

Electronic Supporting Information For

**Elucidating the mechanism and origin of diastereoselectivity in scandium-catalyzed  $\beta$ -C(sp<sup>3</sup>)-H activation and transformation of an aliphatic aldimine**

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## Content

|   |     |
|---|-----|
| Part 1: Calculations for TOF .....  | S2  |
| Part 2: Energy profile for the formation of <i>cis</i> -P3.....                                   | S3  |
| Part 3: Process for the formation of metallacycle 7' without amine .....                          | S4  |
| Part 4: Energy profile for the formation of <i>cis/trans</i> -P3 without AdNH <sub>2</sub> .....  | S5  |
| Part 5: Energy profile of reaction between 21 and R2-Oct .....                                    | S6  |
| Part 6: Energy profiles for the formation of product <i>cis</i> -P3' .....                        | S7  |
| Part 7: Energy profile for the formation of <i>cis/trans</i> -P3' without Bn <sub>2</sub> NH..... | S8  |
| Part 8: Energy profile for the 2,1-insertion between 21 and R2-Oct.....                           | S9  |
| Part 9: ELF analysis for 21 and 21' .....   | S10 |
| Part 10: ELF analysis for <i>trans</i> -ts-10' .....  | S11 |
| Part 11: NCI and AIM analyses for <i>cis</i> -ts-10' and <i>trans</i> -ts-10' .....               | S12 |
| Part 12: Benchmark studies involved in alkene insertion step .....                                | S13 |
| Part 13: Configurational search for diastereoselective transition states .....                    | S14 |
| Part 14: Cartesian Coordinates of all stationary points .....                                     | S15 |

## Part 1: Calculations for TOF

$$\text{TOF} = \frac{k_B T}{h} e^{-\delta E / RT}$$

The energetic span,  $\delta E$ , can be defined as:

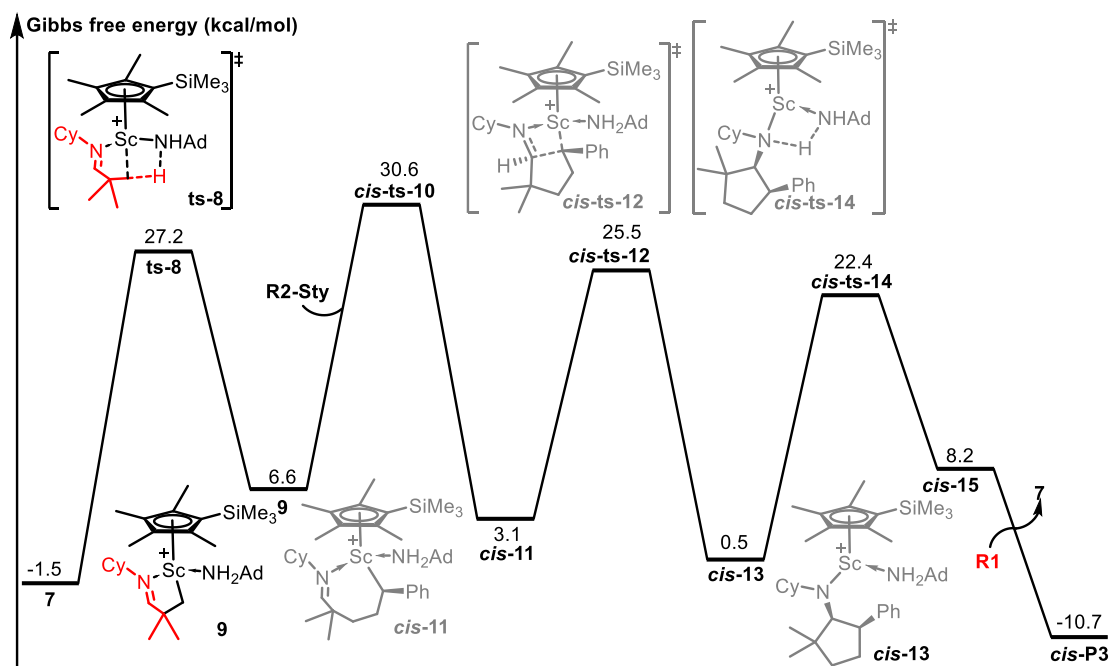
$$\delta E = T_{\text{TDS}} - I_{\text{TDI}}, \text{ if TDS appears after TDI}$$

$$\delta E = T_{\text{TDS}} - I_{\text{TDI}} + \Delta G_{\text{r}}, \text{ if TDS appears before TDI}$$

In the equation,  $k_B$  and  $h$  are the Boltzmann constant and Planck constant, respectively.

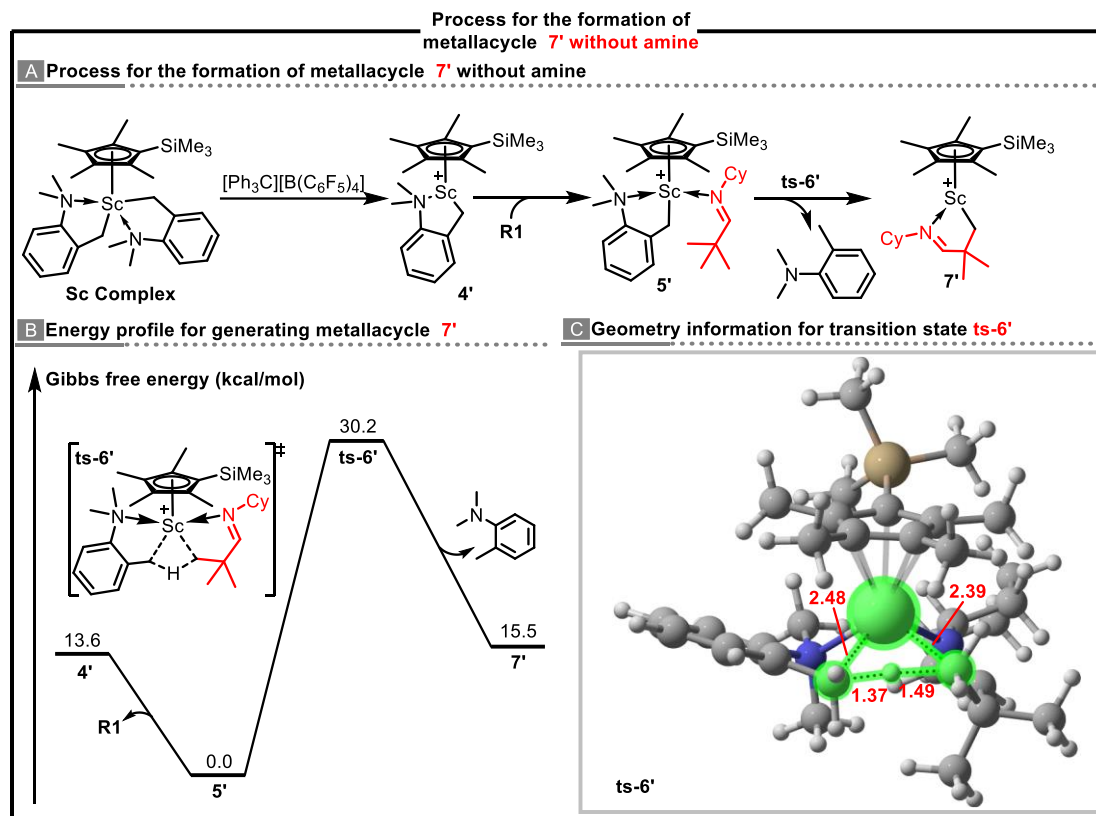
$$k_B = 1.380649 \times 10^{-23} \text{ J/K}, h = 6.62607015 \times 10^{-34} \text{ J}\cdot\text{s}$$

## Part 2: Energy profile for the formation of *cis*-P3



**Fig. S1** Energy profile for the formation of *cis*-P3

### Part 3: Process for the formation of metallacycle 7' without amine



**Fig. S2** (A) Process for the formation of metallacycle 7' without amine, (B) energy profile for generating metallacycle 7' without amine, (C) geometry information for the key transition state

Part 4: Energy profile for the formation of cis/trans-P3 without AdNH<sub>2</sub>

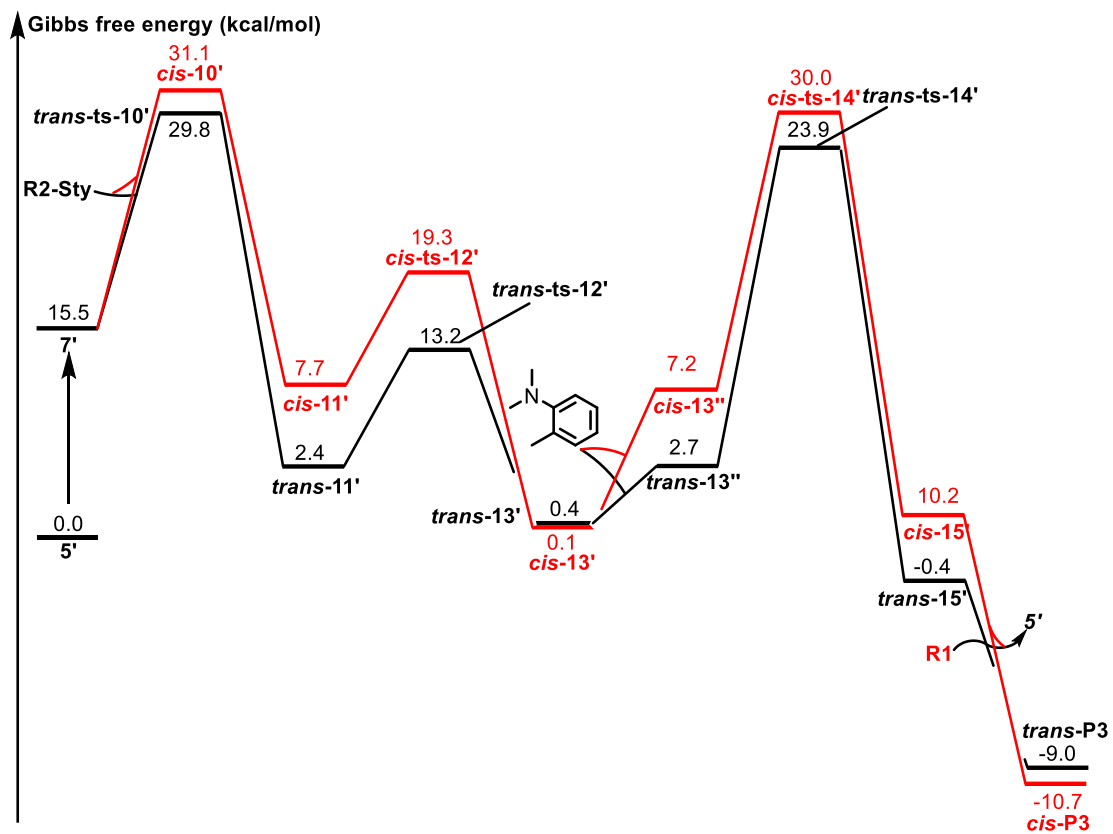


Fig. S3 Energy profile for the reaction between metallacycle intermediate 7' and R2-Sty in the absence of AdNH<sub>2</sub>

## Part 5: Energy profile of reaction between 21 and R2-Oct

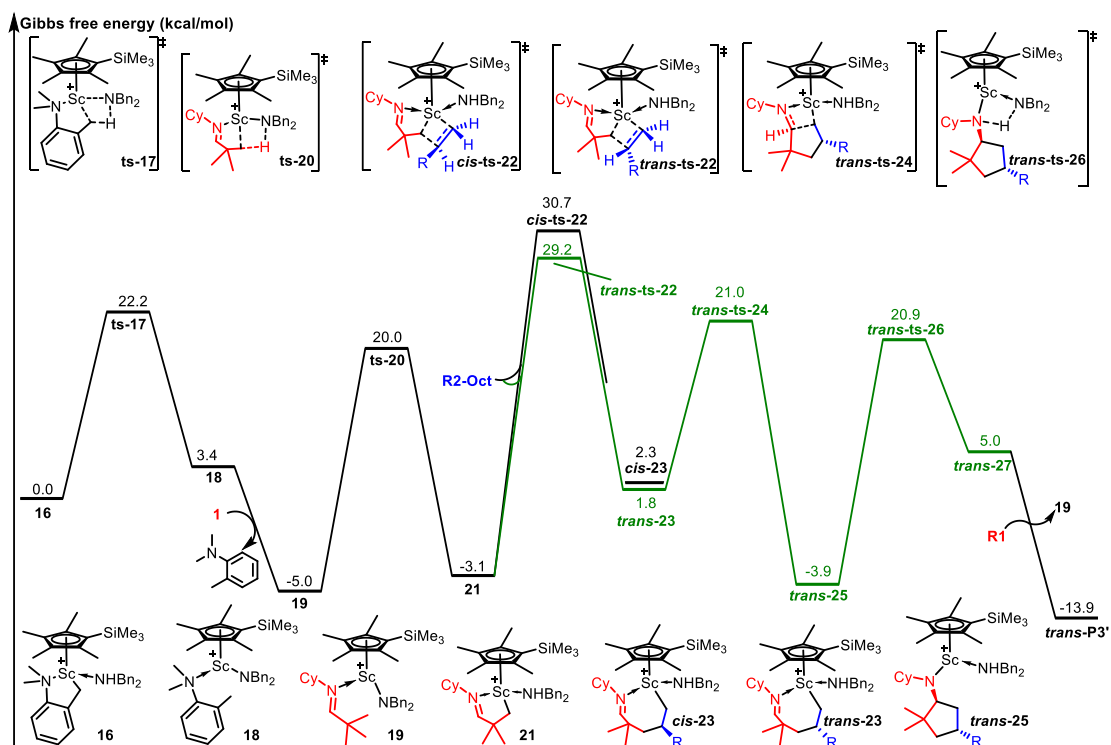


Fig. S4 Energy profiles for the formation of product *trans*-P3'

## Part 6: Energy profiles for the formation of product *cis*-P3'

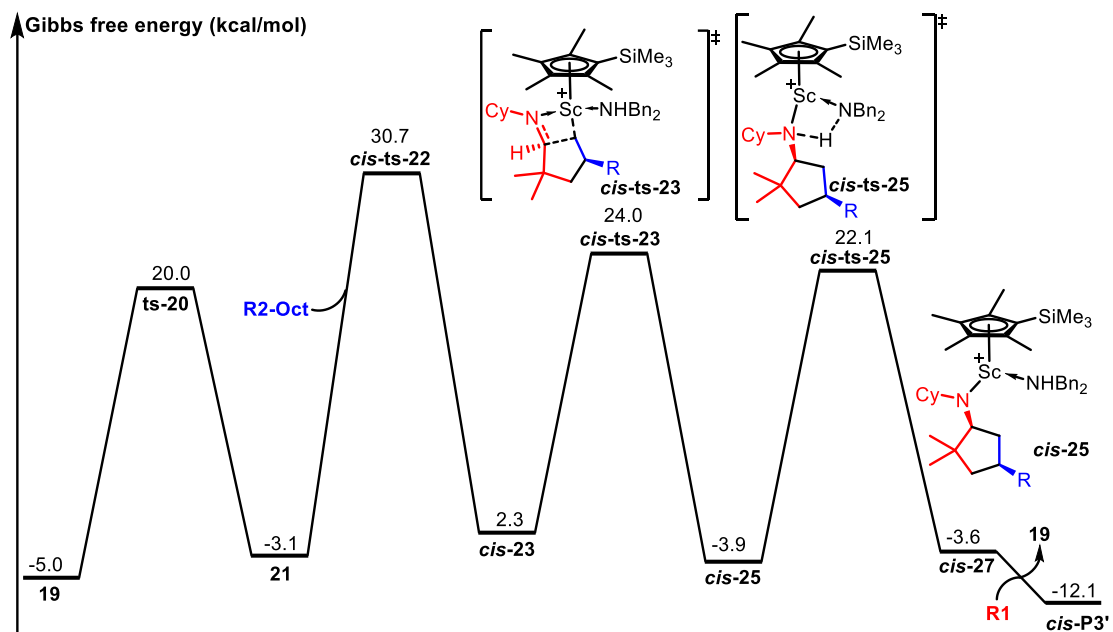


Fig. S5 Energy profiles for the formation of product *cis*-P3'

Part 7: Energy profile for the formation of cis/trans-P3' without Bn<sub>2</sub>NH

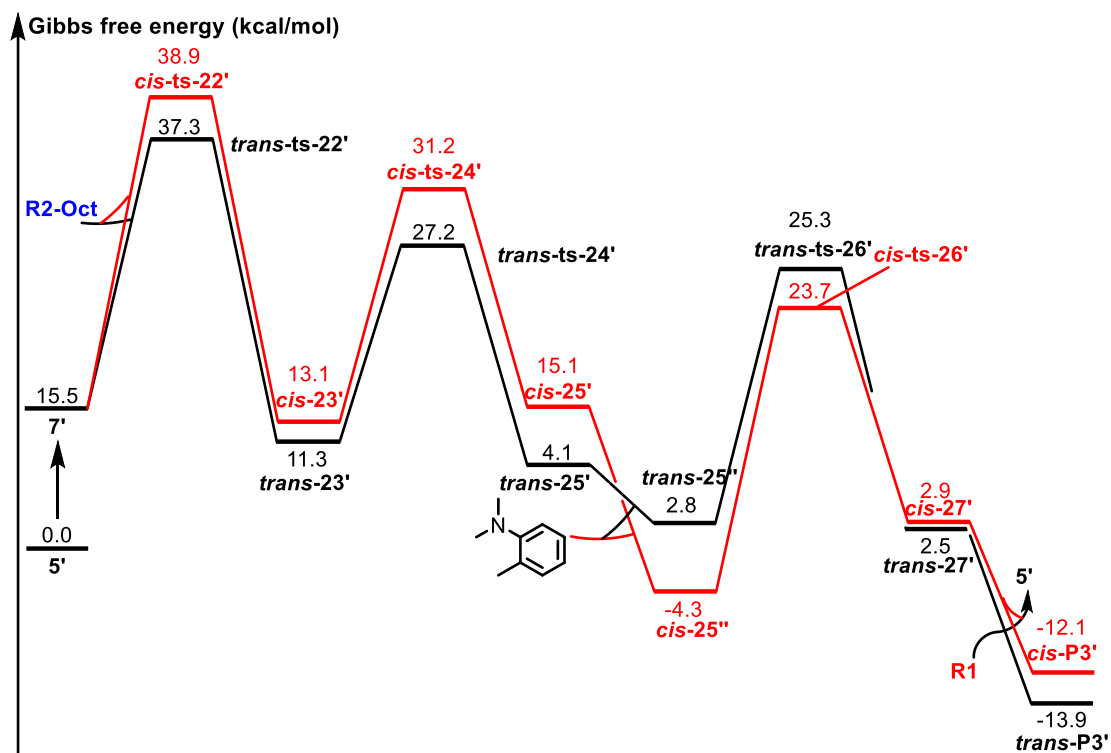
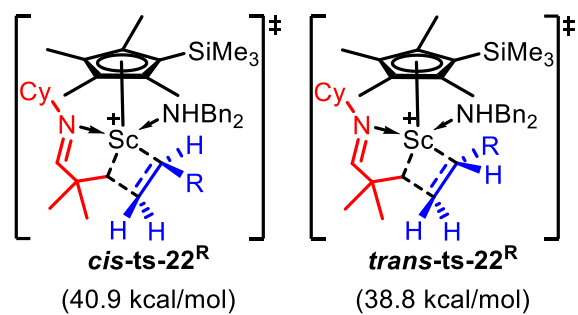


Fig. S6 Energy profile for the reaction between metallacycle intermediate 7' and R2-Oct in the absence of Bn<sub>2</sub>NH

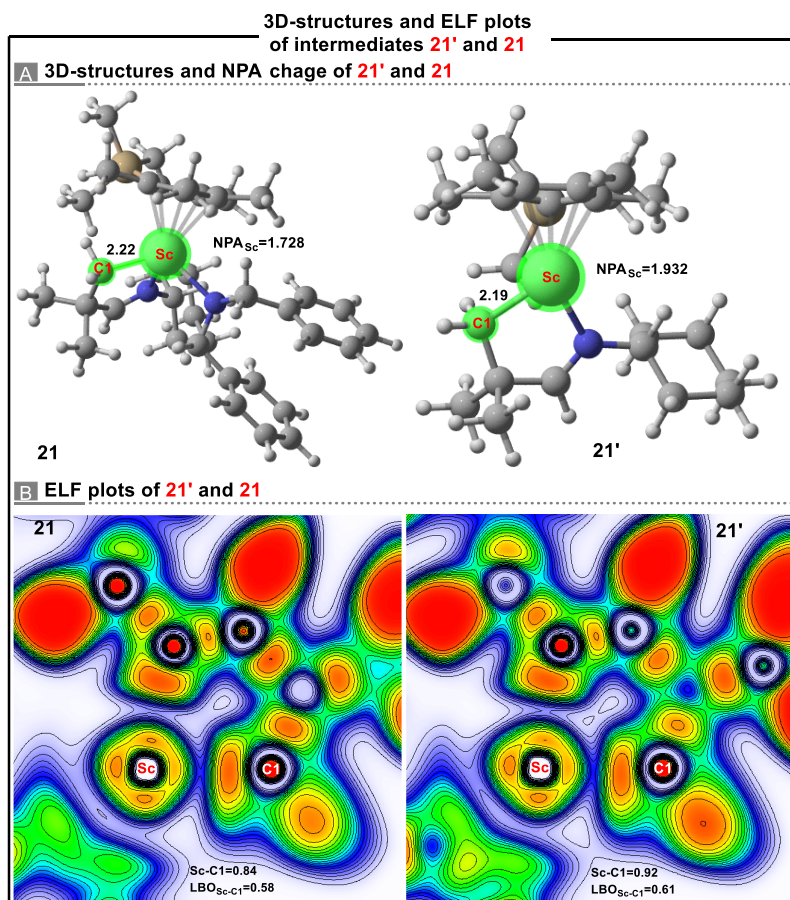


Part 8: Energy profile for the 2,1-insertion between 21 and R2-  
Oct



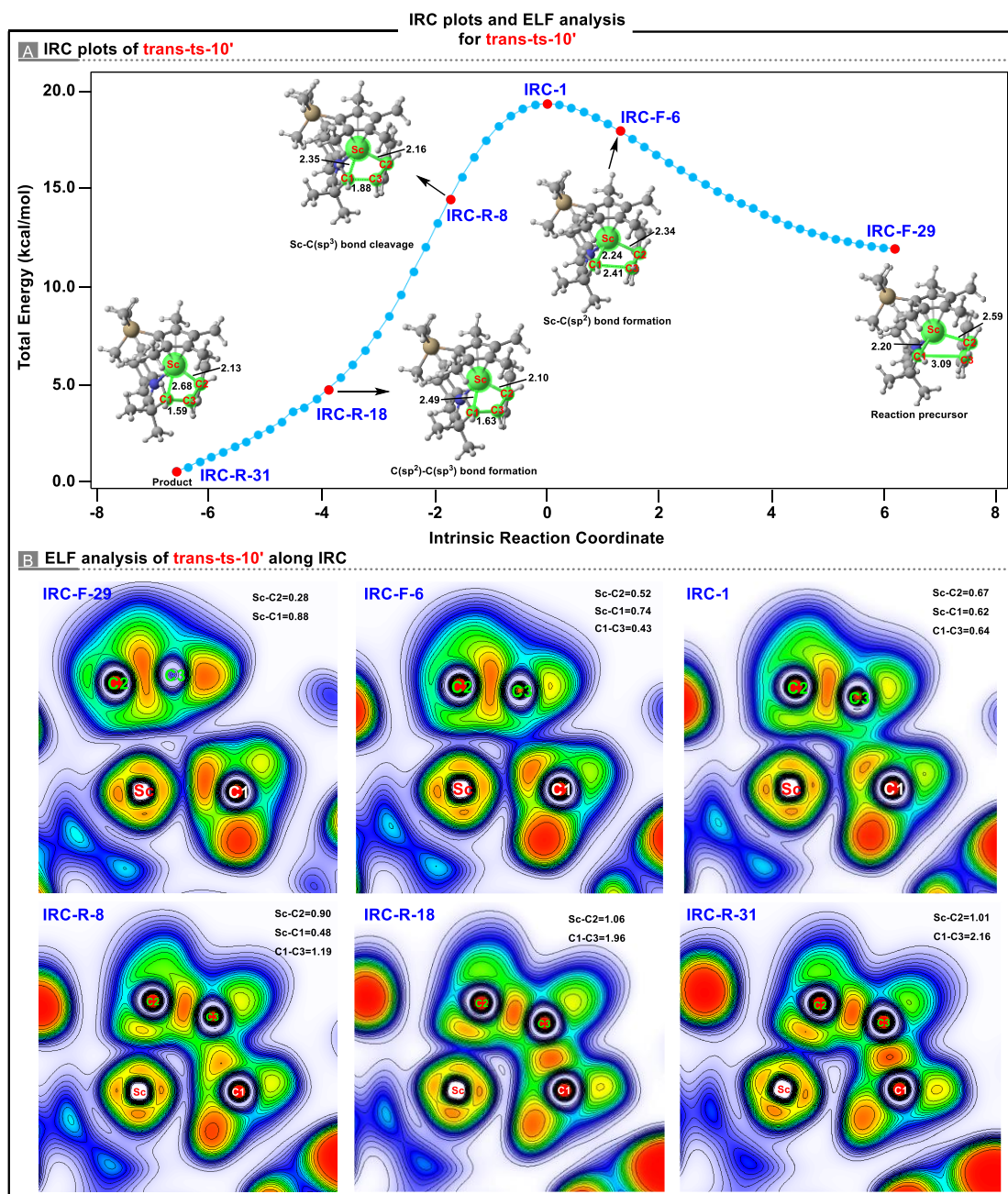
**Fig. S7** Structures and Gibbs free energy barriers of 2,1-insertion for octene

## Part 9: ELF analysis for 21 and 21'



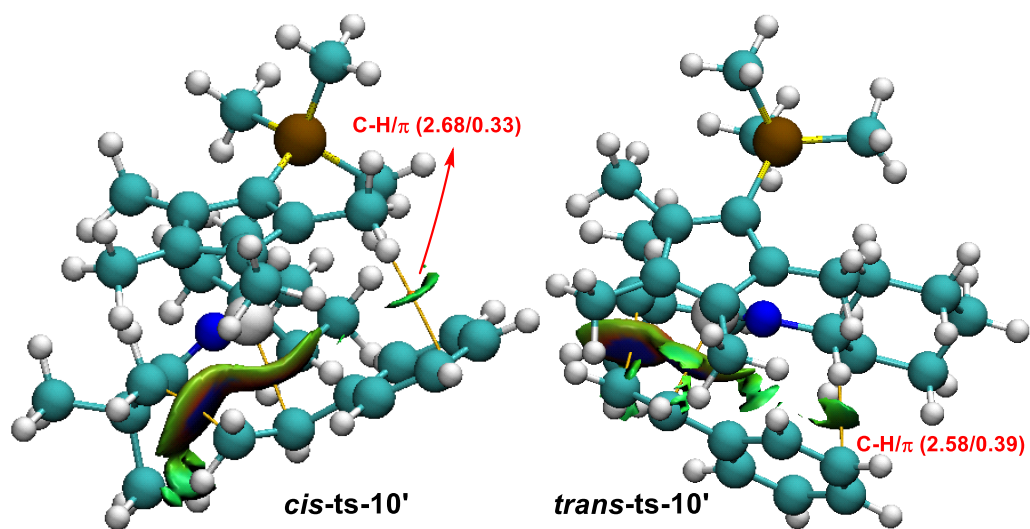
**Fig. S8** (A) 3D-structures and (B) ELF analysis of the key intermediates **21** and **21'**.

## Part 10: ELF analysis for *trans*-*ts*-10'



**Fig. S9** ELF analysis of representative points along the intrinsic reaction coordinates

Part 11: NCI and AIM analyses for *cis*-ts-10' and *trans*-ts-10'



**Fig. S10** NCI and AIM analyses for transition states *cis*-ts-10' and *trans*-ts-10'

## Part 12: Benchmark studies involved in alkene insertion step

**Table S1.** Test of different methods for transition states involved in alkene insertion step

|                     | M06-2X | M06-L | B3LYP | $\omega$ B97X-D |
|---------------------|--------|-------|-------|-----------------|
| <i>cis</i> -ts-10   | 3.6    | 2.8   | 1.3   | 3.5             |
| <i>trans</i> -ts-10 | 0      | 0     | 0     | 0               |

# Part 13: Configurational search for diastereoselective transition states

**Table S2.** Configurational search for diastereoselective transition states

| Amine                   | TS                  | R=SiMe <sub>3</sub> |      |      |      |      |
|-------------------------|---------------------|---------------------|------|------|------|------|
|                         |                     | C1                  | C2   | C3   | C4   | C5   |
| [N]=AdNH <sub>2</sub>   | <i>cis</i> -ts-10   | 0.0                 | -0.1 | -1.8 | -1.9 | -0.5 |
|                         | <i>trans</i> -ts-10 | 0.0                 | 1.6  | 1.6  | 1.7  | 0.3  |
| [NH]=Bn <sub>2</sub> NH | <i>cis</i> -ts-22   | 0.0                 | 1.0  | 4.3  | 2.3  | 4.3  |
|                         | <i>trans</i> -ts-22 | 0.0                 | 1.8  | 1.9  | 4.0  | 1.6  |

## Part 14: Cartesian Coordinates of all stationary points

Sc-Cation

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.85751500 | 0.57416300  | 0.27537800  |
| C  | -1.45087000 | 1.64987600  | -0.58631900 |
| C  | -0.26193100 | 2.22860000  | -0.06673300 |
| C  | 0.07550400  | 1.53187000  | 1.13355400  |
| C  | -0.89990700 | 0.52333200  | 1.34520800  |
| Sc | 0.21844700  | -0.08996200 | -0.68187000 |
| C  | -4.53720200 | -0.06291800 | -1.22727400 |
| C  | -2.78377300 | -2.32316500 | -0.17808800 |
| C  | -4.31678500 | -0.49953000 | 1.78502400  |
| H  | -4.83189900 | 0.98821100  | -1.17220000 |
| H  | -4.12047100 | -0.25174200 | -2.22051300 |
| H  | -5.44592100 | -0.66706800 | -1.13469800 |
| H  | -2.21707300 | -2.74229800 | 0.65978300  |
| H  | -3.64343900 | -2.97902800 | -0.34947600 |
| H  | -2.15751600 | -2.38266900 | -1.08034200 |
| H  | -5.21082500 | -1.12673000 | 1.71116500  |
| H  | -3.72780000 | -0.85573900 | 2.63337400  |
| H  | -4.64140900 | 0.52187600  | 2.00412300  |
| Si | -3.37325100 | -0.55512000 | 0.16270100  |
| C  | -0.91256500 | -0.39580200 | 2.53840100  |
| H  | 0.10315100  | -0.60903100 | 2.88842800  |
| H  | -1.44834900 | 0.06792800  | 3.37381400  |
| H  | -1.40732200 | -1.34757400 | 2.32454100  |
| C  | 1.19444100  | 1.87333200  | 2.07533300  |
| H  | 1.90478700  | 2.56352900  | 1.61638900  |
| H  | 0.79362600  | 2.35295100  | 2.97456100  |
| H  | 1.75322300  | 0.98816000  | 2.39558200  |
| C  | 0.49793700  | 3.39936200  | -0.62089600 |
| H  | 0.31414500  | 3.53570800  | -1.68819500 |
| H  | 0.20863500  | 4.32404700  | -0.11116700 |
| H  | 1.57616300  | 3.27205900  | -0.48446700 |
| C  | -2.14197000 | 2.09662000  | -1.84769700 |
| H  | -2.45416600 | 1.25540600  | -2.47227900 |
| H  | -3.04223700 | 2.67268600  | -1.61269100 |
| H  | -1.49228600 | 2.73467800  | -2.44954600 |
| C  | 4.25146900  | 0.81750300  | 0.74834700  |
| C  | 4.02983400  | -0.36380800 | 1.46968700  |
| C  | 3.12358200  | -1.29401700 | 0.99703700  |
| C  | 2.43385300  | -1.06579300 | -0.20720300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.64968300  | 0.12395000  | -0.97019900 |
| C  | 3.56979100  | 1.05604400  | -0.42751100 |
| H  | 4.96141300  | 1.55054600  | 1.11676100  |
| H  | 4.56601300  | -0.55297100 | 2.39272700  |
| H  | 2.95973500  | -2.21032800 | 1.55248500  |
| H  | 3.75299900  | 1.96914200  | -0.98618300 |
| N  | 1.43675900  | -2.00456700 | -0.70772900 |
| C  | 1.90884200  | -2.78245200 | -1.87604000 |
| H  | 2.62757800  | -3.54035900 | -1.54546100 |
| H  | 1.05686600  | -3.27360100 | -2.35072800 |
| H  | 2.39862700  | -2.12583900 | -2.59278100 |
| C  | 0.88485700  | -2.92175800 | 0.30977500  |
| H  | 0.52999100  | -2.35696300 | 1.17947100  |
| H  | 0.04848900  | -3.46406100 | -0.13439700 |
| H  | 1.63109000  | -3.64950100 | 0.64725800  |
| C  | 1.79709200  | 0.47311800  | -2.11412300 |
| H  | 1.72286700  | -0.26790700 | -2.91332300 |
| H  | 1.98593600  | 1.46815500  | -2.51042000 |
| R1 |             |             |             |
| C  | -3.47762300 | 1.20815100  | 0.65874800  |
| C  | -2.78138000 | -0.00045100 | 0.01499100  |
| H  | -3.38501400 | 1.18296100  | 1.74986400  |
| H  | -3.04362200 | 2.14605500  | 0.29925400  |
| H  | -4.54370800 | 1.20489100  | 0.41027200  |
| C  | -2.89097500 | 0.06990300  | -1.50576800 |
| C  | -3.42558600 | -1.29370000 | 0.53803700  |
| H  | -2.37298900 | -0.77192000 | -1.97186100 |
| H  | -3.94358100 | 0.04787400  | -1.80582600 |
| H  | -2.43663200 | 0.98849600  | -1.88572700 |
| H  | -4.49192000 | -1.30937200 | 0.29120600  |
| H  | -2.95497700 | -2.17331000 | 0.08834300  |
| H  | -3.32930400 | -1.37171300 | 1.62633600  |
| C  | -1.33706900 | 0.00403300  | 0.46070900  |
| H  | -1.19067900 | -0.03126100 | 1.55634700  |
| N  | -0.35554800 | 0.03770800  | -0.33639500 |
| C  | 0.98393100  | 0.01977600  | 0.23098000  |
| C  | 1.70880700  | -1.24629700 | -0.23457200 |
| C  | 1.74599700  | 1.26722000  | -0.22459000 |
| H  | 0.94763800  | 0.01468000  | 1.33711800  |
| C  | 3.15709500  | -1.27297200 | 0.25798400  |
| H  | 1.68533200  | -1.26561200 | -1.33203100 |
| H  | 1.15956900  | -2.12769700 | 0.11437800  |
| C  | 3.19482000  | 1.24642500  | 0.26755300  |



|   |            |             |             |
|---|------------|-------------|-------------|
| H | 1.72292000 | 1.29551000  | -1.32184000 |
| H | 1.22412500 | 2.16236500  | 0.13104700  |
| C | 3.91569300 | -0.02254400 | -0.19213100 |
| H | 3.65853300 | -2.17696000 | -0.10244100 |
| H | 3.16595400 | -1.32237900 | 1.35543500  |
| H | 3.72317800 | 2.13768400  | -0.08607800 |
| H | 3.20557900 | 1.28731600  | 1.36536100  |
| H | 4.94079200 | -0.03943000 | 0.19228000  |
| H | 3.98537700 | -0.01940400 | -1.28831300 |

R2-Sty

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.96041900 | 0.33879300  | 0.00000000  |
| C | -1.95289200 | -0.53484100 | 0.00000000  |
| H | -2.80465200 | 1.41312700  | 0.00000100  |
| H | -3.98951300 | -0.00229200 | 0.00000000  |
| H | -2.18853500 | -1.59816100 | -0.00000100 |
| C | -0.51080500 | -0.22414600 | 0.00000000  |
| C | -0.01488500 | 1.08689200  | 0.00000000  |
| C | 0.40716900  | -1.28035500 | 0.00000000  |
| C | 1.35283900  | 1.32809000  | 0.00000000  |
| H | -0.70268500 | 1.92664100  | 0.00000000  |
| C | 1.77835600  | -1.04122300 | 0.00000000  |
| H | 0.03665600  | -2.30219500 | 0.00000000  |
| C | 2.25641300  | 0.26537100  | 0.00000000  |
| H | 1.71797100  | 2.35029600  | 0.00000000  |
| H | 2.47164100  | -1.87629000 | 0.00000000  |
| H | 3.32446000  | 0.45738800  | 0.00000000  |

R2-Oct

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.97888800 | 0.93013400  | -0.44845400 |
| C | -1.89834800 | 1.97337700  | 0.37337100  |
| H | -1.74918300 | 1.06664100  | -1.50649900 |
| H | -2.11623900 | 1.87098400  | 1.43371800  |
| H | -1.61625800 | 2.96004400  | 0.02054600  |
| C | -2.35409100 | -0.46095600 | -0.02870200 |
| C | -1.24495000 | -1.50015200 | -0.26224100 |
| H | -3.24919100 | -0.77456600 | -0.58104900 |
| H | -2.62065200 | -0.45394700 | 1.03521700  |
| C | 0.05669100  | -1.19785600 | 0.49459100  |
| H | -1.63541000 | -2.47700100 | 0.04205500  |
| H | -1.03413000 | -1.57530700 | -1.33733200 |
| H | -0.18271600 | -0.66278200 | 1.42467300  |
| H | 0.53450500  | -2.13763800 | 0.79735200  |
| C | 1.07130100  | -0.38143400 | -0.30680400 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.32880300 | -0.04817700 | 0.49242100  |
| H | 0.60895700 | 0.55023700  | -0.65516100 |
| H | 1.35186800 | -0.94576500 | -1.20726000 |
| C | 3.35745500 | 0.72576300  | -0.32739400 |
| H | 2.04567600 | 0.53562100  | 1.37734400  |
| H | 2.77660400 | -0.97752400 | 0.86741200  |
| H | 4.24741100 | 0.96442400  | 0.26087900  |
| H | 3.67635300 | 0.14560500  | -1.19920600 |
| H | 2.93456100 | 1.66677700  | -0.69341700 |

Bn<sub>2</sub>NH

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.51391200 | 2.49976400  | -0.38909300 |
| H | -0.64843000 | 3.50243700  | -0.46511400 |
| C | 0.39513100  | 2.21734600  | 0.72419600  |
| H | 1.07817800  | 3.06913700  | 0.81643600  |
| H | -0.13992700 | 2.12937000  | 1.68538900  |
| C | -1.82414600 | 1.86892100  | -0.24164200 |
| H | -2.32987800 | 2.17004900  | 0.69266200  |
| H | -2.44960700 | 2.21211800  | -1.07429400 |
| C | -1.72719700 | 0.35965200  | -0.26335900 |
| C | -1.06047600 | -0.28635600 | -1.30859600 |
| C | -2.25994500 | -0.40412700 | 0.77185400  |
| C | -0.91529700 | -1.66727600 | -1.30583300 |
| H | -0.61936600 | 0.31302600  | -2.10010700 |
| C | -2.12476100 | -1.79261300 | 0.77461400  |
| H | -2.77202100 | 0.09299700  | 1.59238000  |
| C | -1.44629400 | -2.42525200 | -0.26093200 |
| H | -0.37788300 | -2.15633700 | -2.11246400 |
| H | -2.54070900 | -2.37500700 | 1.59111200  |
| H | -1.32727000 | -3.50424800 | -0.25604000 |
| C | 1.21402400  | 0.96379800  | 0.49011300  |
| C | 1.19123300  | -0.10263500 | 1.38524600  |
| C | 1.99534500  | 0.86183300  | -0.66336400 |
| C | 1.92252100  | -1.26115400 | 1.12791600  |
| H | 0.56821200  | -0.04068500 | 2.27414700  |
| C | 2.72990500  | -0.28895300 | -0.92255100 |
| H | 1.99567200  | 1.68677500  | -1.37096800 |
| C | 2.69205900  | -1.35781800 | -0.02729100 |
| H | 1.88008000  | -2.09199100 | 1.82562100  |
| H | 3.32987300  | -0.35682800 | -1.82513500 |
| H | 3.25783100  | -2.26135800 | -0.23220100 |

AdNH<sub>2</sub>

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -2.71373800 | 0.00057600 | -0.11180900 |
|---|-------------|------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.07456800 | -0.81382500 | 0.38369000  |
| H | -3.07446700 | 0.80987700  | 0.39204100  |
| C | -1.25298900 | 0.00006600  | -0.01799200 |
| C | -0.71626300 | -1.24414600 | -0.73989600 |
| C | -0.71631500 | 1.25147400  | -0.72742100 |
| C | -0.72975400 | -0.00722600 | 1.43248500  |
| H | -1.09701800 | -1.24642200 | -1.76833400 |
| H | -1.10343000 | -2.14595900 | -0.24450400 |
| C | 0.81916500  | -1.25151500 | -0.72541200 |
| H | -1.10345400 | 2.14827400  | -0.22299800 |
| H | -1.09715100 | 1.26405500  | -1.75575600 |
| C | 0.81911200  | 1.25873100  | -0.71302700 |
| H | -1.11891000 | -0.89491400 | 1.95096600  |
| H | -1.11896300 | 0.87520100  | 1.95981100  |
| C | 0.80593400  | -0.00725500 | 1.45660400  |
| H | 1.18436400  | -2.14526300 | -1.24429600 |
| C | 1.33830800  | 0.00718800  | -1.43710500 |
| C | 1.32020400  | -1.25807300 | 0.72789500  |
| H | 1.18426900  | 2.15762100  | -1.22298900 |
| C | 1.32018000  | 1.25076200  | 0.74024900  |
| H | 1.15863600  | -0.01240800 | 2.49452700  |
| H | 1.00329400  | 0.01238700  | -2.48184500 |
| H | 2.43560500  | 0.00727700  | -1.44571700 |
| H | 0.96916800  | -2.16209400 | 1.24176400  |
| H | 2.41707300  | -1.27781000 | 0.74621600  |
| H | 2.41705000  | 1.27030000  | 0.75870900  |
| H | 0.96918100  | 2.14963000  | 1.26309400  |

*N,N*-dimethyl-*o*-toluidine

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.62039100 | -0.44499500 | 0.14171800  |
| C | -1.81419500 | -1.57627300 | 0.17823300  |
| C | -0.43224100 | -1.44825900 | 0.07292300  |
| C | 0.16692200  | -0.19248700 | -0.07772700 |
| C | -0.64830300 | 0.95790400  | -0.13794100 |
| C | -2.02919200 | 0.80529100  | -0.01940400 |
| H | -3.69896200 | -0.53280700 | 0.22220300  |
| H | -2.25482400 | -2.56167200 | 0.29360500  |
| H | 0.18641200  | -2.33820300 | 0.11166500  |
| H | -2.65505800 | 1.69261000  | -0.07656300 |
| N | 1.57654800  | -0.04412600 | -0.20341200 |
| C | 2.21218200  | 0.54160300  | 0.97211200  |
| H | 2.22191500  | -0.15829000 | 1.82413400  |
| H | 3.24554200  | 0.80627000  | 0.72965400  |
| H | 1.68965600  | 1.44737000  | 1.28076000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.30225100  | -1.22116000 | -0.64610700 |
| H  | 1.81808900  | -1.64828200 | -1.52694400 |
| H  | 3.31841300  | -0.92235700 | -0.91855100 |
| H  | 2.38095100  | -2.00424200 | 0.12734600  |
| C  | -0.06212700 | 2.32572100  | -0.37392500 |
| H  | 0.15401200  | 2.84740000  | 0.56535700  |
| H  | -0.76422100 | 2.94805600  | -0.93398800 |
| H  | 0.87280600  | 2.24896200  | -0.93408200 |
| 4  |             |             |             |
| C  | -1.22594900 | 2.23053500  | 0.18832300  |
| C  | -1.14340600 | 1.91655700  | 1.58428400  |
| C  | -2.22213000 | 1.05629500  | 1.92618600  |
| C  | -3.01320700 | 0.86583200  | 0.75947400  |
| C  | -2.40136200 | 1.56821300  | -0.30738300 |
| Sc | -0.78114900 | -0.17763800 | 0.31866200  |
| C  | 1.32956900  | 4.06738900  | -0.00482100 |
| C  | 0.43266700  | 2.42617500  | -2.39872500 |
| C  | -1.24403000 | 4.83018800  | -1.44381800 |
| H  | 1.06871100  | 4.65115900  | 0.88177200  |
| H  | 2.06554000  | 3.30923100  | 0.28699500  |
| H  | 1.83685900  | 4.74012500  | -0.70505100 |
| H  | -0.33711000 | 2.29617700  | -3.16436700 |
| H  | 1.26759000  | 2.96187200  | -2.86278700 |
| H  | 0.80100200  | 1.43324300  | -2.11778300 |
| H  | -0.66782500 | 5.48539200  | -2.10482000 |
| H  | -2.13325900 | 4.50105400  | -1.98855100 |
| H  | -1.57408600 | 5.42150600  | -0.58502100 |
| Si | -0.18869400 | 3.37993700  | -0.88686400 |
| C  | -3.03917200 | 1.71264600  | -1.66371000 |
| H  | -3.57111900 | 0.79988300  | -1.95347100 |
| H  | -3.78027900 | 2.52007100  | -1.64724700 |
| H  | -2.31753400 | 1.95075600  | -2.44841500 |
| C  | -4.35577200 | 0.20218100  | 0.68397100  |
| H  | -4.56742400 | -0.38723000 | 1.57700600  |
| H  | -5.13596200 | 0.96649600  | 0.59475400  |
| H  | -4.44166800 | -0.46028000 | -0.18150800 |
| C  | -2.54422800 | 0.52525500  | 3.29358900  |
| H  | -1.64138000 | 0.33902600  | 3.88125300  |
| H  | -3.16366700 | 1.23362100  | 3.85415200  |
| H  | -3.09332200 | -0.41824000 | 3.22947500  |
| C  | -0.18430800 | 2.47494200  | 2.60229700  |
| H  | 0.76683100  | 2.79446700  | 2.17223200  |
| H  | -0.62090300 | 3.35829200  | 3.08048600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.02436100  | 1.75667300  | 3.40160700  |
| C | -4.41303300 | -3.19836400 | 0.29620100  |
| C | -4.33817900 | -2.98431700 | -1.08368900 |
| C | -3.16907600 | -2.48519500 | -1.63567600 |
| C | -2.06320500 | -2.21171700 | -0.81907500 |
| C | -2.11019000 | -2.42329200 | 0.58447800  |
| C | -3.33103800 | -2.90436300 | 1.10581700  |
| H | -5.32345000 | -3.59360300 | 0.73473300  |
| H | -5.18410500 | -3.21102300 | -1.72297200 |
| H | -3.10962900 | -2.33077200 | -2.70719200 |
| H | -3.39403700 | -3.07210400 | 2.17730500  |
| N | -0.79390400 | -1.75124400 | -1.38530300 |
| C | 0.13291800  | -2.89907000 | -1.52484100 |
| H | -0.26371600 | -3.59620000 | -2.27271900 |
| H | 1.11181800  | -2.54106400 | -1.85046700 |
| H | 0.23114800  | -3.42385300 | -0.57496500 |
| C | -0.91052200 | -1.08619900 | -2.69815900 |
| H | -1.65349800 | -0.28593700 | -2.65481400 |
| H | 0.06248400  | -0.66263100 | -2.95802000 |
| H | -1.19433800 | -1.79454100 | -3.48488500 |
| C | -0.99040000 | -2.03700500 | 1.47342600  |
| H | -0.05360700 | -2.56701500 | 1.27244600  |
| H | -1.24856500 | -2.13059500 | 2.52782900  |
| N | 1.38247200  | 0.26908400  | 1.01771400  |
| H | 1.28985100  | 0.10644500  | 2.02653600  |
| H | 1.45226700  | 1.28669700  | 0.93582800  |
| C | 2.69690800  | -0.29053900 | 0.58603500  |
| C | 2.76237000  | -1.78971400 | 0.88959200  |
| C | 2.85543100  | -0.06158500 | -0.91981100 |
| C | 3.83973000  | 0.42440800  | 1.32581000  |
| H | 1.94631900  | -2.30547800 | 0.37204700  |
| H | 2.62788000  | -1.95741900 | 1.96730600  |
| C | 4.11668900  | -2.35200900 | 0.42334900  |
| H | 2.79670300  | 1.01376000  | -1.13820100 |
| H | 2.02574700  | -0.55455000 | -1.45179600 |
| C | 4.20472700  | -0.62200500 | -1.39519100 |
| H | 3.72022000  | 0.28030100  | 2.40819300  |
| H | 3.78459600  | 1.50411000  | 1.12784300  |
| C | 5.19479600  | -0.12953600 | 0.85928600  |
| H | 4.14971600  | -3.42399000 | 0.64278900  |
| C | 4.26662600  | -2.12515500 | -1.08940900 |
| C | 5.25384700  | -1.63324800 | 1.16367000  |
| H | 4.30190300  | -0.45574600 | -2.47308400 |
| C | 5.33977300  | 0.09972800  | -0.65264500 |

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|---|------------|-------------|-------------|
| H | 5.99713900 | 0.39034600  | 1.39216000  |
| H | 3.47468300 | -2.65683400 | -1.63243500 |
| H | 5.22246100 | -2.53522800 | -1.43436600 |
| H | 5.16814900 | -1.80390000 | 2.24354200  |
| H | 6.21990000 | -2.04074400 | 0.84496300  |
| H | 6.30767400 | -0.28071000 | -0.99761700 |
| H | 5.31373000 | 1.17320600  | -0.87637400 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.02265300 | 2.31736800  | 0.34338500  |
| C  | -1.05828800 | 1.68776900  | 1.62661200  |
| C  | -2.25248800 | 0.92328900  | 1.73032700  |
| C  | -3.00103500 | 1.10741600  | 0.52967800  |
| C  | -2.25184500 | 1.95566200  | -0.32170900 |
| Sc | -0.89297000 | -0.06032700 | -0.06319600 |
| C  | 1.77245700  | 3.72388000  | 0.66780100  |
| C  | 0.84496700  | 2.77295000  | -2.08463300 |
| C  | -0.53240200 | 5.15989200  | -0.69991400 |
| H  | 1.51403800  | 4.16892900  | 1.63274200  |
| H  | 2.34627000  | 2.80972800  | 0.85359300  |
| H  | 2.44212400  | 4.42031300  | 0.15136000  |
| H  | 0.14394200  | 2.98549400  | -2.89675800 |
| H  | 1.80578800  | 3.22205300  | -2.35799900 |
| H  | 0.99907000  | 1.68900600  | -2.02761900 |
| H  | 0.20224900  | 5.85993300  | -1.11011600 |
| H  | -1.37090600 | 5.10889600  | -1.39944300 |
| H  | -0.90245400 | 5.57220700  | 0.24322700  |
| Si | 0.26034400  | 3.47762200  | -0.42755700 |
| C  | -2.74450900 | 2.51484900  | -1.63058700 |
| H  | -3.54052300 | 1.90303600  | -2.06170800 |
| H  | -3.16613200 | 3.51330100  | -1.47408000 |
| H  | -1.94990900 | 2.61043000  | -2.37526100 |
| C  | -4.38005100 | 0.57262700  | 0.27348900  |
| H  | -4.52642300 | -0.40094200 | 0.74737200  |
| H  | -5.13406100 | 1.25809600  | 0.67463100  |
| H  | -4.58289600 | 0.45217400  | -0.79456000 |
| C  | -2.70701000 | 0.18493000  | 2.95756900  |
| H  | -1.92125500 | -0.45587700 | 3.37056700  |
| H  | -2.99113300 | 0.89337900  | 3.74290500  |
| H  | -3.57516000 | -0.44190100 | 2.74542900  |
| C  | -0.06362300 | 1.78687700  | 2.75250900  |
| H  | 0.92846300  | 2.09155400  | 2.41780000  |
| H  | -0.39809200 | 2.52860900  | 3.48596400  |
| H  | 0.03621700  | 0.83243600  | 3.27979300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.27503300 | -3.13802100 | 0.97682200  |
| C | -4.61579300 | -2.93883500 | -0.36287900 |
| C | -3.67751200 | -2.41852200 | -1.23860800 |
| C | -2.38253600 | -2.11686500 | -0.79731700 |
| C | -2.00231600 | -2.34314300 | 0.54954700  |
| C | -2.99737300 | -2.83535900 | 1.41627000  |
| H | -5.00439800 | -3.53814700 | 1.67273000  |
| H | -5.60969600 | -3.18340200 | -0.72078300 |
| H | -3.94638100 | -2.25687000 | -2.27620800 |
| H | -2.72919700 | -3.01110800 | 2.45381900  |
| N | -1.39980600 | -1.53500700 | -1.70359700 |
| C | -0.42605300 | -2.53497400 | -2.19471600 |
| H | -0.93036100 | -3.24232200 | -2.86329300 |
| H | 0.36900900  | -2.01931800 | -2.73815900 |
| H | 0.00612100  | -3.08217700 | -1.35813500 |
| C | -1.97671200 | -0.80545400 | -2.85195600 |
| H | -2.77390100 | -0.14107300 | -2.51052000 |
| H | -1.18526800 | -0.21003400 | -3.31561900 |
| H | -2.37920200 | -1.49014600 | -3.60664200 |
| C | -0.60689700 | -2.11544500 | 1.08834000  |
| H | 0.04896600  | -2.92243000 | 0.74641100  |
| H | -0.63974000 | -2.16336700 | 2.17996000  |
| N | 1.15988000  | -0.13343800 | 0.25049300  |
| H | 0.39486300  | -1.12298100 | 0.86546100  |
| H | 1.22396600  | 0.75834400  | 0.75182100  |
| C | 2.55542900  | -0.60884100 | 0.15738500  |
| C | 2.64160900  | -2.08865400 | -0.23846700 |
| C | 3.29909800  | 0.22483300  | -0.90275200 |
| C | 3.25273500  | -0.42375500 | 1.51830800  |
| H | 2.14292700  | -2.23987500 | -1.20314200 |
| H | 2.13375800  | -2.70905500 | 0.51045100  |
| C | 4.11405400  | -2.52680100 | -0.33187800 |
| H | 3.22051800  | 1.29071200  | -0.64764700 |
| H | 2.80288900  | 0.08802900  | -1.87323600 |
| C | 4.77258300  | -0.19970500 | -0.98647000 |
| H | 2.71703800  | -1.00981500 | 2.27837100  |
| H | 3.18829600  | 0.63366100  | 1.81610000  |
| C | 4.72339300  | -0.85619300 | 1.43687500  |
| H | 4.14959800  | -3.58380000 | -0.61703300 |
| C | 4.84212800  | -1.68046400 | -1.38530700 |
| C | 4.78867200  | -2.33647900 | 1.03438400  |
| H | 5.28113300  | 0.41210800  | -1.73940300 |
| C | 5.44195900  | -0.00193100 | 0.38184600  |
| H | 5.19631300  | -0.71531400 | 2.41449000  |

