24682800	2.24168500	-2.87305200
H	-1.22526100	1.95719400	-3.27619700
H	-0.02606800	3.25254300	-3.24469400
H	0.50564700	1.56518400	-3.29965900
C	-2.79455300	2.12599800	-0.90421800
H	-3.42224300	1.62705700	-0.15463500
H	-3.19872100	3.13598300	-1.06066600
H	-2.91909600	1.57860600	-1.84683500
C	-1.68360100	2.44646500	2.08832100
H	-1.19423600	1.93276500	2.92648800
H	-1.81827200	3.49641100	2.38665400

H	-2.68176200	2.00776000	1.96723200
C	1.43977600	2.80685300	1.92800800
H	2.50019100	2.63257200	1.71145300
H	1.33400600	3.86473200	2.20829000
H	1.17124000	2.21497300	2.81221400
C	2.31164500	2.72109400	-1.17281500
H	2.39847000	3.76439200	-1.50982100
H	3.11029600	2.54103300	-0.44481300
H	2.50742300	2.08007200	-2.04121500
C	-1.30578000	-1.01614600	-0.46941300
C	-0.63108300	-0.79135100	-1.70554500
C	1.46917200	-0.77877500	-0.92474500
C	0.74193600	-1.28696000	-1.94553600
H	-1.21406200	-0.34959200	-2.52160000
H	1.04606100	-1.85157100	-2.83404700
C	-2.72925900	-1.12846800	-0.18853800
C	-3.64411300	-1.40891200	-1.21178200
C	-3.20100200	-0.90628700	1.11307200
C	-5.00867600	-1.41701200	-0.94751300
H	-3.27855500	-1.60260000	-2.22059800
C	-4.56164500	-0.93934700	1.38014700
H	-2.47735500	-0.69856900	1.90202000
C	-5.46667700	-1.18091800	0.34587300
H	-5.71700100	-1.61429600	-1.74941500
H	-4.92476300	-0.76797800	2.39157400
H	-6.53504100	-1.19055100	0.55257100
C	2.89146200	-0.96391600	-0.63898900
C	3.53452300	-0.22571200	0.36388900
C	3.65117500	-1.90682400	-1.35223100
C	4.88580000	-0.40602000	0.63611200
C	4.99827800	-2.09233400	-1.07864000
H	3.17366300	-2.50459200	-2.12866300
C	5.62226100	-1.34131500	-0.08395300
H	5.36815200	0.18597600	1.41244900
H	5.56804000	-2.82760300	-1.64400400
H	6.67957200	-1.48746900	0.12811500
H	2.95291600	0.50664800	0.92391300
C	0.90354700	-0.90253100	2.73485300
N	0.53394600	-0.41855400	1.74984000
C	1.40048900	-1.52069000	3.94650900
H	2.48889700	-1.63767900	3.88528000
H	1.15856900	-0.90660900	4.82088200
H	0.94751200	-2.50956500	4.07882500
O	-0.63761400	-2.63162600	0.21153000
H	0.28792200	-2.47324600	-0.09164300
C	-1.16204700	-3.78440300	-0.45900800
H	-0.67084800	-4.67947800	-0.06456600
H	-2.23045500	-3.82468400	-0.23374800
H	-1.01043200	-3.71212100	-1.54379500

IM16

M06/BS1 SCF energy in gas pahse: -1349.207655 a.u.

M06/BS2 SCF energy in THF: -1349.615074 a.u.

M06/BS2 Free energy in THF: -1349.125249 a.u.

Ru	0.00167600	0.42546200	-0.04855500
C	-0.87477500	2.33958700	0.75189300
C	-1.34922800	2.14466600	-0.56871100
C	-0.19622400	2.13756400	-1.45448000
C	0.57267100	2.48421100	0.68482100
C	0.97339600	2.41127400	-0.67437900
C	-0.20839500	2.10767100	-2.94624300
H	-1.18136100	1.80523500	-3.34972200
H	0.01156400	3.10585000	-3.35087100
H	0.55097000	1.42041900	-3.34254900
C	-2.77646600	2.06333900	-0.99319800
H	-3.40370300	1.56643700	-0.24176300
H	-3.18601100	3.06981000	-1.15889800
H	-2.89615500	1.50706700	-1.93113700
C	-1.69233900	2.48348800	1.99061800
H	-1.21391400	1.99356000	2.84922700
H	-1.82823400	3.54219100	2.25568100
H	-2.68930500	2.04261000	1.86996800
C	1.44033000	2.82607700	1.84850600
H	2.49755800	2.61046700	1.65298400
H	1.36274400	3.89824600	2.07926000
H	1.14556000	2.28320200	2.75584700
C	2.33781600	2.62419500	-1.23373700
H	2.45091500	3.66419600	-1.57326200
H	3.12667600	2.42749500	-0.49894500
H	2.52573600	1.97650700	-2.09886000
C	-1.27358800	-1.17614200	-0.41901600
C	-0.61186600	-0.85736900	-1.65513900
C	1.48584000	-0.83916000	-0.86811000
C	0.76142200	-1.35488900	-1.89443100
H	-1.20901800	-0.42088200	-2.45959300
H	1.07745200	-1.91223200	-2.78436300
C	-2.72882900	-1.18169200	-0.17945700
C	-3.63260000	-1.37747300	-1.22801700
C	-3.22200900	-0.96924300	1.11450100
C	-5.00360100	-1.32179800	-0.99624500
H	-3.25618700	-1.56761500	-2.23377100
C	-4.58980600	-0.93366500	1.34901400
H	-2.51376600	-0.81252700	1.92931300
C	-5.48278700	-1.09853100	0.29037000
H	-5.69944600	-1.46211100	-1.82090200
H	-4.96562900	-0.76650300	2.35668800
H	-6.55483500	-1.05731200	0.47207000
C	2.91439600	-1.00426500	-0.59761000
C	3.54264000	-0.26900800	0.41673200
C	3.69415900	-1.90978800	-1.33642900
C	4.90040400	-0.41674400	0.67603000
C	5.04787900	-2.06316100	-1.07576800
H	3.22829200	-2.50249000	-2.12385900
C	5.65698900	-1.31562900	-0.06913000
H	5.37219500	0.17138300	1.46168600
H	5.63534500	-2.76788100	-1.66156300
H	6.71969900	-1.43570700	0.13221200

H	2.94242600	0.43613300	0.99244800
C	0.79001100	-0.75240200	2.85387200
N	0.46793600	-0.36679800	1.80904000
C	1.21866700	-1.23257200	4.15205800
H	2.27852400	-1.51077200	4.12084600
H	1.08329900	-0.45271100	4.90994200
H	0.63297300	-2.10960700	4.44918500
O	-0.66305500	-2.45584500	0.22335000
H	0.30211700	-2.30709800	-0.03244800
C	-1.13506600	-3.70844300	-0.35624800
H	-0.58972000	-4.51271600	0.14098900
H	-2.20162300	-3.76831600	-0.13559200
H	-0.95424600	-3.70087300	-1.43630300

TS19

M06/BS1 SCF energy in gas pahse: -1349.205594 a.u.

M06/BS2 SCF energy in THF: -1349.612417 a.u.

M06/BS2 Free energy in THF: -1349.123154 a.u.

Ru	-0.02551400	0.44072600	-0.02757700
C	-0.77812700	2.39788500	0.70262300
C	-1.22945200	2.21065300	-0.63154600
C	-0.05590200	2.12854000	-1.48181100
C	0.67863200	2.44765400	0.67746700
C	1.10890500	2.32124000	-0.66973000
C	-0.04354500	2.09202300	-2.97304800
H	-1.00935500	1.78500600	-3.39023600
H	0.17548800	3.09201000	-3.37370800
H	0.72567700	1.41163200	-3.36000600
C	-2.64731900	2.19876000	-1.09324400
H	-3.32554400	1.79569500	-0.33031200
H	-2.98481700	3.21626400	-1.33621100
H	-2.78175800	1.58818100	-1.99470300
C	-1.62689300	2.62282700	1.90707600
H	-1.19439400	2.16068700	2.80360400
H	-1.73210400	3.69732700	2.11605700
H	-2.63503100	2.21253100	1.77587900
C	1.55024100	2.73612500	1.85231800
H	2.55347800	2.30905900	1.73072000
H	1.66979200	3.82068200	1.98645900
H	1.12602400	2.34242400	2.78441300
C	2.50932800	2.40001600	-1.17190500
H	2.76753600	3.43867200	-1.42428800
H	3.23496900	2.04540200	-0.43013000
H	2.64895600	1.79547600	-2.07641300
C	-1.27840500	-1.17704400	-0.45690800
C	-0.59159900	-0.82275700	-1.67538400
C	1.46861100	-1.00170000	-0.72863400
C	0.79567600	-1.23872700	-1.89119500
H	-1.18432800	-0.40385000	-2.49069500
H	1.18463100	-1.51859400	-2.87886600
C	-2.74161000	-1.20233900	-0.27460300
C	-3.61435400	-1.35012400	-1.35616000
C	-3.27242200	-1.03923000	1.01151400
C	-4.99176700	-1.29737600	-1.16057100
H	-3.21295500	-1.50555900	-2.35795800
C	-4.64513900	-1.00569900	1.20823200
H	-2.58586000	-0.91541100	1.84966500
C	-5.50800200	-1.12398700	0.11867200
H	-5.66297800	-1.40258000	-2.01051100
H	-5.04924200	-0.87588200	2.21047400
H	-6.58476500	-1.08563300	0.27037500
C	2.90523300	-1.13419600	-0.49413200
C	3.48886100	-0.54672600	0.63754700
C	3.73793600	-1.84075000	-1.37589600
C	4.85633500	-0.63649600	0.86903200
C	5.10206700	-1.94090800	-1.14029000
H	3.30619400	-2.32555300	-2.25199100
C	5.66785900	-1.33478200	-0.02001600
H	5.29235400	-0.16324400	1.74757200
H	5.73109500	-2.49500800	-1.83470800
H	6.73828200	-1.41155400	0.15992400
H	2.84395300	0.00367400	1.32411700
C	0.36760000	-0.66426700	2.99317900
N	0.20697800	-0.30273100	1.90360200
C	0.58097800	-1.12077000	4.35178600
H	1.65081300	-1.26274800	4.54251100
H	0.18988800	-0.38911400	5.06763500
H	0.06791400	-2.07508400	4.51523100
O	-0.63489400	-2.35880900	0.23582600
H	0.37329300	-2.03929900	0.07631900
C	-0.90465900	-3.64664200	-0.38081400
H	-0.44855200	-4.40420600	0.25883000
H	-1.99006200	-3.76525400	-0.40831900
H	-0.48006700	-3.66573600	-1.39051500

IM17

M06/BS1 SCF energy in gas pahse: -1349.297798 a.u.

M06/BS2 SCF energy in THF: -1349.699886 a.u.

M06/BS2 Free energy in THF: -1349.205975 a.u.

Ru	-0.08357200	-0.28645000	0.07453100
C	0.53457700	-1.57535000	1.75487600
C	0.99652800	-2.19477500	0.55926000
C	-0.15330400	-2.48356300	-0.25814600
C	-0.92104200	-1.52622900	1.70158900
C	-1.33632500	-2.11501100	0.47472600
C	-0.12364800	-3.22182200	-1.55355600
H	0.78407300	-3.00581400	-2.13097100
H	-0.13876800	-4.30635700	-1.37666900
H	-0.98883400	-2.98723200	-2.18515900
C	2.40642300	-2.55467500	0.25027800
H	3.11974900	-1.85443500	0.70083300
H	2.63092500	-3.55750300	0.64207000
H	2.60298000	-2.57343000	-0.82797100
C	1.39737800	-1.16987200	2.90122300
H	0.90684300	-0.42785100	3.54159800
H	1.63685700	-2.03778200	3.53184900

H	2.34706200	-0.74058100	2.55522700
C	-1.83781800	-1.05666300	2.77944100
H	-2.74226700	-0.59476500	2.36199900
H	-2.15605300	-1.89927400	3.40967200
H	-1.35849000	-0.32217800	3.43660900
C	-2.74738100	-2.34214900	0.06078400
H	-3.13563600	-3.25784300	0.52963800
H	-3.40028100	-1.51194100	0.35961100
H	-2.84817000	-2.46229700	-1.02445300
C	1.46882200	0.97955400	-1.05194900
C	0.66601500	0.18662900	-1.90958500
C	-1.52297400	1.09187500	-1.11229600
C	-0.76148500	0.26919300	-1.95508600
H	1.11610500	-0.66066800	-2.42746100
H	-1.26121400	-0.51789700	-2.52373900
C	2.90115300	0.66282100	-0.82165800
C	3.66349600	-0.08603800	-1.72300400
C	3.51969700	1.15117700	0.33696500
C	5.00109300	-0.36552100	-1.45887900
H	3.22230700	-0.43788100	-2.65580900
C	4.85137800	0.86437100	0.60476800
H	2.93704100	1.75807600	1.02972500
C	5.59634400	0.09904900	-0.29120300
H	5.58301200	-0.94020000	-2.17690300
H	5.31526100	1.24552100	1.51290100
H	6.64203100	-0.12026400	-0.08535300
C	-2.97863300	0.94532300	-0.95718900
C	-3.58741500	1.48104000	0.18660500
C	-3.78568900	0.29003200	-1.89426500
C	-4.95034000	1.33503900	0.40676000
C	-5.15331700	0.15497500	-1.68191200
H	-3.35057000	-0.09860700	-2.81514800
C	-5.73884800	0.66597100	-0.52753000
H	-5.40331300	1.75209900	1.30446500
H	-5.76675800	-0.34658000	-2.42793400
H	-6.80887700	0.55747800	-0.36309500
H	-2.96858700	2.00810500	0.91512400
C	-0.00695600	2.21888500	2.11087600
N	-0.05224300	1.33498500	1.36525500
C	0.06244800	3.33096300	3.03667500
H	-0.92527300	3.78773200	3.16542700
H	0.42173500	2.99096700	4.01450800
H	0.75332300	4.09105600	2.65485000
O	1.13979400	2.30759700	-0.83263000
H	-1.09713000	2.03745300	-0.78250100
C	1.57540600	3.14801900	-1.89430000
H	1.31546200	4.17200100	-1.61363900
H	2.66303500	3.07462400	-2.03772300
H	1.06343500	2.88491900	-2.83230300

TS20

M06/BS1 SCF energy in gas pahse: -1349.203449 a.u.

M06/BS2 SCF energy in THF: -1349.606525 a.u.

M06/BS2 Free energy in THF: -1349.119576 a.u.

Ru	0.04483800	0.39263000	-0.02253900
C	-0.72284000	2.27654600	0.97599800
C	-1.27408300	2.22238300	-0.32497900
C	-0.17077500	2.22296500	-1.26802200
C	0.72697200	2.35254800	0.84737300
C	1.05205500	2.37404100	-0.53485500
C	-0.28361800	2.31811300	-2.75269900
H	-1.26767700	1.99415800	-3.11234000
H	-0.14610300	3.35731400	-3.08396900
H	0.47816300	1.71042400	-3.25962000
C	-2.71756700	2.25824600	-0.69119500
H	-3.35672100	1.89598000	0.12252100
H	-3.02695500	3.28631200	-0.92826600
H	-2.93845900	1.64092300	-1.57116700
C	-1.46234600	2.35640300	2.26885100
H	-0.99648200	1.73399400	3.04437600
H	-1.47621200	3.38813000	2.64913100
H	-2.50326900	2.02996100	2.16335900
C	1.66549400	2.56900900	1.98644000
H	2.70525300	2.35638200	1.71114500
H	1.62475500	3.61531300	2.32243200
H	1.41155700	1.94642800	2.85424000
C	2.40167100	2.55062200	-1.14137200
H	2.59920900	3.61471000	-1.33500200
H	3.20115600	2.17608500	-0.49133200
H	2.48508800	2.02133800	-2.09894600
C	-1.30487200	-1.17436200	-0.56176500
C	-0.56619200	-0.76435200	-1.71397200
C	1.50706100	-0.80429000	-0.86788100
C	0.76721800	-1.43963300	-1.84188900
H	-1.02753900	-0.21176400	-2.53327900
H	1.09743300	-2.03066000	-2.70412100
C	-2.75723800	-1.07826200	-0.32956300
C	-3.65574900	-1.02421700	-1.39865700
C	-3.25426300	-1.03653500	0.97880000
C	-5.02194200	-0.89366100	-1.16553900
H	-3.27998800	-1.08389400	-2.42092500
C	-4.61833200	-0.92561900	1.21166200
H	-2.55022200	-1.07446100	1.81138300
C	-5.50458500	-0.84363500	0.13773800
H	-5.71154600	-0.84268100	-2.00581100
H	-4.99524700	-0.89374700	2.23224800
H	-6.57308100	-0.74686000	0.31936800
C	2.93385200	-0.95074900	-0.60684900
C	3.50321900	-0.44172300	0.57029900
C	3.77699400	-1.58147700	-1.53704600
C	4.86378200	-0.56767700	0.81801300
C	5.13663000	-1.70579300	-1.29276400
H	3.36021000	-1.96525200	-2.46758100
C	5.68230000	-1.20115800	-0.11355800
H	5.29073900	-0.16826600	1.73636900
H	5.77817300	-2.19212000	-2.02488600
H	6.74991500	-1.29646100	0.07519100

H	2.85314000	0.06042500	1.28609400
C	0.53965300	-1.14633300	2.77428200
N	0.35667400	-0.60516500	1.76584000
C	0.77663300	-1.83309300	4.02840000
H	1.85056800	-1.88251100	4.24076000
H	0.27871300	-1.31106900	4.85311900
H	0.38476900	-2.85501200	3.97684300
O	-0.73896700	-2.48534500	-0.08497500
H	0.23108900	-2.34257700	-0.67406300
C	-1.41489000	-3.64291100	-0.63781800
H	-0.81612500	-4.51329500	-0.36100800
H	-2.40939500	-3.70225400	-0.19178100
H	-1.48822000	-3.54418100	-1.72844400

IM18

M06/BS1 SCF energy in gas pahse: -1349.259865 a.u.

M06/BS2 SCF energy in THF: -1349.657532 a.u.

M06/BS2 Free energy in THF: -1349.166304 a.u.

Ru	0.09878800	0.37915800	-0.03751700
C	-0.79681500	2.20876600	1.05147200
C	-1.29526500	2.21049200	-0.26232000
C	-0.15505300	2.27026000	-1.16497100
C	0.65721900	2.32829000	0.98801600
C	1.03402700	2.43671300	-0.37418600
C	-0.23866700	2.45939000	-2.64267800
H	-1.16126600	2.03784700	-3.05948600
H	-0.23344800	3.52935000	-2.89634600
H	0.60818600	1.99757700	-3.16620400
C	-2.72156500	2.23558700	-0.68583400
H	-3.39313700	1.90375700	0.11400500
H	-3.01334200	3.25807700	-0.96623300
H	-2.91167500	1.59284800	-1.55429000
C	-1.58820800	2.16581700	2.31416600
H	-1.07025000	1.59689800	3.09701500
H	-1.75413700	3.17854700	2.70901700
H	-2.57068200	1.70337600	2.16019300
C	1.53525900	2.51552300	2.17914100
H	2.59900400	2.48303800	1.91664800
H	1.34544000	3.49529800	2.64110100
H	1.35384300	1.75822800	2.95335700
C	2.39804300	2.70493500	-0.91078100
H	2.56278500	3.78737300	-1.00906800
H	3.18822500	2.30755600	-0.26216400
H	2.53844400	2.26267700	-1.90531700
C	-1.23651200	-1.32985400	-0.65596200
C	-0.57158100	-0.76318800	-1.76002700
C	1.50504700	-0.64926900	-0.89211000
C	0.83132000	-1.22449200	-2.08827700
H	-1.11772400	-0.12721000	-2.45572800
H	1.20130300	-0.76338700	-3.01877500
C	-2.68758200	-1.11323300	-0.40585200
C	-3.59600300	-1.02142700	-1.46337500
C	-3.17419000	-1.06163900	0.90566300
C	-4.95527200	-0.84292500	-1.21847500
H	-3.23797800	-1.10835800	-2.48995800
C	-4.52920700	-0.88376100	1.15144600
H	-2.47015300	-1.14771600	1.73414500
C	-5.42406900	-0.76708300	0.08799700
H	-5.65048300	-0.77574000	-2.05316800
H	-4.89374600	-0.83829000	2.17645100
H	-6.48629700	-0.63006900	0.28049500
C	2.90300700	-0.84859600	-0.60789600
C	3.47645600	-0.35849000	0.58311500
C	3.73428700	-1.53245600	-1.51854200
C	4.82268000	-0.54149200	0.85127500
C	5.08215100	-1.71092700	-1.25202500
H	3.31596500	-1.92095700	-2.44618200
C	5.62675700	-1.21645300	-0.06761200
H	5.25403900	-0.15994300	1.77466000
H	5.71412500	-2.23682900	-1.96424600
H	6.68540400	-1.35899700	0.14130600
H	2.83363200	0.16511100	1.28951500
C	0.40900200	-1.31849800	2.70223600
N	0.29295800	-0.68923800	1.73780200
C	0.54255000	-2.12304900	3.89916000
H	1.59959900	-2.28288000	4.13861900
H	0.06023500	-1.62725700	4.74878700
H	0.06663000	-3.09813800	3.74607600
O	-0.71577800	-2.49591100	-0.10203500
H	0.95115800	-2.31578800	-2.20079600
C	-1.29875200	-3.66541300	-0.65655200
H	-0.75608000	-4.51668100	-0.23688300
H	-2.36371200	-3.74777600	-0.39717200
H	-1.19944000	-3.67371900	-1.75423100

TS21

M06/BS1 SCF energy in gas pahse: -1349.205118 a.u.

M06/BS2 SCF energy in THF: -1349.607795 a.u.

M06/BS2 Free energy in THF: -1349.123185 a.u.

Ru	0.04373000	0.31173900	0.09759300
C	-0.75163700	2.02155400	1.29112000
C	-1.06328900	2.23908900	-0.07772400
C	0.19081200	2.32443700	-0.80704400
C	0.69828200	2.00695400	1.41733700
C	1.26558300	2.24917800	0.14113700
C	0.35248200	2.67699700	-2.24838800
H	-0.54706600	2.45179900	-2.83285900
H	0.54978300	3.75191300	-2.36651400
H	1.19472600	2.14196500	-2.70877200
C	-2.42119400	2.45747700	-0.65034900
H	-3.19182600	1.89957500	-0.10472700
H	-2.68428200	3.52417800	-0.61090400
H	-2.48188000	2.14686100	-1.70076100
C	-1.71337500	1.93557500	2.42652000
H	-1.41221900	1.17209900	3.15576300
H	-1.77431100	2.89317100	2.96356800

H	-2.72269100	1.68438800	2.08096600
C	1.45776700	1.88146200	2.69354500
H	2.42613800	1.38859500	2.53878400
H	1.65642100	2.87267600	3.12578100
H	0.90102500	1.30750000	3.44345800
C	2.71667000	2.40877100	-0.15650000
H	3.03664200	3.43806600	0.06074000
H	3.34219500	1.73530200	0.44487600
H	2.94426400	2.21258500	-1.21103200
C	-1.34079800	-1.12637700	-0.73837000
C	-0.56281700	-0.51654900	-1.78948400
C	1.52781900	-0.79954000	-0.92028600
C	0.79532300	-0.99531900	-2.09279600
H	-1.04220700	0.13649400	-2.51930200
H	1.16142900	-1.28011300	-3.09095600
C	-2.80127600	-0.86138800	-0.62786200
C	-3.59795600	-0.59621000	-1.74354300
C	-3.40799300	-0.92473300	0.63256300
C	-4.96191800	-0.35359300	-1.60080300
H	-3.15339200	-0.59227400	-2.73954600
C	-4.76874400	-0.68967900	0.77597200
H	-2.79029800	-1.14459500	1.50435400
C	-5.54907600	-0.39386700	-0.34148000
H	-5.56789700	-0.14312300	-2.47998600
H	-5.22631900	-0.73583100	1.76283300
H	-6.61507500	-0.20681600	-0.22875900
C	2.97751600	-0.92889300	-0.77118000
C	3.52454100	-1.20035400	0.48970800
C	3.83882900	-0.67923300	-1.84782200
C	4.90077900	-1.24121700	0.66694300
C	5.21563500	-0.70110700	-1.66616000
H	3.42344400	-0.43827800	-2.82726500
C	5.74697200	-0.98554500	-0.41034800
H	5.31967800	-1.46194000	1.64676800
H	5.87772300	-0.49248200	-2.50397700
H	6.82582000	-1.00224800	-0.26944700
H	2.84932700	-1.37383600	1.32754900
C	0.15748600	-1.71904600	2.61646400
N	0.13973600	-0.99213600	1.71525600
C	0.17345300	-2.64738000	3.72899900
H	1.20087000	-2.93954500	3.97344000
H	-0.28100900	-2.19212300	4.61587700
H	-0.39434900	-3.54781000	3.46914200
O	-0.96196200	-2.42031700	-0.34402600
H	0.87163900	-1.88856500	-1.00163700
C	-1.56264800	-3.43938100	-1.13410800
H	-1.14716900	-4.39068200	-0.79108100
H	-2.65346700	-3.45102100	-1.00992600
H	-1.32560000	-3.29742200	-2.20148300

TS22

M06/BS1 SCF energy in gas pahse: -1293.86134 a.u.

M06/BS2 SCF energy in THF: -1294.254109 a.u.

M06/BS2 Free energy in THF: -1293.77292 a.u.

Ru	-0.18373600	0.30521400	0.00757300
C	1.12772000	2.26606500	0.23510800
C	0.70092100	2.07103400	-1.12425000
C	-0.73680400	2.14270100	-1.17711200
C	-0.03245000	2.38752500	1.02821000
C	-1.19758700	2.34509500	0.15116700
C	-1.57864700	2.11624900	-2.40668900
H	-1.18526800	1.41598200	-3.15468900
H	-1.62834500	3.11007400	-2.87432300
H	-2.60465400	1.80313800	-2.17814400
C	1.61656200	2.09275200	-2.29950200
H	2.52663700	1.50086500	-2.13203100
H	1.94077600	3.12671500	-2.48830600
H	1.12973300	1.73690300	-3.21503900
C	2.54135300	2.46154900	0.66376200
H	2.69879800	2.20604100	1.71810200
H	2.83169400	3.51503600	0.53661800
H	3.23920200	1.85890100	0.06983200
C	-0.05486500	2.67795000	2.48999600
H	-0.89066400	2.19243800	3.00999800
H	-0.15821400	3.75791000	2.66724600
H	0.87128500	2.35269300	2.97952800
C	-2.60149600	2.70094900	0.51491000
H	-2.86164100	3.67412900	0.07573600
H	-2.73994600	2.79395700	1.59833500
H	-3.33077300	1.96972000	0.14052000
C	1.30671100	-1.08818900	-0.38392100
C	0.65492400	-0.86738600	-1.62980100
C	-1.41798400	-1.03766600	-0.95979900
C	-0.63985600	-1.52305000	-1.93960800
H	1.21593000	-0.33612300	-2.40406700
H	-0.83545700	-2.20113300	-2.77356500
C	2.73738300	-1.02342300	-0.10343400
C	3.66893500	-1.32862100	-1.10700300
C	3.19702800	-0.67870000	1.17478000
C	5.03046400	-1.25214000	-0.84531500
H	3.31304900	-1.62530600	-2.09348400
C	4.55783700	-0.62831700	1.44296700
H	2.46584900	-0.43583100	1.94712000
C	5.47398300	-0.90523700	0.42963400
H	5.74930300	-1.47312300	-1.63144900
H	4.90910300	-0.36043500	2.43739400
H	6.54129800	-0.85390300	0.63566500
C	-2.76904800	-1.25671900	-0.47460600
C	-2.98041200	-0.75658800	0.81818500
C	-3.80733300	-1.89019800	-1.16074400
C	-4.23994300	-0.84832000	1.40409600
C	-5.05861200	-1.99503800	-0.56395400
H	-3.63889400	-2.27265600	-2.16728600
C	-5.27502500	-1.47103400	0.71042700
H	-4.41091600	-0.44352200	2.40188600
H	-5.87693600	-2.47223900	-1.09923200
H	-6.26082500	-1.54474300	1.16521100

C	-1.82127600	-0.13702100	1.50470000
C	-0.64855600	-0.81212500	1.87438200
H	-2.05867200	0.76608800	2.06914000
H	-0.05129600	-0.43879900	2.70827100
H	-0.60123000	-1.88899500	1.72014000
O	0.95419000	-2.83877200	-0.05084300
C	1.46934800	-3.48250900	1.12155500
H	1.21709900	-2.92973900	2.03341100
H	2.55403900	-3.52721300	1.00376500
H	1.06292600	-4.49749400	1.15941300
H	-0.02180500	-2.87608400	-0.12102300

TS23

M06/BS1 SCF energy in gas pahse: -1178.18822 a.u.

M06/BS2 SCF energy in THF: -1178.542691 a.u.

M06/BS2 Free energy in THF: -1178.117502 a.u.

Ru	-0.11572800	0.42042400	0.15676600
C	-0.89549000	2.54559800	0.08098200
C	0.23127700	2.40242500	0.97978200
C	1.42032400	2.11980600	0.19462300
C	-0.44628000	2.18156600	-1.20711000
C	0.99928400	1.93654000	-1.13387600
C	2.80878800	2.02002000	0.72286700
H	2.82245700	1.67769000	1.76487500
H	3.30587500	3.00013300	0.69233900
H	3.42098400	1.31930900	0.14020100
C	0.23689700	2.70924900	2.43640000
H	-0.76630000	2.64415100	2.87275600
H	0.60404400	3.73143700	2.60900200
H	0.89261500	2.02530600	2.98987200
C	-2.27833900	2.93461600	0.48195800
H	-3.02673100	2.55574800	-0.22402500
H	-2.38520900	4.02710400	0.52656800
H	-2.53936200	2.54003900	1.47265800
C	-1.22706400	2.15993600	-2.47481600
H	-0.99607900	1.26722900	-3.07203700
H	-0.98656200	3.03537900	-3.09585200
H	-2.30742600	2.17531900	-2.29069700
C	1.86964100	1.66669300	-2.31148800
H	2.19473000	2.61777100	-2.75873500
H	1.34207100	1.10538000	-3.09107300
H	2.77303900	1.10791600	-2.03780900
C	-1.63896100	-0.56400400	0.75072100
C	-0.92394800	-0.61150400	1.98064000
C	0.96938900	-1.16067300	0.84556800
C	0.29457400	-1.39428900	2.01885900
H	-1.33154400	-0.12385800	2.87441000
H	0.63434800	-1.93073100	2.91222500
C	-2.90239800	-1.06529200	0.34413000
C	-3.68390900	-1.85413800	1.21742800
C	-3.37918200	-0.79377200	-0.95747900
C	-4.90694900	-2.34702700	0.79960300
H	-3.30740400	-2.07026800	2.21627900
C	-4.60394200	-1.28597300	-1.36709700
H	-2.75390500	-0.19656300	-1.62185100
C	-5.36460800	-2.06172700	-0.48841900
H	-5.51052700	-2.95566300	1.46882000
H	-4.97414000	-1.07805700	-2.36832300
H	-6.32686700	-2.45201900	-0.81462300
C	2.32133100	-1.53046900	0.46930500
C	2.65971800	-1.72304700	-0.89540600
C	3.33232700	-1.59998000	1.43814000
C	3.99903800	-1.94782000	-1.22529800
C	4.65517600	-1.84195000	1.08919400
H	3.06843100	-1.42936800	2.48205000
C	4.98906300	-2.01353100	-0.24999300
H	4.26399000	-2.09489700	-2.27254100
H	5.42290400	-1.88879800	1.85862400
H	6.02192300	-2.19773800	-0.53818000
C	1.68707000	-1.68237000	-1.99693200
C	0.39663000	-2.04762100	-1.98300300
H	2.10787100	-1.34688300	-2.94957700
H	-0.20434000	-1.98953400	-2.88984700
H	-0.08360600	-2.48176800	-1.10889500

IM19

M06/BS1 SCF energy in gas pahse: -1178.225121 a.u.

M06/BS2 SCF energy in THF: -1178.574276 a.u.

M06/BS2 Free energy in THF: -1178.150227 a.u.

