# SUPPORTING INFORMATION

# DFT Study on the Biosynthesis of Verrucosane Diterpenoids and Mangicol Sesterterpenoids: Involvement of Secondary-carbocation-free Reaction Cascades

Hajime Sato,[*,†,‡] Bi-Xiao Li,[‡] Taisei Takagi,[‡] Chao Wang,[‡] Kazunori Miyamoto,[‡] Masanobu Uchiyama*,[‡, §]

[†] Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi, 4-4-37 Takeda, Kofu, Yamanashi 400-8510, Japan.

[‡] Graduate School of Pharmaceutical Sciences, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

[§] Research Initiative for Supra-Materials (RISM), Shinshu University, 3-15-1 Tokida, Ueda, Nagano 386-8567, Japan

Email: hsato@yamanashi.ac.jp

Email: uchiyama@mol.f.u-tokyo.ac.jp

## Table of Contents

## 1. Computational Details

All calculations were carried with GRRM11[1-5] based on Gaussian16 program.[6] Structure optimizations were carried out at the M06-2X level in the gas phase using the 6-31+G(d,p) basis set.[7] The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum (no imaginary frequency) or a transition state (single imaginary frequency). Intrinsic reaction coordinates (IRC) calculations[8-11] were performed to track minimum energy paths from transition structures to the corresponding local minima. Single-point energies were calculated at the mPW1PW91/6-31+G(d,p) level[12,13] based on the structures optimized by the M06-2X method. The Gibbs free energy used for discussion in this study was calculated by adding the gas-phase Gibbs free energy correction.

## 2. Cartesian Coordinates and Energies of Computed Structures

**IM0**

Sum of electronic and thermal Free Energies = -781.118377

| | | | |
|---|---|---|---|
| C | -2.63625200 | 1.32079100 | 0.37637700 |
| C | -3.73744500 | 0.37802500 | 0.53316000 |
| C | -4.79029700 | 0.23251100 | -0.43479400 |
| C | -1.48080600 | 0.56957100 | -0.45667100 |
| C | -4.95759400 | 1.05727500 | -1.49148500 |
| C | -0.74124400 | -0.46843300 | 0.30381800 |
| C | -0.79806600 | -1.80075800 | 0.09392700 |
| H | -2.90558600 | 2.21508800 | -0.18554800 |
| H | -4.30956900 | 1.90708800 | -1.68372100 |
| H | -1.91107900 | 0.19745400 | -1.38937700 |
| H | -0.02628000 | -0.09541900 | 1.03564000 |
| H | -2.20478700 | 1.60420200 | 1.33852700 |
| H | -5.48802400 | -0.58607700 | -0.28116800 |
| H | -0.78662800 | 1.38123200 | -0.70221800 |
| H | -5.77109500 | 0.89706900 | -2.19210700 |
| C | -3.65817700 | -0.57475100 | 1.63851500 |
| H | -4.51660700 | -1.23906200 | 1.72436900 |
| H | -2.73399100 | -1.16777100 | 1.42800800 |
| H | -3.43522900 | -0.07866400 | 2.58824100 |
| C | 1.30480000 | -3.13890100 | -0.21396600 |
| H | 0.87310800 | -3.76901300 | -0.99978200 |
| H | 2.01353100 | -3.76889900 | 0.32973300 |
| C | 1.97959800 | -1.94330500 | -0.83079400 |
| H | 1.51256800 | -1.54918500 | -1.73429100 |
| C | 3.04588700 | -1.28419500 | -0.35815500 |
| C | 3.80360100 | -1.68334800 | 0.88139400 |
| H | 4.88011300 | -1.70911600 | 0.67866500 |
| H | 3.65349700 | -0.95268900 | 1.68551600 |
| H | 3.50789500 | -2.66125200 | 1.26422300 |
| C | 3.57152000 | -0.06626600 | -1.08199500 |
| H | 4.56476700 | -0.29752000 | -1.49000400 |
| H | 2.91751000 | 0.16285300 | -1.93068700 |
| C | 2.43186700 | 1.58506100 | 0.49968000 |
| H | 2.10902400 | 0.90861600 | 1.29475900 |
| C | 3.70542000 | 1.18680000 | -0.19367000 |
| H | 4.09164300 | 2.00558000 | -0.80522400 |
| H | 4.46810100 | 1.00050600 | 0.57317500 |
| C | 1.69331700 | 2.68553700 | 0.29573100 |
| C | 1.97954300 | 3.73620500 | -0.74519500 |
| H | 2.80373000 | 3.47201000 | -1.40737100 |
| H | 1.09213700 | 3.90744200 | -1.36652200 |
| H | 2.21744100 | 4.69393900 | -0.26799300 |
| C | 0.51106800 | 3.00303700 | 1.17879800 |
| H | 0.27854900 | 2.17992500 | 1.86277500 |
| H | 0.71721200 | 3.89170900 | 1.78684100 |
| H | -0.38092500 | 3.24434100 | 0.58401800 |
| C | -1.70700700 | -2.44082000 | -0.92244400 |
| H | -2.00492900 | -3.44148600 | -0.59734300 |
| H | -2.61370400 | -1.85864000 | -1.11561500 |
| H | -1.18589700 | -2.55740000 | -1.88099000 |
| C | 0.18716400 | -2.71106300 | 0.77420200 |
| H | 0.65200200 | -2.19061900 | 1.61824600 |
| H | -0.31989000 | -3.60408000 | 1.15862200 |

**TS_0-1**

Sum of electronic and thermal Free Energies = -781.110522

| | | | |
|---|---|---|---|
| C | 2.80909100 | 0.66269200 | 0.18990900 |
| C | 3.97837500 | -0.17289400 | -0.16809300 |
| C | 5.26395100 | 0.38780000 | -0.46362900 |
| C | 1.62036600 | -0.01530300 | 0.89477100 |
| C | 5.55524700 | 1.70483200 | -0.35033800 |
| C | 0.77459000 | -0.86444200 | -0.01530400 |
| C | 0.34400900 | -2.11684400 | 0.19006300 |
| H | 3.13613800 | 1.55135100 | 0.73793000 |

| | | | |
|---|---|---|---|
| H | 4.83706300 | 2.44391000 | -0.00860900 |
| H | 1.97362500 | -0.56386800 | 1.77324300 |
| H | 0.41079900 | -0.34798000 | -0.90584900 |
| H | 2.46183500 | 1.05197400 | -0.78830600 |
| H | 6.03623700 | -0.29987100 | -0.79506500 |
| H | 0.99209700 | 0.79803600 | 1.27906000 |
| H | 6.54634800 | 2.06996500 | -0.60303200 |
| C | 3.82753600 | -1.62814500 | -0.28049800 |
| H | 4.74130800 | -2.14040100 | -0.57501600 |
| H | 3.45564000 | -2.01873700 | 0.67913800 |
| H | 3.00063700 | -1.85136600 | -0.97110700 |
| C | -2.01714800 | -2.98338600 | -0.12579700 |
| H | -1.93431600 | -3.76512300 | 0.63795100 |
| H | -2.68947500 | -3.37786200 | -0.89203100 |
| C | -2.56150500 | -1.72619900 | 0.49598900 |
| H | -2.20312200 | -1.50529500 | 1.50264300 |
| C | -3.39002800 | -0.83425400 | -0.06268100 |
| C | -3.96097500 | -0.96176000 | -1.45128700 |
| H | -5.04145200 | -0.77967800 | -1.43934800 |
| H | -3.52325000 | -0.21303900 | -2.12301300 |
| H | -3.78744600 | -1.94354200 | -1.89399000 |
| C | -3.81429400 | 0.39722900 | 0.70410600 |
| H | -4.89744900 | 0.34968300 | 0.87946300 |
| H | -3.32685800 | 0.40182900 | 1.68502800 |
| C | -2.05784500 | 1.88767700 | -0.37191800 |
| H | -1.64647700 | 1.09155900 | -0.99718400 |
| C | -3.50910100 | 1.72325800 | -0.02037300 |
| H | -3.86285500 | 2.54952100 | 0.60042100 |
| H | -4.09853400 | 1.76708100 | -0.94597200 |
| C | -1.23697600 | 2.89470200 | -0.04297600 |
| C | -1.60925200 | 4.08303700 | 0.80405400 |
| H | -2.60922600 | 4.01070800 | 1.23052300 |
| H | -0.89812800 | 4.19989700 | 1.63021800 |
| H | -1.55985900 | 5.00410900 | 0.21159100 |
| C | 0.17771600 | 2.93799600 | -0.56635100 |
| H | 0.40168600 | 2.05558400 | -1.17558000 |
| H | 0.33271000 | 3.82682700 | -1.18955200 |
| H | 0.90139300 | 3.00505300 | 0.25858300 |
| C | 0.69496900 | -2.95867300 | 1.38882000 |
| H | 0.96162500 | -3.97445600 | 1.07700200 |
| H | 1.51347200 | -2.55559600 | 1.98914700 |
| H | -0.17164100 | -3.05205800 | 2.05322200 |
| C | -0.63165400 | -2.74811100 | -0.77329600 |
| H | -0.75963900 | -2.09505600 | -1.64373600 |
| H | -0.23531800 | -3.70843300 | -1.12881800 |

**IM1**

Sum of electronic and thermal Free
Energies = -781.142992

| | | | |
|---|---|---|---|
| C | -2.54842200 | 1.26530700 | -0.77901900 |
| C | -3.72129700 | 0.51026000 | -0.20558600 |
| C | -3.49235200 | -0.32777200 | 0.81672300 |
| C | -1.33653700 | 0.33678500 | -0.97085500 |
| C | -2.13220300 | -0.44656700 | 1.42077900 |
| C | -0.94490700 | -0.44336900 | 0.29471800 |
| C | -0.83002900 | -1.88167300 | 0.23030900 |
| H | -2.81168400 | 1.71726300 | -1.73946600 |
| H | -1.86103000 | 0.42782300 | 2.02341300 |
| H | -1.56627900 | -0.35227900 | -1.78939500 |
| H | -0.06129600 | -0.00890000 | 0.76949600 |
| H | -2.28329800 | 2.09305500 | -0.10863100 |
| H | -4.29822000 | -0.91405700 | 1.25026000 |
| H | -0.45685500 | 0.91373600 | -1.27649800 |
| H | -2.06660300 | -1.30422100 | 2.09984900 |
| C | -5.07372300 | 0.72815700 | -0.81084400 |
| H | -5.84334000 | 0.13731400 | -0.31079900 |
| H | -5.34975700 | 1.78618300 | -0.74425500 |
| H | -5.06570300 | 0.47051200 | -1.87594000 |
| C | 1.35020000 | -2.90858600 | -0.05307200 |
| H | 0.95717800 | -3.64764900 | -0.75907500 |
| H | 2.13835100 | -3.39769300 | 0.52163600 |
| C | 1.83579500 | -1.68167100 | -0.76552700 |
| H | 1.16995100 | -1.28978200 | -1.53845100 |
| C | 2.96595900 | -0.99878100 | -0.53600200 |
| C | 4.01495800 | -1.39046800 | 0.46985100 |
| H | 5.00669800 | -1.35109500 | 0.00734500 |
| H | 4.03175800 | -0.68541000 | 1.30865200 |
| H | 3.87564700 | -2.39205800 | 0.87781100 |
| C | 3.23936200 | 0.27405000 | -1.29992600 |
| H | 4.15357300 | 0.15356400 | -1.89482100 |
| H | 2.41614200 | 0.46343400 | -1.99835200 |
| C | 2.28665500 | 1.65692300 | 0.61547900 |
| H | 2.34717200 | 1.01523000 | 1.49770900 |
| C | 3.40832600 | 1.49955600 | -0.37592200 |
| H | 3.51189400 | 2.39164500 | -0.99858800 |
| H | 4.35064300 | 1.40743800 | 0.17653600 |
| C | 1.25546200 | 2.51150500 | 0.55815400 |
| C | 1.00697100 | 3.47791000 | -0.57044600 |
| H | 1.66037400 | 3.31262700 | -1.42820900 |
| H | -0.03171000 | 3.40205400 | -0.91651000 |
| H | 1.14442800 | 4.51016700 | -0.22884000 |
| C | 0.26755400 | 2.60543600 | 1.69307200 |
| H | 0.47987700 | 1.87796500 | 2.48280300 |
| H | 0.29206100 | 3.60486200 | 2.14198500 |
| H | -0.76097200 | 2.45633400 | 1.33999700 |
| C | -1.72421100 | -2.67688300 | -0.63197500 |
| H | -1.77300600 | -3.72524700 | -0.33642600 |
| H | -2.72082600 | -2.22251500 | -0.68700200 |
| H | -1.31663200 | -2.62440900 | -1.65397300 |
| C | 0.21258800 | -2.57356400 | 0.99885300 |
| H | 0.64070000 | -1.93127300 | 1.77245400 |
| H | -0.15013000 | -3.51394800 | 1.42271000 |

**TS_1-2**

Sum of electronic and thermal Free
Energies = -781.13262

| | | | |
|---|---|---|---|
| C | 2.09145700 | 1.75716000 | -0.07126300 |
| C | 3.45309300 | 1.12197000 | -0.13531400 |
| C | 3.59189300 | -0.12515800 | -0.61436200 |
| C | 1.08724100 | 0.85033800 | 0.72490300 |
| C | 2.46801900 | -0.91333900 | -1.17285000 |
| C | 0.76861400 | -0.35565800 | -0.05920000 |
| C | 1.38786000 | -1.62045700 | 0.01869800 |
| H | 2.14092600 | 2.72077500 | 0.44109200 |
| H | 1.92057900 | -0.41702100 | -1.97947100 |
| H | 1.50705000 | 0.61170500 | 1.70377100 |
| H | 0.02863700 | -0.22279900 | -0.85049600 |
| H | 1.68365800 | 1.94387400 | -1.07130900 |
| H | 4.56093800 | -0.61504200 | -0.57108500 |
| H | 0.14742900 | 1.40183400 | 0.84898500 |
| H | 2.78690000 | -1.88180500 | -1.56484300 |
| C | 4.60144400 | 1.89874900 | 0.43582400 |
| H | 5.53898100 | 1.34456900 | 0.36754600 |
| H | 4.71862600 | 2.84914300 | -0.09537600 |
| H | 4.41350100 | 2.14301800 | 1.48788000 |
| C | -0.49827900 | -3.25154300 | 0.30067700 |
| H | -0.05328300 | -3.79072600 | 1.14249100 |
| H | -1.09496200 | -3.98626700 | -0.24622700 |
| C | -1.35627400 | -2.12541200 | 0.81911100 |
| H | -1.08911400 | -1.72198200 | 1.79808800 |
| C | -2.43524400 | -1.60170100 | 0.21034200 |
| C | -2.95501400 | -2.08538400 | -1.11715600 |
| H | -4.02438400 | -2.31264000 | -1.04476000 |
| H | -2.85472100 | -1.30718200 | -1.88313000 |
| H | -2.44252100 | -2.97796600 | -1.47830700 |
| C | -3.25427900 | -0.52757100 | 0.88724200 |
| H | -4.16666900 | -1.00054100 | 1.27639000 |
| H | -2.70422200 | -0.13620400 | 1.75113000 |
| C | -2.52912700 | 1.38647800 | -0.65098800 |
| H | -2.12537900 | 0.96167500 | -1.57372300 |
| C | -3.67655600 | 0.63780400 | -0.02542300 |
| H | -4.30273700 | 1.31737300 | 0.55785800 |
| H | -4.32121500 | 0.25499000 | -0.82482800 |
| C | -2.00981800 | 2.55197200 | -0.23607400 |
| C | -2.45614100 | 3.29066800 | 0.99841400 |
| H | -3.18359500 | 2.73783100 | 1.59316300 |
| H | -1.59488400 | 3.51253200 | 1.64037400 |
| H | -2.89661000 | 4.25659900 | 0.72640800 |

| | | | |
|---|---|---|---|
| C | -0.94641600 | 3.26246600 | -1.03333300 |
| H | -0.59347200 | 2.65985400 | -1.87623200 |
| H | -1.34206400 | 4.20105200 | -1.43795400 |
| H | -0.09079200 | 3.53904300 | -0.40456700 |
| C | 2.18133200 | -2.01333800 | 1.24910800 |
| H | 2.79282600 | -2.89352100 | 1.03305700 |
| H | 2.83463500 | -1.21644500 | 1.60285300 |
| H | 1.48573000 | -2.27449800 | 2.05228000 |
| C | 0.62439800 | -2.75741300 | -0.63916800 |
| H | 0.18134500 | -2.40683200 | -1.57997000 |
| H | 1.30965300 | -3.57817800 | -0.87620200 |

**IM2**

Sum of electronic and thermal Free Energies = -781.158944

| | | | |
|---|---|---|---|
| C | -0.56688800 | 1.94362200 | -0.04962900 |
| C | -2.01346000 | 2.37533800 | 0.10907500 |
| C | -2.96656100 | 1.60060200 | 0.64186200 |
| C | -0.31266800 | 0.65612300 | -0.85824600 |
| C | -2.80317300 | 0.18570200 | 1.14383100 |
| C | -0.71754300 | -0.57760200 | -0.07075200 |
| C | -2.24015800 | -0.82406900 | 0.11999100 |
| H | -0.01770500 | 2.75470900 | -0.53988900 |
| H | -2.16465700 | 0.16574400 | 2.04016700 |
| H | -0.84031300 | 0.69036100 | -1.81778900 |
| H | -0.28555600 | -0.49689800 | 0.93829000 |
| H | -0.10460700 | 1.82241400 | 0.94219700 |
| H | -3.96764600 | 2.01974500 | 0.71760200 |
| H | 0.75885300 | 0.62569800 | -1.07593400 |
| H | -3.78254200 | -0.18763800 | 1.46280400 |
| C | -2.31478100 | 3.77574500 | -0.35536200 |
| H | -3.36254500 | 4.03818600 | -0.19795500 |
| H | -1.69366700 | 4.50205500 | 0.18152700 |
| H | -2.08619800 | 3.88829800 | -1.42181000 |
| C | -1.32707500 | -3.03243100 | -0.27514100 |
| H | -1.85518400 | -3.37985100 | -1.16555100 |
| H | -0.89357600 | -3.92041600 | 0.19170900 |
| C | -0.24785000 | -2.02002300 | -0.72457300 |
| H | -0.19676900 | -1.86070400 | -1.80561300 |
| C | 1.05648300 | -2.10087300 | -0.13308200 |
| C | 1.25398000 | -2.65430900 | 1.22379400 |
| H | 1.90111500 | -3.53875800 | 1.12597800 |
| H | 1.81293500 | -1.94630800 | 1.84308700 |
| H | 0.32805500 | -2.94083400 | 1.71818600 |
| C | 2.23994600 | -1.63909100 | -0.88853300 |
| H | 2.53092800 | -2.56739400 | -1.42280000 |
| H | 1.92784300 | -0.95654000 | -1.68611400 |
| C | 3.11836500 | 0.14284800 | 0.71864800 |
| H | 2.96453600 | 0.00215000 | 1.78816000 |
| C | 3.43718400 | -1.09448100 | -0.09283100 |
| H | 4.23340100 | -0.88811500 | -0.81340700 |
| H | 3.83006800 | -1.87648900 | 0.56426600 |
| C | 3.08154600 | 1.40008900 | 0.25201200 |
| C | 3.31351400 | 1.76965300 | -1.18841300 |
| H | 3.51250100 | 0.91263700 | -1.83543100 |
| H | 2.44350400 | 2.30574400 | -1.58771400 |
| H | 4.16233000 | 2.45737500 | -1.26881300 |
| C | 2.84616100 | 2.56752900 | 1.17226400 |
| H | 2.60497300 | 2.24662700 | 2.18810400 |
| H | 3.74340900 | 3.19497900 | 1.21522700 |
| H | 2.03497500 | 3.20387800 | 0.80283500 |
| C | -3.01093000 | -0.74024200 | -1.20359800 |
| H | -4.04488400 | -1.05900500 | -1.03679300 |
| H | -3.04089600 | 0.27957700 | -1.58960200 |
| H | -2.58822100 | -1.38529000 | -1.98044600 |
| C | -2.27233200 | -2.25962000 | 0.65438800 |
| H | -1.90476700 | -2.27456000 | 1.68932500 |
| H | -3.28224200 | -2.67843500 | 0.66197500 |

**TS_2-3**

Sum of electronic and thermal Free Energies = -781.157424

| | | | |
|---|---|---|---|
| C | 1.50434700 | 1.80043100 | -0.79279000 |
| C | 2.94742000 | 1.84099100 | -0.32451300 |
| C | 3.72147300 | 0.75066800 | -0.26391600 |
| C | 0.56116900 | 0.91856100 | 0.04513300 |
| C | 3.29183900 | -0.65459600 | -0.61388700 |
| C | 0.78505700 | -0.56824200 | -0.21030200 |
| C | 2.12470100 | -1.19814000 | 0.23514400 |
| H | 1.10677700 | 2.82044800 | -0.79532300 |
| H | 3.00756600 | -0.71504200 | -1.67588900 |
| H | 0.67677800 | 1.14693700 | 1.11245800 |
| H | 0.72583800 | -0.72760800 | -1.29705000 |
| H | 1.46640600 | 1.45719500 | -1.83757100 |
| H | 4.74601700 | 0.87324600 | 0.08114000 |
| H | -0.47501800 | 1.16653600 | -0.22222700 |
| H | 4.14525500 | -1.32947600 | -0.48781400 |
| C | 3.46631500 | 3.19998600 | 0.06123700 |
| H | 4.50852100 | 3.15925200 | 0.38357700 |
| H | 3.39310700 | 3.89471800 | -0.78323200 |
| H | 2.86845700 | 3.62623900 | 0.87587000 |
| C | 0.41277100 | -2.93029300 | 0.46930900 |
| H | 0.39889800 | -3.28076800 | 1.50297100 |
| H | -0.12482100 | -3.67403200 | -0.12584900 |
| C | -0.28756600 | -1.49343500 | 0.46012200 |
| H | -0.47533300 | -1.16187300 | 1.48426400 |
| C | -1.53849300 | -1.61086200 | -0.26189400 |
| C | -1.54418500 | -1.88627300 | -1.70753000 |
| H | -2.41781100 | -2.46404500 | -2.01758300 |
| H | -1.64334500 | -0.89244500 | -2.18025900 |
| H | -0.61704200 | -2.33184400 | -2.06903500 |
| C | -2.83019300 | -1.48081400 | 0.43816700 |
| H | -3.18864200 | -2.52307400 | 0.54407400 |
| H | -2.67039500 | -1.09224000 | 1.44597500 |
| C | -3.40130400 | 0.72747600 | -0.69481200 |
| H | -3.24987200 | 0.91839100 | -1.75648400 |
| C | -3.89931700 | -0.65173500 | -0.31999000 |
| H | -4.77311400 | -0.59781600 | 0.33679000 |
| H | -4.22567300 | -1.18797700 | -1.21467000 |
| C | -3.15160000 | 1.72693400 | 0.16376700 |
| C | -3.35620900 | 1.62323900 | 1.65196800 |
| H | -3.95796600 | 0.76095000 | 1.94743100 |
| H | -2.38826800 | 1.56512700 | 2.16718400 |
| H | -3.85363100 | 2.52256900 | 2.02751200 |
| C | -2.63021000 | 3.05487200 | -0.31343100 |
| H | -2.43124700 | 3.05630300 | -1.38757300 |
| H | -3.35232500 | 3.84860200 | -0.09447300 |
| H | -1.70538100 | 3.31694500 | 0.21520900 |
| C | 2.41092000 | -1.00247900 | 1.72984900 |
| H | 3.35744100 | -1.49007100 | 1.98455200 |
| H | 2.50795100 | 0.05375300 | 1.98769200 |
| H | 1.63708000 | -1.44131100 | 2.36847600 |
| C | 1.83960100 | -2.67742600 | -0.05349900 |
| H | 1.88781800 | -2.85958700 | -1.13447500 |
| H | 2.55675300 | -3.35119400 | 0.42554100 |

**IM3**

Sum of electronic and thermal Free Energies = -781.16177

| | | | |
|---|---|---|---|
| C | 2.13784600 | 1.43391800 | -1.21866600 |
| C | 3.44239300 | 1.30136500 | -0.45293400 |
| C | 3.89178700 | 0.14018100 | 0.03912300 |
| C | 0.86862700 | 1.01962200 | -0.45481100 |
| C | 3.18758000 | -1.19428100 | -0.04860000 |
| C | 0.74875300 | -0.49613400 | -0.31399100 |
| C | 1.78399500 | -1.21736200 | 0.58262900 |
| H | 2.02379600 | 2.47517300 | -1.53510300 |
| H | 3.10155100 | -1.51245900 | -1.09940700 |
| H | 0.84158100 | 1.50010500 | 0.53148500 |
| H | 0.87442200 | -0.92130700 | -1.32057800 |
| H | 2.19676000 | 0.84107800 | -2.14383000 |
| H | 4.84445800 | 0.14865700 | 0.56454500 |
| H | -0.00743000 | 1.38856600 | -1.00379900 |
| H | 3.80201100 | -1.95192800 | 0.45005600 |
| C | 4.22758700 | 2.57600100 | -0.29485700 |

| | | | |
|---|---|---|---|
| H | 5.15734000 | 2.41489700 | 0.25411700 |
| H | 4.47424500 | 2.99995800 | -1.27494500 |
| H | 3.63698000 | 3.33114400 | 0.23753400 |
| C | -0.32336800 | -2.46432900 | 0.83972400 |
| H | -0.61837500 | -2.41354500 | 1.88874000 |
| H | -0.90097500 | -3.28026000 | 0.38949600 |
| C | -0.60360900 | -0.95212300 | 0.23636200 |
| H | -0.97629100 | -0.32961800 | 1.05289300 |
| C | -1.66016700 | -1.44780900 | -0.58633600 |
| C | -1.41916200 | -1.94914500 | -1.96057100 |
| H | -2.23580200 | -2.57237000 | -2.32588000 |
| H | -1.34626500 | -1.05589900 | -2.60137100 |
| H | -0.46394400 | -2.47010300 | -2.05530400 |
| C | -3.04788000 | -1.41880800 | -0.08314600 |
| H | -3.57119300 | -2.35154100 | -0.31447300 |
| H | -3.06592900 | -1.23173100 | 0.99372700 |
| C | -3.05204100 | 1.08113400 | -0.72705600 |
| H | -2.51992700 | 1.40051100 | -1.62337900 |
| C | -3.78023600 | -0.23691700 | -0.81913400 |
| H | -4.77497100 | -0.18446700 | -0.36762400 |
| H | -3.92598500 | -0.51462800 | -1.86666300 |
| C | -3.00965600 | 1.88219500 | 0.34710500 |
| C | -3.70936400 | 1.58001400 | 1.64548300 |
| H | -4.35598900 | 0.70140700 | 1.59875500 |
| H | -2.97643800 | 1.42666900 | 2.44746100 |
| H | -4.32417000 | 2.43330900 | 1.94925300 |
| C | -2.24227800 | 3.17597900 | 0.32498400 |
| H | -1.74993500 | 3.34362000 | -0.63556700 |
| H | -2.91279200 | 4.01979300 | 0.51925900 |
| H | -1.48240100 | 3.18839300 | 1.11522000 |
| C | 1.82706000 | -0.65742300 | 2.01114500 |
| H | 2.51696000 | -1.25392100 | 2.61703600 |
| H | 2.18517700 | 0.37327400 | 2.02637000 |
| H | 0.84992700 | -0.68312200 | 2.50605500 |
| C | 1.18633200 | -2.63278700 | 0.60124000 |
| H | 1.36469800 | -3.12756200 | -0.36165000 |
| H | 1.61371400 | -3.27182500 | 1.38141500 |