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|----|-------------|-------------|-------------|
| H  | 4.38406500  | -1.82717500 | -2.37150300 |
| H  | 5.88768200  | -2.00114200 | -1.46200600 |
| H  | 4.29015700  | -2.95497500 | 1.79112500  |
| H  | 5.83320400  | -2.66495900 | 0.98249000  |
| H  | 6.49837100  | -0.28915000 | 0.32516800  |
| H  | 5.40736800  | 1.05677900  | 0.66801000  |
| 6  |             |             |             |
| C  | -1.00515600 | 2.36891200  | 0.34463200  |
| C  | -0.93093300 | 1.82661300  | 1.67003700  |
| C  | -2.06454700 | 0.99161700  | 1.87873600  |
| C  | -2.88104200 | 1.04394100  | 0.70723900  |
| C  | -2.24153900 | 1.89174800  | -0.22587400 |
| Sc | -0.65922200 | -0.00260300 | 0.11564100  |
| C  | 1.66974900  | 4.01317600  | 0.45591300  |
| C  | 0.70706000  | 2.88983600  | -2.19931100 |
| C  | -0.81754300 | 5.19780900  | -0.84151500 |
| H  | 1.42876000  | 4.41713200  | 1.44258300  |
| H  | 2.35237900  | 3.16687600  | 0.58759700  |
| H  | 2.22098400  | 4.78433400  | -0.09306600 |
| H  | -0.10461600 | 2.77726900  | -2.92390600 |
| H  | 1.44398100  | 3.56811400  | -2.64278200 |
| H  | 1.19153200  | 1.91617900  | -2.06558200 |
| H  | -0.13992300 | 5.95733700  | -1.24407200 |
| H  | -1.63329600 | 5.06910500  | -1.55741700 |
| H  | -1.23978600 | 5.58288000  | 0.09117000  |
| Si | 0.12865100  | 3.60020800  | -0.54512600 |
| C  | -2.86826000 | 2.39711600  | -1.49805100 |
| H  | -3.70568500 | 1.77244800  | -1.81768200 |
| H  | -3.27455900 | 3.39944600  | -1.32863200 |
| H  | -2.15916100 | 2.46856600  | -2.32719700 |
| C  | -4.24044100 | 0.41949400  | 0.57196900  |
| H  | -4.29450500 | -0.54927500 | 1.07676000  |
| H  | -5.00241400 | 1.06782200  | 1.01803500  |
| H  | -4.51581100 | 0.25913100  | -0.47345000 |
| C  | -2.44384500 | 0.28417100  | 3.15144200  |
| H  | -1.57262700 | 0.05583900  | 3.77094100  |
| H  | -3.11320600 | 0.90910400  | 3.75149900  |
| H  | -2.97448200 | -0.65275500 | 2.94904600  |
| C  | 0.12880700  | 2.08948100  | 2.70691400  |
| H  | 1.11750700  | 2.22287900  | 2.26624500  |
| H  | -0.10715400 | 2.99664800  | 3.27357700  |
| H  | 0.19900600  | 1.26460600  | 3.42041900  |
| C  | -4.53442600 | -3.37544700 | 0.55558600  |



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|---|-------------|-------------|-------------|
| C | -4.71756100 | -2.97266800 | -0.76410200 |
| C | -3.68039700 | -2.35580000 | -1.45458600 |
| C | -2.45541200 | -2.12913100 | -0.82653500 |
| C | -2.25417500 | -2.53705200 | 0.50489800  |
| C | -3.31046600 | -3.15899700 | 1.17762100  |
| H | -5.33823400 | -3.86262200 | 1.09602600  |
| H | -5.66549900 | -3.14327000 | -1.26222700 |
| H | -3.83186400 | -2.05312800 | -2.48476800 |
| H | -3.15980800 | -3.48274900 | 2.20386900  |
| N | -1.35487400 | -1.47012200 | -1.52047600 |
| C | -0.39175500 | -2.46878100 | -2.05327500 |
| H | -0.86317000 | -3.03198500 | -2.86681900 |
| H | 0.49214000  | -1.94769500 | -2.42993000 |
| H | -0.09723300 | -3.17070200 | -1.27342400 |
| C | -1.77103600 | -0.58995000 | -2.63596700 |
| H | -2.61837600 | 0.02184400  | -2.32986200 |
| H | -0.92909000 | 0.06087500  | -2.90027800 |
| H | -2.04468800 | -1.16820600 | -3.52530800 |
| C | -0.94848900 | -2.32641700 | 1.24528800  |
| H | -0.75622900 | -3.15328300 | 1.93217300  |
| H | -0.96979500 | -1.44417000 | 1.91506000  |
| N | 1.30963100  | 0.09887900  | 0.20363100  |
| H | -0.06001400 | -2.28775900 | 0.60469900  |
| H | 1.46652900  | 1.10020600  | 0.36187800  |
| C | 2.63704900  | -0.50804300 | 0.12921300  |
| C | 2.55203100  | -2.03369200 | 0.27081400  |
| C | 3.30320800  | -0.17075600 | -1.22030700 |
| C | 3.53593400  | 0.02783700  | 1.26140500  |
| H | 1.91443100  | -2.43914200 | -0.52695100 |
| H | 2.08967600  | -2.27872500 | 1.23756000  |
| C | 3.94952700  | -2.66571600 | 0.18329700  |
| H | 3.36449200  | 0.92189500  | -1.32293700 |
| H | 2.66215800  | -0.53919500 | -2.03375600 |
| C | 4.70278300  | -0.79429100 | -1.30941200 |
| H | 3.06594700  | -0.19842800 | 2.22780300  |
| H | 3.60325800  | 1.12258200  | 1.17787700  |
| C | 4.93974700  | -0.58966700 | 1.18143700  |
| H | 3.85835900  | -3.75322700 | 0.28153900  |
| C | 4.58305800  | -2.31928000 | -1.17222100 |
| C | 4.82732900  | -2.11529200 | 1.31635800  |
| H | 5.15222000  | -0.54367300 | -2.27668200 |
| C | 5.57562400  | -0.24163400 | -0.17274000 |
| H | 5.55730700  | -0.19092600 | 1.99359600  |
| H | 3.96965100  | -2.72258300 | -1.98853700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.57332600  | -2.78311200 | -1.25071000 |
| H  | 4.39342300  | -2.37642200 | 2.28975500  |
| H  | 5.82352200  | -2.57089300 | 1.27018200  |
| H  | 6.58331800  | -0.66962400 | -0.23324700 |
| H  | 5.67725900  | 0.84607400  | -0.27287300 |
| 7  |             |             |             |
| C  | 2.00635200  | 1.96588100  | -0.57363900 |
| C  | 1.53671600  | 1.85270800  | -1.92281000 |
| C  | 2.09182900  | 0.67717000  | -2.49836700 |
| C  | 2.93124100  | 0.05746600  | -1.52752600 |
| C  | 2.89039500  | 0.85086000  | -0.35461600 |
| Sc | 0.58876400  | 0.02263500  | -0.64247900 |
| C  | 0.48746200  | 4.63584400  | 0.10308300  |
| C  | 1.01416200  | 2.63796500  | 2.31195400  |
| C  | 3.35771700  | 4.18073600  | 1.03983800  |
| H  | 0.78944300  | 5.10228500  | -0.83800000 |
| H  | -0.52745200 | 4.24061100  | -0.01047400 |
| H  | 0.44224100  | 5.42169700  | 0.86471400  |
| H  | 1.69931100  | 1.96220000  | 2.83353700  |
| H  | 0.80179800  | 3.46959400  | 2.99278900  |
| H  | 0.07276300  | 2.10814100  | 2.12752700  |
| H  | 3.22098400  | 4.99648700  | 1.75671000  |
| H  | 4.09549800  | 3.49011900  | 1.45727000  |
| H  | 3.77420300  | 4.60433700  | 0.12127200  |
| Si | 1.71091100  | 3.33682200  | 0.69933300  |
| C  | 3.76931900  | 0.65278700  | 0.85137200  |
| H  | 3.99632300  | -0.40012900 | 1.03906000  |
| H  | 4.72815900  | 1.15955300  | 0.69774700  |
| H  | 3.32605900  | 1.06792900  | 1.75961900  |
| C  | 3.77671000  | -1.16316600 | -1.75739100 |
| H  | 3.22917500  | -1.95325500 | -2.28087200 |
| H  | 4.65151800  | -0.91828300 | -2.36871500 |
| H  | 4.14504400  | -1.58069700 | -0.81712600 |
| C  | 1.94342000  | 0.24298800  | -3.93118700 |
| H  | 0.92516900  | 0.38453900  | -4.30555000 |
| H  | 2.60923800  | 0.82795700  | -4.57408900 |
| H  | 2.20920900  | -0.81005300 | -4.06327200 |
| C  | 0.66840700  | 2.81744700  | -2.68396300 |
| H  | -0.07381300 | 3.30617700  | -2.05194800 |
| H  | 1.27987900  | 3.60784600  | -3.13299700 |
| H  | 0.13522000  | 2.31370700  | -3.49433200 |
| N  | -1.09948700 | 1.03400400  | -0.39370300 |
| H  | -1.01417500 | 2.01315600  | -0.67203200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.48850800 | 0.78933100  | -0.01155600 |
| C | -2.59017300 | -0.51257800 | 0.79808500  |
| C | -3.02497000 | 1.93477200  | 0.86808700  |
| C | -3.39169000 | 0.67763200  | -1.25872800 |
| H | -1.96771800 | -0.41273500 | 1.69814600  |
| H | -2.18573800 | -1.35223700 | 0.20926500  |
| C | -4.04586800 | -0.79787800 | 1.19564600  |
| H | -2.95241800 | 2.87845500  | 0.30865100  |
| H | -2.38610900 | 2.03034500  | 1.75606700  |
| C | -4.48290400 | 1.67238600  | 1.27741000  |
| H | -3.02386700 | -0.13070100 | -1.90557700 |
| H | -3.31669800 | 1.61050000  | -1.83380000 |
| C | -4.84828800 | 0.40612400  | -0.85682700 |
| H | -4.09050300 | -1.73596700 | 1.76058500  |
| C | -4.55861500 | 0.35769500  | 2.06857600  |
| C | -4.91257000 | -0.91006800 | -0.06715900 |
| H | -4.83745000 | 2.49962700  | 1.90183300  |
| C | -5.35665000 | 1.55956700  | 0.01926200  |
| H | -5.46568600 | 0.32680100  | -1.75852000 |
| H | -3.95870800 | 0.43184000  | 2.98422200  |
| H | -5.59393200 | 0.16249500  | 2.37223900  |
| H | -4.56234900 | -1.74123600 | -0.69390700 |
| H | -5.94947600 | -1.13083000 | 0.21236400  |
| H | -6.40060800 | 1.38230600  | 0.30406700  |
| H | -5.32748700 | 2.49949500  | -0.54528500 |
| C | -1.75131000 | -3.84182400 | -1.65113400 |
| C | -0.36666200 | -3.20825500 | -1.87050000 |
| H | -1.66058800 | -4.85143100 | -1.24096100 |
| H | -2.36288700 | -3.24435300 | -0.96836400 |
| H | -2.27470700 | -3.91110900 | -2.60871200 |
| C | -0.51145300 | -1.79795900 | -2.43231800 |
| C | 0.44860000  | -4.08594400 | -2.83805500 |
| H | 0.47595000  | -1.34259700 | -2.61087800 |
| H | -1.00357100 | -1.81179200 | -3.40867900 |
| H | -1.14926500 | -1.16645000 | -1.79584200 |
| H | -0.08348700 | -4.17033000 | -3.78939100 |
| H | 1.43577400  | -3.65599000 | -3.03223700 |
| H | 0.58402300  | -5.09350300 | -2.43520700 |
| C | 0.36227000  | -3.20487100 | -0.55622600 |
| H | 0.48318100  | -4.18725200 | -0.09086400 |
| N | 0.84029400  | -2.16014100 | 0.00016500  |
| C | 1.57591200  | -2.24379200 | 1.28390100  |
| C | 1.07491100  | -1.09905600 | 2.17103200  |
| C | 1.50402900  | -3.57938300 | 2.02134400  |

|      |             |             |             |
|------|-------------|-------------|-------------|
| H    | 2.62588600  | -2.04509400 | 1.02679200  |
| C    | 1.81804100  | -1.03155500 | 3.50686400  |
| H    | 0.00024300  | -1.23697300 | 2.34777000  |
| H    | 1.19959500  | -0.12064800 | 1.66634400  |
| C    | 2.26630600  | -3.49944300 | 3.34851100  |
| H    | 0.45111600  | -3.82695500 | 2.21680200  |
| H    | 1.92627800  | -4.38130100 | 1.40742200  |
| C    | 1.73410900  | -2.37403500 | 4.23445700  |
| H    | 1.39795400  | -0.22757300 | 4.11807900  |
| H    | 2.87167300  | -0.78475800 | 3.32373800  |
| H    | 2.19455600  | -4.46158700 | 3.86243200  |
| H    | 3.33093400  | -3.32839000 | 3.14246200  |
| H    | 2.29883200  | -2.32784600 | 5.16950200  |
| H    | 0.68954400  | -2.58132900 | 4.50025200  |
| ts-8 |             |             |             |
| C    | 1.81552700  | -2.19178600 | -0.00454900 |
| C    | 1.16732200  | -2.68266000 | 1.17581200  |
| C    | 1.65205600  | -1.95727600 | 2.29600300  |
| C    | 2.62931100  | -1.02511900 | 1.83036200  |
| C    | 2.74060700  | -1.18080300 | 0.42653600  |
| Sc   | 0.47678400  | -0.37547600 | 0.84647500  |
| C    | 0.36493300  | -4.12627100 | -1.99249100 |
| C    | 1.04026900  | -1.28169100 | -2.85132500 |
| C    | 3.28686600  | -3.35328500 | -2.43982500 |
| H    | 0.60944600  | -4.99844100 | -1.38075900 |
| H    | -0.65040600 | -3.80504700 | -1.74331900 |
| H    | 0.36317800  | -4.44417200 | -3.04040000 |
| H    | 1.79508400  | -0.49328300 | -2.93930200 |
| H    | 0.81153300  | -1.62569400 | -3.86579800 |
| H    | 0.11982800  | -0.83216700 | -2.45306400 |
| H    | 3.18209000  | -3.71724000 | -3.46674400 |
| H    | 4.04923500  | -2.57002700 | -2.43788100 |
| H    | 3.65318100  | -4.18138700 | -1.82595800 |
| Si   | 1.62637400  | -2.74690100 | -1.80056800 |
| C    | 3.76455900  | -0.47823800 | -0.42281200 |
| H    | 3.95711000  | 0.53912100  | -0.07130200 |
| H    | 4.71700700  | -1.01842600 | -0.38206000 |
| H    | 3.46996100  | -0.42340000 | -1.47388000 |
| C    | 3.44304400  | -0.07453400 | 2.66353500  |
| H    | 3.00105200  | 0.08453400  | 3.65028000  |
| H    | 4.45503000  | -0.46296900 | 2.81828400  |
| H    | 3.53967800  | 0.90430000  | 2.18131400  |
| C    | 1.23660700  | -2.17701600 | 3.72551300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.14836200  | -2.22071300 | 3.84068300  |
| H | 1.64168500  | -3.12111600 | 4.10302500  |
| H | 1.60187800  | -1.38075200 | 4.37757300  |
| C | 0.15518400  | -3.79177000 | 1.26447000  |
| H | -0.63462900 | -3.69300500 | 0.51590600  |
| H | 0.63387200  | -4.76506600 | 1.11767100  |
| H | -0.31366100 | -3.81237400 | 2.25234100  |
| N | -1.51626300 | -0.96621400 | 1.13391200  |
| H | -1.73823900 | -1.80222600 | 1.67550200  |
| C | -2.67025300 | -0.55658300 | 0.32466000  |
| C | -3.84386100 | -0.07801800 | 1.19777200  |
| C | -2.23075600 | 0.58986600  | -0.59574000 |
| C | -3.15034700 | -1.72281100 | -0.55674300 |
| H | -3.50638700 | 0.74054500  | 1.84785600  |
| H | -4.15995100 | -0.90162600 | 1.85196300  |
| C | -5.01277700 | 0.38259900  | 0.31338800  |
| H | -1.40213600 | 0.23656900  | -1.23468000 |
| H | -1.85465900 | 1.43355900  | -0.00008400 |
| C | -3.39226100 | 1.05259900  | -1.48640500 |
| H | -3.45055900 | -2.56310700 | 0.08428200  |
| H | -2.31026100 | -2.06505800 | -1.17797500 |
| C | -4.32529500 | -1.27640500 | -1.44152500 |
| H | -5.83541800 | 0.72577000  | 0.94960300  |
| C | -4.54413200 | 1.53350200  | -0.59064500 |
| C | -5.48334200 | -0.79388500 | -0.55453800 |
| H | -3.05236900 | 1.87337900  | -2.12860500 |
| C | -3.86358800 | -0.12681400 | -2.34959400 |
| H | -4.65516400 | -2.12131800 | -2.05517900 |
| H | -4.21714900 | 2.38499700  | 0.02021300  |
| H | -5.37575200 | 1.88230400  | -1.21352100 |
| H | -5.83604400 | -1.61387400 | 0.08252400  |
| H | -6.32720700 | -0.48263900 | -1.18124400 |
| H | -4.68750500 | 0.19377400  | -2.99749200 |
| H | -3.04873800 | -0.46487200 | -3.00345700 |
| C | -1.52065500 | 3.02553600  | 2.48054100  |
| C | -0.12601900 | 2.37077100  | 2.49622200  |
| H | -1.45824400 | 4.09490200  | 2.25606600  |
| H | -2.18257600 | 2.55884000  | 1.74623200  |
| H | -1.97793200 | 2.91425400  | 3.46786900  |
| C | -0.21787500 | 0.86220200  | 2.78817100  |
| C | 0.73274100  | 3.08632600  | 3.56119400  |
| H | 0.76088200  | 0.52164300  | 3.16506700  |
| H | -0.88123000 | 0.71316400  | 3.64966100  |
| H | -1.09400600 | -0.01907600 | 2.00525300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.28298700  | 2.92927200  | 4.54516600  |
| H  | 1.75020700  | 2.68248200  | 3.58119000  |
| H  | 0.78876600  | 4.16475300  | 3.37971700  |
| C  | 0.52010600  | 2.66080400  | 1.17068900  |
| H  | 0.67609900  | 3.72148800  | 0.93693700  |
| N  | 0.88955900  | 1.76296800  | 0.33672400  |
| C  | 1.50888200  | 2.16273600  | -0.94783900 |
| C  | 0.47668900  | 2.76149200  | -1.91046400 |
| C  | 2.70669800  | 3.10080500  | -0.77876500 |
| H  | 1.87502800  | 1.22805100  | -1.39422200 |
| C  | 1.12417700  | 3.04542300  | -3.26879600 |
| H  | 0.08547700  | 3.69227300  | -1.47595000 |
| H  | -0.37017500 | 2.07660800  | -2.02784000 |
| C  | 3.36248100  | 3.34939100  | -2.13910300 |
| H  | 2.36915700  | 4.06008500  | -0.36576200 |
| H  | 3.42062500  | 2.67602600  | -0.06465400 |
| C  | 2.35611100  | 3.94153200  | -3.12872000 |
| H  | 0.38936400  | 3.50146100  | -3.93815300 |
| H  | 1.41897900  | 2.09107900  | -3.72640400 |
| H  | 4.22138700  | 4.01530700  | -2.01953200 |
| H  | 3.74855400  | 2.39847100  | -2.53160000 |
| H  | 2.82685200  | 4.08849800  | -4.10481500 |
| H  | 2.04400400  | 4.93219800  | -2.77295000 |
| g  |             |             |             |
| C  | 0.80050100  | 2.36861900  | 0.65382100  |
| C  | 0.36126800  | 2.94862400  | -0.58132400 |
| C  | 1.39160300  | 2.80163400  | -1.54981500 |
| C  | 2.49196600  | 2.15177000  | -0.92124000 |
| C  | 2.13129800  | 1.88510700  | 0.42189200  |
| Sc | 0.62516400  | 0.53793700  | -0.98895500 |
| C  | -1.62557700 | 3.32599500  | 2.42099500  |
| C  | -0.27628500 | 0.58945000  | 2.92929900  |
| C  | 1.15836500  | 3.23295600  | 3.57770500  |
| H  | -1.50751100 | 4.34338400  | 2.03692100  |
| H  | -2.44974900 | 2.85068900  | 1.88349400  |
| H  | -1.92317600 | 3.40497700  | 3.47231800  |
| H  | 0.62157200  | 0.18056200  | 3.40644700  |
| H  | -1.09050600 | 0.53108600  | 3.65968000  |
| H  | -0.53487600 | -0.07335400 | 2.09256000  |
| H  | 0.68199000  | 3.29318300  | 4.56166000  |
| H  | 2.10945500  | 2.70885000  | 3.69903500  |
| H  | 1.37517400  | 4.25372600  | 3.24879300  |
| Si | 0.00305700  | 2.37997800  | 2.36247500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.08150900  | 1.31481800  | 1.43872100  |
| H | 3.77004900  | 0.60003700  | 0.98044500  |
| H | 3.69186400  | 2.11258200  | 1.87728800  |
| H | 2.56660400  | 0.81098200  | 2.26166900  |
| C | 3.83274900  | 1.83947300  | -1.52276600 |
| H | 3.85639500  | 2.05741300  | -2.59219600 |
| H | 4.61526400  | 2.43895000  | -1.04598500 |
| H | 4.10330900  | 0.78504300  | -1.39142400 |
| C | 1.33797400  | 3.27797100  | -2.97460400 |
| H | 0.34483800  | 3.14037200  | -3.41398600 |
| H | 1.57832900  | 4.34412600  | -3.04281400 |
| H | 2.04793600  | 2.73555500  | -3.60318900 |
| C | -0.92865500 | 3.68283000  | -0.82649800 |
| H | -1.75989100 | 3.25952600  | -0.25911800 |
| H | -0.83705500 | 4.73332200  | -0.52966800 |
| H | -1.19592400 | 3.68289700  | -1.88843900 |
| N | -1.55214600 | 0.50266600  | -1.79379300 |
| H | -1.84800900 | 1.44776700  | -2.05160200 |
| C | -2.64942500 | -0.14566200 | -1.01980600 |
| C | -3.88254600 | -0.42129300 | -1.89014900 |
| C | -2.11950600 | -1.46529400 | -0.45536900 |
| C | -3.03873300 | 0.77225400  | 0.14051800  |
| H | -3.60221400 | -1.07094200 | -2.73070300 |
| H | -4.25404000 | 0.52283200  | -2.30958800 |
| C | -4.97086200 | -1.09590900 | -1.03605900 |
| H | -1.22883700 | -1.25615800 | 0.15968700  |
| H | -1.80099900 | -2.12924400 | -1.27042900 |
| C | -3.19768000 | -2.14861400 | 0.39879400  |
| H | -3.40845700 | 1.72886300  | -0.25492700 |
| H | -2.14737600 | 0.98549400  | 0.74668500  |
| C | -4.12291000 | 0.10463800  | 1.00017700  |
| H | -5.84732100 | -1.28945000 | -1.66243400 |
| C | -4.42854300 | -2.42199000 | -0.47981700 |
| C | -5.35625400 | -0.16777600 | 0.12562400  |
| H | -2.80206800 | -3.09249700 | 0.78979300  |
| C | -3.58563300 | -1.22169800 | 1.55911000  |
| H | -4.38817000 | 0.77538600  | 1.82439900  |
| H | -4.16481600 | -3.09696600 | -1.30308200 |
| H | -5.20181500 | -2.92075100 | 0.11498200  |
| H | -5.75929700 | 0.77533300  | -0.26234700 |
| H | -6.14336800 | -0.63427800 | 0.72857900  |
| H | -4.35272100 | -1.70248300 | 2.17643300  |
| H | -2.71730400 | -1.03884700 | 2.20469600  |
| C | 0.60196200  | -2.56337700 | -3.35159600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.75913400  | -1.70096000 | -2.81162900 |
| H  | 0.76575800  | -3.63226300 | -3.17903100 |
| H  | -0.34447500 | -2.28201000 | -2.87775000 |
| H  | 0.50825000  | -2.40240900 | -4.42927400 |
| C  | 1.42997100  | -0.19743400 | -2.92243300 |
| C  | 3.04641300  | -2.07605000 | -3.56870800 |
| H  | 2.36221800  | 0.34952600  | -3.11260500 |
| H  | 0.80612700  | -0.02699800 | -3.81228500 |
| H  | -1.43910500 | 0.00917600  | -2.68398000 |
| H  | 2.92592800  | -1.81856700 | -4.62432900 |
| H  | 3.90440200  | -1.51802500 | -3.18006600 |
| H  | 3.26711300  | -3.14728500 | -3.49901200 |
| C  | 1.94629300  | -2.11793700 | -1.37504600 |
| H  | 2.40304900  | -3.10170300 | -1.20421000 |
| N  | 1.58342400  | -1.40220300 | -0.37567200 |
| C  | 1.79556200  | -1.90590700 | 0.99974400  |
| C  | 0.82488400  | -3.03736300 | 1.35893100  |
| C  | 3.24040400  | -2.33880900 | 1.26884500  |
| H  | 1.57459800  | -1.05439500 | 1.65512300  |
| C  | 0.99381300  | -3.43293200 | 2.82889600  |
| H  | 1.03055200  | -3.89978600 | 0.70912600  |
| H  | -0.20894300 | -2.72986300 | 1.16899600  |
| C  | 3.40607100  | -2.69968000 | 2.74685000  |
| H  | 3.48335900  | -3.21895800 | 0.65998500  |
| H  | 3.93157300  | -1.54241200 | 0.97556100  |
| C  | 2.44015100  | -3.81733600 | 3.14495900  |
| H  | 0.31474600  | -4.25599100 | 3.06921600  |
| H  | 0.69762600  | -2.58222000 | 3.45799600  |
| H  | 4.44028900  | -2.99624500 | 2.94244900  |
| H  | 3.20858400  | -1.80910000 | 3.35998000  |
| H  | 2.54473200  | -4.04856800 | 4.20891600  |
| H  | 2.70046900  | -4.73018100 | 2.59311700  |
| 7' |             |             |             |
| C  | -2.22618800 | -0.41941300 | 0.24459300  |
| C  | -2.80702500 | 0.85729500  | -0.05999500 |
| C  | -2.25327700 | 1.83290200  | 0.81530800  |
| C  | -1.32911500 | 1.17249400  | 1.67499200  |
| C  | -1.32105900 | -0.20481600 | 1.33675200  |
| Sc | -0.44860100 | 0.97060700  | -0.59624400 |
| C  | -3.79597800 | -2.05511000 | -1.92098600 |
| C  | -0.94914800 | -2.82809900 | -1.18873600 |
| C  | -3.24492300 | -3.26311000 | 0.83319700  |
| H  | -4.74191400 | -1.58702900 | -1.63734400 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -3.40336900 | -1.53293200 | -2.79898600 |
| H  | -4.01409800 | -3.08376000 | -2.22717200 |
| H  | -0.25999500 | -3.15868300 | -0.40540100 |
| H  | -1.16341600 | -3.69682300 | -1.81994600 |
| H  | -0.41739300 | -2.10144300 | -1.81990000 |
| H  | -3.40804600 | -4.26357700 | 0.42029400  |
| H  | -2.56723500 | -3.35642400 | 1.68550700  |
| H  | -4.20425500 | -2.89186300 | 1.20470200  |
| Si | -2.57015200 | -2.12446000 | -0.49735000 |
| C  | -0.57202500 | -1.24786900 | 2.12046000  |
| H  | 0.40739000  | -0.88571500 | 2.44764300  |
| H  | -1.13571400 | -1.50938800 | 3.02295900  |
| H  | -0.42163700 | -2.16999600 | 1.55467200  |
| C  | -0.52250500 | 1.78623200  | 2.78316600  |
| H  | -0.58239700 | 2.87611000  | 2.76988000  |
| H  | -0.88846100 | 1.44486200  | 3.75697000  |
| H  | 0.53528300  | 1.50717100  | 2.71627700  |
| C  | -2.60743600 | 3.29179000  | 0.86233100  |
| H  | -2.85215400 | 3.68470800  | -0.12748400 |
| H  | -3.47663700 | 3.45750700  | 1.50698200  |
| H  | -1.78285600 | 3.89013300  | 1.25612600  |
| C  | -3.86219600 | 1.14756300  | -1.09583400 |
| H  | -3.67221300 | 0.65045700  | -2.05008100 |
| H  | -4.84124600 | 0.80248700  | -0.74814200 |
| H  | -3.94808500 | 2.21983400  | -1.28353200 |
| C  | 2.27990200  | 2.90741300  | -2.28442400 |
| C  | 2.00288700  | 2.77129500  | -0.77287400 |
| H  | 3.32916900  | 2.71524500  | -2.52999500 |
| H  | 1.66109800  | 2.21041800  | -2.86172000 |
| H  | 2.03664700  | 3.92538800  | -2.60077600 |
| C  | 0.49979300  | 2.94309200  | -0.47135300 |
| C  | 2.87111200  | 3.78724400  | -0.01181500 |
| H  | 0.38939700  | 3.25329100  | 0.57766500  |
| H  | 0.09187200  | 3.76638700  | -1.07250300 |
| H  | 2.57005900  | 4.79872900  | -0.29588100 |
| H  | 2.73437300  | 3.68440100  | 1.06910000  |
| H  | 3.93576500  | 3.66836400  | -0.24140100 |
| C  | 2.46901000  | 1.38641700  | -0.40678600 |
| H  | 3.55060800  | 1.23443200  | -0.29956400 |
| N  | 1.66733800  | 0.39350900  | -0.26991300 |
| C  | 2.20428900  | -0.95453100 | 0.01461100  |
| C  | 2.88120700  | -1.55588400 | -1.22019400 |
| C  | 3.13695100  | -0.98956500 | 1.22763600  |
| H  | 1.33128300  | -1.57332700 | 0.25209700  |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.31573000 | -2.99587800 | -0.93459000 |
| H | 3.75650200 | -0.94374600 | -1.47787400 |
| H | 2.19806900 | -1.52124200 | -2.07711600 |
| C | 3.54188700 | -2.43643800 | 1.51976400  |
| H | 4.04000900 | -0.40148500 | 1.02072500  |
| H | 2.64280600 | -0.53156800 | 2.09185800  |
| C | 4.21629300 | -3.07038300 | 0.30071300  |
| H | 3.82642100 | -3.40749200 | -1.80960400 |
| H | 2.42036600 | -3.61091500 | -0.77094300 |
| H | 4.20690600 | -2.46678000 | 2.38701900  |
| H | 2.64570600 | -3.01407600 | 1.78547400  |
| H | 4.47761700 | -4.11102300 | 0.51233900  |
| H | 5.15604800 | -2.54134800 | 0.09487600  |

trans-ts-10

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.06830200  | -1.49217600 | -1.49358600 |
| C  | 2.94244900  | -1.92322500 | -0.44361700 |
| C  | 3.73419900  | -0.82991900 | -0.02914000 |
| C  | 3.39388400  | 0.29351100  | -0.83331900 |
| C  | 2.36794800  | -0.10394300 | -1.72820200 |
| Sc | 1.32322800  | -0.20143600 | 0.50131400  |
| C  | 0.00258300  | -3.88161300 | -1.80301200 |
| C  | 0.21318100  | -1.83573900 | -4.01354700 |
| C  | 2.56471000  | -3.70729000 | -3.48834700 |
| H  | 0.38916600  | -4.32764000 | -0.88274100 |
| H  | -0.95517100 | -3.40119500 | -1.57756600 |
| H  | -0.21465700 | -4.70404300 | -2.49350300 |
| H  | 0.84397700  | -1.23853400 | -4.67651600 |
| H  | -0.25753200 | -2.61620700 | -4.62165700 |
| H  | -0.59414700 | -1.19138000 | -3.64854200 |
| H  | 2.13961500  | -4.40502300 | -4.21640200 |
| H  | 3.26173900  | -3.04845300 | -4.01478400 |
| H  | 3.13744400  | -4.28699700 | -2.75878500 |
| Si | 1.20759900  | -2.70345300 | -2.66314900 |
| C  | 1.77922300  | 0.77328100  | -2.80212000 |
| H  | 2.00682600  | 1.82641400  | -2.62002900 |
| H  | 2.18840400  | 0.51655900  | -3.78479400 |
| H  | 0.68972100  | 0.68112600  | -2.87632300 |
| C  | 4.14153400  | 1.59789100  | -0.78908500 |
| H  | 3.96091800  | 2.19217900  | -1.68676100 |
| H  | 3.88849200  | 2.21581100  | 0.08218000  |
| H  | 5.21710600  | 1.40299900  | -0.74289500 |
| C  | 4.87385400  | -0.88301400 | 0.94598000  |
| H  | 4.71435400  | -1.63037700 | 1.72900100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.79998900  | -1.15784400 | 0.42842800  |
| H | 5.04658500  | 0.08215500  | 1.43053200  |
| C | 3.16678400  | -3.33027900 | 0.03894000  |
| H | 2.38735500  | -4.01564400 | -0.29838400 |
| H | 4.12061000  | -3.70644800 | -0.34716700 |
| H | 3.21792500  | -3.39883400 | 1.13132500  |
| N | -0.77042100 | -0.66531100 | -0.58842000 |
| H | -0.45180300 | -0.77669900 | -1.55321700 |
| C | -2.20694400 | -0.24038700 | -0.66562100 |
| C | -2.34655700 | 0.90254500  | -1.67505200 |
| C | -3.07373400 | -1.41523300 | -1.15612700 |
| C | -2.69960700 | 0.21488600  | 0.71101300  |
| H | -1.98608800 | 0.57159900  | -2.66076500 |
| H | -1.72693700 | 1.74470800  | -1.36260100 |
| C | -3.81619900 | 1.34419600  | -1.77710700 |
| H | -2.96688200 | -2.26043700 | -0.46590200 |
| H | -2.72051600 | -1.74130900 | -2.14532400 |
| C | -4.54713600 | -0.98886000 | -1.23876200 |
| H | -2.06059200 | 1.03384800  | 1.07242100  |
| H | -2.61418600 | -0.61021200 | 1.42603200  |
| C | -4.16783500 | 0.66270000  | 0.61405200  |
| H | -3.89038700 | 2.16824500  | -2.49536400 |
| C | -4.67809100 | 0.16269900  | -2.24508600 |
| C | -4.30451300 | 1.81065700  | -0.39714800 |
| H | -5.14737200 | -1.84266200 | -1.57027900 |
| C | -5.01904000 | -0.52914100 | 0.14914400  |
| H | -4.50479900 | 0.99350100  | 1.60235800  |
| H | -4.35782500 | -0.16934100 | -3.24029300 |
| H | -5.72533100 | 0.47604800  | -2.32552000 |
| H | -3.73115200 | 2.68543900  | -0.06649600 |
| H | -5.35290400 | 2.12425700  | -0.46386000 |
| H | -6.07584200 | -0.24066800 | 0.10702800  |
| H | -4.92864200 | -1.35229400 | 0.86926000  |
| C | 0.45293600  | 1.50085800  | 3.94407900  |
| C | 1.61782100  | 1.82371900  | 2.99275300  |
| H | 0.00163200  | 2.41771400  | 4.33553700  |
| H | -0.32617100 | 0.92845700  | 3.43213100  |
| H | 0.81920400  | 0.91942000  | 4.79684100  |
| C | 2.35726500  | 0.58359300  | 2.47834700  |
| C | 2.61150000  | 2.75575000  | 3.71685900  |
| H | 3.01607100  | 0.91286500  | 1.65691700  |
| H | 3.04795400  | 0.24546100  | 3.25111000  |
| H | -0.78437200 | -1.62177900 | -0.21900700 |
| H | 3.00996300  | 2.24780700  | 4.59917200  |

|           |             |             |             |
|-----------|-------------|-------------|-------------|
| H         | 3.45078900  | 3.02036900  | 3.06606600  |
| H         | 2.12384100  | 3.67865000  | 4.04776500  |
| C         | 1.04024700  | 2.58872200  | 1.84268800  |
| H         | 0.76513600  | 3.63061100  | 2.04120000  |
| N         | 0.87260900  | 2.08150000  | 0.68255700  |
| C         | 0.35721000  | 2.97843800  | -0.38190500 |
| C         | -0.91873800 | 3.73130400  | 0.01285100  |
| C         | 1.42369900  | 3.98231100  | -0.83485300 |
| H         | 0.13302800  | 2.32988300  | -1.23653100 |
| C         | -1.45363200 | 4.53107500  | -1.17849100 |
| H         | -0.69588700 | 4.43343700  | 0.82541900  |
| H         | -1.66739200 | 3.03083300  | 0.39378600  |
| C         | 0.90870900  | 4.80145500  | -2.02138700 |
| H         | 1.66004400  | 4.64948100  | 0.00614800  |
| H         | 2.34605000  | 3.46003600  | -1.09675300 |
| C         | -0.39901900 | 5.51897900  | -1.68256800 |
| H         | -2.36839800 | 5.05699700  | -0.88917200 |
| H         | -1.72613900 | 3.84437900  | -1.99224100 |
| H         | 1.67243100  | 5.52035400  | -2.33138500 |
| H         | 0.74317900  | 4.12787600  | -2.87395700 |
| H         | -0.77216000 | 6.05823100  | -2.55787000 |
| H         | -0.20846500 | 6.26835000  | -0.90320100 |
| C         | 1.67692800  | -1.46790400 | 2.71404800  |
| C         | 0.69708300  | -2.06907700 | 1.91820400  |
| H         | 1.43486200  | -1.18582200 | 3.73375700  |
| H         | 2.70793700  | -1.78073700 | 2.58145800  |
| H         | 1.03727600  | -2.78268800 | 1.16963100  |
| C         | -0.70029400 | -2.25390700 | 2.35492400  |
| C         | -1.24498800 | -1.64660000 | 3.49837100  |
| C         | -1.52691300 | -3.13311800 | 1.63584500  |
| C         | -2.56483500 | -1.87406300 | 3.87469200  |
| H         | -0.63190500 | -1.00466900 | 4.11995800  |
| C         | -2.84539900 | -3.36552000 | 2.01444500  |
| H         | -1.11863100 | -3.66281100 | 0.77708000  |
| C         | -3.37985400 | -2.72494800 | 3.13001500  |
| H         | -2.95582800 | -1.38989000 | 4.76407900  |
| H         | -3.45522900 | -4.05355800 | 1.43617100  |
| H         | -4.40807900 | -2.90243800 | 3.42631300  |
| cis-ts-10 |             |             |             |
| C         | 0.94411500  | -0.42304300 | -2.41190900 |
| C         | 2.16068800  | -0.67541200 | -1.73746500 |
| C         | 2.66566300  | 0.56366600  | -1.22340800 |
| C         | 1.74666600  | 1.58546400  | -1.63957400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.68797300  | 0.98120200  | -2.36466500 |
| Sc | 0.57393500  | 0.17533500  | 0.01671100  |
| C  | 2.88724400  | -1.98962600 | -1.78505400 |
| H  | 2.21913100  | -2.79911600 | -2.08445900 |
| H  | 3.69021900  | -1.93019900 | -2.53016900 |
| H  | 3.33593700  | -2.26780400 | -0.83026700 |
| N  | -1.70680500 | -0.29245800 | -0.66099500 |
| H  | -2.06310200 | 0.66413700  | -0.60861800 |
| C  | -2.88521500 | -1.17274000 | -0.34110900 |
| C  | -4.15013000 | -0.54759600 | -0.96038900 |
| C  | -2.68654300 | -2.56170600 | -0.96611000 |
| C  | -3.07667700 | -1.31045700 | 1.17459400  |
| H  | -4.00095500 | -0.43413600 | -2.04383100 |
| H  | -4.30575400 | 0.45756100  | -0.54349500 |
| C  | -5.37954500 | -1.42124300 | -0.67313000 |
| H  | -1.77967200 | -3.03771700 | -0.57553400 |
| H  | -2.55962200 | -2.45693000 | -2.05278100 |
| C  | -3.90786700 | -3.44816700 | -0.66508700 |
| H  | -3.19605800 | -0.31907200 | 1.63277500  |
| H  | -2.19394900 | -1.78012100 | 1.62051900  |
| C  | -4.31076800 | -2.18144000 | 1.46497900  |
| H  | -6.26330300 | -0.95328200 | -1.11892200 |
| C  | -5.16319600 | -2.81427900 | -1.28009300 |
| C  | -5.56027700 | -1.53891300 | 0.84734400  |
| H  | -3.73995300 | -4.43790600 | -1.10173400 |
| C  | -4.08740200 | -3.57358400 | 0.85527600  |
| H  | -4.43475400 | -2.26840200 | 2.54938900  |
| H  | -5.05448200 | -2.73952400 | -2.36890600 |
| H  | -6.03531700 | -3.44765900 | -1.08192200 |
| H  | -5.72809400 | -0.54612300 | 1.28386500  |
| H  | -6.44310500 | -2.14735100 | 1.07363600  |
| H  | -4.94534500 | -4.21911300 | 1.07508700  |
| H  | -3.20251100 | -4.04227700 | 1.30364900  |
| C  | 0.33590700  | 1.38133400  | 4.17685300  |
| C  | 0.91965300  | 1.87634000  | 2.84007500  |
| H  | -0.04870300 | 2.22454700  | 4.75794700  |
| H  | -0.47803900 | 0.66537000  | 4.05154400  |
| H  | 1.12776300  | 0.90544100  | 4.76337600  |
| C  | 1.59231400  | 0.78757400  | 2.00910100  |
| C  | 1.92723800  | 3.00715200  | 3.16066300  |
| H  | 2.09770900  | 1.30582800  | 1.16551000  |
| H  | 2.41542000  | 0.32317700  | 2.55737900  |
| H  | -1.53034100 | -0.43227600 | -1.65787500 |
| H  | 2.75207300  | 2.59606100  | 3.74981700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.34352100  | 3.43971800  | 2.24553300  |
| H | 1.45771900  | 3.80686800  | 3.74315500  |
| C | -0.16572600 | 2.51279200  | 2.02982800  |
| H | -0.67391100 | 3.37246600  | 2.48316700  |
| N | -0.46315500 | 2.13207900  | 0.84536100  |
| C | -1.49331100 | 2.91526300  | 0.12238200  |
| C | -2.89036600 | 2.73279200  | 0.72785800  |
| C | -1.17362100 | 4.41067300  | 0.00702800  |
| H | -1.50497300 | 2.52130900  | -0.90245100 |
| C | -3.93948900 | 3.39699800  | -0.16666200 |
| H | -2.90658700 | 3.19104600  | 1.72576800  |
| H | -3.11348700 | 1.67026000  | 0.87502300  |
| C | -2.21098400 | 5.09014400  | -0.89216600 |
| H | -1.20438000 | 4.87200800  | 1.00255100  |
| H | -0.16283600 | 4.55018700  | -0.38525400 |
| C | -3.63053100 | 4.88350200  | -0.35928600 |
| H | -4.93634500 | 3.26045000  | 0.26254100  |
| H | -3.94254300 | 2.89584000  | -1.14614300 |
| H | -1.98451400 | 6.15667500  | -0.97468900 |
| H | -2.13690200 | 4.67145600  | -1.90541300 |
| H | -4.35897800 | 5.33533000  | -1.03830900 |
| H | -3.73164500 | 5.39705600  | 0.60554000  |
| C | 0.38115100  | -1.05198100 | 2.15935600  |
| C | 0.45935300  | -1.97378100 | 1.12027500  |
| H | -0.56976800 | -0.53584400 | 2.29950000  |
| H | 0.94568500  | -1.18562000 | 3.07529600  |
| H | -0.43633700 | -2.15630300 | 0.53534500  |
| C | 1.52698800  | -2.97159600 | 1.00008200  |
| C | 2.74290200  | -2.85516000 | 1.68906500  |
| C | 1.33813500  | -4.09129100 | 0.17605400  |
| C | 3.74111100  | -3.81538000 | 1.54004100  |
| H | 2.92088000  | -1.99990200 | 2.33639600  |
| C | 2.33157200  | -5.05054800 | 0.03104500  |
| H | 0.39771400  | -4.20250200 | -0.35989600 |
| C | 3.54386900  | -4.91379700 | 0.70738700  |
| H | 4.67998900  | -3.69824600 | 2.07254100  |
| H | 2.16177000  | -5.90761800 | -0.61309700 |
| H | 4.32304500  | -5.65903900 | 0.58991800  |
| C | 0.14736400  | -1.44362200 | -3.17791700 |
| H | -0.07452400 | -2.33261300 | -2.57691600 |
| H | -0.79952300 | -1.03146300 | -3.54476400 |
| H | 0.70078300  | -1.77950300 | -4.06101300 |
| C | -0.40855300 | 1.68032900  | -3.12416600 |
| H | -0.45419200 | 2.74490000  | -2.88426000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.23153800 | 1.59662300  | -4.20144400 |
| H  | -1.40742300 | 1.26331000  | -2.94154700 |
| C  | 1.93229300  | 3.06165800  | -1.41180000 |
| H  | 1.88180300  | 3.33397000  | -0.35055800 |
| H  | 2.90768100  | 3.38956000  | -1.78511800 |
| H  | 1.17357100  | 3.64313000  | -1.94006800 |
| Si | 4.44612000  | 0.88301100  | -0.67065700 |
| C  | 5.38821000  | 1.36570100  | -2.22883500 |
| H  | 6.44559600  | 1.53788400  | -2.00449600 |
| H  | 5.32579200  | 0.57047600  | -2.97805000 |
| H  | 4.98658500  | 2.27891200  | -2.67863300 |
| C  | 4.61430400  | 2.27352600  | 0.59561900  |
| H  | 5.68161200  | 2.50224200  | 0.69156100  |
| H  | 4.10653100  | 3.19968500  | 0.31636200  |
| H  | 4.25955700  | 1.96664100  | 1.58398200  |
| C  | 5.25329400  | -0.62878400 | 0.10253800  |
| H  | 4.63667700  | -1.05131800 | 0.90150300  |
| H  | 5.45318500  | -1.42045600 | -0.62339400 |
| H  | 6.21008900  | -0.32402000 | 0.53986300  |