Ru	-0.17213800	0.62753200	0.41199200
C	-1.31179200	2.06704600	-0.90299900
C	-0.69095600	2.82453900	0.14651900
C	0.72677100	2.68943200	0.01240800
C	-0.27371500	1.44688900	-1.67593500
C	0.98889100	1.82596400	-1.09766400
C	1.75974300	3.32749500	0.87620200
H	1.39854200	3.48057200	1.90049400
H	2.04502300	4.31258700	0.47981700
H	2.67241500	2.72019700	0.92800800
C	-1.40164000	3.65075500	1.16289500
H	-2.39455200	3.24529400	1.39120300
H	-1.54195400	4.67912700	0.80054900
H	-0.84185000	3.70927700	2.10416200
C	-2.77397900	2.04518900	-1.19412900
H	-3.06412000	1.17105500	-1.78803300
H	-3.06580700	2.93871800	-1.76383600
H	-3.37501300	2.02849000	-0.27655300
C	-0.43684700	0.69408100	-2.95078900
H	0.23837700	-0.16998800	-3.00053000
H	-0.20033300	1.34225500	-3.80719900
H	-1.46439500	0.33862300	-3.09125900
C	2.33693800	1.52179100	-1.65808900
H	2.69159900	2.36554400	-2.26723100
H	2.31533300	0.63415200	-2.29960400
H	3.08361700	1.34764300	-0.87237400
C	-1.49654100	-0.70104600	0.91572600

C	-0.93410200	-0.45208800	2.20015400
C	1.14195500	-0.66575200	1.01614800
C	0.47861600	-0.41900300	2.25367700
H	-1.53397100	-0.12498200	3.05534000
H	0.99147600	-0.06683200	3.15414000
C	-2.70373600	-1.35379100	0.53237900
C	-3.54533400	-1.95576000	1.49123100
C	-3.05110500	-1.43401000	-0.83059500
C	-4.72133100	-2.56978300	1.09724900
H	-3.26427300	-1.92787500	2.54315400
C	-4.21675400	-2.06919000	-1.22166300
H	-2.36149300	-1.01669100	-1.56413200
C	-5.05706300	-2.62541600	-0.25664100
H	-5.37694900	-3.01958600	1.83935100
H	-4.47636800	-2.13937100	-2.27556300
H	-5.97602700	-3.12130400	-0.56305300
C	2.44579400	-1.19972600	0.75079900
C	2.78946400	-1.74209300	-0.51680600
C	3.41608900	-1.14554000	1.77335700
C	4.10977000	-2.15946100	-0.71259600
C	4.72375500	-1.52316500	1.53400000
H	3.13777700	-0.76410600	2.75463800
C	5.06963000	-2.03013100	0.28030000
H	4.38024000	-2.63058400	-1.65566100
H	5.46899000	-1.44552700	2.32223400
H	6.08927100	-2.35812600	0.08872000
C	1.77359500	-1.96828500	-1.55075400
C	2.02350300	-2.18148900	-2.84728000
H	0.73541000	-1.97563000	-1.21124600
H	1.21737100	-2.39110800	-3.54708400
H	3.02803900	-2.15793000	-3.26871400

IM20

M06/BS1 SCF energy in gas pahse: -1293.863484 a.u.

M06/BS2 SCF energy in MeOH: -1294.258072 a.u.

M06/BS2 Free energy in MeOH: -1293.775574 a.u.

Ru	0.18946300	0.27052400	-0.02829300
C	-1.18016500	2.19478300	-0.23699200
C	-0.77621100	1.98856100	1.12798900
C	0.65494900	2.10014100	1.21237600
C	-0.00875600	2.36505800	-1.00367900
C	1.13836000	2.33641600	-0.10346000
C	1.47437200	2.08726900	2.45750100
H	1.06816500	1.39805800	3.20872200
H	1.51448700	3.08673300	2.91423600
H	2.50554900	1.77465600	2.25186800
C	-1.72048300	1.97076800	2.28117100
H	-2.60686300	1.35180300	2.08505000
H	-2.08274000	2.99183400	2.47051200
H	-1.24716700	1.62229100	3.20674900
C	-2.58799100	2.36760000	-0.69248800
H	-2.72442600	2.09793700	-1.74636900
H	-2.89189400	3.41939400	-0.58326400
H	-3.28925700	1.76445900	-0.10373500
C	0.03252600	2.69108500	-2.45765000
H	0.87945100	2.22587600	-2.97829700
H	0.12759800	3.77601400	-2.60743600
H	-0.88355300	2.36852200	-2.96713200
C	2.53773100	2.74305900	-0.42901800
H	2.75452600	3.71843500	0.02875500
H	2.69873100	2.85515200	-1.50749000
H	3.28208500	2.03114300	-0.04705400
C	-1.29646100	-1.24735400	0.34035500
C	-0.63947700	-0.93580100	1.57313800
C	1.44122000	-1.05675500	0.92917400
C	0.65665800	-1.59863400	1.88158200
H	-1.20114400	-0.39783400	2.33872100
H	0.86483600	-2.27791600	2.71211900
C	-2.74525200	-1.09567300	0.08882500
C	-3.66558600	-1.30863200	1.12248200
C	-3.21991700	-0.76601500	-1.18618200
C	-5.02926400	-1.16666600	0.89119800
H	-3.30494700	-1.58848400	2.11234200
C	-4.58371600	-0.65341100	-1.42480800
H	-2.50008700	-0.57239200	-1.98350100
C	-5.48870500	-0.84432700	-0.38315800
H	-5.73681900	-1.32092500	1.70321300
H	-4.94282000	-0.39753500	-2.41979900
H	-6.55662300	-0.74179700	-0.56524900
C	2.80896600	-1.22127800	0.47194100
C	3.02777200	-0.67186400	-0.79944200
C	3.85325100	-1.83988300	1.16238900
C	4.30124300	-0.70264800	-1.36063300
C	5.11975800	-1.88090000	0.59081400
H	3.67765200	-2.25904000	2.15304900
C	5.34253900	-1.31037100	-0.66270000
H	4.47853800	-0.26242700	-2.34215200
H	5.94390100	-2.34485800	1.12869800
H	6.33973000	-1.33506900	-1.09760000
C	1.85463900	-0.07817800	-1.48522000
C	0.71787700	-0.80843700	-1.88083900
H	2.07110600	0.83145100	-2.04687500
H	0.12977200	-0.46585800	-2.73555400
H	0.75126500	-1.89087000	-1.75185600
O	-0.92140300	-2.72177700	-0.00243000
C	-1.32728400	-3.36265200	-1.23653100
H	-1.12768700	-2.71651500	-2.09382700
H	-2.39424300	-3.56925300	-1.14403800
H	-0.76170100	-4.29481900	-1.29863300
H	0.04387500	-2.77854300	0.24131900

3cat

M06/BS1 SCF energy in gas pahse: -2097.778213 a.u.

M06/BS2 SCF energy in toluene: -2098.29682 a.u.

M06/BS2 Free energy in toluene: -2097.794925 a.u.

Ru	0.87819900	0.19897000	-0.51162900

B	3.39170600	-0.70617800	1.21301300
H	4.32459700	-1.05752700	1.88208400
N	2.46593400	-1.90360200	0.89118500
C	2.64601000	-3.21512000	1.14259200
C	0.86856900	-2.95519500	-0.12052300
C	1.64157000	-3.92897000	0.51697100
H	3.48720200	-3.54091500	1.74290300
H	-0.01865600	-3.06375700	-0.73442200
H	1.49237100	-5.00006800	0.51684300
N	3.86332800	-0.11136600	-0.13169000
C	5.09911600	0.04846700	-0.64392600
C	3.60698200	0.73949800	-2.10270600
C	4.98481100	0.59433200	-1.90944400
H	5.96997100	-0.23956100	-0.06686000
H	3.05844400	1.12305500	-2.95693800
H	5.78305600	0.84769000	-2.59379400
N	2.56413200	0.36941300	1.95023300
C	2.76755100	0.96193000	3.14309300
C	1.78337200	1.91347300	3.33818400
H	3.60752300	0.66622700	3.76051600
C	0.99494900	1.84298200	2.18644000
H	1.65518400	2.56707400	4.19014000
H	0.10323700	2.39968900	1.91334300
N	2.94476400	0.31187600	-1.02707100
N	1.36565000	-1.73883500	0.11724600
N	1.47168500	0.90673500	1.36082300
P	-1.38857600	0.02735500	0.15302700
C	0.78821500	3.27278700	-1.31513000
C	0.09704600	-1.07759500	-3.32491800
C	0.81959200	4.69533900	-1.58401400
H	0.93545600	4.88434800	-2.65720200
H	-0.11534400	5.15637900	-1.24166400
H	1.65685700	5.16463100	-1.05511700
C	-0.32233300	-1.76589500	-4.52782100
H	-1.32283100	-2.19073900	-4.37232800
H	-0.36066500	-1.07561600	-5.37760400
H	0.37567600	-2.57610400	-4.76582200
N	0.72644700	2.13912800	-1.08623200
N	0.40011000	-0.54881900	-2.33996900
C	-2.43710400	-0.98269400	-0.98954500
C	-3.07727200	-0.45114900	-2.11245600
C	-2.50799100	-2.36652400	-0.77805300
C	-3.76286000	-1.27706100	-3.00027400
H	-3.07466200	0.62063000	-2.29483100
C	-3.18077800	-3.19354200	-1.67113600
H	-2.06164600	-2.80094600	0.11621100
C	-3.81037500	-2.65151600	-2.78859200
H	-4.27502500	-0.83689400	-3.85451300
H	-3.23316800	-4.26368500	-1.47868700
H	-4.35443600	-3.29501000	-3.47750800
C	-2.23587700	1.65877800	0.26880500
C	-2.75163400	2.14348800	1.47493200
C	-2.28461100	2.49070800	-0.85909600
C	-3.32418500	3.41133700	1.54515200
H	-2.71139500	1.52909700	2.37275000
C	-2.87553400	3.74729600	-0.79354400
H	-1.84138000	2.15857300	-1.79798800
C	-3.39688600	4.21192700	0.41147800
H	-3.72212400	3.76878600	2.49295200
H	-2.92948700	4.36636200	-1.68854800
H	-3.85710200	5.19666700	0.46549100
C	-1.74959500	-0.78137700	1.75774700
C	-3.08274000	-1.01903000	2.12557400
C	-0.72613600	-1.19250000	2.61496900
C	-3.38167200	-1.64456200	3.32805700
H	-3.89249100	-0.71391700	1.46136600
C	-1.02912200	-1.82415500	3.81910800
H	0.31315600	-1.02921200	2.34041300
C	-2.35252700	-2.04896800	4.17684700
H	-4.41972800	-1.82293000	3.60201000
H	-0.22240300	-2.14315700	4.47615900
H	-2.58649400	-2.54394800	5.11756300

IM21

M06/BS1 SCF energy in gas pahse: -2350.589953 a.u.

M06/BS2 SCF energy in toluene: -2351.175102 a.u.

M06/BS2 Free energy in toluene: -2350.578667 a.u.

Ru	-0.05172700	-0.88341900	-0.17289400
B	1.82794900	-3.46544200	0.04928500
H	2.54523500	-4.42406800	0.13736600
N	1.90790100	-2.60440800	1.33259200
C	2.52415300	-2.86091200	2.50155500
C	1.30189800	-1.04578800	2.71016300
C	2.16772400	-1.88506700	3.41445900
H	3.16683100	-3.72819200	2.59594700
H	0.78800600	-0.14934400	3.03915700
H	2.48555500	-1.79358200	4.44409400
N	0.35594900	-3.89044300	-0.12282700
C	-0.19744300	-5.11743100	-0.06877500
C	-1.78346600	-3.60168600	-0.15171400
C	-1.57235100	-4.98252600	-0.08972100
H	0.43382700	-5.99661100	-0.01678900
H	-2.71337100	-3.04511100	-0.16458600
H	-2.31510700	-5.76813200	-0.06146300
N	2.23527600	-2.58637800	-1.14437000
C	3.21976400	-2.76904300	-2.04370400
C	3.19353300	-1.72361600	-2.94736900
H	3.86270000	-3.63835300	-1.97475600
C	2.13645800	-0.92281400	-2.51602200
H	3.84781000	-1.55844400	-3.79216800
H	1.78891000	0.01981300	-2.92405400
N	-0.61767100	-2.95322900	-0.17972800
N	1.16026400	-1.48160600	1.45228700
N	1.56128800	-1.44783300	-1.42741100
P	0.84776800	1.33964200	-0.02759500
C	-2.08135400	-0.44200700	-1.61167200
C	-0.97967900	-0.65352700	-2.14351300

H	-0.39589000	-0.79676100	-3.04000800
C	-2.42166800	-0.52900700	1.91905000
N	-1.53281200	-0.57885200	1.17928900
C	-3.55911800	-0.41401300	2.80612000
H	-3.73786900	0.64238300	3.04497400
H	-4.45412200	-0.81403100	2.31228500
H	-3.38705100	-0.96499100	3.73703500
C	-3.44522200	-0.37294100	-1.19071900
C	-4.01883800	0.76522600	-0.57447100
C	-4.24570200	-1.50127800	-1.45026600
C	-5.37287800	0.71100900	-0.22197800
C	-5.58169000	-1.52937800	-1.08480400
H	-3.79718300	-2.34766700	-1.96802400
C	-6.14436600	-0.41739500	-0.45903500
H	-5.83922600	1.59315500	0.21409600
H	-6.18791400	-2.40503400	-1.30574300
H	-7.19676100	-0.42052200	-0.18188400
C	2.63429400	1.42131600	-0.45626200
C	3.51957700	0.49214200	0.10810500
C	3.13406400	2.37092600	-1.35089100
C	4.86657600	0.50626400	-0.22768200
H	3.15438900	-0.24975900	0.81702800
C	4.48431600	2.37553000	-1.69352000
H	2.47177300	3.11378900	-1.79248200
C	5.35108700	1.44200100	-1.13891000
H	5.54004400	-0.22341900	0.21826500
H	4.85730100	3.11830200	-2.39636200
H	6.40508400	1.44598500	-1.40999100
C	0.13088700	2.69410100	-1.04495700
C	-0.14338600	3.96016600	-0.51690100
C	-0.10986600	2.47035200	-2.40620300
C	-0.68224200	4.96016800	-1.32265800
H	0.06416800	4.17243300	0.53085500
C	-0.64240500	3.46953800	-3.21162800
H	0.11440900	1.50054100	-2.84630800
C	-0.94208700	4.71479600	-2.66652800
H	-0.89111400	5.93944300	-0.89541700
H	-0.82682800	3.27421300	-4.26626200
H	-1.36732800	5.49633400	-3.29293400
C	0.78879000	2.04487200	1.66862900
C	1.94059400	2.37647600	2.38548500
C	-0.46182600	2.22828100	2.27398800
C	1.84473400	2.84890300	3.69250900
H	2.92230400	2.26054600	1.92936500
C	-0.55532400	2.70913500	3.57399700
H	-1.37138500	2.01532100	1.71164900
C	0.60098200	3.00896400	4.29213900
H	2.75098300	3.09822000	4.24121000
H	-1.53483500	2.85817900	4.02748000
H	0.52982800	3.37933700	5.31300400
C	-3.22294700	1.97116000	-0.34513500
C	-3.53633000	2.96826000	0.48843300
H	-2.29441400	2.04369500	-0.91614400
H	-2.88994500	3.83965100	0.57511100
H	-4.43591100	2.96799900	1.10490100

TS24

M06/BS1 SCF energy in gas pahse: -2350.556419 a.u.

M06/BS2 SCF energy in toluene: -2351.144475 a.u.

M06/BS2 Free energy in toluene: -2350.558647 a.u.

Ru	0.24468200	-0.86529400	0.22458100
B	1.94805500	-3.37828700	-0.77539700
H	2.59100500	-4.31038700	-1.17593400
N	2.76911600	-2.54465200	0.23311200
C	3.97317400	-2.79442200	0.78403100
C	3.09304000	-1.01607300	1.72899900
C	4.22547200	-1.83547300	1.74729300
H	4.55804600	-3.64443400	0.45269200
H	2.86201400	-0.13544000	2.32046000
H	5.10171900	-1.74369400	2.37448100
N	0.66448200	-3.85880700	-0.06382300
C	0.20245800	-5.10169400	0.17241300
C	-1.20958200	-3.62752800	0.98772100
C	-1.00090700	-5.00352800	0.84700300
H	0.76796200	-5.96523200	-0.15734000
H	-2.03024900	-3.09138400	1.45418600
H	-1.63415200	-5.81117300	1.18853300
N	1.52587100	-2.46862400	-1.95141500
C	1.77880200	-2.61585300	-3.26613200
C	1.16703600	-1.58604200	-3.95490500
H	2.37279400	-3.45338900	-3.61214800
C	0.54416700	-0.82981600	-2.96080600
H	1.17360000	-1.40335900	-5.02062000
H	-0.01330800	0.09510000	-3.05743500
N	-0.20047400	-2.95018500	0.43587700
N	2.22522600	-1.44653800	0.80873500
N	0.76225800	-1.36571100	-1.75503200
P	0.87123800	1.39282100	-0.06959600
C	-2.94820200	-0.57854400	-0.19357500
C	-1.68433100	-0.58379600	-0.17239500
H	-2.10488000	-0.80357900	-1.28085200
C	-0.29898300	-0.66660100	3.34791700
N	-0.15663100	-0.65022700	2.19880400
C	-0.44583500	-0.64719100	4.78850300
H	0.11761100	0.19570700	5.20699000
H	-1.49959200	-0.54265200	5.06933600
H	-0.05828900	-1.57598700	5.22190700
C	-4.36876000	-0.66343800	-0.24572500
C	-5.18296500	0.48191200	-0.05616700
C	-4.94275000	-1.92999500	-0.46278100
C	-6.56923400	0.29686000	-0.11313500
C	-6.31563300	-2.07484900	-0.52298800
H	-4.28315700	-2.78849800	-0.58591600
C	-7.12591200	-0.95141300	-0.34508700
H	-7.22582200	1.15573700	0.01013100
H	-6.75883000	-3.05170200	-0.70126200
H	-8.20851100	-1.05315700	-0.39047700

C	2.08332300	1.68411100	-1.41910200
C	3.09198500	0.74211600	-1.65631300
C	2.04408300	2.84822900	-2.19291200
C	4.03726200	0.96023400	-2.65142600
H	3.13324800	-0.17052200	-1.06253500
C	2.98938700	3.06041100	-3.19194200
H	1.27132200	3.59733300	-2.02080300
C	3.98471300	2.11724300	-3.42403500
H	4.81386100	0.21807600	-2.82754500
H	2.94704100	3.96889900	-3.78986600
H	4.72213300	2.28345400	-4.20718300
C	-0.44619900	2.61518900	-0.46699100
C	-0.56606000	3.84344300	0.18818300
C	-1.30110800	2.34795500	-1.54387400
C	-1.52445500	4.77157500	-0.21511600
H	0.10267900	4.09407000	1.00975500
C	-2.24445500	3.27896700	-1.95888500
H	-1.22790800	1.39869000	-2.07432800
C	-2.36119600	4.49524200	-1.28984500
H	-1.60120100	5.72392900	0.30656200
H	-2.89526200	3.05247800	-2.80157800
H	-3.10060400	5.22622700	-1.61199900
C	1.69999300	2.12197300	1.39883100
C	3.05641400	2.45560600	1.38895800
C	0.97593300	2.26824400	2.59077800
C	3.68243100	2.89979800	2.55173800
H	3.63474000	2.36223100	0.47050300
C	1.59999300	2.71884200	3.74748300
H	-0.09246500	2.04820000	2.60294300
C	2.96019500	3.02468300	3.73249300
H	4.74044600	3.15377000	2.52938500
H	1.02227700	2.84985000	4.66194600
H	3.45054300	3.37419500	4.63907200
C	-4.57795600	1.78990600	0.19565800
C	-5.22220800	2.88812800	0.59919300
H	-3.49814300	1.85184700	0.04227900
H	-4.68154500	3.81988000	0.74982900
H	-6.29171100	2.91370700	0.80405500

IM22

M06/BS1 SCF energy in gas pahse: -2350.595424 a.u.

M06/BS2 SCF energy in toluene: -2351.180913 a.u.

M06/BS2 Free energy in toluene: -2350.585694 a.u.

Ru	-0.29715200	0.85655600	0.22573900
B	-2.70961700	2.89903500	-0.35968000
H	-3.59594900	3.66581700	-0.61923300
N	-3.18558600	1.84392900	0.65980300
C	-4.34980300	1.76152900	1.33204300
C	-2.97261900	0.21333600	2.06232700
C	-4.26084500	0.72504800	2.24249000
H	-5.15369600	2.45540300	1.11604300
H	-2.48134700	-0.61083500	2.57022500
H	-5.01649200	0.38892500	2.93941700
N	-1.49862600	3.64345800	0.24680500
C	-1.32833300	4.94736300	0.53909900
C	0.49597300	3.84009900	1.06831500
C	-0.06325800	5.12118900	1.07043400
H	-2.12433500	5.65696700	0.34677600
H	1.47813900	3.50378100	1.38358100
H	0.39045800	6.04331700	1.40725100
N	-2.22806800	2.17861800	-1.64166900
C	-2.63003900	2.35554900	-2.91412800
C	-1.84134400	1.58035700	-3.74468700
H	-3.44930800	3.02976300	-3.13347600
C	-0.95142200	0.94267700	-2.88122700
H	-1.89947500	1.49079400	-4.82058300
H	-0.16170400	0.23400900	-3.10399300
N	-0.37826300	2.96196900	0.57384600
N	-2.33428600	0.88831300	1.10100900
N	-1.19378200	1.30422100	-1.61702500
P	-0.48099900	-1.50205800	-0.21078000
C	2.48897500	1.50990300	-1.05364500
C	1.37720000	1.07893600	-0.48960700
H	2.24015000	2.23254500	-1.84633500
C	0.84841100	0.64026500	3.20435500
N	0.42199500	0.64894500	2.13047900
C	1.38660100	0.58197400	4.54575800
H	1.20276600	-0.40961500	4.97747000
H	2.46782900	0.75889700	4.51614600
H	0.91610800	1.33769800	5.18395700
C	3.91419400	1.26213600	-0.83687700
C	4.41500800	0.36802000	0.13811600
C	4.81951900	1.98815400	-1.62243200
C	5.80103900	0.23440100	0.27506600
C	6.18924900	1.84750600	-1.46172300
H	4.43081900	2.68205200	-2.36783800
C	6.68494700	0.96538400	-0.50546000
H	6.18647000	-0.48749900	0.99409500
H	6.86923900	2.42208400	-2.08738100
H	7.75785000	0.83675000	-0.37887000
C	-1.72136600	-1.87874700	-1.50372500
C	-2.98614000	-1.27510500	-1.44510400
C	-1.41946600	-2.72688500	-2.57184300
C	-3.92245200	-1.51315000	-2.44240900
H	-3.23773700	-0.60819500	-0.61992800
C	-2.35735300	-2.95089400	-3.57650600
H	-0.44714200	-3.21380000	-2.62908300
C	-3.60517400	-2.34224400	-3.51617900
H	-4.90126500	-1.04047400	-2.38553500
H	-2.10817200	-3.60753200	-4.40782700
H	-4.33652800	-2.51731300	-4.30293700
C	1.03352500	-2.37506600	-0.75789500
C	1.47035400	-3.56613900	-0.17066000
C	1.78944100	-1.81830000	-1.79829600
C	2.65522300	-4.16415200	-0.59188800
H	0.88951700	-4.03592800	0.62116200
C	2.96902000	-2.41728600	-2.21872900

H	1.47095400	-0.88894700	-2.26783000
C	3.41022800	-3.58808000	-1.60695900
H	2.98664400	-5.08798600	-0.12174600
H	3.55176300	-1.95909600	-3.01567900
H	4.34046100	-4.05313900	-1.92708900
C	-1.02743600	-2.45527800	1.25639600
C	-2.24774400	-3.13272600	1.29279700
C	-0.21227300	-2.46803800	2.39734300
C	-2.65769000	-3.78507300	2.45352400
H	-2.88875700	-3.14881300	0.41278200
C	-0.61935000	-3.12446800	3.55147000
H	0.76233900	-1.97795600	2.37096700
C	-1.85142200	-3.77607200	3.58539400
H	-3.61213800	-4.30759100	2.46714200
H	0.02982200	-3.14226800	4.42599300
H	-2.17292200	-4.28803500	4.49019300
C	3.51224300	-0.43722500	0.96012200
C	3.75490900	-0.89429100	2.19325200
H	2.56451700	-0.71545600	0.49163800
H	3.05114600	-1.56433500	2.68880800
H	4.67086400	-0.66058600	2.73663000

IM23

M06/BS1 SCF energy in gas pahse: -2350.592908 a.u.

M06/BS2 SCF energy in toluene: -2351.177044 a.u.

M06/BS2 Free energy in toluene: -2350.582126 a.u.

Ru	0.50747700	-0.80401100	0.41750100
B	2.93652300	-2.61043100	-0.68312000
H	3.81220100	-3.29854300	-1.13100400
N	3.51954900	-1.38868700	0.05047200
C	4.80096400	-1.06106300	0.30470500
C	3.46707800	0.37479700	1.28963500
C	4.81698400	0.07112600	1.09789000
H	5.60708300	-1.66609800	-0.09327800
H	3.02511200	1.20397600	1.83264700
H	5.67894000	0.60042300	1.48048500
N	2.07365100	-3.40687500	0.32428800
C	2.19648500	-4.66838300	0.77902300
C	0.45798200	-3.71973000	1.73224700
C	1.18100800	-4.91455000	1.68568100
H	3.00140600	-5.29952400	0.42138300
H	-0.42942300	-3.45766400	2.29961700
H	0.98840700	-5.82894700	2.23009100
N	2.00419300	-2.12324000	-1.81819300
C	2.05379200	-2.41767600	-3.13099200
C	0.95356800	-1.86080700	-3.75572900
H	2.87126600	-3.01243700	-3.52099900
C	0.25043200	-1.22763500	-2.72960400
H	0.69058300	-1.90982100	-4.80342100
H	-0.67853900	-0.66912500	-2.76574200
N	1.00772400	-2.82166200	0.91170900
N	2.69173600	-0.50736100	0.65465300
N	0.89634900	-1.38011900	-1.56736400
P	0.19600100	1.48385300	-0.25536100
C	-2.34684300	-1.98696900	-0.06434800
C	-0.49842800	2.57163200	1.04773100
C	-1.70576100	3.25418400	0.88819200
C	0.18510500	2.68416600	2.26555600
C	-2.23091000	4.01357500	1.93173700
H	-2.24324100	3.19811000	-0.05717100
C	-0.33075700	3.45422800	3.30068100
H	1.14107900	2.17606200	2.39960900
C	-1.54961600	4.11159600	3.13921900
H	-3.17436100	4.53833000	1.79254700
H	0.22520300	3.55569000	4.23211500
H	-1.95774100	4.71169800	3.95011500
C	-0.89539200	1.72535000	-1.70435000
C	-0.46702300	2.39764600	-2.85160100
C	-2.18246000	1.17660700	-1.67896800
C	-1.30726700	2.49384300	-3.95835900
H	0.52679000	2.84032000	-2.89152200
C	-3.02219300	1.27805300	-2.77987400
H	-2.53001500	0.65413500	-0.79089900
C	-2.57907800	1.93115200	-3.92860800
H	-0.96179200	3.01336000	-4.85003900
H	-4.01763900	0.83694700	-2.73691700
H	-3.22726800	2.00304900	-4.79981700
C	1.76815900	2.27742300	-0.74813000
C	2.16310200	3.52393900	-0.25772200
C	2.60146400	1.60172100	-1.65083800
C	3.38518200	4.07247500	-0.63997300
H	1.51963800	4.07543900	0.42631800
C	3.81117500	2.15916100	-2.04047900
H	2.30333700	0.63157800	-2.04916800
C	4.21168300	3.39035700	-1.52489300
H	3.68637200	5.04163300	-0.24687600
H	4.44971400	1.62482800	-2.74135900
H	5.16607000	3.82090800	-1.82181500
C	-1.24791600	-1.30601800	0.19348200
H	-2.04537300	-2.98508400	-0.42171400
C	-3.78352100	-1.70086500	-0.13114500
C	-4.55666800	-2.59029300	-0.89072800
C	-4.41804000	-0.57398600	0.44313700
C	-5.90582900	-2.37066700	-1.12584900
H	-4.07152700	-3.46380900	-1.32638700
C	-5.77030300	-0.35152000	0.15934000
C	-6.51761800	-1.23385700	-0.60865500
H	-6.47318600	-3.07871000	-1.72632800
H	-6.24694100	0.53213500	0.58461100
H	-7.57084200	-1.03734900	-0.79757900
C	-3.75941200	0.40017600	1.32642000
C	-2.88628600	0.13656600	2.30084300
H	-4.07761900	1.43882200	1.18769700
H	-2.47146300	0.94307300	2.90665300
H	-2.56676200	-0.88032400	2.52918000
C	0.17058500	-0.32101800	3.55842400
C	-0.02206800	-0.12431700	4.97937500

H	-0.76245500	-0.83504700	5.36426200
H	0.91895700	-0.27094900	5.52060300
H	-0.38616500	0.89430100	5.16284100
N	0.28971000	-0.44249600	2.41477500

TS25

M06/BS1 SCF energy in gas pahse: -2350.580836 a.u.

M06/BS2 SCF energy in toluene: -2351.163655 a.u.

M06/BS2 Free energy in toluene: -2350.5681 a.u.

Ru	-0.25933400	0.79342200	0.41919700
B	-1.87282700	3.31948600	-0.74598900
H	-2.44531300	4.26467700	-1.21638700
N	-2.86044400	2.38962300	-0.01816300
C	-4.17830200	2.53604900	0.21757200
C	-3.45726100	0.70402600	1.18576400
C	-4.60719600	1.47337800	0.99128600
H	-4.71125200	3.39193500	-0.17969700
H	-3.34883800	-0.24080700	1.70890000
H	-5.60660000	1.28001800	1.35660600
N	-0.79594800	3.77755500	0.26141500
C	-0.45529500	5.01369700	0.67417000
C	0.84364500	3.53482000	1.64959000
C	0.59261500	4.90778000	1.57026600
H	-0.98617700	5.87937500	0.29605000
H	1.59406100	2.99663300	2.21951900
H	1.10500800	5.70852300	2.08598400
N	-1.16309300	2.51377700	-1.86126800
C	-1.12240000	2.76740100	-3.18212600
C	-0.30840500	1.83095000	-3.79177600
H	-1.67474500	3.60603300	-3.58914700
C	0.12855100	1.01519600	-2.74749800
H	-0.05997300	1.75103300	-4.84114700
H	0.78611800	0.15342200	-2.77085900
N	0.00059600	2.86592600	0.86114100
N	-2.40951100	1.26056300	0.57295500
N	-0.39745600	1.42711500	-1.58626700
P	-0.66461400	-1.47550400	-0.21076000
C	2.71261000	1.16328500	-0.39448400
C	-0.32574500	-2.69352200	1.12095500
C	0.66449600	-3.67368600	1.01897400
C	-1.03459900	-2.57791300	2.32472000
C	0.96111800	-4.49520200	2.10474300
H	1.20738200	-3.80393000	0.08419200
C	-0.74812600	-3.40628900	3.40241500
H	-1.83226200	-1.83936700	2.41283100
C	0.26339400	-4.35980600	3.29897400
H	1.73427300	-5.25521100	2.00723200
H	-1.32615600	-3.32132600	4.32215900
H	0.49387800	-5.00619300	4.14353600
C	0.27410800	-2.10805700	-1.65628100
C	-0.37108500	-2.61389800	-2.78842200
C	1.67302000	-2.02141500	-1.66016100
C	0.36615400	-2.99936100	-3.90527000
H	-1.45563000	-2.70192500	-2.80996300
C	2.40737700	-2.41065600	-2.77337800
H	2.19283500	-1.63187600	-0.78741900
C	1.75228300	-2.89196200	-3.90472600
H	-0.15098500	-3.38537500	-4.78161800
H	3.49302800	-2.32752400	-2.75661200
H	2.32375400	-3.18707500	-4.78268000
C	-2.40778800	-1.77014400	-0.68645800
C	-3.14941900	-2.84867500	-0.20033900
C	-3.00870300	-0.87628900	-1.58425700
C	-4.48018900	-3.01267300	-0.57866400
H	-2.69402600	-3.56780200	0.47939300
C	-4.33041100	-1.05211000	-1.97085800
H	-2.44118400	-0.03315900	-1.98095800
C	-5.07258900	-2.11384300	-1.45796100
H	-5.05117200	-3.85292600	-0.18813400
H	-4.78583800	-0.35059100	-2.66735300
H	-6.11244300	-2.24399800	-1.75166200
C	1.63185700	0.64741400	0.20514800
H	2.44273400	1.83188300	-1.22262300
C	4.12614300	0.87971100	-0.23460100
C	5.07127000	1.65242300	-0.92484200
C	4.58379900	-0.25493900	0.48797000
C	6.41521400	1.31790500	-0.91437100
H	4.73047700	2.51933600	-1.49004900
C	5.94227000	-0.60941300	0.43765000
C	6.85752600	0.17754300	-0.23622100
H	7.12677300	1.93428000	-1.46033200
H	6.27095600	-1.49995800	0.97340200
H	7.91096200	-0.09251900	-0.24588800
C	3.63171900	-1.06669400	1.19217700
C	2.48480200	-0.54959200	1.71960900
H	3.80233600	-2.14746800	1.22641300
H	1.73890600	-1.20558800	2.16626400
H	2.49595800	0.47894000	2.09160300
C	-0.37022800	0.38462300	3.57896900
C	-0.46270600	0.24424000	5.01684500
H	-1.40641300	0.66758000	5.37860200
H	-0.42110000	-0.81732100	5.28942600
H	0.36448900	0.76664000	5.50997100
N	-0.30570500	0.45692600	2.42540300

IM24

M06/BS1 SCF energy in gas pahse: -2350.624274 a.u.

M06/BS2 SCF energy in toluene: -2351.206207 a.u.

M06/BS2 Free energy in toluene: -2350.609167 a.u.