**TS_3-4**

Sum of electronic and thermal Free Energies = -781.151727

| | | | |
|---|---|---|---|
| C | 2.37052900 | 1.48746100 | -1.08383700 |
| C | 3.62855500 | 1.09256600 | -0.33203300 |
| C | 3.88074000 | -0.16442600 | 0.05095100 |
| C | 1.04696800 | 1.20891700 | -0.35412300 |
| C | 2.97649700 | -1.35245600 | -0.17961300 |
| C | 0.67001900 | -0.28046500 | -0.38057200 |
| C | 1.57932000 | -1.24957200 | 0.46341500 |
| H | 2.41445300 | 2.55781900 | -1.30560300 |
| H | 2.85133300 | -1.53528900 | -1.25785100 |
| H | 1.09118400 | 1.57622800 | 0.67819900 |
| H | 0.73413300 | -0.62221300 | -1.42100700 |
| H | 2.34920300 | 0.97822500 | -2.05856200 |
| H | 4.81115700 | -0.36042500 | 0.57926800 |
| H | 0.24902400 | 1.76834100 | -0.85609000 |
| H | 3.45998200 | -2.24856600 | 0.22592300 |
| C | 4.59565100 | 2.21139100 | -0.05517500 |
| H | 5.48150700 | 1.85998700 | 0.47711100 |
| H | 4.91832100 | 2.67984900 | -0.99184900 |
| H | 4.11886000 | 2.99628300 | 0.54385100 |
| C | -0.64156100 | -2.43800700 | 0.68855800 |
| H | -0.84421300 | -2.20372500 | 1.73489100 |
| H | -1.22314200 | -3.33174200 | 0.43891700 |
| C | -0.70302100 | -0.51405900 | 0.12125400 |
| H | -0.99189300 | 0.00257500 | 1.03838900 |
| C | -1.62181800 | -1.44928700 | -0.38086900 |
| C | -1.52537200 | -1.97911900 | -1.79673500 |
| H | -2.16482400 | -2.85831300 | -1.90862400 |
| H | -1.88715200 | -1.20744400 | -2.48337400 |
| H | -0.51261600 | -2.24576400 | -2.09649900 |
| C | -3.02705300 | -1.35684000 | 0.17568700 |
| H | -3.53436900 | -2.32368800 | 0.09430400 |
| H | -2.97992100 | -1.09234800 | 1.23855300 |
| C | -3.07710700 | 1.03065500 | -0.74884800 |
| H | -2.66873100 | 1.23922000 | -1.73851200 |
| C | -3.82658900 | -0.27118700 | -0.58897500 |
| H | -4.76825000 | -0.11767300 | -0.05303100 |
| H | -4.09952500 | -0.65569500 | -1.57590700 |
| C | -2.89497200 | 1.95953000 | 0.20556400 |
| C | -3.42369600 | 1.82604400 | 1.60894500 |
| H | -4.05852600 | 0.94974800 | 1.75174900 |
| H | -2.59625000 | 1.77567600 | 2.32897800 |
| H | -4.00692700 | 2.71289300 | 1.87768500 |
| C | -2.15811700 | 3.24164900 | -0.07390500 |
| H | -1.78279200 | 3.28355800 | -1.09913100 |
| H | -2.82203700 | 4.09895200 | 0.08147800 |
| H | -1.31592200 | 3.36937000 | 0.61693800 |
| C | 1.69971700 | -0.82723300 | 1.93290100 |
| H | 2.31509500 | -1.55875400 | 2.46673000 |
| H | 2.19124900 | 0.14157900 | 2.03095200 |
| H | 0.73537700 | -0.77138100 | 2.44835100 |
| C | 0.83747100 | -2.59489100 | 0.35798800 |
| H | 0.95779300 | -3.01616600 | -0.64652100 |
| H | 1.26146000 | -3.32514200 | 1.05683300 |

**IM4**

Sum of electronic and thermal Free Energies = -781.177659

| | | | |
|---|---|---|---|
| C | 2.36411700 | 1.36596200 | -1.02699100 |
| C | 3.54891200 | 0.77831300 | -0.28902000 |
| C | 3.60807300 | -0.52629100 | -0.00449300 |
| C | 1.02376100 | 1.20017300 | -0.29138600 |
| C | 2.55006100 | -1.53368000 | -0.38009400 |
| C | 0.38136600 | -0.18910700 | -0.41050800 |
| C | 1.16306200 | -1.35267600 | 0.29107900 |
| H | 2.54296700 | 2.43253300 | -1.19686100 |
| H | 2.40478600 | -1.54007100 | -1.47121000 |
| H | 1.15006500 | 1.48120400 | 0.76357900 |
| H | 0.36107800 | -0.42878000 | -1.48534200 |
| H | 2.27596600 | 0.90582000 | -2.02189000 |
| H | 4.47443900 | -0.89816100 | 0.53909200 |
| H | 0.32429000 | 1.93030500 | -0.73276200 |
| H | 2.91302100 | -2.53357800 | -0.11875200 |
| C | 4.63259400 | 1.74239200 | 0.10756300 |
| H | 5.44349100 | 1.24088100 | 0.63952400 |
| H | 5.05308600 | 2.23593800 | -0.77615300 |
| H | 4.23376800 | 2.53445400 | 0.75337200 |
| C | -1.08473600 | -2.64827700 | 0.51486200 |
| H | -1.15904700 | -2.50944500 | 1.60131300 |
| H | -1.55652500 | -3.61130200 | 0.28976800 |
| C | -1.05993500 | -0.20663500 | 0.09656300 |
| H | -1.03621400 | -0.10210600 | 1.18997400 |
| C | -1.83130600 | -1.51254600 | -0.19106500 |
| C | -1.98095400 | -1.81965300 | -1.69087000 |
| H | -2.53639000 | -2.75513400 | -1.80803000 |
| H | -2.53815500 | -1.04611200 | -2.22921300 |
| H | -1.02209500 | -1.94406300 | -2.19709800 |
| C | -3.20391600 | -1.15243800 | 0.38599200 |
| H | -4.00470200 | -1.82219400 | 0.05754700 |
| H | -3.17101400 | -1.18506300 | 1.48118000 |
| C | -2.01840800 | 0.89259400 | -0.44004800 |
| H | -1.91620400 | 1.00727000 | -1.52232700 |
| C | -3.47349600 | 0.29127600 | -0.09801200 |
| H | -4.01791600 | 0.87942700 | 0.64688300 |
| H | -4.05285300 | 0.33257600 | -1.02235500 |
| C | -1.97837300 | 2.18398200 | 0.20772500 |
| C | -1.87964900 | 2.31135800 | 1.67226100 |
| H | -2.17993500 | 1.41408900 | 2.21374800 |
| H | -0.80634300 | 2.47497000 | 1.87307300 |
| H | -2.40138900 | 3.19876200 | 2.03919800 |
| C | -2.13170100 | 3.41989700 | -0.57764100 |
| H | -1.78077500 | 3.31984800 | -1.60521300 |
| H | -3.22286500 | 3.59414000 | -0.61776600 |
| H | -1.70083000 | 4.29147100 | -0.07956600 |
| C | 1.36022000 | -1.11023400 | 1.79581300 |
| H | 1.96314600 | -1.92387200 | 2.21324300 |
| H | 1.89853000 | -0.18101600 | 1.99547400 |
| H | 0.41978300 | -1.09260000 | 2.35469200 |

| | | | |
|---|---|---|---|
| C | 0.38971100 | -2.67881700 | 0.08719900 |
| H | 0.45988900 | -2.96943300 | -0.96893900 |
| H | 0.90852200 | -3.46432100 | 0.64823500 |

**TS_4-5**

Sum of electronic and thermal Free
Energies = -781.166925

| | | | |
|---|---|---|---|
| C | 2.18661600 | 1.32121700 | -0.99384300 |
| C | 3.35726600 | 0.57848200 | -0.32757600 |
| C | 3.38343100 | -0.75761800 | -0.16889300 |
| C | 1.11309000 | 0.90914500 | -0.06415100 |
| C | 2.33204300 | -1.76560400 | -0.56029000 |
| C | 0.31248300 | -0.29501700 | -0.35921100 |
| C | 0.99816900 | -1.60597700 | 0.21470300 |
| H | 2.39058800 | 2.39359900 | -0.98139000 |
| H | 2.11913900 | -1.70823100 | -1.63671700 |
| H | 1.22414600 | 1.21703200 | 0.97830000 |
| H | 0.27671900 | -0.41829000 | -1.44986000 |
| H | 1.99331800 | 0.98688400 | -2.01603500 |
| H | 4.26163600 | -1.15593900 | 0.33629000 |
| H | -0.02007300 | 2.03356400 | -0.20907700 |
| H | 2.72603200 | -2.76913400 | -0.37288700 |
| C | 4.42682100 | 1.47719500 | 0.23059400 |
| H | 5.22115500 | 0.90004800 | 0.70655100 |
| H | 4.86456700 | 2.08978100 | -0.56444300 |
| H | 4.01036400 | 2.16503800 | 0.97620300 |
| C | -1.38922300 | -2.62582300 | 0.43462200 |
| H | -1.38625500 | -2.57087800 | 1.53041700 |
| H | -1.97020000 | -3.51512800 | 0.16894600 |
| C | -1.10054100 | -0.18504000 | 0.18205300 |
| H | -1.04196900 | -0.13577500 | 1.28047500 |
| C | -2.02694100 | -1.35889400 | -0.14693000 |
| C | -2.28930400 | -1.54478800 | -1.65354100 |
| H | -2.84479800 | -2.47583000 | -1.80209400 |
| H | -2.90311200 | -0.74074400 | -2.06774600 |
| H | -1.37820200 | -1.61075300 | -2.25558100 |
| C | -3.31709400 | -0.81768800 | 0.51246700 |
| H | -4.21856400 | -1.27573400 | 0.09727200 |
| H | -3.30642800 | -1.03306500 | 1.58652500 |
| C | -1.86323800 | 1.04061000 | -0.29394900 |
| H | -1.90588400 | 1.01054900 | -1.39015300 |
| C | -3.27940100 | 0.73525100 | 0.27618300 |
| H | -3.44240500 | 1.26423200 | 1.21947300 |
| H | -4.05751300 | 1.06592500 | -0.41538700 |
| C | -1.13260900 | 2.32069200 | 0.06991200 |
| C | -1.11287700 | 2.69584900 | 1.54342600 |
| H | -0.92279900 | 1.84254800 | 2.20088900 |
| H | -0.36127000 | 3.46526200 | 1.74192800 |
| H | -2.08484800 | 3.11690900 | 1.82076700 |
| C | -1.44503900 | 3.50571300 | -0.83197000 |
| H | -1.31632200 | 3.25661700 | -1.88824400 |
| H | -2.49307600 | 3.79095200 | -0.68025000 |
| H | -0.82562400 | 4.37338400 | -0.59184100 |
| C | 1.26592400 | -1.54698700 | 1.72483000 |
| H | 1.73397300 | -2.48700900 | 2.03410200 |
| H | 1.94879700 | -0.74106400 | 2.00498600 |
| H | 0.34957400 | -1.43746700 | 2.30814000 |
| C | 0.05190700 | -2.78958400 | -0.09389100 |
| H | 0.02845500 | -2.95469000 | -1.17832700 |
| H | 0.50198400 | -3.68940100 | 0.34150900 |

**IM5**

Sum of electronic and thermal Free
Energies = -781.173762

| | | | |
|---|---|---|---|
| C | 1.99907000 | 1.49705900 | -1.49480300 |
| C | 3.02705500 | 1.16702800 | -0.39125600 |
| C | 3.40365100 | -0.10376800 | -0.04054000 |
| C | 1.23495800 | 1.02979900 | -0.35857000 |
| C | 2.75920300 | -1.38244800 | -0.41714500 |
| C | 0.55723100 | -0.30618200 | -0.40205900 |
| C | 1.37030500 | -1.42896100 | 0.31284800 |
| H | 2.02844400 | 2.55873500 | -1.72495700 |
| H | 2.58479600 | -1.46144700 | -1.49660000 |
| H | 0.98458000 | 1.72779100 | 0.43789000 |
| H | 0.51488400 | -0.59218200 | -1.46072600 |
| H | 2.01132700 | 0.84100700 | -2.36205600 |
| H | 4.18242500 | -0.16004400 | 0.72099600 |
| H | -0.81056600 | 2.60487100 | -0.38649200 |
| H | 3.38128500 | -2.22289300 | -0.09945900 |
| C | 3.64502000 | 2.37381700 | 0.27412500 |
| H | 4.18032300 | 2.10216300 | 1.18565900 |
| H | 4.34571300 | 2.85367800 | -0.41508100 |
| H | 2.88201500 | 3.11408000 | 0.53194400 |
| C | -0.79386700 | -2.77736700 | 0.52589900 |
| H | -0.86546900 | -2.66979300 | 1.61495100 |
| H | -1.23977400 | -3.74814700 | 0.28364300 |
| C | -0.88595200 | -0.28594300 | 0.13157100 |
| H | -0.84025300 | -0.18483100 | 1.22574900 |
| C | -1.57445100 | -1.64843400 | -0.15232000 |
| C | -1.74224800 | -1.95742900 | -1.65211100 |
| H | -2.24736100 | -2.92280100 | -1.75551400 |
| H | -2.36186400 | -1.21437000 | -2.16014700 |
| H | -0.79838300 | -2.03159500 | -2.19984700 |
| C | -2.96347600 | -1.35347700 | 0.43537000 |
| H | -3.72220400 | -2.05886700 | 0.08444400 |
| H | -2.92251000 | -1.43314600 | 1.52832000 |
| C | -1.89742300 | 0.75181200 | -0.38606200 |
| H | -1.82916600 | 0.77572600 | -1.48304000 |
| C | -3.26177800 | 0.10760100 | 0.01258500 |
| H | -3.73064200 | 0.65421500 | 0.83518000 |
| H | -3.96385400 | 0.15021700 | -0.82428300 |
| C | -1.72524000 | 2.21008000 | 0.08433300 |
| C | -1.58325400 | 2.36198000 | 1.60132800 |
| H | -0.67881600 | 1.88600000 | 1.99874800 |
| H | -1.54586200 | 3.41964900 | 1.87702400 |
| H | -2.43665900 | 1.91888900 | 2.12597200 |
| C | -2.87688700 | 3.07630000 | -0.43775100 |
| H | -3.00578800 | 2.95587300 | -1.51813400 |
| H | -3.82171900 | 2.80885500 | 0.04549700 |
| H | -2.69001900 | 4.13422700 | -0.23440000 |
| C | 1.55690200 | -1.18093200 | 1.81838200 |
| H | 2.30332800 | -1.87652100 | 2.21554100 |
| H | 1.89222200 | -0.16365800 | 2.04749500 |
| H | 0.63276400 | -1.35037800 | 2.37154800 |
| C | 0.68426400 | -2.78483000 | 0.08912600 |
| H | 0.75480000 | -3.05539500 | -0.97173600 |
| H | 1.23349600 | -3.55413000 | 0.64417300 |

**TS_5-6**

Sum of electronic and thermal Free
Energies = -781.16124

| | | | |
|---|---|---|---|
| C | 2.21253700 | 1.29586700 | -1.63354100 |
| C | 2.69551400 | 1.25455900 | -0.05991200 |
| C | 3.46906900 | 0.11418400 | -0.24006000 |
| C | 1.25829800 | 1.11940700 | -0.50705800 |
| C | 2.86691500 | -1.24721400 | -0.33939300 |
| C | 0.57293100 | -0.26083700 | -0.44455500 |
| C | 1.46406000 | -1.28549800 | 0.31096600 |
| H | 2.48436800 | 2.26998000 | -2.03029500 |
| H | 2.82912200 | -1.58817200 | -1.38529200 |
| H | 0.67561900 | 1.99523400 | -0.24060300 |
| H | 0.51060600 | -0.60373300 | -1.48672400 |
| H | 2.36568300 | 0.45768300 | -2.30498900 |
| H | 4.55445400 | 0.21738300 | -0.18211500 |
| H | -1.09801000 | 2.60783700 | -0.61830700 |
| H | 3.56207500 | -1.93841000 | 0.15570400 |
| C | 3.24529000 | 2.54165400 | 0.49394400 |
| H | 3.14400700 | 2.52764500 | 1.58277600 |
| H | 4.30183900 | 2.66957500 | 0.24513500 |
| H | 2.68567400 | 3.40072800 | 0.11796600 |
| C | -0.60127500 | -2.76636800 | 0.61423600 |
| H | -0.66650400 | -2.62298200 | 1.69943400 |
| H | -0.99152700 | -3.77090300 | 0.41626200 |
| C | -0.85482500 | -0.29521400 | 0.10830800 |
| H | -0.80783100 | -0.13754600 | 1.19571600 |
| C | -1.46191200 | -1.71481400 | -0.09321700 |
| C | -1.64201200 | -2.10438100 | -1.57310200 |

| | | | |
|---|---|---|---|
| H | -2.08475200 | -3.10428200 | -1.62039000 |
| H | -2.32055600 | -1.42740100 | -2.09811400 |
| H | -0.70777700 | -2.14238100 | -2.14090600 |
| C | -2.85363300 | -1.49489900 | 0.51502400 |
| H | -3.57039700 | -2.26114400 | 0.20530600 |
| H | -2.78473200 | -1.53474700 | 1.60878300 |
| C | -1.95735900 | 0.64234800 | -0.42966400 |
| H | -1.92926400 | 0.61234600 | -1.52801000 |
| C | -3.25835300 | -0.07342500 | 0.05392700 |
| H | -3.71937100 | 0.47378500 | 0.88067600 |
| H | -4.00131300 | -0.10194200 | -0.74767800 |
| C | -1.90490000 | 2.13665900 | -0.03963800 |
| C | -1.62898900 | 2.37458200 | 1.44702900 |
| H | -0.63183600 | 2.03334000 | 1.75148700 |
| H | -1.70153300 | 3.43964300 | 1.68529100 |
| H | -2.35743200 | 1.84880800 | 2.07462000 |
| C | -3.18817300 | 2.85391100 | -0.47560600 |
| H | -3.41861000 | 2.64906700 | -1.52617100 |
| H | -4.04709000 | 2.53976800 | 0.12458000 |
| H | -3.08240800 | 3.93597000 | -0.35795300 |
| C | 1.60913300 | -0.95625100 | 1.81060600 |
| H | 2.39240800 | -1.58031800 | 2.25374700 |
| H | 1.86322600 | 0.09098100 | 2.00194600 |
| H | 0.69014000 | -1.16035200 | 2.35945000 |
| C | 0.86605400 | -2.69758000 | 0.15896900 |
| H | 0.94020900 | -3.00846100 | -0.89124700 |
| H | 1.47130900 | -3.40713000 | 0.73635000 |

**IM6**

Sum of electronic and thermal Free Energies = -781.165183

| | | | |
|---|---|---|---|
| C | 2.55691700 | 1.00587000 | -1.57460900 |
| C | 2.53716500 | 1.30970800 | 0.06723400 |
| C | 3.38526800 | 0.24454300 | -0.42524600 |
| C | 1.24859900 | 1.10959600 | -0.51321400 |
| C | 2.90147500 | -1.20112200 | -0.27400900 |
| C | 0.57506600 | -0.26814900 | -0.45938500 |
| C | 1.48481000 | -1.25891300 | 0.33293700 |
| H | 2.95907500 | 1.89558400 | -2.04888400 |
| H | 2.93732700 | -1.70486400 | -1.24713700 |
| H | 0.61964100 | 1.98963900 | -0.60279000 |
| H | 0.50674400 | -0.62963900 | -1.49411000 |
| H | 2.19744700 | 0.25028700 | -2.26523700 |
| H | 4.45609900 | 0.42721600 | -0.38968500 |
| H | -1.14962400 | 2.59951300 | -0.73156600 |
| H | 3.60776100 | -1.72391000 | 0.37893500 |
| C | 3.04547700 | 2.63338100 | 0.53055200 |
| H | 3.01193600 | 2.61127700 | 1.62612500 |
| H | 4.08226000 | 2.79967200 | 0.23130600 |
| H | 2.41086800 | 3.45435800 | 0.19104600 |
| C | -0.56987700 | -2.75267300 | 0.65227000 |
| H | -0.63658100 | -2.58858200 | 1.73450300 |
| H | -0.95147600 | -3.76409000 | 0.47365800 |
| C | -0.85453300 | -0.29294800 | 0.09218000 |
| H | -0.81185000 | -0.11027800 | 1.17427400 |
| C | -1.44425000 | -1.72524100 | -0.07620700 |
| C | -1.62353000 | -2.14722700 | -1.54684000 |
| H | -2.05337600 | -3.15345100 | -1.57157700 |
| H | -2.31263500 | -1.49050700 | -2.08385500 |
| H | -0.69041500 | -2.18734500 | -2.11661700 |
| C | -2.83670500 | -1.50654100 | 0.53193300 |
| H | -3.54802100 | -2.28111700 | 0.23089600 |
| H | -2.76620500 | -1.53573800 | 1.62576600 |
| C | -1.96720800 | 0.62197400 | -0.46207200 |
| H | -1.95343000 | 0.56320300 | -1.55940400 |
| C | -3.25466600 | -0.09246400 | 0.05835200 |
| H | -3.69720800 | 0.46507200 | 0.88837700 |
| H | -4.01532500 | -0.13220800 | -0.72581100 |
| C | -1.92175800 | 2.12666200 | -0.10816300 |
| C | -1.58100400 | 2.40175400 | 1.35818200 |
| H | -0.56322900 | 2.08419900 | 1.62015900 |
| H | -1.66154400 | 3.47020200 | 1.57770300 |
| H | -2.26798000 | 1.87610900 | 2.03114600 |
| C | -3.23164200 | 2.81905900 | -0.50362100 |
| H | -3.50744100 | 2.58304000 | -1.53645500 |
| H | -4.05885800 | 2.51443400 | 0.14376200 |
| H | -3.13133200 | 3.90479800 | -0.42095100 |
| C | 1.58982800 | -0.90446900 | 1.83008200 |
| H | 2.27994000 | -1.60170800 | 2.31508000 |
| H | 1.96611500 | 0.10669700 | 2.01971400 |
| H | 0.63457800 | -0.98508900 | 2.34793000 |
| C | 0.89751200 | -2.67804600 | 0.19788000 |
| H | 0.97715900 | -2.99919600 | -0.84855700 |
| H | 1.50790900 | -3.37610000 | 0.78284600 |

**TS_6-7**

Sum of electronic and thermal Free Energies = -781.16491

| | | | |
|---|---|---|---|
| C | 2.84576100 | 0.97995300 | -1.59493400 |
| C | 2.54244000 | 1.34795900 | -0.02017600 |
| C | 3.41885000 | 0.21130400 | -0.43681500 |
| C | 1.19259300 | 1.13355900 | -0.30513700 |
| C | 2.89262400 | -1.21580000 | -0.25070300 |
| C | 0.57444400 | -0.22963700 | -0.38609600 |
| C | 1.48311600 | -1.25861800 | 0.36847200 |
| H | 3.36506500 | 1.82688500 | -2.03393800 |
| H | 2.89902400 | -1.72456000 | -1.22197500 |
| H | 0.55234300 | 2.01308900 | -0.35760100 |
| H | 0.53447400 | -0.51949600 | -1.44778400 |
| H | 2.16190900 | 0.46285000 | -2.25661300 |
| H | 4.47365400 | 0.38501900 | -0.24138200 |
| H | -1.18352600 | 2.61775900 | -0.67303300 |
| H | 3.58542800 | -1.76040700 | 0.39764200 |
| C | 3.08204100 | 2.65998400 | 0.47612600 |
| H | 3.11936800 | 2.62706700 | 1.56876500 |
| H | 4.09712500 | 2.83208200 | 0.11183200 |
| H | 2.44528100 | 3.49625200 | 0.17725200 |
| C | -0.58731900 | -2.74613200 | 0.64331000 |
| H | -0.66907200 | -2.56986000 | 1.72309800 |
| H | -0.96645900 | -3.75887500 | 0.46728500 |
| C | -0.88379500 | -0.29082400 | 0.10991900 |
| H | -0.87848300 | -0.13193200 | 1.19658800 |
| C | -1.44704800 | -1.72425700 | -0.10676300 |
| C | -1.55929900 | -2.11655500 | -1.59151000 |
| H | -1.92300100 | -3.14679900 | -1.65694600 |
| H | -2.27409000 | -1.48838600 | -2.12913800 |
| H | -0.61100900 | -2.08137300 | -2.13712100 |
| C | -2.86510100 | -1.53357600 | 0.44911500 |
| H | -3.55285000 | -2.31074800 | 0.10353200 |
| H | -2.83841500 | -1.58499200 | 1.54393600 |
| C | -1.98417000 | 0.62338100 | -0.47065900 |
| H | -1.92677700 | 0.58155000 | -1.56754500 |
| C | -3.28162600 | -0.11550800 | -0.01296600 |
| H | -3.76180600 | 0.42107100 | 0.80976200 |
| H | -4.01090000 | -0.14764800 | -0.82662000 |
| C | -1.97434300 | 2.12251100 | -0.09063000 |
| C | -1.70468300 | 2.37542300 | 1.39428100 |
| H | -0.69951000 | 2.05891300 | 1.70356900 |
| H | -1.80010500 | 3.43967000 | 1.62695700 |
| H | -2.42039000 | 1.83585900 | 2.02459300 |
| C | -3.27499500 | 2.80404900 | -0.53297100 |
| H | -3.50000400 | 2.58389400 | -1.58146200 |
| H | -4.12590700 | 2.47591700 | 0.07063400 |
| H | -3.19389900 | 3.88914200 | -0.42589100 |
| C | 1.60091000 | -0.92562100 | 1.86909400 |
| H | 2.20801700 | -1.69416000 | 2.35703800 |
| H | 2.08733600 | 0.03655000 | 2.05840200 |
| H | 0.63507000 | -0.90829700 | 2.37547800 |
| C | 0.88223400 | -2.66873100 | 0.20571600 |
| H | 0.96945000 | -2.97669300 | -0.84389800 |
| H | 1.48684900 | -3.37652800 | 0.78454800 |