trans-11

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -1.25443000 | 2.56666000 | -0.84095100 |
| C  | -2.00871300 | 2.67520100 | 0.36939800  |
| C  | -3.11083500 | 1.79246200 | 0.30573300  |
| C  | -3.06789700 | 1.12312900 | -0.95378100 |
| C  | -1.92527800 | 1.59284900 | -1.65617400 |
| Sc | -1.03566900 | 0.36391500 | 0.29068600  |
| C  | 1.08334500  | 4.50711000 | -0.02712800 |
| C  | 1.07200300  | 3.32643500 | -2.83090800 |
| C  | -1.07581600 | 5.33563800 | -2.04365000 |
| H  | 0.54515000  | 5.14695200 | 0.67651900  |
| H  | 1.56326300  | 3.70627100 | 0.54646300  |
| H  | 1.88308900  | 5.10895400 | -0.47160600 |
| H  | 0.50243200  | 3.08407000 | -3.73128800 |
| H  | 1.73718600  | 4.16082300 | -3.07893900 |
| H  | 1.71539500  | 2.47075000 | -2.60192100 |
| H  | -0.43497600 | 6.15234300 | -2.38995500 |
| H  | -1.70906500 | 5.02170100 | -2.87881000 |
| H  | -1.72705400 | 5.72647700 | -1.25635700 |
| Si | -0.04299400 | 3.89762900 | -1.41694700 |
| C  | -1.52322000 | 1.20174100 | -3.05530600 |
| H  | -2.09799400 | 0.34617800 | -3.41701500 |
| H  | -1.69436900 | 2.02649200 | -3.75578900 |
| H  | -0.46088200 | 0.93755000 | -3.12271400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.14007000 | 0.19578000  | -1.46077700 |
| H | -5.12855100 | 0.61457700  | -1.25206800 |
| H | -4.07132100 | 0.06419900  | -2.54273200 |
| H | -4.10135300 | -0.79906400 | -1.00133300 |
| C | -4.21548400 | 1.72337500  | 1.32414600  |
| H | -3.83759400 | 1.52126100  | 2.33235700  |
| H | -4.75363500 | 2.67602900  | 1.36171700  |
| H | -4.94063000 | 0.94396400  | 1.07959500  |
| C | -1.76905000 | 3.64198300  | 1.49599500  |
| H | -0.72848600 | 3.64597800  | 1.83029800  |
| H | -2.01449000 | 4.66469000  | 1.18652900  |
| H | -2.39676500 | 3.40399900  | 2.35821100  |
| N | 1.19938000  | 0.88349400  | -0.06099500 |
| H | 1.16399200  | 1.60161700  | -0.78587100 |
| C | 2.48813900  | 0.14791600  | -0.24426700 |
| C | 2.57812800  | -0.39062400 | -1.67290300 |
| C | 3.66329600  | 1.10563800  | 0.00968500  |
| C | 2.55804500  | -1.00372600 | 0.75313400  |
| H | 2.51310700  | 0.43398800  | -2.39635100 |
| H | 1.73312100  | -1.06096800 | -1.85969000 |
| C | 3.90536400  | -1.14744300 | -1.85742900 |
| H | 3.58580000  | 1.50347200  | 1.03159600  |
| H | 3.60419700  | 1.95479900  | -0.68650500 |
| C | 4.99205600  | 0.35514800  | -0.16660000 |
| H | 1.69163100  | -1.66501100 | 0.60706900  |
| H | 2.49650900  | -0.60420700 | 1.76789100  |
| C | 3.87656500  | -1.77031700 | 0.57325900  |
| H | 3.95652800  | -1.53157200 | -2.88222100 |
| C | 5.07724300  | -0.18814600 | -1.60091100 |
| C | 3.97156600  | -2.31356300 | -0.85988900 |
| H | 5.82154100  | 1.04513700  | 0.01923200  |
| C | 5.04576800  | -0.80818300 | 0.83577600  |
| H | 3.90943700  | -2.59634900 | 1.29208200  |
| H | 5.05214800  | 0.63989500  | -2.31999400 |
| H | 6.02672400  | -0.71616000 | -1.74466700 |
| H | 3.15939800  | -3.02545000 | -1.05572500 |
| H | 4.91353200  | -2.85867000 | -0.99157600 |
| H | 5.99892800  | -1.34057200 | 0.73885500  |
| H | 4.98402100  | -0.42316800 | 1.86143100  |
| C | -2.29173700 | -3.69042900 | 2.57176300  |
| C | -2.89269800 | -2.72470200 | 1.53631500  |
| H | -2.26747200 | -4.71135400 | 2.17925400  |
| H | -1.27396600 | -3.41258300 | 2.85434500  |
| H | -2.91249100 | -3.68897800 | 3.47243700  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.20179600 | -1.32975400 | 2.11101800  |
| C | -4.22931300 | -3.33172200 | 1.04056000  |
| H | -3.42269000 | -0.66337100 | 1.26658800  |
| H | -4.15990600 | -1.43986100 | 2.63236700  |
| H | 1.29892600  | 1.40354100  | 0.82046200  |
| H | -4.88253400 | -3.50126500 | 1.90062200  |
| H | -4.74126900 | -2.65380200 | 0.35010500  |
| H | -4.07781800 | -4.29173400 | 0.53797200  |
| C | -2.01996000 | -2.75509400 | 0.31651900  |
| H | -1.92777900 | -3.76207600 | -0.10720600 |
| N | -1.46665800 | -1.78415400 | -0.30679800 |
| C | -0.84016500 | -2.11731100 | -1.62066900 |
| C | 0.19420400  | -3.24672400 | -1.55039000 |
| C | -1.91367600 | -2.44092600 | -2.66467400 |
| H | -0.32438700 | -1.20185500 | -1.95340100 |
| C | 0.83076700  | -3.48972300 | -2.92340000 |
| H | -0.29717200 | -4.17418200 | -1.23245100 |
| H | 0.95454300  | -3.01442100 | -0.79846600 |
| C | -1.27592400 | -2.66898900 | -4.03686000 |
| H | -2.44464400 | -3.34954600 | -2.34712300 |
| H | -2.65248100 | -1.63660900 | -2.69965300 |
| C | -0.23336700 | -3.78715100 | -3.98081600 |
| H | 1.54445100  | -4.31587900 | -2.84962600 |
| H | 1.40540600  | -2.60551500 | -3.23034300 |
| H | -2.05368200 | -2.90152600 | -4.76959600 |
| H | -0.79522500 | -1.73748300 | -4.36805700 |
| H | 0.23497200  | -3.91836100 | -4.96014800 |
| H | -0.73307900 | -4.73362100 | -3.73649600 |
| C | -2.22017800 | -0.66261300 | 3.09670300  |
| C | -1.12646800 | 0.26885000  | 2.53071600  |
| H | -1.77443900 | -1.44112600 | 3.72171000  |
| H | -2.83599900 | -0.08008900 | 3.79208800  |
| H | -1.44404100 | 1.30543000  | 2.70771200  |
| C | 0.22692400  | 0.13736400  | 3.14702500  |
| C | 0.75618200  | -1.07457700 | 3.62599500  |
| C | 1.05607400  | 1.27271100  | 3.26564100  |
| C | 2.02559700  | -1.14521100 | 4.19473200  |
| H | 0.16791300  | -1.98436200 | 3.56184700  |
| C | 2.33335800  | 1.20296500  | 3.81397700  |
| H | 0.66400800  | 2.24205600  | 2.95639800  |
| C | 2.83018500  | -0.01165000 | 4.28760800  |
| H | 2.39066100  | -2.09913000 | 4.56371200  |
| H | 2.93183200  | 2.10601500  | 3.89427000  |
| H | 3.81788300  | -0.06991700 | 4.73207100  |

cis-11

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.54721000 | -0.66503500 | 2.11611400  |
| C  | -2.69664800 | -0.16252800 | 1.42291500  |
| C  | -2.63740900 | 1.24985300  | 1.41246000  |
| C  | -1.47965700 | 1.65232800  | 2.13919200  |
| C  | -0.80059100 | 0.48038600  | 2.56292900  |
| Sc | -0.62718800 | 0.43670300  | 0.12035500  |
| C  | -1.57699600 | -3.68541600 | 1.24320100  |
| C  | 0.18384000  | -2.84339200 | 3.57659000  |
| C  | -2.84114100 | -2.75027000 | 3.90133600  |
| H  | -2.18084900 | -4.54407400 | 1.55373800  |
| H  | -2.05360400 | -3.26533100 | 0.35116000  |
| H  | -0.59455500 | -4.07726400 | 0.95830000  |
| H  | 0.30775900  | -2.24789800 | 4.48479500  |
| H  | 0.15313200  | -3.89723200 | 3.87469100  |
| H  | 1.08560800  | -2.71600200 | 2.96657600  |
| H  | -2.77859800 | -3.75781600 | 4.32435400  |
| H  | -2.79241900 | -2.03136500 | 4.72454600  |
| H  | -3.81703400 | -2.64650600 | 3.41939700  |
| Si | -1.43723600 | -2.46061300 | 2.68750400  |
| C  | 0.45361600  | 0.45754900  | 3.39951700  |
| H  | 0.95038600  | 1.43147600  | 3.39993900  |
| H  | 0.22579300  | 0.20790200  | 4.44114400  |
| H  | 1.18111800  | -0.28246800 | 3.04634800  |
| C  | -1.17275000 | 3.07964800  | 2.50242800  |
| H  | -2.08918400 | 3.58493400  | 2.82184900  |
| H  | -0.47043400 | 3.13314600  | 3.33709300  |
| H  | -0.75264900 | 3.65911900  | 1.67291400  |
| C  | -3.72454700 | 2.15570600  | 0.90608300  |
| H  | -4.15701100 | 1.77983800  | -0.02650200 |
| H  | -4.53486200 | 2.22064800  | 1.64102100  |
| H  | -3.36100400 | 3.17253100  | 0.72993700  |
| C  | -3.90934500 | -0.93895600 | 0.99534800  |
| H  | -3.69200300 | -1.98853600 | 0.79188400  |
| H  | -4.65477000 | -0.90150700 | 1.79928200  |
| H  | -4.36961500 | -0.52049300 | 0.09763700  |
| N  | 0.63823500  | -1.52452700 | 0.09331500  |
| H  | 0.74281800  | -1.79948400 | 1.07293200  |
| C  | 1.86951000  | -1.98461500 | -0.61651900 |
| C  | 3.08623300  | -1.54081000 | 0.20083800  |
| C  | 1.87875500  | -3.51795900 | -0.72701900 |
| C  | 1.93885500  | -1.38063900 | -2.02306700 |
| H  | 3.02656000  | -1.97085700 | 1.21160100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.07014300  | -0.45152700 | 0.30640800  |
| C | 4.38089100  | -1.99679200 | -0.48855200 |
| H | 0.99601500  | -3.85073900 | -1.29183500 |
| H | 1.81496300  | -3.95898000 | 0.27750300  |
| C | 3.16639800  | -3.98246200 | -1.42701300 |
| H | 1.89309300  | -0.28303000 | -1.95764400 |
| H | 1.07366400  | -1.70965000 | -2.61291900 |
| C | 3.23609400  | -1.83083100 | -2.71701300 |
| H | 5.23906300  | -1.66684300 | 0.10702300  |
| C | 4.38040100  | -3.52878700 | -0.60161600 |
| C | 4.45242800  | -1.38085700 | -1.89329300 |
| H | 3.15697900  | -5.07442600 | -1.50317800 |
| C | 3.23471600  | -3.36335000 | -2.83031100 |
| H | 3.27811400  | -1.38532800 | -3.71633600 |
| H | 4.34846500  | -3.98181500 | 0.39685500  |
| H | 5.30550900  | -3.86579600 | -1.08285800 |
| H | 4.48705500  | -0.28628400 | -1.82617900 |
| H | 5.37484600  | -1.70023700 | -2.39155000 |
| H | 4.14421500  | -3.69876900 | -3.34142900 |
| H | 2.38067200  | -3.69570900 | -3.43267400 |
| C | 0.03817900  | 4.03306000  | -3.12719600 |
| C | -0.50021500 | 3.66163500  | -1.73379900 |
| H | 0.72867500  | 4.87925200  | -3.06395700 |
| H | 0.56010400  | 3.19957800  | -3.60379100 |
| H | -0.79687300 | 4.32586800  | -3.76987700 |
| C | -1.52104400 | 2.52671500  | -1.81103100 |
| C | -1.15074000 | 4.91139300  | -1.10803600 |
| H | -1.85625700 | 2.30442600  | -0.78223700 |
| H | -2.42268300 | 2.92751700  | -2.28567400 |
| H | -0.14525100 | -2.09790200 | -0.24017500 |
| H | -1.94107400 | 5.27568200  | -1.77035200 |
| H | -1.59622600 | 4.68571900  | -0.13425900 |
| H | -0.42259300 | 5.71714200  | -0.97605000 |
| C | 0.67332400  | 3.31001800  | -0.86601000 |
| H | 1.46511900  | 4.06940200  | -0.86031500 |
| N | 0.81448200  | 2.25795300  | -0.15106700 |
| C | 2.09303100  | 2.15621600  | 0.61314600  |
| C | 3.29545600  | 2.07071400  | -0.33603500 |
| C | 2.29651600  | 3.28883800  | 1.62508700  |
| H | 2.03143200  | 1.21873000  | 1.18544800  |
| C | 4.60045300  | 1.86832000  | 0.43824700  |
| H | 3.36229400  | 3.00754800  | -0.90429500 |
| H | 3.13673300  | 1.27102400  | -1.06682500 |
| C | 3.59280700  | 3.06750400  | 2.41074900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.35824500  | 4.24763000  | 1.09385200  |
| H | 1.44016600  | 3.35001200  | 2.29979100  |
| C | 4.79919500  | 2.97529500  | 1.47495100  |
| H | 5.44019100  | 1.83783000  | -0.26266200 |
| H | 4.58194000  | 0.89702100  | 0.95150200  |
| H | 3.72531800  | 3.87744900  | 3.13320700  |
| H | 3.50837800  | 2.13687900  | 2.98956200  |
| H | 5.71221800  | 2.79409600  | 2.04899500  |
| H | 4.93083200  | 3.93602600  | 0.96032600  |
| C | -1.05101600 | 1.24777800  | -2.54637900 |
| C | -1.47781500 | -0.06687900 | -1.87055700 |
| H | 0.04692200  | 1.25999500  | -2.60746400 |
| H | -1.39564300 | 1.29299000  | -3.58896400 |
| H | -0.79118700 | -0.85814600 | -2.19990900 |
| C | -2.86086200 | -0.54106600 | -2.11369500 |
| C | -3.94189400 | 0.31529700  | -2.37602600 |
| C | -3.13820100 | -1.91971200 | -2.06749100 |
| C | -5.23830000 | -0.17670500 | -2.52588500 |
| H | -3.77845700 | 1.38456500  | -2.46318000 |
| C | -4.42752600 | -2.41348200 | -2.21696000 |
| H | -2.31474600 | -2.61751300 | -1.91821500 |
| C | -5.49447800 | -1.54132600 | -2.43391200 |
| H | -6.05137900 | 0.51647700  | -2.72052200 |
| H | -4.60106000 | -3.48457100 | -2.17132200 |
| H | -6.50314700 | -1.92282200 | -2.54900000 |

trans-ts-10'

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.26730700 | 0.66207100  | -0.54664800 |
| C  | 2.89208200 | -0.50910400 | 0.01723900  |
| C  | 2.72036500 | -1.59266700 | -0.87175500 |
| C  | 2.01354600 | -1.11953800 | -2.01196700 |
| C  | 1.72920400 | 0.25706600  | -1.81689500 |
| Sc | 0.45560400 | -0.85538200 | -0.03016800 |
| C  | 4.39584400 | 2.66289000  | 0.31655100  |
| C  | 1.74714800 | 2.55985200  | 1.87365000  |
| C  | 1.89852100 | 3.77993600  | -0.94041200 |
| H  | 4.88297400 | 2.51346900  | -0.65184000 |
| H  | 4.86358900 | 1.98806700  | 1.03735400  |
| H  | 4.59874200 | 3.68915100  | 0.63934400  |
| H  | 0.70406900 | 2.22673200  | 1.87384300  |
| H  | 1.76325700 | 3.60827600  | 2.18963200  |
| H  | 2.29076200 | 1.98483300  | 2.63002800  |
| H  | 2.23877800 | 4.72374800  | -0.50034600 |
| H  | 0.81009600 | 3.83506700  | -1.02272600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 2.32135100  | 3.71795200  | -1.94725300 |
| Si | 2.53857500  | 2.39508800  | 0.16532000  |
| C  | 1.05291200  | 1.11923600  | -2.85222600 |
| H  | 0.18027100  | 0.62192800  | -3.29107400 |
| H  | 1.74306000  | 1.34421200  | -3.67274500 |
| H  | 0.71690800  | 2.07068400  | -2.44025900 |
| C  | 1.82004900  | -1.90369800 | -3.27883800 |
| H  | 1.37365700  | -2.89106100 | -3.11335800 |
| H  | 2.79075200  | -2.07536700 | -3.75592500 |
| H  | 1.19923400  | -1.36621500 | -4.00002200 |
| C  | 3.27460200  | -2.97858500 | -0.71753800 |
| H  | 3.46612000  | -3.22530200 | 0.32973200  |
| H  | 4.22569700  | -3.07321100 | -1.25283800 |
| H  | 2.60187700  | -3.73825100 | -1.12960400 |
| C  | 3.70897300  | -0.57855700 | 1.28019800  |
| H  | 3.43113800  | 0.19802800  | 1.99791700  |
| H  | 4.77238800  | -0.45039600 | 1.05317200  |
| H  | 3.59738700  | -1.54495100 | 1.78116200  |
| C  | 0.07460600  | -0.19798800 | 4.20410900  |
| C  | -0.52966600 | -1.00014900 | 3.02744400  |
| H  | -0.71281900 | 0.22793100  | 4.83399300  |
| H  | 0.70903700  | 0.61665900  | 3.84403500  |
| H  | 0.68075500  | -0.86466700 | 4.82361100  |
| C  | 0.61383000  | -1.52531600 | 2.14656200  |
| C  | -1.41371300 | -2.11104000 | 3.62679900  |
| H  | 1.24260300  | -2.20772000 | 2.72126900  |
| H  | 1.28272700  | -0.65453900 | 1.94669200  |
| H  | -0.78401500 | -2.87768700 | 4.08799200  |
| H  | -2.05958400 | -2.58850100 | 2.88563200  |
| H  | -2.06387000 | -1.69671800 | 4.40208000  |
| C  | -1.42726400 | -0.06603100 | 2.26777400  |
| H  | -2.28195000 | 0.34236500  | 2.81641200  |
| N  | -1.22729500 | 0.23208500  | 1.04312500  |
| C  | -2.14590000 | 1.10507300  | 0.28934700  |
| C  | -1.39047500 | 2.35249100  | -0.16997900 |
| C  | -3.45105600 | 1.48050400  | 0.98187900  |
| H  | -2.40181500 | 0.52398100  | -0.60763500 |
| C  | -2.25042900 | 3.16609200  | -1.13804600 |
| H  | -1.13175300 | 2.96084200  | 0.70775100  |
| H  | -0.44406500 | 2.05663400  | -0.64005200 |
| C  | -4.32045400 | 2.29394900  | 0.01641100  |
| H  | -3.24115300 | 2.08362600  | 1.87592300  |
| H  | -3.98411700 | 0.57777000  | 1.30440000  |
| C  | -3.58562800 | 3.53794400  | -0.48884500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.71179800 | 4.06484200  | -1.45432900 |
| H | -2.43571800 | 2.56760500  | -2.04113300 |
| H | -5.25383900 | 2.57567000  | 0.51147100  |
| H | -4.59122700 | 1.65797300  | -0.83738400 |
| H | -4.21344800 | 4.08416600  | -1.19855300 |
| H | -3.39700300 | 4.21339000  | 0.35594700  |
| C | 0.04853300  | -3.20098000 | 0.85362100  |
| C | -0.24486700 | -2.95630700 | -0.49371500 |
| H | -0.74242700 | -3.35583300 | 1.57594800  |
| H | 0.95443700  | -3.76014200 | 1.06526200  |
| H | 0.47546000  | -3.25650600 | -1.24588700 |
| C | -1.50011200 | -2.35788100 | -0.97414200 |
| C | -2.69331600 | -2.36331800 | -0.22100200 |
| C | -1.51070100 | -1.68484800 | -2.21357700 |
| C | -3.84697600 | -1.76968100 | -0.71056100 |
| H | -2.72348000 | -2.88443200 | 0.73116100  |
| C | -2.67610500 | -1.08803400 | -2.70311500 |
| H | -0.61457100 | -1.69053500 | -2.82670100 |
| C | -3.84779800 | -1.13314200 | -1.95757800 |
| H | -4.76204800 | -1.81674600 | -0.12857100 |
| H | -2.66196500 | -0.60413700 | -3.67455600 |
| H | -4.75950600 | -0.68693000 | -2.34028500 |

cis-ts-10'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.43526000  | -0.14142100 | -2.37555700 |
| C  | 1.60772800  | 0.65607400  | -2.38476200 |
| C  | 2.56508900  | 0.04849400  | -1.51976800 |
| C  | 1.99443000  | -1.14187300 | -1.01017100 |
| C  | 0.65448000  | -1.26476600 | -1.50751500 |
| Sc | 0.65426300  | 0.71923600  | -0.07018100 |
| C  | 2.73742100  | -2.17640400 | -0.21640700 |
| H  | 3.50267800  | -1.72621800 | 0.41633000  |
| H  | 3.24159500  | -2.87246200 | -0.89643200 |
| H  | 2.07422000  | -2.75787000 | 0.42903600  |
| C  | 3.97559900  | 0.52879800  | -1.32467100 |
| H  | 4.03084300  | 1.62137200  | -1.26688600 |
| H  | 4.60478700  | 0.22189700  | -2.16732300 |
| H  | 4.41709700  | 0.11894600  | -0.41333200 |
| C  | 1.88276200  | 1.86117200  | -3.23686800 |
| H  | 0.96711700  | 2.29532600  | -3.64585700 |
| H  | 2.51653800  | 1.58361200  | -4.08541700 |
| H  | 2.40668900  | 2.64460600  | -2.68034000 |
| C  | -1.93812100 | 4.08908700  | -1.41964700 |
| C  | -1.20491400 | 3.37603400  | -0.26034300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.95757600 | 4.36941000  | -1.13470000 |
| H | -1.98759400 | 3.45261700  | -2.30813500 |
| H | -1.39457900 | 5.00108000  | -1.68072500 |
| C | 0.18768800  | 2.94394300  | -0.73887700 |
| C | -1.21903100 | 4.32324300  | 0.95649700  |
| H | 0.77365000  | 3.80701700  | -1.05939700 |
| H | 0.02524000  | 2.36360400  | -1.65776200 |
| H | -0.61759800 | 5.21147600  | 0.73892000  |
| H | -0.83550500 | 3.85410500  | 1.86635800  |
| H | -2.23989200 | 4.65808100  | 1.16153700  |
| C | -2.03512200 | 2.18191200  | 0.11090700  |
| H | -3.08603500 | 2.38996900  | 0.34338300  |
| N | -1.58964200 | 0.98519200  | 0.17534000  |
| C | -2.51818900 | -0.08904500 | 0.60193200  |
| C | -3.85009500 | -0.10479600 | -0.15524800 |
| C | -2.76401500 | -0.01539800 | 2.11350300  |
| H | -2.00306800 | -1.03270000 | 0.38382100  |
| C | -4.68432300 | -1.30827000 | 0.29565600  |
| H | -4.41653300 | 0.80975800  | 0.05956900  |
| H | -3.67016400 | -0.12534800 | -1.23613100 |
| C | -3.61659400 | -1.19732600 | 2.57995000  |
| H | -3.27975400 | 0.92976200  | 2.33521200  |
| H | -1.81055900 | 0.01162900  | 2.65280200  |
| C | -4.93398500 | -1.26700900 | 1.80477900  |
| H | -5.63120300 | -1.32381300 | -0.25093000 |
| H | -4.15489100 | -2.23623000 | 0.03960300  |
| H | -3.80459400 | -1.11485200 | 3.65415400  |
| H | -3.05308600 | -2.12703600 | 2.42497700  |
| H | -5.50859600 | -2.14389000 | 2.11603000  |
| H | -5.54164000 | -0.38520700 | 2.04645100  |
| C | 1.49230900  | 2.80758200  | 0.96888500  |
| C | 1.15850700  | 1.82663000  | 1.90686800  |
| H | 1.18516800  | 3.83437200  | 1.10807200  |
| H | 2.44789100  | 2.72348100  | 0.44277900  |
| H | 0.25811100  | 1.95984300  | 2.50422700  |
| C | 1.97016100  | 0.64458400  | 2.22176200  |
| C | 1.33775400  | -0.52860200 | 2.68313100  |
| C | 3.37991200  | 0.64289900  | 2.13702200  |
| C | 2.08116400  | -1.63106600 | 3.10861800  |
| H | 0.25443300  | -0.54335400 | 2.79248200  |
| C | 4.11241800  | -0.45297700 | 2.56753200  |
| H | 3.89593700  | 1.53999600  | 1.80679400  |
| C | 3.46851600  | -1.59025000 | 3.06762200  |
| H | 1.56843500  | -2.51057500 | 3.48520200  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.19678900  | -0.41588500 | 2.53572800  |
| H  | 4.05134400  | -2.43585200 | 3.41619800  |
| C  | -0.80764000 | 0.15380700  | -3.17042800 |
| H  | -0.92666500 | 1.22728500  | -3.35069500 |
| H  | -0.77193800 | -0.33267200 | -4.15125900 |
| H  | -1.70648400 | -0.19758000 | -2.65995200 |
| Si | -0.34531200 | -2.85020100 | -1.28463600 |
| C  | -2.02566500 | -2.77640700 | -2.12701900 |
| H  | -2.69331100 | -2.01499900 | -1.71660800 |
| H  | -1.92789500 | -2.60008100 | -3.20199400 |
| H  | -2.51560100 | -3.74725500 | -1.99382700 |
| C  | -0.57592800 | -3.21843100 | 0.56529300  |
| H  | -1.60611700 | -3.52396600 | 0.77813100  |
| H  | 0.08095000  | -4.03236700 | 0.88768900  |
| H  | -0.34543500 | -2.34578200 | 1.18802800  |
| C  | 0.60430700  | -4.26300100 | -2.08548800 |
| H  | 1.57060400  | -4.43891100 | -1.60627300 |
| H  | 0.02335000  | -5.18842500 | -2.01660200 |
| H  | 0.78386100  | -4.05670500 | -3.14473700 |

trans-11'

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.43998600 | 0.45791100  | -0.27637300 |
| C  | 2.64039200 | -0.90083100 | 0.13819700  |
| C  | 2.45145500 | -1.75771800 | -0.97678900 |
| C  | 2.15776900 | -0.94308400 | -2.10559400 |
| C  | 2.13665800 | 0.41351400  | -1.68094500 |
| Sc | 0.29384500 | -0.63425700 | -0.48154700 |
| C  | 4.67565600 | 1.86532600  | 1.23456100  |
| C  | 1.85667400 | 1.80608100  | 2.46320600  |
| C  | 2.49163500 | 3.58958700  | 0.03059700  |
| H  | 5.26977400 | 1.91745400  | 0.31756500  |
| H  | 4.95106900 | 0.94956100  | 1.76475300  |
| H  | 4.95499100 | 2.71433700  | 1.86666900  |
| H  | 0.92501100 | 1.24209600  | 2.34293600  |
| H  | 1.59538900 | 2.80605900  | 2.82532400  |
| H  | 2.44486000 | 1.32088300  | 3.24842200  |
| H  | 2.83390200 | 4.37068800  | 0.71818400  |
| H  | 1.43310700 | 3.77419900  | -0.17061600 |
| H  | 3.04691400 | 3.70808400  | -0.90387700 |
| Si | 2.83714700 | 1.92749300  | 0.84350000  |
| C  | 1.87972100 | 1.58929300  | -2.58817400 |
| H  | 1.25926000 | 1.30662700  | -3.44361800 |
| H  | 2.81927600 | 1.98706800  | -2.98649300 |
| H  | 1.37596900 | 2.40919100  | -2.07091500 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.98951900  | -1.46016500 | -3.50658200 |
| H | 1.35695400  | -2.35393600 | -3.54294800 |
| H | 2.96185300  | -1.73862200 | -3.92565700 |
| H | 1.55454100  | -0.71166100 | -4.17327000 |
| C | 2.63436600  | -3.24781500 | -0.98358600 |
| H | 2.22232400  | -3.71170200 | -0.08111500 |
| H | 3.69703300  | -3.50890200 | -1.02945100 |
| H | 2.14668000  | -3.70712200 | -1.84712400 |
| C | 3.12937300  | -1.36311700 | 1.48531400  |
| H | 2.78041500  | -0.72035900 | 2.29816900  |
| H | 4.22442500  | -1.35634700 | 1.50772300  |
| H | 2.81329200  | -2.38715600 | 1.70294200  |
| C | -0.32072000 | -1.43851800 | 3.85958000  |
| C | -1.15523000 | -1.84436400 | 2.62564600  |
| H | -0.89678200 | -0.79802500 | 4.53406300  |
| H | 0.58572800  | -0.90038600 | 3.56407200  |
| H | -0.02864400 | -2.33559400 | 4.41284600  |
| C | -0.25899900 | -2.65207800 | 1.66765700  |
| C | -2.35163400 | -2.68629800 | 3.10137100  |
| H | 0.20098200  | -3.43078900 | 2.28741400  |
| H | 0.61387800  | -2.02720500 | 1.39145700  |
| H | -1.99668500 | -3.64750500 | 3.48324600  |
| H | -3.07040200 | -2.88121100 | 2.30087600  |
| H | -2.88077000 | -2.17565200 | 3.91102900  |
| C | -1.70169300 | -0.56443800 | 2.05314400  |
| H | -2.54819800 | -0.14237500 | 2.60372800  |
| N | -1.25001700 | 0.03984900  | 1.02500300  |
| C | -1.92022400 | 1.24504700  | 0.48370200  |
| C | -0.88001200 | 2.33287400  | 0.20771600  |
| C | -3.10207300 | 1.79324100  | 1.27694900  |
| H | -2.31032200 | 0.92077000  | -0.49063100 |
| C | -1.51351700 | 3.49921700  | -0.55250500 |
| H | -0.44816300 | 2.68122900  | 1.15497800  |
| H | -0.03937000 | 1.92846300  | -0.38460400 |
| C | -3.72847700 | 2.96923500  | 0.51930600  |
| H | -2.76555900 | 2.12367300  | 2.26973100  |
| H | -3.85629800 | 1.01126300  | 1.42181800  |
| C | -2.70240000 | 4.06404000  | 0.22697900  |
| H | -0.76644100 | 4.27744600  | -0.73629700 |
| H | -1.85557500 | 3.14104900  | -1.53341400 |
| H | -4.56599900 | 3.37020400  | 1.09641300  |
| H | -4.14177800 | 2.59651200  | -0.42773200 |
| H | -3.16827600 | 4.87926400  | -0.33350400 |
| H | -2.34419600 | 4.48979400  | 1.17326000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.87794200 | -3.32823000 | 0.40861600  |
| C | -0.68990200 | -2.55713900 | -0.89176100 |
| H | -1.92679800 | -3.57555300 | 0.60613700  |
| H | -0.37859200 | -4.29401700 | 0.29530800  |
| H | -0.10534700 | -3.08188100 | -1.64853200 |
| C | -1.74535000 | -1.73149400 | -1.47499600 |
| C | -3.06659500 | -1.60682700 | -0.97878100 |
| C | -1.36699500 | -0.82490100 | -2.50097100 |
| C | -3.95524700 | -0.69665200 | -1.52470000 |
| H | -3.40055500 | -2.26667600 | -0.18331000 |
| C | -2.26884100 | 0.10912500  | -3.03780400 |
| H | -0.39407700 | -0.94411800 | -2.98058900 |
| C | -3.56501500 | 0.17577900  | -2.55523400 |
| H | -4.97296600 | -0.65566900 | -1.14767100 |
| H | -1.94679400 | 0.75822300  | -3.84636900 |
| H | -4.27374700 | 0.88428100  | -2.96935300 |

cis-11'

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -0.55466600 | 2.28556500 | -0.24319300 |
| C  | 0.73410700  | 2.38045400 | 0.39064600  |
| C  | 1.73949700  | 2.01979100 | -0.54626300 |
| C  | 1.08932200  | 1.65973400 | -1.76001900 |
| C  | -0.31290800 | 1.83784200 | -1.58096600 |
| Sc | 0.30904900  | 0.04263900 | -0.08383100 |
| C  | -1.93839100 | 4.57928000 | 1.24391000  |
| C  | -2.63478200 | 1.67078400 | 1.97817800  |
| C  | -3.60208700 | 2.91630700 | -0.65909700 |
| H  | -1.58960300 | 5.25361500 | 0.45597000  |
| H  | -1.22283500 | 4.62372400 | 2.06835100  |
| H  | -2.89600600 | 4.96115600 | 1.61184700  |
| H  | -2.72986800 | 0.63532800 | 1.63101400  |
| H  | -3.59851400 | 1.96556500 | 2.40664500  |
| H  | -1.89766200 | 1.69768200 | 2.78864400  |
| H  | -4.43271500 | 3.43081900 | -0.16422000 |
| H  | -3.97311600 | 1.94139900 | -0.98612200 |
| H  | -3.33824500 | 3.49709400 | -1.54736200 |
| Si | -2.17317600 | 2.84099100 | 0.56557000  |
| C  | -1.32894000 | 1.61802500 | -2.67242300 |
| H  | -0.96354200 | 0.90392100 | -3.41606600 |
| H  | -1.53318800 | 2.55460800 | -3.20214000 |
| H  | -2.28274600 | 1.24952000 | -2.28898700 |
| C  | 1.77171500  | 1.25091700 | -3.03609100 |
| H  | 2.77661700  | 0.86938200 | -2.84393500 |
| H  | 1.85687500  | 2.10560200 | -3.71530200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.21732600  | 0.47202300  | -3.56940200 |
| C | 3.21932100  | 2.12780800  | -0.33307800 |
| H | 3.50307700  | 1.87746400  | 0.69272100  |
| H | 3.54689200  | 3.15592000  | -0.52322300 |
| H | 3.78055700  | 1.46380900  | -0.99438400 |
| C | 1.01464900  | 2.88842300  | 1.78015100  |
| H | 0.18204200  | 2.70232800  | 2.46441800  |
| H | 1.18990900  | 3.96937200  | 1.76400000  |
| H | 1.90996000  | 2.42578000  | 2.20569300  |
| C | -1.45742600 | -1.65107900 | 3.75033400  |
| C | -0.38163300 | -1.90019900 | 2.66877100  |
| H | -2.14452200 | -2.49802900 | 3.83033100  |
| H | -2.03958500 | -0.75075200 | 3.53112300  |
| H | -0.96835300 | -1.52239800 | 4.71954800  |
| C | 0.49075100  | -0.63094600 | 2.54475800  |
| C | 0.45722400  | -3.12250900 | 3.07864500  |
| H | 0.63478800  | -0.24175300 | 3.55855800  |
| H | -0.13141000 | 0.18353100  | 2.10429500  |
| H | 0.99485400  | -2.90203200 | 4.00542300  |
| H | 1.18677700  | -3.39745200 | 2.31209600  |
| H | -0.19111900 | -3.98344400 | 3.26416100  |
| C | -1.15736300 | -2.25651800 | 1.42836200  |
| H | -1.75913000 | -3.16711600 | 1.51515100  |
| N | -1.19373500 | -1.56811400 | 0.35422000  |
| C | -2.09313900 | -1.93493500 | -0.76264000 |
| C | -3.33819600 | -1.04674800 | -0.69360700 |
| C | -2.47893700 | -3.40924600 | -0.86933900 |
| H | -1.54749000 | -1.67006100 | -1.68442000 |
| C | -4.22351800 | -1.26053100 | -1.92264500 |
| H | -3.88864400 | -1.30144800 | 0.22366200  |
| H | -3.03726900 | 0.00336700  | -0.60338100 |
| C | -3.33987900 | -3.61915400 | -2.12108000 |
| H | -3.06842700 | -3.70527300 | 0.00732600  |
| H | -1.58170000 | -4.03770200 | -0.89630100 |
| C | -4.59019200 | -2.73768000 | -2.08396300 |
| H | -5.12418300 | -0.64524100 | -1.83986800 |
| H | -3.68454100 | -0.91814600 | -2.81696000 |
| H | -3.61698000 | -4.67378100 | -2.19857400 |
| H | -2.74739500 | -3.38042200 | -3.01388300 |
| H | -5.17965300 | -2.88244700 | -2.99345600 |
| H | -5.22232400 | -3.04573000 | -1.24119600 |
| C | 1.91405900  | -0.76917300 | 1.93891500  |
| C | 2.01919100  | -1.15079600 | 0.45535100  |
| H | 2.45093500  | -1.48045500 | 2.58228600  |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 2.41612000 | 0.19534100  | 2.09463400  |
| H | 1.56744800 | -2.14763400 | 0.29668200  |
| C | 3.38558900 | -1.13079200 | -0.13178300 |
| C | 3.54980400 | -1.43321700 | -1.49478700 |
| C | 4.53364200 | -0.79278000 | 0.59683500  |
| C | 4.79315500 | -1.36958400 | -2.10983800 |
| H | 2.67411600 | -1.70723200 | -2.08294300 |
| C | 5.78280000 | -0.72044400 | -0.01948500 |
| H | 4.46200900 | -0.57336000 | 1.65789000  |
| C | 5.92074800 | -1.00027000 | -1.37423400 |
| H | 4.88451700 | -1.60256400 | -3.16641700 |
| H | 6.65267600 | -0.44558500 | 0.56905900  |
| H | 6.89272800 | -0.94075300 | -1.85203400 |

trans-ts-10<sup>R</sup>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.85562700  | 0.20235100  | 1.33324900  |
| C  | 2.15151300  | -0.83756500 | 2.02505300  |
| C  | 1.28042900  | -0.24074000 | 2.97601600  |
| C  | 1.44439400  | 1.16830400  | 2.89876700  |
| C  | 2.39035900  | 1.44315400  | 1.88553800  |
| Sc | 0.45529300  | 0.38929800  | 0.68850100  |
| C  | 5.15329800  | -1.65333800 | 0.24531300  |
| C  | 4.27436700  | 0.83072100  | -1.40787200 |
| C  | 5.76908500  | 1.09621600  | 1.23103200  |
| H  | 5.28804800  | -2.05019700 | 1.25656300  |
| H  | 4.57886500  | -2.38349700 | -0.32800500 |
| H  | 6.14602300  | -1.58597000 | -0.21282200 |
| H  | 4.13466000  | 1.91638600  | -1.35955700 |
| H  | 5.18888500  | 0.64594400  | -1.98162400 |
| H  | 3.43559300  | 0.40901300  | -1.96850200 |
| H  | 6.74609200  | 0.91057100  | 0.77275300  |
| H  | 5.58665200  | 2.17251700  | 1.19434200  |
| H  | 5.82979000  | 0.79682700  | 2.28189900  |
| Si | 4.45181000  | 0.09686200  | 0.32544500  |
| C  | 2.90690500  | 2.82071900  | 1.57121800  |
| H  | 2.12351300  | 3.58014800  | 1.66310400  |
| H  | 3.70235500  | 3.10377300  | 2.26926900  |
| H  | 3.31712500  | 2.88819400  | 0.55951800  |
| C  | 0.86128100  | 2.17380000  | 3.84861300  |
| H  | 1.60868600  | 2.45704900  | 4.59757100  |
| H  | 0.54600900  | 3.09475600  | 3.34692800  |
| H  | -0.00131100 | 1.77099800  | 4.38626300  |
| C  | 0.40365500  | -0.94445700 | 3.97446700  |
| H  | 0.38446200  | -2.02610700 | 3.80883900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.77737000  | -0.79232800 | 4.99218300  |
| H | -0.62861600 | -0.57304000 | 3.95323900  |
| C | 2.35520400  | -2.32268500 | 1.87546100  |
| H | 2.78035000  | -2.57852300 | 0.90320100  |
| H | 3.04326000  | -2.70023100 | 2.63982200  |
| H | 1.42121800  | -2.88529300 | 1.99115300  |
| N | -0.90818600 | -1.54218800 | 0.99195700  |
| H | -0.46583700 | -2.23209100 | 0.38011700  |
| C | -2.38785400 | -1.70094000 | 0.81864600  |
| C | -2.75216600 | -3.18641600 | 0.63293200  |
| C | -3.09615500 | -1.19759300 | 2.08485700  |
| C | -2.85938900 | -0.92297000 | -0.41760300 |
| H | -2.40616100 | -3.75797300 | 1.50499900  |
| H | -2.23650300 | -3.59042200 | -0.25006200 |
| C | -4.27324800 | -3.34202100 | 0.46525200  |
| H | -2.82031900 | -0.16044400 | 2.29618900  |
| H | -2.76263200 | -1.80305400 | 2.94021200  |
| C | -4.61791900 | -1.32858000 | 1.91810700  |
| H | -2.35746100 | -1.30830400 | -1.31475400 |
| H | -2.58030200 | 0.13267700  | -0.33155900 |
| C | -4.38111700 | -1.05902700 | -0.57036300 |
| H | -4.51027200 | -4.40205400 | 0.32790500  |
| C | -4.97956700 | -2.80692000 | 1.71932700  |
| C | -4.73506500 | -2.54118400 | -0.76164300 |
| H | -5.10841600 | -0.94307500 | 2.81768500  |
| C | -5.06783400 | -0.51781600 | 0.69302400  |
| H | -4.70411900 | -0.48308100 | -1.44457900 |
| H | -4.68110700 | -3.38882500 | 2.59957500  |
| H | -6.06467500 | -2.91593400 | 1.60949700  |
| H | -4.25391800 | -2.92744600 | -1.66911900 |
| H | -5.81722000 | -2.65419800 | -0.89332300 |
| H | -6.15621300 | -0.58338500 | 0.58268000  |
| H | -4.82149300 | 0.54352900  | 0.83447000  |
| C | -1.09092700 | 1.75291800  | -2.78234800 |
| C | 0.36999600  | 1.56017200  | -2.32810800 |
| H | -1.23648800 | 1.29699300  | -3.76773900 |
| H | -1.79588800 | 1.29532300  | -2.08296200 |
| H | -1.32641400 | 2.81720800  | -2.86356500 |
| C | 0.71712300  | 2.10544100  | -0.92773200 |
| C | 1.27914400  | 2.24714800  | -3.37131500 |
| H | 1.70949000  | 1.69232500  | -0.65243300 |
| H | 0.90633600  | 3.17279200  | -1.00893000 |
| H | -0.68872300 | -1.86912300 | 1.93570200  |
| H | 1.04174900  | 3.31440600  | -3.39572600 |

|                        |             |             |             |
|------------------------|-------------|-------------|-------------|
| H                      | 2.33702100  | 2.13404500  | -3.11903300 |
| H                      | 1.11266900  | 1.83936800  | -4.37400800 |
| C                      | 0.62996300  | 0.08481800  | -2.40109900 |
| H                      | 0.68390900  | -0.34579500 | -3.40892400 |
| N                      | 0.78190700  | -0.65188800 | -1.36971100 |
| C                      | 1.09423400  | -2.08566500 | -1.57823200 |
| C                      | -0.00237900 | -2.85064200 | -2.32571800 |
| C                      | 2.44588200  | -2.27909600 | -2.27204800 |
| H                      | 1.19374100  | -2.52263700 | -0.57567900 |
| C                      | 0.34448500  | -4.34053300 | -2.39250700 |
| H                      | -0.09690200 | -2.44919600 | -3.34303200 |
| H                      | -0.97065400 | -2.70261400 | -1.83715000 |
| C                      | 2.80057300  | -3.76570500 | -2.34317000 |
| H                      | 2.39364700  | -1.86167600 | -3.28697800 |
| H                      | 3.21645000  | -1.72221000 | -1.73453100 |
| C                      | 1.70566200  | -4.56257000 | -3.05511600 |
| H                      | -0.44042000 | -4.87783600 | -2.93199700 |
| H                      | 0.36518100  | -4.74858700 | -1.37200200 |
| H                      | 3.76209100  | -3.89114500 | -2.84911500 |
| H                      | 2.92892800  | -4.15480500 | -1.32268000 |
| H                      | 1.95412000  | -5.62753800 | -3.06014200 |
| H                      | 1.65167300  | -4.24228500 | -4.10370300 |
| C                      | -0.70763600 | 2.74462900  | 0.59739500  |
| C                      | -1.25294900 | 1.71575700  | 1.40944200  |
| H                      | 0.10173200  | 3.31541700  | 1.05322000  |
| H                      | -2.24907400 | 1.37435100  | 1.16085300  |
| H                      | -1.06172800 | 1.76661200  | 2.47554000  |
| C                      | -1.55254200 | 3.58582600  | -0.30447600 |
| C                      | -1.02792000 | 4.77134500  | -0.83429000 |
| C                      | -2.88034700 | 3.25913200  | -0.59777100 |
| C                      | -1.78595700 | 5.57841900  | -1.67576200 |
| H                      | -0.01313400 | 5.06909300  | -0.58092800 |
| C                      | -3.63963900 | 4.05929600  | -1.44461600 |
| H                      | -3.33329100 | 2.36770500  | -0.17544700 |
| C                      | -3.09247200 | 5.21537800  | -1.99638500 |
| H                      | -1.35970100 | 6.49256600  | -2.07527700 |
| H                      | -4.66478600 | 3.78301500  | -1.66855700 |
| H                      | -3.68702400 | 5.84001900  | -2.65454700 |
| cis-ts-10 <sup>R</sup> |             |             |             |
| C                      | 2.00927600  | 1.47340000  | -1.44122000 |
| C                      | 0.78898200  | 1.58981200  | -2.18349600 |
| C                      | 0.57666900  | 0.38071600  | -2.89629300 |
| C                      | 1.65920200  | -0.49374800 | -2.61806700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.52561500  | 0.15988400  | -1.70832700 |
| Sc | 0.43897000  | -0.16508300 | -0.43329000 |
| C  | 2.45373000  | 4.57166000  | -1.18880600 |
| C  | 3.31421800  | 2.73838100  | 1.14981800  |
| C  | 4.78521400  | 2.73180700  | -1.52208100 |
| H  | 2.29214400  | 4.63821000  | -2.26933900 |
| H  | 1.54034300  | 4.90394900  | -0.69094900 |
| H  | 3.24216400  | 5.28749600  | -0.93192200 |
| H  | 3.87030800  | 1.83406400  | 1.42043900  |
| H  | 3.89519700  | 3.59827200  | 1.49987300  |
| H  | 2.36472100  | 2.73026600  | 1.69393600  |
| H  | 5.35872100  | 3.63661600  | -1.29634900 |
| H  | 5.36327200  | 1.87599700  | -1.16689600 |
| H  | 4.69695600  | 2.65368300  | -2.61024500 |
| Si | 3.08343200  | 2.85498300  | -0.72011000 |
| C  | 3.81035900  | -0.42168100 | -1.18075000 |
| H  | 3.70925100  | -1.48888700 | -0.95997200 |
| H  | 4.62325700  | -0.30933700 | -1.90629700 |
| H  | 4.12296000  | 0.06959600  | -0.25453700 |
| C  | 1.92439800  | -1.77682000 | -3.34693500 |
| H  | 1.01742800  | -2.37267900 | -3.48962400 |
| H  | 2.32656500  | -1.55935100 | -4.34288900 |
| H  | 2.66672000  | -2.38838800 | -2.82966500 |
| C  | -0.50994300 | 0.09154900  | -3.89381900 |
| H  | -1.29317000 | 0.85642600  | -3.88301000 |
| H  | -0.10275400 | 0.07813600  | -4.91053400 |
| H  | -0.97603800 | -0.88684000 | -3.72588100 |
| C  | -0.07787100 | 2.81310200  | -2.32382400 |
| H  | 0.05768400  | 3.50475300  | -1.49089200 |
| H  | 0.16463600  | 3.35776000  | -3.24316500 |
| H  | -1.14427300 | 2.56296300  | -2.38013000 |
| N  | -1.90125400 | 0.04144100  | -0.92910800 |
| H  | -2.10952300 | 0.93901600  | -0.48763400 |
| C  | -3.07216900 | -0.84381500 | -0.63487400 |
| C  | -4.38554000 | -0.04337300 | -0.73701300 |
| C  | -3.13367000 | -1.97065400 | -1.67515900 |
| C  | -2.95621600 | -1.40470800 | 0.78981300  |
| H  | -4.47326100 | 0.38120900  | -1.74635000 |
| H  | -4.36406300 | 0.79760200  | -0.02897600 |
| C  | -5.58914700 | -0.95304000 | -0.43583900 |
| H  | -2.19945000 | -2.53931800 | -1.70229300 |
| H  | -3.26544800 | -1.52335300 | -2.67090700 |
| C  | -4.31680400 | -2.90169600 | -1.36434200 |
| H  | -2.94035500 | -0.57411500 | 1.50921900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.01087600 | -1.94609800 | 0.91550600  |
| C | -4.14455100 | -2.33415300 | 1.08027100  |
| H | -6.50880300 | -0.36332800 | -0.50758000 |
| C | -5.62438100 | -2.10250800 | -1.45262700 |
| C | -5.44856000 | -1.52928000 | 0.98068100  |
| H | -4.32887100 | -3.71711400 | -2.09469600 |
| C | -4.15539900 | -3.47564600 | 0.05209400  |
| H | -4.03796100 | -2.74587500 | 2.08937100  |
| H | -5.75650500 | -1.70680200 | -2.46673400 |
| H | -6.47835400 | -2.75679900 | -1.24350500 |
| H | -5.44872200 | -0.71976500 | 1.72163200  |
| H | -6.30446000 | -2.17587200 | 1.20514200  |
| H | -4.98066600 | -4.16303600 | 0.26983000  |
| H | -3.22462700 | -4.05361100 | 0.12111200  |
| C | 0.03006000  | -1.08326300 | 3.48524900  |
| C | 0.96796600  | -0.07086600 | 2.79220800  |
| H | -0.40245300 | -0.64060800 | 4.38800500  |
| H | -0.79364600 | -1.38838000 | 2.83281100  |
| H | 0.58515200  | -1.97420800 | 3.79271900  |
| C | 1.67767800  | -0.59494400 | 1.53101500  |
| C | 2.01210400  | 0.39292100  | 3.82949400  |
| H | 2.08420700  | 0.29029800  | 0.99605900  |
| H | 2.57202500  | -1.14178100 | 1.81539100  |
| H | -1.93097500 | 0.24409700  | -1.93095000 |
| H | 2.60459200  | -0.46839700 | 4.15083400  |
| H | 2.69283400  | 1.13522500  | 3.40536200  |
| H | 1.53248300  | 0.82326500  | 4.71511300  |
| C | 0.09714400  | 1.09718100  | 2.44069300  |
| H | -0.23623600 | 1.72790200  | 3.27435400  |
| N | -0.26270600 | 1.35186100  | 1.24324500  |
| C | -1.10456400 | 2.55181800  | 1.02750400  |
| C | -2.45039800 | 2.48905600  | 1.75594600  |
| C | -0.36321800 | 3.84389600  | 1.37804300  |
| H | -1.30264700 | 2.59714000  | -0.05026100 |
| C | -3.30987400 | 3.69737000  | 1.37312500  |
| H | -2.27866700 | 2.48967400  | 2.83994000  |
| H | -2.97083600 | 1.55317200  | 1.52214500  |
| C | -1.21405000 | 5.05982500  | 1.00204200  |
| H | -0.14844500 | 3.85988600  | 2.45530900  |
| H | 0.59983400  | 3.86094000  | 0.85895200  |
| C | -2.58417300 | 5.00833700  | 1.68312900  |
| H | -4.26678300 | 3.65303000  | 1.90083100  |
| H | -3.53806200 | 3.65121200  | 0.29854200  |
| H | -0.68399700 | 5.97827000  | 1.26978800  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.35024100 | 5.07977000  | -0.08868000 |
| H | -3.19374100 | 5.86063500  | 1.37011500  |
| H | -2.44958900 | 5.09508800  | 2.76924000  |
| C | 0.99526300  | -2.53359200 | 0.70546300  |
| C | 0.28765100  | -2.44768200 | -0.51421700 |
| H | 0.38793300  | -2.60028900 | 1.60222100  |
| H | -0.78459400 | -2.57902200 | -0.44425500 |
| C | 2.27591800  | -3.29454300 | 0.84178000  |
| C | 2.92299900  | -3.86817000 | -0.25651400 |
| C | 2.80291700  | -3.53557500 | 2.11785900  |
| C | 4.08273600  | -4.62067100 | -0.08936500 |
| H | 2.51040400  | -3.75427200 | -1.25210400 |
| C | 3.95374900  | -4.29381700 | 2.29102800  |
| H | 2.30168600  | -3.12150400 | 2.98929300  |
| C | 4.60527500  | -4.83186200 | 1.18280200  |
| H | 4.56908800  | -5.05450700 | -0.95682200 |
| H | 4.34007100  | -4.46793700 | 3.28977800  |
| H | 5.50588200  | -5.42277700 | 1.31234300  |
| H | 0.73030200  | -2.84514900 | -1.41842900 |