Ru	-0.17347300	0.79639400	0.47707100
B	-1.29419100	3.50406800	-0.85677500
H	-1.67099700	4.51525200	-1.38586400
N	-2.48032200	2.73367500	-0.24889900
C	-3.78063100	3.07400100	-0.16086100
C	-3.44150100	1.17694300	0.88657000
C	-4.44147000	2.09772800	0.56186900

H	-4.13751700	3.99135400	-0.61457000
H	-3.52868800	0.23821800	1.42452700
H	-5.49260000	2.05700600	0.81323300
N	-0.29028400	3.82516800	0.27325600
C	0.12455500	5.01149500	0.75733800
C	1.07309200	3.38726000	1.89083400
C	1.00380600	4.78059400	1.79974500
H	-0.23988100	5.93453600	0.32208500
H	1.65165100	2.76164100	2.56305100
H	1.52217800	5.51401800	2.40229600
N	-0.57951400	2.59871200	-1.88724300
C	-0.38817300	2.82260700	-3.20083000
C	0.34242600	1.77470200	-3.72876800
H	-0.78378600	3.72099600	-3.65988200
C	0.56783000	0.92617000	-2.64327200
H	0.66963500	1.64238200	-4.75101500
H	1.10705200	-0.01376100	-2.60472700
N	0.29029600	2.82378400	0.96844400
N	-2.26291500	1.56338800	0.39330500
N	0.00559000	1.42448600	-1.53438700
P	-0.81289700	-1.39171700	-0.20104700
C	2.74028500	0.92384100	-0.13034500
C	-0.85643400	-2.64987300	1.13950700
C	-0.06611600	-3.80142700	1.13233500
C	-1.71110600	-2.42930200	2.22889900
C	-0.11487400	-4.70078500	2.19642200
H	0.58410400	-4.01174900	0.28455700
C	-1.77137700	-3.33358700	3.28153200
H	-2.35747800	-1.55134500	2.23553600
C	-0.96317100	-4.46934900	3.27194600
H	0.50489800	-5.59527200	2.17290500
H	-2.46443700	-3.16292400	4.10471500
H	-1.00835900	-5.17883900	4.09595100
C	0.22421700	-2.17675400	-1.50580300
C	-0.32589000	-2.61078700	-2.71517500
C	1.60974300	-2.28215700	-1.32691000
C	0.49301500	-3.11187100	-3.72454800
H	-1.39980500	-2.54906800	-2.88199200
C	2.42680200	-2.78490300	-2.33119500
H	2.06862400	-1.96675200	-0.39161700
C	1.86851800	-3.19321300	-3.54038400
H	0.04805600	-3.43934000	-4.66225500
H	3.50188800	-2.85020600	-2.16794900
H	2.50527000	-3.57874600	-4.33420200
C	-2.49498100	-1.47993600	-0.92442100
C	-3.37322200	-2.53043900	-0.64598500
C	-2.89087600	-0.47647000	-1.81807500
C	-4.63686500	-2.56196700	-1.23003600
H	-3.07428800	-3.33258100	0.02797200
C	-4.14893700	-0.51585200	-2.40523600
H	-2.21287500	0.34433700	-2.05039700
C	-5.02757900	-1.55354700	-2.10418100
H	-5.31527300	-3.38199700	-1.00213900
H	-4.44755900	0.27248300	-3.09375200
H	-6.01693800	-1.57913500	-2.55711400
C	1.73164600	0.31010900	0.63360300
H	2.46559600	1.71802200	-0.82603800
C	4.07440800	0.51648400	-0.12571000
C	5.03883100	1.12057200	-0.98650100
C	4.52356000	-0.57450600	0.73178500
C	6.32640100	0.67508400	-1.01568700
H	4.71865700	1.94303300	-1.62474500
C	5.89416700	-1.01211000	0.65876000
C	6.76539700	-0.40959800	-0.18645800
H	7.04462700	1.14762800	-1.68337600
H	6.20746100	-1.83244700	1.30376700
H	7.80141400	-0.73559700	-0.24037100
C	3.62563900	-1.13401500	1.58904800
C	2.23545000	-0.64581500	1.68073600
H	3.94278600	-1.92807800	2.26748400
H	1.53690100	-1.47565900	1.87705700
H	2.18257100	-0.06927300	2.63250700
C	-0.65826000	0.35823800	3.58098000
C	-0.95066800	0.20618000	4.99173000
H	-0.09679700	0.51720700	5.60393100
H	-1.81629300	0.81870000	5.26850100
H	-1.17512500	-0.84474300	5.21246300
N	-0.45619100	0.44683000	2.44243100

TS26

M06/BS1 SCF energy in gas pahse: -2350.596304 a.u.

M06/BS2 SCF energy in toluene: -2351.181362 a.u.

M06/BS2 Free energy in toluene: -2350.590987 a.u.

Ru	-0.04342800	-0.81186000	-0.42329600
B	-0.68663100	-3.55494100	1.08996000
H	-0.91195800	-4.57717200	1.68041900
N	-0.10723800	-2.49690300	2.05225300
C	0.12619800	-2.59925800	3.37498600
C	0.73877300	-0.61182700	2.67951300
C	0.67237700	-1.41108700	3.82188500
H	-0.11090600	-3.51810600	3.89807200
H	1.08200200	0.41161400	2.58447700
H	0.97071900	-1.15461900	4.82916400
N	0.34438200	-3.79683600	-0.03619400
C	0.92311600	-4.93882300	-0.45531400
C	1.57508900	-3.27542000	-1.73054200
C	1.72641900	-4.65276300	-1.54374600
H	0.71749900	-5.87291000	0.05406600
H	2.02220400	-2.63093200	-2.48110700
H	2.33258600	-5.33922100	-2.11910700
N	-1.97705300	-3.00254000	0.45078800
C	-3.20497800	-3.55391200	0.37474400
C	-4.00257500	-2.74311300	-0.41062100
H	-3.41504500	-4.48842400	0.88184000
C	-3.16206900	-1.69110800	-0.79043000
H	-5.04171400	-2.89132100	-0.67160200
H	-3.37925400	-0.81971900	-1.40178200

N	0.74242900	-2.76867700	-0.81736100
N	0.26877500	-1.26965600	1.61352000
N	-1.94599400	-1.85126300	-0.26114700
P	-1.02148600	1.26271800	0.12767000
C	0.02189200	2.78525700	0.14048600
C	-0.41608800	4.00655900	-0.38161500
C	1.26496600	2.74373500	0.78363900
C	0.37408600	5.14886700	-0.27563600
H	-1.39137300	4.07719100	-0.86103700
C	2.05314600	3.88288100	0.89278000
H	1.63630700	1.80451800	1.19549500
C	1.60989100	5.08990300	0.35946500
H	0.01364900	6.09103400	-0.68471500
H	3.01883400	3.82434700	1.39313400
H	2.22476300	5.98406300	0.44237600
C	-2.40388300	1.73363300	-0.99249600
C	-3.73190700	1.76281600	-0.56084200
C	-2.12844500	1.99500100	-2.34193700
C	-4.76268800	2.02544100	-1.46104000
H	-3.96884300	1.56996600	0.48487600
C	-3.15558300	2.26832000	-3.23698700
H	-1.09363600	2.00188300	-2.68956300
C	-4.47916100	2.27338700	-2.79874500
H	-5.79248100	2.04166700	-1.10933100
H	-2.92465900	2.49379500	-4.27792600
H	-5.28494000	2.48324000	-3.49953400
C	-1.81008300	1.34928100	1.78896700
C	-1.85571100	2.54666800	2.51121300
C	-2.43576400	0.21458400	2.31994900
C	-2.50842300	2.60585300	3.73882900
H	-1.38159900	3.44505900	2.11756900
C	-3.08851100	0.27776700	3.54554100
H	-2.41292600	-0.72423500	1.76991300
C	-3.12437400	1.47258800	4.25902500
H	-2.53441600	3.54447800	4.28969800
H	-3.56660400	-0.61454600	3.94586600
H	-3.63294200	1.52064200	5.22022100
C	1.87154000	-0.04958800	-0.61624600
C	2.97239000	-0.55929300	0.14292100
H	2.77719700	-1.39236700	0.82103400
C	4.25951500	-0.02935900	0.10442600
C	5.30654100	-0.55696800	0.92032400
C	4.55597800	1.07363100	-0.77618700
C	6.55892200	-0.02003100	0.87238900
H	5.07755500	-1.39384000	1.57885600
C	5.87843900	1.60048300	-0.80021000
C	6.84696000	1.07103100	0.00320300
H	7.35136000	-0.42385600	1.49890500
H	6.09861100	2.43132200	-1.46923200
H	7.85464300	1.48095500	-0.01761900
C	3.53891800	1.57958000	-1.58514300
C	2.25020700	1.04160100	-1.52395100
H	3.74677100	2.41084400	-2.25813900
H	1.45794400	1.46306100	-2.14319900
H	2.19652100	-0.29860600	-1.80296500
C	-0.69875600	-0.68929600	-3.51676300
C	-1.12170400	-0.73466100	-4.90174800
H	-0.29714800	-0.47225400	-5.57382200
H	-1.47316100	-1.74052000	-5.15822800
H	-1.94513500	-0.02725900	-5.06034800
N	-0.40560100	-0.63385900	-2.39486700

IM25

M06/BS1 SCF energy in gas pahse: -2350.659454 a.u.

M06/BS2 SCF energy in toluene: -2351.244486 a.u.

M06/BS2 Free energy in toluene: -2350.644662 a.u.

Ru	-0.72611900	-0.78798900	-0.47558300
B	-2.68319500	-2.64413700	1.19287900
H	-3.44216100	-3.31344300	1.83799500
N	-1.42239200	-2.30345900	2.00720300
C	-1.07951900	-2.69834600	3.24765400
C	0.55268800	-1.51799500	2.38104000
C	0.18348700	-2.21615100	3.53129800
H	-1.76029000	-3.30569200	3.83225600
H	1.47443300	-0.98834300	2.17579500
H	0.75682200	-2.34880300	4.43840400
N	-2.24537500	-3.38155300	-0.08833200
C	-2.59002100	-4.59211700	-0.56592200
C	-1.23634600	-3.60477600	-1.98594500
C	-1.96297300	-4.78112100	-1.78370900
H	-3.25720500	-5.23127200	0.00022300
H	-0.59602000	-3.32456200	-2.81657100
H	-2.01778700	-5.64641500	-2.43001200
N	-3.35858000	-1.32142700	0.76228100
C	-4.63758900	-0.92267700	0.89781900
C	-4.80438900	0.27211200	0.22295400
H	-5.33510300	-1.52774800	1.46465400
C	-3.54886200	0.54833200	-0.32294700
H	-5.70596800	0.86286800	0.13606600
H	-3.22452700	1.38889400	-0.92675200
N	-1.41154900	-2.76856400	-0.95717300
N	-0.41958600	-1.56835300	1.46375300
N	-2.68257700	-0.41311100	0.01962200
P	-0.08628100	1.42558600	0.18894100
C	1.66617000	1.96875900	0.01448400
C	2.07245100	3.03185200	-0.79627000
C	2.63224400	1.31104400	0.78366000
C	3.41373700	3.40528400	-0.85200700
H	1.34557600	3.59561400	-1.37700300
C	3.96735600	1.68457200	0.73260000
H	2.34006500	0.49595700	1.44225200
C	4.36425800	2.73208500	-0.09442400
H	3.70982400	4.24011300	-1.48485400
H	4.70120200	1.14398200	1.32904600
H	5.41160400	3.02551300	-0.13959900
C	-1.01583200	2.72521800	-0.72102200
C	-1.92074500	3.57524100	-0.07937500

C	-0.86966200	2.82241700	-2.11209300
C	-2.67708800	4.48578800	-0.81416800
H	-2.04934100	3.52072000	1.00104900
C	-1.61527200	3.74046400	-2.84230700
H	-0.14742800	2.18467900	-2.62406800
C	-2.53063800	4.56783000	-2.19395000
H	-3.38080000	5.13771300	-0.30025000
H	-1.47194500	3.82457200	-3.91918000
H	-3.11878700	5.28380700	-2.76468800
C	-0.42064000	1.84954800	1.94549200
C	0.28667100	2.88858600	2.56306000
C	-1.43820000	1.20654700	2.65788300
C	-0.00768700	3.26258000	3.86907000
H	1.07343500	3.41121000	2.01900000
C	-1.72825800	1.58103800	3.96580500
H	-2.00784900	0.40453300	2.19478100
C	-1.01228000	2.60634200	4.57449200
H	0.55128000	4.07021400	4.33785700
H	-2.51725000	1.06479200	4.50976000
H	-1.23781500	2.89575800	5.59919400
C	1.70493800	-1.45832500	-1.34017300
C	2.42630800	-2.07611800	-0.34539900
H	1.93678900	-2.78194000	0.32749400
C	3.80570800	-1.80636500	-0.19046900
C	4.56643100	-2.37080500	0.86262200
C	4.44200500	-0.92918700	-1.11979700
C	5.90326900	-2.08706900	0.98676800
H	4.06989200	-3.03836700	1.56796300
C	5.82439100	-0.66728900	-0.97132700
C	6.53778100	-1.23151300	0.05715100
H	6.48263400	-2.52586500	1.79655800
H	6.31001700	0.00032200	-1.68345300
H	7.60074300	-1.02219300	0.16150500
C	3.67222600	-0.32818000	-2.14891400
C	2.32825700	-0.57076500	-2.25092900
H	4.16980800	0.34792500	-2.84416300
H	1.73562900	-0.09574700	-3.03252800
H	0.68509400	-1.81874500	-1.55476000
C	-1.59374600	-0.05613600	-3.44220500
C	-2.09795800	0.26042300	-4.76205800
H	-1.32594600	0.09475000	-5.52183800
H	-2.96457500	-0.36569900	-5.00186500
H	-2.40642500	1.31268400	-4.79502000
N	-1.18911800	-0.26212100	-2.37574800

TS27

M06/BS1 SCF energy in gas pahse: -1255.494153 a.u.

M06/BS2 SCF energy in MeOH: -1255.871198 a.u.

M06/BS2 Free energy in MeOH: -1255.42358 a.u.

Ru	-0.69414800	-0.44669000	-0.01585900
C	-2.01716100	-2.18793200	0.52842600
C	-2.25223900	-1.87732100	-0.83864900
C	-1.00153400	-2.03080100	-1.55714100
C	-0.62824700	-2.55423200	0.67481800
C	-0.02347600	-2.49863500	-0.62886300
C	-0.81390200	-1.89273200	-3.03032400
H	-1.42527800	-1.08419000	-3.45056100
H	-1.09940000	-2.81719700	-3.55198000
H	0.23102900	-1.67955600	-3.28590100
C	-3.59248300	-1.60669000	-1.43558200
H	-4.16006100	-0.85813900	-0.86715900
H	-4.18984800	-2.52928200	-1.44523900
H	-3.52236100	-1.26168800	-2.47345200
C	-3.05299600	-2.18649400	1.59832500
H	-2.62150500	-2.01629400	2.59111800
H	-3.57757400	-3.15197700	1.62747700
H	-3.80538800	-1.40591400	1.42869700
C	0.03073900	-3.06680000	1.91158300
H	1.05257200	-2.67825200	2.01738200
H	0.09678800	-4.16362400	1.89605500
H	-0.52564700	-2.78855900	2.81408900
C	1.36817300	-2.91987000	-0.95711700
H	1.37816900	-3.97682500	-1.25820400
H	2.03956300	-2.81841400	-0.09601800
H	1.79138700	-2.33769600	-1.78448200
C	-2.59521800	1.85053900	1.01799800
C	-3.39752700	2.63758900	1.84906600
C	-4.45349500	3.35003300	1.29527100
C	-4.70832800	3.27571900	-0.07362800
C	-3.89535800	2.50997600	-0.90514000
C	-2.81828700	1.81133700	-0.36737000
H	-3.20760400	2.66077100	2.92040600
H	-5.09383200	3.95259600	1.93558800
H	-5.54780300	3.82278700	-0.49770300
H	-4.08688600	2.46884500	-1.97727400
C	-1.56032100	0.98653300	1.50058200
C	-0.72330700	0.29272000	2.10578500
H	-0.11606900	-0.10724200	2.89994700
C	-1.85544800	1.06103700	-1.20583800
C	-0.49414700	1.39450200	-1.25827500
H	0.09354300	1.16050300	-2.14628400
H	-0.12495600	2.23310700	-0.66302500
H	-2.28293000	0.56759100	-2.08150700
C	1.24193600	0.00808200	0.16777700
C	2.48781400	0.17964200	0.27019900
C	3.90907800	0.30065300	0.37656000
C	4.59168000	-0.61251900	1.19607400
C	4.60473600	1.31478700	-0.32281200
C	5.96825100	-0.54242000	1.31942700
C	5.99416400	1.36085700	-0.17527700
C	6.66445700	0.45197200	0.63201000
H	6.50004500	-1.25524100	1.94486300
H	6.55976200	2.10811400	-0.72872500
H	7.74747100	0.51216500	0.71907900
H	1.64860400	0.99330400	0.84521400
C	3.88216500	2.26719200	-1.16820000
C	4.29323800	3.50367200	-1.45828000

H	2.92789600	1.91865300	-1.57183000
H	3.70871400	4.15408800	-2.10395600
H	5.21462100	3.92287300	-1.05561100
H	4.02175100	-1.37331500	1.72834200

IM26

M06/BS1 SCF energy in gas pahse: -1255.525272 a.u.

M06/BS2 SCF energy in MeOH: -1255.901442 a.u.

M06/BS2 Free energy in MeOH: -1255.448761 a.u.

Ru	-0.49332700	0.23596000	-0.14436300
C	-1.49717500	2.29178200	-0.37359500
C	-1.57870200	1.93066800	0.99353900
C	-0.22557400	1.73361200	1.48166400
C	-0.10169700	2.37073200	-0.74389200
C	0.67628900	2.08581900	0.42352000
C	0.16604800	1.44081100	2.89006600
H	-0.52746600	0.74341300	3.37710200
H	0.17415200	2.36095900	3.49166500
H	1.16862800	0.99853300	2.94109900
C	-2.82572300	1.90719500	1.81075400
H	-3.64957200	1.38354700	1.30900400
H	-3.16414700	2.93562400	2.00019800
H	-2.67125000	1.43794200	2.78898700
C	-2.65657100	2.59225100	-1.25840500
H	-2.44846200	2.35025500	-2.30703400
H	-2.90701200	3.66134900	-1.21114400
H	-3.54964100	2.02948900	-0.96016000
C	0.43948500	2.83193100	-2.05426700
H	1.35621900	2.29138600	-2.32232500
H	0.68877000	3.90150900	-2.01864800
H	-0.28472900	2.69592200	-2.86580300
C	2.15619200	2.20028700	0.54265500
H	2.41728800	3.19837500	0.92249000
H	2.65824600	2.07192000	-0.42256400
H	2.57002800	1.45918800	1.23774100
C	-3.11088000	-1.37292800	-0.91755500
C	-4.23622700	-1.81268500	-1.61994000
C	-5.33747300	-2.27611600	-0.91093900
C	-5.31730000	-2.29625100	0.48274100
C	-4.18837400	-1.87544700	1.18164500
C	-3.06852500	-1.43349700	0.48350400
H	-4.25086800	-1.76350000	-2.70678200
H	-6.22440500	-2.60579800	-1.44708300
H	-6.19022700	-2.64396500	1.03110500
H	-4.17027000	-1.90872200	2.27074700
C	-1.96954600	-0.78275300	-1.54699600
C	-1.07100400	-0.30552400	-2.26043700
H	-0.50006300	-0.03431500	-3.13194900
C	-1.80457600	-1.07245000	1.16210000
C	-0.59563400	-1.73156600	0.91263600
H	0.16500500	-1.74568200	1.69237300
H	-0.54456500	-2.54160200	0.18325200
H	-1.91806800	-0.59305800	2.13781800
C	1.12822100	-0.52496200	-0.70638700
C	2.24995000	-0.82690900	-1.32591900
C	3.64171400	-0.97179600	-0.89020100
C	4.64591300	-0.80089600	-1.84961800
C	3.99741400	-1.20386700	0.45472100
C	5.98588200	-0.82727700	-1.49100800
C	5.35309500	-1.22953800	0.79485600
C	6.34086000	-1.03324800	-0.16071800
H	6.75293800	-0.69315500	-2.25074800
H	5.62660800	-1.44615800	1.82668900
H	7.38923200	-1.06357300	0.12815200
H	2.07954400	-0.88911500	-2.41231000
C	2.97004400	-1.47255600	1.46120900
C	3.01600600	-1.09830300	2.74388400
H	2.11983600	-2.06412500	1.10929000
H	2.24424000	-1.39650000	3.45223700
H	3.83810100	-0.50100000	3.13998900
H	4.36549300	-0.63049200	-2.88913500

TS28

M06/BS1 SCF energy in gas pahse: -2603.371822 a.u.

M06/BS2 SCF energy in solution: -2604.021629 a.u.

M06/BS2 Free energy in solution: -2603.336149 a.u.

Ru	-0.26053900	-0.21928100	-0.04003800
B	-0.89802000	-1.69427900	-2.84272300
H	-1.13884800	-2.23549400	-3.88710300
N	-0.19059500	-2.66468700	-1.88004500
C	0.08611100	-3.97494500	-2.02958000
C	0.66406000	-3.32962500	-0.01318700
C	0.63995000	-4.44521800	-0.85277500
H	-0.13680200	-4.47444800	-2.96505600
H	1.01051500	-3.25211800	1.01145000
H	0.97636300	-5.44904700	-0.63219400
N	-2.19528600	-1.18712200	-2.18096200
C	-3.46402400	-1.23383700	-2.63066700
C	-3.40395800	-0.09860900	-0.75119400
C	-4.27513100	-0.55115900	-1.74296100
H	-3.69236800	-1.75069400	-3.55540300
H	-3.61877500	0.47579400	0.14467700
H	-5.34400600	-0.39964200	-1.80393000
N	0.00329600	-0.46100200	-3.06960300
C	0.39865100	0.08228700	-4.23637400
C	1.03987700	1.27793600	-3.97426800
H	0.18707700	-0.42671900	-5.16950100
C	0.98341600	1.40704000	-2.58585200
H	1.47979700	1.96551000	-4.68347100
H	1.35586100	2.20874100	-1.95949900
N	-2.15505600	-0.48571200	-1.02328100
N	0.16538300	-2.26068900	-0.64053900
N	0.36236000	0.35237200	-2.04233600
P	2.10898300	-0.00840600	0.54994800
C	-0.45993400	1.41682700	1.41827600
C	2.53336300	-0.06980000	2.33505300

C	3.20118100	0.97954900	2.97247700
C	2.18735200	-1.20330400	3.08725000
C	3.51250200	0.89843000	4.32801900
H	3.49436900	1.86432600	2.41028200
C	2.50848700	-1.28693700	4.43560800
H	1.66046700	-2.03296300	2.61402600
C	3.16989200	-0.23144300	5.06026400
H	4.03409900	1.72374400	4.80861000
H	2.23885400	-2.17664900	5.00128100
H	3.41879400	-0.29380200	6.11762500
C	2.91739000	1.54383500	-0.01748400
C	4.14420800	1.49387900	-0.68688200
C	2.32765100	2.79545200	0.21631700
C	4.75414800	2.66256500	-1.13401300
H	4.63034000	0.53759000	-0.86946500
C	2.94372700	3.96020500	-0.22564900
H	1.36795700	2.87321100	0.72281100
C	4.15477300	3.89635100	-0.91024200
H	5.70494600	2.60286900	-1.66001200
H	2.46761000	4.92150200	-0.04121800
H	4.63067000	4.80858100	-1.26460300
C	3.14492900	-1.31946000	-0.20423800
C	4.04976500	-2.07622300	0.54407200
C	3.04432600	-1.54692900	-1.58369900
C	4.81620400	-3.06393300	-0.07035800
H	4.16791100	-1.90113000	1.61165200
C	3.81844900	-2.52423600	-2.19287100
H	2.36087400	-0.95318400	-2.18759600
C	4.69938700	-3.29343800	-1.43546800
H	5.51296500	-3.64993300	0.52590200
H	3.73007400	-2.68841800	-3.26522800
H	5.29968700	-4.06524700	-1.91320400
C	-1.00792000	1.74899500	0.30316800
C	-1.49269400	-1.15983900	1.57965800
C	-0.66575600	-0.34889000	2.11137000
H	-0.02085900	-0.28716000	2.98081700
H	0.21018400	1.80799900	2.17745000
C	-2.69501500	-1.92755500	1.51873300
C	-3.83845500	-1.46476600	2.22475100
C	-2.78049900	-3.09858800	0.74829300
C	-5.01509300	-2.21323400	2.13752900
C	-3.96405100	-3.81255800	0.67410500
H	-1.90224700	-3.43780900	0.20389800
C	-5.08651500	-3.36873900	1.37121900
H	-5.88433400	-1.88491400	2.70552600
H	-4.01018700	-4.72295000	0.08018000
H	-6.01641500	-3.93237200	1.32816700
C	-1.68522800	2.76568700	-0.44546400
C	-1.98388100	2.62452700	-1.81242100
C	-2.01522500	3.98137800	0.21509200
C	-2.57277200	3.65857100	-2.52182100
H	-1.74817800	1.68699200	-2.31159700
C	-2.61899700	5.00185000	-0.52237700
C	-2.88870100	4.85235500	-1.87673400
H	-2.79747300	3.52907000	-3.57841800
H	-2.90014300	5.91877300	-0.00619700
H	-3.36407200	5.66281300	-2.42591100
C	-3.81628900	-0.21433200	2.99466900
C	-4.84715300	0.63118700	3.08058800
H	-2.88971000	0.03551200	3.51304400
H	-4.78951600	1.53679200	3.67996600
H	-5.78631400	0.45377700	2.55596300
C	-1.74930300	4.16583200	1.64605400
C	-1.30378800	5.29973800	2.19190400
H	-1.94517600	3.30397400	2.29079600
H	-1.15829700	5.39582400	3.26544100
H	-1.06381500	6.17375200	1.58611700

TS29

M06/BS1 SCF energy in gas pahse: -1700.303593 a.u.

M06/BS2 SCF energy in solution: -1700.780079 a.u.

M06/BS2 Free energy in solution: -1700.308535 a.u.

Ru	-0.72797400	-0.32732000	0.69951500
B	-2.21894900	-0.16642300	-2.13860300
H	-2.74994500	-0.09936600	-3.21179200
N	-3.00629600	0.63477300	-1.07872500
C	-4.13442100	1.36382900	-1.17578900
C	-3.39341700	1.43795200	0.89353900
C	-4.42296400	1.89853200	0.06781900
H	-4.64981200	1.44592400	-2.12546300
H	-3.20088700	1.62897700	1.94483000
H	-5.25760600	2.53126100	0.33746500
N	-0.78307500	0.39952500	-2.19993400
C	-0.11661000	0.89830400	-3.25789000
C	1.21483600	0.89395000	-1.51197600
C	1.16584500	1.23066400	-2.86387100
H	-0.61086300	0.97785000	-4.21894400
H	2.03773500	0.98161600	-0.80944700
H	1.95674800	1.65224700	-3.46846300
N	-2.12148800	-1.63351300	-1.65633900
C	-2.52539800	-2.78097400	-2.23462100
C	-2.17436500	-3.83846900	-1.41393700
H	-3.03700500	-2.75817000	-3.18957500
C	-1.53713200	-3.23921800	-0.32443300
H	-2.34931900	-4.89226700	-1.58276300
H	-1.07572700	-3.68776400	0.54995800
N	0.03808100	0.39693700	-1.11830000
N	-2.54811800	0.68106600	0.18934000
N	-1.51101400	-1.91383100	-0.48436300
C	0.91991400	-0.94329800	2.01550000
C	1.19177000	-1.30739100	0.80812400
C	0.07986400	1.60854000	1.42845100
C	0.22033800	0.73981800	2.36252700
H	-0.01188200	0.67636900	3.42126700
H	0.85195300	-1.42592500	2.98573600
C	0.39301900	2.78583900	0.68954400
C	1.72106100	3.29161900	0.72457200

C	-0.56960700	3.41463100	-0.11993600
C	2.01637400	4.42385600	-0.03903000
C	-0.24387000	4.53197800	-0.86826600
H	-1.57915000	3.00938400	-0.15200900
C	1.05434300	5.03952200	-0.82800400
H	3.02382300	4.83474700	0.00862000
H	-1.00338800	5.01486700	-1.47935700
H	1.31471700	5.92344800	-1.40684000
C	2.11915500	-1.81461100	-0.14684600
C	1.70029900	-2.29145000	-1.40450900
C	3.50274900	-1.85068500	0.19169600
C	2.60880200	-2.82192500	-2.30124400
H	0.64594900	-2.23389100	-1.66691300
C	4.39693500	-2.36959700	-0.74975700
C	3.96410900	-2.86156500	-1.97232700
H	2.26577700	-3.19151900	-3.26516000
H	5.46075600	-2.35980200	-0.51808700
H	4.68739200	-3.25971500	-2.68131400
C	2.77934000	2.61183200	1.48159100
C	4.04190700	2.49430300	1.05988200
H	2.49710500	2.15683500	2.43262500
H	4.79563800	1.98538300	1.65678000
H	4.36950100	2.89574800	0.10056300
C	3.99435400	-1.33238100	1.47092300
C	5.07007900	-1.78935700	2.11748900
H	3.42317600	-0.51147400	1.91135100
H	5.39934500	-1.34303800	3.05291300
H	5.65263400	-2.63493600	1.75302700
C	-2.57004900	-1.63942300	2.97536500
N	-1.84740300	-1.15655200	2.21252600
C	-3.48400100	-2.24217800	3.92267400
H	-4.43973300	-2.45427900	3.43059600
H	-3.07109600	-3.18044800	4.30904900
H	-3.66459500	-1.56259700	4.76270000

TS30

M06/BS1 SCF energy in gas pahse: -1567.633977 a.u.

M06/BS2 SCF energy in solution: -1568.066974 a.u.

M06/BS2 Free energy in solution: -1567.631815 a.u.

Ru	-0.36357300	-0.13406400	0.33097400
B	0.28059000	2.83701400	-0.76282500
H	0.52787300	3.94419800	-1.15096600
N	-1.13725300	2.40433700	-1.17421800
C	-1.97019500	3.01975800	-2.03380400
C	-2.66261200	0.96321500	-1.70463900
C	-2.96953700	2.13744200	-2.39227200
H	-1.77859200	4.04371900	-2.33204300
H	-3.19607400	0.02088900	-1.70995900
H	-3.80258500	2.31128700	-3.05929300
N	0.41786100	2.75790600	0.76628100
C	0.81683700	3.69287800	1.64499600
C	0.47654400	1.80027400	2.70427800
C	0.86576000	3.12349900	2.90552300
H	1.03658300	4.69838700	1.30637200
H	0.40628200	0.99409300	3.42520200
H	1.14296800	3.59699700	3.83736200
N	1.23477200	1.80245000	-1.39442000
C	2.17402900	1.98157200	-2.33944100
C	2.61234000	0.74408800	-2.77179300
H	2.45114400	2.98423800	-2.64303600
C	1.86344800	-0.16711000	-2.02994000
H	3.36487600	0.52850300	-3.51757500
H	1.91819000	-1.24824100	-2.04909100
N	0.20517400	1.58946400	1.40791500
N	-1.55712800	1.13077000	-0.96731100
N	1.03388600	0.47615200	-1.19904800
C	0.51541300	-1.43874000	2.08022300
C	1.34290200	-1.04050800	1.19672200
C	-2.17752800	-0.13161500	1.43524900
C	-1.32007800	-0.93880100	2.28459100
H	0.51345400	-2.05556500	2.96907700
C	2.73153800	-0.99333000	0.78069700
C	3.43520700	0.20560800	0.95567600
C	3.35290100	-2.09778100	0.16112900
C	4.75121400	0.31561000	0.53422300
H	2.93088700	1.05478900	1.41806900
C	4.68233500	-1.95985000	-0.25311100
C	5.37470000	-0.77050000	-0.07689900
H	5.29286600	1.24675200	0.68623000
H	5.18362500	-2.81915200	-0.69629100
H	6.41029300	-0.69472000	-0.40189500
C	-1.58439000	-1.88995400	-0.50308500
C	-0.41522300	-2.03999400	-0.87729900
C	2.62197000	-3.35021100	-0.06947200
C	2.81153800	-4.16067700	-1.11577400
H	1.86213300	-3.61412000	0.66989600
H	2.25768900	-5.09082800	-1.22004600
H	3.53503200	-3.93446700	-1.89945400
C	-2.97078900	-1.81598600	-0.16560100
C	-3.30219800	-0.82426400	0.77212600
C	-3.96360100	-2.57162900	-0.79462100
C	-4.63988500	-0.55784400	1.03969100
C	-5.29639100	-2.30856100	-0.50113200
H	-3.68971100	-3.32977300	-1.52545100
C	-5.63143700	-1.30028600	0.40190500
H	-4.90662700	0.22574300	1.74786700
H	-6.08037300	-2.87943000	-0.99332500
H	-6.67816700	-1.08948500	0.61100800
H	0.46718600	-2.49825700	-1.29039800
H	-2.37126100	0.89018700	1.77357300
H	-1.09166900	-0.47813800	3.24653300
H	-1.64179500	-1.97922100	2.36567700

IM1S

M06/BS1 SCF energy in gas pahse: -1255.5198 a.u.

M06/BS2 SCF energy in MeOH: -1255.895394 a.u.

M06/BS2 Free energy in MeOH: -1255.44094 a.u.