**IM7**

Sum of electronic and thermal Free Energies = -781.179705

| | | | |
|---|---|---|---|
| C | 3.09788700 | 0.91189400 | -1.56459800 |

| | | | |
|---|---|---|---|
| C | 2.44359200 | 1.48273700 | -0.29014400 |
| C | 3.38288300 | 0.06333500 | -0.42266300 |
| C | 1.22152100 | 1.02106700 | 0.16242400 |
| C | 2.77440300 | -1.31157900 | -0.27700500 |
| C | 0.54883700 | -0.21422100 | -0.25802100 |
| C | 1.40557700 | -1.37088000 | 0.43923200 |
| H | 3.86879300 | 1.57763200 | -1.94056100 |
| H | 2.65500700 | -1.73664500 | -1.28000300 |
| H | 0.79702700 | 1.54538100 | 1.02141000 |
| H | 0.65996300 | -0.36392300 | -1.34104300 |
| H | 2.41632400 | 0.52062800 | -2.31490400 |
| H | 4.27113100 | 0.28704700 | 0.16351900 |
| H | -0.80508600 | 2.52621300 | -0.28645700 |
| H | 3.48720100 | -1.93842700 | 0.26906000 |
| C | 3.09859800 | 2.69303700 | 0.33288300 |
| H | 2.82872800 | 2.79751200 | 1.38616500 |
| H | 4.18735800 | 2.63131200 | 0.26273100 |
| H | 2.78558600 | 3.59533700 | -0.19970400 |
| C | -0.76097900 | -2.76233500 | 0.57710000 |
| H | -0.88104100 | -2.60498800 | 1.65697600 |
| H | -1.16375400 | -3.75740300 | 0.35930700 |
| C | -0.92118300 | -0.30809700 | 0.14354400 |
| H | -0.97061900 | -0.21249200 | 1.23922400 |
| C | -1.53357900 | -1.68464600 | -0.18615600 |
| C | -1.55038700 | -2.00000000 | -1.69370600 |
| H | -1.92462600 | -3.01795800 | -1.84186900 |
| H | -2.21648600 | -1.32841000 | -2.24116000 |
| H | -0.56679600 | -1.94544300 | -2.17013700 |
| C | -2.97978000 | -1.43680100 | 0.27364000 |
| H | -3.68019100 | -2.16828900 | -0.13960900 |
| H | -3.03412600 | -1.51166600 | 1.36638200 |
| C | -1.91425100 | 0.69936500 | -0.45441800 |
| H | -1.74673300 | 0.72780100 | -1.54092500 |
| C | -3.28889000 | 0.01429000 | -0.18350600 |
| H | -3.85520700 | 0.54690700 | 0.58514500 |
| H | -3.90704800 | 0.02801700 | -1.08498400 |
| C | -1.79687600 | 2.15525900 | 0.03080400 |
| C | -1.90346600 | 2.32680300 | 1.54871200 |
| H | -1.12606700 | 1.78946000 | 2.10394100 |
| H | -1.82633200 | 3.38438600 | 1.81664700 |
| H | -2.86851800 | 1.96831300 | 1.92102500 |
| C | -2.83425500 | 3.03327500 | -0.67659800 |
| H | -2.76805200 | 2.92934700 | -1.76406100 |
| H | -3.84857100 | 2.75386000 | -0.37291500 |
| H | -2.69208300 | 4.08797400 | -0.42608300 |
| C | 1.59264700 | -1.13710100 | 1.94690600 |
| H | 2.11329100 | -1.99586600 | 2.38015000 |
| H | 2.19164400 | -0.24624900 | 2.16627500 |
| H | 0.63954900 | -1.03502200 | 2.47071300 |
| C | 0.72886100 | -2.73218700 | 0.19651000 |
| H | 0.83433300 | -3.00305700 | -0.86038500 |
| H | 1.27843400 | -3.49057900 | 0.76649800 |

**IM8**

Sum of electronic and thermal Free Energies = -781.11325

| | | | |
|---|---|---|---|
| C | 0.52466500 | 0.75482500 | -0.17117700 |
| C | -2.48488300 | -0.01444600 | -1.44090900 |
| C | -1.59363900 | -1.73511500 | 1.09642000 |
| C | -1.10136500 | -0.88092400 | 2.03426600 |
| C | 1.24704600 | 1.02264500 | 0.93450600 |
| C | 4.00349200 | 0.32935200 | -0.06465400 |
| H | 0.54445900 | -0.27114300 | -0.54156900 |
| H | -0.06614800 | -0.94160700 | 2.34853500 |
| H | 3.82671900 | 1.29048400 | -0.54881500 |
| C | -2.92615800 | -1.68190100 | 0.62750200 |
| H | -0.91259400 | -2.41929800 | 0.59700000 |
| C | -3.50450100 | -1.10289700 | -1.67222200 |
| H | -3.43197300 | -1.50795500 | -2.68555600 |
| H | -4.52470900 | -0.73881600 | -1.54527900 |
| C | -3.25759300 | -2.29502600 | -0.68331400 |
| H | -2.43310800 | -2.91652700 | -1.03862600 |
| H | -4.16667100 | -2.90290800 | -0.61276400 |
| C | -2.70602800 | 1.20534900 | -0.92724900 |
| H | -1.45909100 | -0.29880000 | -1.67350700 |
| C | -1.58901400 | 2.18607700 | -0.64424700 |
| C | -0.15798400 | 1.79040700 | -1.03446100 |
| H | -0.15245500 | 1.44764000 | -2.07503100 |
| H | 0.44480200 | 2.70414000 | -1.02245400 |
| C | 2.10961400 | -0.03235300 | 1.58280600 |
| H | 1.91039400 | -0.07471300 | 2.66458900 |
| H | 1.88793200 | -1.01718500 | 1.14975300 |
| C | 3.61895400 | 0.24649200 | 1.38760200 |
| H | 4.18035200 | -0.53662600 | 1.90364900 |
| H | 3.87654500 | 1.18556100 | 1.89077200 |
| C | 4.51849700 | -0.65360300 | -0.81563000 |
| C | 4.86729900 | -0.42582400 | -2.26312800 |
| H | 4.32187100 | -1.12293300 | -2.90966300 |
| H | 4.63831100 | 0.59387400 | -2.58064900 |
| C | 4.81546800 | -2.04343200 | -0.31591400 |
| H | 4.30951800 | -2.78492900 | -0.94490400 |
| H | 5.88869200 | -2.25239600 | -0.38962800 |
| H | 4.50814500 | -2.20995200 | 0.71773200 |
| H | -1.84384800 | 3.12539900 | -1.15254200 |
| H | -1.61706700 | 2.42412000 | 0.43020600 |
| C | -4.06599100 | 1.76339900 | -0.58875900 |
| H | -4.89628700 | 1.10395600 | -0.84295700 |
| H | -4.12923700 | 2.00651100 | 0.47904100 |
| H | -4.22191900 | 2.70386500 | -1.12730800 |
| C | -4.02898600 | -1.06600400 | 1.39316900 |
| H | -4.80677500 | -0.67326800 | 0.73635100 |
| H | -4.48377200 | -1.88895100 | 1.96806700 |
| H | -3.71388700 | -0.30809800 | 2.10983100 |
| C | 1.37803600 | 2.41099000 | 1.50734800 |
| H | 0.54254400 | 3.06013400 | 1.24011400 |
| H | 1.45201900 | 2.37760300 | 2.59911900 |
| H | 2.29713700 | 2.88753500 | 1.14324300 |
| H | -1.70606200 | -0.10550400 | 2.49484100 |
| H | 5.93459500 | -0.60727000 | -2.43332600 |

**TS_8-9a**

Sum of electronic and thermal Free Energies = -781.10135

| | | | |
|---|---|---|---|
| C | 0.61440900 | 0.20799600 | -0.49353900 |
| C | -2.18048100 | -1.45469400 | -0.13438700 |
| C | -1.29280400 | 0.94045900 | 1.68830600 |
| C | -0.69391400 | 1.92973300 | 0.88220400 |
| C | 1.21363900 | 1.43490300 | -0.37349000 |
| C | 3.70491900 | -0.08994900 | -0.43331500 |
| H | 0.71969800 | -0.45462000 | 0.36504800 |
| H | 0.11141200 | 2.52859500 | 1.28926900 |
| H | 3.66610800 | -0.12033200 | -1.52272000 |
| C | -2.58353800 | 0.49571600 | 1.54672400 |
| H | -0.66192300 | 0.44704500 | 2.42553400 |
| C | -3.16541600 | -1.81928100 | 0.94973300 |
| H | -3.00412700 | -2.83401400 | 1.32377200 |
| H | -4.19267300 | -1.77305000 | 0.58557700 |
| C | -2.98843100 | -0.81897200 | 2.14664600 |
| H | -2.21123000 | -1.17914900 | 2.82536600 |
| H | -3.92688500 | -0.74044800 | 2.70506900 |
| C | -2.45146700 | -0.86573200 | -1.30771000 |
| H | -1.13647200 | -1.55507500 | 0.16143800 |
| C | -1.38613100 | -0.21755900 | -2.16154200 |
| C | 0.08715200 | -0.40573400 | -1.76392600 |
| H | 0.29380500 | -1.48027200 | -1.69877500 |
| H | 0.69309200 | -0.02039900 | -2.59136600 |
| C | 2.23552300 | 1.64318400 | 0.71750900 |
| H | 2.23841400 | 2.68504900 | 1.06172800 |
| H | 1.99958400 | 0.99845000 | 1.57323600 |
| C | 3.65169400 | 1.27756400 | 0.20022400 |
| H | 4.34178000 | 1.35200100 | 1.04619700 |
| H | 3.97646200 | 2.03200900 | -0.52287500 |
| C | 3.76944400 | -1.25996200 | 0.21866900 |
| C | 3.78707100 | -2.56954100 | -0.52314400 |
| H | 2.95627400 | -3.20936100 | -0.20181900 |
| H | 3.71875800 | -2.42603600 | -1.60393200 |
| C | 3.83054200 | -1.38035700 | 1.71837900 |
| H | 2.94127100 | -1.90154400 | 2.09532100 |
| H | 4.69268400 | -1.98689700 | 2.01541600 |

| | | | |
|---|---|---|---|
| H | 3.90448100 | -0.41750400 | 2.22745300 |
| H | -1.49578800 | -0.56616400 | -3.19596900 |
| H | -1.61276000 | 0.85986600 | -2.19956100 |
| C | -3.82824200 | -0.72470300 | -1.90594700 |
| H | -4.61884700 | -1.15340700 | -1.29011300 |
| H | -4.07046600 | 0.32689200 | -2.10004200 |
| H | -3.85686900 | -1.23544300 | -2.87472500 |
| C | -3.64000400 | 1.24319400 | 0.80274700 |
| H | -4.40245000 | 0.56962200 | 0.40878900 |
| H | -4.13667400 | 1.91484200 | 1.51513900 |
| H | -3.25245600 | 1.85935400 | -0.01185400 |
| C | 1.19032500 | 2.44650500 | -1.48288100 |
| H | 0.36221200 | 2.29314900 | -2.17753800 |
| H | 1.12893600 | 3.46303900 | -1.07985800 |
| H | 2.12544300 | 2.38982400 | -2.05378600 |
| H | -1.24502000 | 2.37868400 | 0.06038000 |
| H | 4.70849900 | -3.12132300 | -0.30734800 |

**IM9a**

Sum of electronic and thermal Free
Energies = -781.13135

| | | | |
|---|---|---|---|
| C | 1.07335465 | 0.61713045 | 0.03012240 |
| C | -1.60157736 | -0.23730206 | -1.69927127 |
| C | -0.88471383 | -1.21255215 | 1.17932575 |
| C | -0.52763180 | 0.00309133 | 1.99618902 |
| C | 0.83762128 | 0.63020242 | 1.58756946 |
| C | 2.74583167 | 0.52377100 | -0.04377248 |
| H | 0.61610425 | -0.31147054 | -0.32571104 |
| H | -0.45225193 | -0.20994905 | 3.07185230 |
| H | 3.09405349 | 1.48313237 | -0.42866075 |
| C | -2.09615629 | -1.54268331 | 0.71321252 |
| H | -0.04514546 | -1.79406453 | 0.78983912 |
| C | -2.49563174 | -1.44828243 | -1.75822675 |
| H | -2.33235205 | -2.02218999 | -2.67601183 |
| H | -3.54856070 | -1.15962269 | -1.75325939 |
| C | -2.21241855 | -2.38683515 | -0.53240352 |
| H | -1.27408903 | -2.92823948 | -0.70355569 |
| H | -3.01580299 | -3.12827341 | -0.46618910 |
| C | -1.92848857 | 0.99431691 | -1.28454286 |
| H | -0.54418740 | -0.46511617 | -1.84811455 |
| C | -0.93209475 | 2.05777072 | -0.86603922 |
| C | 0.57522452 | 1.76538466 | -0.85658925 |
| H | 0.87597574 | 1.56758112 | -1.89031544 |
| H | 1.08713532 | 2.68770020 | -0.55918601 |
| C | 1.98380757 | -0.21754894 | 2.16302352 |
| H | 2.10722767 | -0.02690036 | 3.23293519 |
| H | 1.74897059 | -1.28297429 | 2.06428155 |
| C | 3.23252344 | 0.15568906 | 1.36201084 |
| H | 3.97924339 | -0.64315105 | 1.33455006 |
| H | 3.72508449 | 1.03022246 | 1.79187056 |
| C | 2.64180561 | -0.48437858 | -1.04409631 |
| C | 2.59868826 | -0.14119454 | -2.48782430 |
| H | 2.80538417 | 0.90766858 | -2.69234539 |
| H | 3.34477302 | -0.76564293 | -2.99568772 |
| C | 2.61447280 | -1.93259429 | -0.71671171 |
| H | 1.95943963 | -2.48687485 | -1.39450842 |
| H | 3.63822674 | -2.29532979 | -0.89725652 |
| H | 2.36666299 | -2.14685813 | 0.32045212 |
| H | -1.07199373 | 2.94453847 | -1.49859216 |
| H | -1.24238352 | 2.38341318 | 0.13623739 |
| C | -3.34604948 | 1.48296030 | -1.11038300 |
| H | -4.09331781 | 0.78159378 | -1.48055489 |
| H | -3.56475241 | 1.69974128 | -0.05831952 |
| H | -3.47656498 | 2.42223650 | -1.65954491 |
| C | -3.38305446 | -0.97220381 | 1.23837205 |
| H | -4.03878495 | -0.63494619 | 0.43112423 |
| H | -3.92336187 | -1.76172365 | 1.77386075 |
| H | -3.23447899 | -0.14763013 | 1.93863669 |
| C | 0.94255629 | 2.06086689 | 2.12798326 |
| H | 0.16278356 | 2.71063808 | 1.72411607 |
| H | 0.82801196 | 2.04532652 | 3.21606896 |
| H | 1.91140965 | 2.51938605 | 1.90215338 |
| H | -1.31520151 | 0.75655019 | 1.88502808 |
| H | 1.63105576 | -0.42786371 | -2.91984180 |

**TS_9a-9b**

Sum of electronic and thermal Free
Energies = -781.13096

| | | | |
|---|---|---|---|
| C | 1.01742638 | 0.54143356 | -0.00212920 |
| C | -1.80077857 | -0.35615406 | -1.59560105 |
| C | -1.02663042 | -1.17206416 | 1.26430868 |
| C | -0.59351202 | 0.06517972 | 2.00949000 |
| C | 0.78392368 | 0.61036263 | 1.53821850 |
| C | 2.58757832 | 0.54188925 | -0.15168535 |
| H | 0.65702364 | -0.43683086 | -0.32137643 |
| H | -0.50921327 | -0.09910984 | 3.09330430 |
| H | 2.95210475 | 1.55819472 | -0.32523826 |
| C | -2.26901128 | -1.49677993 | 0.88763190 |
| H | -0.22774340 | -1.78920262 | 0.84839627 |
| C | -2.74144369 | -1.53183328 | -1.57101052 |
| H | -2.61974517 | -2.16202281 | -2.45799675 |
| H | -3.78226837 | -1.20185399 | -1.56152359 |
| C | -2.46607937 | -2.40807256 | -0.29916686 |
| H | -1.56067762 | -3.00405277 | -0.46391313 |
| H | -3.30065161 | -3.10411644 | -0.16264115 |
| C | -2.07968169 | 0.91217201 | -1.26862595 |
| H | -0.75180957 | -0.63128598 | -1.71817362 |
| C | -1.03364915 | 1.95614360 | -0.93737007 |
| C | 0.45848189 | 1.60960395 | -0.96091628 |
| H | 0.72802961 | 1.30605522 | -1.98457955 |
| H | 0.99761983 | 2.54796134 | -0.77583503 |
| C | 1.89836100 | -0.31364807 | 2.05858716 |
| H | 2.08531302 | -0.17059136 | 3.12795195 |
| H | 1.60741348 | -1.36220959 | 1.92394830 |
| C | 3.14994649 | -0.00296844 | 1.23460114 |
| H | 3.81350239 | -0.86771421 | 1.13325704 |
| H | 3.74771830 | 0.80577440 | 1.66007370 |
| C | 3.08715792 | -0.34795401 | -1.17683035 |
| C | 4.06020905 | 0.14415685 | -2.16339943 |
| H | 3.68440450 | 1.07337295 | -2.61123086 |
| H | 4.96257365 | 0.44666396 | -1.60765156 |
| C | 2.64935331 | -1.74890254 | -1.25176520 |
| H | 1.94112853 | -1.78355271 | -2.10013546 |
| H | 3.47489054 | -2.40920111 | -1.53429070 |
| H | 2.13138610 | -2.10243186 | -0.35999691 |
| H | -1.16853778 | 2.81550439 | -1.60824561 |
| H | -1.29110216 | 2.34333041 | 0.05914734 |
| C | -3.47467747 | 1.46720941 | -1.11434192 |
| H | -4.25429507 | 0.76595751 | -1.41119727 |
| H | -3.66395955 | 1.77739724 | -0.07982898 |
| H | -3.58345613 | 2.36263273 | -1.73678266 |
| C | -3.51173967 | -0.84964740 | 1.42942479 |
| H | -4.16849173 | -0.50341605 | 0.62578026 |
| H | -4.07963612 | -1.59197634 | 2.00234396 |
| H | -3.30265657 | -0.01086536 | 2.09663975 |
| C | 0.98443902 | 2.03362788 | 2.06993143 |
| H | 0.23795773 | 2.72093794 | 1.66228100 |
| H | 0.88536694 | 2.04540168 | 3.15961952 |
| H | 1.97387049 | 2.43654791 | 1.82374285 |
| H | -1.34945032 | 0.84769315 | 1.87778445 |
| H | 4.32989943 | -0.58392652 | -2.92725924 |

**IM9b**

Sum of electronic and thermal Free
Energies = -781.13175

| | | | |
|---|---|---|---|
| C | 1.00350500 | 0.24239100 | -0.49336300 |
| C | -1.93102300 | -1.32416400 | -0.91581300 |
| C | -1.06853800 | 0.18525000 | 1.61756300 |
| C | -0.53938800 | 1.53432700 | 1.20018600 |
| C | 0.83515500 | 1.44960900 | 0.48433500 |
| C | 2.51723400 | 0.02194900 | -0.58772900 |
| H | 0.56586600 | -0.62458600 | 0.00076100 |
| H | -0.41184300 | 2.22400300 | 2.04744900 |
| H | 2.99628000 | 0.52680400 | -1.42819300 |
| C | -2.34232100 | -0.22452800 | 1.60513200 |

| | | | |
|---|---|---|---|
| H | -0.32305500 | -0.59438900 | 1.78634600 |
| C | -2.93160100 | -2.02290100 | -0.03320400 |
| H | -2.89094800 | -3.10893500 | -0.16500500 |
| H | -3.95122300 | -1.71578000 | -0.27504700 |
| C | -2.64022200 | -1.69786300 | 1.47374300 |
| H | -1.77447200 | -2.28324600 | 1.80504800 |
| H | -3.50109600 | -2.00944500 | 2.07484600 |
| C | -2.12344300 | -0.20508900 | -1.62601500 |
| H | -0.90924100 | -1.69174200 | -0.80838800 |
| C | -1.00840200 | 0.65387200 | -2.18563200 |
| C | 0.46026500 | 0.29847900 | -1.93658000 |
| H | 0.67021000 | -0.67675400 | -2.39858000 |
| H | 1.05672500 | 1.02944800 | -2.49868100 |
| C | 1.92329200 | 1.15004600 | 1.53415400 |
| H | 2.17106700 | 2.03156000 | 2.13620300 |
| H | 1.57807100 | 0.37845400 | 2.23121500 |
| C | 3.17760600 | 0.66940600 | 0.80629300 |
| H | 3.79212900 | 0.02128500 | 1.44441000 |
| H | 3.84467300 | 1.44562100 | 0.42853200 |
| C | 3.18155500 | -1.16003900 | -0.17908600 |
| C | 4.55447700 | -1.45236700 | -0.67277100 |
| H | 4.44479800 | -2.26110200 | -1.40987500 |
| H | 5.01542800 | -0.59948600 | -1.17241700 |
| C | 2.52227100 | -2.18707000 | 0.67483000 |
| H | 1.96601300 | -2.84080500 | -0.01360300 |
| H | 3.24630500 | -2.79989700 | 1.21287300 |
| H | 1.79074700 | -1.76469800 | 1.36574600 |
| H | -1.13490800 | 0.72893300 | -3.27425900 |
| H | -1.19431500 | 1.67359200 | -1.81774800 |
| C | -3.47559800 | 0.39921300 | -1.91775900 |
| H | -4.30804400 | -0.23207600 | -1.60777400 |
| H | -3.58415700 | 1.37695700 | -1.43329300 |
| H | -3.57558900 | 0.56920600 | -2.99575500 |
| C | -3.52383300 | 0.69703000 | 1.49919700 |
| H | -4.21200700 | 0.38075700 | 0.70977600 |
| H | -4.08649500 | 0.66373700 | 2.43946500 |
| H | -3.24223000 | 1.73729900 | 1.32251400 |
| C | 1.13884700 | 2.78058300 | -0.21222100 |
| H | 0.41337900 | 2.98977800 | -1.00253400 |
| H | 1.09216200 | 3.60333700 | 0.50776700 |
| H | 2.13552000 | 2.79716400 | -0.66985000 |
| H | -1.26063600 | 2.01118700 | 0.52671700 |
| H | 5.20185500 | -1.83497500 | 0.11978400 |

**TS_9b-10a**
Sum of electronic and thermal Free
Energies = -781.11374

| | | | |
|---|---|---|---|
| C | 0.92080467 | 0.58874750 | -0.65791002 |
| C | -2.18779525 | -0.16420521 | -1.62566395 |
| C | -0.91757992 | -1.19605353 | 0.91684200 |
| C | -0.42091675 | 0.03567488 | 1.63054747 |
| C | 1.00448195 | 0.50680021 | 1.29979831 |
| C | 2.29801380 | 0.70314340 | -0.57947344 |
| H | 0.51848524 | -0.40441763 | -0.82466701 |
| H | -0.36192566 | -0.11083895 | 2.72194424 |
| H | 2.70262768 | 1.72038224 | -0.56725014 |
| C | -2.20537502 | -1.52923847 | 0.77206850 |
| H | -0.19530163 | -1.75607686 | 0.32409597 |
| C | -3.11790131 | -1.34603707 | -1.53514864 |
| H | -3.16390465 | -1.88674285 | -2.48534089 |
| H | -4.13674461 | -1.02910849 | -1.30318820 |
| C | -2.62237993 | -2.34206439 | -0.42630999 |
| H | -1.76943293 | -2.91244828 | -0.80976848 |
| H | -3.42585320 | -3.05028131 | -0.20044541 |
| C | -2.39005892 | 1.06707935 | -1.13842545 |
| H | -1.19158723 | -0.41409136 | -1.99342206 |
| C | -1.29285972 | 2.09670458 | -0.96253600 |
| C | 0.15934181 | 1.74680814 | -1.29949466 |
| H | 0.20777587 | 1.51109661 | -2.37188320 |
| H | 0.75618817 | 2.65785524 | -1.17453006 |
| C | 2.01831055 | -0.53390063 | 1.77204179 |
| H | 2.06054404 | -0.41219652 | 2.86251054 |
| H | 1.62346250 | -1.53820551 | 1.59637577 |
| C | 3.41011227 | -0.39325070 | 1.18261961 |
| H | 4.05934896 | -1.22546405 | 1.47364588 |
| H | 3.89416892 | 0.52810612 | 1.52615097 |
| C | 3.29747526 | -0.37320316 | -0.37515874 |
| C | 4.64808271 | 0.03835471 | -0.98332982 |
| H | 4.59723467 | 0.07429727 | -2.07474298 |
| H | 4.97398509 | 1.01615572 | -0.61594968 |
| C | 2.86092144 | -1.73543273 | -0.92494550 |
| H | 2.72299358 | -1.68521386 | -2.00893103 |
| H | 3.63956168 | -2.47483738 | -0.71943014 |
| H | 1.93266112 | -2.10344639 | -0.48168818 |
| H | -1.53529139 | 2.97732658 | -1.57254458 |
| H | -1.35614368 | 2.46250642 | 0.07233427 |
| C | -3.71928514 | 1.59320921 | -0.65503897 |
| H | -4.54885413 | 0.91453061 | -0.85161299 |
| H | -3.69539375 | 1.80662391 | 0.42061508 |
| H | -3.94403321 | 2.54027458 | -1.15848401 |
| C | -3.31522393 | -0.94192821 | 1.59518696 |
| H | -4.13448381 | -0.58013089 | 0.96767459 |
| H | -3.73285750 | -1.72681122 | 2.23650185 |
| H | -2.98685591 | -0.12761284 | 2.24547835 |
| C | 1.25591934 | 1.91624477 | 1.80637587 |
| H | 0.65304374 | 2.65232070 | 1.26907045 |
| H | 0.95151456 | 1.95391480 | 2.85817196 |
| H | 2.30568293 | 2.21190652 | 1.75287964 |
| H | -1.12345111 | 0.86014163 | 1.47383794 |
| H | 5.40746329 | -0.69762598 | -0.70649717 |

**IM10a**
Sum of electronic and thermal Free
Energies = -781.12555

| | | | |
|---|---|---|---|
| C | 0.99161556 | 0.59687665 | -1.53774412 |
| C | -2.19287585 | -0.11408724 | -1.80987609 |
| C | -0.92323817 | -0.95827166 | 0.91338023 |
| C | -0.51934780 | 0.06724452 | 1.94017562 |
| C | 0.90244931 | 0.41791594 | 2.01800552 |
| C | 2.10340831 | 0.77094235 | -0.80778768 |
| H | 0.68986985 | -0.41901793 | -1.78620008 |
| H | -0.67005469 | -0.33294524 | 2.96969199 |
| H | 2.43125182 | 1.79573949 | -0.60240292 |
| C | -2.13543659 | -1.51685803 | 0.81008507 |
| H | -0.21033910 | -1.11923356 | 0.11165457 |
| C | -3.12404556 | -1.25250660 | -1.50090002 |
| H | -3.34680217 | -1.82374068 | -2.40697660 |
| H | -4.08169697 | -0.89760078 | -1.11048206 |
| C | -2.48281753 | -2.23421966 | -0.47003372 |
| H | -1.57901439 | -2.66688745 | -0.91323284 |
| H | -3.18265690 | -3.05466846 | -0.27989399 |
| C | -2.19070695 | 1.08319736 | -1.20955720 |
| H | -1.38831971 | -0.35145674 | -2.50525393 |
| C | -1.09239859 | 2.10919937 | -1.37627060 |
| C | 0.17634424 | 1.71204567 | -2.14247579 |
| H | -0.09341096 | 1.42966667 | -3.16690736 |
| H | 0.80753800 | 2.60320112 | -2.22331742 |
| C | 1.93799650 | -0.61756786 | 1.94141726 |
| H | 2.22461062 | -0.70431554 | 3.00977072 |
| H | 1.51936834 | -1.57924175 | 1.63962975 |
| C | 3.23103798 | -0.27180674 | 1.17321667 |
| H | 3.99256577 | -1.00042005 | 1.46909725 |
| H | 3.60152712 | 0.71162553 | 1.48454541 |
| C | 3.07516636 | -0.30151928 | -0.36349520 |
| C | 4.45594899 | 0.04936798 | -0.95382684 |
| H | 4.41354584 | 0.04725852 | -2.04598118 |
| H | 4.78795130 | 1.04072159 | -0.62883099 |
| C | 2.68391264 | -1.70370492 | -0.84156559 |
| H | 2.68895600 | -1.74895713 | -1.93406392 |
| H | 3.40737103 | -2.43881077 | -0.47521707 |
| H | 1.69072701 | -2.01619377 | -0.50372269 |
| H | -1.51414737 | 3.00776148 | -1.84605451 |
| H | -0.79638223 | 2.43374215 | -0.36349865 |
| C | -3.26510325 | 1.53717802 | -0.25197747 |
| H | -4.19743415 | 0.98151226 | -0.35637370 |
| H | -2.93620167 | 1.43598485 | 0.79174326 |
| H | -3.49098075 | 2.59691794 | -0.40903450 |
| C | -3.23873117 | -1.35412943 | 1.81582450 |

| | | | |
|---|---|---|---|
| H | -4.14700285 | -0.97938265 | 1.33116154 |
| H | -3.49246271 | -2.32616084 | 2.25241231 |
| H | -2.98686386 | -0.67138130 | 2.63139706 |
| C | 1.25317112 | 1.80040983 | 2.39263925 |
| H | 1.14687916 | 2.40812784 | 1.48116727 |
| H | 0.52032785 | 2.20065170 | 3.10138835 |
| H | 2.26904699 | 1.91168261 | 2.76993069 |
| H | -1.13037934 | 0.97863635 | 1.90236030 |
| H | 5.20632843 | -0.68274694 | -0.63878326 |