trans-ts-12

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -1.16691300 | 2.40957300 | -1.21721400 |
| C  | -2.19306400 | 2.49441700 | -0.22610700 |
| C  | -3.17537400 | 1.50467900 | -0.48813900 |
| C  | -2.79023400 | 0.80736400 | -1.67145300 |
| C  | -1.55931200 | 1.35354400 | -2.11411100 |
| Sc | -1.05675700 | 0.27500800 | 0.08040100  |
| C  | 1.15108100  | 4.27709400 | -0.09769700 |
| C  | 1.25294100  | 3.41911500 | -2.97810400 |
| C  | -0.97565000 | 5.29972400 | -2.05601500 |
| H  | 0.60497600  | 4.50209200 | 0.82242000  |
| H  | 1.91234000  | 3.52191800 | 0.12789800  |
| H  | 1.69528900  | 5.18590100 | -0.37830700 |
| H  | 0.74657100  | 3.27885000 | -3.93559000 |
| H  | 1.91838800  | 4.28347300 | -3.08106200 |
| H  | 1.89429700  | 2.54887900 | -2.79960300 |
| H  | -0.33616000 | 6.14749500 | -2.31999100 |
| H  | -1.60218700 | 5.06336200 | -2.92128600 |
| H  | -1.63410700 | 5.61259400 | -1.24036000 |
| Si | 0.05969300  | 3.80878800 | -1.56987600 |
| C  | -0.91206800 | 1.00269100 | -3.42832100 |
| H  | -1.30313900 | 0.06152900 | -3.81995600 |
| H  | -1.12116800 | 1.78044400 | -4.17105300 |
| H  | 0.17750900  | 0.90688500 | -3.37179900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.60523900 | -0.22483900 | -2.40093600 |
| H | -4.64827000 | -0.19156000 | -2.07632600 |
| H | -3.59457100 | -0.03035400 | -3.47670200 |
| H | -3.23568300 | -1.24110400 | -2.22988100 |
| C | -4.50015600 | 1.46027700  | 0.21996800  |
| H | -4.39069900 | 1.65212000  | 1.29199100  |
| H | -5.15336500 | 2.24596800  | -0.17730200 |
| H | -5.02100800 | 0.50956700  | 0.09859000  |
| C | -2.36722500 | 3.55928900  | 0.82359500  |
| H | -1.49735300 | 4.21433200  | 0.89340400  |
| H | -3.22907100 | 4.18673900  | 0.57031200  |
| H | -2.55612700 | 3.14905200  | 1.82271400  |
| N | 1.19565700  | 0.64771900  | -0.47206700 |
| H | 1.17155900  | 0.94322300  | -1.45118900 |
| C | 2.51594300  | -0.02159700 | -0.23362200 |
| C | 2.82781500  | -0.96185200 | -1.39706100 |
| C | 3.62795700  | 1.03552500  | -0.13055800 |
| C | 2.46278000  | -0.80534000 | 1.07600500  |
| H | 2.84707500  | -0.39844600 | -2.34270200 |
| H | 2.03846500  | -1.71044700 | -1.47367100 |
| C | 4.17671500  | -1.65765600 | -1.16072000 |
| H | 3.40168700  | 1.71498100  | 0.70399300  |
| H | 3.65876700  | 1.63251700  | -1.05286000 |
| C | 4.98145000  | 0.34706100  | 0.11136800  |
| H | 1.63549900  | -1.53057400 | 1.04427000  |
| H | 2.25968800  | -0.11356700 | 1.89472500  |
| C | 3.80373600  | -1.51445200 | 1.31643700  |
| H | 4.38017000  | -2.33135800 | -2.00024400 |
| C | 5.28559800  | -0.60158200 | -1.05793400 |
| C | 4.10163100  | -2.46279000 | 0.14609300  |
| H | 5.76273300  | 1.11048400  | 0.18498100  |
| C | 4.91182900  | -0.45531100 | 1.41973900  |
| H | 3.74444300  | -2.07965500 | 2.25309700  |
| H | 5.35509100  | -0.03621900 | -1.99526600 |
| H | 6.25371500  | -1.09005800 | -0.89925800 |
| H | 3.31791900  | -3.22892100 | 0.06972500  |
| H | 5.05020300  | -2.98455400 | 0.31720600  |
| H | 5.87639000  | -0.93947800 | 1.61077200  |
| H | 4.70633600  | 0.21508200  | 2.26387000  |
| C | -3.18746200 | -3.64552200 | 2.26449200  |
| C | -3.19024300 | -2.25429400 | 1.59642300  |
| H | -2.85897400 | -4.42509000 | 1.56957600  |
| H | -2.53511700 | -3.66853800 | 3.14333900  |
| H | -4.20417900 | -3.88943900 | 2.58421900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.55128300 | -1.18863900 | 2.64655100  |
| C | -4.21297800 | -2.24767000 | 0.46308600  |
| H | -4.07091200 | -0.36079300 | 2.15155300  |
| H | -4.25554500 | -1.61944700 | 3.36558600  |
| H | 1.23264300  | 1.53213200  | 0.04612500  |
| H | -5.21980700 | -2.33306200 | 0.88343500  |
| H | -4.15044200 | -1.32169100 | -0.10864300 |
| H | -4.04976600 | -3.07880400 | -0.22956000 |
| C | -1.77234100 | -2.11541600 | 1.03293400  |
| H | -0.99411400 | -2.60692400 | 1.64085400  |
| N | -1.52926500 | -1.88326100 | -0.23343600 |
| C | -0.44335600 | -2.67323000 | -0.87503300 |
| C | -0.84225700 | -4.15694800 | -0.82693000 |
| C | -0.30187900 | -2.20880500 | -2.32483500 |
| H | 0.51201000  | -2.56238700 | -0.33543300 |
| C | 0.10162400  | -5.03374100 | -1.64965200 |
| H | -1.86448800 | -4.24185300 | -1.22200600 |
| H | -0.86763000 | -4.49353000 | 0.21553500  |
| C | 0.58414800  | -3.11660100 | -3.18534600 |
| H | -1.31149700 | -2.18819200 | -2.75539700 |
| H | 0.07132900  | -1.17677200 | -2.35174100 |
| C | 0.13214300  | -4.57402100 | -3.10621100 |
| H | -0.21489000 | -6.07817200 | -1.57688100 |
| H | 1.11543400  | -4.97781400 | -1.22899500 |
| H | 0.56391800  | -2.75719000 | -4.21891300 |
| H | 1.62903900  | -3.06115000 | -2.85570200 |
| H | 0.80094500  | -5.20747000 | -3.69582900 |
| H | -0.87135000 | -4.67509900 | -3.53972100 |
| C | -2.30914600 | -0.65364400 | 3.33339600  |
| C | -1.47142300 | 0.13810400  | 2.34361600  |
| H | -1.73807200 | -1.49413600 | 3.74467600  |
| H | -2.58424400 | -0.02606200 | 4.19096300  |
| H | -2.07273600 | 1.02054300  | 2.04404700  |
| C | -0.16631300 | 0.63056800  | 2.84780100  |
| C | 0.58913200  | -0.08238800 | 3.80283000  |
| C | 0.35924500  | 1.86096200  | 2.40439300  |
| C | 1.78723100  | 0.41716300  | 4.29318300  |
| H | 0.22261500  | -1.03036200 | 4.18165300  |
| C | 1.58139500  | 2.34731700  | 2.87511300  |
| H | -0.23047300 | 2.48737100  | 1.73397500  |
| C | 2.29913400  | 1.63185400  | 3.82690500  |
| H | 2.33143000  | -0.14452800 | 5.04600000  |
| H | 1.94885900  | 3.30753800  | 2.52561900  |
| H | 3.23357800  | 2.02042400  | 4.21689800  |

cis-ts-12

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.77878600  | -2.21837300 | -1.46897800 |
| C  | 1.88849900  | -2.63969400 | -0.67796800 |
| C  | 2.94613600  | -1.70768000 | -0.82353100 |
| C  | 2.53986700  | -0.73989500 | -1.78932500 |
| C  | 1.20665900  | -1.02782800 | -2.16493600 |
| Sc | 1.07470300  | -0.34988700 | 0.23290400  |
| C  | -1.50973400 | -4.17013100 | -0.46323700 |
| C  | -1.96651500 | -2.56004700 | -2.97163000 |
| C  | 0.13811100  | -4.76882800 | -2.98325100 |
| H  | -0.89900700 | -4.90307000 | 0.07012400  |
| H  | -1.86830400 | -3.44039100 | 0.26991900  |
| H  | -2.38909400 | -4.70205300 | -0.84360900 |
| H  | -1.59153100 | -2.17097400 | -3.92104000 |
| H  | -2.72559300 | -3.31620500 | -3.20001500 |
| H  | -2.47890700 | -1.74484900 | -2.45090600 |
| H  | -0.63235100 | -5.46647000 | -3.32625300 |
| H  | 0.63465600  | -4.35109000 | -3.86409400 |
| H  | 0.87990200  | -5.33803700 | -2.41617000 |
| Si | -0.62266500 | -3.39908500 | -1.94716000 |
| C  | 0.42710500  | -0.29382900 | -3.22482200 |
| H  | 0.86921600  | 0.68177200  | -3.43906700 |
| H  | 0.41647700  | -0.86148100 | -4.16190000 |
| H  | -0.61656000 | -0.12790000 | -2.93717600 |
| C  | 3.46401900  | 0.27899300  | -2.38791300 |
| H  | 4.42585700  | -0.18687200 | -2.62299300 |
| H  | 3.06233800  | 0.67605800  | -3.32218100 |
| H  | 3.64851800  | 1.12042200  | -1.71432700 |
| C  | 4.34409900  | -1.91831600 | -0.30893200 |
| H  | 4.36209900  | -2.23682900 | 0.73874900  |
| H  | 4.84186000  | -2.70586800 | -0.88672400 |
| H  | 4.95279300  | -1.01574500 | -0.39321500 |
| C  | 2.07681300  | -3.98957500 | -0.04589500 |
| H  | 1.13028200  | -4.49780500 | 0.13780500  |
| H  | 2.66103300  | -4.61880500 | -0.72787200 |
| H  | 2.63803000  | -3.95648300 | 0.89328600  |
| N  | -1.27023600 | -0.69666600 | 0.39508900  |
| H  | -1.34950300 | -1.31363200 | -0.41587800 |
| C  | -2.57678900 | 0.03572600  | 0.46053700  |
| C  | -2.74447500 | 0.87260000  | -0.80836000 |
| C  | -3.72841900 | -0.98104300 | 0.54887800  |
| C  | -2.63585000 | 0.94658600  | 1.68975200  |
| H  | -2.68316500 | 0.22646700  | -1.69483900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.92505200 | 1.59091900  | -0.86584100 |
| C | -4.09006800 | 1.61195500  | -0.78765700 |
| H | -3.60404600 | -1.59350200 | 1.45422600  |
| H | -3.68961900 | -1.65923200 | -0.31580300 |
| C | -5.07711000 | -0.24407000 | 0.58117400  |
| H | -1.78271800 | 1.63870800  | 1.68106600  |
| H | -2.55288300 | 0.33961300  | 2.59558800  |
| C | -3.97337700 | 1.70497500  | 1.71327200  |
| H | -4.18720200 | 2.20108600  | -1.70644100 |
| C | -5.23037000 | 0.58720500  | -0.70162500 |
| C | -4.12875500 | 2.53950100  | 0.43511000  |
| H | -5.88515500 | -0.97994900 | 0.64591800  |
| C | -5.11961600 | 0.68572400  | 1.80282900  |
| H | -3.99246200 | 2.36069600  | 2.59000200  |
| H | -5.21290500 | -0.06877800 | -1.58081300 |
| H | -6.19722500 | 1.10328000  | -0.69842700 |
| H | -3.32576700 | 3.28479500  | 0.36770500  |
| H | -5.07772000 | 3.08722400  | 0.46010700  |
| H | -6.08206000 | 1.20886400  | 1.83958400  |
| H | -5.03163400 | 0.10012500  | 2.72643100  |
| C | 3.24177800  | 3.12217600  | 2.83753700  |
| C | 3.22035500  | 2.39657700  | 1.48532900  |
| H | 2.66472000  | 4.05127800  | 2.78541600  |
| H | 2.84983600  | 2.52630200  | 3.66417300  |
| H | 4.27232600  | 3.38841900  | 3.08868600  |
| C | 3.97364100  | 1.07280100  | 1.53665800  |
| C | 3.85387600  | 3.33866900  | 0.44481800  |
| H | 3.93890000  | 0.63142000  | 0.53156000  |
| H | 5.02787300  | 1.23643800  | 1.78340000  |
| H | -1.25866400 | -1.34174100 | 1.19476600  |
| H | 4.87372000  | 3.58415300  | 0.75452200  |
| H | 3.88633200  | 2.87312400  | -0.54227100 |
| H | 3.29276000  | 4.27644700  | 0.36517500  |
| C | 1.77900600  | 2.16026300  | 1.00948600  |
| H | 1.05811400  | 2.82629100  | 1.50435400  |
| N | 1.50187900  | 1.71719400  | -0.20927000 |
| C | 0.54752800  | 2.46660900  | -1.06860200 |
| C | -0.31565300 | 3.51947500  | -0.36593600 |
| C | 1.34085700  | 3.15166600  | -2.19278700 |
| H | -0.11697400 | 1.74075600  | -1.55764200 |
| C | -1.25570700 | 4.22250200  | -1.35407900 |
| H | 0.34217800  | 4.27688000  | 0.08268800  |
| H | -0.89259100 | 3.07433700  | 0.45340300  |
| C | 0.40046900  | 3.81573400  | -3.19955900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.99573800  | 3.90937400  | -1.74228600 |
| H | 1.98905500  | 2.42294700  | -2.68255500 |
| C | -0.48400400 | 4.85535700  | -2.51249400 |
| H | -1.83786000 | 4.98103000  | -0.82096300 |
| H | -1.97841500 | 3.50118500  | -1.76006900 |
| H | 0.98172300  | 4.27474200  | -4.00459500 |
| H | -0.23388500 | 3.04656600  | -3.66382100 |
| H | -1.17963800 | 5.30424000  | -3.22745900 |
| H | 0.14829000  | 5.66634500  | -2.12795300 |
| C | 3.28590700  | 0.14236800  | 2.53940000  |
| C | 1.77371500  | 0.34839600  | 2.48977400  |
| H | 3.64904800  | 0.35416800  | 3.55302000  |
| H | 3.55967500  | -0.89679500 | 2.33523900  |
| H | 1.46420100  | 1.20082100  | 3.09047400  |
| C | 0.88656900  | -0.77233200 | 2.80573000  |
| C | 1.13239800  | -2.07665200 | 2.33365000  |
| C | -0.31232800 | -0.56389500 | 3.53182200  |
| C | 0.22165000  | -3.12068300 | 2.56516000  |
| H | 2.09180700  | -2.30438200 | 1.88081500  |
| C | -1.20108800 | -1.59570500 | 3.76457900  |
| H | -0.51468500 | 0.42820300  | 3.92645200  |
| C | -0.95011800 | -2.88483300 | 3.26404500  |
| H | 0.45628200  | -4.12095600 | 2.21832500  |
| H | -2.10092600 | -1.40841800 | 4.34342300  |
| H | -1.65169800 | -3.69074600 | 3.44918400  |

trans-13

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.83016900 | -2.26064300 | -1.08559300 |
| C  | -0.92943800 | -3.21299400 | -0.51436400 |
| C  | 0.29350900  | -3.18345700 | -1.23406600 |
| C  | 0.16793100  | -2.22398000 | -2.27679600 |
| C  | -1.12571400 | -1.64168100 | -2.17707200 |
| Sc | 0.08779900  | -0.92380600 | -0.17165800 |
| C  | -4.09088700 | -1.87923300 | 1.08845600  |
| C  | -4.62737300 | -0.97522200 | -1.74143800 |
| C  | -4.34802200 | -3.95293200 | -1.15766500 |
| H  | -3.58795500 | -2.54940400 | 1.79113800  |
| H  | -3.85800500 | -0.84588200 | 1.36780600  |
| H  | -5.16890400 | -2.01205400 | 1.23043500  |
| H  | -4.49824100 | -1.12538800 | -2.81615500 |
| H  | -5.69178200 | -1.10140200 | -1.51510800 |
| H  | -4.37688100 | 0.06608000  | -1.50958200 |
| H  | -5.43297800 | -3.98553400 | -1.01734400 |
| H  | -4.13391900 | -4.19120200 | -2.20361400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -3.90549200 | -4.73661800 | -0.53656300 |
| Si | -3.68540300 | -2.25006400 | -0.72101900 |
| C  | -1.67198400 | -0.62569700 | -3.14560000 |
| H  | -0.88059100 | 0.00165000  | -3.56514700 |
| H  | -2.17187600 | -1.12053000 | -3.98578000 |
| H  | -2.40503700 | 0.03678700  | -2.68236500 |
| C  | 1.16434900  | -2.03082200 | -3.38474300 |
| H  | 1.14272300  | -2.90002800 | -4.05125700 |
| H  | 0.93918300  | -1.14975700 | -3.98817200 |
| H  | 2.18597400  | -1.92702000 | -3.01080600 |
| C  | 1.41175500  | -4.17282200 | -1.07093700 |
| H  | 1.55542800  | -4.46399900 | -0.02567800 |
| H  | 1.17973500  | -5.08828600 | -1.62733600 |
| H  | 2.36107300  | -3.79169600 | -1.45232800 |
| C  | -1.23315900 | -4.24027100 | 0.54345500  |
| H  | -2.11151300 | -3.98040600 | 1.13836800  |
| H  | -1.42967600 | -5.21160600 | 0.07625200  |
| H  | -0.39381200 | -4.38848100 | 1.23225700  |
| N  | -1.63925800 | 0.58409000  | 0.24723900  |
| H  | -2.39082400 | 0.27023600  | -0.37145200 |
| C  | -1.65358500 | 2.07430800  | 0.23883200  |
| C  | -1.30162600 | 2.56493500  | -1.16784400 |
| C  | -3.05219300 | 2.59255800  | 0.61161400  |
| C  | -0.64753900 | 2.59983200  | 1.26636500  |
| H  | -2.04392200 | 2.18486200  | -1.88375100 |
| H  | -0.32394000 | 2.16568900  | -1.46557000 |
| C  | -1.29228000 | 4.10154900  | -1.19195600 |
| H  | -3.32313700 | 2.22436700  | 1.61160800  |
| H  | -3.79271200 | 2.19857200  | -0.09867700 |
| C  | -3.06160100 | 4.12987900  | 0.58821700  |
| H  | 0.34965100  | 2.18809700  | 1.06451400  |
| H  | -0.94237500 | 2.24766400  | 2.26358200  |
| C  | -0.63672500 | 4.13745700  | 1.23438500  |
| H  | -1.02455500 | 4.44195800  | -2.19812400 |
| C  | -2.69085000 | 4.61727900  | -0.82047100 |
| C  | -0.26476700 | 4.62173400  | -0.17510200 |
| H  | -4.06237600 | 4.48624100  | 0.85303900  |
| C  | -2.03443200 | 4.65847700  | 1.60093600  |
| H  | 0.09787300  | 4.50535700  | 1.95843900  |
| H  | -3.42933700 | 4.26223600  | -1.54970700 |
| H  | -2.70415200 | 5.71272000  | -0.85038100 |
| H  | 0.74040100  | 4.27224300  | -0.44312500 |
| H  | -0.24256600 | 5.71735200  | -0.19783000 |
| H  | -2.03793800 | 5.75449800  | 1.59517200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.30351300 | 4.33725000  | 2.61466600  |
| C | 5.21987000  | -0.53942600 | 1.29785800  |
| C | 4.02071100  | -1.28387100 | 0.69604000  |
| H | 5.35837400  | 0.45272300  | 0.86536200  |
| H | 5.10121000  | -0.41887500 | 2.38097300  |
| H | 6.13769700  | -1.11048100 | 1.12591500  |
| C | 3.85691000  | -2.61593800 | 1.47736300  |
| C | 4.25470700  | -1.58013600 | -0.78226000 |
| H | 3.45798100  | -3.39299100 | 0.81412900  |
| H | 4.81342300  | -2.97942600 | 1.86293000  |
| H | -1.93377700 | 0.28272100  | 1.18260900  |
| H | 5.03017700  | -2.34574900 | -0.89041900 |
| H | 3.33477700  | -1.94652900 | -1.24388700 |
| H | 4.57532500  | -0.70038000 | -1.34537800 |
| C | 2.66634700  | -0.49014700 | 0.97665600  |
| H | 2.92270200  | 0.33495000  | 1.65861200  |
| N | 1.85376600  | 0.01833800  | -0.12485500 |
| C | 2.22180500  | 1.26957300  | -0.81251600 |
| C | 3.59842000  | 1.87479000  | -0.51181700 |
| C | 2.04590700  | 1.11602200  | -2.32772700 |
| H | 1.51184600  | 2.05397700  | -0.50077100 |
| C | 3.76386200  | 3.21848700  | -1.22956600 |
| H | 4.39047100  | 1.19992100  | -0.85124800 |
| H | 3.72684800  | 2.01680700  | 0.56668500  |
| C | 2.21603500  | 2.44907500  | -3.05766100 |
| H | 2.77951600  | 0.38574400  | -2.69514300 |
| H | 1.05310800  | 0.69302900  | -2.54516900 |
| C | 3.57632900  | 3.07107700  | -2.73971000 |
| H | 4.75100400  | 3.63436000  | -1.00577100 |
| H | 3.02603000  | 3.93330000  | -0.84075400 |
| H | 2.09816500  | 2.30644500  | -4.13648700 |
| H | 1.42201800  | 3.14208300  | -2.74039000 |
| H | 3.67808000  | 4.04224600  | -3.23343400 |
| H | 4.36885400  | 2.42419100  | -3.13935500 |
| C | 2.83672500  | -2.32468200 | 2.57213500  |
| C | 1.80770500  | -1.48806400 | 1.80699000  |
| H | 3.26636200  | -1.71211900 | 3.37392500  |
| H | 2.39955500  | -3.21709300 | 3.02703200  |
| H | 1.35662400  | -2.24041000 | 1.11384100  |
| C | 0.71089500  | -0.87065300 | 2.64157200  |
| C | 0.97437000  | 0.22391800  | 3.48064200  |
| C | -0.57718600 | -1.41967200 | 2.64974600  |
| C | -0.01759100 | 0.74291700  | 4.29937800  |
| H | 1.97041800  | 0.65477200  | 3.51138400  |



|        |             |             |             |
|--------|-------------|-------------|-------------|
| C      | -1.58386100 | -0.88629900 | 3.46698700  |
| H      | -0.79151200 | -2.31854400 | 2.06991400  |
| C      | -1.30455100 | 0.19500300  | 4.29067700  |
| H      | 0.20937400  | 1.57990800  | 4.95175800  |
| H      | -2.57010800 | -1.33805100 | 3.47525500  |
| H      | -2.07391600 | 0.60138600  | 4.93842200  |
| cis-13 |             |             |             |
| C      | 0.34115600  | 2.71814000  | -0.91209200 |
| C      | -0.79543900 | 3.15210500  | -0.16335700 |
| C      | -1.97500200 | 2.67786300  | -0.79167000 |
| C      | -1.59337800 | 1.96486000  | -1.96015900 |
| C      | -0.17063900 | 1.95998200  | -2.02364900 |
| Sc     | -0.75130500 | 0.60177600  | -0.06359600 |
| C      | 2.66604300  | 3.44589200  | 1.08105100  |
| C      | 3.35937100  | 2.85000000  | -1.84667200 |
| C      | 1.79950900  | 5.35720500  | -1.15834000 |
| H      | 2.46359200  | 4.38747200  | 1.60170400  |
| H      | 2.23214000  | 2.64516600  | 1.69060600  |
| H      | 3.75205800  | 3.30643000  | 1.08318700  |
| H      | 3.07218500  | 2.90107700  | -2.89994300 |
| H      | 4.25450500  | 3.46841600  | -1.71715400 |
| H      | 3.64659000  | 1.81980500  | -1.61914100 |
| H      | 2.75051800  | 5.89346100  | -1.07937300 |
| H      | 1.43924700  | 5.45594400  | -2.18653200 |
| H      | 1.07951300  | 5.85033800  | -0.49923100 |
| Si     | 2.02913000  | 3.54597100  | -0.71080200 |
| C      | 0.63848200  | 1.34708500  | -3.13801300 |
| H      | 0.09625500  | 0.53296000  | -3.62799600 |
| H      | 0.87398900  | 2.08997200  | -3.90822700 |
| H      | 1.58438000  | 0.93963600  | -2.77281500 |
| C      | -2.56097200 | 1.49966200  | -3.01252100 |
| H      | -3.06390400 | 2.36791900  | -3.45170700 |
| H      | -2.05814500 | 0.97515400  | -3.82676000 |
| H      | -3.33585100 | 0.84146000  | -2.60815500 |
| C      | -3.36907900 | 3.09716300  | -0.41592900 |
| H      | -3.63254800 | 2.84831500  | 0.61857600  |
| H      | -3.47013500 | 4.18374400  | -0.51519800 |
| H      | -4.11442100 | 2.63563900  | -1.06647800 |
| C      | -0.82078500 | 4.16264600  | 0.94970700  |
| H      | 0.15426000  | 4.28313700  | 1.42619900  |
| H      | -1.11208300 | 5.14055100  | 0.54825800  |
| H      | -1.55565200 | 3.91813600  | 1.72466800  |
| N      | 1.40492400  | 0.10227300  | 0.65679000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.78430600  | 1.03011900  | 0.44833900  |
| C | 2.55508700  | -0.84660600 | 0.49883400  |
| C | 2.88567700  | -1.07847600 | -0.97797500 |
| C | 3.77742800  | -0.22703100 | 1.20098900  |
| C | 2.22235900  | -2.18775500 | 1.15682300  |
| H | 3.09718600  | -0.12016400 | -1.46704000 |
| H | 2.02122700  | -1.52227100 | -1.48864100 |
| C | 4.10813900  | -2.00831900 | -1.09510700 |
| H | 3.52933100  | -0.03473600 | 2.25514200  |
| H | 4.00535000  | 0.74361900  | 0.73655300  |
| C | 4.98864200  | -1.16059000 | 1.09533700  |
| H | 1.34020200  | -2.62529500 | 0.67355200  |
| H | 1.97124300  | -2.02720800 | 2.21403500  |
| C | 3.43485800  | -3.13110600 | 1.04514900  |
| H | 4.33530300  | -2.16033300 | -2.15529400 |
| C | 5.31546600  | -1.37317000 | -0.38967300 |
| C | 3.79255200  | -3.35657100 | -0.43146500 |
| H | 5.84322500  | -0.70256700 | 1.60381500  |
| C | 4.64132700  | -2.50199000 | 1.75844300  |
| H | 3.18327200  | -4.08736300 | 1.51566300  |
| H | 5.56899900  | -0.41415800 | -0.85888200 |
| H | 6.18911100  | -2.02689400 | -0.49248000 |
| H | 2.97274300  | -3.85881500 | -0.95480100 |
| H | 4.66584100  | -4.01554500 | -0.50101100 |
| H | 5.49975700  | -3.18088300 | 1.70250900  |
| H | 4.41726800  | -2.34733500 | 2.82119400  |
| C | -5.29571700 | -2.46776200 | 1.00107200  |
| C | -4.41153200 | -1.49307600 | 0.20833700  |
| H | -4.97512700 | -3.50072400 | 0.82770500  |
| H | -5.27441900 | -2.28800500 | 2.07939400  |
| H | -6.33658800 | -2.38211200 | 0.67425200  |
| C | -4.77441300 | -0.03948900 | 0.52552200  |
| C | -4.57671000 | -1.79333700 | -1.27243600 |
| H | -4.23286500 | 0.60426800  | -0.17951600 |
| H | -5.84352600 | 0.16748400  | 0.41505800  |
| H | 1.22846000  | 0.13504900  | 1.66694900  |
| H | -5.62644200 | -1.66869800 | -1.55794700 |
| H | -3.97548200 | -1.11289200 | -1.87798000 |
| H | -4.29004800 | -2.82391100 | -1.50982200 |
| C | -2.94825500 | -1.57628100 | 0.75076200  |
| H | -2.71202600 | -2.62228500 | 0.97699000  |
| N | -1.89269900 | -1.01498300 | -0.08566000 |
| C | -1.12755300 | -1.89677400 | -0.99024500 |
| C | -0.99440100 | -3.35216200 | -0.51809600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.51908800 | -1.88761500 | -2.47938500 |
| H | -0.07908100 | -1.49317300 | -0.98873700 |
| C | -0.00277000 | -4.13778400 | -1.37974700 |
| H | -1.98150000 | -3.82851300 | -0.59317000 |
| H | -0.70205600 | -3.38578600 | 0.53858200  |
| C | -0.48080100 | -2.62561900 | -3.32668600 |
| H | -2.48606500 | -2.37929100 | -2.61228100 |
| H | -1.63661100 | -0.85312700 | -2.81467300 |
| C | -0.35722000 | -4.07765600 | -2.86538200 |
| H | 0.04541700  | -5.17499600 | -1.03378600 |
| H | 0.99922500  | -3.71326800 | -1.24388600 |
| H | -0.76015300 | -2.57807900 | -4.38374600 |
| H | 0.49680700  | -2.12824500 | -3.23556500 |
| H | 0.39665700  | -4.60933200 | -3.45374000 |
| H | -1.31428100 | -4.58874200 | -3.03371000 |
| C | -4.25758900 | 0.18784400  | 1.94941800  |
| C | -3.06963200 | -0.80199100 | 2.11330600  |
| H | -5.03112500 | -0.05171300 | 2.68368400  |
| H | -3.98852800 | 1.22996900  | 2.13394200  |
| H | -3.35672900 | -1.54878700 | 2.85948400  |
| C | -1.76730800 | -0.22461000 | 2.62182300  |
| C | -1.41416200 | 1.12730800  | 2.47425500  |
| C | -0.88196200 | -1.05107200 | 3.33393200  |
| C | -0.25682800 | 1.64912700  | 3.07871900  |
| H | -2.10316300 | 1.81912500  | 1.99109500  |
| C | 0.26184800  | -0.53738300 | 3.93437200  |
| H | -1.12733000 | -2.10275500 | 3.45632300  |
| C | 0.57506200  | 0.82224400  | 3.82283800  |
| H | -0.03712900 | 2.70766800  | 2.99332700  |
| H | 0.90427000  | -1.19312300 | 4.51410100  |
| H | 1.45196900  | 1.22773700  | 4.31683200  |

trans-ts-14

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.16570800 | -2.33057900 | -0.77205600 |
| C  | 1.34770200 | -1.83815700 | -1.84479000 |
| C  | 0.04844100 | -2.41330200 | -1.72859600 |
| C  | 0.03965000 | -3.24504900 | -0.58034600 |
| C  | 1.32954400 | -3.18992300 | 0.01645300  |
| Sc | 0.51266300 | -0.92285900 | 0.25611400  |
| C  | 4.70324100 | -3.97944900 | -0.79003400 |
| C  | 4.89586300 | -1.12169100 | -1.77856700 |
| C  | 4.42716400 | -1.66849400 | 1.23685400  |
| H  | 4.28511000 | -4.68965800 | -0.07126800 |
| H  | 4.46759400 | -4.33667500 | -1.79679000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.79179800  | -3.98946900 | -0.67468800 |
| H  | 4.61361500  | -0.06696400 | -1.71759600 |
| H  | 5.97347200  | -1.18088600 | -1.58939600 |
| H  | 4.72361300  | -1.46553300 | -2.80252300 |
| H  | 5.21758700  | -0.91089600 | 1.23795900  |
| H  | 3.54666000  | -1.23327200 | 1.72295400  |
| H  | 4.77345000  | -2.50476600 | 1.85202900  |
| Si | 4.04331100  | -2.23865400 | -0.52700100 |
| C  | 1.73923300  | -3.99285700 | 1.22341000  |
| H  | 0.93319800  | -4.05519900 | 1.96175800  |
| H  | 1.98504700  | -5.01995000 | 0.93325500  |
| H  | 2.61529600  | -3.56869600 | 1.71948700  |
| C  | -1.09371700 | -4.14752600 | -0.18686600 |
| H  | -2.06804100 | -3.67983400 | -0.35950500 |
| H  | -1.06452800 | -5.06106300 | -0.79055000 |
| H  | -1.03528000 | -4.45393000 | 0.86129700  |
| C  | -1.07112100 | -2.34921800 | -2.72835500 |
| H  | -0.88544300 | -1.60610400 | -3.50579400 |
| H  | -1.17400500 | -3.32279700 | -3.21955000 |
| H  | -2.03269900 | -2.11445900 | -2.26154400 |
| C  | 1.78024300  | -0.95239800 | -2.98379000 |
| H  | 2.57809000  | -0.26820000 | -2.69122200 |
| H  | 2.15496400  | -1.55890600 | -3.81547700 |
| H  | 0.94805300  | -0.35461000 | -3.36777800 |
| C  | -1.56359600 | 0.29046000  | 3.77514700  |
| C  | -1.96520100 | -0.72113100 | 2.70447500  |
| H  | -0.72690300 | 0.91812600  | 3.45093500  |
| H  | -2.40360000 | 0.95302800  | 4.00404800  |
| H  | -1.27150700 | -0.21486500 | 4.70146500  |
| C  | -3.25389300 | -1.46770200 | 3.07570500  |
| C  | -0.83332400 | -1.73798600 | 2.47902500  |
| H  | -3.10089500 | -2.20217200 | 3.87233800  |
| H  | -3.98684900 | -0.73848400 | 3.44126800  |
| H  | -0.77872400 | -2.47741800 | 3.28434000  |
| H  | -0.98758100 | -2.32097600 | 1.55708500  |
| H  | 0.16044500  | -1.25473700 | 2.50194100  |
| C  | -2.36681200 | -0.04681400 | 1.36719400  |
| H  | -2.94180500 | 0.84294700  | 1.65071300  |
| N  | -1.19997700 | 0.36882100  | 0.58225600  |
| C  | -1.39887800 | 1.42087800  | -0.44115700 |
| C  | -1.75605100 | 0.89221200  | -1.83198600 |
| C  | -2.34113300 | 2.55341600  | -0.02055900 |
| H  | -0.40886600 | 1.88905200  | -0.56483500 |
| C  | -1.76834100 | 2.02095700  | -2.86531300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.73291100 | 0.39570900  | -1.80523800 |
| H | -1.01244400 | 0.13831100  | -2.12047800 |
| C | -2.32232900 | 3.67973400  | -1.05711100 |
| H | -3.36662200 | 2.17095700  | 0.05763500  |
| H | -2.04953800 | 2.92621200  | 0.97042000  |
| C | -2.70917600 | 3.14867300  | -2.43848800 |
| H | -2.05405900 | 1.62789400  | -3.84612700 |
| H | -0.74936500 | 2.42388500  | -2.96837400 |
| H | -3.00273700 | 4.47851300  | -0.74767300 |
| H | -1.31586500 | 4.12083500  | -1.10567700 |
| H | -2.69503500 | 3.95611900  | -3.17676200 |
| H | -3.73747400 | 2.76380100  | -2.39912500 |
| C | -3.73502500 | -2.08375000 | 1.75968200  |
| C | -3.34484100 | -1.04746600 | 0.66260700  |
| H | -4.80730000 | -2.28849400 | 1.76047400  |
| H | -3.22822200 | -3.03847000 | 1.58068900  |
| H | -2.79388700 | -1.54632400 | -0.14671300 |
| C | -4.56815600 | -0.39894900 | 0.04745300  |
| C | -5.37065400 | 0.47898000  | 0.78595700  |
| C | -4.95937100 | -0.70932900 | -1.25705600 |
| C | -6.50799200 | 1.05207800  | 0.22506800  |
| H | -5.10753200 | 0.72237200  | 1.81299600  |
| C | -6.09707500 | -0.13876900 | -1.82415100 |
| H | -4.36209200 | -1.40733100 | -1.84020200 |
| C | -6.87242100 | 0.75008000  | -1.08567700 |
| H | -7.11310800 | 1.73336600  | 0.81453200  |
| H | -6.37591200 | -0.39060600 | -2.84231200 |
| H | -7.75761300 | 1.19870400  | -1.52377000 |
| N | 1.17351000  | 0.74651900  | 1.50514500  |
| H | -0.11811500 | 0.82132000  | 1.26042400  |
| H | 1.28376400  | 0.66041700  | 2.51517700  |
| C | 2.05124800  | 1.82799700  | 1.01424400  |
| C | 1.37609800  | 3.21194000  | 1.09795100  |
| C | 3.34919000  | 1.89608800  | 1.83660000  |
| C | 2.42245400  | 1.51347300  | -0.44223400 |
| H | 1.14665300  | 3.42907300  | 2.14986600  |
| H | 0.42326900  | 3.20844900  | 0.55732700  |
| C | 2.29999800  | 4.29286700  | 0.51447800  |
| H | 3.84666000  | 0.92066900  | 1.81556700  |
| H | 3.09442200  | 2.11717800  | 2.88239800  |
| C | 4.28783000  | 2.97900500  | 1.27897900  |
| H | 1.51354500  | 1.44025400  | -1.06836300 |
| H | 2.92829900  | 0.53515300  | -0.46235800 |
| C | 3.34744000  | 2.59389600  | -1.01872900 |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 1.79068300 | 5.26152800 | 0.55782300  |
| C | 3.59488500 | 4.34756700 | 1.33496900  |
| C | 2.62683600 | 3.95008500 | -0.94864800 |
| H | 5.20402300 | 3.00048100 | 1.87829100  |
| C | 4.63392100 | 2.64252000 | -0.17945500 |
| H | 3.58936200 | 2.35167600 | -2.06069100 |
| H | 3.36927000 | 4.61438600 | 2.37442300  |
| H | 4.26229100 | 5.12074500 | 0.93674900  |
| H | 1.70340400 | 3.91585000 | -1.54269600 |
| H | 3.26338300 | 4.72999500 | -1.38193600 |
| H | 5.31401500 | 3.39827100 | -0.58854000 |
| H | 5.15303600 | 1.67607300 | -0.22802200 |

cis-ts-14

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | 0.93217100  | 2.68541600 | -0.32276800 |
| C  | -0.48466500 | 2.94312200 | -0.27538600 |
| C  | -1.03096600 | 2.74266300 | -1.56574700 |
| C  | 0.03449500  | 2.34528400 | -2.43272100 |
| C  | 1.23677300  | 2.33906900 | -1.67874300 |
| Sc | -0.21083400 | 0.57652700 | -0.76186400 |
| C  | 1.74837300  | 5.06599700 | 1.35328100  |
| C  | 1.84658900  | 2.28290400 | 2.66915800  |
| C  | 3.92772500  | 3.11209300 | 0.60250000  |
| H  | 1.87077900  | 5.62898000 | 0.42288800  |
| H  | 0.73823700  | 5.24880300 | 1.72769100  |
| H  | 2.45445100  | 5.47116000 | 2.08508700  |
| H  | 2.16102300  | 1.23935700 | 2.57316500  |
| H  | 2.46213000  | 2.73876300 | 3.45233000  |
| H  | 0.81161000  | 2.29524900 | 3.02256100  |
| H  | 4.49669000  | 3.60156600 | 1.40069100  |
| H  | 4.29447800  | 2.08491900 | 0.52744100  |
| H  | 4.15621700  | 3.63428200 | -0.33029800 |
| Si | 2.10831700  | 3.24031300 | 1.06640900  |
| C  | 2.58972900  | 2.09027400 | -2.27805500 |
| H  | 2.53751600  | 1.35839500 | -3.08901600 |
| H  | 2.99258100  | 3.01864200 | -2.69872800 |
| H  | 3.30139200  | 1.72509300 | -1.53789700 |
| C  | -0.08173600 | 2.13236900 | -3.91597400 |
| H  | -1.10283100 | 1.87051400 | -4.20475700 |
| H  | 0.18384800  | 3.05031000 | -4.45099300 |
| H  | 0.58627400  | 1.34406300 | -4.27579200 |
| C  | -2.43345100 | 3.06365100 | -2.00029300 |
| H  | -3.10064200 | 3.17447800 | -1.14298100 |
| H  | -2.44107800 | 4.01350000 | -2.54538100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.85927000 | 2.31049500  | -2.67197600 |
| C | -1.26133500 | 3.42481200  | 0.92049200  |
| H | -0.67598800 | 3.34394200  | 1.83807300  |
| H | -1.54147300 | 4.47654200  | 0.79673800  |
| H | -2.17933600 | 2.85166600  | 1.06879200  |
| C | -1.02191200 | -3.09760500 | -2.94173700 |
| C | -2.03947800 | -2.08193400 | -2.41990000 |
| H | -0.02811900 | -2.93872300 | -2.51205400 |
| H | -1.33555100 | -4.11366200 | -2.68596500 |
| H | -0.93715500 | -3.03582800 | -4.03183200 |
| C | -3.46089400 | -2.42592100 | -2.89218900 |
| C | -1.65816000 | -0.67398800 | -2.90763400 |
| H | -3.61623400 | -2.19888500 | -3.95120200 |
| H | -3.62603700 | -3.50178500 | -2.75714500 |
| H | -1.85651200 | -0.55522800 | -3.97766800 |
| H | -2.21902300 | 0.12508900  | -2.40062400 |
| H | -0.57325200 | -0.49227000 | -2.82189500 |
| C | -2.17370100 | -2.11673600 | -0.87019200 |
| H | -2.02734900 | -3.16526700 | -0.58096100 |
| N | -1.12294600 | -1.31392400 | -0.24265800 |
| C | -0.83223200 | -1.46467000 | 1.20364700  |
| C | -1.07251000 | -0.14335500 | 1.95866300  |
| C | -1.48422500 | -2.65904600 | 1.90229700  |
| H | 0.25138200  | -1.65188000 | 1.28883400  |
| C | -0.66802200 | -0.23962900 | 3.43155500  |
| H | -2.12114800 | 0.16017000  | 1.87055000  |
| H | -0.46988500 | 0.69090000  | 1.52079700  |
| C | -1.07236400 | -2.71920900 | 3.37559900  |
| H | -2.57355300 | -2.58658000 | 1.83014200  |
| H | -1.18208300 | -3.58052300 | 1.39241700  |
| C | -1.39413900 | -1.41014400 | 4.09616200  |
| H | -0.89402000 | 0.70101000  | 3.94349300  |
| H | 0.41736300  | -0.39523900 | 3.50877300  |
| H | -1.57375000 | -3.56054800 | 3.86240200  |
| H | 0.00786800  | -2.91149600 | 3.44296100  |
| H | -1.11239200 | -1.47414600 | 5.15110700  |
| H | -2.47689600 | -1.22909500 | 4.05826000  |
| C | -4.36804700 | -1.64047600 | -1.95345900 |
| C | -3.70602500 | -1.80842400 | -0.56695600 |
| H | -5.40153000 | -1.99389900 | -1.94985900 |
| H | -4.39649300 | -0.58546900 | -2.24774500 |
| H | -4.09955700 | -2.73703400 | -0.13826700 |
| C | -4.07337000 | -0.71041100 | 0.40191800  |
| C | -3.97494200 | 0.64486900  | 0.06658700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.59657200 | -1.03260400 | 1.65897600  |
| C | -4.38306900 | 1.63771400  | 0.95568000  |
| H | -3.61687500 | 0.93575900  | -0.91787500 |
| C | -4.96960000 | -0.04487400 | 2.56715000  |
| H | -4.72633200 | -2.07801800 | 1.92763200  |
| C | -4.86276900 | 1.29873900  | 2.21863600  |
| H | -4.34726400 | 2.68206200  | 0.65920400  |
| H | -5.36670400 | -0.32746700 | 3.53695900  |
| H | -5.17710800 | 2.07281700  | 2.91054900  |
| N | 1.22857200  | -1.01050400 | -1.19968100 |
| H | 0.06186300  | -1.51591400 | -0.77676100 |
| H | 1.30999200  | -1.19679500 | -2.20023200 |
| C | 2.47914400  | -1.47335500 | -0.55937000 |
| C | 2.35946200  | -2.94137900 | -0.09851100 |
| C | 3.65573300  | -1.39204800 | -1.54904300 |
| C | 2.80162800  | -0.58772900 | 0.64908900  |
| H | 2.14750400  | -3.57058900 | -0.97375400 |
| H | 1.51168200  | -3.05135800 | 0.59109800  |
| C | 3.65601900  | -3.39857200 | 0.58912200  |
| H | 3.75704800  | -0.36382700 | -1.91295400 |
| H | 3.43369100  | -2.02981900 | -2.41677700 |
| C | 4.96292600  | -1.84882000 | -0.88150700 |
| H | 1.98104200  | -0.63776500 | 1.38096000  |
| H | 2.88081700  | 0.45355000  | 0.30933000  |
| C | 4.10175500  | -1.03788300 | 1.33010300  |
| H | 3.54052300  | -4.43477500 | 0.92500700  |
| C | 4.81832600  | -3.30153800 | -0.40854400 |
| C | 3.93820400  | -2.49243900 | 1.79851400  |
| H | 5.78003400  | -1.77401900 | -1.60699000 |
| C | 5.25868500  | -0.94595500 | 0.32472300  |
| H | 4.30385500  | -0.38808100 | 2.19023200  |
| H | 4.63331600  | -3.96081400 | -1.26549300 |
| H | 5.74925300  | -3.63564300 | 0.06477600  |
| H | 3.11380800  | -2.56310800 | 2.52104900  |
| H | 4.84894400  | -2.82437000 | 2.31028100  |
| H | 6.19456600  | -1.25548800 | 0.80427600  |
| H | 5.39403200  | 0.09147200  | -0.00763200 |

trans-15

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.24309000 | -2.18439100 | -0.81023400 |
| C | 1.46097000 | -1.62057600 | -1.87406200 |
| C | 0.14349500 | -2.16150000 | -1.81184600 |
| C | 0.08501600 | -3.04723300 | -0.70941500 |
| C | 1.36123200 | -3.04670200 | -0.07847700 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| Sc | 0.62239700  | -0.75651600 | 0.26768400  |
| C  | 4.69328100  | -3.91256000 | -1.08512400 |
| C  | 5.02888400  | -0.94568100 | -1.62332300 |
| C  | 4.61704400  | -1.94021000 | 1.25523700  |
| H  | 4.22569000  | -4.69650000 | -0.48159700 |
| H  | 4.44500900  | -4.10076300 | -2.13376700 |
| H  | 5.77806700  | -4.00576300 | -0.97120500 |
| H  | 4.72623400  | 0.09075500  | -1.45006600 |
| H  | 6.09546600  | -1.01659000 | -1.38355500 |
| H  | 4.91779900  | -1.16634400 | -2.68847300 |
| H  | 5.60702900  | -1.47371100 | 1.29660800  |
| H  | 3.91899500  | -1.28916500 | 1.78747500  |
| H  | 4.68676600  | -2.89309400 | 1.78808200  |
| Si | 4.12114700  | -2.20012400 | -0.55013800 |
| C  | 1.72227200  | -3.92252000 | 1.09276900  |
| H  | 0.87979600  | -4.04784200 | 1.78037700  |
| H  | 2.00544400  | -4.92474400 | 0.75219200  |
| H  | 2.55993400  | -3.51651200 | 1.66284000  |
| C  | -1.04702500 | -3.98498500 | -0.40016600 |
| H  | -2.02205600 | -3.56403600 | -0.66276400 |
| H  | -0.92929300 | -4.90689800 | -0.98021700 |
| H  | -1.06802000 | -4.27732900 | 0.65403600  |
| C  | -0.92379900 | -1.99730200 | -2.85539400 |
| H  | -0.80911900 | -1.06804800 | -3.41901100 |
| H  | -0.87189900 | -2.82328600 | -3.57345100 |
| H  | -1.92739800 | -2.00896400 | -2.42015100 |
| C  | 1.91195600  | -0.71607700 | -2.99239600 |
| H  | 2.88384200  | -0.26698600 | -2.79362800 |
| H  | 1.99362900  | -1.28181700 | -3.92690200 |
| H  | 1.19797800  | 0.09756500  | -3.17254400 |
| C  | -1.63952300 | 0.09069600  | 3.91783000  |
| C  | -1.99490900 | -0.85276000 | 2.77137000  |
| H  | -0.77152500 | 0.71892900  | 3.67787100  |
| H  | -2.48176000 | 0.74532900  | 4.16087800  |
| H  | -1.38393200 | -0.48019600 | 4.81560400  |
| C  | -3.23510300 | -1.70680000 | 3.06186000  |
| C  | -0.79937600 | -1.76810400 | 2.46236800  |
| H  | -3.03999700 | -2.48840000 | 3.80153000  |
| H  | -4.02276200 | -1.06139600 | 3.46946500  |
| H  | -0.68829900 | -2.55024400 | 3.21960700  |
| H  | -0.92712800 | -2.29270400 | 1.50540900  |
| H  | 0.14990400  | -1.20763000 | 2.50163600  |
| C  | -2.45812500 | -0.10658500 | 1.49719500  |
| H  | -3.14536000 | 0.68268200  | 1.82830300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.29852000 | 0.53081500  | 0.81943500  |
| C | -1.57550500 | 1.60320400  | -0.19416200 |
| C | -1.57421400 | 1.02805000  | -1.60506800 |
| C | -2.80879800 | 2.47077600  | 0.06310900  |
| H | -0.71320200 | 2.27881800  | -0.12003100 |
| C | -1.68039800 | 2.13391300  | -2.65565100 |
| H | -2.40711700 | 0.32494600  | -1.71535800 |
| H | -0.64998300 | 0.45137900  | -1.77375400 |
| C | -2.88206900 | 3.58540000  | -0.98586400 |
| H | -3.72013600 | 1.86701700  | -0.00262900 |
| H | -2.76236100 | 2.89696400  | 1.07308800  |
| C | -2.91369200 | 3.00309400  | -2.39987300 |
| H | -1.71475400 | 1.69313600  | -3.65695000 |
| H | -0.77717200 | 2.76050300  | -2.61171300 |
| H | -3.76938600 | 4.19789100  | -0.80357500 |
| H | -2.01148300 | 4.24789700  | -0.88323100 |
| H | -2.97149100 | 3.80464900  | -3.14179800 |
| H | -3.81710100 | 2.38824100  | -2.51421200 |
| C | -3.64660400 | -2.25464900 | 1.69042000  |
| C | -3.26723100 | -1.14111500 | 0.66223200  |
| H | -4.71003000 | -2.49420100 | 1.63947100  |
| H | -3.10068900 | -3.17636600 | 1.46683300  |
| H | -2.61132500 | -1.55795500 | -0.11474100 |
| C | -4.49475300 | -0.57026700 | -0.01942700 |
| C | -5.47190600 | 0.09979100  | 0.72717700  |
| C | -4.70338300 | -0.72948100 | -1.38954300 |
| C | -6.59818600 | 0.63462300  | 0.11198800  |
| H | -5.34930600 | 0.21150700  | 1.80265300  |
| C | -5.83109400 | -0.19543600 | -2.01254900 |
| H | -3.97678000 | -1.28142200 | -1.98122400 |
| C | -6.77644600 | 0.49797300  | -1.26443000 |
| H | -7.33997700 | 1.15787600  | 0.70653300  |
| H | -5.96913000 | -0.32622700 | -3.08104700 |
| H | -7.65290500 | 0.91929700  | -1.74505900 |
| N | 1.76781900  | 0.30999100  | 1.49256500  |
| H | -0.80045700 | 1.00836000  | 1.57670100  |
| H | 2.09510200  | 0.09577700  | 2.43342300  |
| C | 2.32977400  | 1.57975000  | 1.03720400  |
| C | 1.63256000  | 2.77064800  | 1.72605300  |
| C | 3.84457400  | 1.68920700  | 1.28941200  |
| C | 2.12140900  | 1.67326800  | -0.48420100 |
| H | 1.79671900  | 2.69657500  | 2.80940000  |
| H | 0.54725600  | 2.70271600  | 1.56088700  |
| C | 2.16230700  | 4.10573900  | 1.18598500  |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 4.34913400 | 0.84831500 | 0.79673100  |
| H | 4.03707700 | 1.60043800 | 2.36763100  |
| C | 4.38627200 | 3.02736700 | 0.75721400  |
| H | 1.04989200 | 1.56350600 | -0.74844300 |
| H | 2.66836200 | 0.84863100 | -0.95970600 |
| C | 2.62537600 | 3.01795200 | -1.03394000 |
| H | 1.64706300 | 4.93291300 | 1.68587200  |
| C | 3.67120900 | 4.19152600 | 1.45794100  |
| C | 1.89987100 | 4.17266400 | -0.32681600 |
| H | 5.46244500 | 3.08292500 | 0.95237000  |
| C | 4.13347000 | 3.11800000 | -0.75587200 |
| H | 2.44012500 | 3.06160400 | -2.11334800 |
| H | 3.85871100 | 4.15458100 | 2.53788300  |
| H | 4.06563000 | 5.14649100 | 1.09153300  |
| H | 0.82030500 | 4.12334200 | -0.52719200 |
| H | 2.25589200 | 5.12817700 | -0.72869000 |
| H | 4.51634100 | 4.06916900 | -1.14351900 |
| H | 4.66865700 | 2.31690000 | -1.27999600 |