Ru	-0.47559100	0.15627200	-0.11776000
C	-1.72446000	1.97875900	-0.77139300
C	-1.67323700	1.99575800	0.64386200
C	-0.28007500	2.04572800	1.04033600
C	-0.37323600	2.08451300	-1.27678300
C	0.50559600	2.18735500	-0.15673700
C	0.22118800	2.18228100	2.43808500
H	-0.34314100	1.55528300	3.13995100
H	0.13681700	3.22121700	2.78797300
H	1.27423700	1.88894400	2.51337300
C	-2.84952100	2.07858600	1.55554500
H	-3.64202000	1.36722800	1.28842900
H	-3.28615800	3.08563700	1.50168700
H	-2.57476500	1.90451600	2.60211600
C	-2.95273400	1.93578000	-1.61319200
H	-2.85316700	1.21553100	-2.43593200
H	-3.14467700	2.92001400	-2.06255600
H	-3.83682100	1.65380000	-1.02994500
C	0.00899400	2.22720200	-2.70985700
H	0.99779000	1.79463400	-2.90932400
H	0.05078400	3.28718200	-2.99765900
H	-0.71571300	1.74018400	-3.37343600
C	1.96453600	2.47454200	-0.22215400
H	2.12239800	3.56190500	-0.25364100
H	2.43162600	2.04592200	-1.11615600
H	2.49895200	2.08628200	0.65204100
C	-3.04728200	-1.56530500	-0.63193300
C	-4.18163400	-2.06472400	-1.27463900
C	-5.33845300	-2.28534400	-0.53507500
C	-5.36247000	-2.00779900	0.82972900
C	-4.22436000	-1.52759200	1.47504800
C	-3.05331900	-1.32246300	0.75243600
H	-4.15993900	-2.25010500	-2.34673100
H	-6.23196600	-2.65932800	-1.02963400
H	-6.27611600	-2.16828900	1.39807100
H	-4.24157700	-1.32669900	2.54628700
C	-1.84881600	-1.19046100	-1.31956900
C	-0.87216900	-0.92972200	-2.04416200
H	-0.23215000	-0.91718100	-2.91023600
C	-1.78844400	-0.90014000	1.39188000
C	-0.59597500	-1.61495600	1.24983200
H	0.16643700	-1.52396000	2.01833000
H	-0.55651500	-2.52336700	0.64684000
H	-1.89255700	-0.27113800	2.27918800
C	1.23952800	-0.59668500	-0.33910200
C	2.37403700	-1.03900700	-0.83653600
C	3.79721100	-1.06061900	-0.48370400
C	4.68229400	-1.48517500	-1.48481000
C	4.32790000	-0.59553000	0.73822700
C	6.05668700	-1.43144900	-1.31002000
C	5.71563700	-0.51240700	0.88086800
C	6.57920500	-0.92996500	-0.12269100
H	6.71761200	-1.76708600	-2.10614400
H	6.11836200	-0.13507000	1.82086900
H	7.65526600	-0.86710700	0.02352500
H	2.15904000	-1.41414100	-1.85152700
C	3.50243000	-0.22111700	1.89532700
C	2.55558900	-1.00084100	2.42231600
H	3.76826700	0.71205200	2.40230900
H	2.01514900	-0.71473500	3.32409600
H	2.33636600	-1.98224800	2.00058600
H	4.27627000	-1.85105600	-2.42809900

TS1S

M06/BS1 SCF energy in gas pahse: -1255.508479 a.u.

M06/BS2 SCF energy in MeOH: -1255.881166 a.u.

M06/BS2 Free energy in MeOH: -1255.429522 a.u.

Ru	0.64357700	-0.55588800	-0.03347300
C	1.80294300	-2.23719700	-1.09145900
C	2.44139800	-1.97219900	0.14737100
C	1.48975500	-2.26042200	1.19340700
C	0.44188900	-2.64276300	-0.83369100
C	0.27460300	-2.70757600	0.59348200
C	1.77611800	-2.29164700	2.65553600
H	2.40166200	-1.45510800	2.99033700
H	2.32076800	-3.21346800	2.90495400
H	0.85650300	-2.28676500	3.25178800
C	3.87588400	-1.59173900	0.31251700
H	4.13433100	-0.70058500	-0.27631600
H	4.53420900	-2.40645000	-0.02030000
H	4.12652300	-1.38482700	1.35922800
C	2.48227800	-2.16090200	-2.41365000
H	1.78006600	-2.21617600	-3.25228700
H	3.18106000	-3.00340200	-2.51495300
H	3.06581100	-1.23760700	-2.52030200
C	-0.54980500	-3.10847200	-1.84584200
H	-1.55855800	-2.73877500	-1.62349100
H	-0.59305200	-4.20601700	-1.87885700
H	-0.29452100	-2.76492100	-2.85491700
C	-0.87752100	-3.29574700	1.33761600
H	-0.56268100	-4.21412200	1.85263300
H	-1.69524600	-3.57413500	0.66345800
H	-1.27900800	-2.61519600	2.10054400
C	2.01393100	2.23262700	-0.68175600
C	2.43039200	3.37908900	-1.36836300
C	3.07533600	4.38595100	-0.66460400
C	3.30025800	4.25348400	0.70668700
C	2.87735600	3.11662300	1.38878100
C	2.22045600	2.10360800	0.69544000
H	2.25687100	3.46527000	-2.43934600
H	3.41208800	5.27930600	-1.18579800
H	3.81055900	5.04738400	1.24820700
H	3.05028400	3.01929300	2.46013400
C	1.34276000	1.12335500	-1.29292100
C	0.74669200	0.32188300	-2.04354800
H	0.32584000	-0.09340000	-2.94431900

C	1.72739400	0.86516200	1.35756100
C	0.41825800	0.70100900	1.81565200
H	2.50827200	0.27558300	1.84474100
C	-1.27407700	-0.14353500	-0.02852900
C	-2.52520000	-0.58683800	0.08198900
C	-3.81675000	0.08917500	-0.01531400
C	-3.91678000	1.49863200	0.05691300
C	-4.99335900	-0.66583700	-0.03918800
C	-5.17725400	2.09899300	0.16952500
C	-6.23710300	-0.05164900	0.01662600
H	-4.92674200	-1.75276500	-0.08092800
C	-6.33258300	1.33552600	0.12917300
H	-5.23839000	3.18351000	0.25532600
H	-7.13910400	-0.65998000	0.00117000
H	-7.30681400	1.81425900	0.19610100
H	-2.58188500	-1.63892300	0.38272100
C	-2.71040600	2.28767300	0.07150100
C	-1.60985000	1.92978000	-0.63655800
H	-2.68219700	3.17122000	0.71518400
H	-1.71438500	1.31650200	-1.53594700
H	-0.69148900	2.50922000	-0.57351000
H	-0.31774800	1.48935600	1.66739600
H	0.19750400	0.01453200	2.63404200

IM2S

M06/BS1 SCF energy in gas pahse: -1255.554372 a.u.

M06/BS2 SCF energy in MeOH: -1255.923932 a.u.

M06/BS2 Free energy in MeOH: -1255.468655 a.u.

Ru	0.61069900	-0.52538900	-0.05255900
C	1.38526900	-2.35173400	-1.22383400
C	2.23231100	-2.15131100	-0.09924300
C	1.41612100	-2.31212000	1.07258800
C	0.04545900	-2.60445800	-0.76202100
C	0.07263500	-2.61407200	0.67020400
C	1.88986800	-2.39226600	2.48476900
H	2.90770900	-2.00851600	2.61381000
H	1.90323300	-3.44366300	2.80652300
H	1.23237600	-1.85779600	3.18284700
C	3.70384700	-1.91163500	-0.16539500
H	3.95045800	-1.15329900	-0.92105000
H	4.24884800	-2.82881700	-0.43082800
H	4.10740700	-1.55855700	0.79070200
C	1.85812200	-2.41300300	-2.63455900
H	1.03768400	-2.34056300	-3.35771300
H	2.35939300	-3.37580100	-2.80944500
H	2.58617300	-1.62368800	-2.85993800
C	-1.10351800	-2.97036000	-1.64093900
H	-2.06832500	-2.82243700	-1.14266900
H	-1.04630500	-4.02557300	-1.94332700
H	-1.11985400	-2.36650200	-2.55741000
C	-0.99464900	-3.08200400	1.60467100
H	-0.67436600	-4.00140600	2.11576800
H	-1.92568500	-3.32396400	1.07909800
H	-1.22781000	-2.34532700	2.38571600
C	2.25416300	2.12751500	-0.57104300
C	2.78253200	3.26626800	-1.19179100
C	3.52794600	4.15906000	-0.43561500
C	3.74767300	3.91829300	0.92191300
C	3.21498400	2.79024800	1.53890000
C	2.45061400	1.89560400	0.79456200
H	2.62005600	3.43073500	-2.25557600
H	3.95279200	5.04383000	-0.90481800
H	4.34062900	4.62023200	1.50487700
H	3.38326600	2.61051700	2.60044800
C	1.49380800	1.11133600	-1.23473300
C	0.85563300	0.39074600	-2.03393900
H	0.47230500	0.02883700	-2.97403300
C	1.80344600	0.69064300	1.38175300
C	0.45430100	0.69209600	1.78760000
H	0.12269900	0.04180300	2.59922300
H	-0.12997300	1.60797200	1.69796100
H	2.48454700	0.02510500	1.91714500
C	-1.25582400	0.35310300	-0.15686300
C	-2.42486000	-0.29517900	0.21536700
C	-3.70595400	0.29053900	0.17758400
C	-3.88442900	1.67129400	-0.22726600
C	-4.86247200	-0.43988500	0.55167200
C	-5.19801100	2.25247000	-0.22560900
C	-6.09799300	0.14857300	0.52950400
H	-4.74948500	-1.47891600	0.85854300
C	-6.27588700	1.51022800	0.13898400
H	-5.30398000	3.29302400	-0.52984900
H	-6.97228400	-0.43195500	0.81908100
H	-7.27422700	1.94033000	0.13727700
H	-2.38115400	-1.31403400	0.59499000
C	-2.77241400	2.37618800	-0.58743200
C	-1.44550900	1.75417800	-0.65235200
H	-2.86238400	3.42610900	-0.87236400
H	-1.16799500	1.73963500	-1.73035800
H	-0.67978400	2.44766200	-0.26663800

TS2S

M06/BS1 SCF energy in gas pahse: -1255.528966 a.u.

M06/BS2 SCF energy in MeOH: -1255.902359 a.u.

M06/BS2 Free energy in MeOH: -1255.447487 a.u.

Ru	0.62964100	-0.52068500	-0.09330200
C	1.41407000	-2.37513100	-1.19209500
C	2.27248000	-2.07864700	-0.08728400
C	1.48462900	-2.22278600	1.10532200
C	0.09578700	-2.63231200	-0.69417700
C	0.14079800	-2.55964700	0.74051500
C	1.98678100	-2.24008000	2.50964900
H	3.00839800	-1.85480000	2.59797900
H	2.00455100	-3.27685700	2.87574000
H	1.34498100	-1.67319400	3.19740800
C	3.73539900	-1.80090400	-0.17554900

H	3.96895900	-1.15809600	-1.03432700
H	4.31628800	-2.72740900	-0.28937100
H	4.10599500	-1.28713300	0.71961700
C	1.86745900	-2.51113600	-2.60405600
H	1.04754600	-2.40786600	-3.32447600
H	2.30249300	-3.50994600	-2.75228800
H	2.64444000	-1.78075700	-2.86022200
C	-1.07447200	-3.05292700	-1.51849100
H	-2.02711300	-2.76776900	-1.05505300
H	-1.09005400	-4.14388800	-1.65133500
H	-1.05121800	-2.60357500	-2.51990900
C	-0.90720900	-3.00517400	1.70705500
H	-0.60173900	-3.93874700	2.20158300
H	-1.86375200	-3.21428000	1.21286800
H	-1.08594300	-2.26697800	2.50162400
C	2.28101900	2.15415600	-0.51430000
C	2.87958000	3.27156900	-1.10906300
C	3.60187400	4.14981200	-0.31483100
C	3.72916100	3.91547600	1.05571000
C	3.12337700	2.81122100	1.64697300
C	2.37969900	1.93257700	0.86317500
H	2.79387500	3.42715500	-2.18304900
H	4.08338400	5.01551100	-0.76446100
H	4.30740000	4.60400900	1.66870900
H	3.21761100	2.63859700	2.71880000
C	1.57250000	1.13305800	-1.22461500
C	1.02543300	0.38289000	-2.06225900
H	0.74294900	0.01381000	-3.03511100
C	1.65371500	0.76265800	1.42218500
C	0.26220100	0.79085900	1.63754000
H	-0.18639300	0.19639100	2.43775000
H	-0.28832600	1.70077700	1.39100300
H	2.25490500	0.12899200	2.07675000
C	-1.32576900	0.28824500	-0.38279700
C	-2.47657900	-0.28144200	0.23118100
C	-3.74559800	0.29492300	0.22906800
C	-3.95813100	1.55836600	-0.42963600
C	-4.84786400	-0.33205000	0.88252000
C	-5.25768700	2.13893300	-0.41256100
C	-6.07775400	0.25705800	0.87988600
H	-4.68488600	-1.28748400	1.38014000
C	-6.28441900	1.50557200	0.22619800
H	-5.41180700	3.09410900	-0.91232900
H	-6.91460700	-0.22504900	1.38063300
H	-7.27521000	1.95442600	0.24178700
H	-2.35437300	-1.20588700	0.79439900
C	-2.87412600	2.16934400	-1.05456600
C	-1.61140200	1.56224500	-1.05962500
H	-3.00486300	3.13442500	-1.54328900
H	-1.61879000	0.34713200	-1.62306900
H	-0.77861500	2.06413500	-1.54966100

2cat-Z

M06/BS1 SCF energy in gas pahse: -1041.993143 a.u.

M06/BS2 SCF energy in MeOH: -1042.316271 a.u.

M06/BS2 Free energy in MeOH: -1041.930102 a.u.

Ru	0.50456300	0.02589800	0.03673900
C	1.52800200	-1.67267600	1.12604000
C	0.92903800	-2.16152300	-0.07259200
C	1.57911300	-1.50186200	-1.18486300
C	2.47737000	-0.65542300	0.77717500
C	2.52523400	-0.57184700	-0.66749400
C	1.40469000	-1.84170700	-2.62530600
H	0.36110200	-2.03835200	-2.89895400
H	1.97036800	-2.75490100	-2.85816100
H	1.78342800	-1.05142700	-3.28339900
C	-0.04799400	-3.28831300	-0.13519600
H	-0.90607200	-3.11234700	0.52770500
H	0.42406700	-4.23071900	0.17624400
H	-0.43617300	-3.44280900	-1.14826500
C	1.21391800	-2.18892100	2.48605100
H	1.57554400	-1.52930400	3.28216400
H	1.69248000	-3.16844700	2.62804000
H	0.13465600	-2.32914400	2.62597600
C	3.37042500	0.08219100	1.71677700
H	3.56466000	1.10471000	1.37058000
H	4.34218600	-0.42169500	1.81342800
H	2.94048900	0.15274600	2.72290500
C	3.44736200	0.27852400	-1.47350400
H	4.30176100	-0.30715000	-1.84066600
H	3.85122200	1.10915200	-0.88374400
H	2.93925400	0.70867900	-2.34596400
C	-2.59481900	0.18505300	0.83566900
C	-3.77818400	0.39472500	1.55242700
C	-4.99413400	0.15882800	0.92658100
C	-5.03079100	-0.28143000	-0.39704800
C	-3.85255600	-0.47964600	-1.11037600
C	-2.62659500	-0.23716100	-0.49624400
H	-3.73555900	0.72484000	2.58855800
H	-5.92224700	0.30968700	1.47346400
H	-5.98947100	-0.46794700	-0.87690100
H	-3.88465300	-0.81503500	-2.14684900
C	-1.28329900	0.35712800	1.38450500
C	-0.26366600	0.53570700	2.07328500
H	0.37485800	0.76239300	2.90901700
C	-1.33129600	-0.37221700	-1.21268300
C	-0.67592000	0.72384500	-1.79051300
H	0.00079900	0.51179700	-2.62318400
H	-1.16673400	-1.35075400	-1.66872400
C	1.27112400	3.16984800	0.20235600
C	1.62463700	4.57153200	0.30178700
H	0.90048900	5.18090800	-0.25100400
H	2.62092400	4.74519200	-0.11976300
H	1.62461000	4.89267600	1.34914700
N	0.97582900	2.05419700	0.10709700
C	-1.25061400	2.10933500	-1.79219800
H	-1.73137300	2.36840800	-0.84149400

H	-2.01797700	2.17986400	-2.57785100
H	-0.49047600	2.86612600	-2.01629300

IM1-Z

M06/BS1 SCF energy in gas pahse: -1334.089146 a.u.

M06/BS2 SCF energy in MeOH: -1334.489936 a.u.

M06/BS2 Free energy in MeOH: -1333.983624 a.u.

Ru	0.47923500	0.32918400	0.22533800
C	-0.79529000	1.46802500	-1.30801700
C	-0.06512400	2.39658900	-0.49294300
C	1.32812900	2.20796100	-0.76601500
C	0.14272400	0.64160600	-1.99997400
C	1.46792800	1.11031200	-1.66575900
C	2.44681800	3.05329700	-0.27227200
H	2.18020300	3.61219200	0.63120800
H	2.71620400	3.78587400	-1.04666500
H	3.34584400	2.46453100	-0.05223800
C	-0.67891000	3.47176100	0.33684000
H	-1.60934700	3.12912700	0.80712700
H	-0.92635600	4.34974600	-0.27665300
H	-0.00611900	3.81033100	1.13402800
C	-2.27122900	1.50927700	-1.49306400
H	-2.67001700	0.60545500	-1.96526700
H	-2.51745700	2.36459500	-2.13956700
H	-2.80028000	1.65987500	-0.54361200
C	-0.16871900	-0.32700300	-3.08923000
H	0.47712300	-1.21422000	-3.06290900
H	-0.00882000	0.14980300	-4.06745100
H	-1.20945100	-0.66723300	-3.05554200
C	2.73238600	0.70751500	-2.34271700
H	2.91404700	1.36486800	-3.20576100
H	2.69346100	-0.32051100	-2.72075300
H	3.60404900	0.78637500	-1.68113100
C	-1.55651400	-0.37027500	0.84236800
C	-1.09530800	0.38491500	1.73526200
C	2.36497400	0.41210400	1.51196100
C	1.50969000	1.10730800	2.08318300
H	-1.13624800	0.88519500	2.69013200
H	1.07391300	1.76386100	2.81542200
C	-2.57133100	-1.15727300	0.18649000
C	-3.91715100	-0.97552300	0.59169300
C	-2.27989900	-2.02161000	-0.87629200
C	-4.91331000	-1.67869300	-0.09259400
C	-3.28710500	-2.70633700	-1.54032200
H	-1.24725800	-2.14246700	-1.20061900
C	-4.61091600	-2.53037900	-1.14766100
H	-5.94557400	-1.56508900	0.23489600
H	-3.03962700	-3.37731900	-2.36038700
H	-5.40947000	-3.06533000	-1.65762700
C	3.45361200	-0.36363400	0.99922500
C	3.10037000	-1.35931200	0.07412500
C	4.79073400	-0.13163000	1.33013800
C	4.10355400	-2.09688900	-0.54483200
C	5.78192200	-0.88039200	0.70511200
H	5.04473800	0.64342300	2.05112100
C	5.43933500	-1.85351300	-0.23161000
H	3.84078200	-2.86258900	-1.27483100
H	6.82750000	-0.69511100	0.94052400
H	6.22130100	-2.42656900	-0.72537400
C	1.66112300	-1.57817000	-0.18883500
C	0.74472300	-1.90333400	0.81728000
H	1.40836700	-1.88803000	-1.20711900
H	-0.17330800	-2.37813100	0.47548400
C	1.03633900	-2.19255400	2.25533300
H	0.96445600	-3.27836400	2.40952900
H	0.28496200	-1.73104700	2.91064900
H	2.02777000	-1.87371100	2.58802900
C	-4.25641100	-0.08565600	1.71101500
C	-5.20963000	0.85679200	1.71214000
H	-3.66805700	-0.21964300	2.62143800
H	-5.35529000	1.40814700	2.64340500
C	-6.09006200	1.26515100	0.57970000
H	-5.78324000	0.82494600	-0.37660500
H	-6.09583800	2.35793000	0.47052500
H	-7.13404700	0.97238400	0.76337900

IM2-Z

M06/BS1 SCF energy in gas pahse: -1334.118629 a.u.

M06/BS2 SCF energy in MeOH: -1334.508927 a.u.

M06/BS2 Free energy in MeOH: -1333.997027 a.u.

Ru	-0.49210500	0.43149500	-0.08586000
C	0.16251400	2.59543400	-0.61537400
C	-0.44407700	1.92229100	-1.75036900
C	-1.82394300	1.68367600	-1.45598500
C	-0.81492200	2.69668600	0.39471300
C	-2.05068300	2.12280900	-0.12554900
C	-2.84581300	1.13428800	-2.39093900
H	-2.40731600	0.42322900	-3.10182200
H	-3.31017800	1.94180400	-2.97526700
H	-3.64727300	0.61290200	-1.85355000
C	0.19044600	1.72533800	-3.08481000
H	1.28502800	1.71996600	-3.02488200
H	-0.09278600	2.54616700	-3.75993900
H	-0.13448400	0.78973900	-3.55738200
C	1.55063000	3.14107500	-0.61185600
H	1.86777600	3.45978100	0.38740600
H	1.61885800	4.01679500	-1.27275300
H	2.28526800	2.40669600	-0.97000900
C	-0.69617500	3.38416300	1.71314000
H	-1.05641800	2.76385200	2.54570000
H	-1.29280100	4.30756000	1.72564100
H	0.33936300	3.66589600	1.93469300
C	-3.39168700	2.22008400	0.52123100
H	-3.98140700	3.00937700	0.03383300
H	-3.31972700	2.48513400	1.58287900
H	-3.96641500	1.28759900	0.43779200

C	1.29495100	-0.34972500	0.04483600
C	0.90995700	-0.87685400	-1.20022400
C	-1.18721600	-1.38917600	-0.73333200
C	-0.15979600	-1.87333200	-1.43835400
H	1.51928600	-0.51938500	-2.04561600
H	-0.03440000	-2.77619800	-2.04103900
C	2.54097100	-0.19305000	0.70345700
C	3.66361700	-1.00831100	0.36307900
C	2.67027300	0.80448200	1.69568500
C	4.87360200	-0.74926100	1.01449800
C	3.87866000	1.04128800	2.31581500
H	1.78470200	1.39189400	1.93924200
C	4.98321000	0.25857300	1.96460800
H	5.73214400	-1.38280600	0.80099900
H	3.97359400	1.81578700	3.07318200
H	5.93964200	0.42269100	2.45794500
C	-2.47837700	-1.84291000	-0.24839300
C	-2.82680500	-1.26368100	0.98369700
C	-3.32728800	-2.76925500	-0.85210400
C	-4.03345500	-1.59086700	1.59161300
C	-4.53219700	-3.09652600	-0.23546300
H	-3.05388600	-3.21276400	-1.80909400
C	-4.88544400	-2.50895800	0.97697200
H	-4.30844000	-1.13619400	2.54372000
H	-5.20740700	-3.80602500	-0.70945700
H	-5.83367600	-2.76251000	1.44644500
C	-1.85186700	-0.30688500	1.57220700
C	-0.56755500	-0.64309200	2.02004500
H	-2.28254100	0.59335000	2.01655800
H	-0.08759400	0.08797800	2.67544600
C	-0.04568600	-2.04295500	2.15141100
H	-0.40576500	-2.45482700	3.10575600
H	1.05042300	-2.07352100	2.18142600
H	-0.39275900	-2.70565800	1.35290600
C	3.53875300	-2.12706300	-0.57385300
C	4.41454600	-2.47755100	-1.52991100
H	2.64014000	-2.73802700	-0.46445500
H	4.16832000	-3.37288000	-2.10432500
C	5.66453800	-1.78114600	-1.94246700
H	6.55312400	-2.35569500	-1.64193300
H	5.75611300	-0.77269000	-1.52400800
H	5.71204200	-1.70234900	-3.03633700

TS2-Z

M06/BS1 SCF energy in gas pahse: -1334.112504 a.u.

M06/BS2 SCF energy in MeOH: -1334.503312 a.u.

M06/BS2 Free energy in MeOH: -1333.989062 a.u.

Ru	0.53628000	0.44703000	0.18145200
C	-0.10349900	2.54512200	0.81455700
C	0.57721000	2.72361800	-0.40982000
C	1.92463700	2.22690500	-0.23929500
C	0.82917600	1.94317400	1.76091800
C	2.09404900	1.79910500	1.10948400
C	3.01358500	2.34207500	-1.24817900
H	2.62631700	2.37698600	-2.27378600
H	3.57240100	3.27492500	-1.08464900
H	3.73406600	1.51732500	-1.17857800
C	0.07652900	3.36872700	-1.65772700
H	-0.98627600	3.62679800	-1.58796000
H	0.62356300	4.30051800	-1.86070400
H	0.21147200	2.72465800	-2.54012600
C	-1.50539900	2.94092600	1.13516000
H	-1.97489500	2.23620800	1.83338700
H	-1.53339100	3.93256400	1.60796500
H	-2.13845700	2.97638200	0.24054300
C	0.55596600	1.66287200	3.19938600
H	1.13736100	0.80610600	3.55981400
H	0.82375700	2.53092000	3.81877700
H	-0.50319300	1.44550500	3.38158700
C	3.36856600	1.31846500	1.71443200
H	4.00304500	2.16978600	1.99902500
H	3.19352600	0.72074200	2.61649700
H	3.94366700	0.69718700	1.01509800
C	1.51483500	-0.46866200	-1.45538600
C	0.11958000	-0.93451800	-1.58686900
H	-0.41641600	-0.37888000	-2.36119600
C	-1.19479100	-0.49877300	-0.13837900
C	-0.92689000	-1.01470900	1.14350400
H	1.78517900	0.27280700	-2.21564200
C	2.63154800	-1.33631600	-1.00323700
C	2.52634800	-1.79568200	0.32434300
C	3.73126800	-1.68605900	-1.77867800
C	3.49667500	-2.63722800	0.85913300
C	4.71650000	-2.50739300	-1.22959700
H	3.82211600	-1.32275500	-2.80289100
C	4.59721000	-2.98143900	0.07514800
H	3.41060200	-2.99430100	1.88447800
H	5.58646200	-2.77780000	-1.82449900
H	5.37698700	-3.61624000	0.49103000
C	1.28864900	-1.30805400	0.90443200
C	0.23463700	-1.81647700	1.56011700
H	0.14060900	-2.69367000	2.20666500
C	-2.48572500	-0.19219100	-0.71711900
C	-2.59806100	0.88607400	-1.61148000
C	-3.63721100	-0.95949900	-0.39442800
C	-3.81408900	1.24298800	-2.16341300
H	-1.69680400	1.45020500	-1.85170000
C	-4.85599600	-0.58064700	-0.97284100
C	-4.95017500	0.50180000	-1.83553100
H	-3.88228300	2.08298700	-2.85130700
H	-5.73840300	-1.18377700	-0.76884400
H	-5.91262500	0.75731500	-2.27445200
H	-1.73013000	-0.80322400	1.86163300
C	-0.16939200	-2.42354700	-1.64889600
H	0.12213800	-2.96355700	-0.74388900
H	0.40769400	-2.84367400	-2.48368600
H	-1.23219100	-2.60579200	-1.84530600

C	-3.56835700	-2.15240500	0.45896900
C	-4.44355700	-2.51234600	1.41089400
H	-2.71790600	-2.81565800	0.28383400
H	-4.25419600	-3.46610000	1.90767800
C	-5.63148600	-1.76002700	1.90546100
H	-5.63713300	-0.71137700	1.58668000
H	-5.66972300	-1.78526200	3.00205700
H	-6.56730400	-2.22243600	1.55820300

IM3-Z

M06/BS1 SCF energy in gas pahse: -1334.152065 a.u.

M06/BS2 SCF energy in MeOH: -1334.543954 a.u.

M06/BS2 Free energy in MeOH: -1334.025512 a.u.

Ru	0.53747900	0.55137300	0.28193800
C	-0.66803000	2.45264000	-0.25786400
C	0.08715100	2.66328200	0.93118900
C	1.49369800	2.53503300	0.61326600
C	0.25493600	2.13792600	-1.30702600
C	1.59907600	2.20810000	-0.76770000
C	2.63096800	2.75436400	1.55231900
H	2.36637300	2.50162300	2.58638400
H	2.94444100	3.80771800	1.54343400
H	3.50114800	2.14640000	1.27670300
C	-0.46573400	2.98749200	2.27772100
H	-1.46996900	2.56870700	2.41815200
H	-0.54256400	4.07499700	2.41729700
H	0.17124100	2.60008700	3.08228200
C	-2.15295300	2.52405800	-0.37359000
H	-2.53726300	1.85623000	-1.15453100
H	-2.47638400	3.54603500	-0.61593100
H	-2.64370400	2.23973400	0.56664100
C	-0.06668500	2.01869100	-2.75738700
H	0.49261700	1.21275900	-3.25078800
H	0.20141300	2.95122000	-3.27483700
H	-1.13477700	1.84549900	-2.92836800
C	2.85351500	2.10491300	-1.56479600
H	3.09406600	3.07537700	-2.02237200
H	2.76215800	1.37667600	-2.38037900
H	3.71155300	1.80981600	-0.94891200
C	-0.86514800	-1.19241900	-0.08147300
C	-0.77002300	-0.89690400	1.30691900
C	1.60503600	-0.71891500	1.24192700
C	0.45636700	-0.75446400	2.04564600
H	-1.68000300	-0.58786700	1.82461300
H	0.41573500	-0.49148400	3.10583800
C	-2.19281500	-1.04881200	-0.74230600
C	-3.42518700	-1.30723800	-0.09728300
C	-2.21382000	-0.62889800	-2.07970600
C	-4.61100600	-1.08431800	-0.81183000
C	-3.39756800	-0.40708400	-2.76676600
H	-1.26786900	-0.43484100	-2.58404000
C	-4.61056500	-0.62488100	-2.12032000
H	-5.55462900	-1.32597000	-0.32525400
H	-3.37229500	-0.07158000	-3.80215000
H	-5.55225100	-0.46768700	-2.64214900
C	2.81458800	-1.30352000	0.78405700
C	2.73133700	-1.30253000	-0.62969800
C	3.90161600	-1.87432200	1.45846300
C	3.80765200	-1.77466000	-1.37512500
C	4.96320400	-2.33620400	0.69707700
H	3.93429300	-1.90320500	2.54562100
C	4.92065100	-2.27232400	-0.70303500
H	3.76981700	-1.77386200	-2.46435500
H	5.84452100	-2.74319200	1.18754800
H	5.77072200	-2.63943100	-1.27502600
C	1.38218200	-0.91528700	-1.10843600
C	0.22313600	-1.92930600	-0.88728900
H	1.37449300	-0.52437600	-2.13402500
H	-0.21262400	-2.14517400	-1.87192700
C	0.56737100	-3.27801000	-0.26887400
H	1.33876600	-3.78901300	-0.85987400
H	-0.33249200	-3.90773500	-0.25928100
H	0.92855700	-3.21023400	0.76401700
C	-3.51866300	-1.91546000	1.24277100
C	-4.34563100	-1.55242300	2.23324000
H	-2.85713300	-2.76883300	1.42006000
H	-4.32935100	-2.16368500	3.13793500
C	-5.27411800	-0.38486100	2.26037600
H	-6.32395200	-0.70405400	2.18527900
H	-5.08291200	0.32476700	1.44596500
H	-5.18803800	0.15221300	3.21436200

TS3-Z

M06/BS1 SCF energy in gas pahse: -1334.14199 a.u.

M06/BS2 SCF energy in MeOH: -1334.533821 a.u.

M06/BS2 Free energy in MeOH: -1334.018195 a.u.

Ru	-0.48760200	0.68788300	-0.18670200
C	0.90572800	2.29367700	0.65500800
C	-0.20352200	2.07870300	1.53453500
C	-1.42029000	2.40274000	0.81624600
C	0.39032300	2.67521000	-0.61796900
C	-1.04737600	2.78160500	-0.51062500
C	-2.79107100	2.42811200	1.40216500
H	-2.93826100	1.61950200	2.12938100
H	-2.97408000	3.37608000	1.92809200
H	-3.56592000	2.32377100	0.63349500
C	-0.13032300	1.75641100	2.98833700
H	0.77468400	1.19161600	3.24108200
H	-0.11746800	2.67973700	3.58493400
H	-0.99752600	1.17431000	3.32522100
C	2.35364000	2.13162200	0.96838600
H	2.84472200	1.43158600	0.27596100
H	2.86964700	3.09803100	0.88394900
H	2.51887600	1.74953500	1.98068300
C	1.20830000	2.96796000	-1.82991600
H	0.66765500	2.72216500	-2.75288100

H	1.47738900	4.03260600	-1.88052800
H	2.14240300	2.39091700	-1.82724200
C	-1.96703700	3.22531400	-1.59670600
H	-2.07215600	4.31935100	-1.59371600
H	-1.59417700	2.93631600	-2.58739000
H	-2.96875400	2.79458000	-1.47951500
C	-1.50991500	-1.12055000	0.86392100
C	-0.34577700	-2.09534900	0.68182000
H	0.02562800	-2.38572000	1.67380500
C	0.76261300	-1.27888000	-0.01201200
C	0.59130500	-0.84673300	-1.34782800
H	-1.43533600	-0.59376300	1.82371500
C	-2.92516000	-1.47037300	0.49406700
C	-3.11018200	-1.00347300	-0.80698500
C	-3.92916200	-2.17277900	1.14379500
C	-4.28223100	-1.21803300	-1.52338900
C	-5.12856300	-2.35763800	0.45420500
H	-3.79789300	-2.56100500	2.15299800
C	-5.30219600	-1.88689500	-0.85207700
H	-4.41429200	-0.86739300	-2.54462300
H	-5.94916600	-2.88130600	0.94054700
H	-6.25338900	-2.05297800	-1.35337200
C	-1.77485600	-0.49874500	-1.03765300
C	-0.69779800	-0.63732500	-1.93398100
H	-0.79026900	-0.41236700	-2.99948600
H	1.46405500	-0.56882500	-1.93891500
C	2.10560600	-1.29363700	0.61957300
C	2.16901600	-1.10519900	2.00947200
C	3.31682100	-1.46892700	-0.09263100
C	3.37283000	-1.04331100	2.69318300
H	1.24181700	-0.96962000	2.56755500
C	4.52364600	-1.40658900	0.61941300
C	4.56410100	-1.18322900	1.98764200
H	3.38110400	-0.89034700	3.77075100
H	5.44932500	-1.58507800	0.07442400
H	5.52054900	-1.14740300	2.50503500
C	-0.64653200	-3.38410100	-0.07064100
H	0.27275400	-3.97552600	-0.17592600
H	-1.37766600	-3.98809100	0.48169800
H	-1.04889300	-3.20700100	-1.07513600
C	3.36828100	-1.83377000	-1.52095000
C	4.16914900	-1.30141600	-2.45470000
H	2.70073400	-2.64549700	-1.82558400
H	4.12389800	-1.74219100	-3.45267100
C	5.10635700	-0.15113800	-2.29952400
H	6.15483800	-0.48187300	-2.32973300
H	4.95724700	0.39087400	-1.35761700
H	4.98806500	0.55857500	-3.12923100

IM4-Z

M06/BS1 SCF energy in gas pahse: -1334.165891 a.u.