**TS_10a-10b**

Sum of electronic and thermal Free Energies = -781.12350

| | | | |
|---|---|---|---|
| C | 1.01720827 | 0.55714594 | -1.59756621 |
| C | -2.19273305 | -0.04653561 | -1.82111559 |
| C | -0.95023583 | -1.06411209 | 0.99276558 |
| C | -0.52246109 | -0.24262997 | 2.20947378 |
| C | 0.81517462 | 0.35139406 | 2.02320494 |
| C | 2.11103760 | 0.76904353 | -0.85189849 |
| H | 0.70941718 | -0.46760627 | -1.80191413 |
| H | -0.42708799 | -0.91803148 | 3.07897325 |
| H | 2.42387468 | 1.80603466 | -0.68765394 |
| C | -2.18440585 | -1.54331174 | 0.80759080 |
| H | -0.20729708 | -1.19621918 | 0.21304289 |
| C | -3.16150091 | -1.14728506 | -1.49294754 |
| H | -3.44263009 | -1.68217324 | -2.40528934 |
| H | -4.08942229 | -0.75923075 | -1.06328286 |
| C | -2.52820921 | -2.17818266 | -0.51692696 |
| H | -1.62580321 | -2.59336228 | -0.97961833 |
| H | -3.23043350 | -3.00559250 | -0.36699795 |
| C | -2.09803150 | 1.14134113 | -1.21041283 |
| H | -1.45495176 | -0.29869976 | -2.58288696 |
| C | -1.00634619 | 2.14368672 | -1.51075028 |
| C | 0.22907505 | 1.65268105 | -2.27435524 |
| H | -0.06832959 | 1.30735689 | -3.27088415 |
| H | 0.88763097 | 2.51332427 | -2.43132123 |
| C | 1.97455396 | -0.54087265 | 1.97945546 |
| H | 2.23843275 | -0.50513684 | 3.06244292 |
| H | 1.66153148 | -1.57288826 | 1.79421404 |
| C | 3.23196860 | -0.14993562 | 1.19595928 |
| H | 4.03595310 | -0.81682067 | 1.52542230 |
| H | 3.54992162 | 0.86505671 | 1.45950392 |
| C | 3.08722939 | -0.26756426 | -0.33878325 |
| C | 4.46790046 | 0.06586968 | -0.93836117 |
| H | 4.43075907 | 0.01365422 | -2.02959191 |
| H | 4.79082032 | 1.07386621 | -0.65781843 |
| C | 2.71296347 | -1.69675095 | -0.74227695 |
| H | 2.73586503 | -1.80238825 | -1.83041036 |
| H | 3.43390637 | -2.40690454 | -0.32447572 |
| H | 1.71496609 | -1.99478769 | -0.40517660 |
| H | -1.44350932 | 2.99224199 | -2.05464802 |
| H | -0.66926447 | 2.57040506 | -0.55311734 |
| C | -3.05545839 | 1.62097383 | -0.14949713 |
| H | -3.95655883 | 1.01273724 | -0.06960006 |
| H | -2.56754940 | 1.62551721 | 0.83617446 |
| H | -3.36344609 | 2.65295397 | -0.35114556 |
| C | -3.30321531 | -1.42028535 | 1.80185496 |
| H | -4.19095056 | -0.98295996 | 1.33195040 |
| H | -3.59390391 | -2.41499182 | 2.15721794 |
| H | -3.04823438 | -0.81427326 | 2.67408827 |
| C | 0.94614340 | 1.81173590 | 2.10149152 |
| H | 0.22861858 | 2.26341122 | 1.40427982 |
| H | 0.59336995 | 2.11172374 | 3.10142710 |
| H | 1.94837049 | 2.19440222 | 1.92440433 |
| H | -1.25763713 | 0.52856360 | 2.45644408 |
| H | 5.22208933 | -0.64521555 | -0.58584048 |

**IM10b**

Sum of electronic and thermal Free Energies = -781.13116

| | | | |
|---|---|---|---|
| C | 1.05794309 | 0.60436818 | -2.02272670 |
| C | -1.99746214 | 0.03252142 | -1.65772325 |
| C | -0.55685602 | -1.63982999 | 1.56739899 |
| C | -0.22088851 | -1.42123059 | 3.07165286 |
| C | 0.51115525 | -0.48119086 | 2.25954724 |
| C | 1.84363388 | 0.87137951 | -0.97829843 |
| H | 1.06827631 | -0.40337895 | -2.43635971 |
| H | 0.32126624 | -2.26953702 | 3.48221281 |
| H | 1.87497012 | 1.89662986 | -0.59411044 |
| C | -1.79537328 | -1.30750293 | 1.04227350 |
| H | 0.01935298 | -2.39541707 | 1.04612326 |
| C | -2.96866134 | -1.01863615 | -1.20166345 |
| H | -3.30232269 | -1.62357820 | -2.05109638 |
| H | -3.86892534 | -0.59372851 | -0.75213826 |
| C | -2.26294144 | -1.97400754 | -0.21339250 |
| H | -1.42642317 | -2.48069355 | -0.70403067 |
| H | -2.96871816 | -2.75582644 | 0.11098003 |
| C | -2.04342742 | 1.35829321 | -1.46782836 |
| H | -1.13119375 | -0.37990846 | -2.16867820 |
| C | -0.91707664 | 2.26404843 | -1.91407165 |
| C | 0.20038013 | 1.62427257 | -2.74406755 |
| H | -0.23897953 | 1.16532045 | -3.63557561 |
| H | 0.84811198 | 2.43009897 | -3.10568134 |
| C | 1.97811619 | -0.82824844 | 2.03584890 |
| H | 2.38152762 | -0.77884087 | 3.05835112 |
| H | 2.07207716 | -1.88059399 | 1.74722206 |
| C | 2.89419648 | 0.05338688 | 1.17835594 |
| H | 3.90640101 | -0.22103497 | 1.49911875 |
| H | 2.77831761 | 1.10672648 | 1.46405051 |
| C | 2.86958447 | -0.05977744 | -0.36491334 |
| C | 4.24523558 | 0.43886473 | -0.86111291 |
| H | 4.27906849 | 0.44074191 | -1.95365731 |
| H | 4.44190947 | 1.45893645 | -0.51415094 |
| C | 2.68907287 | -1.51377041 | -0.80539738 |
| H | 2.87132619 | -1.62435344 | -1.87778740 |
| H | 3.40349854 | -2.16173529 | -0.28597490 |
| H | 1.67510332 | -1.87887053 | -0.60043087 |
| H | -1.35127254 | 3.09143010 | -2.48997849 |
| H | -0.48479187 | 2.73562372 | -1.01775093 |
| C | -3.19120941 | 2.10178676 | -0.83179151 |
| H | -4.00563187 | 1.45635014 | -0.49757289 |
| H | -2.84474263 | 2.70080539 | 0.02030757 |
| H | -3.61434054 | 2.81084577 | -1.55122946 |
| C | -2.75890731 | -0.37369926 | 1.67921989 |
| H | -2.69155756 | 0.58561973 | 1.14713204 |
| H | -3.78035053 | -0.73706904 | 1.53576711 |
| H | -2.58565116 | -0.19535843 | 2.73803582 |
| C | 0.12036404 | 0.96591438 | 2.14531011 |
| H | 0.18838042 | 1.30662074 | 1.10758582 |
| H | -0.87161604 | 1.17526935 | 2.54220501 |
| H | 0.84018361 | 1.54279652 | 2.73668638 |
| H | -1.05428337 | -1.07754429 | 3.67449072 |
| H | 5.04709362 | -0.20717537 | -0.48786865 |

**TS_10b-10c**

Sum of electronic and thermal Free Energies = -781.12380

| | | | |
|---|---|---|---|
| C | 1.08220080 | 0.33667631 | -1.72305482 |
| C | -2.27664493 | 0.06809754 | -1.51957016 |
| C | -0.90286663 | -1.89775394 | 1.00411279 |
| C | 0.04422436 | -1.53431772 | 2.13290850 |
| C | 0.77772723 | -0.26298238 | 1.92281911 |
| C | 2.10487983 | 0.80993657 | -1.00430563 |
| H | 0.87574065 | -0.73383290 | -1.73868005 |
| H | 0.74489374 | -2.34715967 | 2.33513058 |
| H | 2.28519732 | 1.89001465 | -1.03766055 |
| C | -2.20342638 | -1.59133992 | 0.93203065 |
| H | -0.44210352 | -2.46599158 | 0.19910916 |
| C | -3.45663732 | -0.75493556 | -1.08415762 |
| H | -4.00132470 | -1.10509420 | -1.96847426 |
| H | -4.16827025 | -0.16997652 | -0.49615568 |
| C | -3.00177038 | -1.99249167 | -0.28242603 |
| H | -2.39908655 | -2.64267396 | -0.92517153 |
| H | -3.88205749 | -2.56603419 | 0.03012331 |
| C | -2.02900497 | 1.36355953 | -1.27878379 |
| H | -1.54880852 | -0.48945252 | -2.11049848 |
| C | -0.81442391 | 2.07660146 | -1.83434999 |

| | | | |
|---|---|---|---|
| C | 0.22876704 | 1.24191551 | -2.58815537 |
| H | -0.25929920 | 0.65956772 | -3.37526756 |
| H | 0.89557539 | 1.94288776 | -3.10033251 |
| C | 2.21396467 | -0.21520637 | 2.20320053 |
| H | 2.22661362 | 0.34537762 | 3.16160166 |
| H | 2.59625141 | -1.21580223 | 2.40951524 |
| C | 3.16208184 | 0.54831699 | 1.24649366 |
| H | 4.16037681 | 0.41081423 | 1.67491196 |
| H | 2.95793695 | 1.62388762 | 1.27383912 |
| C | 3.15339931 | 0.05009545 | -0.22177675 |
| C | 4.52268118 | 0.42181233 | -0.82651486 |
| H | 4.54975890 | 0.17055173 | -1.88993604 |
| H | 4.71841155 | 1.49445856 | -0.72682253 |
| C | 2.96806771 | -1.46524427 | -0.30479035 |
| H | 3.06979361 | -1.80429319 | -1.33905409 |
| H | 3.72450038 | -1.98462936 | 0.29304104 |
| H | 1.97698374 | -1.78673902 | 0.04352699 |
| H | -1.17791191 | 2.86680074 | -2.50505804 |
| H | -0.31202009 | 2.61257666 | -1.01355177 |
| C | -2.93749160 | 2.27954554 | -0.49669337 |
| H | -3.84937961 | 1.79636939 | -0.14485667 |
| H | -2.41140053 | 2.69708010 | 0.37242785 |
| H | -3.23336775 | 3.13439095 | -1.11455777 |
| C | -2.95287180 | -0.78431290 | 1.95615710 |
| H | -3.09070898 | 0.24371990 | 1.59669909 |
| H | -3.95126075 | -1.20163137 | 2.11588949 |
| H | -2.45202502 | -0.73493608 | 2.92711346 |
| C | 0.01924327 | 0.94824413 | 1.59610170 |
| H | -0.56629406 | 0.75438876 | 0.68150122 |
| H | -0.73337048 | 1.09967525 | 2.38567181 |
| H | 0.63953326 | 1.83505077 | 1.47693838 |
| H | -0.53690029 | -1.36525605 | 3.05670456 |
| H | 5.32792277 | -0.12095464 | -0.32111028 |

**IM10c**

Sum of electronic and thermal Free Energies = -781.12919

| | | | |
|---|---|---|---|
| C | 1.25181766 | -0.22208890 | -1.70482985 |
| C | -2.54780704 | 0.30713607 | -1.39163339 |
| C | -1.26175860 | -1.85351170 | 0.48595397 |
| C | 0.03553500 | -1.85367881 | 1.24036776 |
| C | 0.62217298 | -0.53754373 | 1.58422723 |
| C | 1.77769893 | 0.59220786 | -0.77470165 |
| H | 1.73089764 | -1.18835255 | -1.86949404 |
| H | 0.80510449 | -2.47462053 | 0.76850689 |
| H | 1.32543067 | 1.57675088 | -0.62292274 |
| C | -2.47940579 | -1.62248568 | 0.99501392 |
| H | -1.15810432 | -1.99051549 | -0.58804181 |
| C | -3.69162509 | 0.04393881 | -0.45285339 |
| H | -4.64143506 | 0.18993731 | -0.98171236 |
| H | -3.69657992 | 0.74280950 | 0.39148962 |
| C | -3.65393073 | -1.41506651 | 0.06775428 |
| H | -3.58809671 | -2.09347418 | -0.78963086 |
| H | -4.58966520 | -1.64097430 | 0.58784940 |
| C | -1.71812396 | 1.35599195 | -1.46820210 |
| H | -2.39794049 | -0.49730709 | -2.11385088 |
| C | -0.62276350 | 1.39002025 | -2.52700275 |
| C | 0.17042841 | 0.09215219 | -2.70536314 |
| H | -0.50369606 | -0.76729459 | -2.78742990 |
| H | 0.68494863 | 0.12531095 | -3.67637794 |
| C | 1.99836880 | -0.48631513 | 2.10828334 |
| H | 1.87636189 | -0.20624431 | 3.16905094 |
| H | 2.47079851 | -1.47036594 | 2.07166304 |
| C | 2.89595787 | 0.59257223 | 1.46149760 |
| H | 3.86287262 | 0.56040924 | 1.97393864 |
| H | 2.47516852 | 1.58725016 | 1.64656790 |
| C | 3.09591051 | 0.38636292 | -0.05101433 |
| C | 4.06117624 | 1.48740730 | -0.53426627 |
| H | 4.23245813 | 1.40023112 | -1.61011956 |
| H | 3.65819570 | 2.48537065 | -0.33346978 |
| C | 3.72657252 | -0.98122701 | -0.33032857 |
| H | 4.01125458 | -1.06891207 | -1.38225941 |
| H | 4.63394399 | -1.10507805 | 0.26917365 |
| H | 3.05531304 | -1.81631575 | -0.10163529 |
| H | -1.08068921 | 1.64328411 | -3.49060416 |
| H | 0.06849768 | 2.21361042 | -2.31321813 |
| C | -1.84683483 | 2.61115906 | -0.64472538 |
| H | -2.60027599 | 2.53901124 | 0.14238609 |
| H | -0.88728767 | 2.88847742 | -0.18958978 |
| H | -2.12950248 | 3.44840642 | -1.29344806 |
| C | -2.78241194 | -1.44420858 | 2.45791022 |
| H | -3.22175074 | -0.45539339 | 2.64183165 |
| H | -3.53274735 | -2.17774570 | 2.77000099 |
| H | -1.91507545 | -1.56348360 | 3.11298213 |
| C | -0.24195498 | 0.64210562 | 1.68070068 |
| H | -0.89920822 | 0.69818528 | 0.80499835 |
| H | -0.91538427 | 0.45295855 | 2.53460968 |
| H | 0.30014161 | 1.56906009 | 1.86039950 |
| H | -0.07788203 | -2.30071041 | 2.25187487 |
| H | 5.02614925 | 1.40028010 | -0.02473402 |

**TS_10c-11**

Sum of electronic and thermal Free Energies = -781.12499

| | | | |
|---|---|---|---|
| C | 1.15218754 | -0.33528269 | -1.44692788 |
| C | -2.62834260 | 0.31559037 | -1.42545877 |
| C | -1.25201336 | -1.81003822 | 0.37844437 |
| C | 0.07257566 | -1.79937906 | 1.08151895 |
| C | 0.73002317 | -0.46153564 | 1.31150251 |
| C | 1.70263209 | 0.48955855 | -0.50900624 |
| H | 1.59631360 | -1.32553797 | -1.56600838 |
| H | 0.79086344 | -2.48421095 | 0.61902572 |
| H | 1.26875982 | 1.48673515 | -0.41206816 |
| C | -2.45130274 | -1.56449194 | 0.92735220 |
| H | -1.20826998 | -2.00554972 | -0.69109206 |
| C | -3.77996137 | 0.03483037 | -0.50541070 |
| H | -4.72843992 | 0.12102022 | -1.04877260 |
| H | -3.82442321 | 0.75129334 | 0.32183467 |
| C | -3.66930188 | -1.41078076 | 0.04483615 |
| H | -3.61449067 | -2.10357506 | -0.80208710 |
| H | -4.57663642 | -1.65662381 | 0.60477951 |
| C | -1.78238536 | 1.35166071 | -1.46033298 |
| H | -2.45167056 | -0.49478406 | -2.13517449 |
| C | -0.60773962 | 1.33297502 | -2.43011931 |
| C | 0.14682149 | 0.00250774 | -2.50103761 |
| H | -0.53196087 | -0.84297235 | -2.64814662 |
| H | 0.77060902 | -0.00550795 | -3.41267289 |
| C | 2.04314434 | -0.52258571 | 2.04511005 |
| H | 1.79019978 | -0.34264290 | 3.10071848 |
| H | 2.46543714 | -1.52871873 | 1.98190641 |
| C | 3.03530343 | 0.52085078 | 1.54910909 |
| H | 4.01323001 | 0.38920217 | 2.02182529 |
| H | 2.68870441 | 1.52990640 | 1.80240447 |
| C | 3.12818416 | 0.37204925 | 0.02277503 |
| C | 3.94133031 | 1.53774935 | -0.56290518 |
| H | 4.00741975 | 1.46717168 | -1.65213320 |
| H | 3.49553811 | 2.50374690 | -0.30565681 |
| C | 3.79783559 | -0.95202732 | -0.36120902 |
| H | 3.95637981 | -1.01152627 | -1.44201459 |
| H | 4.77773428 | -1.01890589 | 0.12009825 |
| H | 3.22110927 | -1.83222559 | -0.05878943 |
| H | -0.96680080 | 1.56666014 | -3.43920528 |
| H | 0.09195401 | 2.13922711 | -2.18038264 |
| C | -1.93940480 | 2.62030199 | -0.66441849 |
| H | -2.73279439 | 2.56177835 | 0.08305000 |
| H | -1.00533513 | 2.89923703 | -0.16125050 |
| H | -2.18498623 | 3.44842833 | -1.33954795 |
| C | -2.69739144 | -1.32788955 | 2.39286521 |
| H | -3.08855004 | -0.31588138 | 2.55897228 |
| H | -3.46386271 | -2.02123938 | 2.75339737 |
| H | -1.81232360 | -1.45907327 | 3.01922286 |
| C | -0.15956787 | 0.69569798 | 1.61033632 |
| H | -0.95317444 | 0.79218464 | 0.86769010 |
| H | -0.64333278 | 0.45934676 | 2.57040053 |
| H | 0.38643365 | 1.63124948 | 1.73766875 |
| H | -0.03484204 | -2.16942661 | 2.11765958 |
| H | 4.95862592 | 1.51743112 | -0.15991545 |

**IM11**

Sum of electronic and thermal Free Energies = -781.13573

| | | | |
|---|---|---|---|
| C | 0.76502300 | 0.71677500 | -1.11976600 |
| C | -2.26515500 | 1.54962900 | -0.33966300 |
| C | -1.25040900 | -1.37290600 | -1.13560100 |
| C | 0.02345900 | -2.08880300 | -0.77246800 |
| C | 0.84134600 | -1.41665000 | 0.35742900 |
| C | 1.20292800 | 0.09818200 | 0.07776100 |
| H | 0.85230100 | 0.13506700 | -2.03893200 |
| H | 0.65728600 | -2.18776000 | -1.66393400 |
| H | 0.96780800 | 0.71090200 | 0.95066500 |
| C | -2.45772200 | -1.48249800 | -0.55463100 |
| H | -1.18559500 | -0.66934300 | -1.96990200 |
| C | -3.50411300 | 0.75707300 | -0.03822100 |
| H | -4.39107200 | 1.36377500 | -0.25799800 |
| H | -3.56164600 | 0.48514800 | 1.02032200 |
| C | -3.56161900 | -0.51715000 | -0.91788600 |
| H | -3.47926000 | -0.22087700 | -1.96989300 |
| H | -4.53856100 | -0.99373400 | -0.79240000 |
| C | -1.39489400 | 2.12626300 | 0.49975800 |
| H | -2.07273700 | 1.63562800 | -1.41037900 |
| C | -0.14910500 | 2.82355700 | -0.03551000 |
| C | 0.41943700 | 2.13805400 | -1.27952000 |
| H | -0.21093100 | 2.25827700 | -2.16630200 |
| H | 1.38249600 | 2.59792900 | -1.58873700 |
| C | 2.20059300 | -2.12555400 | 0.56298900 |
| H | 2.13190500 | -2.88892200 | 1.34298400 |
| H | 2.51475900 | -2.63378300 | -0.35495700 |
| C | 3.17627100 | -1.01338400 | 0.91988700 |
| H | 4.22859400 | -1.30177600 | 0.82281400 |
| H | 3.01987100 | -0.67718200 | 1.95178400 |
| C | 2.86164600 | 0.14690200 | -0.04244500 |
| C | 3.38708000 | 1.48302300 | 0.46118600 |
| H | 3.12318200 | 2.31873400 | -0.19572900 |
| H | 3.02829700 | 1.70175100 | 1.47100900 |
| C | 3.39141400 | -0.15127400 | -1.44967400 |
| H | 3.23632100 | 0.68516200 | -2.13984800 |
| H | 4.47092300 | -0.31522000 | -1.38387200 |
| H | 2.94930200 | -1.05016400 | -1.88860000 |
| H | -0.36189800 | 3.87162700 | -0.27406200 |
| H | 0.61655400 | 2.85068000 | 0.74877500 |
| C | -1.54510100 | 2.18122700 | 1.99498400 |
| H | -2.45755700 | 1.70068500 | 2.34819000 |
| H | -0.68899100 | 1.70813800 | 2.49391200 |
| H | -1.56671900 | 3.22409800 | 2.33193700 |
| C | -2.81193900 | -2.48645800 | 0.50752900 |
| H | -3.09580400 | -1.98565100 | 1.44161800 |
| H | -3.68404000 | -3.06352100 | 0.18290200 |
| H | -2.00624700 | -3.18642300 | 0.72827500 |
| C | 0.04805000 | -1.39970400 | 1.67032200 |
| H | -0.86014500 | -0.79489300 | 1.57358500 |
| H | -0.23825100 | -2.41629800 | 1.95352100 |
| H | 0.65442600 | -0.98551900 | 2.48309100 |
| H | -0.17857900 | -3.11511400 | -0.44396200 |
| H | 4.48086500 | 1.44074900 | 0.49537000 |

**TS_11-12**

Sum of electronic and thermal Free Energies = -781.11708

| | | | |
|---|---|---|---|
| C | 0.38472400 | 0.78323200 | -0.91008100 |
| C | -1.42476600 | 1.62740600 | -0.43734900 |
| C | -1.54125200 | -1.44059200 | -1.20027600 |
| C | -0.33968700 | -2.21212400 | -0.74756900 |
| C | 0.47941400 | -1.53170200 | 0.39798500 |
| C | 1.04835400 | -0.07188700 | 0.14386300 |
| H | 0.06446000 | 0.22113700 | -1.78023200 |
| H | 0.32301800 | -2.38972900 | -1.60168300 |
| H | 0.98630200 | 0.45569700 | 1.10679800 |
| C | -2.70893800 | -1.26012300 | -0.57339000 |
| H | -1.40431700 | -0.82702800 | -2.08893900 |
| C | -2.79599700 | 1.11290300 | -0.01147900 |
| H | -3.43973700 | 2.00526600 | -0.00963000 |
| H | -2.76134900 | 0.75806100 | 1.02428800 |
| C | -3.44307000 | 0.01966300 | -0.88602400 |
| H | -3.36171300 | 0.28517600 | -1.94629300 |
| H | -4.50759300 | -0.03951300 | -0.64018300 |
| C | -0.71039400 | 2.45544900 | 0.43308100 |
| H | -1.37853800 | 1.89947300 | -1.49294700 |
| C | 0.60244800 | 2.99529900 | -0.03107200 |
| C | 0.94287600 | 2.15802300 | -1.25226500 |
| H | 0.45558800 | 2.54199600 | -2.15240200 |
| H | 2.00935800 | 2.11481800 | -1.46619400 |
| C | 1.74140700 | -2.40421300 | 0.63843200 |
| H | 1.59567700 | -3.09014900 | 1.47800600 |
| H | 1.94989100 | -3.02243600 | -0.24089800 |
| C | 2.88178300 | -1.42561000 | 0.87170900 |
| H | 3.87094700 | -1.85897200 | 0.69255300 |
| H | 2.86960000 | -1.05995400 | 1.90707600 |
| C | 2.61082000 | -0.24230700 | -0.07701000 |
| C | 3.45663800 | 0.94545000 | 0.39401300 |
| H | 3.44696500 | 1.81019200 | -0.27360700 |
| H | 3.15538800 | 1.27223300 | 1.39586800 |
| C | 2.96474600 | -0.61824900 | -1.52198600 |
| H | 2.78299800 | 0.20249600 | -2.22380300 |
| H | 4.02828200 | -0.86727400 | -1.58767500 |
| H | 2.40034500 | -1.48683300 | -1.87265700 |
| H | 0.55266200 | 4.08100900 | -0.18036600 |
| H | 1.33842300 | 2.82912700 | 0.76834100 |
| C | -1.10504300 | 2.67366000 | 1.84537800 |
| H | -0.54258000 | 3.49497800 | 2.29278000 |
| H | -2.17867300 | 2.83292700 | 1.96527500 |
| H | -0.85143700 | 1.75740600 | 2.40464300 |
| C | -3.26491700 | -2.09897200 | 0.54166400 |
| H | -3.39756900 | -1.52922500 | 1.46964500 |
| H | -4.25770700 | -2.45770100 | 0.24806200 |
| H | -2.64455700 | -2.96915100 | 0.75881800 |
| C | -0.34041200 | -1.46946000 | 1.69320300 |
| H | -1.16528700 | -0.75294100 | 1.61321600 |
| H | -0.76164600 | -2.44601100 | 1.94660600 |
| H | 0.30044700 | -1.15968300 | 2.52674000 |
| H | -0.61155800 | -3.20564000 | -0.36874500 |
| H | 4.50151100 | 0.62517000 | 0.46258600 |