cis-15

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | 1.09852200  | 2.62582500 | -0.20345100 |
| C  | -0.32786600 | 2.82733000 | -0.25038300 |
| C  | -0.76009800 | 2.70633300 | -1.58858500 |
| C  | 0.39048900  | 2.42819500 | -2.39765100 |
| C  | 1.52958500  | 2.42358800 | -1.55808200 |
| Sc | 0.20655100  | 0.47868000 | -0.93205500 |
| C  | 1.75614100  | 4.88304500 | 1.71934200  |
| C  | 1.75182300  | 2.01194200 | 2.82098400  |
| C  | 3.99455600  | 2.97643100 | 1.00437200  |
| H  | 1.99735100  | 5.52415600 | 0.86595100  |
| H  | 0.70573200  | 5.04349700 | 1.97480700  |
| H  | 2.36232200  | 5.21305200 | 2.56910400  |
| H  | 1.94358800  | 0.95098500 | 2.63295900  |
| H  | 2.40379500  | 2.32028100 | 3.64550800  |
| H  | 0.71998200  | 2.11370000 | 3.16916300  |
| H  | 4.49590700  | 3.37755900 | 1.89205400  |
| H  | 4.35996600  | 1.95617100 | 0.85882200  |
| H  | 4.30494700  | 3.58109600 | 0.14838200  |
| Si | 2.14111300  | 3.08473500 | 1.31611400  |
| C  | 2.93944500  | 2.26584300 | -2.05024600 |
| H  | 2.97061800  | 1.69385200 | -2.98105900 |
| H  | 3.38820000  | 3.24622000 | -2.24637100 |
| H  | 3.57010500  | 1.75199600 | -1.32308900 |
| C  | 0.38437700  | 2.29442600 | -3.89536000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.60226000 | 2.00150300  | -4.26549300 |
| H | 0.63989700  | 3.24777100  | -4.37026500 |
| H | 1.11069900  | 1.55384500  | -4.24439600 |
| C | -2.12226500 | 3.05085600  | -2.12313900 |
| H | -2.83629100 | 3.21120400  | -1.31245000 |
| H | -2.06549800 | 3.98238400  | -2.69609300 |
| H | -2.53371000 | 2.29232000  | -2.79833700 |
| C | -1.20399500 | 3.21955000  | 0.90805900  |
| H | -0.70181200 | 3.06170400  | 1.86446900  |
| H | -1.46820400 | 4.28140300  | 0.84653500  |
| H | -2.13174500 | 2.64560000  | 0.93156300  |
| C | -0.97874600 | -2.96920000 | -2.98587100 |
| C | -1.99919200 | -1.94203500 | -2.49489000 |
| H | 0.00934200  | -2.80842300 | -2.53924900 |
| H | -1.30909600 | -3.98467400 | -2.74837800 |
| H | -0.86394100 | -2.89817700 | -4.07253300 |
| C | -3.40394800 | -2.22781300 | -3.04583300 |
| C | -1.54931600 | -0.52649200 | -2.90550100 |
| H | -3.48776600 | -1.99047600 | -4.11031400 |
| H | -3.62372600 | -3.29557400 | -2.92477400 |
| H | -1.86477600 | -0.28293600 | -3.92487400 |
| H | -1.97016700 | 0.25444700  | -2.25706700 |
| H | -0.44877500 | -0.46420900 | -2.93819300 |
| C | -2.24096500 | -2.02376200 | -0.96214600 |
| H | -2.19651700 | -3.08918300 | -0.70750100 |
| N | -1.10839000 | -1.37180500 | -0.23458100 |
| C | -0.99996500 | -1.53891600 | 1.25621600  |
| C | -1.22461800 | -0.20468400 | 1.96996400  |
| C | -1.82311500 | -2.68268400 | 1.84787300  |
| H | 0.05058700  | -1.81076500 | 1.43781200  |
| C | -1.00134500 | -0.33743700 | 3.47694800  |
| H | -2.23260700 | 0.17308000  | 1.76861400  |
| H | -0.51950700 | 0.55357000  | 1.57264300  |
| C | -1.59967000 | -2.77609600 | 3.36093700  |
| H | -2.88576800 | -2.51874000 | 1.64876100  |
| H | -1.53746700 | -3.62640400 | 1.36888700  |
| C | -1.88977400 | -1.44258700 | 4.05045700  |
| H | -1.20406900 | 0.62021100  | 3.96624600  |
| H | 0.05288900  | -0.58057000 | 3.67260900  |
| H | -2.22921400 | -3.56996000 | 3.77262900  |
| H | -0.55772200 | -3.06457900 | 3.55663500  |
| H | -1.73265700 | -1.53140400 | 5.12918900  |
| H | -2.94294600 | -1.17218600 | 3.89559500  |
| C | -4.31767500 | -1.39709000 | -2.15401700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.74959700 | -1.60763400 | -0.72985800 |
| H | -5.36888200 | -1.68769500 | -2.20680000 |
| H | -4.26275900 | -0.34098200 | -2.44023100 |
| H | -4.21675200 | -2.51799100 | -0.33863700 |
| C | -4.14495600 | -0.50365400 | 0.22415300  |
| C | -3.98166000 | 0.84670600  | -0.09494600 |
| C | -4.79271600 | -0.81968200 | 1.42371700  |
| C | -4.44319700 | 1.84661500  | 0.75862400  |
| H | -3.51731500 | 1.12976500  | -1.03473300 |
| C | -5.22379800 | 0.17457400  | 2.29789900  |
| H | -4.97787500 | -1.86178900 | 1.67231200  |
| C | -5.04921800 | 1.51570700  | 1.96784700  |
| H | -4.33870900 | 2.89058500  | 0.47698600  |
| H | -5.71871600 | -0.10004000 | 3.22394400  |
| H | -5.40407800 | 2.29524600  | 2.63337100  |
| N | 1.58482100  | -0.80128600 | -1.60843700 |
| H | -0.31772100 | -1.90825500 | -0.60818300 |
| H | 1.78089800  | -0.99295000 | -2.59042100 |
| C | 2.60731600  | -1.41885100 | -0.76354600 |
| C | 2.26989900  | -2.89091700 | -0.43547500 |
| C | 4.00050800  | -1.38792700 | -1.41550700 |
| C | 2.67747600  | -0.62560600 | 0.54955000  |
| H | 2.22692200  | -3.46396500 | -1.37118600 |
| H | 1.27213800  | -2.95105000 | 0.02629700  |
| C | 3.31040400  | -3.49372100 | 0.52093500  |
| H | 4.25704700  | -0.35204900 | -1.66828800 |
| H | 3.96494400  | -1.95624400 | -2.35544000 |
| C | 5.05417800  | -1.98877900 | -0.47087500 |
| H | 1.68326400  | -0.62383700 | 1.04209300  |
| H | 2.93214000  | 0.41532600  | 0.31583200  |
| C | 3.71372500  | -1.22152400 | 1.51269400  |
| H | 3.04222700  | -4.53231000 | 0.74305000  |
| C | 4.69143700  | -3.44573900 | -0.14888600 |
| C | 3.33772800  | -2.67789800 | 1.82292100  |
| H | 6.03580500  | -1.95015200 | -0.95500500 |
| C | 5.09169400  | -1.17582300 | 0.83152800  |
| H | 3.73765600  | -0.63241900 | 2.43705100  |
| H | 4.68340200  | -4.04497400 | -1.06716100 |
| H | 5.44581200  | -3.87999700 | 0.51770200  |
| H | 2.35513200  | -2.71735200 | 2.31506700  |
| H | 4.06456500  | -3.10876400 | 2.52085400  |
| H | 5.85054300  | -1.58439800 | 1.50871400  |
| H | 5.37278900  | -0.13647300 | 0.61838100  |

cis-ts-12'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.61367100 | 0.86093700  | -1.27773900 |
| C  | -2.55024600 | -0.18751000 | -0.95824800 |
| C  | -2.19962400 | -1.35101800 | -1.68486000 |
| C  | -1.05746400 | -1.03788600 | -2.48131900 |
| C  | -0.70772200 | 0.31867200  | -2.24208000 |
| Sc | -0.35394300 | -0.87045700 | -0.11382800 |
| C  | -1.43357600 | 2.59887700  | 1.23817800  |
| C  | -0.60771100 | 3.84652700  | -1.45022200 |
| C  | -3.52254100 | 3.25367300  | -0.93943300 |
| H  | -2.21406700 | 2.05820300  | 1.78363600  |
| H  | -0.47940900 | 2.10141700  | 1.45182600  |
| H  | -1.37866800 | 3.61212800  | 1.64901800  |
| H  | -0.70328900 | 3.82200600  | -2.53948200 |
| H  | -0.88766600 | 4.85151600  | -1.11617200 |
| H  | 0.44498700  | 3.70239800  | -1.19292200 |
| H  | -3.57063800 | 4.32279800  | -0.70865300 |
| H  | -3.79351800 | 3.12735000  | -1.99197500 |
| H  | -4.27687700 | 2.74947400  | -0.33146700 |
| Si | -1.77676100 | 2.62885700  | -0.61682900 |
| C  | 0.39856700  | 1.01746100  | -2.97824700 |
| H  | 1.24541200  | 0.34474200  | -3.14118900 |
| H  | 0.04632300  | 1.35415800  | -3.95966100 |
| H  | 0.76631900  | 1.89241000  | -2.44301000 |
| C  | -0.44250400 | -1.92043700 | -3.53189800 |
| H  | -0.88316700 | -1.69801900 | -4.50950900 |
| H  | 0.63650700  | -1.76411500 | -3.62108600 |
| H  | -0.61568500 | -2.98095000 | -3.33097100 |
| C  | -2.95404900 | -2.65200900 | -1.70537100 |
| H  | -3.43108800 | -2.86772900 | -0.74443300 |
| H  | -3.74924200 | -2.62413300 | -2.45781400 |
| H  | -2.30360100 | -3.49552100 | -1.95449400 |
| C  | -3.81243900 | -0.03770000 | -0.15626900 |
| H  | -3.69068200 | 0.63762300  | 0.69421700  |
| H  | -4.60669300 | 0.36693500  | -0.79296200 |
| H  | -4.16316500 | -0.99985100 | 0.22591300  |
| C  | 3.24819100  | -3.48534500 | 0.71242000  |
| C  | 2.46001500  | -2.54618700 | -0.20729900 |
| H  | 4.13533600  | -2.98189900 | 1.10875600  |
| H  | 2.66403900  | -3.86225200 | 1.55515200  |
| H  | 3.58847800  | -4.35374100 | 0.14151200  |
| C  | 1.14057800  | -3.18642300 | -0.65480300 |
| C  | 3.32354200  | -2.21947300 | -1.43573600 |
| H  | 0.71420200  | -2.54110400 | -1.44550700 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| H            | 1.30356200  | -4.14436500 | -1.15734300 |
| H            | 3.56575500  | -3.13848000 | -1.97733000 |
| H            | 2.80005800  | -1.53464600 | -2.10784300 |
| H            | 4.26316300  | -1.74745600 | -1.13221000 |
| C            | 2.10818400  | -1.21812200 | 0.49021100  |
| H            | 2.73157500  | -0.97575700 | 1.35696600  |
| N            | 1.60923800  | -0.20775300 | -0.24261900 |
| C            | 2.03075000  | 1.18206800  | 0.01547600  |
| C            | 2.25113600  | 1.56878200  | 1.48215100  |
| C            | 3.29014300  | 1.50059100  | -0.80110300 |
| H            | 1.21670400  | 1.81832400  | -0.36084700 |
| C            | 2.57244700  | 3.06329000  | 1.58333400  |
| H            | 3.09369500  | 1.00441300  | 1.90408500  |
| H            | 1.36360800  | 1.32243700  | 2.07676100  |
| C            | 3.66012100  | 2.98143800  | -0.69157100 |
| H            | 4.11151900  | 0.87775000  | -0.41619500 |
| H            | 3.13025700  | 1.21230600  | -1.84486500 |
| C            | 3.81978000  | 3.41003200  | 0.76776700  |
| H            | 2.70944000  | 3.34418100  | 2.63191600  |
| H            | 1.71567300  | 3.64167100  | 1.20836900  |
| H            | 4.57755200  | 3.18011600  | -1.25349500 |
| H            | 2.86881600  | 3.58266000  | -1.16085300 |
| H            | 4.02650000  | 4.48258200  | 0.82868900  |
| H            | 4.68552600  | 2.89336800  | 1.20318400  |
| C            | 0.15323000  | -3.32113600 | 0.53496200  |
| C            | 0.50299500  | -2.26580000 | 1.57640700  |
| H            | 0.17031300  | -4.33059700 | 0.95711100  |
| H            | -0.88404200 | -3.22814800 | 0.15968000  |
| H            | 1.32166300  | -2.55133500 | 2.22558700  |
| C            | -0.52652200 | -1.52565400 | 2.31867100  |
| C            | -1.91130300 | -1.62942600 | 2.07165300  |
| C            | -0.10118900 | -0.57860000 | 3.28579400  |
| C            | -2.82722700 | -0.85897000 | 2.80596400  |
| H            | -2.30091200 | -2.39661600 | 1.40589300  |
| C            | -1.01125700 | 0.18196500  | 3.99362500  |
| H            | 0.96234500  | -0.48688400 | 3.48917100  |
| C            | -2.38700200 | 0.04089900  | 3.76040400  |
| H            | -3.88985900 | -0.99836600 | 2.63923600  |
| H            | -0.65676700 | 0.88328100  | 4.74194800  |
| H            | -3.09928100 | 0.62448400  | 4.33307600  |
| trans-ts-12' |             |             |             |
| C            | -1.99620200 | -1.24828700 | -0.02968800 |
| C            | -1.63017600 | -1.62785100 | 1.30786600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.59623900 | -2.59235500 | 1.23441400  |
| C  | -0.30383900 | -2.82641000 | -0.14184100 |
| C  | -1.17178800 | -2.01536700 | -0.92100100 |
| Sc | 0.24905700  | -0.43297900 | 0.27983300  |
| C  | -4.94217600 | -1.62181700 | -0.60919300 |
| C  | -4.07047200 | 0.99100100  | 0.72022900  |
| C  | -3.39288400 | 0.49755100  | -2.21091700 |
| H  | -4.70049100 | -2.40631700 | -1.33244400 |
| H  | -5.08848200 | -2.09605600 | 0.36600500  |
| H  | -5.88976800 | -1.16417000 | -0.90971200 |
| H  | -3.26496800 | 1.69289500  | 0.95819800  |
| H  | -4.89098300 | 1.57343300  | 0.28746900  |
| H  | -4.43427500 | 0.56118600  | 1.65681600  |
| H  | -4.19713700 | 1.22947500  | -2.33805100 |
| H  | -2.44213100 | 1.02862400  | -2.31355900 |
| H  | -3.46386200 | -0.21921500 | -3.03248300 |
| Si | -3.57742300 | -0.33366200 | -0.52970000 |
| C  | -1.28283100 | -2.02415100 | -2.42267000 |
| H  | -0.60329700 | -2.75340100 | -2.86684000 |
| H  | -2.29782900 | -2.30072900 | -2.72567800 |
| H  | -1.05420700 | -1.04655800 | -2.85808700 |
| C  | 0.64008100  | -3.90457200 | -0.59761500 |
| H  | 1.65511700  | -3.76200300 | -0.20976800 |
| H  | 0.29133000  | -4.87464500 | -0.22778100 |
| H  | 0.70326800  | -3.97205300 | -1.68425400 |
| C  | 0.03291200  | -3.37134700 | 2.35497300  |
| H  | -0.27432700 | -3.00758100 | 3.33781000  |
| H  | -0.26831300 | -4.42228500 | 2.29171200  |
| H  | 1.12921400  | -3.35643700 | 2.31601500  |
| C  | -2.25792700 | -1.10528500 | 2.57174600  |
| H  | -2.30858200 | -0.01197700 | 2.57621600  |
| H  | -3.28025400 | -1.48205000 | 2.68338000  |
| H  | -1.69925400 | -1.41886400 | 3.45714500  |
| C  | 3.93237900  | 0.30849800  | -2.81270900 |
| C  | 3.05493700  | -0.59923500 | -1.92883400 |
| H  | 3.31768800  | 1.01636000  | -3.37853600 |
| H  | 4.65003300  | 0.87551800  | -2.21058500 |
| H  | 4.49349200  | -0.30151900 | -3.52581600 |
| C  | 3.93980700  | -1.47156800 | -1.00868700 |
| C  | 2.15144000  | -1.44623900 | -2.81682500 |
| H  | 3.50582400  | -2.47720500 | -0.94353800 |
| H  | 4.94516100  | -1.58646000 | -1.42367700 |
| H  | 2.75924900  | -2.13137400 | -3.41563200 |
| H  | 1.46198400  | -2.04717100 | -2.21866700 |



|         |             |             |             |
|---------|-------------|-------------|-------------|
| H       | 1.55658500  | -0.82031600 | -3.48765700 |
| C       | 2.25466300  | 0.36804300  | -1.06279800 |
| H       | 2.88653600  | 1.15696200  | -0.63963800 |
| N       | 0.98891600  | 0.70991600  | -1.32135000 |
| C       | 0.57875700  | 2.08731600  | -0.96615100 |
| C       | 0.04654400  | 2.77976400  | -2.22398400 |
| C       | -0.48191500 | 2.08468200  | 0.14831200  |
| H       | 1.44964900  | 2.64902900  | -0.59089600 |
| C       | -0.51588500 | 4.17072700  | -1.92769800 |
| H       | -0.73320700 | 2.14488200  | -2.66158300 |
| H       | 0.85842300  | 2.82896800  | -2.95686000 |
| C       | -1.03623700 | 3.48578100  | 0.42978700  |
| H       | -1.32635100 | 1.43578700  | -0.15092900 |
| H       | -0.06150000 | 1.72259900  | 1.10694000  |
| C       | -1.59599200 | 4.11024600  | -0.84718300 |
| H       | -0.91578100 | 4.60656900  | -2.84724800 |
| H       | 0.29408200  | 4.83021000  | -1.58946300 |
| H       | -1.79574400 | 3.43179900  | 1.21569000  |
| H       | -0.21929600 | 4.10738100  | 0.81888000  |
| H       | -1.98211900 | 5.11062900  | -0.63325800 |
| H       | -2.44352300 | 3.50762100  | -1.20319800 |
| C       | 3.97611300  | -0.87182300 | 0.39792800  |
| C       | 2.53767000  | -0.69670500 | 0.85201800  |
| H       | 4.50146500  | 0.09041800  | 0.39432500  |
| H       | 4.52668100  | -1.52382400 | 1.08366800  |
| H       | 2.12036200  | -1.69594500 | 1.07559100  |
| C       | 2.13909100  | 0.27452100  | 1.88911200  |
| C       | 2.62918600  | 1.60238100  | 1.92328100  |
| C       | 1.07625900  | -0.03909500 | 2.76646500  |
| C       | 2.06390700  | 2.55087500  | 2.75990500  |
| H       | 3.47208200  | 1.88380500  | 1.29969700  |
| C       | 0.49673200  | 0.93176000  | 3.59866700  |
| H       | 0.76515600  | -1.07468100 | 2.87561200  |
| C       | 0.97825500  | 2.23077700  | 3.58878900  |
| H       | 2.46814300  | 3.55816300  | 2.77061600  |
| H       | -0.31190400 | 0.64859300  | 4.26498700  |
| H       | 0.54235100  | 2.98544200  | 4.23365300  |
| cis-13' |             |             |             |
| C       | -2.41553100 | -0.39316100 | -0.99948400 |
| C       | -2.35703400 | -1.77489500 | -0.60287800 |
| C       | -1.33170800 | -2.41670200 | -1.34093300 |
| C       | -0.76964400 | -1.45463400 | -2.24109000 |
| C       | -1.44833900 | -0.22497100 | -2.05112600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Sc | -0.25082400 | -0.61498700 | -0.02766300 |
| C  | -2.93703800 | 1.02582500  | 1.65538600  |
| C  | -3.39371900 | 2.59006100  | -0.91867700 |
| C  | -5.31301500 | 0.32286100  | -0.17287500 |
| H  | -2.96276400 | 0.06813200  | 2.18572300  |
| H  | -1.92369000 | 1.44099500  | 1.75811000  |
| H  | -3.59618300 | 1.71206600  | 2.19906600  |
| H  | -3.60206600 | 2.58164800  | -1.99163300 |
| H  | -4.13341600 | 3.23898300  | -0.43819800 |
| H  | -2.41165700 | 3.04695100  | -0.76109400 |
| H  | -5.94688600 | 1.10182200  | 0.26273100  |
| H  | -5.64860900 | 0.15181000  | -1.19977100 |
| H  | -5.47688200 | -0.59628000 | 0.39476600  |
| Si | -3.52106200 | 0.88252700  | -0.14508300 |
| C  | -1.18137800 | 1.01752200  | -2.85688800 |
| H  | -0.22042900 | 0.94779200  | -3.37286000 |
| H  | -1.95640600 | 1.14843900  | -3.61915400 |
| H  | -1.17119700 | 1.92489600  | -2.24805000 |
| C  | 0.30347900  | -1.73366200 | -3.25652200 |
| H  | -0.13475600 | -1.89686500 | -4.24651200 |
| H  | 1.01206800  | -0.90513200 | -3.33976500 |
| H  | 0.87164000  | -2.63196400 | -3.00003600 |
| C  | -0.95178300 | -3.87054900 | -1.28689000 |
| H  | -1.25082200 | -4.33678500 | -0.34509100 |
| H  | -1.43906700 | -4.42543000 | -2.09504100 |
| H  | 0.12704200  | -4.01510400 | -1.40420300 |
| C  | -3.28980100 | -2.45357900 | 0.36300300  |
| H  | -3.49898600 | -1.84228600 | 1.24598600  |
| H  | -4.24867100 | -2.65536900 | -0.12560500 |
| H  | -2.89574500 | -3.41385500 | 0.70330700  |
| C  | 5.20947200  | 0.14037600  | -0.29062600 |
| C  | 3.80727500  | -0.16960500 | -0.83143800 |
| H  | 5.31161600  | 1.20647600  | -0.06288600 |
| H  | 5.43202000  | -0.42506800 | 0.62042900  |
| H  | 5.96936300  | -0.11982000 | -1.03404700 |
| C  | 3.68213300  | -1.69202700 | -1.15297700 |
| C  | 3.57731000  | 0.65281700  | -2.09577400 |
| H  | 3.38612000  | -1.86206000 | -2.19225100 |
| H  | 4.64785000  | -2.18803400 | -1.01206500 |
| H  | 4.26797400  | 0.31591700  | -2.87537500 |
| H  | 2.55482800  | 0.52909300  | -2.46380600 |
| H  | 3.76098700  | 1.71739400  | -1.93194800 |
| C  | 2.76729300  | 0.08041500  | 0.32001700  |
| H  | 3.15688900  | 0.84462800  | 1.00675500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.40602900  | 0.41889600  | -0.07673300 |
| C | 0.87578900  | 1.77486000  | 0.04445800  |
| C | 0.92577100  | 2.36219700  | 1.46513000  |
| C | 1.39648500  | 2.79659000  | -0.97424500 |
| H | -0.22760300 | 1.68316400  | -0.19347000 |
| C | 0.19575400  | 3.70545000  | 1.55676700  |
| H | 1.97493800  | 2.50314000  | 1.75768500  |
| H | 0.49348100  | 1.64123100  | 2.16907100  |
| C | 0.66900300  | 4.13869900  | -0.87160900 |
| H | 2.46349400  | 2.94921500  | -0.76325300 |
| H | 1.32024800  | 2.38320700  | -1.98364700 |
| C | 0.74823100  | 4.70793200  | 0.54441300  |
| H | 0.27304900  | 4.09815300  | 2.57505300  |
| H | -0.87566100 | 3.55224600  | 1.35932600  |
| H | 1.09115100  | 4.84205600  | -1.59510200 |
| H | -0.38695500 | 4.00374100  | -1.14864800 |
| H | 0.20127600  | 5.65301900  | 0.60812700  |
| H | 1.79621800  | 4.92762700  | 0.78723200  |
| C | 2.65059200  | -2.26627700 | -0.17800400 |
| C | 2.70885500  | -1.31463900 | 1.02039200  |
| H | 2.82172700  | -3.31423500 | 0.08507500  |
| H | 1.65367700  | -2.22826600 | -0.65723100 |
| H | 3.65111100  | -1.48595300 | 1.55550200  |
| C | 1.56188100  | -1.41631700 | 1.99996800  |
| C | 0.47554500  | -2.28610500 | 1.78943200  |
| C | 1.50893700  | -0.56245700 | 3.11206200  |
| C | -0.65470200 | -2.25093100 | 2.62589100  |
| H | 0.52511100  | -3.04995000 | 1.01326700  |
| C | 0.39657300  | -0.53394400 | 3.94399200  |
| H | 2.34558400  | 0.10369600  | 3.30611700  |
| C | -0.70311900 | -1.36157600 | 3.69286100  |
| H | -1.47006600 | -2.94479000 | 2.45097000  |
| H | 0.37860100  | 0.14212700  | 4.79271500  |
| H | -1.57098200 | -1.33279800 | 4.34250800  |

trans-13'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.37164500 | -0.59883100 | -0.70132500 |
| C  | -2.19401700 | -1.92475200 | -0.17131600 |
| C  | -1.23429200 | -2.60240200 | -0.95547600 |
| C  | -0.79467100 | -1.71158800 | -1.98450900 |
| C  | -1.50606200 | -0.49315200 | -1.84729100 |
| Sc | -0.10305400 | -0.61938800 | 0.10158200  |
| C  | -5.37715600 | -0.28567600 | -0.96257000 |
| C  | -4.03168400 | 0.63169900  | 1.63597600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.68603900 | 2.24293700  | -0.95847300 |
| H  | -5.30352800 | -0.34061800 | -2.05281600 |
| H  | -5.53415300 | -1.29990300 | -0.58465200 |
| H  | -6.26326800 | 0.30630400  | -0.71268800 |
| H  | -3.09527800 | 0.83882000  | 2.16401300  |
| H  | -4.72315100 | 1.44871500  | 1.86705400  |
| H  | -4.45853200 | -0.28372100 | 2.05430200  |
| H  | -4.48628800 | 2.86016700  | -0.53609700 |
| H  | -2.73645000 | 2.73457000  | -0.72986900 |
| H  | -3.81177600 | 2.23557900  | -2.04468200 |
| Si | -3.83536200 | 0.51012200  | -0.23801400 |
| C  | -1.39053700 | 0.67044700  | -2.79364000 |
| H  | -0.40393100 | 0.70460200  | -3.26149900 |
| H  | -2.13941000 | 0.59090900  | -3.58950600 |
| H  | -1.54517500 | 1.62406100  | -2.28973200 |
| C  | 0.18031000  | -2.08153400 | -3.06859700 |
| H  | 1.10569200  | -2.51469600 | -2.67079500 |
| H  | -0.26031300 | -2.83056100 | -3.73497900 |
| H  | 0.45131200  | -1.21825100 | -3.67817100 |
| C  | -0.84925700 | -4.05290500 | -0.86825600 |
| H  | -0.82167600 | -4.42903400 | 0.15743200  |
| H  | -1.57689100 | -4.66272600 | -1.41387000 |
| H  | 0.12611600  | -4.24113300 | -1.32580700 |
| C  | -2.92118900 | -2.51828500 | 1.00702900  |
| H  | -2.73022100 | -1.97733200 | 1.94085700  |
| H  | -4.00397200 | -2.50284700 | 0.84762600  |
| H  | -2.63314000 | -3.56080200 | 1.15925900  |
| C  | 4.02311000  | 2.57710500  | -1.09953600 |
| C  | 3.48676800  | 1.17565900  | -1.39805800 |
| H  | 3.21912600  | 3.27246500  | -0.83882100 |
| H  | 4.72734800  | 2.54943200  | -0.26085000 |
| H  | 4.54954600  | 2.98421800  | -1.96850100 |
| C  | 4.66846400  | 0.16708100  | -1.57805700 |
| C  | 2.59296600  | 1.19970900  | -2.63707200 |
| H  | 4.54202600  | -0.38266800 | -2.51732200 |
| H  | 5.63380800  | 0.67683300  | -1.63415900 |
| H  | 3.17640400  | 1.47106200  | -3.52240900 |
| H  | 2.14358100  | 0.21510900  | -2.81622100 |
| H  | 1.77786200  | 1.92046600  | -2.52069900 |
| C  | 2.71548100  | 0.60392800  | -0.16842500 |
| H  | 3.19264600  | 1.03785100  | 0.72923800  |
| N  | 1.28272100  | 0.78541000  | -0.03269900 |
| C  | 0.82855200  | 1.96454600  | 0.70807500  |
| C  | 0.35901600  | 3.14106900  | -0.15588500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.32568200 | 1.55786300  | 1.64910900  |
| H | 1.65090200  | 2.31370100  | 1.35647500  |
| C | -0.10394400 | 4.32299400  | 0.70241100  |
| H | -0.46563700 | 2.78720700  | -0.79186100 |
| H | 1.16019400  | 3.44965400  | -0.83285000 |
| C | -0.79678000 | 2.72268000  | 2.52837100  |
| H | -1.21064200 | 1.23381100  | 1.05469800  |
| H | -0.00484600 | 0.72961100  | 2.30550900  |
| C | -1.21386400 | 3.92059600  | 1.67636900  |
| H | -0.44306200 | 5.14046000  | 0.05954100  |
| H | 0.75337700  | 4.70495400  | 1.27269500  |
| H | -1.61647400 | 2.40193900  | 3.17822000  |
| H | 0.03774100  | 3.00618300  | 3.18156600  |
| H | -1.47282300 | 4.76191800  | 2.32551800  |
| H | -2.12340300 | 3.66368300  | 1.11827500  |
| C | 4.60254800  | -0.82617100 | -0.40066000 |
| C | 3.09795200  | -0.89380800 | -0.14761100 |
| H | 5.11360700  | -0.42629800 | 0.48324200  |
| H | 5.04743200  | -1.79552000 | -0.63455500 |
| H | 2.64870700  | -1.38356800 | -1.02840800 |
| C | 2.53043600  | -1.52682800 | 1.09651300  |
| C | 2.89055800  | -1.08026000 | 2.37541400  |
| C | 1.46957900  | -2.44311200 | 0.99577300  |
| C | 2.17822900  | -1.48765100 | 3.49797300  |
| H | 3.72110100  | -0.38949900 | 2.48868700  |
| C | 0.72961300  | -2.83614800 | 2.12595900  |
| H | 1.25965200  | -2.90768200 | 0.03081900  |
| C | 1.07611000  | -2.34072500 | 3.37839200  |
| H | 2.47297900  | -1.12652000 | 4.47797700  |
| H | -0.08296100 | -3.54923500 | 2.02431200  |
| H | 0.51877500  | -2.64101100 | 4.25872800  |

trans-P3

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.47673800 | -1.07920400 | 1.46710900  |
| C | -2.94138000 | -0.39791200 | 0.20890000  |
| H | -3.23597900 | -2.14847800 | 1.48600400  |
| H | -3.05772200 | -0.62132000 | 2.36951500  |
| H | -4.56724000 | -0.99343400 | 1.51682600  |
| C | -3.23033200 | 1.10809900  | 0.20813400  |
| C | -3.55218600 | -1.05625700 | -1.03503000 |
| H | -4.28412100 | 1.33127100  | 0.01121900  |
| H | -2.98578300 | 1.52191100  | 1.19577000  |
| H | -4.63600000 | -0.89842600 | -1.04403100 |
| H | -3.13691900 | -0.64597000 | -1.95975200 |

|        |             |             |             |
|--------|-------------|-------------|-------------|
| H      | -3.36396200 | -2.13253800 | -1.04866400 |
| C      | -1.39044000 | -0.40761400 | 0.15321700  |
| H      | -1.04871100 | -0.14997500 | 1.17146000  |
| N      | -0.90088800 | -1.71657200 | -0.26971700 |
| C      | 0.51384100  | -2.06785700 | -0.06144900 |
| C      | 1.36828300  | -1.69427900 | -1.27617600 |
| C      | 1.14917300  | -1.53931900 | 1.23213500  |
| H      | 0.52852600  | -3.16680300 | 0.00011100  |
| C      | 2.81021400  | -2.18091000 | -1.11690200 |
| H      | 1.37509100  | -0.60547300 | -1.38761500 |
| H      | 0.90368300  | -2.11351500 | -2.17464700 |
| C      | 2.58784000  | -2.03890200 | 1.38538700  |
| H      | 1.16370000  | -0.44184200 | 1.21006000  |
| H      | 0.53808500  | -1.83815400 | 2.09375800  |
| C      | 3.43032300  | -1.63804500 | 0.17242700  |
| H      | 3.40707200  | -1.88307900 | -1.98541900 |
| H      | 2.82315400  | -3.27959300 | -1.08576600 |
| H      | 3.02720100  | -1.64174200 | 2.30641000  |
| H      | 2.58950300  | -3.13398700 | 1.47875900  |
| H      | 4.45896600  | -1.99686300 | 0.28490600  |
| H      | 3.47379000  | -0.54103100 | 0.11477900  |
| C      | -2.28181100 | 1.67555700  | -0.85278000 |
| C      | -1.00498500 | 0.77683900  | -0.78778300 |
| H      | -2.04281000 | 2.72756300  | -0.68023700 |
| H      | -2.73703400 | 1.60708400  | -1.84489200 |
| H      | -0.79342900 | 0.35781400  | -1.77794600 |
| C      | 0.19815900  | 1.58275000  | -0.34267000 |
| C      | 0.27680700  | 2.10866700  | 0.95324600  |
| C      | 1.23527200  | 1.87683400  | -1.23131800 |
| C      | 1.37307800  | 2.86473400  | 1.35674000  |
| H      | -0.52834600 | 1.91978800  | 1.65984200  |
| C      | 2.33661400  | 2.63243900  | -0.83347700 |
| H      | 1.18080200  | 1.50143500  | -2.25036600 |
| C      | 2.41367800  | 3.12300000  | 0.46631200  |
| H      | 1.41523100  | 3.25391500  | 2.36939600  |
| H      | 3.13316900  | 2.83684600  | -1.54230600 |
| H      | 3.27169800  | 3.70806000  | 0.78122600  |
| H      | -1.45786500 | -2.40918500 | 0.22349200  |
| cis-P3 |             |             |             |
| C      | -3.53679000 | -0.97944900 | 1.47070900  |
| C      | -2.85133800 | -0.85797700 | 0.10328200  |
| H      | -3.08510900 | -1.78056700 | 2.06561900  |
| H      | -3.45691100 | -0.04757400 | 2.03993900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.60115400 | -1.20468900 | 1.34639000  |
| C | -3.54124800 | 0.25352000  | -0.74946000 |
| C | -2.93182700 | -2.21901800 | -0.59330200 |
| H | -3.98203400 | -0.15345800 | -1.66458300 |
| H | -4.35781300 | 0.70716000  | -0.17604600 |
| H | -3.97188100 | -2.55976000 | -0.61207800 |
| H | -2.59254900 | -2.16807400 | -1.63309400 |
| H | -2.34176100 | -2.97824900 | -0.06634900 |
| C | -1.39107000 | -0.34267300 | 0.32796300  |
| H | -1.06765900 | -0.59531300 | 1.35091800  |
| N | -0.42937500 | -0.83457200 | -0.65727400 |
| C | 0.92916100  | -1.03809400 | -0.14407400 |
| C | 1.06952400  | -2.28376700 | 0.74246200  |
| C | 1.91379800  | -1.11547300 | -1.31070500 |
| H | 1.19052100  | -0.15545400 | 0.45537300  |
| C | 2.50460200  | -2.45202900 | 1.24877300  |
| H | 0.78894000  | -3.16473200 | 0.14452100  |
| H | 0.36822100  | -2.23414700 | 1.58390500  |
| C | 3.35261800  | -1.28312000 | -0.81919500 |
| H | 1.63829400  | -1.97187700 | -1.94485300 |
| H | 1.80999400  | -0.21365400 | -1.92175400 |
| C | 3.49295900  | -2.51227100 | 0.08144200  |
| H | 2.58725400  | -3.35071400 | 1.86915700  |
| H | 2.75899700  | -1.59780600 | 1.89080400  |
| H | 4.03887200  | -1.35245100 | -1.66975500 |
| H | 3.63775200  | -0.38508100 | -0.25383700 |
| H | 4.51891800  | -2.59908900 | 0.45446800  |
| H | 3.29107200  | -3.41565800 | -0.51052800 |
| C | -2.45852000 | 1.30135600  | -1.03957200 |
| C | -1.55053600 | 1.19865400  | 0.18708300  |
| H | -2.85530200 | 2.30770900  | -1.19831800 |
| H | -1.89202700 | 1.00881100  | -1.92881100 |
| H | -2.12225700 | 1.54037600  | 1.06201000  |
| C | -0.25156600 | 1.96260800  | 0.16427000  |
| C | 0.48623100  | 2.14193600  | -1.00955400 |
| C | 0.28266000  | 2.44908800  | 1.36210800  |
| C | 1.73020200  | 2.76790200  | -0.98102100 |
| H | 0.09679400  | 1.76536800  | -1.94935000 |
| C | 1.52532100  | 3.07481000  | 1.39607600  |
| H | -0.28241800 | 2.32208500  | 2.28291500  |
| C | 2.25773600  | 3.23189300  | 0.22168600  |
| H | 2.29081500  | 2.88990200  | -1.90319700 |
| H | 1.92116100  | 3.44061900  | 2.33857900  |
| H | 3.22783600  | 3.71841900  | 0.24269600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.74243000 | -1.71747000 | -1.04764100 |
| 16 |             |             |             |
| C  | -1.18500100 | 2.27040500  | -0.17448300 |
| C  | -1.61555000 | 2.04728200  | 1.17534500  |
| C  | -2.86644800 | 1.37951700  | 1.15607300  |
| C  | -3.24460000 | 1.18675500  | -0.20664800 |
| C  | -2.21870600 | 1.72623400  | -1.02181400 |
| Sc | -1.22073300 | -0.17472600 | 0.19413000  |
| C  | 1.01785400  | 4.40065000  | 0.57489500  |
| C  | 1.34235400  | 2.85507200  | -2.02303700 |
| C  | -0.92029400 | 4.88056500  | -1.69959800 |
| H  | 0.34831500  | 4.88608700  | 1.29043900  |
| H  | 1.69857900  | 3.75092800  | 1.13309800  |
| H  | 1.62754900  | 5.18449100  | 0.11169900  |
| H  | 0.94414100  | 2.09332800  | -2.70017900 |
| H  | 1.70701900  | 3.68180700  | -2.64184600 |
| H  | 2.21331600  | 2.43655000  | -1.50852300 |
| H  | -0.27900600 | 5.74966300  | -1.87917200 |
| H  | -1.29576500 | 4.54286400  | -2.66884300 |
| H  | -1.77401800 | 5.20857000  | -1.09924600 |
| Si | 0.06429400  | 3.54514800  | -0.80797100 |
| C  | -2.29989600 | 1.87092900  | -2.51860100 |
| H  | -2.86121800 | 1.05856700  | -2.98644000 |
| H  | -2.82201500 | 2.79789600  | -2.77845400 |
| H  | -1.31171900 | 1.90978100  | -2.98564600 |
| C  | -4.56098200 | 0.63207000  | -0.67035500 |
| H  | -4.92819100 | -0.14922300 | 0.00045300  |
| H  | -5.31412300 | 1.42690300  | -0.70432200 |
| H  | -4.49692000 | 0.20385400  | -1.67463300 |
| C  | -3.70575100 | 1.07362900  | 2.36152000  |
| H  | -3.10243300 | 0.70084600  | 3.19448700  |
| H  | -4.21501600 | 1.98002100  | 2.70718000  |
| H  | -4.47074300 | 0.32753800  | 2.13772700  |
| C  | -0.94042800 | 2.45873400  | 2.45601700  |
| H  | 0.09888500  | 2.74674000  | 2.30487600  |
| H  | -1.45903800 | 3.31454300  | 2.90265300  |
| H  | -0.96507000 | 1.64936100  | 3.19475800  |
| C  | -5.17484800 | -2.68854400 | 1.21175200  |
| C  | -5.18190600 | -2.93323000 | -0.16409900 |
| C  | -4.02199600 | -2.74206700 | -0.89702400 |
| C  | -2.84848100 | -2.31585400 | -0.26465000 |
| C  | -2.79950900 | -2.10173500 | 1.13545900  |
| C  | -4.01013900 | -2.27808900 | 1.83789400  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.07884200 | -2.83264900 | 1.79434900  |
| H | -6.08585900 | -3.26827900 | -0.66040400 |
| H | -4.03196100 | -2.92743700 | -1.96510000 |
| H | -4.00357600 | -2.10740800 | 2.91043000  |
| N | -1.62041300 | -2.08907700 | -1.03369500 |
| C | -0.73534300 | -3.27344200 | -0.95048900 |
| H | -1.23077100 | -4.13555500 | -1.41210200 |
| H | 0.19810100  | -3.07671300 | -1.48335900 |
| H | -0.52411200 | -3.51362400 | 0.09240300  |
| C | -1.85864300 | -1.77121900 | -2.45761900 |
| H | -2.63728400 | -1.01116400 | -2.53966400 |
| H | -0.93312300 | -1.38918800 | -2.89738000 |
| H | -2.16308200 | -2.65818600 | -3.02408800 |
| C | -1.57239200 | -1.61057200 | 1.82040100  |
| H | -0.74764200 | -2.33450600 | 1.78788100  |
| H | -1.77240800 | -1.35621300 | 2.86175700  |
| N | 1.04945300  | -0.45583200 | 0.33367500  |
| H | 1.13280500  | -1.35193700 | 0.81941700  |
| C | 1.69786300  | 0.57104700  | 1.20386300  |
| H | 1.44414300  | 1.54767900  | 0.78267700  |
| H | 1.20732500  | 0.49356700  | 2.18174700  |
| C | 1.68346100  | -0.61314400 | -1.00336200 |
| H | 0.92047900  | -1.01661800 | -1.68419000 |
| H | 1.93198600  | 0.38405200  | -1.37032700 |
| C | 3.19564300  | 0.44898200  | 1.33405800  |
| C | 3.77025900  | -0.66006300 | 1.96068400  |
| C | 4.02295800  | 1.43399100  | 0.79734000  |
| C | 5.15117300  | -0.79903700 | 2.01431800  |
| H | 3.13362200  | -1.42912300 | 2.39442400  |
| C | 5.40969900  | 1.30551700  | 0.86287800  |
| H | 3.58234200  | 2.31100600  | 0.32810600  |
| C | 5.97350500  | 0.18459200  | 1.46217900  |
| H | 5.58953100  | -1.67124900 | 2.48776400  |
| H | 6.04542600  | 2.07861400  | 0.44401600  |
| H | 7.05216500  | 0.07621900  | 1.50697200  |
| C | 2.91004000  | -1.50082800 | -1.02798300 |
| C | 4.10308300  | -1.02784600 | -1.57321100 |
| C | 2.87086400  | -2.79370800 | -0.50010000 |
| C | 5.24272700  | -1.82768600 | -1.57793900 |
| H | 4.14766400  | -0.01648700 | -1.96898600 |
| C | 4.00929500  | -3.59375500 | -0.49994100 |
| H | 1.95427600  | -3.18772700 | -0.06537900 |
| C | 5.19924900  | -3.11027800 | -1.03834500 |
| H | 6.16852100  | -1.44167700 | -1.99178200 |

|       |             |             |             |
|-------|-------------|-------------|-------------|
| H     | 3.96596200  | -4.59350400 | -0.08053700 |
| H     | 6.08907400  | -3.73072300 | -1.03598400 |
| ts-17 |             |             |             |
| C     | 2.16475000  | 1.98333000  | -0.31322000 |
| C     | 2.01647500  | 1.42500800  | -1.62069500 |
| C     | 2.75989700  | 0.21548300  | -1.68882500 |
| C     | 3.43205500  | 0.04032300  | -0.43868200 |
| C     | 3.06899000  | 1.11906300  | 0.40350000  |
| Sc    | 0.99418100  | -0.11562700 | -0.04149300 |
| C     | 0.07057100  | 4.30923300  | -0.59756500 |
| C     | 1.04860600  | 3.47359400  | 2.16183000  |
| C     | 2.95861400  | 4.88721500  | 0.19827400  |
| H     | 0.32429400  | 4.60654100  | -1.61822700 |
| H     | -0.75286500 | 3.58982000  | -0.64292600 |
| H     | -0.29776600 | 5.19923300  | -0.07655700 |
| H     | 0.47174400  | 2.56094700  | 2.35422300  |
| H     | 1.91279300  | 3.47623000  | 2.83076000  |
| H     | 0.41698600  | 4.32342400  | 2.44027000  |
| H     | 2.64458900  | 5.86491100  | 0.57696600  |
| H     | 3.84408300  | 4.57746600  | 0.76034800  |
| H     | 3.25105400  | 5.00888400  | -0.84905400 |
| Si    | 1.55578600  | 3.64500600  | 0.34832300  |
| C     | 3.64648500  | 1.39389100  | 1.76913500  |
| H     | 4.37841800  | 0.63230500  | 2.04757800  |
| H     | 4.16919800  | 2.35591500  | 1.76993600  |
| H     | 2.89156800  | 1.44141500  | 2.55902800  |
| C     | 4.43753900  | -1.03568500 | -0.14819700 |
| H     | 4.16660700  | -1.97971400 | -0.62754900 |
| H     | 5.42136700  | -0.74017600 | -0.52850900 |
| H     | 4.54216700  | -1.22817200 | 0.92255900  |
| C     | 2.93074900  | -0.65472300 | -2.90239600 |
| H     | 2.00696300  | -0.73654300 | -3.48316500 |
| H     | 3.69722700  | -0.24207500 | -3.56678500 |
| H     | 3.24234500  | -1.66452800 | -2.62507300 |
| C     | 1.28240200  | 2.02797200  | -2.78526900 |
| H     | 0.36790000  | 2.53699600  | -2.48194100 |
| H     | 1.92102100  | 2.76485300  | -3.28540000 |
| H     | 1.02108700  | 1.27190900  | -3.53049900 |
| C     | 2.97438300  | -4.48172700 | -0.75917000 |
| C     | 3.30693300  | -4.35299300 | 0.58959600  |
| C     | 2.62869100  | -3.43897100 | 1.38162100  |
| C     | 1.60204200  | -2.65928400 | 0.83847700  |
| C     | 1.22051900  | -2.79878300 | -0.51354300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.95110200  | -3.71276900 | -1.29303500 |
| H | 3.50600300  | -5.18738700 | -1.38832700 |
| H | 4.09575600  | -4.95820900 | 1.02250100  |
| H | 2.89914400  | -3.33673400 | 2.42607300  |
| H | 1.67735800  | -3.82870700 | -2.33788000 |
| N | 0.89595600  | -1.67135700 | 1.64881000  |
| C | -0.42337000 | -2.19752400 | 2.07928500  |
| H | -0.27158500 | -3.06391900 | 2.73312800  |
| H | -0.96862700 | -1.42307800 | 2.62277300  |
| H | -1.00845000 | -2.50114900 | 1.21309200  |
| C | 1.63730300  | -1.22181500 | 2.84399600  |
| H | 2.66337300  | -0.96563000 | 2.57467400  |
| H | 1.13861000  | -0.33595300 | 3.24939300  |
| H | 1.64681300  | -1.99228400 | 3.62318500  |
| C | 0.06590800  | -2.04137800 | -1.13801800 |
| H | -0.85142600 | -2.63668800 | -1.02093400 |
| H | 0.23412300  | -1.95833700 | -2.21780400 |
| N | -1.01026700 | 0.36511100  | -0.43507200 |
| H | -0.66729100 | -0.91371900 | -0.68616300 |
| C | -1.68590800 | 0.83930600  | -1.65211100 |
| H | -1.67984400 | 1.93755300  | -1.65637000 |
| H | -1.07336100 | 0.51256100  | -2.50146800 |
| C | -1.53328100 | 0.84960100  | 0.83629400  |
| H | -0.75288300 | 0.68198100  | 1.61529400  |
| H | -1.64067000 | 1.94485600  | 0.79499000  |
| C | -3.10331300 | 0.34489500  | -1.82752000 |
| C | -3.34594300 | -0.90846800 | -2.39306500 |
| C | -4.18045300 | 1.10209500  | -1.36697700 |
| C | -4.64058000 | -1.41583300 | -2.45835000 |
| H | -2.51311200 | -1.49471500 | -2.77842800 |
| C | -5.47698300 | 0.60045000  | -1.43124200 |
| H | -3.99827300 | 2.08167800  | -0.93003700 |
| C | -5.70716400 | -0.66376900 | -1.96907700 |
| H | -4.81866400 | -2.39245300 | -2.89719500 |
| H | -6.30608900 | 1.19228800  | -1.05741900 |
| H | -6.71681500 | -1.05840000 | -2.01760200 |
| C | -2.82348800 | 0.25029700  | 1.37643400  |
| C | -3.54167000 | 0.97696500  | 2.32727600  |
| C | -3.30437900 | -0.99454400 | 0.97200500  |
| C | -4.72359900 | 0.47098500  | 2.86258600  |
| H | -3.18130100 | 1.95417900  | 2.64175100  |
| C | -4.48944700 | -1.49908700 | 1.49763500  |
| H | -2.78119600 | -1.55060400 | 0.20020800  |
| C | -5.20161900 | -0.76869600 | 2.44640900  |