M06/BS2 SCF energy in MeOH: -1334.560722 a.u.

M06/BS2 Free energy in MeOH: -1334.045163 a.u.

Ru	-0.46298800	0.70987900	-0.01755100
C	0.95851600	2.34482400	0.36058600
C	0.04679200	2.24442000	1.45574400
C	-1.29357900	2.49304700	0.94483400
C	0.19028500	2.60264900	-0.83071800
C	-1.19892900	2.73562700	-0.45516100
C	-2.54376500	2.50046200	1.75705000
H	-2.47331900	1.81990200	2.61478400
H	-2.75010600	3.50433100	2.15459900
H	-3.41321200	2.19278200	1.16221200
C	0.40722400	2.03471400	2.88727300
H	1.34647100	1.47720800	2.98927000
H	0.53592800	2.99845000	3.40040800
H	-0.37038900	1.47970500	3.42714800
C	2.43933300	2.19843300	0.42500300
H	2.84416300	1.75883300	-0.49599000
H	2.91522100	3.18038400	0.55867300
H	2.75284600	1.55813600	1.25874000
C	0.74228200	2.82126100	-2.19786700
H	0.03833800	2.50177700	-2.97634400
H	0.95135400	3.88744600	-2.36508100
H	1.68287500	2.27797200	-2.35226700
C	-2.32149900	3.05214600	-1.38229900
H	-2.42160100	4.13841900	-1.51751000
H	-2.16204100	2.61274300	-2.37544100
H	-3.27974400	2.67734100	-1.00297900
C	-1.53836000	-1.37012300	0.48229200
C	-0.28497700	-2.21991100	0.57959900
H	-0.04933700	-2.40288400	1.63657700
C	0.80430800	-1.29529000	-0.00867300
C	0.58979300	-0.75194200	-1.28748500
H	-1.39401000	-0.52883200	1.25920400
C	-3.02968100	-1.72676100	0.43194800
C	-3.22490000	-1.09237900	-0.80348000
C	-4.04844000	-2.35752400	1.11097900
C	-4.46199800	-1.02434400	-1.41940300
C	-5.30793200	-2.29202000	0.49489500
H	-3.91255000	-2.87390000	2.05882600
C	-5.50868200	-1.64242400	-0.72600900
H	-4.62762200	-0.54738100	-2.38314700
H	-6.15967700	-2.76115700	0.98375400
H	-6.50940900	-1.62784300	-1.15302100
C	-1.78610000	-0.81215600	-0.91705800
C	-0.74357200	-0.60603700	-1.81247800
H	-0.90955100	-0.25811400	-2.83105200
H	1.42667400	-0.38144400	-1.87780100
C	2.14185400	-1.31531200	0.62406100
C	2.20283800	-1.13989900	2.01524600
C	3.34816800	-1.46023300	-0.09921100
C	3.41058900	-1.07236100	2.69269900
H	1.27315000	-1.01541900	2.57317800
C	4.55797400	-1.40199200	0.60693300
C	4.59948900	-1.19913600	1.97880700
H	3.42489100	-0.92883600	3.77143000

H	5.48436000	-1.56223500	0.05756600
H	5.55742400	-1.16372100	2.49363600
C	-0.34100200	-3.55507800	-0.14558700
H	0.63153300	-4.06187500	-0.08979000
H	-1.09032200	-4.21444900	0.31153200
H	-0.59960100	-3.43101500	-1.20531100
C	3.37133100	-1.76527800	-1.54074300
C	4.15736900	-1.20076900	-2.46838800
H	2.67853500	-2.54628900	-1.86855800
H	4.07856300	-1.59246800	-3.48467500
C	5.11830100	-0.07402700	-2.28668700
H	6.15906000	-0.41670800	-2.38029200
H	5.01726000	0.41543600	-1.31044400
H	4.97712100	0.68352300	-3.06980800

TS8-Z

M06/BS1 SCF energy in gas pahse: -1334.061913 a.u.

M06/BS2 SCF energy in MeOH: -1334.459987 a.u.

M06/BS2 Free energy in MeOH: -1333.960668 a.u.

Ru	0.89745500	-0.55016100	0.01187500
C	2.35599400	-2.22336800	-0.41506900
C	2.55994000	-1.80281700	0.92569900
C	1.32135600	-2.00490900	1.65358400
C	0.99990700	-2.70050300	-0.53707900
C	0.38654500	-2.60840400	0.76079100
C	1.11293400	-1.78637000	3.11429300
H	1.67598200	-0.92241700	3.48873300
H	1.44087000	-2.66043000	3.69476000
H	0.05530300	-1.61385300	3.34819500
C	3.87217700	-1.38674400	1.50082000
H	4.37751500	-0.63121200	0.88504100
H	4.54262800	-2.25508500	1.56648000
H	3.77136000	-0.98323800	2.51484000
C	3.39112700	-2.22195100	-1.48523700
H	2.95074800	-2.12905400	-2.48445500
H	3.96687800	-3.15808500	-1.46401900
H	4.10020300	-1.39424100	-1.35892600
C	0.39450900	-3.33897000	-1.74196700
H	-0.67710600	-3.11439500	-1.82486900
H	0.49948900	-4.43234000	-1.70414700
H	0.87616400	-2.99855100	-2.66609800
C	-0.96303800	-3.12499700	1.12723700
H	-0.87587300	-4.14777200	1.52042700
H	-1.63857500	-3.16535000	0.26437100
H	-1.44310300	-2.51651900	1.90320600
C	2.67434300	1.79020000	-1.13599200
C	3.44837800	2.56847300	-2.00189700
C	4.38688600	3.44366400	-1.47086500
C	4.54806200	3.54489500	-0.08955100
C	3.76322800	2.78351200	0.77291500
C	2.81077300	1.91049500	0.25537100
H	3.32539800	2.46552800	-3.07838700
H	5.00614300	4.04202800	-2.13547400
H	5.29243500	4.22537600	0.31899100
H	3.88552600	2.87332700	1.85226200
C	1.72281000	0.81380200	-1.57664500
C	0.93087400	0.04308200	-2.15010500
H	0.35670500	-0.42882300	-2.92946900
C	1.90411500	1.11273200	1.11870200
C	0.52381200	1.35924900	1.21768500
H	0.03739700	1.00105900	2.12975000
H	2.38254400	0.66595400	1.99301800
C	-1.06662800	-0.29140800	-0.22278400
C	-2.32259700	-0.30091900	-0.34910000
C	-3.74638400	-0.33801700	-0.46836500
C	-4.32855500	-1.32354400	-1.28028300
C	-4.54459000	0.60946100	0.21750800
C	-5.70553900	-1.39207000	-1.41139800
C	-5.93021800	0.51648400	0.06154600
C	-6.50148400	-0.46593300	-0.73919000
H	-6.15927400	-2.16028700	-2.03284100
H	-6.56943500	1.20562400	0.61002300
H	-7.58462600	-0.51700600	-0.83137500
H	-1.56594600	0.61565600	-0.92048200
C	-3.91947700	1.61317600	1.08490900
C	-4.24231300	2.91180300	1.17866500
H	-3.09755800	1.24554400	1.70583300
H	-3.67673700	3.50163700	1.90355600
H	-3.68244500	-2.02875800	-1.80184900
C	-0.15792700	2.52861000	0.56615600
H	0.05585400	3.43882800	1.14629800
H	0.18441200	2.71481100	-0.45826700
H	-1.24875600	2.41179700	0.54973900
C	-5.25710900	3.66386500	0.38856200
H	-5.60833200	3.10684000	-0.48730300
H	-6.13336800	3.91574000	1.00361500
H	-4.84192000	4.61927500	0.04280200

TS3S

M06/BS1 SCF energy in gas pahse: -732.0633426 a.u.

M06/BS2 SCF energy in THF: -732.2568692 a.u.

M06/BS2 Free energy in THF: -732.0211402 a.u.

C	-1.47406400	0.23289400	-0.30667800
C	-0.56976100	-0.61669700	-0.81281200
C	1.76480600	-0.63883600	0.01734600
C	0.86468100	-0.29589500	-0.91158200
H	-0.92036400	-1.56835900	-1.21725400
H	1.18752700	0.24472600	-1.80653600
C	-2.91475400	-0.04639800	-0.15995700
C	-3.83175300	1.01035200	-0.18302900
C	-3.39790600	-1.35022100	-0.00256400
C	-5.19464600	0.76693800	-0.07385100
H	-3.45812600	2.02574500	-0.30213100
C	-4.76079700	-1.59272100	0.10053900
H	-2.69325000	-2.17846700	0.06310100
C	-5.66512900	-0.53492200	0.06418100

H	-5.89498400	1.60023800	-0.10030600
H	-5.11971100	-2.61314700	0.22464900
H	-6.73343500	-0.72505700	0.15197200
C	3.20235500	-0.36062800	-0.00023300
C	4.01429500	-0.93458400	0.98481800
C	3.81014900	0.46411000	-0.95670400
C	5.38446300	-0.70642100	1.01216400
C	5.17760300	0.69280200	-0.93184700
H	3.20203700	0.94253900	-1.72333200
C	5.97290200	0.10826300	0.05165800
H	5.99420600	-1.16652700	1.78808200
H	5.62828900	1.33954300	-1.68312500
H	7.04556900	0.29269000	0.06995400
H	3.55467200	-1.57493100	1.73869900
O	-1.06656800	1.49536400	0.05215000
C	-1.00416500	1.69283500	1.44965700
H	-0.25404000	1.02464300	1.89989200
H	-0.70745700	2.73282800	1.61385400
H	-1.97896400	1.51302300	1.92919700
H	1.41089900	-1.19764000	0.88944500

TS4S

M06/BS1 SCF energy in gas pahse: -2350.556509 a.u.

M06/BS2 SCF energy in toluene: -2351.14457 a.u.

M06/BS2 Free energy in toluene: -2350.553775 a.u.

Ru	-0.37593100	0.86932000	0.42504900
B	-1.95397200	3.32570100	-0.86738400
H	-2.54349600	4.24171900	-1.37356200
N	-2.92921900	2.39884200	-0.11648000
C	-4.26253100	2.51104800	0.04351000
C	-3.54063100	0.74967500	1.13291300
C	-4.70058700	1.47106900	0.84056600
H	-4.79795400	3.33109600	-0.42039000
H	-3.43308500	-0.16089900	1.71195500
H	-5.71162500	1.26119400	1.16160800
N	-0.90252700	3.84253900	0.14296600
C	-0.60883000	5.09575600	0.53998800
C	0.65333300	3.66796500	1.63251300
C	0.38780700	5.03404500	1.49703500
H	-1.13331600	5.94022100	0.10877000
H	1.35684000	3.15647900	2.28249100
H	0.85507100	5.85761000	2.01969100
N	-1.21016800	2.50359300	-1.94467200
C	-1.08701700	2.73212200	-3.26622600
C	-0.23155100	1.78699900	-3.80172200
H	-1.61581200	3.55829900	-3.72656100
C	0.14308700	0.99664400	-2.71219700
H	0.07888300	1.68477900	-4.83268100
H	0.79668700	0.13092900	-2.67221600
N	-0.12803900	2.96148000	0.81107700
N	-2.47711200	1.31172100	0.55408300
N	-0.45922200	1.43062100	-1.59892700
P	-0.79840000	-1.40144500	-0.09561200
C	-0.20039200	0.42413600	3.57364700
C	-0.14119500	0.20283900	5.00390300
H	-0.22686700	-0.87112600	5.21118700
H	0.80764200	0.56429400	5.41539800
H	-0.96085800	0.72728500	5.50751900
N	-0.27122100	0.54908000	2.42429300
C	-0.72541300	-2.61763500	1.28569000
C	-0.07890200	-3.85140200	1.17472200
C	-1.43497600	-2.33938900	2.46118000
C	-0.12071500	-4.77118400	2.22023400
H	0.45288500	-4.10985900	0.26088800
C	-1.48630800	-3.26067200	3.50032300
H	-1.97150900	-1.39623800	2.55722700
C	-0.82070500	-4.47894300	3.38449600
H	0.38710900	-5.72800100	2.11377200
H	-2.06064700	-3.03330500	4.39788600
H	-0.86050600	-5.20325100	4.19578800
C	0.32307300	-2.13246300	-1.35291700
C	-0.12104600	-2.47748400	-2.63188900
C	1.68316700	-2.27918800	-1.04824900
C	0.77923300	-2.93269500	-3.59267000
H	-1.17596000	-2.38581000	-2.88639800
C	2.57870400	-2.74200200	-2.00408700
H	2.04064000	-2.05236500	-0.04253500
C	2.12883500	-3.05902000	-3.28467000
H	0.41822300	-3.19533300	-4.58528300
H	3.63130100	-2.85606100	-1.74780200
H	2.82982700	-3.41922600	-4.03537100
C	-2.47499000	-1.70522500	-0.78774600
C	-3.23558000	-2.81140400	-0.39768100
C	-3.01045600	-0.81099300	-1.72395200
C	-4.51276300	-3.00701300	-0.91583100
H	-2.83578100	-3.52762400	0.31915900
C	-4.28264000	-1.01316000	-2.24427800
H	-2.43490800	0.05623200	-2.04567100
C	-5.04059500	-2.10706200	-1.83408800
H	-5.09522900	-3.87044500	-0.59948900
H	-4.68655500	-0.30590000	-2.96651400
H	-6.04091300	-2.25890300	-2.23536500
C	1.60745400	0.65881200	0.19315700
C	2.82561400	0.44732300	-0.06819800
C	4.18506500	0.28479400	-0.43840300
C	5.20387700	0.13626500	0.53789300
C	4.49790600	0.27025100	-1.81176300
C	6.51350500	-0.04216600	0.08165500
C	5.80454600	0.10345900	-2.23003600
H	3.69058200	0.39164500	-2.53277600
C	6.81010100	-0.05354200	-1.27371500
H	7.31097400	-0.19568000	0.80606100
H	6.04631100	0.09079300	-3.29007600
H	7.84090600	-0.19631800	-1.59262900
H	2.12421500	1.71844800	0.18111000
C	4.87973600	0.16269900	1.96443900
C	5.74406800	0.44307800	2.94293700

H	3.83845700	-0.04613400	2.21861600
H	5.43575000	0.43889800	3.98529600
H	6.78436500	0.70250000	2.75054500

TS5S

M06/BS1 SCF energy in gas pahse: -2217.843413 a.u.

M06/BS2 SCF energy in toluene: -2218.395251 a.u.

M06/BS2 Free energy in toluene: -2217.85211 a.u.

Ru	-0.28531800	0.77571500	0.45318400
B	-1.34805800	3.50696900	-0.73138400
H	-1.73645300	4.52256200	-1.23904800
N	-2.48611700	2.79176900	0.01878300
C	-3.76696200	3.15575400	0.21964000
C	-3.38175100	1.24991900	1.23933600
C	-4.38175400	2.19454900	1.00074000
H	-4.14358300	4.07981200	-0.20299500
H	-3.43204200	0.32258600	1.80117100
H	-5.40523200	2.17986500	1.34931700
N	-0.19542900	3.78051500	0.25667900
C	0.39954200	4.93437000	0.61625100
C	1.41223300	3.25283300	1.60426600
C	1.43495100	4.64543800	1.48602300
H	0.04067600	5.87830900	0.22309000
H	2.05670400	2.59178500	2.17448800
H	2.11226000	5.34165300	1.96137200
N	-0.80538400	2.53476100	-1.81940000
C	-0.68520200	2.71019300	-3.14915700
C	-0.06559800	1.59979500	-3.69408000
H	-1.04782100	3.62238500	-3.60779700
C	0.18044600	0.76122200	-2.60478200
H	0.18006800	1.42260900	-4.73224400
H	0.64139400	-0.22057900	-2.56114500
N	0.42304200	2.74310700	0.86604300
N	-2.24126900	1.61759300	0.64498600
N	-0.27961900	1.33313400	-1.48610400
P	-1.17365300	-1.34932400	0.11873000
C	2.83762000	0.02616600	-0.02699600
C	-1.25506600	-2.09349100	1.78487500
C	-1.37923500	-3.46455600	2.03304000
C	-1.13986900	-1.21422600	2.86879700
C	-1.40491800	-3.93895200	3.33989000
H	-1.44589000	-4.16462100	1.19910600
C	-1.15711600	-1.68805500	4.17647600
H	-1.05981700	-0.13103800	2.70012600
C	-1.29442300	-3.05297600	4.40950300
H	-1.50774800	-5.00628800	3.52559200
H	-1.06733800	-0.99395600	5.00947900
H	-1.31260100	-3.42949600	5.43023700
C	-0.15808200	-2.52241800	-0.85504400
C	-0.40586300	-2.72100500	-2.21555100
C	0.99508000	-3.08275800	-0.28517600
C	0.49024500	-3.44874500	-2.99484000
H	-1.30701300	-2.30800500	-2.67020000
C	1.89329700	-3.80074300	-1.06811700
H	1.17531200	-2.98544900	0.78800200
C	1.64465900	-3.97877900	-2.42711500
H	0.28042800	-3.60613700	-4.05124600
H	2.78190400	-4.23462800	-0.61264300
H	2.34237600	-4.54669800	-3.03930100
C	-2.85134800	-1.43884800	-0.59708600
C	-3.82253500	-2.31079200	-0.09865000
C	-3.18211500	-0.56882300	-1.64449300
C	-5.10472400	-2.31403400	-0.63880600
H	-3.58702900	-2.98041100	0.72757000
C	-4.46178100	-0.58149900	-2.18612800
H	-2.44318500	0.13601400	-2.02913500
C	-5.42508800	-1.45071400	-1.68109600
H	-5.85587200	-2.99303800	-0.23990800
H	-4.71077000	0.09837400	-2.99851700
H	-6.42994200	-1.45158100	-2.09894300
C	1.61398500	0.17949500	0.24614400
C	4.18597700	-0.24851900	-0.37950400
C	4.45400800	-0.65171500	-1.70097600
C	5.23573700	-0.08928400	0.55989600
C	5.75106400	-0.90988900	-2.10274900
H	3.62049200	-0.75012500	-2.39575400
C	6.53566800	-0.36177400	0.12271200
C	6.79000000	-0.76046200	-1.18194100
H	5.95993300	-1.22368500	-3.12265100
H	7.35975200	-0.28261200	0.82908100
H	7.81441200	-0.96816400	-1.48535500
C	4.95333000	0.33427900	1.93196800
C	5.83257300	0.90554000	2.75860100
H	3.93019500	0.17649200	2.27938800
H	5.55169800	1.18524100	3.77082700
H	6.85610000	1.13330400	2.46366300
H	1.87924100	-0.98603900	0.22808100

TS6S

M06/BS1 SCF energy in gas pahse: -2217.846676 a.u.

M06/BS2 SCF energy in toluene: -2218.398442 a.u.

M06/BS2 Free energy in toluene: -2217.855513 a.u.

Ru	-0.35866800	0.85164300	0.34823700
B	-2.05465400	3.22889500	-0.85235600
H	-2.68692700	4.10961500	-1.36687400
N	-2.94081000	2.37477700	0.07246200
C	-4.23633400	2.51459800	0.41332800
C	-3.37447000	0.81663200	1.50626700
C	-4.55928500	1.53544000	1.33438900
H	-4.83098600	3.30866400	-0.02265000
H	-3.18100700	-0.04794700	2.13271100
H	-5.51337200	1.36734100	1.81479900
N	-0.88278100	3.79948300	-0.02143200
C	-0.52040000	5.07248000	0.22809000
C	0.89134400	3.70644500	1.21202300
C	0.61398000	5.06274600	1.01929800

H	-1.09789000	5.89388000	-0.17936800
H	1.69489900	3.23298700	1.76837400
H	1.16112900	5.91427300	1.40012500
N	-1.44682800	2.29952200	-1.94110600
C	-1.51193100	2.38352800	-3.28370800
C	-0.75287900	1.36591700	-3.83378100
H	-2.09186000	3.17170700	-3.74864300
C	-0.23041700	0.67818300	-2.73613100
H	-0.59258500	1.15330500	-4.88196800
H	0.41308300	-0.19556900	-2.69330700
N	-0.01850400	2.95433200	0.58450000
N	-2.40333800	1.32763900	0.74291500
N	-0.66513700	1.24768100	-1.60471500
P	-0.84817500	-1.41397900	0.17750300
C	2.80959000	0.27627600	-0.18560700
C	-0.50880500	-2.10746100	1.83100700
C	-0.33759700	-3.47190100	2.08204600
C	-0.38984800	-1.19881300	2.88902900
C	-0.06424200	-3.91520400	3.37134100
H	-0.41217600	-4.18779700	1.26248500
C	-0.11008300	-1.63983000	4.17829900
H	-0.53637100	-0.12306600	2.71629900
C	0.05018200	-3.00147900	4.41681400
H	0.06449300	-4.97889300	3.56189800
H	-0.01860500	-0.92409300	4.99270000
H	0.26729900	-3.35307300	5.42347100
C	0.12293300	-2.46620900	-0.96141900
C	-0.41442500	-2.92700600	-2.16651600
C	1.46338600	-2.74149800	-0.66226500
C	0.37774300	-3.64121900	-3.06122000
H	-1.45984800	-2.73556000	-2.40709000
C	2.24820500	-3.46473900	-1.55238300
H	1.88839300	-2.41059900	0.28661300
C	1.70803100	-3.90928800	-2.75774300
H	-0.05259000	-4.00036900	-3.99416100
H	3.28457200	-3.68669000	-1.30095800
H	2.32229200	-4.47766800	-3.45354400
C	-2.59484600	-1.79131300	-0.20608900
C	-3.34744200	-2.68935600	0.55350800
C	-3.21000200	-1.10117400	-1.25980700
C	-4.69622700	-2.88765300	0.27144500
H	-2.88818100	-3.22612600	1.38277200
C	-4.55256100	-1.31246900	-1.54653400
H	-2.64049700	-0.38471500	-1.85542900
C	-5.29962900	-2.20001100	-0.77562400
H	-5.27686900	-3.58214500	0.87566100
H	-5.02159400	-0.77487000	-2.36845900
H	-6.35467400	-2.35560400	-0.99268700
C	1.58765900	0.53342300	0.00943200
C	4.18970100	0.04676600	-0.42371800
C	4.56509800	-0.62869400	-1.59963900
C	5.16759100	0.50205600	0.49746400
C	5.89997400	-0.87038900	-1.86833300
H	3.78427000	-0.95761500	-2.28461300
C	6.50692100	0.23751300	0.19935200
C	6.86748700	-0.43221400	-0.96209000
H	6.19220800	-1.39760000	-2.77331400
H	7.27658500	0.54113300	0.90648400
H	7.91989600	-0.62624500	-1.16093300
C	4.77509200	1.21516100	1.71448700
C	5.54241500	2.09294600	2.36535900
H	3.77078400	1.00680900	2.09023200
H	5.19586200	2.57949500	3.27372700
H	6.53537000	2.37311900	2.01545300
H	2.10850200	1.48963300	-0.47363000

TS7S

M06/BS1 SCF energy in gas pahse: -2217.874285 a.u.

M06/BS2 SCF energy in toluene: -2218.417837 a.u.

M06/BS2 Free energy in toluene: -2217.866073 a.u.

Ru	0.32876300	0.91078500	-0.27378900
B	3.12551800	2.42358900	0.05887100
H	4.16727700	2.98903900	0.24841000
N	3.28812700	1.31957400	-0.99531800
C	4.37314800	0.96643100	-1.70857800
C	2.66850000	-0.27364900	-2.30821100
C	4.02105500	-0.05587200	-2.57059500
H	5.31786000	1.47428500	-1.55273100
H	2.00496200	-1.01225800	-2.74464100
H	4.65131500	-0.56864000	-3.28407500
N	2.04169500	3.41492700	-0.41034400
C	2.12549100	4.74753800	-0.58429100
C	0.04654100	4.10578000	-0.85982900
C	0.86702900	5.23494800	-0.88137800
H	3.08005000	5.24972100	-0.48019600
H	-1.02562700	4.04631200	-1.00975000
H	0.58193800	6.25871900	-1.08111800
N	2.61523200	1.79308600	1.38424900
C	3.11831000	1.88720500	2.62913400
C	2.23642000	1.29374300	3.51559600
H	4.07068400	2.37808700	2.79085500
C	1.17949300	0.85046300	2.72009000
H	2.33869200	1.20084900	4.58801600
H	0.26885700	0.32544100	2.99113400
N	0.76133700	3.01085400	-0.58500600
N	2.22687900	0.55959800	-1.35902600
N	1.42665900	1.14772100	1.43812600
P	0.10425900	-1.42455700	0.10656800
C	-2.50656300	1.67836900	0.94425700
C	-0.97213300	-2.27831500	-1.10892900
C	-1.92234300	-3.23114700	-0.73357800
C	-0.80726100	-1.98819000	-2.47008900
C	-2.70533300	-3.86160700	-1.69788000
H	-2.05359100	-3.48726500	0.31648900
C	-1.57837500	-2.62737100	-3.43311600
H	-0.06449500	-1.25407800	-2.78757400
C	-2.53750300	-3.56141700	-3.04531900

H	-3.44471500	-4.59858400	-1.39054400
H	-1.43210400	-2.39639200	-4.48665400
H	-3.14679100	-4.06060700	-3.79608700
C	-0.57962700	-1.88815500	1.73819900
C	0.18810300	-2.55592900	2.69583500
C	-1.88456500	-1.49200600	2.06452300
C	-0.33194100	-2.80133100	3.96416100
H	1.19968700	-2.88115700	2.45762600
C	-2.40237300	-1.74599600	3.32805200
H	-2.50212500	-0.98391800	1.32356000
C	-1.62204400	-2.39363000	4.28418700
H	0.27643600	-3.31909400	4.70308800
H	-3.41908900	-1.43901100	3.56687300
H	-2.02545300	-2.58641300	5.27635200
C	1.68863300	-2.33487000	-0.01115800
C	1.79736300	-3.51569300	-0.75042900
C	2.82591100	-1.82193600	0.62746300
C	3.02698000	-4.15799700	-0.87002200
H	0.92383900	-3.93862100	-1.24513100
C	4.04776500	-2.47163700	0.51382700
H	2.76111800	-0.90257200	1.20872200
C	4.15300500	-3.63455900	-0.24573400
H	3.10030400	-5.07297900	-1.45463700
H	4.92479300	-2.06034000	1.01002800
H	5.11453400	-4.13439900	-0.34620200
C	-1.36332600	1.30741400	0.36042800
H	-2.43893300	1.85352600	2.02266600
C	-3.83387900	1.63569800	0.35087100
C	-4.94608500	2.08976200	1.06967900
C	-4.06209100	0.94828200	-0.88037200
C	-6.23431000	1.86639700	0.60752400
H	-4.78909200	2.60439500	2.01687500
C	-5.37958300	0.67300200	-1.29194400
C	-6.45859100	1.14618700	-0.57139400
H	-7.08102200	2.23060200	1.18618900
H	-5.53368700	0.11691300	-2.21631100
H	-7.47324200	0.95566800	-0.91244300
C	-2.93513700	0.49112500	-1.62898600
C	-1.75721500	1.22436200	-1.61167100
H	-2.99390200	-0.46218900	-2.16180100
H	-0.92234600	0.89026200	-2.25202600
H	-1.87351500	2.30785300	-1.56183400

TS8S

M06/BS1 SCF energy in gas pahse: -2217.883207 a.u.

M06/BS2 SCF energy in toluene: -2218.42813 a.u.

M06/BS2 Free energy in toluene: -2217.876053 a.u.

Ru	-0.13445200	-0.71718300	-0.41919500
B	-0.67061900	-3.55024400	0.91414900
H	-0.83995400	-4.60458600	1.46375000
N	-0.00004600	-2.54436400	1.88451800
C	0.32415500	-2.68796400	3.18445800
C	0.79398600	-0.63800700	2.54596100
C	0.83991700	-1.49183500	3.64976700
H	0.16055200	-3.63715100	3.68071900
H	1.10723300	0.39534900	2.44775300
H	1.19579000	-1.26719400	4.64595700
N	0.24164200	-3.71452700	-0.32067300
C	0.75668300	-4.82419800	-0.88561300
C	1.29255300	-3.07038900	-2.09335400
C	1.44315300	-4.45922200	-2.02887500
H	0.59423700	-5.79410700	-0.43035000
H	1.66757100	-2.36866300	-2.83248400
H	1.97394100	-5.10336100	-2.71654700
N	-2.01052300	-2.94839900	0.45220200
C	-3.25071300	-3.47323100	0.51220300
C	-4.12552800	-2.60544300	-0.11185500
H	-3.41314100	-4.43321900	0.98823900
C	-3.31803700	-1.54860300	-0.54166100
H	-5.19279000	-2.72099300	-0.24298300
H	-3.59819800	-0.64383800	-1.07118400
N	0.56719700	-2.63157600	-1.06118400
N	0.28292700	-1.28175500	1.48991400
N	-2.04429700	-1.75813600	-0.19615500
P	-1.09895900	1.35064000	-0.00155200
C	-0.13730600	2.90695000	0.03768900
C	-0.06512800	3.77027600	-1.05815800
C	0.62253900	3.18718100	1.17883300
C	0.77328500	4.88252900	-1.02156900
H	-0.66352100	3.57236600	-1.94816200
C	1.45767600	4.29644800	1.21457000
H	0.54357300	2.54137800	2.05525200
C	1.54057700	5.14159000	0.10934200
H	0.81856400	5.55236800	-1.87844900
H	2.04083500	4.50896700	2.10866000
H	2.19342000	6.01195000	0.13699800
C	-1.91845900	1.32977000	-1.63763900
C	-3.13781800	1.90284900	-1.98901400
C	-1.29894700	0.43393600	-2.52583000
C	-3.71665700	1.60034500	-3.22112900
H	-3.64658300	2.56662000	-1.28934900
C	-1.88467900	0.11160600	-3.74423700
H	-0.27877300	0.01895000	-2.32586100
C	-3.09717400	0.70613100	-4.09059500
H	-4.66504000	2.05617700	-3.49889100
H	-1.40444300	-0.59545200	-4.41762400
H	-3.56342700	0.46620200	-5.04392100
C	-2.37891400	1.62102000	1.26753900
C	-2.95089400	2.88723000	1.44637000
C	-2.79175700	0.55690200	2.07625400
C	-3.93892100	3.07865200	2.40401100
H	-2.61025500	3.73034100	0.84310000
C	-3.77605000	0.75621700	3.03923400
H	-2.34371200	-0.42886800	1.94909600
C	-4.35164200	2.01227900	3.19968400
H	-4.38231000	4.06372000	2.53659300
H	-4.09131300	-0.07439100	3.66762500

H	-5.12122400	2.16478700	3.95413600
C	1.80862900	0.01262100	-0.55526200
C	2.88354000	-0.67375200	0.09650900
H	2.66057800	-1.62071300	0.59196700
C	4.18942400	-0.19465700	0.17425300
C	5.20610300	-0.91844800	0.86744600
C	4.53558100	1.05843900	-0.44879900
C	6.47529500	-0.42587700	0.94535300
H	4.94133900	-1.86673600	1.33345300
C	5.87259600	1.53555600	-0.34756000
C	6.81149800	0.81525500	0.33274400
H	7.24514800	-0.98013000	1.47794600
H	6.12761000	2.48186400	-0.82273300
H	7.83125800	1.18653400	0.41004100
C	3.54981200	1.74987300	-1.15002900
C	2.24913300	1.24412000	-1.23351700
H	3.79185000	2.69059000	-1.64376300
H	1.50117700	1.80715500	-1.79081900
H	2.19002500	0.00618000	-1.76651900

TS9S

M06/BS1 SCF energy in gas pahse: -2603.377737 a.u.

M06/BS2 SCF energy in toluene: -2604.025935 a.u.

M06/BS2 Free energy in toluene: -2603.339325 a.u.