**IM12**

Sum of electronic and thermal Free Energies = -781.12447

| | | | |
|---|---|---|---|
| C | 0.19200000 | 0.79237800 | -0.85422800 |
| C | -1.20575300 | 1.46624700 | -0.35333400 |
| C | -1.48922500 | -1.59516900 | -1.22353800 |
| C | -0.26031000 | -2.33887000 | -0.80903100 |
| C | 0.51590100 | -1.63479500 | 0.35294600 |
| C | 0.95885900 | -0.10360400 | 0.17082500 |
| H | 0.01442600 | 0.23402500 | -1.76781100 |
| H | 0.40819900 | -2.45373500 | -1.66904400 |
| H | 0.80185900 | 0.35010100 | 1.16410800 |
| C | -2.62877000 | -1.42908200 | -0.54510800 |
| H | -1.36815900 | -0.93500000 | -2.07870500 |
| C | -2.55219400 | 0.90533000 | 0.16639600 |
| H | -3.19542200 | 1.78081600 | 0.31731200 |
| H | -2.40619400 | 0.45844100 | 1.15685000 |
| C | -3.31035900 | -0.09767700 | -0.73266100 |
| H | -3.28011800 | 0.23346200 | -1.77752400 |
| H | -4.35960700 | -0.11488900 | -0.42105000 |
| C | -0.74783900 | 2.66313500 | 0.34665300 |
| H | -1.46963500 | 2.00422000 | -1.30472500 |
| C | 0.60106500 | 3.03971100 | -0.07214400 |
| C | 0.91119800 | 2.10678700 | -1.23651900 |
| H | 0.46290000 | 2.51012800 | -2.15280000 |
| H | 1.97227600 | 2.00077300 | -1.42056900 |
| C | 1.84369000 | -2.41336300 | 0.55010600 |
| H | 1.73854800 | -3.18289200 | 1.32066300 |
| H | 2.13281200 | -2.92814800 | -0.37170600 |
| C | 2.87338400 | -1.35672800 | 0.90484100 |
| H | 3.90682600 | -1.68484800 | 0.75541900 |

| | | | |
|---|---|---|---|
| H | 2.77530000 | -1.06144500 | 1.95840800 |
| C | 2.52561400 | -0.15276500 | 0.00860700 |
| C | 3.29231600 | 1.05472600 | 0.57005100 |
| H | 3.27795700 | 1.95184500 | -0.05354200 |
| H | 2.92753200 | 1.31545000 | 1.57167200 |
| C | 2.96468900 | -0.46039000 | -1.43296100 |
| H | 2.80989000 | 0.37273300 | -2.12309900 |
| H | 4.03376000 | -0.69508400 | -1.44990900 |
| H | 2.43250200 | -1.32259400 | -1.84412100 |
| H | 0.72724500 | 4.12008300 | -0.20329200 |
| H | 1.22996900 | 2.77242900 | 0.80335700 |
| C | -1.51107300 | 3.42508700 | 1.34096100 |
| H | -0.93232700 | 4.23483100 | 1.78397000 |
| H | -2.40383800 | 3.84316000 | 0.85210900 |
| H | -1.89961800 | 2.74743400 | 2.11161600 |
| C | -3.17401700 | -2.31795800 | 0.53572600 |
| H | -3.29399200 | -1.79610000 | 1.49317900 |
| H | -4.17208600 | -2.65744700 | 0.23578300 |
| H | -2.55492700 | -3.20064000 | 0.69997900 |
| C | -0.26775600 | -1.72976300 | 1.66982500 |
| H | -1.14338000 | -1.07727300 | 1.67908300 |
| H | -0.60363900 | -2.75341500 | 1.85854100 |
| H | 0.37607300 | -1.43384400 | 2.50563200 |
| H | -0.48068300 | -3.35457800 | -0.45656400 |
| H | 4.34703900 | 0.78258400 | 0.68229600 |

**TS_12-13**
Sum of electronic and thermal Free
Energies = -781.12089

| | | | |
|---|---|---|---|
| C | 0.08134700 | 0.79392000 | -0.80854300 |
| C | -1.26823900 | 1.32411400 | -0.17319900 |
| C | -1.31497600 | -1.76384900 | -1.23068700 |
| C | -0.05223100 | -2.40941900 | -0.76008900 |
| C | 0.64773800 | -1.61039600 | 0.39157600 |
| C | 0.96416200 | -0.05067800 | 0.18575000 |
| H | -0.10937700 | 0.22216900 | -1.70896200 |
| H | 0.64138300 | -2.51025100 | -1.60077900 |
| H | 0.80665200 | 0.39556600 | 1.18148500 |
| C | -2.47342800 | -1.63720900 | -0.57564100 |
| H | -1.21531900 | -1.14100200 | -2.11568700 |
| C | -2.62221800 | 0.68202000 | 0.16957700 |
| H | -3.33541900 | 1.50270200 | 0.28854500 |
| H | -2.52600000 | 0.22178900 | 1.15991100 |
| C | -3.22572200 | -0.35390800 | -0.81000900 |
| H | -3.12772200 | -0.00417900 | -1.84399900 |
| H | -4.29426700 | -0.43820400 | -0.58656800 |
| C | -0.98558100 | 2.61796000 | 0.35822400 |
| H | -1.57413100 | 2.23209200 | -0.93207900 |
| C | 0.36721200 | 3.08746600 | -0.06294700 |
| C | 0.70431900 | 2.14899700 | -1.21753400 |
| H | 0.20129400 | 2.50850800 | -2.12534000 |
| H | 1.76167100 | 2.10071600 | -1.44003000 |
| C | 2.03643600 | -2.26969900 | 0.61107100 |
| H | 2.00085200 | -3.00458300 | 1.42074200 |
| H | 2.35539600 | -2.80746800 | -0.28729100 |
| C | 2.98650900 | -1.12160700 | 0.89787700 |
| H | 4.03802400 | -1.37305600 | 0.72712300 |
| H | 2.89583700 | -0.79801800 | 1.94369800 |
| C | 2.52299700 | 0.02389800 | -0.02319900 |
| C | 3.21451000 | 1.29840600 | 0.48831100 |
| H | 3.13725200 | 2.17096000 | -0.16347300 |
| H | 2.84275200 | 1.56991900 | 1.48398500 |
| C | 2.94300300 | -0.28639200 | -1.46854200 |
| H | 2.66124100 | 0.49568900 | -2.17869800 |
| H | 4.03121900 | -0.39201200 | -1.52226200 |
| H | 2.50402400 | -1.22134000 | -1.82719300 |
| H | 0.39571700 | 4.15673000 | -0.28633700 |
| H | 1.03410800 | 2.90943000 | 0.79507400 |
| C | -1.84978600 | 3.46914900 | 1.21435800 |
| H | -1.95578000 | 4.46950200 | 0.78571000 |
| H | -2.82409900 | 3.04789900 | 1.44843900 |
| H | -1.29406700 | 3.59674000 | 2.15331500 |
| C | -2.98667900 | -2.52566900 | 0.52177400 |
| H | -3.16971700 | -1.98782800 | 1.46013300 |
| H | -3.94984500 | -2.94294600 | 0.20615100 |
| H | -2.31376800 | -3.35818300 | 0.72968200 |
| C | -0.13956300 | -1.74392500 | 1.70320900 |
| H | -1.06471100 | -1.16309800 | 1.69452400 |
| H | -0.39536300 | -2.78732600 | 1.90889700 |
| H | 0.47018800 | -1.38185500 | 2.53839700 |
| H | -0.21177500 | -3.42364400 | -0.37261800 |
| H | 4.28489500 | 1.09551100 | 0.59748700 |

**IM13**
Sum of electronic and thermal Free
Energies = -781.13966

| | | | |
|---|---|---|---|
| C | 0.01006000 | 0.84672300 | -0.82239700 |
| C | -1.33613400 | 1.17200500 | -0.31005600 |
| C | -0.87364400 | -1.95583000 | -0.99056900 |
| C | 0.16952200 | -2.42014400 | -0.03318800 |
| C | 0.64020000 | -1.23508000 | 0.87755300 |
| C | 1.01814400 | 0.12023900 | 0.18775000 |
| H | -0.05671700 | 0.26425400 | -1.73889800 |
| H | 1.01872900 | -2.83306400 | -0.58266300 |
| H | 1.11100700 | 0.81509000 | 1.03245700 |
| C | -2.16102600 | -1.69436100 | -0.73273100 |
| H | -0.48802400 | -1.60136500 | -1.94513800 |
| C | -2.65904700 | 0.69851700 | -0.78064400 |
| H | -3.00794900 | 1.56073700 | -1.38202300 |
| H | -3.33660600 | 0.73130900 | 0.08786100 |
| C | -2.81058400 | -0.61685300 | -1.56170100 |
| H | -2.32631500 | -0.52870900 | -2.53933900 |
| H | -3.87903300 | -0.78071800 | -1.73496100 |
| C | -1.31802400 | 2.42850100 | 0.51585800 |
| H | -2.13485700 | 3.04622800 | 0.11400600 |
| C | 0.04164200 | 3.07508700 | 0.18905900 |
| C | 0.46891800 | 2.32571400 | -1.07794400 |
| H | -0.06849000 | 2.72010600 | -1.94870200 |
| H | 1.52944300 | 2.38143200 | -1.30610300 |
| C | 2.01816400 | -1.61512900 | 1.45195500 |
| H | 2.25475900 | -0.96839300 | 2.30672000 |
| H | 2.03863800 | -2.64970500 | 1.80897000 |
| C | 2.98637100 | -1.35203200 | 0.30027100 |
| H | 2.98292300 | -2.18887700 | -0.40494600 |
| H | 4.01849300 | -1.23673600 | 0.64179900 |
| C | 2.47685300 | -0.05527500 | -0.39647500 |
| C | 3.40065800 | 1.09377500 | 0.04481400 |
| H | 3.09932000 | 2.07813500 | -0.31999600 |
| H | 3.44927200 | 1.14634900 | 1.13854700 |
| C | 2.52222000 | -0.23407700 | -1.91717900 |
| H | 2.24472900 | 0.67104800 | -2.46732100 |
| H | 3.54022700 | -0.49615800 | -2.22071600 |
| H | 1.86810300 | -1.05127700 | -2.24410300 |
| H | -0.04678100 | 4.15112200 | 0.03199100 |
| H | 0.75408700 | 2.91934400 | 1.00475000 |
| C | -1.62229400 | 2.23327400 | 2.01532400 |
| H | -1.72476900 | 3.22095300 | 2.46899300 |
| H | -2.55073300 | 1.68114800 | 2.18312700 |
| H | -0.80307100 | 1.71039800 | 2.50925800 |
| C | -2.96509100 | -2.23357600 | 0.41684600 |
| H | -3.37579200 | -1.44048100 | 1.05533700 |
| H | -3.82166700 | -2.79021200 | 0.02040300 |
| H | -2.38831100 | -2.91026000 | 1.04814700 |
| C | -0.37601700 | -0.99847300 | 1.99155300 |
| H | -1.31840100 | -0.57670000 | 1.61651600 |
| H | -0.62598000 | -1.93198200 | 2.50493100 |
| H | 0.03067000 | -0.31005600 | 2.73878100 |
| H | -0.18770300 | -3.21145700 | 0.63475300 |
| H | 4.41546300 | 0.91046300 | -0.32103900 |

**TS_13-14a**
Sum of electronic and thermal Free
Energies = -781.13286

| | | | |
|---|---|---|---|
| C | 0.08739000 | 1.08660900 | -0.71727200 |
| C | -1.38565000 | 0.94695200 | -0.56272300 |

| | | | |
|---|---|---|---|
| C | -0.49975700 | -1.87502700 | -0.79504600 |
| C | 0.54433400 | -2.20918000 | 0.21129600 |
| C | 0.90546100 | -0.93961900 | 1.03198800 |
| C | 1.17097400 | 0.35582700 | 0.21883500 |
| H | 0.34578700 | 0.84794200 | -1.75203500 |
| H | 1.43522800 | -2.60492400 | -0.28434200 |
| H | 1.35615400 | 1.08964100 | 1.01169700 |
| C | -1.82910300 | -1.86204000 | -0.63944000 |
| H | -0.12280400 | -1.45282700 | -1.72876900 |
| C | -2.36275700 | 0.41993700 | -1.58137800 |
| H | -1.96565300 | 0.80379400 | -2.53483700 |
| H | -3.31411500 | 0.93046200 | -1.41433900 |
| C | -2.61471700 | -1.11199600 | -1.69573500 |
| H | -2.33469100 | -1.45813100 | -2.69353400 |
| H | -3.68812100 | -1.28379500 | -1.58836100 |
| C | -1.92601500 | 1.93724300 | 0.40911100 |
| H | -2.47639400 | 2.58447500 | -0.30816500 |
| C | -0.71459600 | 2.74476100 | 0.87059400 |
| C | 0.19683700 | 2.61862000 | -0.35443400 |
| H | -0.18327900 | 3.23876200 | -1.17471200 |
| H | 1.23327700 | 2.89608900 | -0.17118800 |
| C | 2.30963900 | -1.12382100 | 1.63716800 |
| H | 2.45005300 | -0.40951700 | 2.45730800 |
| H | 2.43918700 | -2.12728000 | 2.05462700 |
| C | 3.28166800 | -0.82536300 | 0.48470300 |
| H | 3.53579000 | -1.74508000 | -0.05167100 |
| H | 4.22355300 | -0.40929900 | 0.85179300 |
| C | 2.56463400 | 0.16998000 | -0.48560800 |
| C | 3.34827700 | 1.48752000 | -0.56730200 |
| H | 2.90930800 | 2.18614500 | -1.28795000 |
| H | 3.41238600 | 1.98062500 | 0.40943600 |
| C | 2.51781500 | -0.42259500 | -1.90164900 |
| H | 2.08067400 | 0.26604100 | -2.63317800 |
| H | 3.54335700 | -0.61338500 | -2.23252100 |
| H | 1.98449800 | -1.37415500 | -1.95349700 |
| H | -0.97200500 | 3.77773600 | 1.11075100 |
| H | -0.26101200 | 2.29561100 | 1.75987500 |
| C | -2.96681900 | 1.46400800 | 1.43085900 |
| H | -3.46787800 | 2.33439900 | 1.85725300 |
| H | -3.72710600 | 0.82383700 | 0.97379000 |
| H | -2.48229700 | 0.91534200 | 2.24006400 |
| C | -2.60605800 | -2.46719400 | 0.49385000 |
| H | -3.21298700 | -1.71443200 | 1.01306100 |
| H | -3.30471400 | -3.21378100 | 0.09950100 |
| H | -1.96559600 | -2.95564800 | 1.22922200 |
| C | -0.15103900 | -0.71508000 | 2.10691400 |
| H | -1.14788200 | -0.59518600 | 1.66714000 |
| H | -0.20054200 | -1.57179100 | 2.78690100 |
| H | 0.07407700 | 0.17322000 | 2.70727000 |
| H | 0.21079400 | -2.97894900 | 0.91477400 |
| H | 4.36983500 | 1.28679900 | -0.90375200 |

**IM14a**

Sum of electronic and thermal Free Energies = -781.19549

| | | | |
|---|---|---|---|
| C | 0.25709000 | 0.94024700 | -1.21590800 |
| C | -1.03323600 | 0.14246600 | -0.81345200 |
| C | -0.90942300 | -0.52738100 | 0.46623600 |
| C | -0.15241700 | 0.04153600 | 1.57727200 |
| C | 1.25473300 | 0.66220900 | 1.20943800 |
| C | 1.49265200 | 0.63865000 | -0.33095900 |
| H | 0.50971200 | 0.64080400 | -2.23786900 |
| H | -0.08226500 | -0.66020900 | 2.41336200 |
| H | 2.17881300 | 1.46868000 | -0.53681600 |
| C | -1.59138000 | -1.83725400 | 0.48179600 |
| H | -0.69421100 | -2.49445200 | 0.42003200 |
| C | -1.61533700 | -0.92344200 | -1.77565400 |
| H | -0.81272800 | -1.40996800 | -2.33082100 |
| H | -2.28240900 | -0.47150200 | -2.51304400 |
| C | -2.33862800 | -1.92974300 | -0.86251700 |
| H | -2.32332100 | -2.94628600 | -1.26006000 |
| H | -3.38830100 | -1.65973900 | -0.71655600 |
| C | -2.16549500 | 1.30440500 | -0.57237100 |
| H | -2.59479400 | 1.37063800 | -1.57818200 |
| C | -1.36174400 | 2.56647700 | -0.31073000 |
| C | -0.14097100 | 2.44035200 | -1.21648200 |
| H | -0.42009400 | 2.74128200 | -2.23135000 |
| H | 0.68884400 | 3.08310400 | -0.91153300 |
| C | 2.34192400 | -0.28227700 | 1.75576600 |
| H | 3.29295300 | 0.26174600 | 1.78697700 |
| H | 2.13218500 | -0.61457700 | 2.77763300 |
| C | 2.41292300 | -1.40226200 | 0.73198400 |
| H | 1.56210200 | -2.08804100 | 0.86406300 |
| H | 3.31828800 | -2.01083800 | 0.81372000 |
| C | 2.31684500 | -0.68520200 | -0.63296000 |
| C | 3.72010300 | -0.26452100 | -1.10091900 |
| H | 3.65944200 | 0.30907300 | -2.03243900 |
| H | 4.22404700 | 0.36191300 | -0.35769900 |
| C | 1.74525600 | -1.64483300 | -1.67717200 |
| H | 1.61296400 | -1.17926700 | -2.65919000 |
| H | 2.43840200 | -2.48181600 | -1.80785700 |
| H | 0.79157800 | -2.07775300 | -1.36100100 |
| H | -1.96968800 | 3.45003700 | -0.53048800 |
| H | -1.09215400 | 2.63649500 | 0.74864900 |
| C | -3.30372300 | 1.07019800 | 0.41775600 |
| H | -3.97319000 | 1.93397200 | 0.37829200 |
| H | -3.90254700 | 0.18931800 | 0.17881500 |
| H | -2.95568700 | 0.98856500 | 1.45312300 |
| C | -2.36530500 | -2.22791000 | 1.74389000 |
| H | -2.74345800 | -3.24534100 | 1.62849200 |
| H | -1.74238900 | -2.20082300 | 2.64045400 |
| H | -3.22066300 | -1.56304800 | 1.88835600 |
| C | 1.40918000 | 2.04378900 | 1.85197600 |
| H | 0.70531000 | 2.78431200 | 1.46894500 |
| H | 1.27491500 | 1.97796200 | 2.93725700 |
| H | 2.41814300 | 2.42271900 | 1.66608100 |
| H | -0.79518300 | 0.87219400 | 1.92361100 |
| H | 4.34710200 | -1.14217300 | -1.28489800 |

**TS_11-15a**

Sum of electronic and thermal Free Energies = -781.129668

| | | | |
|---|---|---|---|
| C | 0.63807419 | -0.64140182 | -0.85881165 |
| C | -2.66559292 | 0.20998893 | -1.86405373 |
| C | -0.87193472 | -1.62407680 | 0.60119875 |
| C | 0.22710169 | -1.54768346 | 1.64523785 |
| C | 1.06772568 | -0.24737019 | 1.61629582 |
| C | 1.25117488 | 0.23539292 | 0.13478737 |
| H | 0.98528468 | -1.67250577 | -0.84169173 |
| H | 0.89542112 | -2.39882401 | 1.47097307 |
| H | 0.86548752 | 1.25348015 | 0.02433417 |
| C | -2.14840434 | -1.12696803 | 0.73321192 |
| H | -0.80170325 | -2.43834668 | -0.12126091 |
| C | -3.79514972 | -0.26121711 | -1.00268990 |
| H | -4.65373535 | -0.58427824 | -1.59739657 |
| H | -4.14886544 | 0.50088868 | -0.30335289 |
| C | -3.23983420 | -1.49325794 | -0.23634138 |
| H | -2.87753352 | -2.23021892 | -0.96044474 |
| H | -4.04874510 | -1.96504912 | 0.33609366 |
| C | -1.80124585 | 1.20095383 | -1.62557677 |
| H | -2.41665838 | -0.49568402 | -2.65861322 |
| C | -0.46767411 | 1.17718044 | -2.35523191 |
| C | 0.20568024 | -0.19315470 | -2.20456721 |
| H | -0.36896153 | -0.98616734 | -2.69005404 |
| H | 1.17897860 | -0.20050058 | -2.74033132 |
| C | 2.50073629 | -0.44280249 | 2.16290686 |
| H | 2.55850616 | -0.21826224 | 3.23187869 |
| H | 2.83359151 | -1.47808407 | 2.03408076 |
| C | 3.35164350 | 0.49894683 | 1.31395399 |
| H | 4.42575320 | 0.29886008 | 1.38052118 |
| H | 3.19538163 | 1.53992656 | 1.62147565 |
| C | 2.83885215 | 0.30721355 | -0.12804933 |
| C | 3.17601570 | 1.49065216 | -1.03009340 |
| H | 2.77588766 | 1.36579082 | -2.04306340 |
| H | 2.78863205 | 2.42782009 | -0.61853093 |
| C | 3.43235737 | -0.97950966 | -0.72021108 |
| H | 3.11937308 | -1.14794481 | -1.75642221 |
| H | 4.52214942 | -0.88923233 | -0.72985420 |

| | | | |
|---|---|---|---|
| H | 3.18402683 | -1.87170914 | -0.13674199 |
| H | -0.59458628 | 1.37650346 | -3.42473258 |
| H | 0.19048749 | 1.96584268 | -1.97491095 |
| C | -2.00820008 | 2.32676315 | -0.65068410 |
| H | -2.99884811 | 2.31585130 | -0.19309604 |
| H | -1.25117188 | 2.32022246 | 0.14393291 |
| H | -1.90014099 | 3.28462646 | -1.17207429 |
| C | -2.60397947 | -0.28560636 | 1.88553113 |
| H | -2.68778200 | 0.76485949 | 1.58175426 |
| H | -3.60608965 | -0.59913748 | 2.19275211 |
| H | -1.93553054 | -0.33702785 | 2.74346424 |
| C | 0.40179363 | 0.89739355 | 2.39143907 |
| H | -0.52936114 | 1.22097327 | 1.92307919 |
| H | 0.18937235 | 0.59546399 | 3.42193201 |
| H | 1.06720839 | 1.76585981 | 2.42890618 |
| H | -0.17968676 | -1.69304944 | 2.65264897 |
| H | 4.26258071 | 1.58696892 | -1.12296831 |

**IM15a**

Sum of electronic and thermal Free Energies = -781.165108

| | | | |
|---|---|---|---|
| C | -0.63360200 | 2.26857273 | -1.27573821 |
| C | -0.02581972 | 4.79852882 | -3.27303536 |
| C | -0.53595576 | 3.75349067 | -0.83526270 |
| C | -0.26361746 | 3.64656097 | 0.69058666 |
| C | 0.40791623 | 2.26929786 | 0.95593438 |
| C | 0.35755738 | 1.48375059 | -0.39451792 |
| H | -1.63816406 | 1.97585720 | -0.94686522 |
| H | -1.22752030 | 3.69817121 | 1.20682799 |
| H | 1.35398318 | 1.49276752 | -0.86105309 |
| C | 0.46771900 | 4.66844362 | -1.53537142 |
| H | -1.51263883 | 4.22331386 | -1.00133736 |
| C | 0.15262640 | 6.29793322 | -3.11951851 |
| H | -0.64591462 | 6.88950183 | -3.56610388 |
| H | 1.11134768 | 6.66478414 | -3.48654979 |
| C | 0.11117142 | 6.17791912 | -1.58317664 |
| H | -0.89506016 | 6.34480773 | -1.19180761 |
| H | 0.82091003 | 6.80404881 | -1.03681955 |
| C | 0.91786005 | 3.86414172 | -3.68624250 |
| H | -1.05361725 | 4.44975355 | -3.20019161 |
| C | 0.65241595 | 2.39825146 | -3.54626149 |
| C | -0.60019849 | 1.96933481 | -2.78268311 |
| H | -1.49242143 | 2.38396118 | -3.26803457 |
| H | -0.68182334 | 0.88709507 | -2.91237591 |
| C | -0.40225174 | 1.36468719 | 1.90825621 |
| H | -0.20823426 | 1.58807725 | 2.96237036 |
| H | -1.47771097 | 1.50554379 | 1.73748283 |
| C | 0.00622571 | -0.04762880 | 1.49338107 |
| H | -0.66230383 | -0.81961872 | 1.88674808 |
| H | 1.01130859 | -0.28130807 | 1.86133348 |
| C | -0.01110651 | -0.01190065 | -0.05651450 |
| C | 1.02366402 | -0.96840724 | -0.65495682 |
| H | 0.99385191 | -0.95198442 | -1.75182290 |
| H | 2.03707254 | -0.69765085 | -0.33831527 |
| C | -1.41307231 | -0.45007951 | -0.51334877 |
| H | -1.56053498 | -0.37461548 | -1.59436571 |
| H | -1.55597476 | -1.50120271 | -0.24594618 |
| H | -2.20942367 | 0.11691706 | -0.02017216 |
| H | 0.61555289 | 2.00652646 | -4.57431105 |
| H | 1.55138222 | 1.93774806 | -3.11255804 |
| C | 2.23880206 | 4.23070461 | -4.26246229 |
| H | 2.45661425 | 5.29642758 | -4.24395004 |
| H | 3.05268433 | 3.67008990 | -3.79352822 |
| H | 2.20909107 | 3.91152705 | -5.31396971 |
| C | 1.94163994 | 4.47343462 | -1.24342878 |
| H | 2.08959214 | 4.74350341 | -0.19404881 |
| H | 2.28925020 | 3.44617105 | -1.37652122 |
| H | 2.56467276 | 5.15248417 | -1.83068066 |
| C | 1.83204204 | 2.40901687 | 1.51096299 |
| H | 2.50961196 | 2.90661136 | 0.81391181 |
| H | 1.82277050 | 2.98295310 | 2.44350240 |
| H | 2.26777797 | 1.43050148 | 1.72999612 |
| H | 0.32804052 | 4.48454322 | 1.07537858 |
| H | 0.83553709 | -1.99788953 | -0.33400344 |