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|----|-------------|-------------|-------------|
| H  | -5.27513800 | 1.05017800  | 3.59593000  |
| H  | -4.86398500 | -2.45751600 | 1.15291700  |
| H  | -6.12878400 | -1.15956100 | 2.85204000  |
| 18 |             |             |             |
| C  | -2.13920800 | 1.97562900  | 0.13794200  |
| C  | -1.79000300 | 1.59286200  | 1.47177000  |
| C  | -2.37402400 | 0.32568100  | 1.74711900  |
| C  | -3.12864600 | -0.07820500 | 0.60940700  |
| C  | -2.98310400 | 0.92743200  | -0.38037400 |
| Sc | -0.70232000 | 0.03603300  | -0.08881100 |
| C  | -0.86020400 | 4.87494000  | 0.13684800  |
| C  | -0.72797900 | 3.11837300  | -2.35341300 |
| C  | -3.40678400 | 4.31540500  | -1.40073800 |
| H  | -1.42160100 | 5.20293500  | 1.01617700  |
| H  | 0.14047500  | 4.56791000  | 0.45193500  |
| H  | -0.74151500 | 5.74444000  | -0.51907700 |
| H  | -0.96122200 | 2.12338000  | -2.75347900 |
| H  | -0.87491700 | 3.84560900  | -3.15779300 |
| H  | 0.33074400  | 3.12743700  | -2.07855300 |
| H  | -3.22559900 | 5.34095400  | -1.73876800 |
| H  | -3.86407300 | 3.77238600  | -2.23108900 |
| H  | -4.12936400 | 4.35661100  | -0.58016400 |
| Si | -1.77605900 | 3.55513800  | -0.84259700 |
| C  | -3.76235100 | 0.98542100  | -1.66902900 |
| H  | -4.19344300 | 0.01599600  | -1.92797900 |
| H  | -4.59959400 | 1.68151800  | -1.56004400 |
| H  | -3.16402200 | 1.33061700  | -2.51859600 |
| C  | -4.07020000 | -1.24782600 | 0.58033500  |
| H  | -3.70921000 | -2.07547000 | 1.19726500  |
| H  | -5.04744100 | -0.94422400 | 0.97200900  |
| H  | -4.23317900 | -1.63487300 | -0.42879700 |
| C  | -2.36678200 | -0.36912000 | 3.08024800  |
| H  | -1.49151900 | -0.09401200 | 3.67656500  |
| H  | -3.25305500 | -0.08679200 | 3.65868500  |
| H  | -2.38315100 | -1.45837100 | 2.97316300  |
| C  | -1.07648700 | 2.40397000  | 2.52169200  |
| H  | -0.67615000 | 3.33181500  | 2.11762700  |
| H  | -1.78105100 | 2.66986700  | 3.31723300  |
| H  | -0.25295100 | 1.85947300  | 2.99548800  |
| C  | -2.43126500 | -4.74965200 | 1.49656400  |
| C  | -2.89632700 | -4.74439600 | 0.18512400  |
| C  | -2.36722000 | -3.84719000 | -0.73646500 |
| C  | -1.38276600 | -2.93905900 | -0.34847700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.88979900 | -2.94660000 | 0.96548800  |
| C | -1.43068800 | -3.86121400 | 1.87382300  |
| H | -2.83663200 | -5.44844000 | 2.21969700  |
| H | -3.66774700 | -5.43966200 | -0.12711800 |
| H | -2.73424800 | -3.85772300 | -1.75644300 |
| H | -1.05198000 | -3.87299000 | 2.89218900  |
| N | -0.80833000 | -1.99293400 | -1.30588700 |
| C | 0.42524100  | -2.60458500 | -1.88106100 |
| H | 0.16284100  | -3.56625700 | -2.33555800 |
| H | 0.84529900  | -1.94885400 | -2.64510100 |
| H | 1.17786800  | -2.76603800 | -1.10907300 |
| C | -1.71620300 | -1.66946100 | -2.43213700 |
| H | -2.71768300 | -1.46478800 | -2.05586900 |
| H | -1.33872400 | -0.78020300 | -2.95120600 |
| H | -1.76196600 | -2.48625500 | -3.16038200 |
| C | 0.18368400  | -1.99270100 | 1.43532900  |
| H | 0.79551700  | -2.44419200 | 2.21966900  |
| H | -0.24617400 | -1.10021500 | 1.92806700  |
| N | 1.01436400  | 0.97348200  | -0.30766500 |
| H | 0.89558800  | -1.69337300 | 0.65789800  |
| C | 1.71330100  | 2.04707600  | 0.39163000  |
| H | 2.07498500  | 2.79243400  | -0.33389900 |
| H | 0.98718800  | 2.55043400  | 1.03694900  |
| C | 1.57162500  | 0.62337500  | -1.60344800 |
| H | 0.76610700  | 0.15102300  | -2.20957800 |
| H | 1.81204500  | 1.53797600  | -2.16793200 |
| C | 2.86885800  | 1.57251200  | 1.24832900  |
| C | 2.60543600  | 0.81409600  | 2.39301300  |
| C | 4.19238800  | 1.81447800  | 0.88972600  |
| C | 3.64387200  | 0.28709800  | 3.15307100  |
| H | 1.57096800  | 0.62397800  | 2.67856300  |
| C | 5.23821300  | 1.29095400  | 1.64852600  |
| H | 4.40824700  | 2.39877700  | -0.00119800 |
| C | 4.96675700  | 0.52158800  | 2.77590600  |
| H | 3.42628000  | -0.29873800 | 4.04082300  |
| H | 6.26556700  | 1.47943000  | 1.35411300  |
| H | 5.78068400  | 0.11174200  | 3.36487600  |
| C | 2.77160300  | -0.31230300 | -1.67401900 |
| C | 3.36297600  | -0.51599200 | -2.92498400 |
| C | 3.26686700  | -1.01173500 | -0.57484600 |
| C | 4.41657500  | -1.41077600 | -3.07825600 |
| H | 2.99147700  | 0.03335900  | -3.78817700 |
| C | 4.32877400  | -1.90397000 | -0.72418000 |
| H | 2.84701300  | -0.83598900 | 0.40987900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.90183500  | -2.11167700 | -1.97484500 |
| H  | 4.86323600  | -1.55711400 | -4.05644200 |
| H  | 4.71282700  | -2.42771400 | 0.14575900  |
| H  | 5.72677800  | -2.80685500 | -2.08976800 |
| 19 |             |             |             |
| C  | -2.53340100 | -0.53997200 | -1.46455800 |
| C  | -1.71901500 | -0.11632600 | -2.56774800 |
| C  | -1.65822300 | 1.29937300  | -2.56897800 |
| C  | -2.46415700 | 1.78187200  | -1.48714700 |
| C  | -3.01691500 | 0.65956300  | -0.83110700 |
| Sc | -0.54885700 | 0.50174300  | -0.54442900 |
| C  | -2.33353400 | -3.60090700 | -2.11838600 |
| C  | -2.90484500 | -2.75861900 | 0.72200500  |
| C  | -5.02506800 | -2.29645300 | -1.44611200 |
| H  | -2.46500000 | -3.45113000 | -3.19250900 |
| H  | -1.26156200 | -3.67045200 | -1.90782400 |
| H  | -2.78107800 | -4.56647100 | -1.85948900 |
| H  | -3.39980400 | -2.08850300 | 1.43183400  |
| H  | -3.32366300 | -3.75855800 | 0.87962800  |
| H  | -1.84123400 | -2.80974600 | 0.98490000  |
| H  | -5.42605000 | -3.30662000 | -1.31717500 |
| H  | -5.57949400 | -1.63011400 | -0.77946200 |
| H  | -5.22091600 | -1.98415800 | -2.47607100 |
| Si | -3.18102500 | -2.27864600 | -1.08415100 |
| C  | -4.08306100 | 0.74235800  | 0.22551300  |
| H  | -4.03042600 | 1.67974400  | 0.78459900  |
| H  | -5.07192800 | 0.70986600  | -0.24580300 |
| H  | -4.03927800 | -0.08558100 | 0.93823300  |
| C  | -2.76809300 | 3.21680700  | -1.15177100 |
| H  | -2.07775100 | 3.90815200  | -1.64215300 |
| H  | -3.77784500 | 3.48519700  | -1.47935200 |
| H  | -2.71472300 | 3.40286400  | -0.07341500 |
| C  | -0.93239800 | 2.12922700  | -3.59421100 |
| H  | 0.12176200  | 1.84435400  | -3.69082000 |
| H  | -1.39085100 | 2.00359400  | -4.57978100 |
| H  | -0.96708800 | 3.19346400  | -3.35190800 |
| C  | -1.04197700 | -0.98285200 | -3.59208900 |
| H  | -0.56221200 | -1.85500600 | -3.14190600 |
| H  | -1.76342400 | -1.34469100 | -4.33254500 |
| H  | -0.27350900 | -0.42087200 | -4.12937300 |
| N  | 1.07288400  | -0.43495300 | -1.16430200 |
| C  | 2.04896900  | -0.44761300 | -2.24817800 |
| H  | 1.84913300  | -1.29813400 | -2.91898400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.91075500  | 0.46681000  | -2.83950200 |
| C | 0.82767800  | -1.71554800 | -0.53679600 |
| H | -0.24932800 | -1.75807700 | -0.21388800 |
| H | 0.88831100  | -2.53926400 | -1.26870200 |
| C | 3.48182500  | -0.51334300 | -1.76313300 |
| C | 4.17492200  | 0.66128800  | -1.46302300 |
| C | 4.10174000  | -1.74121400 | -1.52907300 |
| C | 5.44809700  | 0.61232700  | -0.90172600 |
| H | 3.71520900  | 1.62428000  | -1.67750900 |
| C | 5.37562200  | -1.79663000 | -0.96979400 |
| H | 3.57630600  | -2.66194200 | -1.77350700 |
| C | 6.04695800  | -0.61989300 | -0.64585700 |
| H | 5.97639700  | 1.53295500  | -0.67324500 |
| H | 5.84394200  | -2.75827000 | -0.78679100 |
| H | 7.03942100  | -0.66310000 | -0.20935100 |
| C | 1.63716500  | -2.06505100 | 0.70553700  |
| C | 2.47663400  | -1.13547400 | 1.31932400  |
| C | 1.47288300  | -3.32556300 | 1.28466700  |
| C | 3.15083000  | -1.46663200 | 2.49329800  |
| H | 2.61440500  | -0.16251000 | 0.85540300  |
| C | 2.13873300  | -3.65371800 | 2.46206100  |
| H | 0.81918300  | -4.05468500 | 0.80886100  |
| C | 2.98087500  | -2.72336700 | 3.06921000  |
| H | 3.82016600  | -0.74461500 | 2.95068100  |
| H | 2.00514100  | -4.63636000 | 2.90276800  |
| H | 3.50779700  | -2.98101200 | 3.98192900  |
| C | 2.85327000  | 3.52633300  | 0.62057800  |
| C | 1.33349400  | 3.54898900  | 0.38302500  |
| H | 3.10655000  | 3.97493800  | 1.58548800  |
| H | 3.24524000  | 2.50423800  | 0.59683400  |
| H | 3.35336600  | 4.10493300  | -0.16172800 |
| C | 0.99350900  | 2.94504500  | -0.97468900 |
| C | 0.80983800  | 4.99275700  | 0.47470000  |
| H | -0.09163400 | 2.95902300  | -1.14283800 |
| H | 1.43726200  | 3.52715700  | -1.78763300 |
| H | 1.40401000  | 1.92815200  | -1.05591000 |
| H | 1.30939400  | 5.60952100  | -0.27756000 |
| H | -0.26901400 | 5.03265600  | 0.29434300  |
| H | 1.01329000  | 5.42637300  | 1.45819600  |
| C | 0.69365700  | 2.76860500  | 1.49197300  |
| H | 0.92396400  | 3.11626600  | 2.50871400  |
| N | -0.07522100 | 1.76178300  | 1.34024200  |
| C | -0.60726500 | 1.14002000  | 2.57373500  |
| C | -1.80285100 | 1.93099800  | 3.10775500  |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -0.99534500 | -0.30377500 | 2.26919600 |
| H | 0.18820700  | 1.13156200  | 3.33220600 |
| C | -2.40229900 | 1.24747300  | 4.33937400 |
| H | -2.55684300 | 1.99946900  | 2.31226500 |
| H | -1.48850300 | 2.95406100  | 3.34266100 |
| C | -1.58906900 | -0.98851900 | 3.50359900 |
| H | -1.77034400 | -0.30868100 | 1.47241500 |
| H | -0.11502500 | -0.86286100 | 1.93000500 |
| C | -2.78577100 | -0.20402000 | 4.04213700 |
| H | -3.27269900 | 1.81240200  | 4.68378200 |
| H | -1.66740800 | 1.26652400  | 5.15437000 |
| H | -1.86737900 | -2.01730900 | 3.26236100 |
| H | -0.80624200 | -1.04427900 | 4.27092200 |
| H | -3.17515100 | -0.68426500 | 4.94399100 |
| H | -3.59557900 | -0.21995000 | 3.29901300 |

ts-20

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.29942900 | -1.92855000 | 0.15095100  |
| C  | 1.47102200 | -2.45233000 | 1.19593500  |
| C  | 1.70290500 | -1.71039000 | 2.38254600  |
| C  | 2.70309900 | -0.72873500 | 2.10111700  |
| C  | 3.08479700 | -0.87849800 | 0.74507100  |
| Sc | 0.71534600 | -0.16997200 | 0.77144400  |
| C  | 1.36544700 | -3.98994800 | -2.02251100 |
| C  | 2.51651000 | -1.36737800 | -2.94415500 |
| C  | 4.33750100 | -3.41050800 | -1.56208800 |
| H  | 1.37706200 | -4.84055100 | -1.33744000 |
| H  | 0.34372400 | -3.60035700 | -2.07575900 |
| H  | 1.62450600 | -4.36209300 | -3.01950300 |
| H  | 2.68491400 | -1.88025400 | -3.89750600 |
| H  | 1.52943800 | -0.89458700 | -3.00269900 |
| H  | 3.27183800 | -0.57963900 | -2.86683200 |
| H  | 4.53568900 | -3.90403500 | -2.51878200 |
| H  | 5.11217300 | -2.65379500 | -1.41059200 |
| H  | 4.43500500 | -4.15783900 | -0.76932300 |
| Si | 2.61461600 | -2.65883100 | -1.56875000 |
| C  | 4.27865900 | -0.20918900 | 0.12206500  |
| H  | 4.52390400 | 0.73509900  | 0.61302800  |
| H  | 5.15497700 | -0.85784400 | 0.23162200  |
| H  | 4.14876800 | -0.01953700 | -0.94618400 |
| C  | 3.29348900 | 0.25217300  | 3.07545100  |
| H  | 2.62348900 | 0.43847500  | 3.91892300  |
| H  | 4.23616400 | -0.12442200 | 3.48595300  |
| H  | 3.50289200 | 1.21523300  | 2.59909900  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.05651300  | -1.97312600 | 3.71537700  |
| H | -0.03143300 | -2.07036400 | 3.63633600  |
| H | 1.43696800  | -2.90403100 | 4.14728500  |
| H | 1.26437700  | -1.17266200 | 4.42880300  |
| C | 0.55389300  | -3.63993700 | 1.11872000  |
| H | -0.03210200 | -3.65023400 | 0.19829600  |
| H | 1.13265300  | -4.56933700 | 1.15133300  |
| H | -0.13814700 | -3.65714400 | 1.96427200  |
| N | -1.25256400 | -0.80648000 | 0.43047800  |
| C | -2.21569500 | -1.75612900 | 0.99632900  |
| H | -1.97795000 | -2.76600600 | 0.64244800  |
| H | -2.05847200 | -1.75323500 | 2.08336200  |
| C | -1.27733900 | -0.68179100 | -1.03003000 |
| H | -0.27571900 | -0.33070700 | -1.37885000 |
| H | -1.37564900 | -1.68608100 | -1.46539600 |
| C | -3.66034000 | -1.44904400 | 0.66705900  |
| C | -4.22415600 | -0.22637700 | 1.03741500  |
| C | -4.43547700 | -2.36746200 | -0.03706500 |
| C | -5.52960300 | 0.08738300  | 0.68080600  |
| H | -3.62856200 | 0.48723700  | 1.60176800  |
| C | -5.75101100 | -2.06303300 | -0.38673600 |
| H | -4.00529400 | -3.32418500 | -0.32505900 |
| C | -6.29581600 | -0.83224700 | -0.03684000 |
| H | -5.95325000 | 1.04589900  | 0.96350600  |
| H | -6.34500000 | -2.78537900 | -0.93737700 |
| H | -7.31615000 | -0.58916500 | -0.31498100 |
| C | -2.31658300 | 0.24806900  | -1.62426700 |
| C | -2.25980200 | 1.62190000  | -1.38210100 |
| C | -3.35506100 | -0.26050200 | -2.40210800 |
| C | -3.24301000 | 2.47171600  | -1.88010500 |
| H | -1.44362100 | 2.03109600  | -0.79200700 |
| C | -4.34245500 | 0.58584800  | -2.89996400 |
| H | -3.41029300 | -1.32846500 | -2.59293300 |
| C | -4.29133300 | 1.95192100  | -2.63613100 |
| H | -3.19058600 | 3.53727800  | -1.67965800 |
| H | -5.15584100 | 0.17418000  | -3.48849700 |
| H | -5.06202400 | 2.61082000  | -3.02181200 |
| C | -2.11111900 | 2.79252600  | 2.17182100  |
| C | -0.65891900 | 2.33663700  | 2.41570900  |
| H | -2.17616700 | 3.88191100  | 2.08846700  |
| H | -2.52813000 | 2.35309500  | 1.26046700  |
| H | -2.72862500 | 2.48293500  | 3.02046500  |
| C | -0.56683100 | 0.80910400  | 2.51848200  |
| C | -0.12740700 | 3.03395500  | 3.68376100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.36724900  | 0.55922500  | 3.05447400  |
| H  | -1.34634100 | 0.43532900  | 3.19414900  |
| H  | -1.15205800 | 0.12849900  | 1.30206100  |
| H  | -0.72574000 | 2.71697900  | 4.54228400  |
| H  | 0.91612400  | 2.76216400  | 3.87301600  |
| H  | -0.19439900 | 4.12408100  | 3.60543400  |
| C  | 0.14713500  | 2.84395600  | 1.25960800  |
| H  | 0.13956400  | 3.93137000  | 1.09952300  |
| N  | 0.80441200  | 2.10224900  | 0.44875900  |
| C  | 1.50630700  | 2.77730500  | -0.66494200 |
| C  | 2.86945900  | 3.29108400  | -0.19797400 |
| C  | 1.63993400  | 1.79793500  | -1.82589600 |
| H  | 0.89932300  | 3.63435200  | -0.99070700 |
| C  | 3.66196100  | 3.88905900  | -1.36243700 |
| H  | 3.42390100  | 2.45096900  | 0.23781900  |
| H  | 2.72477200  | 4.02943500  | 0.59881200  |
| C  | 2.44931000  | 2.38717800  | -2.98211300 |
| H  | 2.16057800  | 0.89726400  | -1.45604600 |
| H  | 0.64378700  | 1.49815000  | -2.17630700 |
| C  | 3.81509100  | 2.88114400  | -2.50304900 |
| H  | 4.64096700  | 4.22101200  | -1.00620400 |
| H  | 3.14079900  | 4.78023300  | -1.73539800 |
| H  | 2.55868300  | 1.63706900  | -3.77107700 |
| H  | 1.88871800  | 3.22505000  | -3.41609200 |
| H  | 4.36442000  | 3.33122400  | -3.33461000 |
| H  | 4.41125400  | 2.02661900  | -2.15413100 |
| 21 |             |             |             |
| C  | 2.87587100  | 1.35099700  | 0.50683300  |
| C  | 1.74566000  | 1.59871200  | 1.35540100  |
| C  | 0.97949700  | 2.65344900  | 0.79776300  |
| C  | 1.59655000  | 3.04714100  | -0.42557800 |
| C  | 2.76786400  | 2.26727000  | -0.59516900 |
| Sc | 0.93587500  | 0.66285100  | -0.79675700 |
| C  | 5.90172000  | 1.60441000  | 0.76485100  |
| C  | 4.49370600  | -0.21235500 | 2.69177600  |
| C  | 4.74352400  | -1.03161000 | -0.28760400 |
| H  | 6.10736800  | 1.90589100  | -0.26470500 |
| H  | 5.70673200  | 2.50863400  | 1.34984300  |
| H  | 6.80948600  | 1.13830400  | 1.16152800  |
| H  | 3.80518900  | -1.02536800 | 2.93146900  |
| H  | 5.50719400  | -0.57700500 | 2.89175600  |
| H  | 4.30122400  | 0.61120100  | 3.38608200  |
| H  | 5.63530700  | -1.59776500 | -0.00002600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.89522000  | -1.72290600 | -0.31154400 |
| H  | 4.90260500  | -0.65796600 | -1.30488100 |
| Si | 4.46059400  | 0.39879300  | 0.90700800  |
| C  | 3.76117900  | 2.46402000  | -1.70762200 |
| H  | 4.40843500  | 3.32193100  | -1.49557500 |
| H  | 4.40298300  | 1.58937100  | -1.83804200 |
| H  | 3.26645500  | 2.65133400  | -2.66536700 |
| C  | 1.13455800  | 4.15242600  | -1.33458200 |
| H  | 0.04635100  | 4.26663600  | -1.32177500 |
| H  | 1.56417800  | 5.11296900  | -1.03055900 |
| H  | 1.44106900  | 3.97273800  | -2.36868000 |
| C  | -0.10729100 | 3.40725900  | 1.51453300  |
| H  | -0.89473500 | 2.77038000  | 1.92481200  |
| H  | 0.33080400  | 3.95313300  | 2.35689900  |
| H  | -0.58005800 | 4.14933200  | 0.86649800  |
| C  | 1.41270800  | 0.93992900  | 2.66836700  |
| H  | 1.73830600  | -0.10234900 | 2.70397300  |
| H  | 1.89398200  | 1.45916600  | 3.50474800  |
| H  | 0.33351900  | 0.96398400  | 2.85551800  |
| C  | 0.49045200  | -1.93277800 | -3.85584900 |
| C  | 1.62641000  | -1.59158700 | -2.86946300 |
| H  | 0.28343000  | -3.00761700 | -3.88673700 |
| H  | -0.43339600 | -1.40694800 | -3.60564200 |
| H  | 0.79552000  | -1.61959100 | -4.85816300 |
| C  | 1.79412900  | -0.06591100 | -2.71142800 |
| C  | 2.90510200  | -2.28653300 | -3.37926600 |
| H  | 2.86095100  | 0.13331600  | -2.52215100 |
| H  | 1.57272800  | 0.43180300  | -3.66441800 |
| H  | 3.17762300  | -1.85500800 | -4.34613300 |
| H  | 3.74072400  | -2.13676200 | -2.69087500 |
| H  | 2.75480400  | -3.36361500 | -3.51573900 |
| C  | 1.25875600  | -2.23354800 | -1.55810000 |
| H  | 1.23574500  | -3.33055500 | -1.53148000 |
| N  | 0.94435000  | -1.56060800 | -0.51301900 |
| C  | 0.53723400  | -2.24499000 | 0.73060000  |
| C  | -0.44768800 | -3.40339400 | 0.54257500  |
| C  | 1.76365000  | -2.71006800 | 1.51784400  |
| H  | 0.02836700  | -1.47519800 | 1.33712700  |
| C  | -0.89059400 | -3.92280800 | 1.91403800  |
| H  | 0.03720300  | -4.22172900 | -0.00306800 |
| H  | -1.31297100 | -3.08617100 | -0.05091300 |
| C  | 1.34420200  | -3.24739100 | 2.88749900  |
| H  | 2.26665100  | -3.49882400 | 0.93994600  |
| H  | 2.47370200  | -1.88292200 | 1.61209500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.31396700  | -4.37111000 | 2.74577100  |
| H | -1.59762000 | -4.74681100 | 1.78548800  |
| H | -1.42605600 | -3.12489600 | 2.44768200  |
| H | 2.22460800  | -3.59821100 | 3.43365000  |
| H | 0.91148400  | -2.42628600 | 3.47656500  |
| H | -0.01371800 | -4.71004800 | 3.73247200  |
| H | 0.78741300  | -5.23075000 | 2.25407300  |
| N | -1.38549900 | 0.52614200  | -0.58063300 |
| H | -1.45850700 | 0.11702100  | 0.35600700  |
| C | -1.98858700 | -0.45730100 | -1.53445700 |
| H | -1.85485800 | -0.04346400 | -2.53901300 |
| H | -1.39324400 | -1.37122400 | -1.47335000 |
| C | -2.17930200 | 1.79452800  | -0.54528900 |
| H | -1.49590600 | 2.61199200  | -0.30707700 |
| H | -2.55549100 | 1.97095100  | -1.55759200 |
| C | -3.33371400 | 1.77154000  | 0.43497600  |
| C | -4.60741600 | 2.16510400  | 0.02641300  |
| C | -3.15041200 | 1.34942900  | 1.75495900  |
| C | -5.67924100 | 2.12791400  | 0.91402400  |
| H | -4.76749800 | 2.47784100  | -1.00188800 |
| C | -4.21948400 | 1.30767000  | 2.64415100  |
| H | -2.16825100 | 1.03503300  | 2.10596000  |
| C | -5.48889400 | 1.69615200  | 2.22373900  |
| H | -6.66630300 | 2.42671500  | 0.57689100  |
| H | -4.06034500 | 0.97429900  | 3.66443100  |
| H | -6.32527400 | 1.66212500  | 2.91375000  |
| C | -3.44770000 | -0.75426700 | -1.28806700 |
| C | -3.84860500 | -1.36454200 | -0.09604700 |
| C | -4.41220500 | -0.38619500 | -2.22344800 |
| C | -5.19588000 | -1.57305100 | 0.16963300  |
| H | -3.10493100 | -1.65454600 | 0.64606100  |
| C | -5.76435300 | -0.61044200 | -1.96811400 |
| H | -4.10630300 | 0.08645100  | -3.15386000 |
| C | -6.15680200 | -1.19494200 | -0.76865800 |
| H | -5.49945200 | -2.02934000 | 1.10606900  |
| H | -6.50837000 | -0.31984900 | -2.70257400 |
| H | -7.20916200 | -1.35929700 | -0.56225500 |

trans-ts-22

|   |            |             |            |
|---|------------|-------------|------------|
| C | 3.05814700 | 0.21375800  | 1.41426000 |
| C | 2.07979100 | -0.60495600 | 2.06608800 |
| C | 1.18237100 | 0.23301100  | 2.78114000 |
| C | 1.58497500 | 1.58220100  | 2.57436000 |
| C | 2.72298000 | 1.57290300  | 1.73354700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Sc | 0.87609000  | 0.68942700  | 0.28066000  |
| C  | 6.05297100  | 0.73758400  | 1.75592800  |
| C  | 5.20661500  | -2.06901200 | 1.20787600  |
| C  | 5.05154100  | 0.07631700  | -1.03654300 |
| H  | 6.13294600  | 1.76743000  | 1.40105100  |
| H  | 5.81785700  | 0.76154800  | 2.82453400  |
| H  | 7.03746400  | 0.27239800  | 1.64060400  |
| H  | 4.65201800  | -2.84183900 | 0.67268900  |
| H  | 6.26786100  | -2.20868000 | 0.97439300  |
| H  | 5.08505500  | -2.24905600 | 2.28077800  |
| H  | 6.03705900  | -0.29384200 | -1.33837200 |
| H  | 4.30304500  | -0.39581300 | -1.67930800 |
| H  | 5.03605800  | 1.15501000  | -1.22754300 |
| Si | 4.77986600  | -0.27457600 | 0.79900100  |
| C  | 3.52394100  | 2.79820600  | 1.38560300  |
| H  | 4.26919600  | 3.00152100  | 2.16199500  |
| H  | 4.05922900  | 2.68942800  | 0.43718500  |
| H  | 2.89574000  | 3.69128000  | 1.31335000  |
| C  | 1.03328200  | 2.79468900  | 3.26768900  |
| H  | 0.03476800  | 2.61481700  | 3.67460000  |
| H  | 1.67935800  | 3.07918600  | 4.10492100  |
| H  | 0.96993700  | 3.66320700  | 2.60266100  |
| C  | 0.19548700  | -0.23871500 | 3.81343900  |
| H  | -0.33122500 | -1.14947600 | 3.51666900  |
| H  | 0.72225200  | -0.46382400 | 4.74750800  |
| H  | -0.55621400 | 0.52025500  | 4.04553600  |
| C  | 2.05720100  | -2.10795000 | 2.15015500  |
| H  | 2.51041600  | -2.57759700 | 1.27599000  |
| H  | 2.60991100  | -2.45626000 | 3.03029700  |
| H  | 1.03633100  | -2.49172600 | 2.24833300  |
| C  | 0.33699000  | 1.72144900  | -3.55018700 |
| C  | 1.62731500  | 1.35508200  | -2.78650600 |
| H  | 0.24620000  | 1.11246700  | -4.45584700 |
| H  | -0.55021800 | 1.55506900  | -2.93354100 |
| H  | 0.35828100  | 2.76865700  | -3.85807900 |
| C  | 1.80293200  | 2.04195100  | -1.41521000 |
| C  | 2.82876400  | 1.68876600  | -3.69577200 |
| H  | 2.63154100  | 1.51303900  | -0.90260700 |
| H  | 2.20877100  | 3.04089800  | -1.57260100 |
| H  | 2.85480300  | 2.76690500  | -3.87631200 |
| H  | 3.77388600  | 1.39458200  | -3.23183300 |
| H  | 2.74437700  | 1.18558700  | -4.66514800 |
| C  | 1.56756200  | -0.13641800 | -2.63264400 |
| H  | 1.73037500  | -0.72165300 | -3.54569900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.30282600  | -0.71284000 | -1.52565200 |
| C | 1.27341500  | -2.19383200 | -1.48593700 |
| C | 0.48407500  | -2.88360200 | -2.60666300 |
| C | 2.70500100  | -2.73292700 | -1.45787700 |
| H | 0.79896500  | -2.46252800 | -0.53016100 |
| C | 0.46898300  | -4.39757400 | -2.36279800 |
| H | 0.96135100  | -2.68964300 | -3.57496100 |
| H | -0.53949100 | -2.50019500 | -2.66975600 |
| C | 2.71697200  | -4.24329500 | -1.22413300 |
| H | 3.17902800  | -2.49951900 | -2.42239500 |
| H | 3.27338200  | -2.20337200 | -0.69051300 |
| C | 1.88809900  | -4.96550300 | -2.28842000 |
| H | -0.10040700 | -4.88940400 | -3.15619700 |
| H | -0.05516100 | -4.60852600 | -1.41970800 |
| H | 3.74778600  | -4.60996300 | -1.22257200 |
| H | 2.30179800  | -4.45685400 | -0.22889500 |
| H | 1.85482500  | -6.03860600 | -2.08048200 |
| H | 2.37372700  | -4.84431300 | -3.26532300 |
| C | 0.28841500  | 3.16506100  | -0.31455700 |
| C | -0.62564900 | 2.40469100  | 0.44477100  |
| H | 1.09765700  | 3.63286000  | 0.24867900  |
| H | -0.63368300 | 2.51573700  | 1.52375400  |
| H | -1.60054800 | 2.22798000  | -0.00359700 |
| C | -0.20641100 | 4.02934000  | -1.45355300 |
| C | -0.71956700 | 5.38362600  | -0.92395900 |
| H | -1.01183700 | 3.51643100  | -1.98712700 |
| H | 0.58768900  | 4.23385200  | -2.17627400 |
| C | -1.96585900 | 5.33855100  | -0.03594900 |
| H | 0.09476000  | 5.88142800  | -0.38315200 |
| H | -0.93383500 | 6.00892800  | -1.79910200 |
| H | -1.75116500 | 4.78748600  | 0.88726500  |
| H | -2.20250600 | 6.36570800  | 0.26755700  |
| C | -3.19693500 | 4.73583000  | -0.71058500 |
| C | -4.43280600 | 4.76077200  | 0.18678600  |
| H | -2.99955100 | 3.69546100  | -1.00584300 |
| H | -3.40847300 | 5.28037000  | -1.64148500 |
| C | -5.65800900 | 4.14146600  | -0.47947900 |
| H | -4.20796000 | 4.22758800  | 1.11991300  |
| H | -4.65045300 | 5.79734500  | 0.47097200  |
| H | -6.53324700 | 4.17778500  | 0.17368300  |
| H | -5.90728300 | 4.66979900  | -1.40472300 |
| H | -5.47553900 | 3.09228300  | -0.73645400 |
| N | -1.16048000 | -0.56706200 | 0.23112300  |
| H | -0.89357000 | -1.54805900 | 0.34392600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.84629500 | -0.45761200 | -1.08948200 |
| H | -2.06831900 | 0.60252400  | -1.24845700 |
| H | -1.12503700 | -0.75033500 | -1.85496900 |
| C | -2.10206100 | -0.25281900 | 1.34843900  |
| H | -1.52267900 | 0.19046700  | 2.16050600  |
| H | -2.79150600 | 0.51863200  | 0.99236100  |
| C | -2.88801900 | -1.44637000 | 1.84832600  |
| C | -4.27675200 | -1.37931400 | 1.95937400  |
| C | -2.24250900 | -2.63680000 | 2.19408000  |
| C | -5.00794600 | -2.48356700 | 2.38782200  |
| H | -4.79276900 | -0.46451200 | 1.68073900  |
| C | -2.96963400 | -3.74438400 | 2.61959700  |
| H | -1.15797900 | -2.71497300 | 2.12654100  |
| C | -4.35711500 | -3.67061300 | 2.71318100  |
| H | -6.08911600 | -2.41898600 | 2.45482100  |
| H | -2.45243300 | -4.66198900 | 2.88037000  |
| H | -4.92740700 | -4.53390500 | 3.03948600  |
| C | -3.11686800 | -1.26395700 | -1.21338700 |
| C | -3.08237800 | -2.65945300 | -1.13347700 |
| C | -4.34430600 | -0.62291600 | -1.36902500 |
| C | -4.25798400 | -3.39804800 | -1.17930600 |
| H | -2.13168600 | -3.17568100 | -1.00765200 |
| C | -5.52549100 | -1.36098700 | -1.43041100 |
| H | -4.37764800 | 0.46250200  | -1.43486200 |
| C | -5.48347300 | -2.74744000 | -1.32652300 |
| H | -4.22156900 | -4.47934400 | -1.09813700 |
| H | -6.47612000 | -0.85195600 | -1.55096100 |
| H | -6.40204800 | -3.32375100 | -1.36163900 |

cis-ts-22

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.96362100 | -0.38731200 | 1.37849300  |
| C  | 1.83963500 | -0.98244700 | 2.03675300  |
| C  | 1.12585700 | 0.03157300  | 2.72898500  |
| C  | 1.79499200 | 1.26880700  | 2.51083900  |
| C  | 2.91338000 | 1.01720400  | 1.67842700  |
| Sc | 0.93757300 | 0.53181100  | 0.22956600  |
| C  | 6.02287600 | -0.48768900 | 1.62620400  |
| C  | 4.57998600 | -3.07034900 | 1.23574100  |
| C  | 4.81105100 | -1.03859700 | -1.10163400 |
| H  | 6.31602500 | 0.47570200  | 1.20286100  |
| H  | 5.83415000 | -0.34907000 | 2.69523100  |
| H  | 6.87583900 | -1.16652000 | 1.52319400  |
| H  | 3.84693300 | -3.72377700 | 0.75947200  |
| H  | 5.57437300 | -3.44710000 | 0.97230500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 4.47038100  | -3.17557300 | 2.31987600  |
| H  | 5.66452400  | -1.64807600 | -1.41654700 |
| H  | 3.94430000  | -1.33484100 | -1.69897800 |
| H  | 5.04804700  | 0.00486000  | -1.33852100 |
| Si | 4.53102200  | -1.24503500 | 0.75414800  |
| C  | 3.96490300  | 2.02887800  | 1.31037100  |
| H  | 4.78017100  | 2.01563600  | 2.04109800  |
| H  | 4.40434200  | 1.82817900  | 0.32694700  |
| H  | 3.56679100  | 3.04458000  | 1.29172300  |
| C  | 1.48307000  | 2.54678800  | 3.23432900  |
| H  | 0.40714900  | 2.69828900  | 3.36193300  |
| H  | 1.92723200  | 2.52763800  | 4.23588400  |
| H  | 1.88724700  | 3.42199600  | 2.72010500  |
| C  | 0.06497700  | -0.20060700 | 3.77000400  |
| H  | -0.64886400 | -0.98092600 | 3.49389600  |
| H  | 0.53631200  | -0.51657500 | 4.70766600  |
| H  | -0.50048100 | 0.70901900  | 3.98870700  |
| C  | 1.53157100  | -2.44910900 | 2.17283600  |
| H  | 1.78309400  | -3.01702000 | 1.27603300  |
| H  | 2.10099700  | -2.88619200 | 3.00091100  |
| H  | 0.47409200  | -2.61633400 | 2.39841300  |
| C  | 0.54809700  | 1.51549900  | -3.63016400 |
| C  | 1.71560400  | 0.82897500  | -2.89382800 |
| H  | 0.33060500  | 1.00401000  | -4.57287300 |
| H  | -0.36340700 | 1.51894400  | -3.02544200 |
| H  | 0.81433800  | 2.55045300  | -3.86705700 |
| C  | 2.09664800  | 1.50899400  | -1.56687000 |
| C  | 2.93168100  | 0.81110800  | -3.84529400 |
| H  | 2.79804200  | 0.83220100  | -1.03483100 |
| H  | 2.70631000  | 2.37864500  | -1.79933200 |
| H  | 3.21519200  | 1.83916200  | -4.08645700 |
| H  | 3.79068500  | 0.31722000  | -3.38404900 |
| H  | 2.69474200  | 0.29689900  | -4.78270100 |
| C  | 1.29757400  | -0.59334100 | -2.66570000 |
| H  | 1.25781900  | -1.23670300 | -3.55273200 |
| N  | 0.98687600  | -1.04551600 | -1.51337000 |
| C  | 0.63819700  | -2.47947500 | -1.38652200 |
| C  | -0.34355400 | -3.02426100 | -2.43210100 |
| C  | 1.91606200  | -3.32315700 | -1.39621500 |
| H  | 0.17763700  | -2.59722600 | -0.39358500 |
| C  | -0.68846500 | -4.48012900 | -2.09888900 |
| H  | 0.11858100  | -2.99531400 | -3.42635200 |
| H  | -1.25219700 | -2.41607300 | -2.48250900 |
| C  | 1.60395600  | -4.78781500 | -1.08490000 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.37451500  | -3.23973400 | -2.39226400 |
| H | 2.63252700  | -2.90784400 | -0.68378500 |
| C | 0.57047700  | -5.35008300 | -2.06364900 |
| H | -1.40232800 | -4.86514700 | -2.83226900 |
| H | -1.18735200 | -4.52082000 | -1.11976800 |
| H | 2.52525600  | -5.37692900 | -1.11557700 |
| H | 1.21302800  | -4.86408200 | -0.06017300 |
| H | 0.31271300  | -6.37792100 | -1.79340300 |
| H | 1.00876300  | -5.38506800 | -3.06941900 |
| C | 0.74379000  | 3.01118800  | -0.72367900 |
| C | -0.14912200 | 2.55396300  | 0.26868600  |
| H | 0.36838300  | 3.06939400  | -1.74105900 |
| H | -0.06087200 | 2.97808600  | 1.26372300  |
| H | -1.16182500 | 2.31606600  | -0.04218800 |
| C | 1.69502700  | 4.13652400  | -0.37088900 |
| C | 1.10362000  | 5.51307700  | -0.73575100 |
| H | 2.66512100  | 4.04374400  | -0.86522900 |
| H | 1.87797100  | 4.11488100  | 0.70781100  |
| C | -0.21058800 | 5.86773000  | -0.02527700 |
| H | 1.87077200  | 6.25362800  | -0.48825300 |
| H | 0.96310500  | 5.57168700  | -1.82338500 |
| H | -0.23573200 | 5.37589900  | 0.95655600  |
| H | -0.23626600 | 6.94405700  | 0.17792800  |
| C | -1.47039900 | 5.50006400  | -0.81320700 |
| C | -2.73751400 | 5.55639300  | 0.03505700  |
| H | -1.37485600 | 4.49163000  | -1.23491600 |
| H | -1.56797800 | 6.17983400  | -1.67020100 |
| C | -3.99153100 | 5.20363700  | -0.75937500 |
| H | -2.62549600 | 4.86292000  | 0.87975400  |
| H | -2.84091900 | 6.55736800  | 0.47149600  |
| H | -4.88868000 | 5.23754300  | -0.13642500 |
| H | -4.13426100 | 5.89795200  | -1.59284000 |
| H | -3.91165100 | 4.19486300  | -1.18066400 |
| N | -1.34331900 | -0.24528400 | 0.15698100  |
| H | -1.27240400 | -1.25932100 | 0.26569100  |
| C | -2.03136800 | -0.01821300 | -1.14750000 |
| H | -2.07103800 | 1.06346300  | -1.31351700 |
| H | -1.39489200 | -0.43729300 | -1.92956900 |
| C | -2.18343000 | 0.24560500  | 1.29217100  |
| H | -1.51240600 | 0.58936400  | 2.08279300  |
| H | -2.73571400 | 1.12341000  | 0.94291200  |
| C | -3.16117300 | -0.77722400 | 1.83004300  |
| C | -4.50348300 | -0.43988900 | 2.00087500  |
| C | -2.74605500 | -2.07231400 | 2.15192700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.41587100 | -1.37963000 | 2.47230000  |
| H | -4.84256800 | 0.55761100  | 1.73459100  |
| C | -3.65541900 | -3.01642800 | 2.61856300  |
| H | -1.70334000 | -2.36208200 | 2.02733500  |
| C | -4.99501700 | -2.67105700 | 2.77849400  |
| H | -6.45934200 | -1.10531400 | 2.58783200  |
| H | -3.31767100 | -4.01880500 | 2.86091300  |
| H | -5.70674000 | -3.40523000 | 3.14096800  |
| C | -3.43117800 | -0.58419300 | -1.22469200 |
| C | -3.65365800 | -1.95545600 | -1.06464100 |
| C | -4.52331700 | 0.26223800  | -1.40511900 |
| C | -4.94469500 | -2.46765600 | -1.06589700 |
| H | -2.81396100 | -2.62951500 | -0.90188300 |
| C | -5.82055100 | -0.24896200 | -1.41924300 |
| H | -4.36077900 | 1.33078600  | -1.52713200 |
| C | -6.03244300 | -1.61223500 | -1.24344800 |
| H | -5.10478600 | -3.53110500 | -0.92230400 |
| H | -6.66278900 | 0.42073800  | -1.55917600 |
| H | -7.04169100 | -2.01045300 | -1.24311000 |

trans-23

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.87342000 | 0.10900200  | -1.84796200 |
| C  | -2.12086300 | -1.04566800 | -2.24540900 |
| C  | -0.90536100 | -0.61900800 | -2.84176100 |
| C  | -0.88037500 | 0.80423000  | -2.82571200 |
| C  | -2.07715800 | 1.25017100  | -2.21546900 |
| Sc | -0.84158800 | 0.05939100  | -0.44593100 |
| C  | -5.51420200 | 1.41447700  | -2.66619700 |
| C  | -5.62007500 | -1.40961300 | -1.62761900 |
| C  | -5.05126200 | 0.89786900  | 0.30645200  |
| H  | -5.26718900 | 2.46020200  | -2.46910300 |
| H  | -5.21124600 | 1.17868500  | -3.69087100 |
| H  | -6.60306400 | 1.31646500  | -2.60728200 |
| H  | -5.41014000 | -2.14818600 | -0.84923700 |
| H  | -6.69333000 | -1.19455200 | -1.58398000 |
| H  | -5.41686200 | -1.86649000 | -2.60060600 |
| H  | -6.12134700 | 0.81427000  | 0.52454600  |
| H  | -4.50657900 | 0.33980300  | 1.07458700  |
| H  | -4.78117800 | 1.95514100  | 0.39407700  |
| Si | -4.71786200 | 0.23657700  | -1.42950500 |
| C  | -2.47381100 | 2.69812300  | -2.13774100 |
| H  | -3.03993900 | 2.98448200  | -3.03095200 |
| H  | -3.09850200 | 2.91823500  | -1.26601400 |
| H  | -1.59218500 | 3.34291000  | -2.09263900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.16848700  | 1.69794600  | -3.42818000 |
| H | 1.00483400  | 1.12192300  | -3.83279300 |
| H | -0.25293000 | 2.27901500  | -4.25476500 |
| H | 0.57025300  | 2.41177700  | -2.70008900 |
| C | 0.08619800  | -1.53059500 | -3.50607100 |
| H | 0.15126800  | -2.49960800 | -2.99775700 |
| H | -0.22052000 | -1.74281700 | -4.53618800 |
| H | 1.09054000  | -1.10046600 | -3.55420100 |
| C | -2.50606900 | -2.49875400 | -2.14654700 |
| H | -3.40440800 | -2.64685300 | -1.54975800 |
| H | -2.70035600 | -2.91577000 | -3.14108400 |
| H | -1.70572100 | -3.10569300 | -1.70247400 |
| C | -0.75202900 | 1.92222300  | 3.78429500  |
| C | -1.93281200 | 1.63858300  | 2.83291300  |
| H | -0.84055800 | 1.31745300  | 4.69295300  |
| H | 0.21128900  | 1.70449400  | 3.31556900  |
| H | -0.76149500 | 2.97349100  | 4.08083900  |
| C | -1.95977700 | 2.50278800  | 1.54719700  |
| C | -3.24129000 | 1.91496500  | 3.61109200  |
| H | -2.55917900 | 1.95064700  | 0.80551000  |
| H | -2.55669900 | 3.39171900  | 1.78685600  |
| H | -3.24654600 | 2.95819600  | 3.93725100  |
| H | -4.11904300 | 1.74983400  | 2.97882600  |
| H | -3.32505600 | 1.28274100  | 4.50047500  |
| C | -1.92902600 | 0.14813100  | 2.61887900  |
| H | -2.13589700 | -0.41060900 | 3.53908800  |
| N | -1.73813700 | -0.50883300 | 1.53922800  |
| C | -1.88708800 | -1.98551700 | 1.56852400  |
| C | -1.35898600 | -2.69387500 | 2.81960700  |
| C | -3.35039500 | -2.36200700 | 1.32360800  |
| H | -1.30840600 | -2.36365800 | 0.70377000  |
| C | -1.46593800 | -4.21010200 | 2.62884200  |
| H | -1.97094400 | -2.42006100 | 3.68683400  |
| H | -0.33110900 | -2.38683500 | 3.03946100  |
| C | -3.50202400 | -3.87743800 | 1.17265000  |
| H | -3.94070500 | -2.00213500 | 2.17845300  |
| H | -3.71676800 | -1.83447400 | 0.43825900  |
| C | -2.91903500 | -4.61990400 | 2.37726000  |
| H | -1.06952800 | -4.71958500 | 3.51109500  |
| H | -0.84346900 | -4.51923600 | 1.77680300  |
| H | -4.55768900 | -4.13068600 | 1.03540900  |
| H | -2.97771300 | -4.20068400 | 0.26338200  |
| H | -2.98686400 | -5.70019000 | 2.22188300  |
| H | -3.51405800 | -4.38772400 | 3.26984900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.66715200 | 2.99046100  | 0.85880400  |
| C | 0.18300700  | 1.82735000  | 0.33646700  |
| H | -1.04284000 | 3.52489900  | -0.02540700 |
| H | 0.95378900  | 2.19485500  | -0.35140300 |
| H | 0.74635100  | 1.37775400  | 1.18120100  |
| C | 0.09223400  | 4.05912800  | 1.68148200  |
| C | 0.74983300  | 5.16217300  | 0.84150900  |
| H | 0.84672500  | 3.58294200  | 2.31768400  |
| H | -0.61095300 | 4.55467500  | 2.36453100  |
| C | 1.84245600  | 4.71617600  | -0.13455700 |
| H | -0.03362900 | 5.68862700  | 0.28148200  |
| H | 1.18199600  | 5.90036900  | 1.52895300  |
| H | 1.41055100  | 4.08910700  | -0.92577500 |
| H | 2.23603800  | 5.60428800  | -0.64467300 |
| C | 3.00438100  | 3.98229400  | 0.53109600  |
| C | 4.07656500  | 3.52610800  | -0.45529700 |
| H | 2.63378000  | 3.10157900  | 1.07351100  |
| H | 3.45821600  | 4.64045700  | 1.28541600  |
| C | 5.28054000  | 2.90698600  | 0.24949400  |
| H | 3.63553900  | 2.80058300  | -1.15593500 |
| H | 4.40216800  | 4.37755500  | -1.06515800 |
| H | 6.02920100  | 2.54467700  | -0.46113800 |
| H | 5.76471300  | 3.63941300  | 0.90255400  |
| H | 4.97241600  | 2.06171300  | 0.87702600  |
| N | 1.14281100  | -1.14639800 | -0.36734700 |
| H | 1.08060400  | -2.00063100 | -0.92226300 |
| C | 1.45909300  | -1.53689200 | 1.05127300  |
| H | 0.97154200  | -0.80701600 | 1.70851100  |
| H | 0.98069800  | -2.50672200 | 1.21830200  |
| C | 2.17160700  | -0.28010300 | -1.01623900 |
| H | 1.68177300  | 0.22665200  | -1.85589200 |
| H | 2.44891800  | 0.49820700  | -0.29986000 |
| C | 3.41872400  | -0.99729600 | -1.49225800 |
| C | 4.66265700  | -0.42075300 | -1.23600200 |
| C | 3.36767900  | -2.21231100 | -2.17954300 |
| C | 5.83501000  | -1.04790100 | -1.64485800 |
| H | 4.71255800  | 0.51484500  | -0.68703300 |
| C | 4.53945300  | -2.84553900 | -2.58455100 |
| H | 2.41574600  | -2.68862000 | -2.40158600 |
| C | 5.77710400  | -2.26651300 | -2.31566100 |
| H | 6.79416600  | -0.58968700 | -1.42488800 |
| H | 4.48413900  | -3.79187200 | -3.11278100 |
| H | 6.68984300  | -2.76266600 | -2.62850100 |
| C | 2.92183900  | -1.60660300 | 1.40919600  |

|   |            |             |            |
|---|------------|-------------|------------|
| C | 3.67685200 | -2.74242900 | 1.10734500 |
| C | 3.54434400 | -0.50907300 | 2.00573200 |
| C | 5.04243700 | -2.76672500 | 1.36308400 |
| H | 3.19502200 | -3.60110500 | 0.64580400 |
| C | 4.91136400 | -0.53606900 | 2.27643000 |
| H | 2.95828600 | 0.37496300  | 2.25448700 |
| C | 5.66158500 | -1.66050100 | 1.94485800 |
| H | 5.62509800 | -3.64544600 | 1.10782500 |
| H | 5.38790900 | 0.31948100  | 2.74437700 |
| H | 6.72755900 | -1.67972600 | 2.14636700 |