Ru	-0.25579600	-0.59593500	-0.51190500
B	-1.57414600	-3.50255000	-0.98133900
H	-2.06429300	-4.58405600	-1.16464700
N	-2.31498100	-2.42691600	-1.79585300
C	-3.30129500	-2.57228600	-2.70130500
C	-2.59738600	-0.49577200	-2.71622800
C	-3.52179400	-1.35377400	-3.31460200
H	-3.76591200	-3.54049700	-2.84594400
H	-2.43953700	0.56321200	-2.88746900
H	-4.24691200	-1.11749100	-4.08114000
N	-0.09877800	-3.49382200	-1.43963700
C	0.64816900	-4.48966200	-1.95400300
C	1.85384300	-2.65783400	-1.84142500
C	1.91183400	-3.99944300	-2.22636900
H	0.21754700	-5.47440300	-2.09328600
H	2.62867100	-1.89932100	-1.84644400
H	2.75243500	-4.53452200	-2.64676000
N	-1.62304600	-3.14383700	0.51715400
C	-2.06064900	-3.90318300	1.54080600
C	-1.83113200	-3.22531000	2.72236500
H	-2.50309500	-4.87362500	1.34800100
C	-1.22973400	-2.02897700	2.32297300
H	-2.06451800	-3.54621500	3.72846900
H	-0.88372600	-1.20343600	2.93363400
N	0.64085500	-2.36192400	-1.37017800
N	-1.87545200	-1.14762000	-1.80015000
N	-1.10842600	-1.98079800	0.99220700
P	-1.60449100	1.15639800	0.38321100
C	1.26875500	0.66999600	0.35034000
C	-1.19335900	2.84993100	-0.20717900
C	-0.92052600	3.90341500	0.67073000
C	-1.14675000	3.09622200	-1.58579600
C	-0.61801300	5.17270500	0.18001300
H	-0.95294700	3.74404800	1.74776900
C	-0.86166300	4.36492000	-2.07499000
H	-1.34307600	2.28677300	-2.28878100
C	-0.59465800	5.40824800	-1.18966700
H	-0.41325800	5.98202100	0.87831200
H	-0.84434200	4.53993300	-3.14912500
H	-0.37167500	6.40302900	-1.57084700
C	-1.65415000	1.39624200	2.20991800
C	-2.82119900	1.89031200	2.80495600
C	-0.52298200	1.20470400	3.01309300
C	-2.85614500	2.17932600	4.16522200
H	-3.71167100	2.06262600	2.20239500
C	-0.56024600	1.49414300	4.37327000
H	0.39865200	0.81658200	2.58318400
C	-1.72726000	1.98184400	4.95305700
H	-3.77352600	2.56201500	4.60845800
H	0.32837900	1.33356000	4.98085200
H	-1.75637000	2.20855300	6.01700500
C	-3.38093600	0.95141200	-0.02100700
C	-4.12860600	1.92623200	-0.68393300
C	-4.00040100	-0.24641900	0.35935500
C	-5.46861600	1.69482800	-0.98825100
H	-3.67184400	2.87383300	-0.96654200
C	-5.33699300	-0.46988300	0.05873100
H	-3.43505800	-1.01011900	0.89464500
C	-6.07180000	0.49719200	-0.62453900
H	-6.04125000	2.46122100	-1.50736500
H	-5.80704900	-1.40518400	0.35696200
H	-7.11810700	0.31800300	-0.86478400
C	1.53556400	-0.54962200	0.64630200
C	1.70421600	1.12320200	-1.74172000
C	0.64967600	0.45196400	-2.04725600
H	1.23836600	1.70427000	0.66932400
C	2.82975000	1.97799300	-1.66175300
C	4.15033800	1.46829100	-1.78985200
C	2.62786500	3.33361300	-1.32670000
C	5.21821300	2.33464800	-1.55419100
C	3.70531900	4.16876300	-1.09551800
H	1.60664700	3.70579000	-1.24369100
C	5.00222200	3.66219900	-1.20045700
H	6.23383000	1.96187900	-1.67682900
H	3.54168500	5.21285700	-0.83812600
H	5.85495400	4.31462900	-1.02191500
C	2.40551400	-1.48440700	1.29446400
C	2.03413400	-2.83129200	1.45457900
C	3.64018000	-1.02423400	1.83421000
C	2.84254800	-3.71211600	2.15243600
H	1.09284800	-3.17068600	1.02922800
C	4.44168700	-1.94134100	2.51811900
C	4.04838600	-3.26282500	2.68724500

H	2.53987300	-4.74981200	2.27233400
H	5.40641500	-1.61236400	2.90119200
H	4.69647700	-3.95164600	3.22599100
C	4.37862500	0.06883400	-2.15475100
C	5.36519200	-0.68518800	-1.66286900
H	3.67631500	-0.36231000	-2.87096700
H	5.49956100	-1.71798800	-1.97709900
H	6.06453800	-0.30639400	-0.91673900
C	4.08859100	0.36000800	1.65307400
C	4.86505600	1.03521600	2.50482000
H	3.76180000	0.86169100	0.74030300
H	5.17964300	2.05384500	2.28727900
H	5.20211600	0.61286600	3.45127600
H	0.28304100	0.35214900	-3.07484000

TS10S

M06/BS1 SCF energy in gas pahse: -2603.358841 a.u.

M06/BS2 SCF energy in toluene: -2604.010729 a.u.

M06/BS2 Free energy in toluene: -2603.321454 a.u.

Ru	0.04858500	0.41037000	-0.46170700
B	1.72725900	1.95310400	-2.76458800
H	2.34012000	2.51664200	-3.62921900
N	1.17473200	0.60072800	-3.28158700
C	1.27132200	0.05558500	-4.50662800
C	0.11126200	-1.28501900	-3.21143800
C	0.60318200	-1.15549500	-4.50946300
H	1.80978700	0.57590000	-5.28997700
H	-0.47386400	-2.08964600	-2.77896000
H	0.48554600	-1.84751400	-5.33197900
N	0.52323000	2.80272200	-2.31613900
C	0.05186700	3.95155900	-2.83702600
C	-1.40650600	3.14078000	-1.41154700
C	-1.18464100	4.21432600	-2.27698900
H	0.62850500	4.48840000	-3.58085600
H	-2.25388500	2.95440400	-0.75895300
H	-1.83634500	5.05505700	-2.47211400
N	2.62741600	1.63232500	-1.56713800
C	3.94155400	1.87119100	-1.40333900
C	4.36974000	1.22429200	-0.25990900
H	4.47568400	2.47774000	-2.12508000
C	3.22769200	0.58656600	0.22383600
H	5.36340900	1.21203800	0.16653200
H	3.12326700	-0.03016900	1.10703400
N	-0.36406600	2.30283900	-1.43102700
N	0.46703000	-0.22534900	-2.47181000
N	2.17961000	0.83534500	-0.56663000
C	-1.86570600	-0.03734400	-0.97572400
C	-2.34941600	0.41132000	0.12328700
C	0.40591200	1.27042200	1.48382400
C	-1.03377800	1.09426900	1.44761800
H	0.91884900	0.50318700	2.06247600
H	-1.34644700	0.31244100	2.14138200
H	-1.59820600	2.02565000	1.52333300
C	1.05133600	2.59092500	1.66208800
C	2.22688800	2.68086700	2.45005500
C	0.54334700	3.78106100	1.13234200
C	2.87658400	3.91351800	2.60848100
C	1.19269800	4.99607900	1.29358400
H	-0.38090400	3.76242900	0.56572200
C	2.37663500	5.06449900	2.02195100
H	3.77814900	3.94764200	3.21707100
H	0.76544900	5.89344900	0.84968300
H	2.89351200	6.01282800	2.15175700
C	2.78331700	1.56968500	3.15693600
C	3.30586400	0.68252100	3.79505400
H	3.78298600	-0.08192700	4.37241500
P	0.34499700	-1.84853600	0.36818700
C	-0.15300000	-2.03533100	2.12836100
C	-1.43072900	-2.47466800	2.49205600
C	0.71163100	-1.59109300	3.13888300
C	-1.83867100	-2.44823900	3.82312700
H	-2.12028700	-2.85626900	1.74252700
C	0.30069900	-1.55989500	4.46646300
H	1.72477200	-1.26855300	2.89770000
C	-0.98005100	-1.98067000	4.81216000
H	-2.83506400	-2.80066300	4.08369200
H	0.98739900	-1.20240800	5.23192200
H	-1.30196400	-1.95632700	5.85126100
C	-0.60335900	-3.16566900	-0.51926500
C	0.06690300	-4.25398600	-1.09262200
C	-1.99581700	-3.08463000	-0.68080400
C	-0.62968000	-5.21906500	-1.81382800
H	1.14525000	-4.35425500	-0.99203600
C	-2.68877400	-4.05377100	-1.39737200
H	-2.55220900	-2.25361900	-0.25390900
C	-2.00684900	-5.12125600	-1.97312100
H	-0.08588200	-6.05242700	-2.25435900
H	-3.76849000	-3.96961000	-1.50565500
H	-2.54867400	-5.87628800	-2.53913900
C	2.04652400	-2.51996500	0.27960100
C	2.52281200	-3.43167600	1.22777300
C	2.82855400	-2.23782600	-0.84792000
C	3.76981000	-4.02686200	1.06648600
H	1.91094900	-3.69484800	2.08969200
C	4.07053000	-2.84062000	-1.00904000
H	2.46766300	-1.54046400	-1.60414300
C	4.54557100	-3.73058000	-0.04998000
H	4.13063800	-4.73334700	1.81154500
H	4.67056300	-2.60909700	-1.88696900
H	5.51991500	-4.19889500	-0.17637200
H	-2.23234600	-0.46146100	-1.90265500
C	-3.64479600	0.66678900	0.75574400
C	-3.89064000	0.53507900	2.12943800
C	-4.72994500	0.97167100	-0.11081100
C	-5.16202500	0.71025400	2.65495400
H	-3.08746900	0.26997400	2.81247400
C	-5.99955200	1.15026400	0.45096200

C	-6.22380200	1.02209100	1.81298400
H	-5.31973600	0.60235900	3.72598600
H	-6.81905000	1.42747900	-0.21002100
H	-7.22208200	1.17427100	2.21792900
C	-4.57468000	1.11518800	-1.56519700
C	-5.47206800	0.69876100	-2.46159800
H	-3.66567600	1.60228000	-1.92522500
H	-5.32862400	0.86887200	-3.52608400
H	-6.37635900	0.16530400	-2.16945900

TS11S

M06/BS1 SCF energy in gas pahse: -2603.350593 a.u.

M06/BS2 SCF energy in toluene: -2604.003057 a.u.

M06/BS2 Free energy in toluene: -2603.315983 a.u.

Ru	0.31575500	-0.24754200	0.05226300
B	0.84839700	-1.91299900	-2.67024800
H	1.03600400	-2.52295800	-3.68773100
N	0.15624300	-0.56655700	-2.98057900
C	-0.09783600	-0.02061400	-4.18380000
C	-0.57748100	1.43255100	-2.61084100
C	-0.57822100	1.26161100	-3.99568400
H	0.08962300	-0.59028300	-5.08647200
H	-0.87068500	2.30112600	-2.03585000
H	-0.88189300	1.97578300	-4.74881100
N	2.17834400	-1.57900400	-1.97820900
C	3.42624700	-1.75700400	-2.45037000
C	3.50378800	-0.51582300	-0.64455900
C	4.31199700	-1.09619700	-1.62253700
H	3.58659600	-2.34355200	-3.34729900
H	3.79497000	0.09883900	0.19739400
H	5.38838400	-1.03941900	-1.70864700
N	-0.02709900	-2.72332400	-1.70865700
C	-0.55673300	-3.95033000	-1.86233700
C	-1.16760400	-4.31793700	-0.67796200
H	-0.44725700	-4.47373200	-2.80494300
C	-0.94890600	-3.23025800	0.16876100
H	-1.69578200	-5.23540800	-0.45599700
H	-1.25057100	-3.10675900	1.20226500
N	2.21921600	-0.81651700	-0.85486600
N	-0.13916600	0.32358000	-2.00002200
N	-0.26811000	-2.26887100	-0.45987000
C	1.25000500	1.65266400	0.30934200
C	0.49077500	1.49203800	1.34258900
C	1.26319100	-1.16690500	1.99582200
C	0.63606600	-0.02894600	2.54110500
H	0.68622800	-2.08766200	1.90061300
H	-0.39009800	-0.11614400	2.88411900
H	1.23408300	0.60712800	3.19578300
C	2.71095900	-1.35029900	2.11691000
C	3.31057300	-2.57525300	1.73734200
C	3.54787900	-0.34592300	2.62695700
C	4.69138700	-2.75642000	1.88161700
C	4.91691100	-0.53332300	2.75982400
H	3.12931500	0.61740700	2.91777200
C	5.49443800	-1.74436900	2.38651200
H	5.12321400	-3.70956300	1.58284400
H	5.53446600	0.26794400	3.16083900
H	6.56551000	-1.90073800	2.49485800
C	2.54752500	-3.64082200	1.17783800
C	1.95003800	-4.57894700	0.70132400
H	1.42299900	-5.40385600	0.27057000
H	-0.18400800	2.08869700	1.95131400
C	2.04874000	2.57016600	-0.44571400
C	2.43400900	2.30181900	-1.77281600
C	2.40662100	3.81585300	0.14371200
C	3.13072500	3.24029000	-2.51500700
H	2.17198900	1.34415400	-2.21589600
C	3.12356400	4.73597700	-0.62402500
C	3.47509000	4.46177600	-1.93957000
H	3.41648000	3.01517500	-3.54021200
H	3.42743600	5.67476100	-0.16329300
H	4.03550900	5.19773400	-2.51289600
C	2.04229900	4.13976200	1.52663100
C	1.66935700	5.35155700	1.94543900
H	2.08827700	3.31910100	2.24805100
H	1.44321400	5.54906600	2.99064500
H	1.57248100	6.19108700	1.25705600
P	-2.07266400	0.16426300	0.42734700
C	-2.64594500	0.16608800	2.17685300
C	-3.11111800	1.33068700	2.79558800
C	-2.54704600	-1.00358600	2.94590600
C	-3.46830300	1.32170100	4.14252100
H	-3.20968300	2.25433500	2.22774700
C	-2.91392600	-1.01458400	4.28518600
H	-2.17387300	-1.92194900	2.49329500
C	-3.37364600	0.15376900	4.88864600
H	-3.83110700	2.23770900	4.60479900
H	-2.83696600	-1.93573000	4.85926700
H	-3.65791100	0.15059000	5.93883100
C	-2.77435500	1.76216900	-0.17241500
C	-4.10763700	1.79102600	-0.59753100
C	-2.06627600	2.96947500	-0.10549700
C	-4.71177800	2.99151800	-0.95723000
H	-4.68733300	0.87046900	-0.64332600
C	-2.67286100	4.16802500	-0.46643400
H	-1.02548700	2.98509200	0.21148800
C	-3.99684600	4.18209800	-0.89440000
H	-5.74870600	2.99196000	-1.28719100
H	-2.10241800	5.09364400	-0.41420700
H	-4.47028500	5.12016100	-1.17744600
C	-3.15418100	-1.06231300	-0.41341900
C	-4.13967900	-1.78541400	0.26369300
C	-3.01521600	-1.23691600	-1.79706900
C	-4.94207400	-2.69390400	-0.42156300
H	-4.30128100	-1.63728300	1.32926100
C	-3.82489800	-2.13695700	-2.47726000
H	-2.28289500	-0.65531900	-2.35347400

C	-4.78221100	-2.87790500	-1.78925300
H	-5.70509000	-3.24961600	0.12029700
H	-3.70615700	-2.25815100	-3.55246400
H	-5.41294000	-3.58615000	-2.32298500

TS12S

M06/BS1 SCF energy in gas pahse: -2603.363232 a.u.

M06/BS2 SCF energy in toluene: -2604.015156 a.u.

M06/BS2 Free energy in toluene: -2603.326949 a.u.

Ru	0.13488000	-0.58012900	-0.58073600
B	1.35810200	-3.54430400	-0.92237500
H	1.81652900	-4.64786000	-1.04553400
N	1.40332400	-3.11477800	0.55974400
C	1.79183900	-3.84891600	1.62114600
C	0.98432100	-1.93029300	2.31868800
C	1.54522600	-3.12664300	2.77255200
H	2.21503400	-4.83561200	1.47258500
H	0.63459600	-1.08023300	2.89333900
H	1.74020200	-3.41978700	3.79513500
N	-0.11652100	-3.51718000	-1.38074800
C	-0.90412300	-4.52081600	-1.81216100
C	-2.05983900	-2.65670100	-1.76116600
C	-2.16462100	-4.01425100	-2.07004200
H	-0.50210600	-5.52241200	-1.91016600
H	-2.82237600	-1.88510300	-1.78016900
H	-3.03326000	-4.54957800	-2.42828400
N	2.13212800	-2.53473000	-1.78511000
C	3.10938200	-2.75438900	-2.68593100
C	3.38250500	-1.56788200	-3.33910300
H	3.53288400	-3.74563000	-2.79697500
C	2.49801200	-0.65030500	-2.76930300
H	4.11551900	-1.39006900	-4.11390400
H	2.39040900	0.40856300	-2.97893700
N	-0.82316000	-2.36395800	-1.34987800
N	0.90340200	-1.92401100	0.98338000
N	1.74646700	-1.23906200	-1.83445400
C	-1.65818400	-0.45447400	0.55659300
C	-1.37944900	0.75793600	0.22295000
C	-0.72688900	0.35103600	-2.39157100
C	-1.51385100	1.36053100	-1.78806400
H	0.17201200	0.71611700	-2.89258700
H	-0.98056000	2.28134000	-1.53845800
H	-1.38536500	1.77208000	0.61040500
C	-2.52918600	-1.33891800	1.26783800
C	-2.18669100	-2.68398900	1.50319000
C	-3.74309300	-0.82335100	1.80778400
C	-2.99186000	-3.49699500	2.28124500
H	-1.27015500	-3.07690900	1.07100600
C	-4.53727500	-1.66846400	2.58476700
C	-4.16661700	-2.98436000	2.83010900
H	-2.71050900	-4.53302300	2.45589800
H	-5.48012100	-1.28687600	2.97392500
H	-4.80871200	-3.62088500	3.43624500
C	-4.17568400	0.54826100	1.53092600
C	-4.82811500	1.33980500	2.38506000
H	-3.94068500	0.93383900	0.53900900
H	-5.13711500	2.34123400	2.09076600
H	-5.06440800	1.03157300	3.40351800
P	1.59621200	1.08875100	0.34731900
C	1.38009000	2.84008200	-0.17410900
C	1.38978900	3.89770800	0.74024500
C	1.29044500	3.13632100	-1.54083600
C	1.31065000	5.21565300	0.29499100
H	1.47998800	3.69835000	1.80663700
C	1.20497800	4.45021300	-1.98442700
H	1.31151900	2.32984300	-2.27506400
C	1.21600200	5.49529200	-1.06397500
H	1.33790300	6.02841300	1.01928800
H	1.14097200	4.65915500	-3.05048700
H	1.15902900	6.52597700	-1.40835200
C	1.61464500	1.23578100	2.18676000
C	2.82214100	1.21568400	2.89269200
C	0.42357600	1.39593700	2.90985300
C	2.83535000	1.31892300	4.28118500
H	3.76738100	1.11344500	2.36396000
C	0.43989300	1.50684500	4.29518200
H	-0.53661300	1.41632100	2.40082800
C	1.64684500	1.45791600	4.98739100
H	3.78610700	1.29160000	4.81015000
H	-0.49847500	1.62481600	4.83394600
H	1.65972800	1.53498000	6.07272700
C	3.36102300	0.76148700	-0.04033900
C	4.18562700	1.72569200	-0.62346000
C	3.89790100	-0.49617800	0.26998400
C	5.51596200	1.43029500	-0.91447100
H	3.79919700	2.71790800	-0.85114700
C	5.22751400	-0.78092000	-0.00891300
H	3.27622700	-1.25686700	0.74200300
C	6.03819200	0.17944600	-0.61137800
H	6.14659700	2.19017100	-1.37213900
H	5.63193000	-1.76009900	0.24110100
H	7.07841800	-0.04761600	-0.83709700
H	-1.22539500	-0.43723800	-2.95833800
C	-2.96307100	1.53228800	-1.87716300
C	-3.77879600	0.61580000	-2.55003600
C	-3.56839200	2.67139500	-1.28486900
C	-5.15366300	0.79084600	-2.61557500
H	-3.32125200	-0.23367100	-3.05413100
C	-4.95489800	2.83934500	-1.36286400
C	-5.74422500	1.90089100	-2.01418600
H	-5.76685100	0.06715200	-3.14800200
H	-5.40329400	3.71697500	-0.90122900
H	-6.82161300	2.04163700	-2.06463400
C	-2.79410300	3.63286400	-0.57175200
C	-2.13911800	4.44076700	0.04763300
H	-1.57219000	5.17675700	0.57865600

TS13S

M06/BS1 SCF energy in gas pahse: -1700.305212 a.u.

M06/BS2 SCF energy in toluene: -1700.779175 a.u.

M06/BS2 Free energy in toluene: -1700.308105 a.u.

Ru	0.91262300	-0.68526400	0.05948200
B	3.44863200	1.03975000	-0.81954000
H	4.38841100	1.69704100	-1.17439400
N	3.68166600	-0.46020800	-1.10701700
C	4.73303200	-1.09561400	-1.65923000
C	3.13434000	-2.54848100	-1.25586600
C	4.42942000	-2.44027600	-1.76990000
H	5.61976100	-0.53836300	-1.93715200
H	2.49685700	-3.42068300	-1.15366100
H	5.05222300	-3.22764300	-2.17194700
N	2.17231900	1.45390100	-1.59557700
C	2.02416400	2.38250300	-2.55972600
C	0.11379200	1.33935200	-2.26279600
C	0.71947100	2.34777500	-3.01533700
H	2.86773600	2.99507600	-2.85505100
H	-0.91141700	0.98471600	-2.26927700
H	0.27127400	2.96155400	-3.78459500
N	3.19459400	1.22350100	0.69237900
C	3.83807600	1.98089300	1.60432600
C	3.22371700	1.80941900	2.83130500
H	4.69159500	2.58098500	1.31131100
C	2.18442700	0.90766600	2.57703200
H	3.49023300	2.26894700	3.77344900
H	1.43445700	0.49997600	3.24851700
N	0.99463200	0.80725700	-1.41199200
N	2.69553600	-1.35060700	-0.86188400
N	2.17561600	0.56513300	1.28899900
C	-1.04367100	-0.75127200	1.01520100
C	-0.75614600	0.47713600	0.79964200
C	-0.32657200	-1.81513700	-1.16598700
C	-1.55143100	-1.84918400	-0.77648700
H	-1.35843600	-1.46757000	1.76259200
C	-1.10170100	1.86274100	0.83334600
C	-0.11735400	2.85382900	0.66141800
C	-2.45194500	2.24363300	1.08605900
C	-0.43788900	4.19588000	0.74875000
H	0.90708600	2.54980500	0.46352500
C	-2.74622300	3.60867000	1.14102000
C	-1.75928400	4.57222200	0.98644100
H	0.33469400	4.95020200	0.61883100
H	-3.77965700	3.91851400	1.28645700
H	-2.02552100	5.62644100	1.03514100
C	-3.51400200	1.24756700	1.24715200
C	-4.66069500	1.43433100	1.90706900
H	-3.34238600	0.27456900	0.78512300
H	-5.40345800	0.64122900	1.96222800
H	-4.89869200	2.35834300	2.43288200
C	1.54052000	-3.00359900	2.16697100
N	1.23011400	-2.18375900	1.41124500
C	1.94940600	-4.02499500	3.10931800
H	1.83024900	-5.02156500	2.66989700
H	3.00236400	-3.88362600	3.37752500
H	1.34594500	-3.96908100	4.02183500
C	-2.95059600	-2.03833200	-0.63818200
C	-3.86731000	-1.16887900	-1.28695300
C	-3.42578800	-3.03166800	0.24132800
C	-5.22763300	-1.32240000	-1.01321800
C	-4.77783500	-3.15888600	0.49900000
H	-2.70190900	-3.68823900	0.72317300
C	-5.67793200	-2.29249400	-0.12556600
H	-5.94192300	-0.68098200	-1.52693400
H	-5.13840100	-3.92858700	1.17742100
H	-6.74472200	-2.38883100	0.06752500
H	0.04114100	-2.31930800	-2.06470400
C	-3.39470800	-0.13466200	-2.21007700
C	-3.94520200	1.07692900	-2.32467400
H	-2.52953200	-0.39338400	-2.82406900
H	-3.56524700	1.80657600	-3.03655300
H	-4.78133400	1.39221200	-1.69994200

TS14S

M06/BS1 SCF energy in gas pahse: -1700.294542 a.u.

M06/BS2 SCF energy in toluene: -1700.773067 a.u.

M06/BS2 Free energy in toluene: -1700.301291 a.u.

Ru	0.18201500	-0.50107400	0.48376600
B	2.42007200	-1.99203700	-1.29496400
H	3.22809700	-2.55795000	-1.97674800
N	1.86097300	-2.93307200	-0.19554600
C	2.20278200	-4.18799300	0.14521900
C	0.76161300	-3.41110400	1.61027300
C	1.51731900	-4.54045900	1.29542400
H	2.91446700	-4.73978100	-0.45734100
H	0.06936000	-3.24210400	2.42804500
H	1.55799100	-5.48089000	1.82774000
N	1.22900200	-1.50549300	-2.14348000
C	0.98316100	-1.70392100	-3.45191800
C	-0.76957300	-0.76525700	-2.51987100
C	-0.28618700	-1.23829200	-3.74039400
H	1.73201300	-2.17298900	-4.07872200
H	-1.73158300	-0.31833400	-2.29293700
H	-0.79455200	-1.24334900	-4.69506900
N	3.04646200	-0.80183900	-0.55204800
C	4.33873100	-0.43989600	-0.44085400
C	4.44902700	0.50442600	0.56210500
H	5.08509700	-0.88962800	-1.08485100
C	3.14572300	0.65988800	1.03979000
H	5.34216600	1.01242500	0.89914400
H	2.77195800	1.31994600	1.81479300
N	0.15426700	-0.92184100	-1.56540100
N	0.97776800	-2.45046800	0.70618200
N	2.30931900	-0.12783900	0.35902200
C	-1.62696600	-1.41916900	0.62877400

C	-2.28190700	-0.31898900	0.48964800
C	0.12369000	1.60808500	0.38172800
C	-1.29694100	1.24138600	0.19890600
H	0.32650100	1.96823000	1.39358000
H	-1.87110600	1.72997900	0.98911300
H	-1.68594600	1.46308100	-0.79924600
C	0.87719900	2.39241300	-0.61323100
C	1.75721300	3.40207200	-0.14656200
C	0.75275800	2.22393000	-1.99608900
C	2.49160600	4.17056200	-1.05962800
C	1.48421200	2.99153200	-2.89088400
H	0.07001000	1.47390700	-2.38651800
C	2.36441800	3.96453800	-2.42397100
H	3.15771000	4.94005800	-0.67453700
H	1.36243400	2.83040700	-3.96016400
H	2.93996900	4.56916200	-3.12135400
C	1.90680000	3.70160900	1.24305200
C	2.05608400	3.98325600	2.41150500
H	2.19735800	4.28577400	3.42781300
H	-1.87782100	-2.46325700	0.77902200
C	-3.67462200	0.15956600	0.52993500
C	-4.10811600	0.88269600	1.64588000
C	-4.56554200	-0.09728600	-0.53163000
C	-5.40795900	1.35902900	1.72882300
H	-3.40805200	1.06070900	2.46443400
C	-5.87476500	0.38922200	-0.42426500
C	-6.29257700	1.11425600	0.68157300
H	-5.73276100	1.90971500	2.60894600
H	-6.57982600	0.16478000	-1.22320800
H	-7.31727600	1.47605900	0.73524100
C	-4.16072200	-0.86757600	-1.71561500
C	-4.59187700	-0.63329900	-2.95749500
H	-3.45908300	-1.68717900	-1.54942600
H	-4.27703300	-1.25740100	-3.79145900
H	-5.26869200	0.18832200	-3.19124000
C	0.27695900	-0.11375000	3.66954800
N	0.22908000	-0.24511400	2.52087900
C	0.34702900	0.04193300	5.10782600
H	0.65838500	1.06065900	5.36392900
H	-0.63194600	-0.15078200	5.56025900
H	1.07362200	-0.66291300	5.52700700

TS15S

M06/BS1 SCF energy in gas pahse: -1700.289745 a.u.

M06/BS2 SCF energy in toluene: -1700.769176 a.u.

M06/BS2 Free energy in toluene: -1700.295681 a.u.

Ru	0.61583400	-0.33869000	0.65164300
B	2.03535300	-0.68763600	-2.19361700
H	2.55519100	-0.81778800	-3.26708700
N	1.53521500	-2.05360500	-1.66118800
C	1.58009400	-3.28411000	-2.20789400
C	0.52754200	-3.38285300	-0.27933300
C	0.94770600	-4.17113400	-1.35444400
H	2.06169700	-3.43655400	-3.16667500
H	-0.03159800	-3.65323400	0.61133300
H	0.80779900	-5.23469900	-1.49237100
N	0.82250200	0.25704700	-2.27730400
C	0.31609500	0.86959200	-3.36325100
C	-0.92917800	1.34840500	-1.62099500
C	-0.80725000	1.58102500	-2.99048500
H	0.80094400	0.75074400	-4.32508900
H	-1.68248000	1.70914900	-0.93114100
H	-1.44946200	2.18582000	-3.61572900
N	3.02193900	-0.09310500	-1.16840700
C	4.32799600	0.21120000	-1.27781700
C	4.76896100	0.70564400	-0.06232300
H	4.84602500	0.05264600	-2.21625700
C	3.63598300	0.67791300	0.75463800
H	5.76430300	1.04269300	0.19427900
H	3.52289900	0.98917700	1.78842600
N	0.05977800	0.55853100	-1.19144600
N	0.88442700	-2.11253300	-0.47963600
N	2.59068800	0.19915400	0.07561800
C	-1.48155500	-0.84017700	0.76433400
C	-1.05153800	-0.76867800	1.97684900
C	0.31344700	1.70057800	1.71497200
C	-0.22848100	0.86639100	2.71351200
H	1.38801000	1.89038700	1.73526800
H	0.45764400	0.42225200	3.43283800
H	-1.19235100	1.12429700	3.15659500
C	-0.49042400	2.73870400	1.07009400
C	0.12104700	3.67805900	0.20452300
C	-1.87456000	2.83833000	1.27103300
C	-0.65086700	4.67122400	-0.41009500
C	-2.63278500	3.82069800	0.64817000
H	-2.37951600	2.12882200	1.92533800
C	-2.01976900	4.74442800	-0.19552400
H	-0.15509700	5.38106200	-1.06926800
H	-3.70506400	3.86931100	0.82716900
H	-2.60606800	5.52161600	-0.68070500
C	1.51195400	3.60691000	-0.09925300
C	2.68483300	3.55311100	-0.39250100
H	3.72039400	3.51686600	-0.65851600
C	2.24611900	-2.01589600	2.83521500
N	1.60603900	-1.36263600	2.12596900
C	3.05752300	-2.83390700	3.71249600
H	2.83476500	-2.60890200	4.76122900
H	2.86087900	-3.89612900	3.52949300
H	4.11955600	-2.63711800	3.52813600
H	-1.09502300	-1.39370900	2.86445000
C	-2.52584500	-1.16318000	-0.15051600
C	-2.24512100	-1.53673600	-1.48024500
C	-3.87491100	-1.16675900	0.31092100
C	-3.25913900	-1.91836600	-2.33886100
H	-1.21334300	-1.53093500	-1.82358600
C	-4.87792700	-1.52894400	-0.59235200
C	-4.58104300	-1.90843500	-1.89345400

H	-3.02488900	-2.20855800	-3.36052600
H	-5.91586400	-1.48986400	-0.26664700
H	-5.38704600	-2.18488600	-2.57040100
C	-4.21895100	-0.79642200	1.68515300
C	-5.26496100	-1.27234800	2.36590700
H	-3.55249900	-0.08766800	2.18046000
H	-5.47821800	-0.93961200	3.37874600
H	-5.93912400	-2.02023800	1.94993400

TS16S

M06/BS1 SCF energy in gas pahse: -1700.294792 a.u.

M06/BS2 SCF energy in toluene: -1700.772401 a.u.

M06/BS2 Free energy in toluene: -1700.300847 a.u.