**TS_15a-15b**

Sum of electronic and thermal Free Energies = -781.157416

| | | | |
|---|---|---|---|
| C | -0.33071687 | 2.23716632 | -1.22000361 |
| C | -0.27947193 | 4.73171177 | -3.24078422 |
| C | -0.04781975 | 3.71151426 | -0.70643661 |
| C | 0.79026361 | 3.52308130 | 0.58295850 |
| C | 0.63771180 | 2.06142821 | 1.00793232 |
| C | 0.50087179 | 1.28739609 | -0.32425298 |
| H | -1.37733087 | 2.06886415 | -0.94901739 |
| H | 0.49977894 | 4.22445685 | 1.37346449 |
| H | 1.48611875 | 1.11495157 | -0.78807533 |
| C | 0.53769610 | 4.80138421 | -1.62529972 |
| H | -1.02831708 | 4.10922197 | -0.42526879 |
| C | -0.41546531 | 6.23837751 | -3.15561261 |
| H | -1.38683644 | 6.61903328 | -3.46891408 |
| H | 0.36671519 | 6.78091143 | -3.68676199 |
| C | -0.17947890 | 6.18432763 | -1.63501654 |
| H | -1.12313072 | 6.12709855 | -1.08843201 |
| H | 0.43479854 | 6.98524652 | -1.21581902 |
| C | 0.77971750 | 4.00143940 | -3.76768428 |
| H | -1.17550841 | 4.17840315 | -2.96815659 |
| C | 0.88490024 | 2.53223464 | -3.51377621 |
| C | -0.25020779 | 1.89846003 | -2.72197089 |
| H | -1.20059282 | 2.11188592 | -3.22537223 |
| H | -0.12788749 | 0.81701734 | -2.80155483 |
| C | -0.69006981 | 1.72496576 | 1.70905790 |
| H | -0.65023884 | 1.93875760 | 2.78188939 |
| H | -1.51058311 | 2.32583214 | 1.29633587 |
| C | -0.90356022 | 0.23268325 | 1.40336675 |
| H | -1.96619414 | -0.02364296 | 1.36206073 |
| H | -0.46731869 | -0.38357802 | 2.19681066 |
| C | -0.18607585 | -0.07251840 | 0.04462117 |
| C | 0.88871335 | -1.15748661 | 0.22057369 |
| H | 1.36174200 | -1.39220380 | -0.73957829 |
| H | 1.67589547 | -0.85435710 | 0.91486139 |
| C | -1.20273131 | -0.62005756 | -0.96957025 |
| H | -0.72893140 | -0.93692874 | -1.90428507 |
| H | -1.67844674 | -1.50858877 | -0.54301227 |
| H | -2.00422934 | 0.08815046 | -1.20461963 |
| H | 0.97933035 | 2.05489893 | -4.49919043 |
| H | 1.85744493 | 2.35321075 | -3.02898501 |
| C | 1.87048973 | 4.60000389 | -4.58298084 |
| H | 1.87480415 | 5.68775804 | -4.60282229 |
| H | 2.85283662 | 4.22138243 | -4.28642033 |
| H | 1.69691084 | 4.24973242 | -5.61047940 |
| C | 2.04230273 | 5.01250694 | -1.60455085 |
| H | 2.28277362 | 5.43533224 | -0.62464469 |
| H | 2.62604354 | 4.09519156 | -1.72285946 |
| H | 2.35997824 | 5.75040478 | -2.34383577 |
| C | 1.81974589 | 1.65436163 | 1.89230076 |
| H | 2.75173288 | 1.60854494 | 1.31762686 |
| H | 1.95142465 | 2.38848486 | 2.69461497 |
| H | 1.66522333 | 0.68359053 | 2.36827277 |
| H | 1.85284018 | 3.68470459 | 0.38357013 |
| H | 0.43926549 | -2.07869916 | 0.60523929 |

**IM15b**

Sum of electronic and thermal Free Energies = -781.156058

| | | | |
|---|---|---|---|
| C | -0.23532676 | 2.18302949 | -1.30538528 |
| C | -0.26616132 | 4.61009767 | -3.31963699 |
| C | 0.06406339 | 3.63454793 | -0.72979323 |
| C | 1.06008561 | 3.40593423 | 0.42277551 |
| C | 0.78330815 | 1.99583124 | 0.94166504 |
| C | 0.46550543 | 1.19132259 | -0.33453340 |
| H | -1.31453074 | 2.05871105 | -1.19922594 |
| H | 0.98071220 | 4.17020235 | 1.20514172 |
| H | 1.39955716 | 0.85387907 | -0.81030155 |
| C | 0.42620563 | 4.82317649 | -1.64153271 |

| | | | |
|---|---|---|---|
| H | -0.88292413 | 3.94644528 | -0.27662760 |
| C | -0.64863806 | 6.07222212 | -3.25715366 |
| H | -1.62777276 | 6.30067132 | -3.67595436 |
| H | 0.09418241 | 6.73980014 | -3.69425336 |
| C | -0.57390013 | 6.01626949 | -1.72138800 |
| H | -1.53820815 | 5.73067920 | -1.29542545 |
| H | -0.20226720 | 6.91276269 | -1.21761031 |
| C | 0.94200116 | 4.04974159 | -3.70828217 |
| H | -1.08233599 | 3.92833135 | -3.09295034 |
| C | 1.23043628 | 2.61045669 | -3.41026466 |
| C | 0.08634882 | 1.83072087 | -2.77688830 |
| H | -0.80122663 | 1.91884029 | -3.41372314 |
| H | 0.35187093 | 0.77009815 | -2.80846933 |
| C | -0.51416095 | 1.81948867 | 1.75222043 |
| H | -0.39564997 | 2.10719979 | 2.80181024 |
| H | -1.31951770 | 2.43945380 | 1.33533322 |
| C | -0.84844008 | 0.33138244 | 1.56675358 |
| H | -1.91244470 | 0.12401460 | 1.71425951 |
| H | -0.30858749 | -0.26988365 | 2.30581737 |
| C | -0.38279556 | -0.04705821 | 0.12398695 |
| C | 0.50701735 | -1.29793803 | 0.14247953 |
| H | 0.77940240 | -1.59773912 | -0.87620234 |
| H | 1.43253119 | -1.12827018 | 0.70105054 |
| C | -1.60368192 | -0.35494537 | -0.75622645 |
| H | -1.33547578 | -0.47883050 | -1.81164476 |
| H | -2.05726462 | -1.29416890 | -0.42496517 |
| H | -2.38021759 | 0.41319609 | -0.68319211 |
| H | 1.54333370 | 2.14923749 | -4.35635000 |
| H | 2.13013779 | 2.58173464 | -2.77353157 |
| C | 2.00633619 | 4.79791861 | -4.43132080 |
| H | 1.85061860 | 5.87395045 | -4.47367929 |
| H | 3.00142320 | 4.57389118 | -4.03694484 |
| H | 1.98434332 | 4.41827336 | -5.46237502 |
| C | 1.83817068 | 5.37129608 | -1.52206316 |
| H | 1.92917787 | 5.74240158 | -0.49553022 |
| H | 2.62824752 | 4.63276989 | -1.67331911 |
| H | 2.00303987 | 6.22252245 | -2.18584549 |
| C | 1.98678268 | 1.48257224 | 1.73627671 |
| H | 2.87188170 | 1.39429529 | 1.09645992 |
| H | 2.22409973 | 2.17701530 | 2.54934021 |
| H | 1.80019724 | 0.50555895 | 2.18740509 |
| H | 2.09179861 | 3.42247502 | 0.05091454 |
| H | -0.01887006 | -2.13679167 | 0.60944754 |

**TS_15b-15c**
Sum of electronic and thermal Free Energies = -781.154202

| | | | |
|---|---|---|---|
| C | -0.07860769 | -0.09234706 | -0.01981466 |
| C | 0.65702059 | -1.76191434 | 2.51613425 |
| C | -0.04714563 | 0.70693434 | 1.34678165 |
| C | -1.21110654 | 1.70547837 | 1.24899599 |
| C | -1.27194141 | 2.09546268 | -0.22752465 |
| C | -0.94535405 | 0.78542873 | -0.97849539 |
| H | 0.95132379 | -0.11422278 | -0.37938639 |
| H | -1.08309032 | 2.57411258 | 1.90518367 |
| H | -1.87967075 | 0.23802527 | -1.16529890 |
| C | 0.09124907 | -0.01384039 | 2.69827492 |
| H | 0.87364927 | 1.30042523 | 1.29219234 |
| C | 1.52895196 | -1.50663661 | 3.72238569 |
| H | 2.51424393 | -1.96791265 | 3.67304623 |
| H | 1.05546214 | -1.76170034 | 4.67083012 |
| C | 1.47663231 | -0.00042237 | 3.41268719 |
| H | 2.26337018 | 0.27628620 | 2.70670110 |
| H | 1.49686090 | 0.67846278 | 4.27006799 |
| C | -0.68407932 | -2.10193790 | 2.45959697 |
| H | 1.19040629 | -1.68085801 | 1.57279829 |
| C | -1.42256946 | -1.98869068 | 1.15815328 |
| C | -0.57030760 | -1.56437608 | -0.03234665 |
| H | 0.26977154 | -2.26142138 | -0.12879294 |
| H | -1.16238795 | -1.71447916 | -0.93908753 |
| C | -0.15357241 | 3.03864604 | -0.71021492 |
| H | -0.36867855 | 4.08984373 | -0.49248048 |
| H | 0.80008213 | 2.79488930 | -0.22284974 |
| C | -0.05802475 | 2.73617398 | -2.21040536 |
| H | 0.90773707 | 3.02638800 | -2.63499998 |
| H | -0.82191265 | 3.29955543 | -2.75661931 |
| C | -0.31238261 | 1.20463186 | -2.35579376 |
| C | -1.30896067 | 0.92151348 | -3.48766877 |
| H | -1.44905492 | -0.15674182 | -3.62722073 |
| H | -2.28806764 | 1.36436727 | -3.27767686 |
| C | 1.00294915 | 0.48874488 | -2.68917988 |
| H | 0.89765511 | -0.60241532 | -2.65129486 |
| H | 1.31245694 | 0.75385569 | -3.70468701 |
| H | 1.81853533 | 0.78328176 | -2.01932032 |
| H | -1.89149628 | -2.96431721 | 0.97501682 |
| H | -2.26415432 | -1.29463894 | 1.31426901 |
| C | -1.45572492 | -2.62799155 | 3.62006431 |
| H | -0.94363076 | -2.53662849 | 4.57611831 |
| H | -2.45404113 | -2.18649441 | 3.68168594 |
| H | -1.59648653 | -3.69895949 | 3.42013389 |
| C | -0.98926697 | 0.28497854 | 3.72279310 |
| H | -0.90833762 | 1.35794001 | 3.92939347 |
| H | -2.00699074 | 0.09568623 | 3.37777503 |
| H | -0.81998406 | -0.23639157 | 4.66690000 |
| C | -2.64625583 | 2.67434165 | -0.57281326 |
| H | -3.43811302 | 1.94182461 | -0.38141980 |
| H | -2.84945961 | 3.56137844 | 0.03652284 |
| H | -2.71592135 | 2.97348571 | -1.62147882 |
| H | -2.16176205 | 1.22590302 | 1.51735455 |
| H | -0.94735272 | 1.33849606 | -4.43305285 |

**IM15c**
Sum of electronic and thermal Free Energies = -781.161237

| | | | |
|---|---|---|---|
| C | -0.45091221 | -0.29837471 | -0.09438743 |
| C | 0.41728858 | -1.97891418 | 2.23394450 |
| C | -0.12349692 | 0.59045209 | 1.13278888 |
| C | -1.30425424 | 1.57561770 | 1.17916916 |
| C | -1.56765743 | 1.91664069 | -0.30477446 |
| C | -0.93259979 | 0.74064676 | -1.12966390 |
| H | 0.45817387 | -0.79109292 | -0.45623285 |
| H | -1.08674834 | 2.47236716 | 1.76897425 |
| H | -1.70312256 | 0.28152898 | -1.76036699 |
| C | 0.32278838 | -0.09328773 | 2.42047780 |
| H | 0.76101335 | 1.17966165 | 0.85111907 |
| C | 1.67626751 | -1.87670503 | 3.05629736 |
| H | 2.47017295 | -2.55570948 | 2.74887808 |
| H | 1.51062710 | -1.96905449 | 4.13019771 |
| C | 1.83473421 | -0.41505250 | 2.60123917 |
| H | 2.34797306 | -0.36283012 | 1.63689637 |
| H | 2.31601038 | 0.26637074 | 3.30918410 |
| C | -0.90121603 | -1.92081399 | 2.63493985 |
| H | 0.60121131 | -2.05905945 | 1.16660145 |
| C | -1.97388062 | -1.68308810 | 1.61195190 |
| C | -1.53206028 | -1.39406982 | 0.16861140 |
| H | -1.19443696 | -2.33173931 | -0.28737197 |
| H | -2.44548840 | -1.12762027 | -0.37043025 |
| C | -0.80870785 | 3.17190659 | -0.79411020 |
| H | -1.43115677 | 4.07053792 | -0.74064820 |
| H | 0.07488829 | 3.35790827 | -0.16962230 |
| C | -0.37860287 | 2.81549052 | -2.21812702 |
| H | 0.38347211 | 3.48739740 | -2.62581018 |
| H | -1.24457802 | 2.85804235 | -2.89118678 |
| C | 0.12020459 | 1.35956002 | -2.10874709 |
| C | 0.08615908 | 0.62985976 | -3.45434488 |
| H | 0.40655445 | -0.41357135 | -3.34627687 |
| H | -0.92353816 | 0.63180102 | -3.87738208 |
| C | 1.57559258 | 1.36523858 | -1.60948868 |
| H | 1.94145901 | 0.36019882 | -1.37135790 |
| H | 2.21921628 | 1.75408698 | -2.40435098 |
| H | 1.73179350 | 2.00831091 | -0.73842105 |
| H | -2.61636370 | -2.57402398 | 1.61705991 |
| H | -2.61535047 | -0.88217393 | 2.00141534 |
| C | -1.35772486 | -2.18395926 | 4.03172189 |
| H | -0.54987475 | -2.22551407 | 4.76054487 |
| H | -2.11905146 | -1.47025857 | 4.35660132 |
| H | -1.83767055 | -3.17088748 | 4.01112348 |
| C | -0.22942099 | 0.51386644 | 3.69190859 |

| | | | |
|---|---|---|---|
| H | 0.18185814 | 1.53116969 | 3.71622354 |
| H | -1.31697683 | 0.60217851 | 3.70692355 |
| H | 0.11718312 | 0.00479228 | 4.59338522 |
| C | -3.06740691 | 2.06725584 | -0.57111854 |
| H | -3.60355469 | 1.13381618 | -0.36208939 |
| H | -3.49718277 | 2.85320052 | 0.05892503 |
| H | -3.25714946 | 2.33264852 | -1.61600779 |
| H | -2.19516234 | 1.11086957 | 1.61616125 |
| H | 0.75537299 | 1.10893702 | -4.17582808 |

**TS_15c-16**

Sum of electronic and thermal Free Energies = -781.14541

| | | | |
|---|---|---|---|
| C | 0.17009800 | -0.01401900 | -0.89630600 |
| C | -2.88639600 | -0.44602600 | -1.24816200 |
| C | -0.34517300 | -0.17186100 | 0.55080400 |
| C | 0.26859100 | 0.98484600 | 1.33416400 |
| C | 1.68664000 | 1.12958700 | 0.72206400 |
| C | 1.65252500 | 0.33594800 | -0.63647000 |
| H | 0.07380300 | -0.95482800 | -1.44520300 |
| H | 0.30615100 | 0.81469500 | 2.41360300 |
| H | 2.00942700 | 0.98566700 | -1.44264700 |
| C | -1.44576200 | -0.95416000 | 1.00922800 |
| H | 0.18062300 | -1.13625200 | 0.95933500 |
| C | -3.32666900 | -1.64633400 | -0.46358000 |
| H | -3.68712500 | -2.47143500 | -1.08183200 |
| H | -4.09847000 | -1.41977800 | 0.27570700 |
| C | -2.01550500 | -2.11784300 | 0.24823000 |
| H | -1.30876100 | -2.46201300 | -0.51178000 |
| H | -2.22480500 | -2.93780000 | 0.94375900 |
| C | -2.88228500 | 0.81294600 | -0.79501600 |
| H | -2.23218300 | -0.68924300 | -2.08464500 |
| C | -1.83645100 | 1.77936500 | -1.30296700 |
| C | -0.51367300 | 1.12573800 | -1.74665000 |
| H | -0.63930100 | 0.71239600 | -2.75233400 |
| H | 0.21017000 | 1.93686900 | -1.86137700 |
| C | 2.77765700 | 0.40820600 | 1.55158100 |
| H | 3.31415200 | 1.10113200 | 2.20658100 |
| H | 2.33134700 | -0.35658400 | 2.20168400 |
| C | 3.67585500 | -0.25558400 | 0.50531700 |
| H | 4.33840100 | -1.02081000 | 0.92216100 |
| H | 4.31062800 | 0.49983700 | 0.02499200 |
| C | 2.68791700 | -0.82813100 | -0.53067700 |
| C | 3.34260600 | -1.08115500 | -1.89096200 |
| H | 2.61021200 | -1.44455000 | -2.62180700 |
| H | 3.78890000 | -0.16398600 | -2.28750600 |
| C | 2.13480500 | -2.16989800 | -0.01651300 |
| H | 1.29832600 | -2.53962100 | -0.62189100 |
| H | 2.92180500 | -2.92756600 | -0.07799800 |
| H | 1.83058500 | -2.14305900 | 1.03727700 |
| H | -2.21635700 | 2.38474300 | -2.13548500 |
| H | -1.63921200 | 2.50111700 | -0.50009900 |
| C | -3.76523500 | 1.33901600 | 0.30566200 |
| H | -4.52768000 | 0.62902800 | 0.63056700 |
| H | -3.17685600 | 1.65551600 | 1.17678500 |
| H | -4.28455000 | 2.23609400 | -0.04944300 |
| C | -1.98508800 | -0.75792200 | 2.38270400 |
| H | -1.46683700 | -1.44997900 | 3.06172200 |
| H | -1.86389500 | 0.25760400 | 2.75539300 |
| H | -3.03881900 | -1.05085600 | 2.40271300 |
| C | 2.04762500 | 2.60376500 | 0.52928100 |
| H | 1.35373900 | 3.09900200 | -0.15908400 |
| H | 2.01745600 | 3.13893900 | 1.48408200 |
| H | 3.05708000 | 2.70564100 | 0.11881200 |
| H | -0.33341200 | 1.88492100 | 1.15811600 |
| H | 4.13296100 | -1.83375300 | -1.81055600 |

**IM16**

Sum of electronic and thermal Free Energies = -781.182053

| | | | |
|---|---|---|---|
| C | 0.08238511 | -0.50131125 | -0.93878675 |
| C | -2.44197493 | -0.14874780 | -0.41857351 |
| C | -0.92321346 | -0.33419804 | 0.25053123 |
| C | -0.35389535 | 0.86649674 | 1.04078529 |
| C | 1.17596530 | 0.79127194 | 0.86236975 |
| C | 1.34544505 | 0.34667262 | -0.60628716 |
| H | 0.32246111 | -1.56201652 | -1.04260055 |
| H | -0.67681534 | 0.90716775 | 2.08314540 |
| H | 1.33747960 | 1.23041807 | -1.26066560 |
| C | -1.24663339 | -1.59766118 | 1.16822694 |
| H | -0.61107448 | -2.41855475 | 0.81686423 |
| C | -3.40907174 | -0.61392416 | 0.64110545 |
| H | -4.43124457 | -0.71650134 | 0.26749217 |
| H | -3.42019761 | 0.05444536 | 1.51020152 |
| C | -2.74402369 | -1.95356826 | 0.98204841 |
| H | -2.89242257 | -2.64899365 | 0.14889636 |
| H | -3.15848688 | -2.42296324 | 1.87610547 |
| C | -2.32130984 | 1.14039864 | -0.99759815 |
| H | -2.38907745 | -0.90656642 | -1.20810027 |
| C | -1.34201553 | 1.24795964 | -2.10182838 |
| C | -0.51472813 | -0.02700481 | -2.28950629 |
| H | -1.12997556 | -0.80646736 | -2.75034907 |
| H | 0.29628257 | 0.17114613 | -2.99534455 |
| C | 1.94342017 | -0.33021633 | 1.59376805 |
| H | 2.12857507 | -0.11185327 | 2.65095444 |
| H | 1.38856525 | -1.27414927 | 1.53700449 |
| C | 3.21885996 | -0.48437489 | 0.76029975 |
| H | 3.71493960 | -1.44304939 | 0.93854317 |
| H | 3.94382853 | 0.29654203 | 1.01074514 |
| C | 2.75161707 | -0.34536065 | -0.71796204 |
| C | 3.70791840 | 0.55037086 | -1.51495473 |
| H | 3.40737615 | 0.60989738 | -2.56747721 |
| H | 3.73017563 | 1.56824325 | -1.11119246 |
| C | 2.71595867 | -1.72726105 | -1.38264780 |
| H | 2.24646943 | -1.69552728 | -2.37310574 |
| H | 3.73869222 | -2.09241018 | -1.51549121 |
| H | 2.18722806 | -2.46805428 | -0.77225764 |
| H | -1.91504956 | 1.50309272 | -3.01013062 |
| H | -0.72318179 | 2.13855166 | -1.91529282 |
| C | -3.04269170 | 2.31731187 | -0.49058371 |
| H | -3.11574885 | 2.28812472 | 0.60178185 |
| H | -2.62620409 | 3.26441367 | -0.83478474 |
| H | -4.07914392 | 2.22813823 | -0.85437829 |
| C | -1.02389409 | -1.40640701 | 2.67616839 |
| H | -1.13912939 | -2.37961360 | 3.16076573 |
| H | -0.04381240 | -1.01911043 | 2.94673102 |
| H | -1.78124759 | -0.74090384 | 3.10542724 |
| C | 1.79094389 | 2.15770327 | 1.17792253 |
| H | 1.37248623 | 2.93396780 | 0.52686610 |
| H | 1.58533309 | 2.43952239 | 2.21606287 |
| H | 2.87454809 | 2.16552908 | 1.04379059 |
| H | -0.65139305 | 1.82413152 | 0.59304894 |
| H | 4.72715627 | 0.15297598 | -1.47926001 |

**TS_16-17**

Sum of electronic and thermal Free Energies = -781.182487

| | | | |
|---|---|---|---|
| C | -0.17528800 | -0.34123100 | -0.97217300 |
| C | 2.35922200 | -0.48874100 | -0.38756600 |
| C | 0.98237800 | 0.39334700 | -0.21146400 |
| C | 0.48079300 | 0.49527800 | 1.25076500 |
| C | -1.05778100 | 0.42186300 | 1.20005100 |
| C | -1.35613900 | -0.52697900 | 0.02229000 |
| H | -0.47259500 | 0.27530800 | -1.82369400 |
| H | 0.84343400 | 1.38168200 | 1.77576700 |
| H | -1.34983200 | -1.56843800 | 0.37394900 |
| C | 1.53813800 | 1.76267000 | -0.80266600 |
| H | 1.09019700 | 1.88221900 | -1.79581400 |
| C | 3.46992600 | 0.46327300 | -0.01608700 |
| H | 4.46926900 | 0.06625000 | -0.21382900 |
| H | 3.41136400 | 0.75287200 | 1.04044900 |
| C | 3.08530800 | 1.63135500 | -0.93323400 |
| H | 3.37594700 | 1.38707900 | -1.96032600 |
| H | 3.59080700 | 2.56133100 | -0.66702000 |
| C | 2.07793400 | -1.75685600 | 0.19817200 |

| | | | |
|---|---|---|---|
| H | 2.35605600 | -0.63045300 | -1.47845200 |
| C | 1.00349300 | -2.52567600 | -0.45865500 |
| C | 0.24974200 | -1.72324400 | -1.52406500 |
| H | 0.86413200 | -1.62275700 | -2.42520400 |
| H | -0.64007200 | -2.28310600 | -1.82544800 |
| C | -1.81413800 | 1.68461000 | 0.74069700 |
| H | -1.89302800 | 2.45314900 | 1.51702300 |
| H | -1.30983000 | 2.12879000 | -0.12527900 |
| C | -3.15937700 | 1.13472600 | 0.25885800 |
| H | -3.68423700 | 1.83859200 | -0.39380000 |
| H | -3.82457800 | 0.93304800 | 1.10437000 |
| C | -2.80300300 | -0.18455200 | -0.48815500 |
| C | -3.76769100 | -1.31325000 | -0.10433200 |
| H | -3.54972200 | -2.22708600 | -0.66956800 |
| H | -3.70005400 | -1.55098500 | 0.96265800 |
| C | -2.89769900 | 0.03778300 | -2.00350600 |
| H | -2.49794500 | -0.80979000 | -2.57262200 |
| H | -3.94791700 | 0.15525400 | -2.28691700 |
| H | -2.37631000 | 0.94616000 | -2.32404000 |
| H | 1.48621400 | -3.42300000 | -0.88673100 |
| H | 0.35058400 | -2.93209500 | 0.32728900 |
| C | 2.76643200 | -2.25586600 | 1.39508900 |
| H | 2.90454500 | -1.44689200 | 2.12206200 |
| H | 2.28684800 | -3.12293700 | 1.84924500 |
| H | 3.78709600 | -2.52808100 | 1.07996400 |
| C | 1.25992800 | 3.02905300 | 0.01861200 |
| H | 1.87036600 | 3.04842000 | 0.92784500 |
| H | 1.55554400 | 3.89353300 | -0.58210300 |
| H | 0.22023900 | 3.16818300 | 0.30638400 |
| C | -1.58830700 | -0.06508800 | 2.55139100 |
| H | -1.18860400 | -1.05736100 | 2.79166100 |
| H | -1.28822400 | 0.62210600 | 3.34972600 |
| H | -2.67766200 | -0.13540600 | 2.57083400 |
| H | 0.81646300 | -0.36484900 | 1.84643300 |
| H | -4.80171200 | -1.02560400 | -0.31894900 |

**IM17**

Sum of electronic and thermal Free Energies = -781.192722

| | | | |
|---|---|---|---|
| C | -0.14731334 | -0.22867175 | -1.01067082 |
| C | 2.44009154 | -0.55462049 | -0.36208805 |
| C | 1.03995863 | 0.42493612 | -0.27678271 |
| C | 0.59092625 | 0.72382700 | 1.17048012 |
| C | -0.92144405 | 0.43120468 | 1.24592334 |
| C | -1.23942756 | -0.50352781 | 0.05290025 |
| H | -0.50522892 | 0.49209485 | -1.75298645 |
| H | 0.81268641 | 1.75935054 | 1.44806632 |
| H | -1.15411260 | -1.55256315 | 0.37382809 |
| C | 1.75164451 | 1.62519769 | -0.96521936 |
| H | 1.92930650 | 1.32370293 | -2.00667076 |
| C | 3.48977586 | 0.34033395 | 0.26745821 |
| H | 4.49102047 | 0.03454061 | -0.04482376 |
| H | 3.45767127 | 0.29449914 | 1.35909233 |
| C | 3.10669260 | 1.75916610 | -0.23819432 |
| H | 3.86446579 | 2.17677641 | -0.90474491 |
| H | 3.01185436 | 2.44920978 | 0.60596246 |
| C | 1.88649658 | -1.75545173 | 0.13403530 |
| H | 2.55773909 | -0.61191610 | -1.44650642 |
| C | 0.99126511 | -2.48023784 | -0.80457961 |
| C | 0.26516197 | -1.50581138 | -1.76384956 |
| H | 0.90517596 | -1.25955359 | -2.61689773 |
| H | -0.61371219 | -2.01085921 | -2.17355083 |
| C | -1.81991991 | 1.64476950 | 0.94247286 |
| H | -1.92145219 | 2.31734773 | 1.80074902 |
| H | -1.39473476 | 2.22900402 | 0.11733235 |
| C | -3.13896267 | 1.01029831 | 0.49609395 |
| H | -3.76697447 | 1.70317001 | -0.07159672 |
| H | -3.72482111 | 0.69626573 | 1.36622302 |
| C | -2.73296012 | -0.22511861 | -0.36033759 |
| C | -3.60318492 | -1.44101232 | -0.02182521 |
| H | -3.35049085 | -2.29700840 | -0.65880387 |
| H | -3.47264697 | -1.74509973 | 1.02247880 |
| C | -2.92069220 | 0.10783130 | -1.84723178 |
| H | -2.50979324 | -0.66608287 | -2.50523156 |
| H | -3.98981904 | 0.18632031 | -2.06547127 |
| H | -2.46884066 | 1.06842050 | -2.11838555 |
| H | 1.64219831 | -3.14663672 | -1.39445148 |
| H | 0.30620788 | -3.13056671 | -0.25440024 |
| C | 2.04486173 | -2.25232224 | 1.51194380 |
| H | 1.06141265 | -2.29910893 | 1.99912260 |
| H | 2.38589658 | -3.29579841 | 1.45034553 |
| H | 2.74500614 | -1.67688225 | 2.11473237 |
| C | 0.95444318 | 2.92476833 | -1.00505900 |
| H | 0.72525861 | 3.30632399 | -0.00657049 |
| H | 1.55079981 | 3.68538815 | -1.51755520 |
| H | 0.01914461 | 2.81271234 | -1.56128086 |
| C | -1.28698343 | -0.17233746 | 2.60495255 |
| H | -0.75883675 | -1.11801634 | 2.77447995 |
| H | -1.01617941 | 0.51310453 | 3.41486369 |
| H | -2.35649678 | -0.37873551 | 2.68937396 |
| H | 1.12694259 | 0.10846635 | 1.90086614 |
| H | -4.66260227 | -1.21205826 | -0.17388873 |