cis-23

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.53904200 | 0.20772400  | -1.92455500 |
| C  | -1.56645100 | -0.74444200 | -2.37065000 |
| C  | -0.43062400 | -0.04485800 | -2.85787600 |
| C  | -0.67584500 | 1.35120500  | -2.72090400 |
| C  | -1.96427700 | 1.50713200  | -2.15384600 |
| Sc | -0.57325700 | 0.42084000  | -0.40701000 |
| C  | -5.37439500 | 1.05682700  | -2.74475400 |
| C  | -4.98744900 | -1.78909600 | -1.87885700 |
| C  | -4.83026500 | 0.47027300  | 0.20314200  |
| H  | -5.38939600 | 2.10560900  | -2.43957300 |
| H  | -4.97969700 | 1.00203400  | -3.76394300 |
| H  | -6.41081500 | 0.70515700  | -2.76884400 |
| H  | -4.63932500 | -2.53999900 | -1.16513900 |
| H  | -6.08094200 | -1.76707500 | -1.81524400 |
| H  | -4.72668300 | -2.12382600 | -2.88742600 |
| H  | -5.88201700 | 0.23697900  | 0.39968300  |
| H  | -4.22245000 | -0.05908100 | 0.94300200  |
| H  | -4.69733100 | 1.54650000  | 0.35755800  |
| Si | -4.38532000 | -0.02849800 | -1.56127900 |
| C  | -2.67968700 | 2.82515600  | -2.04297300 |
| H  | -3.34928300 | 2.95438100  | -2.89963700 |
| H  | -3.28625400 | 2.90627300  | -1.13500900 |
| H  | -1.97937400 | 3.66053200  | -2.05467800 |
| C  | 0.21223800  | 2.47114100  | -3.18894900 |
| H  | 1.17950300  | 2.09858500  | -3.53598600 |
| H  | -0.24834800 | 3.00171900  | -4.02859500 |
| H  | 0.39693800  | 3.20569200  | -2.39747200 |
| C  | 0.72762700  | -0.68803800 | -3.56704800 |
| H  | 0.90728400  | -1.71065500 | -3.21308200 |
| H  | 0.51716300  | -0.77143500 | -4.63879600 |
| H  | 1.65795200  | -0.12007700 | -3.47317900 |
| C  | -1.67895300 | -2.24669700 | -2.41441100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.59883700 | -2.60198900 | -1.95319300 |
| H | -1.67118000 | -2.60272700 | -3.45049700 |
| H | -0.84362300 | -2.74353700 | -1.90279000 |
| C | -0.95220500 | 1.80202200  | 4.06807300  |
| C | -1.97936000 | 1.46295600  | 2.96864200  |
| H | -1.05641000 | 1.12014300  | 4.91759400  |
| H | 0.07585300  | 1.74230900  | 3.69910200  |
| H | -1.12936600 | 2.81911700  | 4.42954200  |
| C | -1.98297800 | 2.50785000  | 1.82965600  |
| C | -3.38422700 | 1.45916300  | 3.61693300  |
| H | -2.49791000 | 2.08288200  | 0.95058000  |
| H | -2.63515000 | 3.31755700  | 2.18075700  |
| H | -3.56494400 | 2.43422600  | 4.07670200  |
| H | -4.16337800 | 1.28209400  | 2.87014000  |
| H | -3.46913200 | 0.69832700  | 4.39901100  |
| C | -1.72839800 | 0.02380200  | 2.60478500  |
| H | -1.89092100 | -0.64488200 | 3.45710500  |
| N | -1.38743700 | -0.49830100 | 1.48837900  |
| C | -1.31689200 | -1.98366000 | 1.39744200  |
| C | -0.81561400 | -2.71829900 | 2.64412600  |
| C | -2.68280200 | -2.52298000 | 0.97030300  |
| H | -0.60136400 | -2.20943200 | 0.58641000  |
| C | -0.73346100 | -4.22223100 | 2.36121100  |
| H | -1.51612900 | -2.57051900 | 3.47448000  |
| H | 0.15819100  | -2.32539200 | 2.96029500  |
| C | -2.62042100 | -4.02872100 | 0.70876600  |
| H | -3.40035200 | -2.30809400 | 1.77556800  |
| H | -3.02282000 | -1.97783300 | 0.08569100  |
| C | -2.09458500 | -4.77524400 | 1.93625800  |
| H | -0.36682200 | -4.73799400 | 3.25353700  |
| H | -0.00161500 | -4.40466800 | 1.56583300  |
| H | -3.61136800 | -4.39590500 | 0.42350600  |
| H | -1.95068200 | -4.21871200 | -0.14159900 |
| H | -2.01636100 | -5.84494100 | 1.72226600  |
| H | -2.81071200 | -4.66494000 | 2.76116000  |
| C | -0.64426100 | 3.13638700  | 1.40745400  |
| C | 0.24924700  | 2.14136500  | 0.65866400  |
| H | -0.15827500 | 3.47887200  | 2.33355100  |
| H | 1.01625700  | 2.67894600  | 0.08755900  |
| H | 0.81299200  | 1.51868700  | 1.39054700  |
| C | -0.87543900 | 4.40522600  | 0.56295900  |
| C | 0.10738700  | 5.55944900  | 0.80686400  |
| H | -1.88837100 | 4.78908700  | 0.74108600  |
| H | -0.83344700 | 4.13175600  | -0.49773500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.56324800  | 5.31068600  | 0.38538500  |
| H | -0.27041000 | 6.42752500  | 0.25554500  |
| H | 0.08131900  | 5.84016500  | 1.86887900  |
| H | 1.57479400  | 4.72328900  | -0.54506400 |
| H | 2.03264300  | 6.26924100  | 0.13321300  |
| C | 2.43981100  | 4.62578600  | 1.43635300  |
| C | 3.80045000  | 4.20916000  | 0.88335000  |
| H | 1.93836400  | 3.73866800  | 1.84059500  |
| H | 2.58350200  | 5.31092300  | 2.28258600  |
| C | 4.67300300  | 3.51854000  | 1.92745500  |
| H | 3.64429100  | 3.53790600  | 0.02497700  |
| H | 4.32010200  | 5.08969400  | 0.48595700  |
| H | 5.65249400  | 3.24501100  | 1.52412500  |
| H | 4.84035300  | 4.17152000  | 2.78934500  |
| H | 4.19098100  | 2.60495000  | 2.29680000  |
| N | 1.55903400  | -0.50992400 | -0.44957900 |
| H | 1.57118600  | -1.19092300 | -1.20741200 |
| C | 1.98008500  | -1.19358300 | 0.80250000  |
| H | 2.95288700  | -0.79303000 | 1.10942600  |
| H | 1.27264000  | -0.92798200 | 1.60047100  |
| C | 2.54972200  | 0.53859300  | -0.84056600 |
| H | 2.14030500  | 1.07235900  | -1.70658000 |
| H | 2.60655600  | 1.25830400  | -0.02065100 |
| C | 3.92925800  | -0.01071000 | -1.12886300 |
| C | 5.03805300  | 0.56134500  | -0.50361600 |
| C | 4.12512800  | -1.07584700 | -2.01280600 |
| C | 6.32238200  | 0.08948100  | -0.76422700 |
| H | 4.89401200  | 1.38346500  | 0.19315100  |
| C | 5.40612800  | -1.55306200 | -2.26978900 |
| H | 3.28054800  | -1.54274200 | -2.51460900 |
| C | 6.50809700  | -0.96947900 | -1.64750200 |
| H | 7.17435300  | 0.54648300  | -0.27171200 |
| H | 5.54473200  | -2.37904900 | -2.95933400 |
| H | 7.50661400  | -1.34242700 | -1.84945500 |
| C | 2.10208600  | -2.70146600 | 0.71394400  |
| C | 1.72224400  | -3.46036400 | -0.39315400 |
| C | 2.64016100  | -3.36269900 | 1.82392400  |
| C | 1.88245600  | -4.84753000 | -0.39684400 |
| H | 1.29326900  | -3.00195100 | -1.28094000 |
| C | 2.79901800  | -4.74254700 | 1.82480700  |
| H | 2.94610300  | -2.78296000 | 2.69174700  |
| C | 2.42141200  | -5.49180400 | 0.70986800  |
| H | 1.58507400  | -5.41757200 | -1.27081200 |
| H | 3.22461100  | -5.23447400 | 2.69307500  |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| H           | 2.54966600  | -6.56869700 | 0.70628900  |
| trans-ts-24 |             |             |             |
| C           | 2.86672500  | -0.61351500 | -1.76618100 |
| C           | 1.99105000  | 0.30249700  | -2.42930500 |
| C           | 0.75055000  | -0.34726000 | -2.68217600 |
| C           | 0.83230100  | -1.67034200 | -2.16451900 |
| C           | 2.12591800  | -1.83427200 | -1.60300600 |
| Sc          | 0.99176600  | -0.11339600 | -0.21081200 |
| C           | 5.45445100  | -1.98931800 | -2.58525900 |
| C           | 5.50124900  | 1.00481800  | -2.36245300 |
| C           | 5.33162400  | -0.71610800 | 0.19097300  |
| H           | 5.34684700  | -2.94714300 | -2.07091800 |
| H           | 4.97037500  | -2.07187600 | -3.56329300 |
| H           | 6.52358200  | -1.82443000 | -2.75413600 |
| H           | 5.30966100  | 1.93598800  | -1.82320600 |
| H           | 6.58702800  | 0.86136200  | -2.38323000 |
| H           | 5.16899900  | 1.13180000  | -3.39721400 |
| H           | 6.42350700  | -0.79420500 | 0.21854300  |
| H           | 5.02753000  | 0.13801700  | 0.80048200  |
| H           | 4.92221500  | -1.61984400 | 0.65413500  |
| Si          | 4.75390500  | -0.54735700 | -1.59123000 |
| C           | 2.68386500  | -3.16103800 | -1.16209400 |
| H           | 3.09512200  | -3.69056500 | -2.02904500 |
| H           | 3.49046300  | -3.05485900 | -0.43289900 |
| H           | 1.91851200  | -3.80885000 | -0.72879400 |
| C           | -0.18090200 | -2.76796000 | -2.33446200 |
| H           | -1.18212000 | -2.38141300 | -2.54534000 |
| H           | 0.09723700  | -3.41093500 | -3.17681900 |
| H           | -0.24580800 | -3.40809300 | -1.44885600 |
| C           | -0.34833900 | 0.20860600  | -3.54043600 |
| H           | -0.40562300 | 1.29989900  | -3.47220400 |
| H           | -0.15179800 | -0.02374800 | -4.59293100 |
| H           | -1.33232900 | -0.20511600 | -3.30453400 |
| C           | 2.28765200  | 1.71117200  | -2.87459100 |
| H           | 3.15762900  | 2.12538400  | -2.36545200 |
| H           | 2.48911700  | 1.74546600  | -3.95118200 |
| H           | 1.44159100  | 2.38462600  | -2.68912700 |
| C           | 1.15706300  | -1.19042300 | 4.41914300  |
| C           | 2.03030900  | -1.11958000 | 3.15667700  |
| H           | 1.32181800  | -0.30483900 | 5.04211700  |
| H           | 0.08945800  | -1.24513000 | 4.18907500  |
| H           | 1.42119600  | -2.06918400 | 5.01355700  |
| C           | 1.98438600  | -2.41467200 | 2.33291100  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.48195300  | -0.83676700 | 3.58766600  |
| H | 2.70528100  | -2.30184400 | 1.51139600  |
| H | 2.33936800  | -3.24898500 | 2.95059100  |
| H | 3.82372800  | -1.63344500 | 4.25469800  |
| H | 4.14276900  | -0.79011100 | 2.72023700  |
| H | 3.55515400  | 0.11210300  | 4.12964600  |
| C | 1.57466500  | 0.09668700  | 2.35011800  |
| H | 0.89260700  | 0.74483600  | 2.91590700  |
| N | 2.25227300  | 0.61449700  | 1.34866500  |
| C | 2.12699100  | 2.04416600  | 1.00377100  |
| C | 1.63512900  | 2.98102500  | 2.11282400  |
| C | 3.48955900  | 2.51376000  | 0.48919600  |
| H | 1.42184600  | 2.15985800  | 0.12966800  |
| C | 1.59992500  | 4.43612600  | 1.63172900  |
| H | 2.33603000  | 2.88291700  | 2.95358900  |
| H | 0.64851800  | 2.70120700  | 2.48942300  |
| C | 3.44909500  | 3.95937500  | -0.00228400 |
| H | 4.20480200  | 2.41524000  | 1.31704300  |
| H | 3.82055100  | 1.83092900  | -0.29682000 |
| C | 2.95916000  | 4.89453000  | 1.10310300  |
| H | 1.26713800  | 5.07708700  | 2.45272100  |
| H | 0.85077200  | 4.53780900  | 0.83258700  |
| H | 4.44184400  | 4.25814000  | -0.35209100 |
| H | 2.77388700  | 4.03277000  | -0.86698500 |
| H | 2.89392400  | 5.92239300  | 0.73562100  |
| H | 3.68517900  | 4.89333800  | 1.92608100  |
| C | 0.58616800  | -2.69393100 | 1.74556900  |
| C | -0.03773200 | -1.35755900 | 1.35482600  |
| H | 0.73496000  | -3.25127900 | 0.81308600  |
| H | -0.70162500 | -1.50929400 | 0.48190900  |
| H | -0.69637700 | -0.95111400 | 2.13056300  |
| C | -0.28311200 | -3.60057300 | 2.65375500  |
| C | -1.78853900 | -3.54753500 | 2.37622400  |
| H | -0.11764200 | -3.34696400 | 3.70509200  |
| H | 0.07571300  | -4.63108600 | 2.53599200  |
| C | -2.20242300 | -3.89036700 | 0.94583400  |
| H | -2.30066800 | -4.22495000 | 3.07012500  |
| H | -2.16260000 | -2.54151900 | 2.61195300  |
| H | -1.63995700 | -3.26667600 | 0.23981000  |
| H | -1.93224500 | -4.92923400 | 0.71313600  |
| C | -3.69369200 | -3.67049400 | 0.68902700  |
| C | -4.05425900 | -3.68120700 | -0.79485500 |
| H | -3.99468400 | -2.70330100 | 1.12056800  |
| H | -4.27910800 | -4.43235500 | 1.22004900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.55481800 | -3.56031500 | -1.04317600 |
| H | -3.53380700 | -2.84897200 | -1.29173600 |
| H | -3.67267800 | -4.60145800 | -1.25503600 |
| H | -5.78593900 | -3.55514000 | -2.11116600 |
| H | -6.09377800 | -4.39480700 | -0.58447500 |
| H | -5.94855100 | -2.63324100 | -0.61322100 |
| N | -1.09444000 | 1.02097200  | -0.41747300 |
| H | -1.05894300 | 1.63956300  | -1.22939400 |
| C | -1.31840400 | 1.87217000  | 0.79848800  |
| H | -0.91346400 | 1.31584700  | 1.65150900  |
| H | -0.71181600 | 2.77344000  | 0.66403400  |
| C | -2.19211900 | 0.03747800  | -0.66160000 |
| H | -1.77489300 | -0.76407200 | -1.28189300 |
| H | -2.44861300 | -0.41306000 | 0.30230100  |
| C | -3.45736700 | 0.57201200  | -1.29979200 |
| C | -4.68664500 | 0.13653900  | -0.80235500 |
| C | -3.44285300 | 1.45686600  | -2.37980000 |
| C | -5.87939400 | 0.57734200  | -1.36783300 |
| H | -4.70865300 | -0.53549700 | 0.05256200  |
| C | -4.63422500 | 1.90835900  | -2.94047800 |
| H | -2.50427300 | 1.81662300  | -2.79297500 |
| C | -5.85587100 | 1.46975800  | -2.43613500 |
| H | -6.82590800 | 0.23249500  | -0.96387100 |
| H | -4.60677800 | 2.60121500  | -3.77511000 |
| H | -6.78394500 | 1.82297100  | -2.87304100 |
| C | -2.74774400 | 2.24144500  | 1.10624300  |
| C | -3.39940200 | 3.24910600  | 0.39156500  |
| C | -3.44521200 | 1.54256800  | 2.09162200  |
| C | -4.73784200 | 3.53056600  | 0.63656300  |
| H | -2.86216000 | 3.80014200  | -0.37708700 |
| C | -4.78453400 | 1.82880600  | 2.34733600  |
| H | -2.93862100 | 0.76519700  | 2.66071600  |
| C | -5.43281200 | 2.81752400  | 1.61403900  |
| H | -5.24080000 | 4.30538600  | 0.06768000  |
| H | -5.31826700 | 1.28102900  | 3.11690200  |
| H | -6.47735700 | 3.03921500  | 1.80643200  |

cis-24

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.04473600 | 0.00652300  | -1.65258900 |
| C  | -2.10503700 | -0.91397100 | -2.21443500 |
| C  | -1.00971500 | -0.18088000 | -2.74622500 |
| C  | -1.24570000 | 1.20315100  | -2.51530300 |
| C  | -2.49015400 | 1.31975300  | -1.84107600 |
| Sc | -0.98031000 | 0.11546100  | -0.27096300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -5.85394800 | 0.78880200  | -2.50777500 |
| C  | -5.43631300 | -2.03932800 | -1.60366900 |
| C  | -5.37189800 | 0.23759000  | 0.46927600  |
| H  | -5.83941800 | 1.85228700  | -2.25902700 |
| H  | -5.45980400 | 0.67102300  | -3.52197000 |
| H  | -6.89994900 | 0.46553800  | -2.51591400 |
| H  | -5.06939300 | -2.78231500 | -0.89117600 |
| H  | -6.53035000 | -2.04989200 | -1.54671200 |
| H  | -5.15966000 | -2.36263800 | -2.61158500 |
| H  | -6.43882200 | 0.04308800  | 0.62091200  |
| H  | -4.80691400 | -0.31767900 | 1.22144200  |
| H  | -5.20331900 | 1.30498700  | 0.64420900  |
| Si | -4.88531700 | -0.26357100 | -1.27790100 |
| C  | -3.21896500 | 2.61278800  | -1.58554400 |
| H  | -3.75237000 | 2.92136600  | -2.49152900 |
| H  | -3.96026100 | 2.50688700  | -0.78984700 |
| H  | -2.55013300 | 3.42764400  | -1.30739000 |
| C  | -0.40659200 | 2.32166700  | -3.07109300 |
| H  | 0.61596000  | 2.33826300  | -2.67596000 |
| H  | -0.32477800 | 2.22161200  | -4.15850100 |
| H  | -0.85466100 | 3.29583500  | -2.86472800 |
| C  | 0.07195100  | -0.74233200 | -3.62119300 |
| H  | 0.26994300  | -1.79623200 | -3.40128700 |
| H  | -0.24340300 | -0.70065600 | -4.67014000 |
| H  | 1.01092100  | -0.18593000 | -3.55333700 |
| C  | -2.22569300 | -2.41277000 | -2.31114800 |
| H  | -2.93992300 | -2.81105800 | -1.59036200 |
| H  | -2.56167500 | -2.71596600 | -3.30907400 |
| H  | -1.26417800 | -2.91025200 | -2.13496400 |
| C  | -0.88587300 | 1.99539400  | 4.14932300  |
| C  | -1.78865100 | 1.65721700  | 2.95267200  |
| H  | -0.96655400 | 1.22086700  | 4.91860200  |
| H  | 0.16811600  | 2.07585300  | 3.86491100  |
| H  | -1.18999100 | 2.94583800  | 4.59616600  |
| C  | -1.84205500 | 2.82510700  | 1.96884900  |
| C  | -3.19776200 | 1.32771000  | 3.46697400  |
| H  | -2.53588900 | 2.58200800  | 1.14793600  |
| H  | -2.24280400 | 3.71395300  | 2.47183400  |
| H  | -3.58079800 | 2.17357000  | 4.04530900  |
| H  | -3.87675100 | 1.12778700  | 2.63663700  |
| H  | -3.18325600 | 0.44819000  | 4.11938900  |
| C  | -1.22334500 | 0.39387900  | 2.29535400  |
| H  | -0.39682800 | -0.04392000 | 2.87042500  |
| N  | -1.95397000 | -0.40527700 | 1.53161100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.72531100 | -1.86388900 | 1.50353200  |
| C | -1.05019300 | -2.46851800 | 2.74071200  |
| C | -3.08353200 | -2.53150300 | 1.27797800  |
| H | -1.10054500 | -2.13311200 | 0.60837900  |
| C | -0.93800400 | -3.99290300 | 2.62185900  |
| H | -1.67372600 | -2.20634500 | 3.60679600  |
| H | -0.05926900 | -2.04800800 | 2.92676100  |
| C | -2.97120700 | -4.04945600 | 1.14963100  |
| H | -3.72184100 | -2.27126500 | 2.13328300  |
| H | -3.54454500 | -2.08857100 | 0.39286700  |
| C | -2.29866200 | -4.64763100 | 2.38482200  |
| H | -0.46958300 | -4.38984400 | 3.52664800  |
| H | -0.26858100 | -4.24642200 | 1.78638600  |
| H | -3.96564200 | -4.48131500 | 1.00131300  |
| H | -2.38046000 | -4.30231200 | 0.25726700  |
| H | -2.18348300 | -5.72960700 | 2.27457600  |
| H | -2.93764900 | -4.47989900 | 3.26123000  |
| C | -0.44783400 | 3.09034600  | 1.38931300  |
| C | 0.11087000  | 1.74231800  | 0.92247400  |
| H | 0.18052800  | 3.48269900  | 2.20026600  |
| H | 0.47091000  | 1.83447400  | -0.12960800 |
| H | 0.99145500  | 1.42095600  | 1.48862300  |
| C | -0.50497900 | 4.16833600  | 0.29212400  |
| C | 0.70125300  | 5.10452600  | 0.17135100  |
| H | -1.39075900 | 4.79200600  | 0.46871300  |
| H | -0.66323300 | 3.67865200  | -0.67715500 |
| C | 2.01235100  | 4.47315100  | -0.31497200 |
| H | 0.41901200  | 5.89820900  | -0.52896600 |
| H | 0.87249300  | 5.60084300  | 1.13598000  |
| H | 1.79267300  | 3.70474800  | -1.07232200 |
| H | 2.59916100  | 5.24053100  | -0.83443800 |
| C | 2.90104900  | 3.87115100  | 0.77230500  |
| C | 4.23622900  | 3.38190300  | 0.21541600  |
| H | 2.38943000  | 3.03737700  | 1.27106200  |
| H | 3.08532400  | 4.62573000  | 1.54858200  |
| C | 5.09981000  | 2.68761400  | 1.26403700  |
| H | 4.04542600  | 2.69980600  | -0.62527700 |
| H | 4.78104300  | 4.23357300  | -0.20931300 |
| H | 6.05395500  | 2.35148200  | 0.84722500  |
| H | 5.31741200  | 3.36099700  | 2.09857000  |
| H | 4.58785000  | 1.80872600  | 1.67373600  |
| N | 1.17308600  | -0.89908300 | -0.47753100 |
| H | 1.09089800  | -1.64060600 | -1.17682100 |
| C | 1.54304100  | -1.53396100 | 0.83132300  |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 1.18519600 | -0.85815500 | 1.61431400  |
| H | 0.97029600 | -2.46258200 | 0.90002900  |
| C | 2.20284200 | 0.06054700  | -0.98571200 |
| H | 1.70647800 | 0.70323400  | -1.72246100 |
| H | 2.49518800 | 0.70339700  | -0.14819700 |
| C | 3.44178500 | -0.56738000 | -1.59637900 |
| C | 4.70431600 | -0.13854200 | -1.18447200 |
| C | 3.35720400 | -1.57224000 | -2.56295800 |
| C | 5.85723300 | -0.70465200 | -1.71941200 |
| H | 4.78798500 | 0.61826600  | -0.41018600 |
| C | 4.50851700 | -2.14397600 | -3.09657200 |
| H | 2.39200900 | -1.93192900 | -2.90637000 |
| C | 5.76347000 | -1.71141200 | -2.67611600 |
| H | 6.82927100 | -0.36739900 | -1.37388000 |
| H | 4.42258100 | -2.92628700 | -3.84363000 |
| H | 6.66155800 | -2.15805400 | -3.08957700 |
| C | 3.00335700 | -1.81234000 | 1.07934700  |
| C | 3.63990300 | -2.89849300 | 0.47295700  |
| C | 3.73653500 | -0.96536100 | 1.90931200  |
| C | 5.00168600 | -3.10130300 | 0.65308600  |
| H | 3.07016800 | -3.57106100 | -0.16391800 |
| C | 5.10093700 | -1.17457300 | 2.10479900  |
| H | 3.23897100 | -0.13229400 | 2.40340400  |
| C | 5.73475200 | -2.23510900 | 1.46581600  |
| H | 5.49463500 | -3.93292800 | 0.16084000  |
| H | 5.66526300 | -0.50777400 | 2.74886400  |
| H | 6.79863400 | -2.39587000 | 1.60642900  |

trans-25

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.56978700 | -1.05817400 | -2.00819500 |
| C  | 1.95575400 | 0.01710500  | -2.73828300 |
| C  | 0.64514400 | -0.37273100 | -3.10897600 |
| C  | 0.41681000 | -1.68542900 | -2.59817000 |
| C  | 1.60670300 | -2.11988000 | -1.95652600 |
| Sc | 0.77848100 | -0.31298100 | -0.57228300 |
| C  | 5.23056100 | -2.33921900 | -2.70631900 |
| C  | 5.25736400 | 0.43607800  | -1.40065700 |
| C  | 4.46713200 | -1.99232400 | 0.26981800  |
| H  | 4.73736000 | -3.31466400 | -2.76186700 |
| H  | 5.20989400 | -1.89428600 | -3.70557000 |
| H  | 6.27596600 | -2.50463300 | -2.42835700 |
| H  | 4.78354100 | 1.15333700  | -0.72144200 |
| H  | 6.27136700 | 0.25846800  | -1.02607200 |
| H  | 5.34693100 | 0.90197000  | -2.38473300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.24092600  | -1.49171500 | 0.86169700  |
| H  | 3.51894700  | -1.90339300 | 0.80963400  |
| H  | 4.72447200  | -3.05534800 | 0.22577600  |
| Si | 4.37300300  | -1.22725200 | -1.45831500 |
| C  | 1.82526200  | -3.51761700 | -1.44300100 |
| H  | 1.99792500  | -4.19932200 | -2.28337500 |
| H  | 2.69159200  | -3.57993500 | -0.78263100 |
| H  | 0.95872500  | -3.89792000 | -0.89208600 |
| C  | -0.83000900 | -2.50149600 | -2.80214100 |
| H  | -1.73624000 | -1.90374300 | -2.65647000 |
| H  | -0.87111100 | -2.90865000 | -3.81808900 |
| H  | -0.87514600 | -3.34551800 | -2.10805300 |
| C  | -0.27309500 | 0.35713400  | -4.05031800 |
| H  | -0.35424900 | 1.42799200  | -3.84017700 |
| H  | 0.09874800  | 0.26290700  | -5.07614300 |
| H  | -1.27936500 | -0.07002800 | -4.03602900 |
| C  | 2.60282400  | 1.31652100  | -3.14322400 |
| H  | 3.04496100  | 1.85243600  | -2.29685100 |
| H  | 3.40436100  | 1.14107600  | -3.86819400 |
| H  | 1.87841200  | 1.97990100  | -3.62376500 |
| C  | 0.00480200  | -2.89443800 | 4.19089200  |
| C  | 0.12686100  | -2.88963400 | 2.66176100  |
| H  | 0.70045400  | -2.18548100 | 4.64955200  |
| H  | -1.00370400 | -2.63498100 | 4.52452000  |
| H  | 0.23956700  | -3.88849100 | 4.58489800  |
| C  | -0.91029900 | -3.86563100 | 2.03253200  |
| C  | 1.53116200  | -3.35103900 | 2.27832600  |
| H  | -0.43825100 | -4.39749300 | 1.19662200  |
| H  | -1.23658600 | -4.62767300 | 2.74900600  |
| H  | 1.64884100  | -4.41020400 | 2.53159900  |
| H  | 1.69940600  | -3.23484200 | 1.20521600  |
| H  | 2.30763200  | -2.79209200 | 2.80488700  |
| C  | -0.25070200 | -1.46792500 | 2.06321000  |
| H  | -0.68103900 | -0.86834900 | 2.88513400  |
| N  | 0.76242400  | -0.67707500 | 1.38120900  |
| C  | 1.51244500  | 0.33884100  | 2.11327900  |
| C  | 2.48621200  | -0.16826000 | 3.18370200  |
| C  | 2.30613800  | 1.15256300  | 1.07395900  |
| H  | 0.80619600  | 1.03261200  | 2.61209500  |
| C  | 3.26297300  | 0.98079200  | 3.83071200  |
| H  | 3.19657300  | -0.85868500 | 2.71194800  |
| H  | 1.93354500  | -0.73382800 | 3.93953400  |
| C  | 3.12320200  | 2.29100400  | 1.68897000  |
| H  | 2.99526000  | 0.46766300  | 0.54677600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.63479300  | 1.63160500  | 0.33014800  |
| C | 4.05339700  | 1.75859400  | 2.77779300  |
| H | 3.93526200  | 0.58772600  | 4.59874500  |
| H | 2.56454000  | 1.66108200  | 4.33630500  |
| H | 3.68704700  | 2.81005500  | 0.90672100  |
| H | 2.42763600  | 3.02489900  | 2.11547000  |
| H | 4.59893600  | 2.58763600  | 3.23787700  |
| H | 4.80139300  | 1.09441600  | 2.32234100  |
| C | -2.08409500 | -3.03678300 | 1.48925200  |
| C | -1.36819000 | -1.76233200 | 1.03972600  |
| H | -2.54249100 | -3.54793000 | 0.63458100  |
| H | -0.89686400 | -1.98910100 | 0.05439500  |
| H | -2.04054600 | -0.90892900 | 0.90603200  |
| C | -3.17787600 | -2.77924300 | 2.53140000  |
| C | -4.37352500 | -1.93818300 | 2.06805000  |
| H | -2.74094700 | -2.29831600 | 3.41471600  |
| H | -3.54568700 | -3.75692900 | 2.86777200  |
| C | -5.07819500 | -2.42144300 | 0.78920900  |
| H | -5.09262200 | -1.92283500 | 2.89360200  |
| H | -4.07028600 | -0.89135200 | 1.92693700  |
| H | -5.00958800 | -3.51532300 | 0.71127600  |
| H | -6.14727100 | -2.19100400 | 0.86460700  |
| C | -4.55766000 | -1.77015500 | -0.49414400 |
| C | -5.38340000 | -2.09875700 | -1.73539700 |
| H | -3.51212500 | -2.06058100 | -0.67667400 |
| H | -4.56000000 | -0.67918900 | -0.35315300 |
| C | -4.89943400 | -1.33330600 | -2.96454200 |
| H | -5.35097100 | -3.17814600 | -1.92693500 |
| H | -6.43351300 | -1.85023200 | -1.54000200 |
| H | -5.51603200 | -1.54141200 | -3.84231400 |
| H | -4.92778500 | -0.25317500 | -2.77948700 |
| H | -3.86724600 | -1.60361200 | -3.21534100 |
| N | -0.81450500 | 1.37690100  | -0.65048400 |
| H | -0.95798500 | 1.52440700  | 0.35252900  |
| C | -2.13191300 | 0.94365700  | -1.20935600 |
| H | -2.07157100 | 1.02227600  | -2.29624900 |
| H | -2.29173000 | -0.11286300 | -0.96992800 |
| C | -0.41273600 | 2.69878300  | -1.23051600 |
| H | 0.29518700  | 2.51973500  | -2.04544600 |
| H | -1.30535300 | 3.16567000  | -1.66541700 |
| C | 0.18855600  | 3.65171000  | -0.22487700 |
| C | 1.38057000  | 4.31776600  | -0.51591000 |
| C | -0.48120600 | 3.94378200  | 0.96780900  |
| C | 1.89245000  | 5.26898900  | 0.36470800  |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 1.90260500  | 4.10313600 | -1.44558200 |
| C | 0.03960300  | 4.88070900 | 1.85634200  |
| H | -1.43730800 | 3.47184600 | 1.18908500  |
| C | 1.22482800  | 5.54907400 | 1.55383900  |
| H | 2.81531200  | 5.78580900 | 0.12280600  |
| H | -0.49226200 | 5.10476100 | 2.77503400  |
| H | 1.62324600  | 6.28703800 | 2.24184000  |
| C | -3.28593700 | 1.76070100 | -0.67955200 |
| C | -3.55772600 | 1.77447000 | 0.69394800  |
| C | -4.10309100 | 2.49240700 | -1.54035100 |
| C | -4.62720300 | 2.50782000 | 1.19616700  |
| H | -2.93749500 | 1.19909800 | 1.38218500  |
| C | -5.17795400 | 3.22599000 | -1.03960900 |
| H | -3.90020900 | 2.48454800 | -2.60837100 |
| C | -5.44016300 | 3.23459500 | 0.32648600  |
| H | -4.83240500 | 2.50581700 | 2.26147900  |
| H | -5.80703300 | 3.79236400 | -1.71798100 |
| H | -6.27690400 | 3.80476700 | 0.71573200  |

cis-25

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.26299900 | -0.52331800 | -1.49276600 |
| C  | -2.40734200 | -1.47219100 | -2.15638200 |
| C  | -1.47512000 | -0.76517000 | -2.95058100 |
| C  | -1.74814200 | 0.63169500  | -2.81662900 |
| C  | -2.85689800 | 0.78064700  | -1.94230100 |
| Sc | -1.12181000 | -0.10062100 | -0.54097100 |
| C  | -6.28489500 | -0.77119400 | -1.70162700 |
| C  | -4.81102300 | -2.63812400 | 0.22036300  |
| C  | -5.07537500 | 0.33075200  | 0.89941900  |
| H  | -6.35211900 | 0.22857300  | -2.14083200 |
| H  | -6.18033300 | -1.49152900 | -2.51858200 |
| H  | -7.22836200 | -0.97668200 | -1.18639900 |
| H  | -3.90068600 | -2.86254800 | 0.78483000  |
| H  | -5.65532000 | -2.72868300 | 0.91200700  |
| H  | -4.93293400 | -3.40682300 | -0.54668200 |
| H  | -5.82814600 | -0.05936900 | 1.59237900  |
| H  | -4.15437900 | 0.50157700  | 1.46696900  |
| H  | -5.43338800 | 1.29847500  | 0.53716300  |
| Si | -4.83694500 | -0.89857700 | -0.50958000 |
| C  | -3.51149800 | 2.08455500  | -1.56895800 |
| H  | -4.51910100 | 2.14691300  | -1.99450600 |
| H  | -3.60572100 | 2.20313200  | -0.48628600 |
| H  | -2.94349300 | 2.93853500  | -1.94516800 |
| C  | -1.04265000 | 1.70298000  | -3.60508300 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.03194700  | 1.75734200  | -3.39291300 |
| H | -1.14698400 | 1.50625700  | -4.67697800 |
| H | -1.46638000 | 2.68943600  | -3.41128900 |
| C | -0.46080600 | -1.33078300 | -3.90582600 |
| H | -0.07049100 | -2.30124400 | -3.58731100 |
| H | -0.90896200 | -1.47405900 | -4.89508100 |
| H | 0.38809400  | -0.65296200 | -4.03443100 |
| C | -2.54282400 | -2.97147700 | -2.11009200 |
| H | -2.46381800 | -3.37930200 | -1.09730900 |
| H | -3.51805800 | -3.27559100 | -2.50327500 |
| H | -1.78422800 | -3.45388100 | -2.73028300 |
| C | -0.33877100 | 3.87199400  | 3.16321100  |
| C | -1.04898800 | 3.21607100  | 1.97172300  |
| H | -0.30508700 | 3.19442700  | 4.02296000  |
| H | 0.69191000  | 4.15184700  | 2.92082300  |
| H | -0.87030200 | 4.77735600  | 3.47269300  |
| C | -1.00236200 | 4.17033500  | 0.76187900  |
| C | -2.50176000 | 2.93615200  | 2.34329200  |
| H | -1.79916400 | 3.90316900  | 0.05035000  |
| H | -1.16396900 | 5.21377000  | 1.05337800  |
| H | -3.05279400 | 3.88193700  | 2.38058400  |
| H | -2.98033800 | 2.29006500  | 1.60323700  |
| H | -2.59585600 | 2.46450700  | 3.32310700  |
| C | -0.20311200 | 1.95691600  | 1.48937500  |
| H | 0.61185500  | 1.81345600  | 2.22030600  |
| N | -0.87417000 | 0.68062700  | 1.27386800  |
| C | -0.87026300 | -0.30722800 | 2.34845500  |
| C | -1.34268800 | 0.14763900  | 3.73341400  |
| C | -1.74478700 | -1.50516100 | 1.93709000  |
| H | 0.17016900  | -0.67884200 | 2.49833900  |
| C | -1.18402400 | -0.98559400 | 4.75168200  |
| H | -2.39961600 | 0.43327700  | 3.66726500  |
| H | -0.78125100 | 1.03362100  | 4.04771000  |
| C | -1.61176700 | -2.67419400 | 2.91742000  |
| H | -2.78771500 | -1.16460600 | 1.90721800  |
| H | -1.51379600 | -1.89230000 | 0.92272000  |
| C | -1.98448400 | -2.22107100 | 4.33152300  |
| H | -1.50648500 | -0.64659700 | 5.74016700  |
| H | -0.12162300 | -1.25072200 | 4.83854400  |
| H | -2.24724500 | -3.50760800 | 2.60061700  |
| H | -0.57537000 | -3.03986200 | 2.90588300  |
| H | -1.82782400 | -3.03916200 | 5.04033200  |
| H | -3.05530700 | -1.97998700 | 4.35317500  |
| C | 0.34611400  | 3.93838600  | 0.08400300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.42398500  | 2.40868800  | 0.14488300  |
| H | 1.14224400  | 4.35977600  | 0.71288100  |
| H | -0.22512400 | 2.07109800  | -0.70117400 |
| H | 1.42228100  | 1.99176100  | -0.01892100 |
| C | 0.43299600  | 4.54458100  | -1.31859300 |
| C | 1.83437500  | 4.82446000  | -1.87063500 |
| H | -0.11999000 | 5.49191100  | -1.31734500 |
| H | -0.10834900 | 3.88263600  | -2.00966600 |
| C | 2.84122500  | 3.66205400  | -1.84730100 |
| H | 1.71230800  | 5.17725300  | -2.90027400 |
| H | 2.26972700  | 5.66641200  | -1.31689000 |
| H | 2.32470600  | 2.69933600  | -1.98603900 |
| H | 3.51198100  | 3.76214100  | -2.70911900 |
| C | 3.71738300  | 3.62059100  | -0.59213900 |
| C | 4.87229500  | 2.62525900  | -0.68299500 |
| H | 3.11823900  | 3.39433200  | 0.30137000  |
| H | 4.12958700  | 4.62620700  | -0.43114900 |
| C | 5.83928500  | 2.75618900  | 0.48986700  |
| H | 4.47816300  | 1.60197100  | -0.72873000 |
| H | 5.41392900  | 2.79331700  | -1.62268300 |
| H | 6.64874200  | 2.02396100  | 0.42515300  |
| H | 6.28587800  | 3.75533000  | 0.51518100  |
| H | 5.32243100  | 2.59662000  | 1.44204700  |
| N | 0.58639800  | -1.57662200 | -0.35658400 |
| H | 0.83208500  | -1.45969600 | 0.63142400  |
| C | 1.64175600  | -0.86908500 | -1.13841900 |
| H | 1.79839100  | -1.41044200 | -2.07515000 |
| H | 1.26122200  | 0.13172600  | -1.42421300 |
| C | 0.55174500  | -3.04542800 | -0.60403300 |
| H | -0.20268700 | -3.46313000 | 0.07227000  |
| H | 0.20205000  | -3.20249400 | -1.62635600 |
| C | 1.89154100  | -3.70324100 | -0.38754300 |
| C | 2.61276700  | -4.21816500 | -1.46283600 |
| C | 2.44980900  | -3.73873500 | 0.89365200  |
| C | 3.88561400  | -4.75299300 | -1.26518000 |
| H | 2.17974400  | -4.19947000 | -2.46078300 |
| C | 3.72111000  | -4.26199600 | 1.09200400  |
| H | 1.89106000  | -3.34299200 | 1.74177600  |
| C | 4.44208500  | -4.76803100 | 0.00936100  |
| H | 4.43996100  | -5.15398700 | -2.10743000 |
| H | 4.15117300  | -4.27876000 | 2.08789400  |
| H | 5.43414500  | -5.17935300 | 0.16359200  |
| C | 2.93480600  | -0.70881400 | -0.37465900 |
| C | 2.91578100  | -0.12107800 | 0.89427700  |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 4.13798200 | -1.18201800 | -0.89336100 |
| C | 4.08338000 | -0.02475500 | 1.64359100  |
| H | 1.98045300 | 0.25765300  | 1.30601600  |
| C | 5.30889100 | -1.08252800 | -0.14428700 |
| H | 4.15626400 | -1.65893800 | -1.86926300 |
| C | 5.28248000 | -0.51100700 | 1.12459300  |
| H | 4.05890700 | 0.43166600  | 2.62804500  |
| H | 6.23933700 | -1.46634300 | -0.54944700 |
| H | 6.19450300 | -0.43912200 | 1.70799200  |

trans-ts-26

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.84994300  | -1.54502400 | -1.58844600 |
| C  | 2.23897100  | -0.75342300 | -2.62333400 |
| C  | 0.95277400  | -1.27870000 | -2.90342800 |
| C  | 0.74531500  | -2.40642800 | -2.05644500 |
| C  | 1.92107700  | -2.59606900 | -1.27909900 |
| Sc | 0.95923400  | -0.49508700 | -0.54211200 |
| C  | 5.74240100  | -2.42779100 | -1.99140600 |
| C  | 5.18470100  | 0.44003600  | -1.01746900 |
| C  | 4.73581900  | -1.88360600 | 0.87803500  |
| H  | 5.43259400  | -3.47635400 | -1.95049900 |
| H  | 5.71360400  | -2.10819000 | -3.03746800 |
| H  | 6.77864300  | -2.36605900 | -1.64544000 |
| H  | 4.47198400  | 1.12722500  | -0.54607600 |
| H  | 6.12894600  | 0.52703900  | -0.46952600 |
| H  | 5.36668800  | 0.77993700  | -2.03963200 |
| H  | 5.60880000  | -1.40323700 | 1.33147400  |
| H  | 3.85578100  | -1.58389100 | 1.45744800  |
| H  | 4.86362300  | -2.96338700 | 0.99357600  |
| Si | 4.62076500  | -1.35745500 | -0.93198000 |
| C  | 2.19197200  | -3.81951300 | -0.44603300 |
| H  | 2.56277700  | -4.61994800 | -1.09572900 |
| H  | 2.94438100  | -3.64034900 | 0.32129100  |
| H  | 1.29077000  | -4.19386000 | 0.04638700  |
| C  | -0.47226700 | -3.28900700 | -2.06861500 |
| H  | -1.39706500 | -2.70316600 | -2.11299500 |
| H  | -0.46309000 | -3.94783300 | -2.94322500 |
| H  | -0.52060800 | -3.92186700 | -1.17870100 |
| C  | 0.01958200  | -0.82809700 | -3.99027500 |
| H  | -0.03127000 | 0.26093400  | -4.07742700 |
| H  | 0.35812200  | -1.21388800 | -4.95770200 |
| H  | -0.99325000 | -1.20341900 | -3.82624600 |
| C  | 2.87066300  | 0.39190100  | -3.37171000 |
| H  | 3.21825500  | 1.19404100  | -2.71509300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.73945900  | 0.04277800  | -3.93932400 |
| H | 2.16474500  | 0.82297500  | -4.08577800 |
| C | -0.19938600 | -1.86673800 | 4.47932600  |
| C | -0.03852500 | -2.04834700 | 2.96312300  |
| H | 0.37456800  | -1.01814400 | 4.85655900  |
| H | -1.24614100 | -1.71335700 | 4.75710800  |
| H | 0.15324300  | -2.76213000 | 5.00062300  |
| C | -0.82899500 | -3.31169400 | 2.49931600  |
| C | 1.44213600  | -2.24614100 | 2.64498400  |
| H | -0.21365900 | -3.88367000 | 1.79326300  |
| H | -1.04867000 | -3.98105200 | 3.33791600  |
| H | 1.80849500  | -3.15995500 | 3.12588500  |
| H | 1.61290100  | -2.37000400 | 1.56988700  |
| H | 2.06110500  | -1.41291200 | 2.98726700  |
| C | -0.69140800 | -0.85184300 | 2.14916000  |
| H | -1.31017400 | -0.26881200 | 2.84831200  |
| N | 0.18426200  | 0.04634700  | 1.38474900  |
| C | 0.85956600  | 1.20333000  | 2.01317400  |
| C | 1.04433900  | 1.18753100  | 3.53060300  |
| C | 2.22064500  | 1.38351500  | 1.32569300  |
| H | 0.27277100  | 2.11039600  | 1.79550600  |
| C | 1.73788000  | 2.47447200  | 3.99100600  |
| H | 1.65838600  | 0.33186600  | 3.83079900  |
| H | 0.07208600  | 1.08396600  | 4.02240800  |
| C | 2.95691600  | 2.64033000  | 1.79754700  |
| H | 2.83445900  | 0.48441200  | 1.51061500  |
| H | 2.09179800  | 1.49172200  | 0.22628500  |
| C | 3.10271200  | 2.63165600  | 3.31993700  |
| H | 1.84546400  | 2.46485200  | 5.07933600  |
| H | 1.10885900  | 3.33837100  | 3.73773100  |
| H | 3.93439400  | 2.71350600  | 1.30997700  |
| H | 2.37450600  | 3.51817000  | 1.49030300  |
| H | 3.58844400  | 3.55405400  | 3.65112100  |
| H | 3.75390700  | 1.80022700  | 3.62223100  |
| C | -2.10373300 | -2.84085700 | 1.78250900  |
| C | -1.63047300 | -1.53941600 | 1.14234200  |
| H | -2.39335000 | -3.56294700 | 1.00959000  |
| H | -1.06404000 | -1.80713300 | 0.22253100  |
| H | -2.44015100 | -0.88261800 | 0.82014900  |
| C | -3.29691600 | -2.66228700 | 2.72931900  |
| C | -4.56145000 | -2.04264200 | 2.12240800  |
| H | -2.99962700 | -2.05512100 | 3.59286700  |
| H | -3.54502300 | -3.65341600 | 3.12977300  |
| C | -5.10394100 | -2.71099300 | 0.84803100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.33455100 | -2.07387400 | 2.89728000  |
| H | -4.39638600 | -0.97518900 | 1.92032700  |
| H | -4.94900400 | -3.79756700 | 0.89967900  |
| H | -6.18969600 | -2.56255600 | 0.81328500  |
| C | -4.52483900 | -2.16400600 | -0.45969200 |
| C | -5.25342300 | -2.64497800 | -1.71148800 |
| H | -3.46227500 | -2.42864300 | -0.55311500 |
| H | -4.57061500 | -1.06402700 | -0.43324900 |
| C | -4.66019500 | -2.03712400 | -2.98041900 |
| H | -5.21194000 | -3.73978100 | -1.76455300 |
| H | -6.31420800 | -2.37790800 | -1.63531400 |
| H | -5.20618200 | -2.34819500 | -3.87428300 |
| H | -4.68632400 | -0.94247200 | -2.93272800 |
| H | -3.61430500 | -2.34093500 | -3.10794900 |
| N | -0.73542900 | 0.77932400  | -0.91246700 |
| H | -0.54419900 | 0.60148400  | 0.37550400  |
| C | -2.05455400 | 0.56107300  | -1.53022100 |
| H | -1.93007900 | 0.46367000  | -2.61587700 |
| H | -2.44670700 | -0.39401500 | -1.17061700 |
| C | 0.05889500  | 1.83075100  | -1.54630800 |
| H | 1.09718400  | 1.45629800  | -1.74550300 |
| H | -0.32581700 | 2.00051000  | -2.56148000 |
| C | 0.23977100  | 3.16793000  | -0.84864500 |
| C | 1.37322400  | 3.92366400  | -1.16543400 |
| C | -0.69087900 | 3.68440300  | 0.05265100  |
| C | 1.57479800  | 5.17707200  | -0.59622900 |
| H | 2.10550100  | 3.52772500  | -1.86801200 |
| C | -0.48264500 | 4.93514700  | 0.63354600  |
| H | -1.57824000 | 3.11211300  | 0.30326400  |
| C | 0.64581400  | 5.68422300  | 0.31121900  |
| H | 2.45864800  | 5.75165300  | -0.85283000 |
| H | -1.21272700 | 5.32578500  | 1.33512700  |
| H | 0.80098700  | 6.65838800  | 0.76281300  |
| C | -3.03795200 | 1.67182700  | -1.24437200 |
| C | -3.70273300 | 1.73655800  | -0.01561600 |
| C | -3.23329200 | 2.69519900  | -2.17202800 |
| C | -4.53383800 | 2.81124400  | 0.28544400  |
| H | -3.55602300 | 0.94783300  | 0.71936600  |
| C | -4.06014600 | 3.77645900  | -1.87289300 |
| H | -2.73421700 | 2.64720000  | -3.13734200 |
| C | -4.70767400 | 3.83780400  | -0.64255100 |
| H | -5.04675900 | 2.84912500  | 1.24108400  |
| H | -4.19876400 | 4.56827700  | -2.60154800 |
| H | -5.35210500 | 4.67844800  | -0.40790000 |

cis-ts-26

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.51091500 | -0.07645700 | -1.40508600 |
| C  | -2.71797000 | -0.95890000 | -2.22455000 |
| C  | -1.78615000 | -0.18824500 | -2.95775000 |
| C  | -1.99655000 | 1.18676500  | -2.62820300 |
| C  | -3.07004300 | 1.25929700  | -1.69731800 |
| Sc | -1.28417600 | 0.08897100  | -0.56526200 |
| C  | -6.49105600 | -0.41119700 | -1.73542400 |
| C  | -5.03710600 | -2.32614900 | 0.16832200  |
| C  | -5.45426300 | 0.57313800  | 0.98070600  |
| H  | -6.57621400 | 0.61296700  | -2.11077800 |
| H  | -6.31780200 | -1.06914200 | -2.59259000 |
| H  | -7.44916500 | -0.68742400 | -1.28441800 |
| H  | -4.14737700 | -2.53941000 | 0.76888200  |
| H  | -5.90813000 | -2.47342600 | 0.81600100  |
| H  | -5.09677000 | -3.06820200 | -0.63117700 |
| H  | -6.31865200 | 0.16512200  | 1.51575000  |
| H  | -4.62596600 | 0.62430900  | 1.69488000  |
| H  | -5.71078100 | 1.59072200  | 0.67650000  |
| Si | -5.09817400 | -0.55870400 | -0.48185400 |
| C  | -3.68871600 | 2.52652300  | -1.16737400 |
| H  | -4.69267000 | 2.65754900  | -1.58561600 |
| H  | -3.78900400 | 2.52120000  | -0.07903600 |
| H  | -3.10301300 | 3.40531900  | -1.44408200 |
| C  | -1.26976500 | 2.32652200  | -3.28662200 |
| H  | -0.18136000 | 2.20792500  | -3.24016200 |
| H  | -1.54103700 | 2.37886200  | -4.34614000 |
| H  | -1.52170800 | 3.28611200  | -2.83328100 |
| C  | -0.79250600 | -0.67889300 | -3.97082700 |
| H  | -0.41883600 | -1.67846100 | -3.73367900 |
| H  | -1.25021400 | -0.72552000 | -4.96472300 |
| H  | 0.06825500  | -0.00807600 | -4.03844400 |
| C  | -2.89560100 | -2.44989700 | -2.34450500 |
| H  | -2.78170000 | -2.97307200 | -1.38954400 |
| H  | -3.89782800 | -2.67911300 | -2.72093500 |
| H  | -2.17881000 | -2.87452500 | -3.05009600 |
| C  | -0.17716100 | 3.20453300  | 3.53935900  |
| C  | -0.76091000 | 2.60115000  | 2.25498300  |
| H  | -0.07692800 | 2.44387500  | 4.31986600  |
| H  | 0.81408100  | 3.63553200  | 3.36875300  |
| H  | -0.82765800 | 3.99749000  | 3.92066300  |
| C  | -0.78345500 | 3.66517500  | 1.14245300  |
| C  | -2.18265200 | 2.12242500  | 2.53517500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.50277100 | 3.35791900  | 0.36088300  |
| H | -1.09758800 | 4.64891400  | 1.50619200  |
| H | -2.82040800 | 2.98819100  | 2.74441000  |
| H | -2.62141200 | 1.60364400  | 1.67559500  |
| H | -2.24611400 | 1.45142600  | 3.39601700  |
| C | 0.24005400  | 1.50784700  | 1.68808100  |
| H | 1.06367400  | 1.40335100  | 2.40778300  |
| N | -0.29919000 | 0.18710200  | 1.34724600  |
| C | -0.49551900 | -0.87181800 | 2.36378400  |
| C | -0.13403100 | -0.52940900 | 3.80957200  |
| C | -1.92157400 | -1.42750100 | 2.26888800  |
| H | 0.17728600  | -1.70475500 | 2.08720600  |
| C | -0.33577000 | -1.75739200 | 4.70558000  |
| H | -0.76121300 | 0.29213600  | 4.17416700  |
| H | 0.90697900  | -0.19457000 | 3.86827900  |
| C | -2.12095200 | -2.65126000 | 3.16175900  |
| H | -2.63753500 | -0.63932200 | 2.53751000  |
| H | -2.14051900 | -1.70439400 | 1.21768600  |
| C | -1.76238600 | -2.30197000 | 4.60844900  |
| H | -0.09626400 | -1.49862800 | 5.74078900  |
| H | 0.37073800  | -2.54228400 | 4.40353100  |
| H | -3.15250700 | -3.00990200 | 3.09337300  |
| H | -1.47146100 | -3.46513100 | 2.81091900  |
| H | -1.87504500 | -3.18250600 | 5.24746900  |
| H | -2.46615600 | -1.54532700 | 4.98054300  |
| C | 0.61279600  | 3.65235500  | 0.52235700  |
| C | 0.82861200  | 2.14277200  | 0.39869400  |
| H | 1.33396200  | 4.04920800  | 1.25056000  |
| H | 0.24392400  | 1.84370400  | -0.50953400 |
| H | 1.85338900  | 1.81857600  | 0.19559000  |
| C | 0.71026200  | 4.45858700  | -0.77248900 |
| C | 2.10999700  | 4.88782100  | -1.22021700 |
| H | 0.10252800  | 5.36433400  | -0.65317200 |
| H | 0.23600400  | 3.87942300  | -1.57659100 |
| C | 3.12835800  | 3.75678700  | -1.44706800 |
| H | 1.99071900  | 5.46129400  | -2.14531800 |
| H | 2.51898700  | 5.59054000  | -0.48268300 |
| H | 2.60704800  | 2.82795900  | -1.72806600 |
| H | 3.76092800  | 4.00899000  | -2.30589800 |
| C | 4.05139600  | 3.50196500  | -0.25391100 |
| C | 5.11671400  | 2.44267500  | -0.52561000 |
| H | 3.47081100  | 3.21423100  | 0.63503100  |
| H | 4.54408700  | 4.44868200  | 0.00683900  |
| C | 6.09516400  | 2.29489500  | 0.63544200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.63630700  | 1.47712400  | -0.72900400 |
| H | 5.66520400  | 2.71625300  | -1.43606400 |
| H | 6.85018300  | 1.53263300  | 0.42676000  |
| H | 6.60979100  | 3.24039600  | 0.83515300  |
| H | 5.56983000  | 1.99776200  | 1.54937100  |
| N | 0.53869400  | -1.03704600 | -0.73231300 |
| H | 0.42160900  | -0.44488400 | 0.46955500  |
| C | 1.70375300  | -0.59925800 | -1.50775700 |
| H | 1.73824700  | -1.12690000 | -2.47057400 |
| H | 1.58181700  | 0.46786800  | -1.75208600 |
| C | 0.26472200  | -2.48952900 | -0.82207400 |
| H | -0.45568300 | -2.74919500 | -0.02916400 |
| H | -0.22707900 | -2.71099500 | -1.78063400 |
| C | 1.48238600  | -3.38152000 | -0.71287300 |
| C | 2.00742900  | -3.97107200 | -1.86233900 |
| C | 2.13599800  | -3.57338700 | 0.50616200  |
| C | 3.18073700  | -4.72076600 | -1.80416900 |
| H | 1.49879100  | -3.83535900 | -2.81446900 |
| C | 3.31256400  | -4.31002600 | 0.56778500  |
| H | 1.73636800  | -3.11812600 | 1.40968500  |
| C | 3.83997600  | -4.88216900 | -0.59002500 |
| H | 3.58001700  | -5.17187700 | -2.70679300 |
| H | 3.82126100  | -4.43735000 | 1.51785300  |
| H | 4.75951500  | -5.45620100 | -0.54186500 |
| C | 3.03496300  | -0.78353600 | -0.79549800 |
| C | 3.17592500  | -0.51538400 | 0.57017500  |
| C | 4.15057400  | -1.21980400 | -1.50894500 |
| C | 4.40250300  | -0.67993200 | 1.20549300  |
| H | 2.31470200  | -0.20941800 | 1.16002200  |
| C | 5.38147400  | -1.38519800 | -0.87633600 |
| H | 4.05083200  | -1.45574700 | -2.56545200 |
| C | 5.51107200  | -1.11582700 | 0.48284900  |
| H | 4.49282900  | -0.47285800 | 2.26757200  |
| H | 6.23610300  | -1.73649900 | -1.44568900 |
| H | 6.46788100  | -1.24830000 | 0.97744100  |