Ru	0.83078700	-0.65271900	0.00528500
B	3.43735000	1.05801000	0.69897400
H	4.40254500	1.71466900	0.97788400
N	3.09091100	1.20740300	-0.79947200
C	3.69077000	1.93165700	-1.76677100
C	1.97203900	0.85567200	-2.61623000
C	3.00656600	1.73624700	-2.95215200
H	4.56615200	2.52764000	-1.53664800
H	1.17848200	0.44312700	-3.23228600
H	3.22405100	2.16760900	-3.91985300
N	2.21591900	1.50462100	1.54057800
C	2.12879300	2.47090600	2.47455700
C	0.18568600	1.46792000	2.29044100
C	0.84308300	2.48614900	2.98227100
H	2.99717600	3.07307800	2.71405100
H	-0.85138000	1.15448700	2.34218400
H	0.43910200	3.14009400	3.74270900
N	3.67383600	-0.43485700	1.00476100
C	4.76031900	-1.06859600	1.48513400
C	4.46020100	-2.41021000	1.63210500
H	5.66691400	-0.51266800	1.69257700
C	3.13084600	-2.51641500	1.21622300
H	5.10639600	-3.19687900	1.99682600
H	2.49238900	-3.39226700	1.17132200
N	1.01865100	0.87852700	1.42875200
N	2.03228500	0.54693700	-1.32103400
N	2.66642000	-1.32077200	0.84296800
C	-0.83034100	0.54862500	-0.64395100
C	-1.17522800	-0.67137400	-0.86181400
C	-0.29828600	-1.80535800	1.49149000
C	-1.48156600	-1.98016000	0.72809600
H	0.31612100	-2.70683500	1.56964600
C	1.28134000	-3.05166900	-2.05603500
N	1.04641700	-2.19932100	-1.30823500
C	1.58609900	-4.11407500	-2.99216800
H	1.54709100	-3.73889200	-4.02082000
H	2.59226100	-4.50356700	-2.80111900
H	0.86719200	-4.93415600	-2.88787500
H	-1.57659900	-1.27477300	-1.67152100
C	-1.12212100	1.94270000	-0.71573800
C	-0.09575300	2.90561600	-0.63172200
C	-2.46535600	2.36759900	-0.94311600
C	-0.36781200	4.25118800	-0.78476500
H	0.92395000	2.57618900	-0.45481700
C	-2.70880400	3.73767900	-1.07275900
C	-1.68122700	4.66765400	-1.00460300
H	0.43707600	4.97980000	-0.72156200
H	-3.73468000	4.07766900	-1.20337100
H	-1.90718500	5.72741800	-1.10710000
C	-3.56900100	1.40957200	-1.02042400
C	-4.68579100	1.58210600	-1.73245700
H	-3.44906500	0.48530800	-0.45620200
H	-5.47095000	0.82897900	-1.73182800
H	-4.85576200	2.45893800	-2.35648500
H	-0.35326500	-1.25182900	2.43112100
H	-1.46485000	-2.82132900	0.03095900
C	-2.83364500	-1.55662800	1.09776200
C	-3.07387900	-0.77014300	2.22961900
C	-3.93720400	-1.95912200	0.30416400
C	-4.35865800	-0.36953500	2.56656800
H	-2.24008200	-0.48880100	2.87068500
C	-5.22967700	-1.55783800	0.66074600
C	-5.43906700	-0.76039600	1.77787400
H	-4.52188700	0.23876300	3.45335900
H	-6.06718900	-1.87973200	0.04504400
H	-6.44875100	-0.45345500	2.04135000
C	-3.76240400	-2.74591400	-0.87255800
C	-3.63026400	-3.40477500	-1.87953000
H	-3.56566600	-4.00125900	-2.76543100

TS17S

M06/BS1 SCF energy in gas pahse: -1567.62564 a.u.

M06/BS2 SCF energy in toluene: -1568.058252 a.u.

M06/BS2 Free energy in toluene: -1567.626122 a.u.

Ru	-0.30956000	0.01839000	-0.38021800
B	-0.16728100	-2.99627100	0.81649800
H	-0.08783700	-4.10651200	1.26413900
N	-1.62104000	-2.51236200	0.80063300
C	-2.73472400	-3.21612700	1.07519000
C	-3.29170100	-1.26471000	0.24329000
C	-3.83306800	-2.45169200	0.73717000
H	-2.65598800	-4.21488900	1.48814800
H	-3.81763300	-0.39682900	-0.13296900
H	-4.87865900	-2.71067900	0.83170200
N	0.34876500	-2.95975000	-0.63609900
C	0.83279700	-3.95587300	-1.39742100
C	0.80570100	-2.09892600	-2.56476200
C	1.14158000	-3.44853400	-2.64681000
H	0.91755300	-4.95684900	-0.99105200
H	0.91108200	-1.32797100	-3.31804900
H	1.54992500	-3.97785600	-3.49673500
N	0.68510100	-2.02008100	1.64142100
C	1.45233300	-2.26844000	2.71501100

C	2.06387100	-1.09069000	3.10519000
H	1.50459900	-3.27064900	3.12366300
C	1.61128900	-0.14549200	2.18926600
H	2.74617300	-0.93657400	3.92962500
H	1.88621800	0.90016200	2.12068800
N	0.32500400	-1.81064900	-1.34748000
N	-1.95212200	-1.30381300	0.28470500
N	0.77490000	-0.71079900	1.30510200
C	0.78645400	0.97781700	-2.24781000
C	1.51450000	0.86862000	-1.21799100
C	-1.89232200	1.11022200	-1.42623400
C	-1.17092400	0.60926700	-2.34412000
H	-1.22920500	0.11257900	-3.30386600
H	0.78862700	1.15901200	-3.31309800
C	2.82265000	0.92755200	-0.60128500
C	3.47899900	-0.28663000	-0.35132700
C	3.41899700	2.15312900	-0.23234000
C	4.72216100	-0.30053600	0.26005800
H	2.99191400	-1.22159000	-0.63220700
C	4.67294600	2.10562400	0.39034800
C	5.31487300	0.90188000	0.64163700
H	5.22786200	-1.24675900	0.43964000
H	5.16544000	3.04253300	0.64592900
H	6.29287700	0.90183400	1.11853400
C	-1.24043100	1.38848600	1.12576400
C	-0.13455300	2.00847200	0.52532000
H	-0.30040700	2.78850300	-0.22048300
H	0.81883100	2.08650600	1.04087300
C	2.75882700	3.43452000	-0.50868900
C	2.92418200	4.55567700	0.19741800
H	2.08006600	3.44990600	-1.36442700
H	2.42075200	5.47768100	-0.08260500
H	3.56106500	4.60092000	1.08042500
H	-1.12668100	0.91616200	2.10351200
C	-2.59564400	1.80748800	0.72800700
C	-2.87385900	1.78128800	-0.65065300
C	-3.55626700	2.28216300	1.61229500
C	-4.07397900	2.30004400	-1.15361300
C	-4.76320800	2.76693400	1.11409200
H	-3.35761300	2.28808800	2.68300400
C	-5.01542200	2.78950700	-0.25974200
H	-4.27350200	2.27641700	-2.22297500
H	-5.51671800	3.13981700	1.80471900
H	-5.96232900	3.17515300	-0.63057400

TS18S

M06/BS1 SCF energy in gas pahse: -1567.636071 a.u.

M06/BS2 SCF energy in toluene: -1568.065647 a.u.

M06/BS2 Free energy in toluene: -1567.634778 a.u.

Ru	-0.53362100	-0.03831000	0.39653800
B	-3.13224600	-1.71428000	-0.53629900
H	-4.09190200	-2.35938500	-0.85831100
N	-3.14846300	-0.33805400	-1.21080700
C	-3.99382900	0.12501800	-2.15158800
C	-2.31228900	1.51672700	-1.92792900
C	-3.49981300	1.31965800	-2.63640500
H	-4.88231300	-0.43911000	-2.40971400
H	-1.60687600	2.33656800	-2.00434100
H	-3.93167900	1.95850100	-3.39455600
N	-1.82987500	-2.42867800	-0.96553600
C	-1.67228300	-3.59365900	-1.61714300
C	0.29864200	-2.72687400	-1.19607100
C	-0.31992500	-3.82706700	-1.78801600
H	-2.54051400	-4.16985900	-1.91419200
H	1.35603100	-2.51144500	-1.09902800
H	0.15143600	-4.67082200	-2.27337900
N	-3.07866900	-1.56916200	0.99744800
C	-3.86405200	-2.15384800	1.91879900
C	-3.30375200	-1.96036700	3.16774000
H	-4.76385300	-2.67469100	1.61356700
C	-2.13791900	-1.23975700	2.91370300
H	-3.67962000	-2.29729900	4.12399400
H	-1.39258600	-0.89736100	3.62221200
N	-0.61850300	-1.88625200	-0.70316400
N	-2.10554800	0.51291200	-1.06773600
N	-2.00849900	-1.00071100	1.60151000
C	2.24820800	-0.50923400	0.86119100
C	1.11889700	-0.78172600	1.41940300
C	0.69522300	1.43783900	-0.54284200
C	1.23491400	0.33043000	-0.86304900
H	1.59526600	-0.29503700	-1.66880200
C	-1.19425900	1.89262700	1.27227500
C	-0.25207300	1.28710000	2.11896700
H	0.75767900	1.69687100	2.17265800
H	-0.57693700	0.77924100	3.02321000
H	-2.25867300	1.80730800	1.50278700
C	-0.75435500	3.03468500	0.44986500
C	0.35174700	2.80688600	-0.39403700
C	-1.31654600	4.30439600	0.50658200
C	0.93916800	3.85621500	-1.11657200
C	-0.74606400	5.33834600	-0.23198600
H	-2.18340100	4.49098700	1.13851900
C	0.38239300	5.12231100	-1.02894000
H	1.79084400	3.65731200	-1.76430000
H	-1.18268900	6.33390500	-0.18172100
H	0.81126300	5.94546300	-1.59557100
H	1.04895000	-1.34147300	2.35732700
C	3.62502400	-0.29718400	0.61087800
C	4.42380300	-1.27467000	-0.04164300
C	4.18999200	0.93765700	0.99517300
C	5.76670900	-0.97221000	-0.27484300
C	5.52060500	1.21108000	0.74714600
C	6.30648600	0.24981200	0.10574300
H	6.40594500	-1.72576000	-0.73137600
H	5.95375500	2.15992300	1.05429400
H	7.35859000	0.45220300	-0.08568100
C	3.86322100	-2.57256000	-0.42176900

C	4.24977400	-3.28422300	-1.48444000
H	3.07503300	-2.96647500	0.22303800
H	3.80949500	-4.25444900	-1.70300100
H	5.00834900	-2.92553800	-2.17972000
H	3.54998500	1.67265600	1.48276500

TS19S

M06/BS1 SCF energy in gas pahse: -1567.624126 a.u.

M06/BS2 SCF energy in toluene: -1568.055864 a.u.

M06/BS2 Free energy in toluene: -1567.624338 a.u.

Ru	0.49337000	-0.08690700	-0.24450600
B	3.54479400	-1.06759700	0.37639000
H	4.65783300	-1.43739400	0.62311400
N	3.45782700	0.46444500	0.34177900
C	4.43145100	1.38708000	0.43711900
C	2.54232200	2.38044400	-0.08517200
C	3.88846500	2.63159300	0.17893400
H	5.44322600	1.08458000	0.67968900
H	1.75228100	3.08200700	-0.32687400
H	4.39180500	3.58862500	0.18134700
N	2.55011000	-1.59744400	1.42821700
C	2.77779700	-2.41864200	2.46827100
C	0.62512900	-2.02307600	2.31832100
C	1.57024800	-2.71378400	3.07451500
H	3.78824200	-2.73508400	2.69822700
H	-0.45250400	-1.99852100	2.43440500
H	1.39628300	-3.34289100	3.93652600
N	3.08556800	-1.57231900	-1.00950600
C	3.71921500	-2.35681300	-1.89894100
C	2.89848800	-2.53597200	-2.99822300
H	4.71404500	-2.72819000	-1.68344000
C	1.75070100	-1.80554200	-2.69544200
H	3.10233200	-3.11117100	-3.89087800
H	0.84064000	-1.69623900	-3.27517500
N	1.22439100	-1.34481900	1.33103400
N	2.29258400	1.06834600	0.01853100
N	1.87455100	-1.22152600	-1.49731400
C	-1.70277900	-1.08971000	0.12175900
C	-0.72614500	-1.62384300	-0.58585900
C	-0.34282700	1.09136600	1.25502300
C	-1.55089900	0.15079500	1.13711900
C	-0.37007600	1.67694700	-1.32059800
C	-0.03269300	0.82096900	-2.15917700
C	-0.74911700	2.76580600	-0.47953100
C	-0.61991000	2.49779100	0.89414800
C	-1.10418700	4.03675400	-0.94020500
C	-0.79195100	3.53385000	1.80741700
C	-1.30337500	5.05127000	-0.01262100
H	-1.19282200	4.22692900	-2.00803200
C	-1.13483800	4.80365300	1.35063200
H	-0.67090900	3.34470600	2.87351300
H	-1.57157500	6.04874900	-0.35316400
H	-1.27443500	5.61123400	2.06622300
H	0.17077200	0.40829400	-3.13223800
H	0.20118000	0.96721200	2.19734400
H	-1.73405600	-0.32146800	2.11275800
H	-2.42713700	0.75838900	0.87640700
H	-0.67423700	-2.48484300	-1.24508600
C	-3.11227300	-1.56881300	0.07099400
C	-3.37450700	-2.82938800	0.61143000
C	-4.15646200	-0.78275400	-0.45184200
C	-4.67566300	-3.31455200	0.66432700
H	-2.54767500	-3.42226400	1.00409700
C	-5.45646000	-1.29486100	-0.39151600
C	-5.71839700	-2.53955600	0.16627000
H	-4.87172700	-4.29645300	1.08976400
H	-6.26743800	-0.71457100	-0.82936300
H	-6.73923900	-2.91491100	0.19322400
C	-3.88245500	0.51168300	-1.09150300
C	-4.70428400	1.56387700	-1.08782700
H	-2.92221900	0.59434000	-1.61015600
H	-4.44760300	2.48373700	-1.60844700
H	-5.65961000	1.55089400	-0.56358800

2cat-I

M06/BS1 SCF energy in gas pahse: -1041.986689 a.u.

M06/BS2 SCF energy in MeOH: -1042.309528 a.u.

M06/BS2 Free energy in MeOH: -1041.921283 a.u.

Ru	0.52432600	0.07553600	0.03614700
C	2.24467700	-0.58367600	1.33274700
C	1.97557500	-1.60648400	0.37472900
C	2.20792000	-1.03888700	-0.93128400
C	2.54774000	0.63451900	0.63651200
C	2.54541900	0.33945300	-0.78071400
C	2.28036000	-1.80635300	-2.20580100
H	1.57024200	-2.64033500	-2.24464300
H	3.28553100	-2.24040700	-2.30642800
H	2.11471200	-1.17742600	-3.08814900
C	1.77584700	-3.04476800	0.71422300
H	1.00098700	-3.17934200	1.48036400
H	2.70646400	-3.47660000	1.11103600
H	1.48922100	-3.64146000	-0.15793100
C	2.30369300	-0.81898100	2.80194000
H	2.35015000	0.11028200	3.38047900
H	3.21416200	-1.38874800	3.03735100
H	1.45183200	-1.41004700	3.16047600
C	2.94302900	1.93154600	1.25631900
H	2.64587500	2.78280600	0.63258300
H	4.03203300	1.98782700	1.39302400
H	2.48036800	2.07282500	2.24072300
C	2.91347900	1.28099500	-1.87589100
H	3.98606100	1.21822500	-2.10753500
H	2.69598800	2.32040300	-1.60345000
H	2.36117000	1.06164500	-2.79816400
C	-2.63269800	-0.03194200	0.84114800
C	-3.81191100	0.40596600	1.45589400

C	-5.02874000	0.11701000	0.85667200
C	-5.07045200	-0.60119100	-0.33961600
C	-3.89646400	-1.03818700	-0.94517100
C	-2.66825300	-0.73796000	-0.36030400
H	-3.76286900	0.95932700	2.39182400
H	-5.95413600	0.44906100	1.32224000
H	-6.02942500	-0.81865900	-0.80554900
H	-3.93485200	-1.59580200	-1.88097500
C	-1.32529600	0.20230400	1.36865500
C	-0.32268700	0.54388900	2.02107500
H	0.24315500	0.87186900	2.87516100
C	-1.37196300	-1.19025000	-0.94964200
C	-0.69172100	-0.37724800	-1.84260600
H	0.00354200	-0.82107900	-2.55427700
H	-1.13629900	0.56770900	-2.15274800
C	-0.42101700	3.12358100	-0.65885500
C	-0.82417200	4.48878400	-0.93078900
H	-0.02926700	5.02241100	-1.46343200
H	-1.03346700	5.01489500	0.00707400
H	-1.72890000	4.50084000	-1.54846400
N	-0.09688100	2.03312600	-0.44174800
C	-1.16996900	-2.67508500	-0.87762600
H	-0.25240700	-3.00094200	-1.37757700
H	-2.01555200	-3.17717100	-1.37230300
H	-1.16086300	-3.02976500	0.16135500

IM1-I

M06/BS1 SCF energy in gas pahse: -1334.083348 a.u.

M06/BS2 SCF energy in MeOH: -1334.484077 a.u.

M06/BS2 Free energy in MeOH: -1333.973619 a.u.

Ru	-0.39981600	0.39026200	-0.13139300
C	0.78988700	1.03975500	1.72272000
C	0.11837000	2.16839500	1.14773400
C	-1.28923200	1.93983700	1.27913700
C	-0.18912400	0.08408300	2.12708800
C	-1.49172600	0.64655300	1.85096200
C	-2.37336700	2.90864500	0.96725500
H	-2.06356500	3.66183500	0.23497700
H	-2.65914200	3.44007600	1.88655200
H	-3.27349300	2.41441900	0.58261700
C	0.79447700	3.41251200	0.68305300
H	1.71600700	3.18348200	0.13117600
H	1.07440900	4.04505400	1.53750300
H	0.15102400	4.01473200	0.03085200
C	2.24709000	0.98974600	2.01489600
H	2.61131700	-0.02576200	2.20442700
H	2.44031400	1.58886200	2.91767300
H	2.84441000	1.42415800	1.20399000
C	0.11189200	-1.12264900	2.94908100
H	-0.74466300	-1.79737500	3.03221300
H	0.38392900	-0.81496600	3.96918900
H	0.95977100	-1.69301200	2.54796700
C	-2.81418100	0.12492700	2.29967000
H	-3.12744900	0.63942600	3.21961300
H	-2.78837500	-0.94745400	2.52073000
H	-3.59965900	0.28916900	1.55003000
C	1.68728700	-0.07390100	-0.85896200
C	1.21156100	0.88336700	-1.51743100
C	-2.18261300	0.82534500	-1.46642000
C	-1.31646000	1.67474700	-1.73380900
H	1.25866500	1.61838500	-2.30559300
H	-0.86324700	2.53083300	-2.20206200
C	2.73749100	-0.95996300	-0.42299000
C	4.07922800	-0.55973800	-0.63056100
C	2.47603700	-2.14496600	0.27452100
C	5.10028600	-1.34512000	-0.09567700
C	3.50748200	-2.92434200	0.77826800
H	1.44243500	-2.44596000	0.43414200
C	4.82572700	-2.51502100	0.60488400
H	6.13053600	-1.02445100	-0.24541300
H	3.28246000	-3.84545400	1.31211400
H	5.64216500	-3.10954600	1.00943200
C	-3.30354600	-0.04687100	-1.31221500
C	-3.05619200	-1.28992000	-0.70084400
C	-4.59613600	0.33745200	-1.67242500
C	-4.14108900	-2.11839800	-0.42085700
C	-5.66358400	-0.50878600	-1.39406400
H	-4.75682600	1.30666600	-2.14160200
C	-5.43397500	-1.72869500	-0.76561400
H	-3.98800300	-3.08406000	0.05666800
H	-6.67585200	-0.20992200	-1.65628000
H	-6.26933400	-2.38803400	-0.53990700
C	-1.65246600	-1.68970800	-0.42852300
C	-0.65911300	-1.46656100	-1.38369000
H	0.24208700	-2.07811900	-1.34621700
H	-0.90669600	-1.09601400	-2.37916800
C	-1.45698500	-2.78237400	0.58294400
H	-1.79034000	-3.73291500	0.13986700
H	-0.40607000	-2.91658900	0.85441600
H	-2.04130100	-2.63420300	1.49834600
C	4.43073400	0.66609300	-1.39433400
C	4.95019600	1.72716800	-0.77062200
H	5.24861200	2.61900100	-1.32064300
H	5.12207100	1.73089200	0.30599300
C	4.26761000	0.59514600	-2.88392900
H	4.98322600	-0.12508500	-3.30647000
H	3.26972100	0.24144700	-3.17641800
H	4.44935700	1.56840500	-3.35488800

TS1-I

M06/BS1 SCF energy in gas pahse: -1334.069732 a.u.

M06/BS2 SCF energy in MeOH: -1334.466042 a.u.

M06/BS2 Free energy in MeOH: -1333.958465 a.u.

Ru	-0.38995000	0.36336600	-0.26981700
C	0.36551200	2.52199500	-0.26363700
C	-0.40289900	2.27179800	-1.44830900

C	-1.75239500	1.98016300	-1.05677500
C	-0.48640900	2.33599600	0.86337500
C	-1.81458400	2.01501700	0.36384700
C	-2.90831000	1.75152100	-1.96712700
H	-2.59534800	1.33571600	-2.93178800
H	-3.42729900	2.69915700	-2.17063400
H	-3.64030900	1.06086700	-1.52999600
C	0.08905600	2.42847700	-2.84538200
H	1.16278800	2.22179600	-2.92593400
H	-0.07015700	3.46027700	-3.18943900
H	-0.44146100	1.77115300	-3.54542300
C	1.78758600	2.96494000	-0.26066600
H	2.23048700	2.93928100	0.74052900
H	1.86093300	3.99686500	-0.63224800
H	2.41115100	2.33931600	-0.91347300
C	-0.15705300	2.72533700	2.26470700
H	-0.75481000	2.18416000	3.00440500
H	-0.35869300	3.79691200	2.40883700
H	0.90125200	2.56498300	2.50167200
C	-3.09000500	1.98848400	1.13996300
H	-3.76539200	2.76939700	0.76400300
H	-2.92855500	2.19105100	2.20368500
H	-3.62351700	1.03169100	1.04783900
C	1.64594400	-0.33040500	-0.36024400
C	1.23107200	-0.44176200	-1.56831400
C	-1.55544900	-1.15783600	-1.23075600
C	-0.66310000	-0.93122900	-2.10602000
H	1.57424600	-0.36108500	-2.59042000
H	-0.45623600	-0.86732600	-3.16391800
C	2.77504100	-0.42717100	0.52825300
C	3.96409500	-1.04423900	0.07402600
C	2.73868800	0.14437300	1.80815800
C	5.08056000	-1.03478700	0.90910400
C	3.85718600	0.13417800	2.62719900
H	1.81076600	0.60810100	2.14389900
C	5.03525300	-0.45067200	2.17134300
H	5.99811300	-1.50188300	0.55327500
H	3.81316000	0.58245700	3.61760100
H	5.92146200	-0.45848100	2.80272500
C	-2.66969300	-1.70323400	-0.51902000
C	-2.64522900	-1.48282000	0.87204500
C	-3.74323100	-2.35658400	-1.12554400
C	-3.74927600	-1.86288600	1.63261200
C	-4.82925100	-2.74476500	-0.34871800
H	-3.73576100	-2.52346000	-2.20102900
C	-4.83469300	-2.48715600	1.01971100
H	-3.76726700	-1.69381700	2.70771800
H	-5.68162000	-3.23346800	-0.81528700
H	-5.69295400	-2.77931000	1.62123000
C	-1.39357700	-0.94504200	1.45846000
C	-0.15354000	-1.45315200	1.03623000
H	0.68013500	-1.37269100	1.73180700
H	-0.09879800	-2.30673600	0.35670400
C	-1.46596200	-0.39799000	2.85586500
H	-2.26000700	0.34209000	2.99869800
H	-1.67746100	-1.23218700	3.54163000
H	-0.50712900	0.02660000	3.17167400
C	4.04610900	-1.71353300	-1.25041700
C	4.73814000	-1.15573500	-2.24654700
H	4.84319200	-1.64994000	-3.21195100
H	5.23747500	-0.19485300	-2.12583400
C	3.38591200	-3.05675700	-1.35697800
H	3.85274800	-3.76859500	-0.66103500
H	2.32016700	-3.00751500	-1.08968600
H	3.46951100	-3.46577900	-2.37054600

IM2-I

M06/BS1 SCF energy in gas pahse: -1334.110546 a.u.

M06/BS2 SCF energy in MeOH: -1334.500579 a.u.

M06/BS2 Free energy in MeOH: -1333.987541 a.u.

Ru	0.34228500	0.35378900	0.16092300
C	-0.30645700	2.51490600	0.78427600
C	0.25116200	1.76806700	1.88941300
C	1.63334800	1.51483100	1.61692000
C	0.70444800	2.66630200	-0.18701600
C	1.91522400	2.03199900	0.32345300
C	2.61244300	0.87861900	2.54294600
H	2.14367100	0.09297300	3.14850300
H	3.03598300	1.62234300	3.23321500
H	3.44441300	0.42017000	1.99472700
C	-0.43832200	1.48862600	3.18070700
H	-1.52664700	1.41998900	3.06130600
H	-0.24209500	2.30176800	3.89500200
H	-0.08257000	0.55933200	3.64283000
C	-1.67587500	3.10527600	0.76844300
H	-1.95786600	3.46503300	-0.22767000
H	-1.72987300	3.96437800	1.45268200
H	-2.44353200	2.38837800	1.09063400
C	0.60892000	3.50441800	-1.41767600
H	1.39227800	3.27053400	-2.14588700
H	0.71609200	4.56850800	-1.16186700
H	-0.35848200	3.39250100	-1.92376600
C	3.29745700	2.14466000	-0.23254400
H	3.93641100	2.68682000	0.47816700
H	3.32337100	2.70550700	-1.17262700
H	3.76882700	1.16544800	-0.40199500
C	-1.43258100	-0.47166000	0.00888100
C	-1.00300200	-1.09034500	1.19253000
C	1.13317500	-1.45176100	0.70931900
C	0.12941700	-2.02649700	1.37664200
H	-1.63452200	-0.83692600	2.05731500
H	0.04752800	-2.97027400	1.92141400
C	-2.70399900	-0.24090400	-0.58968000
C	-3.83953200	-1.02861400	-0.25085900
C	-2.84139100	0.82165800	-1.50848800
C	-5.07192100	-0.67359000	-0.79727100
C	-4.06852200	1.13844600	-2.05603100

H	-1.94727300	1.39350000	-1.76200500
C	-5.18867500	0.39214100	-1.68466000
H	-5.94785800	-1.26469800	-0.53499400
H	-4.16443500	1.95781300	-2.76454900
H	-6.16355200	0.63466000	-2.10366400
C	2.41689700	-1.80659700	0.13622700
C	2.61232100	-1.23070900	-1.13554000
C	3.40127200	-2.60361000	0.71145000
C	3.81234300	-1.44697000	-1.80487500
C	4.60068600	-2.81273100	0.03147100
H	3.23970600	-3.03131300	1.70063700
C	4.80361700	-2.23580900	-1.21694600
H	3.98719900	-1.01196300	-2.78822800
H	5.38311600	-3.41685700	0.48585800
H	5.74403000	-2.39377500	-1.74088600
C	1.48952400	-0.42467400	-1.69980700
C	0.16901900	-0.92925300	-1.71415400
H	-0.52885600	-0.50973600	-2.43999600
H	-0.02852300	-1.96600700	-1.43282900
C	1.82289200	0.56202800	-2.78654500
H	2.68589600	1.19077100	-2.54788000
H	2.07206600	0.00645600	-3.70325000
H	0.96239300	1.19839000	-3.02506000
C	-3.76256000	-2.22088100	0.63041100
C	-4.38962900	-2.22143700	1.81020400
H	-4.38561600	-3.10105200	2.45229100
H	-4.93224200	-1.34860300	2.17186900
C	-3.06165100	-3.42829800	0.07655200
H	-3.58928300	-3.80122100	-0.81312200
H	-2.03236100	-3.20778600	-0.23814100
H	-3.02820500	-4.23756000	0.81483500

TS2-I

M06/BS1 SCF energy in gas pahse: -1334.110382 a.u.

M06/BS2 SCF energy in MeOH: -1334.500573 a.u.

M06/BS2 Free energy in MeOH: -1333.987334 a.u.

Ru	0.35811400	0.35299500	0.18035300
C	-0.32378600	2.49844200	0.78811400
C	0.63940600	2.66190500	-0.22968600
C	1.88684500	2.07207300	0.23856000
C	0.30592900	1.79671400	1.88562500
C	1.67957100	1.57782200	1.55574300
C	3.23968900	2.20461900	-0.37982100
H	3.20891900	2.71948500	-1.34563600
H	3.88720700	2.80057200	0.27852400
H	3.73576600	1.23339800	-0.52141300
C	0.46409800	3.46513300	-1.47409700
H	-0.52827600	3.32726700	-1.92297000
H	0.56866700	4.53719300	-1.25291000
H	1.21103000	3.22219800	-2.23694900
C	-1.71541300	3.03428400	0.81559300
H	-2.44235600	2.28828800	1.16598600
H	-1.78121800	3.89478300	1.49677900
H	-2.04501600	3.37509200	-0.17254500
C	-0.32199400	1.51617600	3.20768800
H	0.04983800	0.58412800	3.65108600
H	-0.08873100	2.32710200	3.91318600
H	-1.41419000	1.45315800	3.13747000
C	2.72816000	1.00194800	2.44389900
H	3.23648900	1.79915500	3.00557300
H	2.30684400	0.30069000	3.17446900
H	3.49238000	0.46456500	1.86865700
C	1.42952900	-0.45537000	-1.63872300
C	0.10433000	-0.99820500	-1.60873600
H	-0.03636500	-2.04215800	-1.31557100
H	-0.59116400	-0.63920700	-2.36873600
C	-1.39388900	-0.52558600	-0.01459100
C	-0.99546100	-1.12410300	1.19086000
C	2.58623400	-1.24143400	-1.11368100
C	2.44426400	-1.79214900	0.17636500
C	3.75883100	-1.46611000	-1.82705200
C	3.44950000	-2.58050500	0.72617500
C	4.77512800	-2.24017600	-1.26237500
H	3.89301300	-1.04891800	-2.82438100
C	4.62175300	-2.79726100	0.00230000
H	3.32753800	-2.99474000	1.72652000
H	5.69544000	-2.40519200	-1.81878900
H	5.42326300	-3.39195700	0.43539800
C	1.17237100	-1.42732900	0.76865100
C	0.16552200	-2.00413400	1.43339500
H	0.09952300	-2.93374600	2.00439400
C	-2.67511700	-0.26775600	-0.59771100
C	-2.80255000	0.79645500	-1.51326100
C	-3.82162700	-1.02796800	-0.24177100
C	-4.02973800	1.14000000	-2.04588900
H	-1.90086700	1.35147200	-1.77885500
C	-5.05437900	-0.64431300	-0.77088000
C	-5.16160600	0.42070400	-1.65904800
H	-4.11540500	1.96091300	-2.75411300
H	-5.93873500	-1.21606700	-0.49424900
H	-6.13653400	0.68448100	-2.06460900
H	-1.69047600	-0.90533300	2.01471400
C	1.70046300	0.48286400	-2.78584700
H	2.56580800	1.12970000	-2.61407200
H	1.91293800	-0.10771000	-3.68988500
H	0.82360200	1.10254700	-3.00853500
C	-3.76767100	-2.21760700	0.64583700
C	-4.39917100	-2.20000100	1.82350700
H	-4.41513500	-3.07626200	2.47005100
H	-4.92602400	-1.31489000	2.17873400
C	-3.08870700	-3.44331000	0.10527000
H	-3.60530200	-3.79892800	-0.79772000
H	-2.04604000	-3.25326200	-0.18362900
H	-3.09653500	-4.25451100	0.84201800

IM3-I

M06/BS1 SCF energy in gas pahse: -1334.148555 a.u.

M06/BS2 SCF energy in MeOH: -1334.538444 a.u.

M06/BS2 Free energy in MeOH: -1334.020683 a.u.

Ru	-0.47451600	0.49882400	-0.31723000
C	0.77979900	2.38884900	0.12149600
C	0.00557600	2.56600700	-1.05926500
C	-1.39355600	2.48362000	-0.69963100
C	-0.11976800	2.15891400	1.20914700
C	-1.47568700	2.23447700	0.69978100
C	-2.55823000	2.68457700	-1.60853300
H	-2.33019400	2.39720900	-2.64243600
H	-2.86234900	3.74107900	-1.62211300
H	-3.42337900	2.09436000	-1.28177000
C	0.53663900	2.82376400	-2.42849300
H	1.50973500	2.34135000	-2.58867300
H	0.67604100	3.90137900	-2.59388400
H	-0.14819000	2.46321400	-3.20579100
C	2.26476400	2.42898400	0.23358500
H	2.63595300	1.72168300	0.98711400
H	2.60247400	3.43304600	0.52857800
H	2.75358500	2.18402700	-0.71729000
C	0.31204100	2.12521800	2.63579400
H	-0.50625500	1.87688700	3.31843300
H	0.69103200	3.11533900	2.92741400
H	1.13052000	1.41068100	2.80299100
C	-2.74479400	2.22542500	1.48508100
H	-3.24734800	3.19950900	1.40635500
H	-2.56547200	2.03965700	2.54900200
H	-3.45104900	1.46428600	1.12533600
C	0.94990800	-1.24205900	-0.05472700
C	0.81198000	-0.89197500	-1.42630700
C	-1.56185400	-0.77005200	-1.26538100
C	-0.44460600	-0.75817200	-2.11089500
H	1.68828500	-0.53359000	-1.96661900
H	-0.44846700	-0.44983200	-3.15977700
C	2.28470500	-1.10680000	0.59447300
C	3.52450400	-1.06329700	-0.09533500
C	2.31561100	-0.96148400	1.99112700
C	4.69181800	-0.79797900	0.63148700
C	3.48427400	-0.70890800	2.69485800
H	1.38560300	-1.03108200	2.54946900
C	4.68574200	-0.60334200	2.00575200
H	5.63509500	-0.78186700	0.08737900
H	3.45138900	-0.59956600	3.77717700
H	5.61570300	-0.40311500	2.53361700
C	-2.74129300	-1.39074300	-0.79546700
C	-2.64151500	-1.42657800	0.61823800
C	-3.83013900	-1.94775900	-1.47947500
C	-3.72344400	-1.91317700	1.35097800
C	-4.88897700	-2.43112400	-0.72935400
H	-3.86585200	-1.94200000	-2.56698000
C	-4.83762800	-2.39733500	0.67057400
H	-3.69791900	-1.94335400	2.43862600
H	-5.77190800	-2.82694100	-1.22581600
H	-5.68262000	-2.77999900	1.24005600
C	-1.29147800	-1.05175100	1.12439700
C	-0.15480200	-2.01461900	0.67738500
H	0.26356400	-2.56516700	1.53318200
H	-0.55467900	-2.77006400	-0.01595700
C	-1.27267000	-0.77036900	2.60680300
H	-2.08868700	-0.10499700	2.91627300
H	-1.39266700	-1.71810700	3.16052200
H	-0.33566700	-0.32457000	2.94790200
C	3.72471500	-1.38607200	-1.53661700
C	4.31827200	-0.51322300	-2.35840800
H	4.54145400	-0.76900800	-3.39341700
H	4.62391500	0.47642000	-2.01873000
C	3.36177400	-2.77539700	-1.97502500
H	3.95699100	-3.51283900	-1.41833600
H	2.30822700	-3.01855000	-1.77722400
H	3.55177000	-2.91946300	-3.04474000

TS3-I

M06/BS1 SCF energy in gas pahse: -1334.135531 a.u.