**TS_17-18a**

Sum of electronic and thermal Free Energies = -781.192127

| | | | |
|---|---|---|---|
| C | -0.13603171 | -0.39259913 | -0.90992341 |
| C | 2.30215960 | -0.21047879 | -0.04222923 |
| C | 0.94410658 | 0.48475907 | -0.21333091 |
| C | 0.39048152 | 0.79639251 | 1.21199055 |
| C | -1.09610226 | 0.39823391 | 1.24707130 |
| C | -1.29865764 | -0.61313096 | 0.09228011 |
| H | -0.48599712 | 0.15197421 | -1.79056515 |
| H | 0.53828144 | 1.84642285 | 1.48866824 |
| H | -1.21488468 | -1.63493014 | 0.49057131 |
| C | 1.43582976 | 1.73864112 | -0.98593979 |
| H | 1.72011383 | 1.38115233 | -1.98951812 |
| C | 3.31306260 | 0.85140142 | 0.37902233 |
| H | 4.32199078 | 0.63530090 | 0.01949317 |
| H | 3.35731926 | 0.90186497 | 1.47159816 |
| C | 2.72259660 | 2.14970695 | -0.23305806 |
| H | 3.43194418 | 2.64728577 | -0.89767783 |
| H | 2.47549833 | 2.86108195 | 0.56055196 |
| C | 2.40405111 | -1.61305635 | 0.14984244 |
| H | 2.63365759 | -0.57844747 | -1.10404667 |
| C | 1.25721808 | -2.44048546 | -0.30427714 |
| C | 0.42740905 | -1.73920569 | -1.39195880 |
| H | 1.05967844 | -1.61257217 | -2.28176875 |
| H | -0.39458819 | -2.39793571 | -1.68636118 |
| C | -2.08208114 | 1.52153317 | 0.87677858 |
| H | -2.27503786 | 2.20266545 | 1.71246273 |
| H | -1.68006168 | 2.11854249 | 0.05182282 |
| C | -3.32197302 | 0.76668942 | 0.39598386 |
| H | -3.99360949 | 1.39380670 | -0.19815918 |
| H | -3.90344430 | 0.40230962 | 1.24952404 |
| C | -2.77253962 | -0.42795418 | -0.43411397 |
| C | -3.58925778 | -1.69852687 | -0.17203578 |
| H | -3.22993672 | -2.53460023 | -0.78382732 |
| H | -3.52857822 | -1.99713924 | 0.88034765 |
| C | -2.86426825 | -0.09121780 | -1.92797747 |
| H | -2.37392406 | -0.84579310 | -2.55427391 |
| H | -3.91638281 | -0.05290057 | -2.22525065 |
| H | -2.42774359 | 0.88713974 | -2.15987334 |
| H | 1.59564474 | -3.43702863 | -0.60048003 |
| H | 0.64036411 | -2.58069188 | 0.60246915 |
| C | 3.61992091 | -2.24880766 | 0.69853178 |
| H | 4.48702138 | -1.58788613 | 0.69772003 |
| H | 3.37490458 | -2.45673530 | 1.75353633 |
| H | 3.84397985 | -3.20643889 | 0.22608321 |
| C | 0.46473971 | 2.89369626 | -1.17178450 |
| H | 0.15374981 | 3.31881252 | -0.21285231 |
| H | 0.94860772 | 3.69095973 | -1.74304741 |
| H | -0.42925993 | 2.59010563 | -1.72518912 |
| C | -1.45237936 | -0.19187048 | 2.61565298 |
| H | -0.83758638 | -1.07396403 | 2.83184585 |
| H | -1.28027754 | 0.54191358 | 3.41017917 |
| H | -2.49971462 | -0.50002913 | 2.66886055 |
| H | 0.93564701 | 0.20538793 | 1.96208890 |

| | | | |
|---|---|---|---|
| H | -4.64448962 | -1.53671323 | -0.41388120 |

**IM18a**

Sum of electronic and thermal Free Energies = -781.202928

| | | | |
|---|---|---|---|
| C | -0.18395100 | -0.12422200 | -1.15817300 |
| C | 2.15764100 | -0.10264700 | -0.11449300 |
| C | 0.92694200 | 0.58653200 | -0.35979600 |
| C | 0.62210100 | 0.28520600 | 1.22650000 |
| C | -0.85082200 | -0.19934300 | 1.26127800 |
| C | -1.27473300 | -0.62145900 | -0.17118400 |
| H | -0.58424700 | 0.60467100 | -1.86733000 |
| H | 0.81564000 | 1.20556800 | 1.78207700 |
| H | -1.28373300 | -1.71557000 | -0.22374100 |
| C | 1.31634000 | 2.05610600 | -0.63999500 |
| H | 1.56044600 | 2.07013700 | -1.71277000 |
| C | 3.24966600 | 0.85442400 | 0.25369800 |
| H | 4.03157500 | 0.71068900 | -0.50553700 |
| H | 3.71802100 | 0.61462500 | 1.21402600 |
| C | 2.61369200 | 2.25233300 | 0.16971500 |
| H | 3.27996500 | 2.98034300 | -0.29606200 |
| H | 2.37966400 | 2.63109700 | 1.16943400 |
| C | 2.41230300 | -1.53522400 | -0.41762500 |
| H | 3.16014900 | -1.41867700 | -1.22570400 |
| C | 1.19619000 | -2.24219700 | -1.02046400 |
| C | 0.41303300 | -1.30635100 | -1.94481100 |
| H | 1.07708500 | -0.93696300 | -2.73812400 |
| H | -0.39741600 | -1.85067700 | -2.43899100 |
| C | -1.82354300 | 0.94898200 | 1.59497400 |
| H | -1.86688800 | 1.16129000 | 2.66819000 |
| H | -1.51240000 | 1.86631800 | 1.08456300 |
| C | -3.14667500 | 0.46931200 | 1.00119200 |
| H | -3.87494800 | 1.27828000 | 0.89179200 |
| H | -3.60477200 | -0.28474000 | 1.65037400 |
| C | -2.76788400 | -0.15396700 | -0.36844400 |
| C | -3.65956200 | -1.36016100 | -0.68444800 |
| H | -3.40329800 | -1.79890300 | -1.65542300 |
| H | -3.55516700 | -2.13920300 | 0.07874600 |
| C | -2.95804500 | 0.88847000 | -1.47578300 |
| H | -2.64762000 | 0.50818700 | -2.45499500 |
| H | -4.01817700 | 1.14758800 | -1.54900900 |
| H | -2.41034700 | 1.81518000 | -1.27482300 |
| H | 1.54528700 | -3.12483000 | -1.56378800 |
| H | 0.55578500 | -2.61501100 | -0.21148900 |
| C | 3.09166200 | -2.31801500 | 0.71362000 |
| H | 4.00258600 | -1.83022300 | 1.06817400 |
| H | 2.40540000 | -2.44247500 | 1.55774700 |
| H | 3.35954100 | -3.31355400 | 0.35410500 |
| C | 0.28099000 | 3.13854200 | -0.37612200 |
| H | 0.05409400 | 3.22630300 | 0.69054800 |
| H | 0.67364200 | 4.10405500 | -0.70585700 |
| H | -0.64912600 | 2.95877000 | -0.92074700 |
| C | -0.99290100 | -1.34158700 | 2.27261400 |
| H | -0.36164800 | -2.19403000 | 1.99505300 |
| H | -0.70867000 | -1.01625600 | 3.27872500 |
| H | -2.02425600 | -1.70081600 | 2.31622800 |
| H | 1.26177300 | -0.48599600 | 1.68970800 |
| H | -4.71260900 | -1.06356700 | -0.71861700 |

**TS_18a-18b**

Sum of electronic and thermal Free Energies = -781.193397

| | | | |
|---|---|---|---|
| C | -0.11397000 | -0.27935500 | -1.07464100 |
| C | 2.22532100 | 0.03065500 | -0.16062700 |
| C | 0.84110900 | 0.49025100 | -0.05664900 |
| C | 0.37254100 | -0.03398700 | 1.36389300 |
| C | -1.10485000 | -0.47406800 | 1.23799100 |
| C | -1.37734700 | -0.69478500 | -0.27647300 |
| H | -0.35822000 | 0.43660000 | -1.86225400 |
| H | 0.53253100 | 0.73917600 | 2.11928600 |
| H | -1.53390800 | -1.76749300 | -0.44905800 |
| C | 0.92714500 | 2.04738200 | -0.26186800 |
| H | 0.15874200 | 2.35369300 | -0.97515800 |
| C | 3.17447100 | 1.15558000 | -0.17522600 |
| H | 4.14919800 | 0.91436000 | -0.60433600 |
| H | 3.33474900 | 1.45323300 | 0.87615000 |
| C | 2.32951800 | 2.23600600 | -0.88523300 |
| H | 2.31618900 | 2.03514400 | -1.96198500 |
| H | 2.73440700 | 3.23862800 | -0.73548800 |
| C | 2.62315100 | -1.37034500 | -0.36019100 |
| H | 3.31110100 | -1.30097600 | -1.22321500 |
| C | 1.44492500 | -2.26119200 | -0.75076200 |
| C | 0.57168300 | -1.48644900 | -1.73907600 |
| H | 1.20440000 | -1.15003300 | -2.57238200 |
| H | -0.19708200 | -2.13083000 | -2.17350400 |
| C | -2.13676300 | 0.59296400 | 1.65876900 |
| H | -2.34779100 | 0.56173700 | 2.73225500 |
| H | -1.77985000 | 1.60090000 | 1.42395700 |
| C | -3.34420200 | 0.26878700 | 0.77946700 |
| H | -4.09666200 | 1.06290200 | 0.76792100 |
| H | -3.84110000 | -0.64070300 | 1.13716200 |
| C | -2.73375600 | 0.02518700 | -0.61945200 |
| C | -3.62187600 | -0.87241300 | -1.48403300 |
| H | -3.16038000 | -1.06352800 | -2.46000400 |
| H | -3.79991700 | -1.83688300 | -0.99696700 |
| C | -2.57532000 | 1.37941600 | -1.32559400 |
| H | -2.16071700 | 1.27959100 | -2.33369000 |
| H | -3.56018700 | 1.84337200 | -1.43254600 |
| H | -1.94833100 | 2.07683200 | -0.75970700 |
| H | 1.83265000 | -3.18273200 | -1.19350600 |
| H | 0.86567700 | -2.55426300 | 0.13304400 |
| C | 3.48834300 | -1.89597200 | 0.81458900 |
| H | 4.34423000 | -1.24766900 | 1.01506500 |
| H | 2.89044200 | -1.98964700 | 1.72376900 |
| H | 3.86052000 | -2.88568300 | 0.54408800 |
| C | 0.79167100 | 2.91735400 | 0.99000100 |
| H | 1.57649100 | 2.71666300 | 1.72810300 |
| H | 0.87448200 | 3.96840200 | 0.70254900 |
| H | -0.17062800 | 2.79072600 | 1.48807400 |
| C | -1.32485400 | -1.74414200 | 2.07058000 |
| H | -0.70919000 | -2.57451000 | 1.70749500 |
| H | -1.07285500 | -1.56646800 | 3.12133300 |
| H | -2.36853100 | -2.06741700 | 2.02847200 |
| H | 0.97136900 | -0.89725000 | 1.67550300 |
| H | -4.59347400 | -0.40111300 | -1.66323000 |

**IM18b**

Sum of electronic and thermal Free Energies = -781.197656

| | | | |
|---|---|---|---|
| C | -0.92315778 | 0.67030304 | 2.51548034 |
| C | -2.49779029 | 0.43493203 | 4.25953602 |
| C | -2.43055427 | 0.01862986 | 2.87959773 |
| C | -2.24169925 | -1.46902243 | 2.54045422 |
| C | -1.29438408 | -1.55211266 | 1.33826316 |
| C | -0.33056595 | -0.34933610 | 1.49537074 |
| H | -1.14703070 | 1.63569161 | 2.06359046 |
| H | -3.20681873 | -1.95251171 | 2.36180263 |
| H | 0.60519600 | -0.70692454 | 1.94365832 |
| C | -3.55401247 | 0.80860431 | 2.14539049 |
| H | -3.22123432 | 1.09844845 | 1.14580945 |
| C | -3.43533457 | 1.55757919 | 4.44314961 |
| H | -3.09649243 | 2.29739884 | 5.17367755 |
| H | -4.33023935 | 1.07760901 | 4.88811230 |
| C | -3.73403398 | 2.06154602 | 3.02462018 |
| H | -3.00884892 | 2.83767375 | 2.76047236 |
| H | -4.73006063 | 2.49769397 | 2.93467151 |
| C | -1.61544064 | -0.05027105 | 5.34641451 |
| H | -1.58409202 | 0.74146854 | 6.10422329 |
| C | -0.19047633 | -0.22437806 | 4.76906534 |
| C | 0.01013719 | 0.87500732 | 3.72262273 |
| H | -0.17357293 | 1.84961768 | 4.19498878 |
| H | 1.04084756 | 0.89449710 | 3.35728889 |
| C | -1.94604181 | -1.32286549 | -0.03896427 |
| H | -2.39062107 | -2.23895105 | -0.44121336 |
| H | -2.74477193 | -0.57529930 | 0.02150899 |

| | | | |
|---|---|---|---|
| C | -0.79364076 | -0.78354006 | -0.88703591 |
| H | -1.13433530 | -0.27800752 | -1.79540296 |
| H | -0.14568814 | -1.60622205 | -1.20766961 |
| C | -0.00830367 | 0.18140726 | 0.04370723 |
| C | 1.49937412 | 0.09191557 | -0.21836447 |
| H | 2.05641739 | 0.78303817 | 0.42447951 |
| H | 1.87180654 | -0.92131370 | -0.03317940 |
| C | -0.46039394 | 1.62249354 | -0.22380050 |
| H | 0.03821688 | 2.34237288 | 0.43473129 |
| H | -0.20243475 | 1.89271844 | -1.25165540 |
| H | -1.54467863 | 1.74842089 | -0.12025183 |
| H | 0.52995158 | -0.14626545 | 5.58725192 |
| H | -0.06390732 | -1.21608758 | 4.32115198 |
| C | -2.18362217 | -1.31163042 | 6.04275111 |
| H | -3.16038526 | -1.11201284 | 6.48916570 |
| H | -2.27428263 | -2.15719637 | 5.36033973 |
| H | -1.49481658 | -1.58707914 | 6.84431557 |
| C | -4.85516482 | 0.01214931 | 2.02028258 |
| H | -5.19240768 | -0.37830514 | 2.98826359 |
| H | -5.64599532 | 0.65391908 | 1.62481330 |
| H | -4.75070367 | -0.83526390 | 1.33871286 |
| C | -0.55644485 | -2.89579487 | 1.35056887 |
| H | 0.01752055 | -3.01933122 | 2.27583240 |
| H | -1.26713613 | -3.72539848 | 1.27753773 |
| H | 0.14230954 | -2.98210613 | 0.51426394 |
| H | -1.78228264 | -1.98978754 | 3.38268243 |
| H | 1.72469424 | 0.34668340 | -1.25885808 |

**TS_18b-14b**

Sum of electronic and thermal Free Energies = -781.190082

| | | | |
|---|---|---|---|
| C | -0.80559996 | 0.65673622 | 2.68196660 |
| C | -2.24474782 | 0.46336522 | 3.94590665 |
| C | -2.73418664 | -0.19146835 | 2.81460927 |
| C | -2.44200410 | -1.58993830 | 2.40562683 |
| C | -1.30512640 | -1.59283990 | 1.35429897 |
| C | -0.37376530 | -0.35782570 | 1.59735143 |
| H | -1.04741438 | 1.63407824 | 2.27674709 |
| H | -3.33917478 | -2.05432023 | 1.98410856 |
| H | 0.58084917 | -0.75997124 | 1.95543979 |
| C | -3.75798762 | 0.67016264 | 2.10779104 |
| H | -3.65943682 | 0.63415429 | 1.02007010 |
| C | -2.88846665 | 1.83304051 | 4.05411289 |
| H | -2.16878711 | 2.60407477 | 4.34777214 |
| H | -3.62696316 | 1.77125482 | 4.86472185 |
| C | -3.54827486 | 2.08156005 | 2.68857096 |
| H | -2.89337497 | 2.67231654 | 2.04175253 |
| H | -4.49032909 | 2.62690048 | 2.77255224 |
| C | -1.57289502 | -0.12450668 | 5.18367543 |
| H | -1.54414625 | 0.70531797 | 5.90122147 |
| C | -0.11997376 | -0.41975264 | 4.79175040 |
| C | 0.20976566 | 0.72055465 | 3.83386729 |
| H | 0.13448119 | 1.67727041 | 4.36120718 |
| H | 1.21400391 | 0.65856429 | 3.40305516 |
| C | -1.77716652 | -1.43854866 | -0.10469890 |
| H | -2.07240242 | -2.39993582 | -0.53609913 |
| H | -2.64450352 | -0.77226007 | -0.17507304 |
| C | -0.57180772 | -0.80458394 | -0.79564216 |
| H | -0.80608510 | -0.39345112 | -1.78152433 |
| H | 0.21679844 | -1.55152541 | -0.94051994 |
| C | -0.09187236 | 0.29134355 | 0.18322470 |
| C | 1.40093940 | 0.58775574 | 0.01796010 |
| H | 1.73910956 | 1.34503216 | 0.73506055 |
| H | 2.00179657 | -0.31559623 | 0.16550286 |
| C | -0.87711769 | 1.58199146 | -0.09632492 |
| H | -0.52188745 | 2.42684557 | 0.50299649 |
| H | -0.73657278 | 1.86192316 | -1.14388810 |
| H | -1.95405540 | 1.46969583 | 0.06811947 |
| H | 0.54069998 | -0.45381642 | 5.66105300 |
| H | -0.04548361 | -1.38795958 | 4.27857986 |
| C | -2.33825990 | -1.27000949 | 5.85055095 |
| H | -3.38105201 | -0.99664841 | 6.03666117 |
| H | -2.32375986 | -2.18891772 | 5.26147090 |
| H | -1.87850268 | -1.49375568 | 6.81625152 |
| C | -5.14151889 | 0.09923579 | 2.48995773 |
| H | -5.28197497 | 0.09465594 | 3.57624415 |
| H | -5.91551796 | 0.73272082 | 2.05110730 |
| H | -5.28727828 | -0.91728888 | 2.11875372 |
| C | -0.52522725 | -2.90627074 | 1.49729656 |
| H | -0.06955694 | -2.99092249 | 2.48972028 |
| H | -1.19075510 | -3.76332544 | 1.35392364 |
| H | 0.27585491 | -2.97583154 | 0.75630451 |
| H | -2.13084782 | -2.17837730 | 3.27038901 |
| H | 1.60882233 | 0.96921810 | -0.98663100 |

**IM14b**

Sum of electronic and thermal Free Energies = -781.19441

| | | | |
|---|---|---|---|
| C | -0.57727078 | 0.63296855 | 2.80801795 |
| C | -2.00554255 | 0.52191049 | 3.64066128 |
| C | -2.82803090 | -0.23549820 | 2.71893580 |
| C | -2.52402405 | -1.60220161 | 2.33663608 |
| C | -1.25744572 | -1.56757979 | 1.37681930 |
| C | -0.30879892 | -0.34004241 | 1.62437603 |
| H | -0.55107177 | 1.65726428 | 2.43172260 |
| H | -3.34843177 | -2.09082190 | 1.81060819 |
| H | 0.66938231 | -0.78493804 | 1.84162767 |
| C | -3.92609134 | 0.57441670 | 2.15889192 |
| H | -4.09647604 | 0.37219856 | 1.09528190 |
| C | -2.71249291 | 1.88442725 | 3.78161327 |
| H | -1.99724997 | 2.70067771 | 3.91611504 |
| H | -3.34145552 | 1.85911132 | 4.67982754 |
| C | -3.57406274 | 2.02901645 | 2.51875261 |
| H | -3.00425926 | 2.49102282 | 1.70996520 |
| H | -4.46799808 | 2.63477818 | 2.68205218 |
| C | -1.59679839 | -0.10402985 | 5.02108030 |
| H | -1.51741275 | 0.77802008 | 5.67069260 |
| C | -0.17594253 | -0.63019808 | 4.83839408 |
| C | 0.43826410 | 0.44728880 | 3.95349652 |
| H | 0.52914546 | 1.37715465 | 4.52642197 |
| H | 1.42801840 | 0.20468021 | 3.55826860 |
| C | -1.66212732 | -1.47152093 | -0.10898243 |
| H | -1.87318634 | -2.45967826 | -0.52875708 |
| H | -2.56569248 | -0.86482095 | -0.24050250 |
| C | -0.46457149 | -0.77278103 | -0.75215036 |
| H | -0.67083896 | -0.40507236 | -1.76121189 |
| H | 0.38310324 | -1.46485529 | -0.82572853 |
| C | -0.13300320 | 0.36598742 | 0.23077454 |
| C | 1.29702642 | 0.88306604 | 0.06800762 |
| H | 1.53179742 | 1.64536485 | 0.82064476 |
| H | 2.02464876 | 0.07117604 | 0.16850651 |
| C | -1.10501798 | 1.52729796 | -0.02348968 |
| H | -0.89202237 | 2.39996202 | 0.60111789 |
| H | -1.00571262 | 1.85460530 | -1.06268446 |
| H | -2.15100497 | 1.24243959 | 0.12603300 |
| H | 0.33936751 | -0.76087890 | 5.79349109 |
| H | -0.17619863 | -1.60245930 | 4.32741916 |
| C | -2.60440711 | -1.04216885 | 5.67978821 |
| H | -3.59439418 | -0.58014424 | 5.75475767 |
| H | -2.71011103 | -1.99907670 | 5.16264847 |
| H | -2.27601880 | -1.26535480 | 6.69804162 |
| C | -5.18839330 | 0.07467638 | 2.93697014 |
| H | -5.09080731 | 0.24767677 | 4.01157598 |
| H | -6.03820005 | 0.65536647 | 2.57223773 |
| H | -5.38579915 | -0.98467056 | 2.76239419 |
| C | -0.51804177 | -2.89388558 | 1.60454009 |
| H | -0.09000248 | -2.95165149 | 2.60978009 |
| H | -1.19388815 | -3.74344532 | 1.46589835 |
| H | 0.30110867 | -2.99461410 | 0.88653938 |
| H | -2.23695718 | -2.18321354 | 3.21615181 |
| H | 1.43472093 | 1.34029282 | -0.91675193 |

## 3. 3D Representation of All Computed Structures

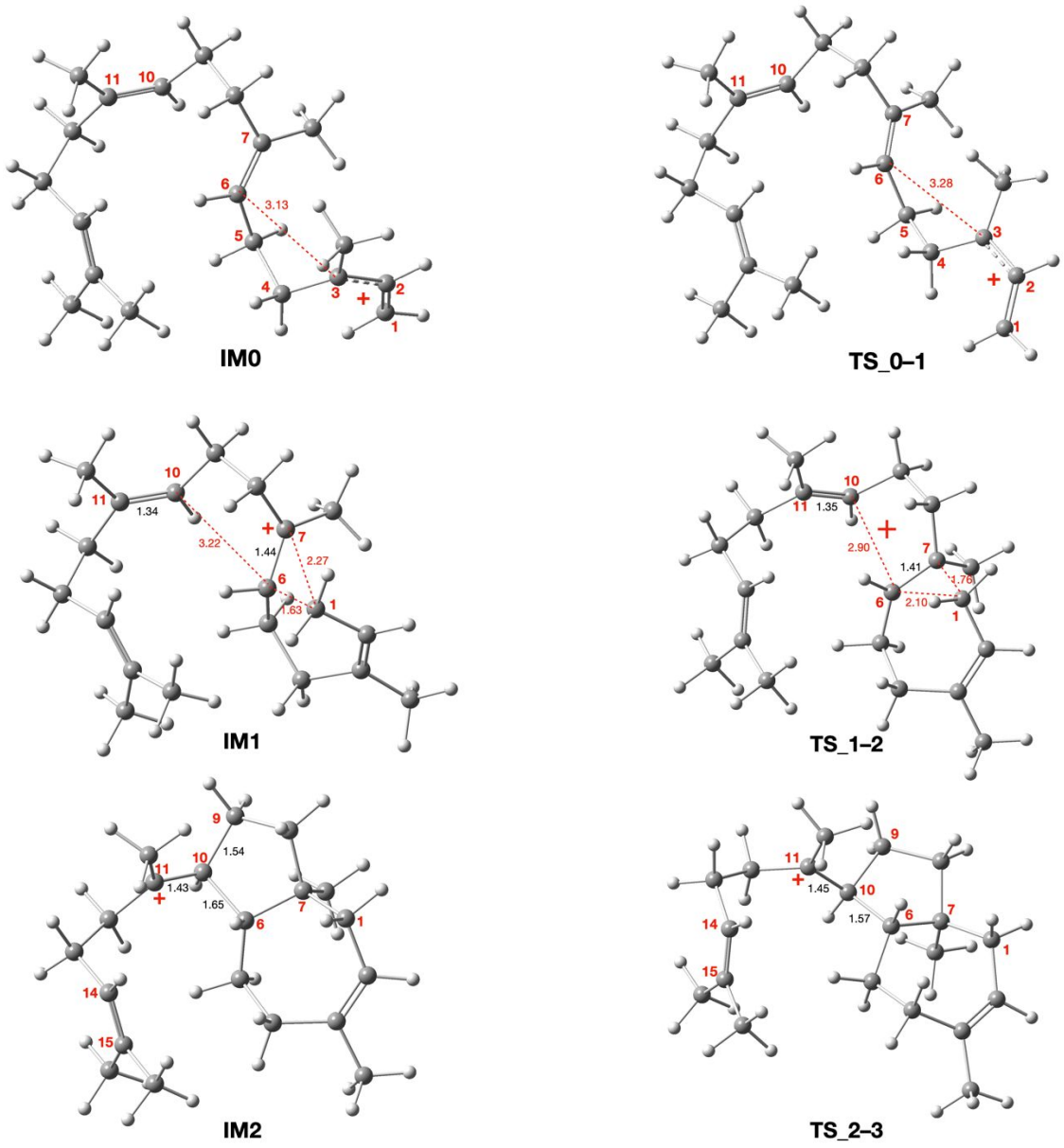



**Figure S1. 3D representation of IM0, TS_0–1, IM1, TS_1–2, IM2 and TS_2–3. Atomic distances are shown in Å.**

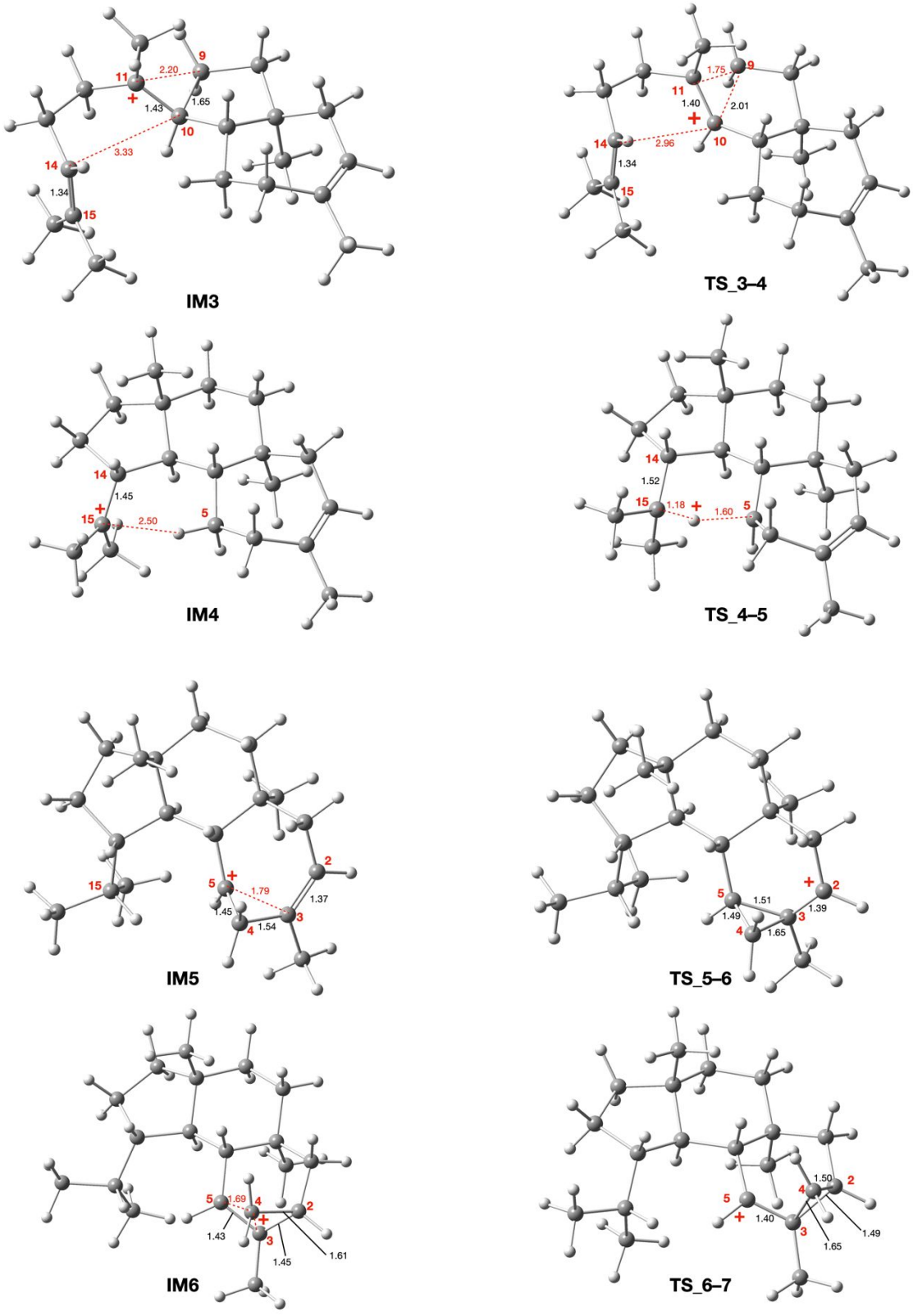



**Figure S2. 3D representation of IM3, TS_3–4, IM4, TS_4–5, IM5, TS_5–6, IM6 and TS_6–7. Atomic distances are shown in Å.**

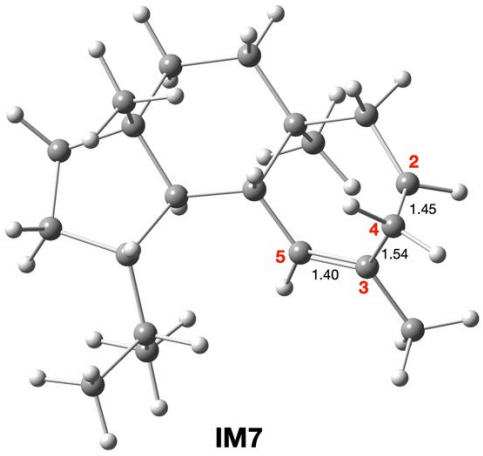



**Figure S3. 3D representation of IM7. Atomic distances are shown in Å.**

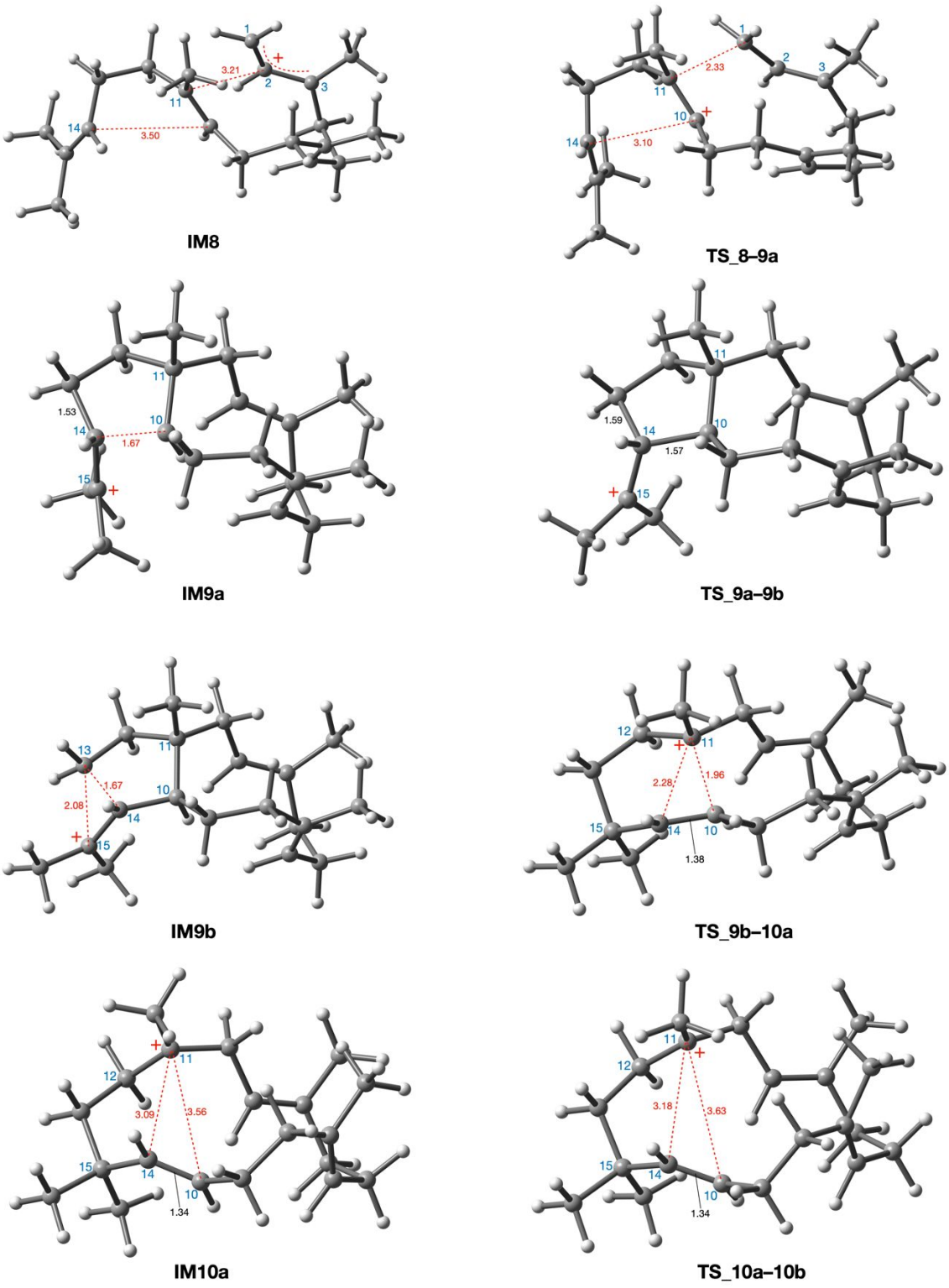



**Figure S4. 3D representation of IM8, TS_8–9a, IM9a, TS_9a–9b, IM9b, TS_9b–10a, IM10a and TS_10a–10b. Atomic distances are shown in Å.**

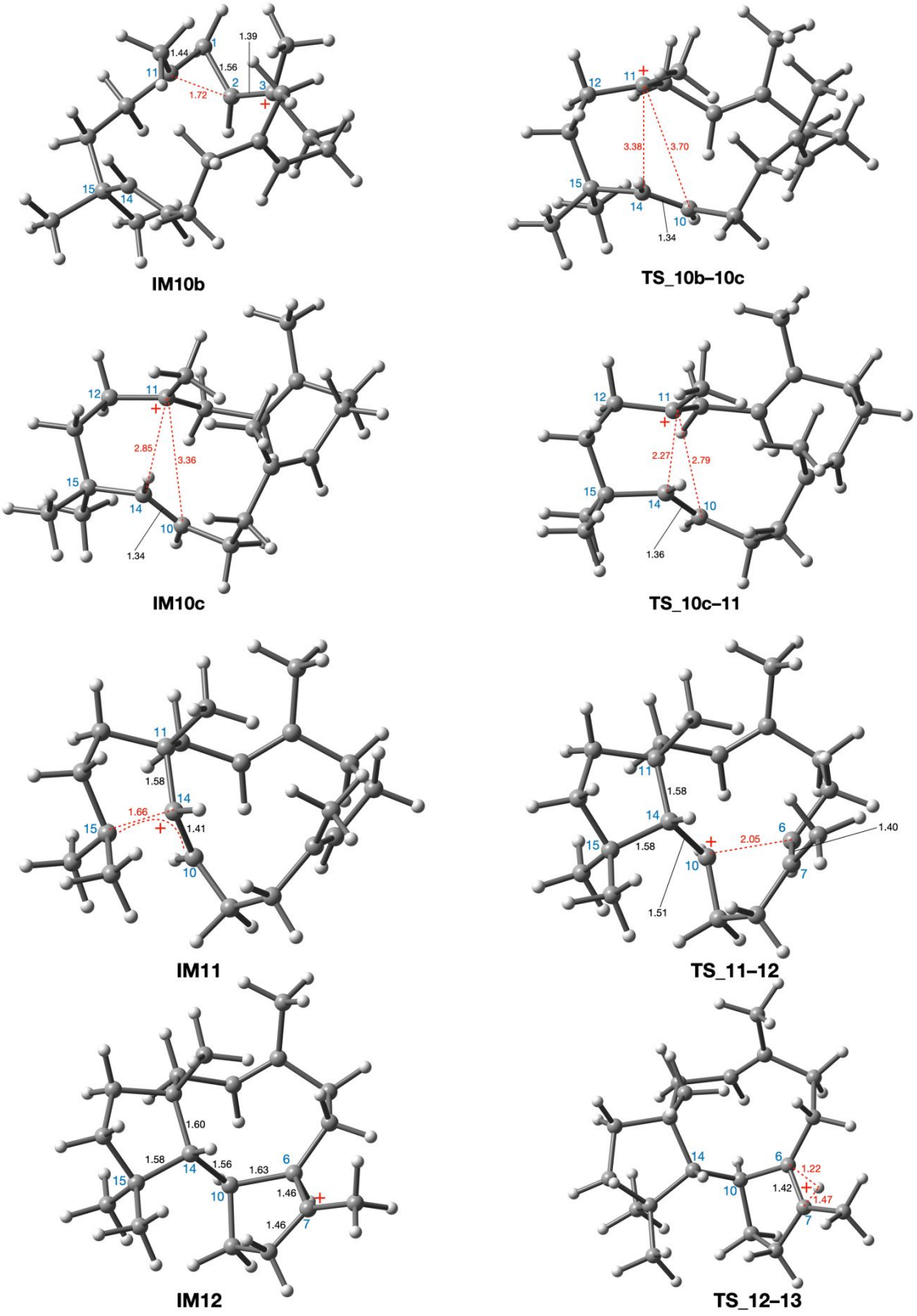
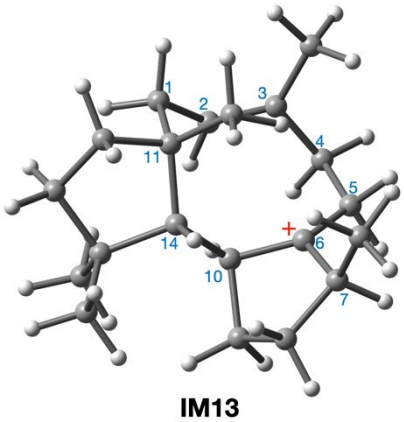
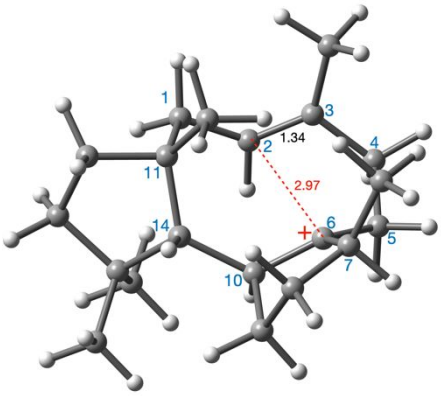



**Figure S5. 3D representation of IM10b, TS_10b–10c, IM10c, TS_10c–**

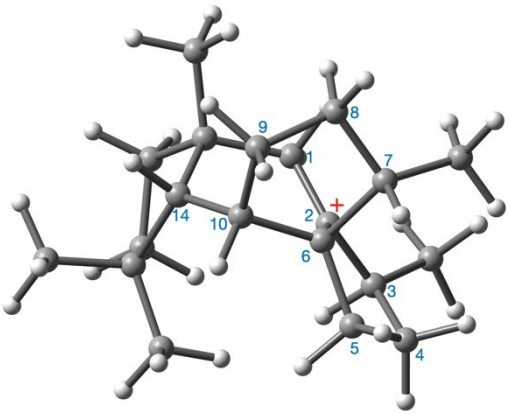
11, IM11, TS_11–12, IM12 and TS_12–13. Atomic distances are shown in Å.



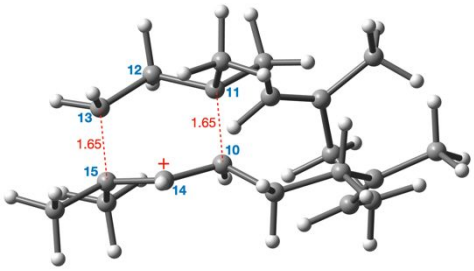

IM13



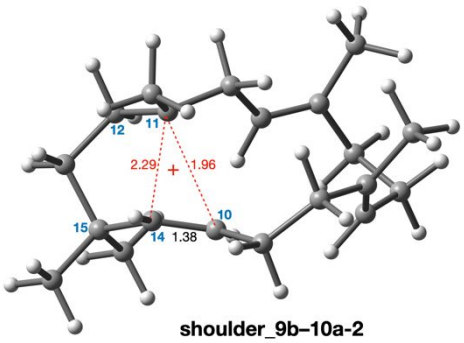

TS_13–14a




IM14a




shoulder_9b–10a-1




shoulder_9b–10a-2

Figure S6. 3D representation of IM13, TS_13–14a, IM14a, shoulder_9b–10a-1 and shoulder_9b–10a-2. Atomic distances are shown in Å.

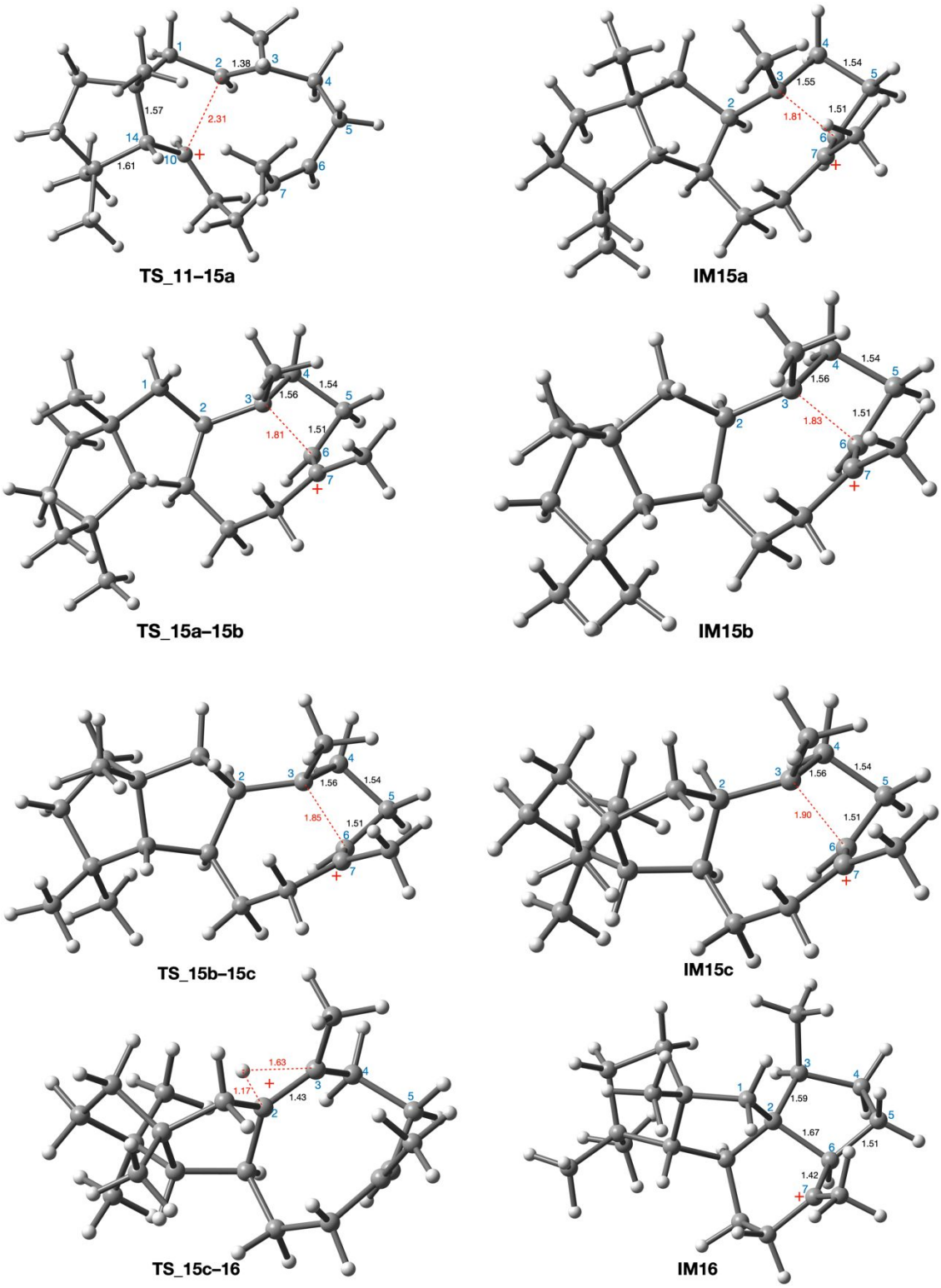
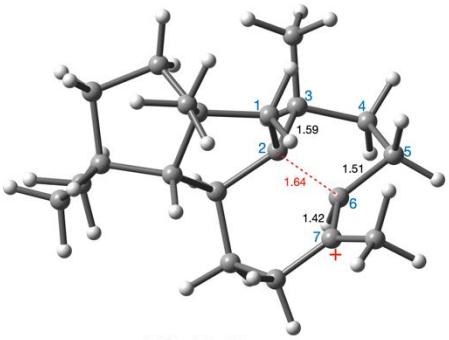
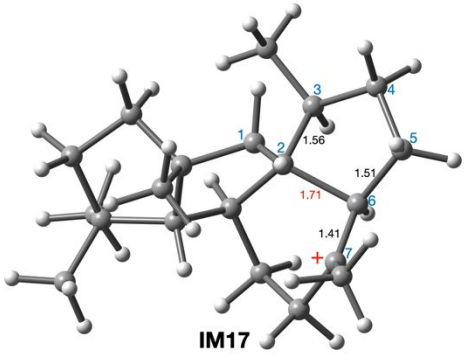



**Figure S7. 3D representation of TS_11–15a, IM15a, TS_15a–15b,**

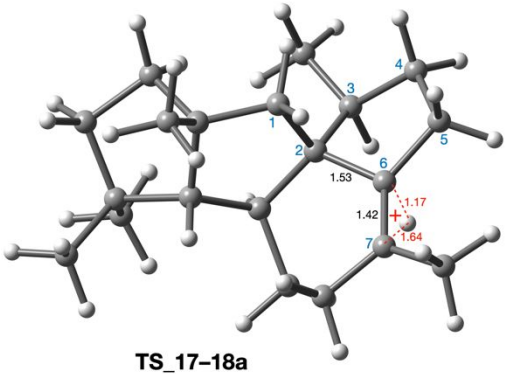
**IM15b, TS_15b–15c, IM15c, TS_15c–16, and IM16. Atomic distances are shown in Å.**



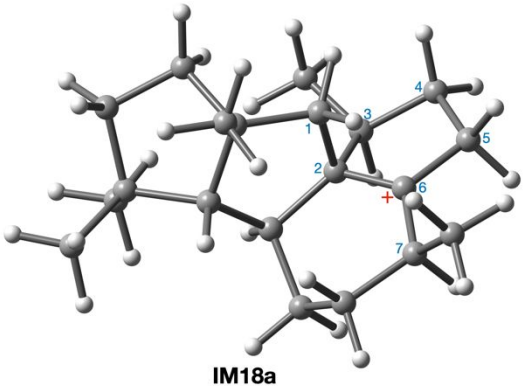

TS_16–17



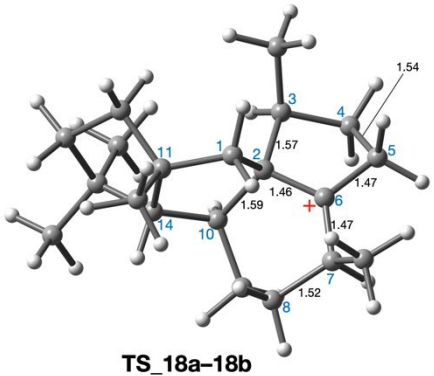

IM17



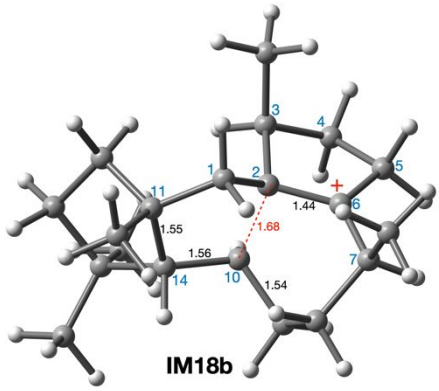

TS_17–18a



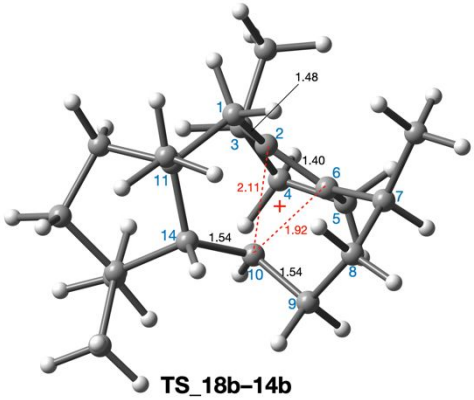
IM18a



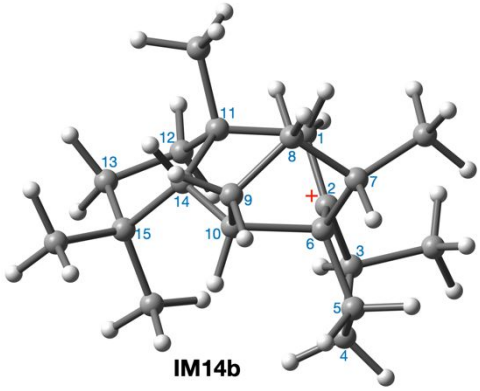

TS_18a–18b




IM18b




TS_18b–14b



IM14b

**Figure S8. 3D representation of TS_16–17, IM17, TS_17–18a, TS_18a–18b, IM18b, TS_18b–14b, and IM14b. Atomic distances are shown in Å.**

## 4. References


(1) Maeda S.; Osada Y.; Morokuma K.; Ohno K. GRRM 11, Version 11.03, **2012**.

(2) Maeda, S.; Ohno, K.; Morokuma, K. Systematic exploration of the mechanism of chemical reactions: the global reaction route mapping (GRRM) strategy using the ADDF and AFIR methods. *Phys. Chem. Chem. Phys.* **2013**, *15*, 3683–3701.

(3) Ohno, K.; Maeda, S. A scaled hypersphere search method for the topography of reaction pathways on the potential energy surface. *Chem. Phys. Lett.* **2004**, *384*, 277–282.

(4) Maeda, S.; Ohno, K. Global Mapping of Equilibrium and Transition Structures on Potential Energy Surfaces by the Scaled Hypersphere Search Method: Applications to ab Initio Surfaces of Formaldehyde and Propyne Molecules. *J. Phys. Chem. A* **2005**, *109*, 5742–5753.

(5) Ohno, K.; Maeda, S. Global Reaction Route Mapping on Potential Energy Surfaces of Formaldehyde, Formic Acid, and Their Metal-Substituted Analogues. *J. Phys. Chem. A* **2006**, *110*, 8933–8941.

(6) Gaussian16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.;

Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

(7) Zhao,Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, *120*, 215–241.

(8) Fukui, K. The path of chemical reactions - the IRC approach. *Acc. Chem. Res.* **2002**, *14*, 363–368.

(9) Page, M.; Doubleday, C.; McIver, J. W., Jr. Following steepest descent reaction paths. The use of higher energy derivatives with ab initio electronic structure methods. *J. Chem. Phys.* **1990**, *93*, 5634–5642.

(10) Ishida, K.; Morokuma, K.; Komornicki, A. The intrinsic reaction coordinate. An ab initio calculation for HNC→HCN and $H^-$ + $CH_4$→$CH_4$ + $H^-$. *J. Chem. Phys.* **1977**, *66*, 2153–2156.

(11) Gonzalez, C.; Schlegel, H. B. Reaction path following in mass-weighted internal coordinates. *J. Phys. Chem.* **1990**, *94*, 5523–5527.

(12) Adamo, C.; Barone, V. Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. *J. Chem. Phys.* **1998**, *108*, 664–675.

(13) Matsuda, S. P. T.; Wilson, W. K.; Xiong, Q. Mechanistic insights into triterpene synthesis from quantum mechanical calculations. Detection of systematic errors in B3LYP cyclization energies. *Org. Biomol. Chem.* **2006**, *4*, 530–543.