M06/BS2 SCF energy in MeOH: -1334.526915 a.u.

M06/BS2 Free energy in MeOH: -1334.009842 a.u.

Ru	-0.42964800	0.67721700	-0.24876400
C	1.01436000	2.37714000	0.14338800
C	0.07542300	2.30198400	1.22327900
C	-1.24808000	2.52514600	0.68268000
C	0.28640600	2.59709700	-1.06399500
C	-1.11386900	2.70971600	-0.72538900
C	-2.53013900	2.65280000	1.43663200
H	-2.40400500	2.43813200	2.50335700
H	-2.92546100	3.67496200	1.35721300
H	-3.29890800	1.97203100	1.04485200
C	0.46240000	2.22993900	2.66130800
H	1.26140000	1.49504400	2.83288700
H	0.84765400	3.20413600	2.99532600
H	-0.38147300	1.97655400	3.31165900
C	2.49000800	2.24279100	0.28581300
H	2.97079300	1.95645700	-0.65758900
H	2.93067600	3.19866900	0.60428500
H	2.75761400	1.48964200	1.03859700
C	0.85908200	2.73622400	-2.43337600
H	0.17408200	2.34890300	-3.19835400
H	1.05436100	3.79090800	-2.67279400
H	1.80785400	2.19495400	-2.53408900
C	-2.22537100	3.00649700	-1.67347800
H	-2.35098100	4.09193300	-1.79600600
H	-2.03752900	2.58566100	-2.66936600
H	-3.17852900	2.60074600	-1.31236200
C	-1.40058700	-1.18974200	0.99177400
C	-0.19802300	-2.09109900	0.72716200
H	-0.47143200	-2.94382500	0.08550200
H	0.19873000	-2.51354400	1.66050700
C	0.87153000	-1.26764800	-0.00062500

C	0.62736600	-0.90364600	-1.34299100
C	-2.77995300	-1.67571000	0.61261200
C	-3.03905700	-1.19118000	-0.66591700
C	-3.69765600	-2.49205100	1.26045200
C	-4.20025200	-1.49700300	-1.36625700
C	-4.88621900	-2.77439800	0.58707900
H	-3.51467200	-2.89789200	2.25433600
C	-5.13591800	-2.28192700	-0.69888900
H	-4.38579100	-1.13129400	-2.37384900
H	-5.63977300	-3.39231500	1.07125600
H	-6.07684700	-2.52546400	-1.18768200
C	-1.73818700	-0.61364900	-0.91802900
C	-0.70093000	-0.78524200	-1.85891600
H	-0.86700900	-0.62872400	-2.92819300
H	1.45672500	-0.62807500	-1.99427900
C	2.23656600	-1.21303200	0.57767200
C	2.34378400	-1.01208500	1.96354400
C	3.43320000	-1.30300200	-0.17481600
C	3.56477600	-0.84312000	2.59938100
H	1.43439700	-0.96044200	2.56071300
C	4.65567500	-1.11915300	0.48296800
C	4.73374900	-0.87806500	1.84809600
H	3.60025900	-0.68577800	3.67561100
H	5.56820100	-1.20391500	-0.10550100
H	5.70338900	-0.74618900	2.32365000
C	-1.41638700	-0.59512700	2.38572100
H	-2.17104700	0.19170200	2.49357500
H	-1.69360000	-1.40660400	3.08255000
H	-0.44692700	-0.20523100	2.70782700
C	3.50385300	-1.68306300	-1.61274600
C	4.11567300	-0.89198500	-2.50065700
H	4.23720400	-1.19308500	-3.54032500
H	4.53585900	0.07224200	-2.21455800
C	2.98068000	-3.04217600	-1.97928300
H	3.54629600	-3.82046000	-1.44776200
H	1.92729400	-3.18015100	-1.69518300
H	3.07227100	-3.22863100	-3.05538700

IM4-I

M06/BS1 SCF energy in gas pahse: -1334.158214 a.u.

M06/BS2 SCF energy in MeOH: -1334.552282 a.u.

M06/BS2 Free energy in MeOH: -1334.035439 a.u.

Ru	0.25138700	0.88286000	-0.03262400
C	-1.48198200	2.22973600	0.03737800
C	-0.65091700	2.59128300	-1.06319200
C	0.65267000	2.97623200	-0.54563800
C	-0.68791500	2.34929200	1.23973000
C	0.61877400	2.84909900	0.87224600
C	1.80012000	3.47596700	-1.35553200
H	1.76479500	3.10384900	-2.38647200
H	1.79510700	4.57412100	-1.40630400
H	2.76189100	3.16887600	-0.92613000
C	-1.06952200	2.65272200	-2.49297000
H	-1.91864900	1.98967200	-2.69629600
H	-1.37887500	3.67427500	-2.75710000
H	-0.25557600	2.37732200	-3.17510100
C	-2.91256800	1.82538100	-0.03787700
H	-3.21343600	1.23005700	0.83262700
H	-3.56098800	2.71260300	-0.07286400
H	-3.11962500	1.22153900	-0.93102000
C	-1.18583900	2.16115400	2.63219900
H	-0.38243300	1.87424200	3.32174200
H	-1.61725200	3.09852700	3.01110300
H	-1.96903700	1.39491800	2.69406600
C	1.72571800	3.18575800	1.80973000
H	1.67494500	4.24398100	2.10350100
H	1.67889700	2.59083200	2.72939300
H	2.70893000	3.01739500	1.35341900
C	1.71927600	-1.37275200	-0.79873100
C	0.44315800	-2.19486500	-0.76631700
H	0.57323300	-3.11038600	-0.16621900
H	0.13938800	-2.51817400	-1.76977400
C	-0.66052500	-1.35714900	-0.10144900
C	-0.39219600	-0.81727900	1.16559600
C	3.15823700	-1.84612100	-0.62062200
C	3.37086600	-1.01871900	0.49711100
C	4.15943300	-2.64265900	-1.14479000
C	4.60113200	-0.92239300	1.13305000
C	5.40029800	-2.55176700	-0.50614400
H	4.01475900	-3.30424400	-1.99623400
C	5.61686200	-1.71118100	0.59445900
H	4.77936000	-0.28569000	1.99710800
H	6.23060200	-3.15203200	-0.87358700
H	6.60759900	-1.68333300	1.04369200
C	1.94511100	-0.69725500	0.56829800
C	0.97495000	-0.56442400	1.54406800
H	1.22392600	-0.25192700	2.55771500
H	-1.19104900	-0.59669500	1.87195200
C	-2.04358000	-1.49810700	-0.61355600
C	-2.24784500	-1.31459300	-1.99053300
C	-3.16953700	-1.73810700	0.20735000
C	-3.51482700	-1.32542000	-2.55495900
H	-1.38575000	-1.11927700	-2.63074400
C	-4.44080900	-1.74249500	-0.37978200
C	-4.62347700	-1.53178300	-1.73966700
H	-3.63569400	-1.17506700	-3.62596300
H	-5.29911900	-1.94739700	0.25869500
H	-5.62544100	-1.54808100	-2.16338700
C	1.64324900	-0.33101600	-1.91561500
H	2.51812300	0.32734300	-1.92614400
H	1.55517000	-0.81755200	-2.89858000
H	0.70070300	0.29242400	-1.88961300
C	-3.09349200	-2.05661900	1.65957600
C	-3.77480500	-1.32831100	2.55171700
H	-3.78461200	-1.58896000	3.60930800
H	-4.37019200	-0.46465100	2.25282900
C	-2.32827400	-3.28612700	2.05444300

H	-2.76653600	-4.17431300	1.57810500
H	-1.27726200	-3.24880100	1.73437500
H	-2.34740000	-3.43615200	3.13990200

TS4-I

M06/BS1 SCF energy in gas pahse: -1334.102998 a.u.

M06/BS2 SCF energy in MeOH: -1334.49243 a.u.

M06/BS2 Free energy in MeOH: -1333.980227 a.u.

Ru	0.35522700	0.32229700	0.05364000
C	-0.42066000	2.04160000	1.35787200
C	0.61275100	1.27022700	2.04255300
C	1.85261900	1.49940200	1.36542500
C	0.18434300	2.70879100	0.27027300
C	1.58610200	2.35442800	0.26565400
C	3.19376600	1.00545400	1.79212300
H	3.10766100	0.18411600	2.51350200
H	3.76773600	1.80866600	2.27609400
H	3.78935700	0.63604900	0.94547400
C	0.46355900	0.52660500	3.32269800
H	-0.58755300	0.41392500	3.61225000
H	0.98233700	1.04970000	4.13836200
H	0.89833900	-0.48159800	3.25208400
C	-1.82197100	2.19486800	1.84518600
H	-2.49184800	2.57333300	1.06450900
H	-1.85855500	2.90182600	2.68589700
H	-2.24083900	1.24380200	2.20055300
C	-0.42883400	3.71627000	-0.64217800
H	-0.19272600	3.51985400	-1.69735300
H	-0.04949400	4.72398200	-0.41624100
H	-1.51996600	3.75115800	-0.54447100
C	2.62354500	3.03391700	-0.55444500
H	2.89691500	3.97944000	-0.06142000
H	2.27627900	3.28955900	-1.56156800
H	3.54193300	2.44037900	-0.63644200
C	-1.41162700	-0.58317300	-0.04397600
C	-1.12786100	-1.49632600	0.99080000
C	1.12174400	-1.45985300	0.52936800
C	0.13580800	-2.16732900	1.14290300
H	-1.92061000	-1.64264600	1.74001800
H	0.19929300	-3.15495000	1.60646400
C	-2.69067500	-0.20923800	-0.57186900
C	-3.89088600	-0.93790100	-0.32587000
C	-2.76018600	0.98074300	-1.32889200
C	-5.09713900	-0.38782900	-0.75876800
C	-3.96617400	1.50007700	-1.76002500
H	-1.82143400	1.48899000	-1.55550900
C	-5.14279200	0.81667400	-1.45533300
H	-6.01645400	-0.93760900	-0.56310100
H	-3.99574700	2.42105400	-2.33852200
H	-6.10214000	1.20748400	-1.78931900
C	2.45126000	-1.76330800	0.05414000
C	2.76035800	-1.10560000	-1.15766400
C	3.38863000	-2.58546900	0.67618100
C	4.02944100	-1.25784000	-1.70584000
C	4.65459700	-2.73077500	0.11615800
H	3.13471200	-3.07739500	1.61509800
C	4.97140500	-2.06586800	-1.06471500
H	4.29482800	-0.76593900	-2.64055400
H	5.39983500	-3.35233200	0.60763900
H	5.96323100	-2.17685300	-1.49843900
C	1.68409800	-0.28756000	-1.78839800
C	0.37944000	-0.79008900	-1.92370200
H	-0.29125800	-0.29709500	-2.63103100
H	0.14931700	-1.83889600	-1.73161000
C	2.10178000	0.77871900	-2.76257500
H	2.98242300	1.34139800	-2.44107000
H	2.35681700	0.29956800	-3.71997100
H	1.28157400	1.47891000	-2.96617000
C	-3.93022000	-2.26664100	0.33520300
C	-4.61352500	-2.42950400	1.47357900
H	-4.69974300	-3.40647800	1.94719000
H	-5.11156300	-1.59603100	1.96792700
C	-3.28831400	-3.41335300	-0.39400800
H	-3.80286400	-3.58970500	-1.34933600
H	-2.23409800	-3.22180900	-0.63761100
H	-3.34200300	-4.33566200	0.19538900

IM5-I

M06/BS1 SCF energy in gas pahse: -1334.131458 a.u.

M06/BS2 SCF energy in MeOH: -1334.523967 a.u.

M06/BS2 Free energy in MeOH: -1334.011653 a.u.

Ru	0.37538600	0.29432300	-0.11982400
C	-0.70266800	1.57200400	1.46294800
C	0.15573700	0.58498300	2.06987000
C	1.51344100	0.94481000	1.76040700
C	0.11820100	2.51700200	0.78077300
C	1.48165100	2.13538700	0.97674100
C	2.73150700	0.29906700	2.32662800
H	2.57150400	-0.76718700	2.52790900
H	3.00337800	0.77003500	3.28254900
H	3.59965000	0.38110300	1.66025800
C	-0.25886800	-0.49055500	3.01330200
H	-1.27169300	-0.85384200	2.80476000
H	-0.24023200	-0.12891000	4.05150700
H	0.41217600	-1.35754600	2.95696900
C	-2.16238800	1.71328400	1.72756200
H	-2.69933900	2.20196900	0.90596700
H	-2.31218500	2.31844100	2.63344500
H	-2.64321600	0.74487800	1.90050700
C	-0.34257300	3.75408500	0.08699300
H	0.23140600	3.95499800	-0.82757200
H	-0.22419700	4.63459900	0.73603600
H	-1.40109200	3.69637600	-0.19161100
C	2.66422800	2.97106900	0.63378000
H	2.88031200	3.65019000	1.47209200
H	2.49285400	3.59862100	-0.24835900

H	3.56930500	2.37333600	0.46890200
C	-1.28032200	-0.80016100	-0.45209400
C	-1.12141900	-2.20201600	-0.27126500
C	1.08016200	-1.51894400	0.00472600
C	0.16465600	-2.59576800	0.03773000
H	-1.91542300	-2.92607000	-0.45251600
H	0.46825700	-3.64404100	0.08114800
C	-2.55947700	-0.18446300	-0.75694000
C	-3.83162800	-0.68513900	-0.35928500
C	-2.52546800	1.00868000	-1.51565800
C	-4.97508900	0.03162300	-0.71074700
C	-3.67225800	1.70802900	-1.84920100
H	-1.55561600	1.36341500	-1.86556200
C	-4.90754600	1.21872800	-1.43391600
H	-5.94491600	-0.34499200	-0.38595700
H	-3.60904300	2.61690300	-2.44413600
H	-5.82245800	1.75198500	-1.68459600
C	2.48980000	-1.66795500	-0.24954000
C	3.02464500	-0.67434900	-1.11439500
C	3.32309400	-2.65885600	0.28846200
C	4.40435500	-0.64336200	-1.33447200
C	4.68612400	-2.61922300	0.04709000
H	2.89952100	-3.41680600	0.94763200
C	5.22257100	-1.60654800	-0.75461700
H	4.84354800	0.10948200	-1.98670300
H	5.34311000	-3.36269400	0.49277300
H	6.29436700	-1.57940700	-0.94063300
C	2.09058000	0.26461400	-1.77174300
C	0.84749200	-0.15946100	-2.26780200
H	0.32753900	0.52712200	-2.94125700
H	0.62022700	-1.21395700	-2.42119400
C	2.63530500	1.56409300	-2.29295500
H	3.37087200	2.02902300	-1.63073900
H	3.13361700	1.37897200	-3.25661700
H	1.82787600	2.28159900	-2.48368800
C	-4.03932800	-1.93821300	0.41841300
C	-3.81493000	-2.00440500	1.73270500
H	-4.01580300	-2.91522900	2.29513100
H	-3.46464900	-1.14611700	2.30519900
C	-4.60605000	-3.08990100	-0.35988500
H	-5.59834300	-2.84220600	-0.76358000
H	-3.98181300	-3.33812000	-1.23170800
H	-4.70773900	-3.98498000	0.26421600

1a

M06/BS1 SCF energy in gas pahse: -385.4828087 a.u.

M06/BS2 SCF energy in MeOH: -385.5864434 a.u.

M06/BS2 Free energy in MeOH: -385.4785744 a.u.

M06/BS2 SCF energy in toluene: -385.5879309 a.u.

M06/BS2 Free energy in toluene: -385.4800619 a.u.

C	-1.25318400	-1.62733500	0.00453700
C	-2.23670800	-2.33047700	0.01537800
H	-3.10654600	-2.95155000	0.02691800
C	-0.07302500	-0.82384200	-0.00642000
C	-0.14194700	0.58677500	-0.05967000
C	1.17339100	-1.46277600	0.04697400
C	1.05890600	1.30386500	-0.07331200
C	2.34696300	-0.72725400	0.04430400
H	1.19986500	-2.54982000	0.09175900
C	2.28714100	0.66344100	-0.01821500
H	1.02332500	2.38966900	-0.14726400
H	3.30859000	-1.23508500	0.08420200
H	3.20348500	1.25093300	-0.03264000
C	-1.44514500	1.25349900	-0.10939500
C	-1.67754700	2.54566100	0.13076700
H	-2.28922200	0.60578700	-0.35254400
H	-2.68160000	2.95687000	0.06346300
H	-0.89096800	3.24385200	0.41642400

2a

M06/BS1 SCF energy in gas pahse: -308.1457409 a.u.

M06/BS2 SCF energy in MeOH: -308.2303267 a.u.

M06/BS2 Free energy in MeOH: -308.1515927 a.u.

M06/BS2 SCF energy in THF: -308.2317235 a.u.

M06/BS2 Free energy in THF: -308.1529895 a.u.

C	2.01665700	0.00031800	-0.00004700
C	3.22529500	-0.00017100	0.00005300
H	4.29401400	-0.00012200	0.00022200
C	0.58905800	0.00015000	-0.00002400
C	-0.11969500	-1.20865400	-0.00000300
C	-0.11997200	1.20879200	-0.00002700
C	-1.50732900	-1.20498100	0.00001300
C	-1.50760600	1.20479600	-0.00001100
H	0.43386700	2.14579800	-0.00004300
C	-2.20470600	-0.00017200	0.00000900
H	-2.04940900	-2.14898300	0.00002900
H	-2.04990200	2.14867400	-0.00001400
H	-3.29314800	-0.00029700	0.00002200
H	0.43435800	-2.14553400	0.00000000

MeCN

M06/BS1 SCF energy in gas pahse: -132.6568451 a.u.

M06/BS2 SCF energy in MeOH: -132.7028415 a.u.

M06/BS2 Free energy in MeOH: -132.6813475 a.u.

M06/BS2 SCF energy in THF: -132.702456 a.u.

M06/BS2 Free energy in THF: -132.680962 a.u.

M06/BS2 SCF energy in toluene: -132.6990469 a.u.

M06/BS2 Free energy in toluene: -132.6775529 a.u.

C	-0.27729500	0.00014700	-0.00000800
N	-1.43731200	-0.00006500	0.00000200
C	1.17499600	-0.00003200	-0.00004500
H	1.55847700	0.86820000	-0.54673500
H	1.55822900	0.03950400	1.02524200
H	1.55827300	-0.90793600	-0.47819900

MeOH

M06/BS1 SCF energy in gas pahse: -115.6440535 a.u.

M06/BS2 SCF energy in MeOH: -115.697227 a.u.

M06/BS2 Free energy in MeOH: -115.668641 a.u.

M06/BS2 SCF energy in THF: -115.6929545 a.u.

M06/BS2 Free energy in THF: -115.6643685 a.u.

C	0.65435400	-0.01988000	0.00000300
H	1.07904600	0.98922800	-0.00075100
H	1.03303000	-0.54452500	-0.89294000
H	1.03316500	-0.54327200	0.89362900
O	-0.74243500	0.12229100	0.00000400
H	-1.13188700	-0.76047700	0.00000700

1b

M06/BS1 SCF energy in gas pahse: -693.7381347 a.u.

M06/BS2 SCF energy in MeOH: -693.9097577 a.u.

M06/BS2 Free energy in MeOH: -693.6882827 a.u.

C	-2.91742900	0.66362000	0.00414400
C	-4.21889800	0.97395000	-0.36431900
C	-5.13094000	-0.08207400	-0.31906800
C	-4.75097400	-1.37288400	0.06200400
C	-3.43487600	-1.67972300	0.42972300
C	-2.53982600	-0.62984400	0.40459300
H	-4.52767600	1.96942400	-0.67731800
H	-6.16950500	0.09949000	-0.59220800
H	-5.50495500	-2.15871700	0.07541700
H	-3.15875900	-2.69176600	0.72141200
C	-1.53812300	1.13620200	0.10644600
C	-0.65150100	2.04303300	-0.32567300
H	-0.93235800	2.98163300	-0.80155000
C	-1.09891800	-0.21254200	0.67664400
C	0.11708500	-0.72160600	-0.07539800
H	0.52490500	-1.63390500	0.37866100
H	-0.87315300	-0.15164300	1.75408100
C	1.16050300	0.38847400	-0.09159600
C	0.75381600	1.67667100	-0.21866000
H	1.50189100	2.46165500	-0.33144500
C	2.58557400	0.03325800	-0.04260800
C	3.03879400	-1.18643700	-0.56503400
C	3.53867800	0.90308100	0.50753000
C	4.38918200	-1.51112800	-0.56255100
H	2.32503400	-1.88271200	-1.00423300
C	4.88774800	0.57832700	0.51238700
H	3.20718000	1.83492700	0.96405000
C	5.32165900	-0.62990500	-0.02553500
H	4.71579600	-2.46004100	-0.98533900
H	5.60572400	1.26956700	0.95133900
H	6.37939300	-0.88689800	-0.01715300
H	-0.16283300	-0.97385000	-1.11389200

2b

M06/BS1 SCF energy in gas pahse: -771.071044 a.u.

M06/BS2 SCF energy in MeOH: -771.2618329 a.u.

M06/BS2 Free energy in MeOH: -771.0111609 a.u.

C	-3.25159200	0.59333200	0.36341100
C	-4.50268600	1.17617600	0.22012700
C	-5.49057500	0.36288700	-0.33827500
C	-5.22875900	-0.95155300	-0.73850800
C	-3.96281500	-1.53199700	-0.59433600
C	-2.99321500	-0.73305600	-0.02314400
H	-4.71896800	2.20195800	0.51228200
H	-6.49486200	0.76216200	-0.47302400
H	-6.03767500	-1.53779600	-1.17228900
H	-3.77854700	-2.55642600	-0.91383000
C	-1.84920300	0.79904500	0.72288500
C	-0.87835200	1.70840100	0.88357900
H	-1.06626000	2.77219100	1.02382300
C	-1.54360200	-0.67409900	0.44367200
C	-0.32789500	-0.76635300	-0.45753300
H	-0.00893000	-1.79932300	-0.64575400
H	-1.37138000	-1.24623000	1.37097800
C	0.79477100	0.05181700	0.16988600
C	0.49180800	1.21642900	0.79279000
H	1.29482800	1.81762500	1.21980700
C	2.17745900	-0.45345700	0.07868400
C	3.26624400	0.36142200	-0.30998200
C	2.42777500	-1.79033800	0.41897600
C	4.55108000	-0.19645100	-0.32882400
C	3.70939500	-2.31812200	0.41257400
H	1.59267900	-2.41615200	0.73461300
C	4.78088200	-1.51328000	0.03667200
H	5.38033800	0.41871500	-0.67577700
H	3.87220600	-3.35640700	0.69651000
H	5.79104700	-1.91799500	0.00824500
H	-0.56298600	-0.32823200	-1.44369100
C	3.07509300	1.74702300	-0.75813700
C	3.97022300	2.72981300	-0.63717400
H	2.11319000	1.96836400	-1.22450700
H	3.77395700	3.72477200	-1.02996300
H	4.92513700	2.58694100	-0.13148200

(1*Z*,3*E*) *s-cis*-**3b**

M06/BS1 SCF energy in gas pahse: -732.0728775 a.u.

M06/BS2 SCF energy in THF: -732.2651984 a.u.

M06/BS2 Free energy in THF: -732.0288124 a.u.

C	-1.42915700	-0.00290300	-0.09401400
C	-0.57459300	-1.04923600	-0.11466200
C	1.71980000	-0.00441500	-0.14241800
C	0.87135100	-1.05263700	-0.08301400
H	-1.03880300	-2.03363900	-0.17237800
H	1.30249200	-2.05337900	-0.00306000
C	-2.89377300	-0.13158800	-0.08541800
C	-3.68300000	0.90417800	-0.60318000
C	-3.53636100	-1.26669800	0.42693100

C	-5.06704100	0.79677600	-0.62943400
H	-3.18966100	1.78867100	-1.00250100
C	-4.91922800	-1.37402600	0.39485500
H	-2.94432500	-2.06161800	0.87877000
C	-5.69171100	-0.34373300	-0.13496900
H	-5.66239200	1.60853100	-1.04436100
H	-5.39920200	-2.26314600	0.80066200
H	-6.77680100	-0.42739900	-0.15433100
C	3.17552400	-0.07322000	-0.09958900
C	3.90224100	1.12570900	-0.12844900
C	3.89945600	-1.27409700	-0.03283900
C	5.28988200	1.13183000	-0.08757500
C	5.28479400	-1.27005100	0.00653200
H	3.37048000	-2.22624900	-0.01553800
C	5.98964300	-0.06783500	-0.01967800
H	5.82756600	2.07846900	-0.11087100
H	5.82363900	-2.21513100	0.05661100
H	7.07765700	-0.06919500	0.01096900
H	3.35577500	2.06782800	-0.18462700
O	-0.94480600	1.28124200	-0.13629600
C	-1.05120200	1.96686200	1.09836000
H	-0.47315400	1.45112200	1.88052000
H	-0.63912800	2.96856300	0.94378500
H	-2.09858700	2.05067300	1.42444400
H	1.30313500	0.99646700	-0.24635000

(1*Z*,3*E*) *s-trans*-**3b**

M06/BS1 SCF energy in gas pahse: -732.0777784 a.u.

M06/BS2 SCF energy in THF: -732.2706253 a.u.

M06/BS2 Free energy in THF: -732.0350423 a.u.

C	-1.55074800	0.37801200	-0.09722900
C	-0.46645200	-0.42748900	-0.06913300
C	1.94957200	-0.80749500	-0.05864700
C	0.89452300	0.03226900	-0.06966400
H	-0.62931500	-1.50628200	-0.07769500
H	1.04073600	1.11351900	-0.08394000
C	-2.94114700	-0.09466300	-0.07434900
C	-3.95054000	0.66984900	-0.67409900
C	-3.29236700	-1.31022000	0.52762900
C	-5.26421200	0.22100000	-0.69037000
H	-3.68397100	1.61336200	-1.14720900
C	-4.60505000	-1.75939100	0.50510200
H	-2.52941200	-1.89523500	1.03971300
C	-5.59727700	-0.99672900	-0.10490400
H	-6.03368800	0.82417200	-1.16959000
H	-4.85861200	-2.70552200	0.98055200
H	-6.62786400	-1.34687300	-0.11648400
C	3.36168400	-0.45496600	-0.05417200
C	4.31571200	-1.48203500	-0.03252200
C	3.82344200	0.87028900	-0.07166500
C	5.67562600	-1.20298400	-0.02781500
C	5.18100800	1.14993000	-0.06695200
H	3.10688100	1.69066100	-0.09149300
C	6.11568100	0.11594500	-0.04470600
H	6.39536700	-2.01986100	-0.01108300
H	5.51635500	2.18585600	-0.08150200
H	7.18082100	0.34034500	-0.04154900
H	3.97298200	-2.51735000	-0.01995200
O	-1.36666300	1.73317800	-0.22684100
C	-1.70138700	2.46871300	0.93433200
H	-1.05327700	2.17897000	1.77618400
H	-1.54169300	3.52524700	0.70031300
H	-2.75122000	2.31536100	1.22556200
H	1.74081700	-1.88200200	-0.05212800

(1*E*,3*E*) *s-trans*-**3b**

M06/BS1 SCF energy in gas pahse: -732.0745349 a.u.

M06/BS2 SCF energy in toluene: -732.2678876 a.u.

M06/BS2 Free energy in toluene: -732.0320046 a.u.

C	1.82689300	-1.21991900	-0.01504400
C	0.56270600	-0.75892200	-0.10085400
H	1.96713100	-2.30142600	0.07632300
H	0.38311700	0.31346800	-0.20157200
C	-0.58463800	-1.62641000	-0.09409300
C	-1.88440800	-1.25954400	-0.12380500
H	-0.39448200	-2.70121800	-0.12664400
C	-2.40824000	0.11509600	-0.05070500
C	-3.45273800	0.50128100	-0.90145500
C	-1.90773000	1.04765400	0.86427800
C	-3.96119300	1.79132800	-0.85621800
H	-3.85079400	-0.22672800	-1.60746700
C	-2.41738100	2.34025000	0.90714800
H	-1.12821400	0.74296900	1.56162400
C	-3.44292900	2.71686100	0.04624100
H	-4.76662900	2.07899400	-1.52998200
H	-2.01945800	3.05327300	1.62740200
H	-3.84417200	3.72812000	0.08355200
C	3.05357100	-0.43564600	-0.03260200
C	4.28561800	-1.10171000	0.02991000
C	3.06858800	0.96579800	-0.10884900
C	5.48471800	-0.40215500	0.01508300
H	4.29162500	-2.19060200	0.08988100
C	4.26517100	1.66521700	-0.12273600
H	2.12850600	1.51432300	-0.15755100
C	5.48093300	0.98628800	-0.06143500
H	6.42763000	-0.94470200	0.06346400
H	4.25168000	2.75243300	-0.18245900
H	6.41863500	1.53900700	-0.07279400
O	-2.80654000	-2.25438600	-0.32685300
C	-3.82359300	-2.34970000	0.65152600
H	-4.46363900	-1.45600500	0.67671700
H	-4.43165300	-3.21883700	0.38511500
H	-3.38905600	-2.50258700	1.65087400

4b

M06/BS1 SCF energy in gas pahse: -385.5828075 a.u.

M06/BS2 SCF energy in toluene: -385.6828871 a.u.

M06/BS2 Free energy in toluene: -385.5663971 a.u.

C	0.00000000	2.42420200	0.70627500
C	0.00000000	1.23952600	1.39731500
C	0.00000000	0.00000000	0.71286200
C	0.00000000	0.00000000	-0.71286200
C	0.00000000	1.23952600	-1.39731500
C	0.00000000	2.42420200	-0.70627500
H	0.00000000	1.23283900	2.48768300
H	0.00000000	3.37013300	1.24522200
H	0.00000000	1.23283900	-2.48768300
H	0.00000000	3.37013300	-1.24522200
C	0.00000000	-1.23952600	-1.39731500
C	0.00000000	-2.42420200	-0.70627500
H	0.00000000	-1.23283900	-2.48768300
H	0.00000000	-3.37013300	-1.24522200
C	0.00000000	-1.23952600	1.39731500
C	0.00000000	-2.42420200	0.70627500
H	0.00000000	-1.23283900	2.48768300
H	0.00000000	-3.37013300	1.24522200

PPh_3

M06/BS1 SCF energy in gas pahse: -1035.716317 a.u.

M06/BS2 SCF energy in toluene: -1035.92035 a.u.

M06/BS2 Free energy in toluene: -1035.694351 a.u.

P	-0.01459900	-0.02970400	-1.27155200
C	0.23144100	1.60212600	-0.44504600
C	1.29950600	-1.03418800	-0.46090600
C	-1.53665600	-0.62201400	-0.41718400
C	-0.54439800	2.66640700	-0.91891100
C	1.12298500	1.83443000	0.60476000
C	-0.44313500	3.92937800	-0.34905300
H	-1.24185000	2.49702200	-1.74106800
C	0.45223000	4.15091400	0.69423100
H	-1.06030800	4.74528900	-0.72226700
C	1.23520700	3.10365800	1.16617100
H	0.54141600	5.14175000	1.13711400
H	1.93697200	3.27094800	1.98207000
H	1.73332400	1.01680600	0.98886000
C	1.09126300	-1.89857400	0.61578800
C	2.59382100	-0.90134000	-0.97744800
C	3.65808800	-1.59691800	-0.41783200
H	2.76719100	-0.23407800	-1.82396300
C	3.43894000	-2.45599900	0.65578200
H	4.66007200	-1.47429400	-0.82659400
C	2.15490800	-2.60811300	1.16695500
H	4.26953300	-3.00843600	1.09231000
H	1.97762900	-3.28114700	2.00466300
H	0.09068600	-2.01778700	1.03119200
C	-2.31802800	-1.56933300	-1.08603400
C	-1.94470800	-0.18068700	0.84589100
C	-3.47814300	-2.07201100	-0.50547400
H	-2.01402900	-1.90804400	-2.07778500
C	-3.87558200	-1.62288200	0.74970700
H	-4.07680100	-2.80862600	-1.03935500
C	-3.10689300	-0.67819600	1.42483800
H	-4.78824000	-2.00718500	1.20281400
H	-3.41551600	-0.32623100	2.40863300
H	-1.34617900	0.55962600	1.37924400