trans-27

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.56576500 | -1.69361000 | -1.67060900 |
| C  | 2.00793500 | -0.87651000 | -2.71803800 |
| C  | 0.68164400 | -1.30306200 | -2.97355500 |
| C  | 0.39240100 | -2.38451200 | -2.09018400 |
| C  | 1.56648800 | -2.65990200 | -1.33248400 |
| Sc | 0.70255400 | -0.39970400 | -0.69059600 |
| C  | 5.41675300 | -2.60453500 | -2.28060600 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.94216100  | 0.18132100  | -1.04560700 |
| C  | 4.58198700  | -2.32406500 | 0.65763400  |
| H  | 5.10823400  | -3.65439200 | -2.29328800 |
| H  | 5.32481000  | -2.21437200 | -3.29859300 |
| H  | 6.47268900  | -2.56493700 | -1.99612000 |
| H  | 4.15380500  | 0.86879900  | -0.71676000 |
| H  | 5.77943100  | 0.28168900  | -0.34744000 |
| H  | 5.29018000  | 0.51483200  | -2.02678600 |
| H  | 5.54173400  | -1.97468100 | 1.05238400  |
| H  | 3.80261300  | -2.00501200 | 1.35738900  |
| H  | 4.61036700  | -3.41690200 | 0.65710800  |
| Si | 4.36066800  | -1.61803900 | -1.08001600 |
| C  | 1.78005000  | -3.92570200 | -0.54947500 |
| H  | 2.10537400  | -4.71350000 | -1.23829700 |
| H  | 2.54565100  | -3.82025300 | 0.21791700  |
| H  | 0.86449900  | -4.27775400 | -0.06917200 |
| C  | -0.89508600 | -3.16304200 | -2.06343900 |
| H  | -1.76612600 | -2.50393700 | -2.15706200 |
| H  | -0.93951100 | -3.87755700 | -2.89225300 |
| H  | -1.00610200 | -3.72964500 | -1.13379200 |
| C  | -0.24064600 | -0.78211000 | -4.03684600 |
| H  | -0.14055300 | 0.29755700  | -4.17863000 |
| H  | -0.02743600 | -1.26176100 | -4.99808000 |
| H  | -1.28538100 | -0.98930200 | -3.79122000 |
| C  | 2.74288100  | 0.16146000  | -3.52864500 |
| H  | 3.21933900  | 0.93282200  | -2.91840500 |
| H  | 3.53452200  | -0.31279800 | -4.11899700 |
| H  | 2.06762900  | 0.65790800  | -4.22966100 |
| C  | -0.32075600 | -2.28518600 | 4.36755200  |
| C  | -0.21758700 | -2.26855200 | 2.83651500  |
| H  | 0.25380400  | -1.47972900 | 4.82921700  |
| H  | -1.35953700 | -2.19173800 | 4.69680800  |
| H  | 0.06354700  | -3.23407800 | 4.75377300  |
| C  | -1.11863900 | -3.39988200 | 2.24602900  |
| C  | 1.23622900  | -2.50647800 | 2.42745900  |
| H  | -0.57093100 | -3.91874000 | 1.45092800  |
| H  | -1.36095200 | -4.15189100 | 3.00408700  |
| H  | 1.52132500  | -3.53944900 | 2.65279000  |
| H  | 1.38454100  | -2.35896700 | 1.35365300  |
| H  | 1.93460600  | -1.85147600 | 2.95387400  |
| C  | -0.82315900 | -0.95146400 | 2.23402800  |
| H  | -1.37179100 | -0.42727800 | 3.02866900  |
| N  | 0.06860400  | 0.01476400  | 1.53626100  |
| C  | 0.99375800  | 0.96902400  | 2.23527200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.24941000  | 0.76007400  | 3.72434000  |
| C | 2.30210600  | 1.01693700  | 1.44233900  |
| H | 0.53906600  | 1.96431700  | 2.14645200  |
| C | 2.16609500  | 1.87584500  | 4.24170400  |
| H | 1.73655200  | -0.20135000 | 3.90970600  |
| H | 0.30073900  | 0.76321000  | 4.27113200  |
| C | 3.24886500  | 2.09482600  | 1.97497600  |
| H | 2.78583400  | 0.02612700  | 1.46413300  |
| H | 2.08211100  | 1.28005900  | 0.38626000  |
| C | 3.48901500  | 1.90008300  | 3.47328500  |
| H | 2.34613900  | 1.73309600  | 5.31062000  |
| H | 1.66254900  | 2.84482300  | 4.12676900  |
| H | 4.19237300  | 2.07390700  | 1.42160100  |
| H | 2.78890900  | 3.07597200  | 1.79657200  |
| H | 4.13510100  | 2.69658900  | 3.85295600  |
| H | 4.01966200  | 0.95212300  | 3.63611700  |
| C | -2.37524200 | -2.75330400 | 1.64013200  |
| C | -1.82349600 | -1.41382100 | 1.16035100  |
| H | -2.72606300 | -3.34794600 | 0.78888200  |
| H | -1.28454300 | -1.60268500 | 0.20816700  |
| H | -2.58277300 | -0.65961500 | 0.93585500  |
| C | -3.54225100 | -2.60740800 | 2.62239800  |
| C | -4.77203100 | -1.86605500 | 2.08030100  |
| H | -3.20592500 | -2.10002300 | 3.53548800  |
| H | -3.84264400 | -3.61709400 | 2.92887500  |
| C | -5.33863200 | -2.38751300 | 0.74863100  |
| H | -5.54906500 | -1.93109200 | 2.84875600  |
| H | -4.55245100 | -0.79377200 | 1.97926000  |
| H | -5.21843500 | -3.47853500 | 0.69424900  |
| H | -6.41931500 | -2.20398700 | 0.73443200  |
| C | -4.75004400 | -1.73942600 | -0.50871800 |
| C | -5.48209800 | -2.12354100 | -1.79209400 |
| H | -3.68868700 | -1.99986800 | -0.62352300 |
| H | -4.78859200 | -0.64492200 | -0.39813600 |
| C | -4.89068400 | -1.43261300 | -3.01811500 |
| H | -5.44540600 | -3.21226400 | -1.92197200 |
| H | -6.54181500 | -1.85897500 | -1.69445500 |
| H | -5.43589400 | -1.68814900 | -3.92982200 |
| H | -4.91967900 | -0.34359600 | -2.90127500 |
| H | -3.84381400 | -1.72418500 | -3.16473400 |
| N | -0.62944500 | 0.97252300  | -1.21198300 |
| H | -0.60302800 | 0.64003000  | 1.07949800  |
| C | -1.98056400 | 1.05356200  | -1.76021700 |
| H | -1.94120300 | 1.10670500  | -2.85915800 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -2.50425100 | 0.12446100 | -1.49647100 |
| C | 0.32404300  | 1.95324800 | -1.69549500 |
| H | 1.31894600  | 1.45022700 | -1.83315600 |
| H | 0.08215800  | 2.27010500 | -2.72411900 |
| C | 0.63489000  | 3.17256900 | -0.83308300 |
| C | 1.78389200  | 3.91372800 | -1.13205700 |
| C | -0.15640100 | 3.56303400 | 0.24567500  |
| C | 2.13123900  | 5.02726100 | -0.37441200 |
| H | 2.40982300  | 3.61914400 | -1.97306700 |
| C | 0.19229500  | 4.67827900 | 1.00985500  |
| H | -1.05808400 | 3.00610600 | 0.48189900  |
| C | 1.33351200  | 5.41280500 | 0.70316700  |
| H | 3.02366100  | 5.59249900 | -0.62233200 |
| H | -0.43975700 | 4.97485300 | 1.84127100  |
| H | 1.60093000  | 6.28119000 | 1.29595500  |
| C | -2.76533600 | 2.23909900 | -1.24190000 |
| C | -3.47443200 | 2.15506100 | -0.04093800 |
| C | -2.70847900 | 3.46541900 | -1.90512900 |
| C | -4.09054600 | 3.27918400 | 0.50277400  |
| H | -3.54312700 | 1.19953900 | 0.47474100  |
| C | -3.31947300 | 4.59428700 | -1.36451100 |
| H | -2.17422500 | 3.54012100 | -2.84967500 |
| C | -4.00473900 | 4.50489200 | -0.15558300 |
| H | -4.64138900 | 3.19922200 | 1.43466500  |
| H | -3.25960700 | 5.54368100 | -1.88655100 |
| H | -4.48080700 | 5.38358900 | 0.26681800  |

cis-27

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.34655100 | 1.25018200  | -0.92797700 |
| C  | -3.21813300 | 0.27658500  | -1.98158500 |
| C  | -2.19692400 | 0.69244000  | -2.86606600 |
| C  | -1.67314100 | 1.93245500  | -2.38503400 |
| C  | -2.41222300 | 2.29673600  | -1.22671300 |
| Sc | -1.13417700 | 0.18875100  | -0.71796700 |
| C  | -5.94544600 | 2.70489500  | -0.44854700 |
| C  | -5.73533500 | -0.21266700 | 0.47888800  |
| C  | -4.32684100 | 1.94231800  | 2.03629100  |
| H  | -5.46136400 | 3.68458100  | -0.50172500 |
| H  | -6.24557600 | 2.42331800  | -1.46240500 |
| H  | -6.85049600 | 2.80758600  | 0.15835900  |
| H  | -5.08844800 | -1.04959600 | 0.76048400  |
| H  | -6.47126100 | -0.08291700 | 1.27969500  |
| H  | -6.27916800 | -0.49566000 | -0.42521100 |
| H  | -5.25695900 | 2.22996700  | 2.53951700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -3.89606600 | 1.12280600  | 2.62065700  |
| H  | -3.65063200 | 2.79811300  | 2.09665900  |
| Si | -4.79690200 | 1.40857900  | 0.28360000  |
| C  | -2.39987400 | 3.67421100  | -0.62033500 |
| H  | -2.95627000 | 4.35476800  | -1.27498300 |
| H  | -2.88172000 | 3.69755000  | 0.35792900  |
| H  | -1.39492300 | 4.08705200  | -0.50669400 |
| C  | -0.64194400 | 2.78150500  | -3.07751400 |
| H  | 0.16688900  | 2.18287100  | -3.50856600 |
| H  | -1.09832000 | 3.34498000  | -3.89851900 |
| H  | -0.19197000 | 3.50565000  | -2.39326000 |
| C  | -1.76765300 | -0.00800700 | -4.12304100 |
| H  | -1.70039700 | -1.09071000 | -3.98368200 |
| H  | -2.48264400 | 0.17889300  | -4.93090900 |
| H  | -0.79282200 | 0.34942000  | -4.46558700 |
| C  | -4.06759300 | -0.94884100 | -2.18703600 |
| H  | -4.14630200 | -1.56905700 | -1.28882000 |
| H  | -5.08604300 | -0.66339200 | -2.47027800 |
| H  | -3.66929100 | -1.56791800 | -2.99380900 |
| C  | 1.38561800  | 3.05912600  | 3.14001900  |
| C  | 0.68127100  | 2.50623100  | 1.89150100  |
| H  | 1.10588100  | 2.47881500  | 4.02573600  |
| H  | 2.47494200  | 3.01626700  | 3.05072900  |
| H  | 1.09965100  | 4.10078000  | 3.31352600  |
| C  | 1.06360700  | 3.34009300  | 0.65817400  |
| C  | -0.82335100 | 2.54504600  | 2.13351900  |
| H  | 0.40233700  | 3.08408100  | -0.18650900 |
| H  | 0.96174700  | 4.41762800  | 0.82951400  |
| H  | -1.13909300 | 3.58527100  | 2.27051400  |
| H  | -1.39399000 | 2.15800600  | 1.28263000  |
| H  | -1.12619400 | 1.99527300  | 3.02983300  |
| C  | 1.31003800  | 1.11107700  | 1.57518200  |
| H  | 1.78456300  | 0.72286800  | 2.47873300  |
| N  | 0.39105400  | 0.04813500  | 1.04531300  |
| C  | -0.33729000 | -0.86476300 | 2.01195700  |
| C  | 0.04005900  | -0.67511800 | 3.48413100  |
| C  | -1.85342800 | -0.76813500 | 1.77508900  |
| H  | -0.04683400 | -1.88708500 | 1.73215000  |
| C  | -0.79667600 | -1.57293700 | 4.39791900  |
| H  | -0.10588000 | 0.36859400  | 3.78500200  |
| H  | 1.10277500  | -0.90153100 | 3.61510400  |
| C  | -2.68404300 | -1.60193600 | 2.76025000  |
| H  | -2.17633600 | 0.27872800  | 1.82698700  |
| H  | -2.10843300 | -1.17120700 | 0.77045700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.28786800 | -1.30936200 | 4.20456200  |
| H | -0.50300700 | -1.40032900 | 5.43679500  |
| H | -0.58206400 | -2.62697400 | 4.17653900  |
| H | -3.74782200 | -1.40686000 | 2.59457100  |
| H | -2.51756600 | -2.66836900 | 2.56023300  |
| H | -2.88124200 | -1.92942600 | 4.88188100  |
| H | -2.51205800 | -0.26191800 | 4.44909000  |
| C | 2.48197000  | 2.91025800  | 0.29050300  |
| C | 2.39559100  | 1.38514600  | 0.49603500  |
| H | 3.18224500  | 3.35289900  | 1.00918700  |
| H | 2.07018300  | 0.94799000  | -0.45901100 |
| H | 3.34794200  | 0.90187300  | 0.73758100  |
| C | 2.88378600  | 3.35444200  | -1.12158600 |
| C | 4.38589400  | 3.43831400  | -1.40964000 |
| H | 2.44675200  | 4.34426100  | -1.30697700 |
| H | 2.41026500  | 2.67173300  | -1.84564400 |
| C | 5.17541900  | 2.14516900  | -1.15265300 |
| H | 4.50468700  | 3.74573800  | -2.45384700 |
| H | 4.81860800  | 4.24760800  | -0.80673400 |
| H | 4.51612700  | 1.27543600  | -1.28098000 |
| H | 5.96244400  | 2.03644700  | -1.90857500 |
| C | 5.83952900  | 2.09147900  | 0.22448500  |
| C | 6.53704600  | 0.76277100  | 0.50123200  |
| H | 5.10045700  | 2.27855700  | 1.01561000  |
| H | 6.56793300  | 2.91033900  | 0.29755700  |
| C | 7.25951700  | 0.74513200  | 1.84501300  |
| H | 5.79229100  | -0.04303400 | 0.46689400  |
| H | 7.24971900  | 0.55486100  | -0.30776500 |
| H | 7.74481300  | -0.21670800 | 2.02914700  |
| H | 8.02899700  | 1.52220700  | 1.88468400  |
| H | 6.55948800  | 0.93097900  | 2.66610600  |
| N | -0.53867000 | -1.56467800 | -1.40378100 |
| H | 1.03331600  | -0.58106600 | 0.55826200  |
| C | 0.67643100  | -1.14850000 | -2.07186500 |
| H | 0.63677100  | -1.39271900 | -3.14625900 |
| H | 0.72173000  | -0.02145400 | -2.08800400 |
| C | -1.10464900 | -2.83758700 | -1.84321800 |
| H | -2.19410700 | -2.77638700 | -1.74526400 |
| H | -0.88258600 | -3.00684500 | -2.90793400 |
| C | -0.62058100 | -4.01852000 | -1.02954400 |
| C | 0.35963100  | -4.88973300 | -1.50057100 |
| C | -1.11032500 | -4.18952600 | 0.26764100  |
| C | 0.86475000  | -5.89509800 | -0.67701500 |
| H | 0.74659900  | -4.76943000 | -2.50950100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.60519500 | -5.18435300 | 1.09787200  |
| H | -1.90053400 | -3.53070200 | 0.62359200  |
| C | 0.39307800  | -6.03715200 | 0.62533200  |
| H | 1.63185100  | -6.56478800 | -1.05200400 |
| H | -0.99600700 | -5.30370400 | 2.10415700  |
| H | 0.79022900  | -6.81707100 | 1.26657900  |
| C | 2.01906900  | -1.59639600 | -1.50526200 |
| C | 3.18578600  | -1.15310500 | -2.13673600 |
| C | 2.12807600  | -2.39703300 | -0.36825000 |
| C | 4.43629700  | -1.50339300 | -1.64168700 |
| H | 3.11238400  | -0.52174000 | -3.02092600 |
| C | 3.38387800  | -2.75184200 | 0.12876000  |
| H | 1.22864200  | -2.77287700 | 0.11149100  |
| C | 4.53849700  | -2.30709100 | -0.50487700 |
| H | 5.33409900  | -1.14464700 | -2.13612600 |
| H | 3.45074200  | -3.38981700 | 1.00441800  |
| H | 5.51534800  | -2.58405600 | -0.12151100 |

trans-P3'

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.03190900 | -3.50839000 | 1.03323300  |
| C | -0.07886900 | -2.33105300 | 0.85713000  |
| H | -1.94855900 | -3.17573600 | 1.53021100  |
| H | -1.30582700 | -3.93690500 | 0.06289300  |
| H | -0.57670900 | -4.30014600 | 1.63783400  |
| C | 1.13758500  | -2.66063800 | -0.01710900 |
| C | 0.36674300  | -1.82321300 | 2.23463500  |
| H | 1.87733500  | -3.28482500 | 0.49674500  |
| H | 0.80017100  | -3.21408000 | -0.90561900 |
| H | 0.96339300  | -2.58634500 | 2.74466700  |
| H | 0.97623800  | -0.91486600 | 2.16454500  |
| H | -0.50198000 | -1.60180900 | 2.86207000  |
| C | -0.72994600 | -1.19319500 | 0.03682300  |
| H | -1.25182000 | -1.67387800 | -0.80159700 |
| N | -1.72755000 | -0.45524000 | 0.79715200  |
| C | -2.51810600 | 0.50097300  | 0.01959500  |
| C | -3.63682600 | -0.20961200 | -0.74860500 |
| C | -3.11615000 | 1.53628100  | 0.97280700  |
| H | -1.89236500 | 1.04568800  | -0.71507100 |
| C | -4.52915000 | 0.78850200  | -1.49109100 |
| H | -4.23142900 | -0.77652200 | -0.01988300 |
| H | -3.21617100 | -0.93654100 | -1.45220700 |
| C | -4.00945900 | 2.53877600  | 0.24258100  |
| H | -3.69866600 | 0.99921500  | 1.73411300  |
| H | -2.30684400 | 2.06041000  | 1.49716600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.11868200 | 1.82245500  | -0.52975600 |
| H | -5.32796500 | 0.25718100  | -2.01857200 |
| H | -3.93626800 | 1.30722500  | -2.25713800 |
| H | -4.43530700 | 3.25240700  | 0.95523800  |
| H | -3.39883700 | 3.12003300  | -0.46175800 |
| H | -5.73321900 | 2.54603500  | -1.07561000 |
| H | -5.78102500 | 1.31257400  | 0.18303400  |
| C | 1.70596100  | -1.29651900 | -0.44942600 |
| C | 0.46160300  | -0.37433700 | -0.53450500 |
| H | 2.36447300  | -0.94023700 | 0.35273500  |
| H | 0.59567900  | 0.54650000  | 0.04744400  |
| H | 0.27013000  | -0.06171300 | -1.56738400 |
| C | 2.52403400  | -1.36805000 | -1.73628700 |
| C | 3.18161500  | -0.05349100 | -2.17006800 |
| H | 1.86832600  | -1.72507900 | -2.54281900 |
| H | 3.30717600  | -2.12924800 | -1.61427900 |
| C | 4.18233300  | 0.52945300  | -1.15632300 |
| H | 3.69218600  | -0.23409300 | -3.12222400 |
| H | 2.40624900  | 0.69540100  | -2.38165800 |
| H | 4.62495400  | -0.28606300 | -0.56664800 |
| H | 5.01620300  | 0.99774900  | -1.69344200 |
| C | 3.59130500  | 1.57735600  | -0.21106500 |
| C | 4.61459900  | 2.13687400  | 0.77442900  |
| H | 2.74830400  | 1.15418300  | 0.34992200  |
| H | 3.17480000  | 2.40070100  | -0.80807000 |
| C | 4.02266900  | 3.20415300  | 1.69121400  |
| H | 5.02117800  | 1.31455000  | 1.37676400  |
| H | 5.46123100  | 2.55601300  | 0.21581800  |
| H | 4.76580400  | 3.59309800  | 2.39208900  |
| H | 3.63698800  | 4.04691300  | 1.10866200  |
| H | 3.19057600  | 2.79771500  | 2.27525400  |
| H | -1.24164800 | 0.06323700  | 1.52743800  |

cis-P3'

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.73809600 | -3.25491700 | 1.61318500  |
| C | -1.10911000 | -2.57923000 | 0.29414000  |
| H | 0.33972000  | -3.45043700 | 1.64104700  |
| H | -0.99039200 | -2.61234300 | 2.46405500  |
| H | -1.26499400 | -4.20688900 | 1.73845400  |
| C | -2.57371300 | -2.05058100 | 0.28013900  |
| C | -0.88460000 | -3.56117700 | -0.85905300 |
| H | -3.10151400 | -2.43329300 | -0.60389900 |
| H | -3.14402800 | -2.37755500 | 1.15619500  |
| H | -1.55756800 | -4.41892900 | -0.75782100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.09222900 | -3.09539800 | -1.83004600 |
| H | 0.14647800  | -3.92553500 | -0.86437400 |
| C | -0.25599600 | -1.29023800 | 0.10193000  |
| H | -0.07143200 | -0.87625800 | 1.10388900  |
| N | 1.04891200  | -1.52517000 | -0.49794500 |
| C | 1.99439400  | -0.41883700 | -0.33511400 |
| C | 2.64520600  | -0.46874300 | 1.05085800  |
| C | 3.07239200  | -0.50119200 | -1.41639200 |
| H | 1.49268500  | 0.56492900  | -0.43908900 |
| C | 3.68666500  | 0.63853600  | 1.22406700  |
| H | 3.11964600  | -1.45313000 | 1.15864600  |
| H | 1.88243900  | -0.39647700 | 1.83429800  |
| C | 4.12141500  | 0.60045100  | -1.25530200 |
| H | 3.55075800  | -1.48797200 | -1.34626800 |
| H | 2.60444100  | -0.43869500 | -2.40709300 |
| C | 4.75826400  | 0.55755600  | 0.13516500  |
| H | 4.14327200  | 0.57315100  | 2.21696800  |
| H | 3.19063400  | 1.61747700  | 1.16744400  |
| H | 4.88698400  | 0.50559300  | -2.03215200 |
| H | 3.64139400  | 1.57811400  | -1.39990100 |
| H | 5.48361600  | 1.37007200  | 0.24777500  |
| H | 5.31248700  | -0.38426700 | 0.24697400  |
| C | -2.50185300 | -0.51118900 | 0.18185800  |
| C | -1.20253200 | -0.31660300 | -0.60684000 |
| H | -2.34841000 | -0.11203900 | 1.19625800  |
| H | -1.35823400 | -0.63679900 | -1.64906400 |
| H | -0.82001800 | 0.70527700  | -0.62787000 |
| C | -3.76774600 | 0.11831800  | -0.40236600 |
| C | -3.97080700 | 1.61721500  | -0.14003100 |
| H | -4.63784000 | -0.41481100 | 0.00334900  |
| H | -3.77661300 | -0.06630900 | -1.48644900 |
| C | -2.84120900 | 2.53425000  | -0.63779100 |
| H | -4.91524300 | 1.90972500  | -0.61202700 |
| H | -4.11002200 | 1.77717500  | 0.93810500  |
| H | -2.37486900 | 2.08419300  | -1.52489200 |
| H | -3.25767000 | 3.49141600  | -0.97325500 |
| C | -1.77067100 | 2.82081200  | 0.42010100  |
| C | -0.49277500 | 3.43000500  | -0.15360600 |
| H | -1.51342600 | 1.89761100  | 0.95440500  |
| H | -2.18853800 | 3.49397300  | 1.18056900  |
| C | 0.60624600  | 3.56878900  | 0.89614300  |
| H | -0.13092200 | 2.79800700  | -0.97652300 |
| H | -0.71816300 | 4.40702500  | -0.59930800 |
| H | 1.52165300  | 3.99170800  | 0.47285300  |



|     |             |             |             |
|-----|-------------|-------------|-------------|
| H   | 0.28542600  | 4.21348800  | 1.72049100  |
| H   | 0.85369700  | 2.58824700  | 1.32003700  |
| H   | 0.92156300  | -1.70319800 | -1.49269700 |
| 21' |             |             |             |
| C   | -1.72926300 | -0.95517000 | 0.05510500  |
| C   | -1.32877500 | -1.27224900 | -1.28480600 |
| C   | -2.07317200 | -0.46498700 | -2.18700500 |
| C   | -2.94988400 | 0.35830300  | -1.42067700 |
| C   | -2.74503900 | 0.05824400  | -0.04925000 |
| Sc  | -0.65705200 | 0.99688000  | -0.81870300 |
| C   | -2.92509700 | -2.39838700 | 2.46345800  |
| C   | -0.31487600 | -3.42336500 | 1.37918400  |
| C   | -0.38703000 | -0.71251600 | 2.86975200  |
| H   | -3.54444500 | -1.56303300 | 2.79703700  |
| H   | -3.51214600 | -2.99702500 | 1.76038700  |
| H   | -2.70921200 | -3.02380900 | 3.33570200  |
| H   | 0.72422300  | -3.27503200 | 1.07586300  |
| H   | -0.30095200 | -3.98181200 | 2.32129600  |
| H   | -0.80012000 | -4.05706000 | 0.63074800  |
| H   | -0.06010600 | -1.28629100 | 3.74337300  |
| H   | 0.50018900  | -0.25863100 | 2.41656400  |
| H   | -1.03181700 | 0.09494500  | 3.23142800  |
| Si  | -1.30746000 | -1.84905200 | 1.67599100  |
| C   | -3.52404000 | 0.66489900  | 1.08404100  |
| H   | -4.47184100 | 0.13485900  | 1.22677700  |
| H   | -2.97097700 | 0.61630700  | 2.02499000  |
| H   | -3.75698200 | 1.71624300  | 0.89519800  |
| C   | -3.94940600 | 1.34315100  | -1.96072100 |
| H   | -3.63618900 | 1.76735100  | -2.91816800 |
| H   | -4.91660100 | 0.85678400  | -2.12288500 |
| H   | -4.11455200 | 2.16862000  | -1.26342100 |
| C   | -1.97169900 | -0.51610700 | -3.68770500 |
| H   | -0.93374100 | -0.48152100 | -4.03759400 |
| H   | -2.40262700 | -1.44703300 | -4.06889400 |
| H   | -2.51127200 | 0.30907200  | -4.15661800 |
| C   | -0.31199000 | -2.29548800 | -1.71846200 |
| H   | 0.47373900  | -2.43633700 | -0.97275100 |
| H   | -0.78745000 | -3.26977800 | -1.87545000 |
| H   | 0.16007100  | -2.01622200 | -2.66567700 |
| C   | 1.11870700  | 4.16347300  | 0.17850800  |
| C   | 0.76193400  | 2.93538600  | 1.04353200  |
| H   | 2.16259600  | 4.46594900  | 0.30826000  |
| H   | 0.95164400  | 3.96059300  | -0.88626200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.48236400  | 5.00223000  | 0.47354200  |
| C | -0.69202700 | 2.48469400  | 0.78239300  |
| C | 1.00674300  | 3.27757700  | 2.52374600  |
| H | -1.02940100 | 1.89050200  | 1.64662900  |
| H | -1.35167700 | 3.35972300  | 0.74134400  |
| H | 0.32723300  | 4.08031500  | 2.82114200  |
| H | 0.80677800  | 2.41144100  | 3.16214900  |
| H | 2.03417200  | 3.61415000  | 2.70269600  |
| C | 1.75049600  | 1.87040700  | 0.63865700  |
| H | 2.76862600  | 1.95435600  | 1.03926100  |
| N | 1.45805400  | 0.92355000  | -0.17671200 |
| C | 2.46723800  | -0.08333700 | -0.57131600 |
| C | 3.77233500  | 0.51582000  | -1.10135300 |
| C | 2.72614600  | -1.04582300 | 0.58820400  |
| H | 2.00647000  | -0.66088800 | -1.38797100 |
| C | 4.71526100  | -0.60987900 | -1.54142400 |
| H | 4.26021200  | 1.10005900  | -0.31116800 |
| H | 3.56168200  | 1.19951800  | -1.93144500 |
| C | 3.67639500  | -2.16366200 | 0.15740700  |
| H | 3.16504900  | -0.48040700 | 1.42269800  |
| H | 1.77252100  | -1.45045800 | 0.94297900  |
| C | 4.98237000  | -1.58805300 | -0.39542100 |
| H | 5.65214600  | -0.18084800 | -1.90699600 |
| H | 4.26329600  | -1.14941600 | -2.38437900 |
| H | 3.87350300  | -2.82814100 | 1.00335200  |
| H | 3.18907600  | -2.77111600 | -0.61777200 |
| H | 5.63752400  | -2.39518300 | -0.73462100 |
| H | 5.51319300  | -1.06317000 | 0.40944500  |

cis-ts-22'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.68211400  | -1.90831200 | -0.62486100 |
| C  | 1.42511600  | -1.14549500 | -1.81341100 |
| C  | 0.12311600  | -1.46208600 | -2.28491400 |
| C  | -0.42953600 | -2.45197900 | -1.42249800 |
| C  | 0.51021300  | -2.71187400 | -0.39310700 |
| Sc | -0.10831400 | -0.38637500 | -0.04357200 |
| C  | 3.66830000  | -3.92495000 | 0.56622300  |
| C  | 4.77104500  | -1.36841000 | -0.59464300 |
| C  | 3.17603500  | -1.26969500 | 2.03087400  |
| H  | 2.97685200  | -4.41797900 | 1.25304200  |
| H  | 3.62810000  | -4.45217500 | -0.39179800 |
| H  | 4.67861100  | -4.04355700 | 0.97076000  |
| H  | 4.79670200  | -0.27656500 | -0.63139100 |
| H  | 5.68090700  | -1.69735800 | -0.08133800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 4.81792800  | -1.74421800 | -1.62082100 |
| H  | 4.13031600  | -1.34624400 | 2.56235500  |
| H  | 2.92875800  | -0.20539000 | 1.94134100  |
| H  | 2.41393500  | -1.75079100 | 2.65489000  |
| Si | 3.30210600  | -2.09333100 | 0.33600700  |
| C  | 0.30777400  | -3.69605000 | 0.73107700  |
| H  | 0.61118400  | -4.70528500 | 0.43344700  |
| H  | 0.89448700  | -3.42524200 | 1.61397600  |
| H  | -0.74179200 | -3.74470300 | 1.03859700  |
| C  | -1.71109600 | -3.19122600 | -1.68131000 |
| H  | -2.55027800 | -2.52526600 | -1.90891500 |
| H  | -1.58685100 | -3.85085500 | -2.54679900 |
| H  | -1.99532100 | -3.81880600 | -0.83391700 |
| C  | -0.52972400 | -0.94623000 | -3.53552400 |
| H  | -0.23894200 | 0.08459700  | -3.75636000 |
| H  | -0.24935000 | -1.55603200 | -4.40117500 |
| H  | -1.62024900 | -0.97601900 | -3.45752200 |
| C  | 2.38746900  | -0.24987400 | -2.54689600 |
| H  | 3.05928100  | 0.28362600  | -1.87234100 |
| H  | 3.01180600  | -0.84045900 | -3.22605000 |
| H  | 1.86117500  | 0.48850600  | -3.15856800 |
| C  | -1.36939600 | 2.01215800  | 3.11561200  |
| C  | -0.19526800 | 1.08678300  | 2.72878600  |
| H  | -1.00035000 | 2.87456700  | 3.67743900  |
| H  | -1.90820300 | 2.39041400  | 2.24234900  |
| H  | -2.07019300 | 1.46903400  | 3.75710600  |
| C  | -0.67719300 | -0.25513300 | 2.13858000  |
| C  | 0.64140000  | 0.82622000  | 4.00044600  |
| H  | 0.22179300  | -0.92351800 | 2.01817200  |
| H  | -1.27073100 | -0.76772200 | 2.89474200  |
| H  | 0.01186200  | 0.34139100  | 4.75134200  |
| H  | 1.49459600  | 0.17589100  | 3.79182300  |
| H  | 1.01316700  | 1.76442100  | 4.42470300  |
| C  | 0.65061700  | 1.87870900  | 1.77285500  |
| H  | 1.08730400  | 2.80347500  | 2.16973600  |
| N  | 0.84288500  | 1.53957400  | 0.55593400  |
| C  | 1.66226300  | 2.39174900  | -0.33145300 |
| C  | 1.19249900  | 3.84708800  | -0.38773000 |
| C  | 3.13997400  | 2.29590200  | 0.05232700  |
| H  | 1.54253900  | 1.96761200  | -1.33735700 |
| C  | 2.05168200  | 4.62388600  | -1.39076800 |
| H  | 1.29061300  | 4.31098100  | 0.60198600  |
| H  | 0.13294100  | 3.88516600  | -0.66500900 |
| C  | 3.99987400  | 3.07836100  | -0.94179100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.26893200  | 2.70860400  | 1.06312100  |
| H | 3.43719000  | 1.24174300  | 0.09777400  |
| C | 3.53756200  | 4.53469000  | -1.03444600 |
| H | 1.72627100  | 5.66719600  | -1.42300000 |
| H | 1.89319000  | 4.21027000  | -2.39555500 |
| H | 5.05120700  | 3.02370300  | -0.64542800 |
| H | 3.92271000  | 2.60773500  | -1.93184800 |
| H | 4.13474400  | 5.07325800  | -1.77553100 |
| H | 3.70751300  | 5.02805200  | -0.06837300 |
| C | -2.48580300 | -0.13502600 | 0.89283100  |
| C | -2.23388600 | 0.22507800  | -0.45027100 |
| H | -2.73756500 | 0.65170200  | 1.59655200  |
| H | -2.58911900 | -0.43620100 | -1.23570500 |
| H | -2.18858600 | 1.28558700  | -0.70354500 |
| C | -3.15302600 | -1.46138900 | 1.19124600  |
| C | -4.68808400 | -1.34528100 | 1.27418200  |
| H | -2.79668600 | -1.87572700 | 2.13808300  |
| H | -2.89228700 | -2.18095200 | 0.40703700  |
| C | -5.38596500 | -0.86091600 | -0.00438900 |
| H | -5.05535400 | -2.34023300 | 1.54415000  |
| H | -4.95349100 | -0.68528000 | 2.11033600  |
| H | -4.80385000 | -1.17308100 | -0.88275900 |
| H | -6.35614300 | -1.36146600 | -0.09790800 |
| C | -5.62377800 | 0.64904600  | -0.05497700 |
| C | -6.13536000 | 1.12304200  | -1.41248100 |
| H | -4.69899000 | 1.18867400  | 0.18506000  |
| H | -6.34814800 | 0.91962600  | 0.72525900  |
| C | -6.42565200 | 2.62071600  | -1.44157500 |
| H | -5.38967000 | 0.87441700  | -2.17947600 |
| H | -7.04214800 | 0.56325500  | -1.67296200 |
| H | -6.78138900 | 2.94319100  | -2.42306300 |
| H | -7.19053500 | 2.88374500  | -0.70446200 |
| H | -5.52520100 | 3.19717300  | -1.20479300 |

trans-ts-22'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.78811200  | -1.87232200 | -0.58381900 |
| C  | 1.44159000  | -1.26315100 | -1.83564800 |
| C  | 0.14196300  | -1.70045700 | -2.20967400 |
| C  | -0.32656600 | -2.59860600 | -1.20840800 |
| C  | 0.66972900  | -2.69508800 | -0.20597700 |
| Sc | -0.05041300 | -0.36080200 | -0.12562200 |
| C  | 3.93930000  | -3.72275300 | 0.55163100  |
| C  | 4.84383000  | -1.16246500 | -0.74050000 |
| C  | 3.37273800  | -1.06239500 | 1.97412400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.27712500  | -4.24598400 | 1.24485600  |
| H  | 3.92652800  | -4.26224200 | -0.40032800 |
| H  | 4.95561500  | -3.77982000 | 0.95446800  |
| H  | 4.80290000  | -0.07722400 | -0.85855000 |
| H  | 5.79199000  | -1.39977400 | -0.24594700 |
| H  | 4.87455700  | -1.61090100 | -1.73801400 |
| H  | 4.36049200  | -1.05457800 | 2.44697900  |
| H  | 3.03692800  | -0.02321300 | 1.88751300  |
| H  | 2.69092900  | -1.58714800 | 2.65304800  |
| Si | 3.46322000  | -1.92050300 | 0.29390200  |
| C  | 0.57620300  | -3.57267400 | 1.01534700  |
| H  | 0.86894100  | -4.60171300 | 0.78190100  |
| H  | 1.22926900  | -3.21986900 | 1.81831700  |
| H  | -0.44258300 | -3.60730800 | 1.41450100  |
| C  | -1.60747500 | -3.38173700 | -1.27136400 |
| H  | -2.48028800 | -2.75965900 | -1.49846700 |
| H  | -1.54590200 | -4.13962100 | -2.05903300 |
| H  | -1.80395900 | -3.90546200 | -0.33287200 |
| C  | -0.58060000 | -1.36957200 | -3.48509400 |
| H  | -0.40664300 | -0.33876500 | -3.80632800 |
| H  | -0.24618400 | -2.02281000 | -4.29805000 |
| H  | -1.66054900 | -1.51092300 | -3.38335500 |
| C  | 2.30836800  | -0.37121800 | -2.68517400 |
| H  | 2.96900700  | 0.25789800  | -2.08421400 |
| H  | 2.94463100  | -0.96910600 | -3.34662100 |
| H  | 1.70629600  | 0.28023200  | -3.32545900 |
| C  | -1.40721200 | 1.91864500  | 3.03474500  |
| C  | -0.20117900 | 1.03402300  | 2.66379100  |
| H  | -1.06119400 | 2.84546000  | 3.50179000  |
| H  | -2.00203000 | 2.17981000  | 2.15680100  |
| H  | -2.04468100 | 1.40127000  | 3.75553300  |
| C  | -0.59927900 | -0.33777100 | 2.06896900  |
| C  | 0.64028900  | 0.81254500  | 3.94093000  |
| H  | 0.35093800  | -0.91809400 | 1.92281300  |
| H  | -1.12174800 | -0.91856100 | 2.82933500  |
| H  | 0.03556000  | 0.28336800  | 4.68204600  |
| H  | 1.53327700  | 0.21699200  | 3.73416800  |
| H  | 0.95156400  | 1.76721100  | 4.37764600  |
| C  | 0.62123100  | 1.87123000  | 1.72269000  |
| H  | 1.02857700  | 2.80106800  | 2.13849700  |
| N  | 0.82692400  | 1.56164800  | 0.50059100  |
| C  | 1.63246700  | 2.42796700  | -0.38342300 |
| C  | 1.16720900  | 3.88472800  | -0.41411900 |
| C  | 3.11452800  | 2.31926700  | -0.02242300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.49998200  | 2.01322800  | -1.39315200 |
| C | 2.01777700  | 4.67244900  | -1.41624100 |
| H | 1.27947800  | 4.33265300  | 0.58140200  |
| H | 0.10477200  | 3.93126900  | -0.67769000 |
| C | 3.96547100  | 3.11384700  | -1.01421100 |
| H | 3.25736400  | 2.71234600  | 0.99447700  |
| H | 3.40603600  | 1.26322500  | -0.00220200 |
| C | 3.50766100  | 4.57298600  | -1.08010400 |
| H | 1.69588100  | 5.71720700  | -1.42984300 |
| H | 1.84548400  | 4.27345500  | -2.42464500 |
| H | 5.01982800  | 3.05064400  | -0.73030600 |
| H | 3.87589100  | 2.65727800  | -2.00999000 |
| H | 4.09732000  | 5.12002800  | -1.82098400 |
| H | 3.69176800  | 5.05192900  | -0.10939200 |
| C | -2.38852800 | -0.62325700 | 0.78191500  |
| C | -2.24757600 | -0.03980800 | -0.49964000 |
| H | -2.25387600 | -1.71064500 | 0.81706400  |
| H | -2.32926400 | -0.67981200 | -1.37371500 |
| H | -2.59575000 | 0.98370800  | -0.63077500 |
| C | -3.44371200 | -0.15636300 | 1.76109000  |
| C | -4.74382100 | -0.95930500 | 1.54505800  |
| H | -3.63899800 | 0.90966300  | 1.61959400  |
| H | -3.13614200 | -0.30424400 | 2.79815600  |
| C | -5.40415100 | -0.81812900 | 0.17213400  |
| H | -4.53777600 | -2.01803200 | 1.74517100  |
| H | -5.45216400 | -0.63241100 | 2.31555900  |
| H | -4.73408100 | -1.19682700 | -0.60962600 |
| H | -6.29108300 | -1.46261800 | 0.15339400  |
| C | -5.82534900 | 0.60862300  | -0.17205500 |
| C | -6.50955000 | 0.71094000  | -1.53334900 |
| H | -4.95017800 | 1.27194600  | -0.16820400 |
| H | -6.50056800 | 0.98759700  | 0.60778000  |
| C | -6.92611100 | 2.13839200  | -1.87552600 |
| H | -5.82815500 | 0.32805200  | -2.30424500 |
| H | -7.38835700 | 0.05484100  | -1.54619100 |
| H | -7.41316800 | 2.19207700  | -2.85223000 |
| H | -7.62537100 | 2.52955900  | -1.13022900 |
| H | -6.05725600 | 2.80427900  | -1.89689300 |

cis-23'

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.51146800  | -2.13251600 | -0.41331500 |
| C | 1.49646200  | -1.41307100 | -1.65415700 |
| C | 0.20021200  | -1.52816900 | -2.22779500 |
| C | -0.58798300 | -2.35976500 | -1.38346500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.20513200  | -2.71808600 | -0.26263200 |
| Sc | -0.03139300 | -0.30120000 | -0.10609100 |
| C  | 3.03513600  | -4.23653100 | 1.25017700  |
| C  | 4.61001900  | -1.93985700 | 0.07460500  |
| C  | 2.62439900  | -1.41300100 | 2.37892200  |
| H  | 2.22550600  | -4.55527600 | 1.91054600  |
| H  | 3.01134100  | -4.86385300 | 0.35410200  |
| H  | 3.98005600  | -4.42954400 | 1.76819000  |
| H  | 4.77879400  | -0.86497800 | -0.02938600 |
| H  | 5.38242700  | -2.32450000 | 0.74907100  |
| H  | 4.76495900  | -2.40527600 | -0.90310100 |
| H  | 3.46145600  | -1.52260100 | 3.07578000  |
| H  | 2.50378500  | -0.34124500 | 2.17255500  |
| H  | 1.72225300  | -1.76424500 | 2.89438000  |
| Si | 2.93685700  | -2.41142900 | 0.80029600  |
| C  | -0.23231600 | -3.61117300 | 0.87077500  |
| H  | 0.14184000  | -4.62944500 | 0.72633500  |
| H  | 0.14351700  | -3.25876400 | 1.83784000  |
| H  | -1.32026700 | -3.67036800 | 0.94281100  |
| C  | -1.96813300 | -2.83791200 | -1.72865200 |
| H  | -2.61752900 | -2.01177400 | -2.03342700 |
| H  | -1.92032300 | -3.54231700 | -2.56600800 |
| H  | -2.44804700 | -3.35562900 | -0.89522500 |
| C  | -0.26231900 | -0.96596800 | -3.54138100 |
| H  | 0.30032100  | -0.07350200 | -3.82648600 |
| H  | -0.13628100 | -1.70206500 | -4.34279100 |
| H  | -1.32168000 | -0.69715300 | -3.50412500 |
| C  | 2.66506300  | -0.76078500 | -2.34264400 |
| H  | 3.37911200  | -0.33116500 | -1.64017400 |
| H  | 3.20644300  | -1.50183200 | -2.94079400 |
| H  | 2.34404300  | 0.02833400  | -3.02857500 |
| C  | -1.75630800 | 3.04210700  | 2.31673100  |
| C  | -0.62199000 | 2.00323400  | 2.30379900  |
| H  | -1.35980400 | 4.03410700  | 2.55024400  |
| H  | -2.27358200 | 3.09644200  | 1.35485800  |
| H  | -2.48648100 | 2.78216300  | 3.08868200  |
| C  | -1.18689800 | 0.57480500  | 2.15976300  |
| C  | 0.14997800  | 2.08792500  | 3.64068000  |
| H  | -0.33230500 | -0.14710900 | 2.11111100  |
| H  | -1.59952500 | 0.31176900  | 3.13988400  |
| H  | -0.54526300 | 1.93429200  | 4.47037400  |
| H  | 0.93233300  | 1.32385000  | 3.69494500  |
| H  | 0.61503500  | 3.06940600  | 3.76903300  |
| C  | 0.37739900  | 2.42558800  | 1.26229300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.68599100  | 3.47206800  | 1.34751400  |
| N | 0.90569900  | 1.67938700  | 0.37134400  |
| C | 1.96567300  | 2.22382400  | -0.51194400 |
| C | 1.91711400  | 3.73048100  | -0.76848100 |
| C | 3.32525500  | 1.81365800  | 0.05993800  |
| H | 1.83364800  | 1.72429400  | -1.48398000 |
| C | 3.02979200  | 4.11291300  | -1.75038400 |
| H | 2.08583400  | 4.28320300  | 0.16404500  |
| H | 0.93207300  | 4.01788100  | -1.15385300 |
| C | 4.46319200  | 2.22844700  | -0.87574500 |
| H | 3.44081100  | 2.30260300  | 1.03780300  |
| H | 3.33503700  | 0.73316400  | 0.24353400  |
| C | 4.40181100  | 3.72361400  | -1.19618200 |
| H | 2.98717100  | 5.18700200  | -1.94938800 |
| H | 2.86130500  | 3.60506700  | -2.70926100 |
| H | 5.42430500  | 1.96886800  | -0.42196100 |
| H | 4.38776700  | 1.65861300  | -1.81136200 |
| H | 5.18682000  | 3.98559900  | -1.91102500 |
| H | 4.59779100  | 4.29972900  | -0.28238800 |
| C | -2.34688400 | 0.30938000  | 1.14187800  |
| C | -1.99449300 | 0.52641400  | -0.35448900 |
| H | -3.12207200 | 1.02008800  | 1.45838400  |
| H | -2.76303000 | 0.09078500  | -0.99585800 |
| H | -1.92080200 | 1.59904600  | -0.58760100 |
| C | -2.90326900 | -1.11334500 | 1.38198600  |
| C | -4.43298000 | -1.24210200 | 1.37094600  |
| H | -2.55123100 | -1.49349300 | 2.35001700  |
| H | -2.49227600 | -1.79024500 | 0.62080700  |
| C | -5.13892600 | -0.94382300 | 0.04140000  |
| H | -4.66638400 | -2.26990300 | 1.66942700  |
| H | -4.84857800 | -0.59594300 | 2.15631800  |
| H | -4.53424600 | -1.33608700 | -0.78846800 |
| H | -6.07958000 | -1.50644800 | 0.01211100  |
| C | -5.47388800 | 0.52751700  | -0.21075800 |
| C | -6.12280600 | 0.75048500  | -1.57540700 |
| H | -4.57400900 | 1.15091400  | -0.14552800 |
| H | -6.15299500 | 0.87801500  | 0.57854800  |
| C | -6.48287100 | 2.21205000  | -1.82446100 |
| H | -5.43586900 | 0.40027600  | -2.35751100 |
| H | -7.02160900 | 0.12642200  | -1.65427300 |
| H | -6.94271400 | 2.35146700  | -2.80589100 |
| H | -7.18707300 | 2.57479900  | -1.06945200 |
| H | -5.59112700 | 2.84595500  | -1.77900800 |



trans-23'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.27156700 | -2.20848600 | 0.23488000  |
| C  | -1.27908100 | -1.82568700 | 1.61539200  |
| C  | 0.05364900  | -1.89494000 | 2.11329400  |
| C  | 0.89769300  | -2.35016100 | 1.06037600  |
| C  | 0.09202900  | -2.53089600 | -0.09336900 |
| Sc | -0.01099000 | -0.14825400 | 0.41410400  |
| C  | -2.62082600 | -4.20777200 | -1.65890600 |
| C  | -4.39028400 | -2.34068500 | -0.07247400 |
| C  | -2.66168400 | -1.22183300 | -2.36516200 |
| H  | -1.79455900 | -4.32528900 | -2.36369600 |
| H  | -2.49855000 | -4.94972700 | -0.86428200 |
| H  | -3.54799000 | -4.43871200 | -2.19300500 |
| H  | -4.66445800 | -1.33431400 | 0.25373300  |
| H  | -5.15808600 | -2.67414600 | -0.77888900 |
| H  | -4.43415400 | -3.00373000 | 0.79638100  |
| H  | -3.55725300 | -1.32149400 | -2.98757300 |
| H  | -2.62366700 | -0.18812500 | -2.00326600 |
| H  | -1.79505200 | -1.39058600 | -3.01444400 |
| Si | -2.72621900 | -2.47039200 | -0.94533200 |
| C  | 0.57918500  | -3.07918200 | -1.40884600 |
| H  | 0.45952700  | -4.16724600 | -1.43531600 |
| H  | 0.02454300  | -2.66875600 | -2.25843400 |
| H  | 1.63980600  | -2.86945600 | -1.57014300 |
| C  | 2.35625400  | -2.66966900 | 1.19294300  |
| H  | 2.86744700  | -1.96576500 | 1.85583000  |
| H  | 2.49121700  | -3.67314100 | 1.61075600  |
| H  | 2.86416800  | -2.64950100 | 0.22524700  |
| C  | 0.51582300  | -1.60081400 | 3.51343700  |
| H  | -0.15698800 | -0.91674200 | 4.03616300  |
| H  | 0.56495900  | -2.52123200 | 4.10436500  |
| H  | 1.51547400  | -1.15696500 | 3.51750800  |
| C  | -2.47820300 | -1.42026200 | 2.43472200  |
| H  | -3.19237800 | -0.82692700 | 1.85748300  |
| H  | -3.01423600 | -2.30215100 | 2.80038700  |
| H  | -2.18690300 | -0.83681400 | 3.31218200  |
| C  | 1.28685700  | 3.12332400  | -2.31428000 |
| C  | 0.24039800  | 1.99892800  | -2.22696900 |
| H  | 0.78862000  | 4.08213800  | -2.48672800 |
| H  | 1.88036700  | 3.20290100  | -1.40101900 |
| H  | 1.96144600  | 2.94417000  | -3.15388200 |
| C  | 0.85250700  | 0.58341200  | -2.06125700 |
| C  | -0.58805800 | 2.00300700  | -3.53482400 |
| H  | 0.00904700  | -0.11088400 | -1.82619900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.11225600  | 0.23121400  | -3.06605400 |
| H | 0.08518100  | 1.85623500  | -4.38367200 |
| H | -1.33003800 | 1.19840800  | -3.53711800 |
| H | -1.10561200 | 2.95601900  | -3.67607400 |
| C | -0.74916800 | 2.39380000  | -1.16207000 |
| H | -1.17720000 | 3.39378200  | -1.29123700 |
| N | -1.14465000 | 1.65292300  | -0.20120700 |
| C | -2.22302200 | 2.08177200  | 0.71499700  |
| C | -2.29959700 | 3.57938500  | 1.00723500  |
| C | -3.56034600 | 1.54979800  | 0.18988600  |
| H | -2.02226800 | 1.56538200  | 1.66965800  |
| C | -3.40525900 | 3.83993800  | 2.03671900  |
| H | -2.54745200 | 4.12796800  | 0.09031900  |
| H | -1.33059900 | 3.94653000  | 1.36299300  |
| C | -4.68159300 | 1.82952800  | 1.19230300  |
| H | -3.77192300 | 2.04342300  | -0.76958900 |
| H | -3.47407500 | 0.47630000  | -0.01518200 |
| C | -4.75521700 | 3.31859100  | 1.53700900  |
| H | -3.46223000 | 4.91104400  | 2.24753200  |
| H | -3.14679900 | 3.34354800  | 2.98128600  |
| H | -5.63397600 | 1.47810900  | 0.78526800  |
| H | -4.49546000 | 1.25271900  | 2.10899000  |
| H | -5.52826200 | 3.49213600  | 2.29056300  |
| H | -5.04926600 | 3.88213400  | 0.64213500  |
| C | 2.12605300  | 0.32012700  | -1.18670000 |
| C | 1.96714800  | 0.68972400  | 0.30773500  |
| H | 2.24146000  | -0.77577500 | -1.23607300 |
| H | 2.80693100  | 0.30560200  | 0.89110800  |
| H | 1.95257900  | 1.78455500  | 0.42593800  |
| C | 3.39893800  | 0.88569500  | -1.87434400 |
| C | 4.59593600  | -0.07232500 | -1.84403000 |
| H | 3.67172400  | 1.84132400  | -1.41506000 |
| H | 3.18429900  | 1.09774300  | -2.92866000 |
| C | 5.12024100  | -0.44852100 | -0.45743700 |
| H | 4.31920200  | -0.98848300 | -2.38280800 |
| H | 5.41165400  | 0.38519100  | -2.41748300 |
| H | 4.33857100  | -0.97136000 | 0.10767200  |
| H | 5.93408600  | -1.17405200 | -0.57880100 |
| C | 5.63113900  | 0.73144000  | 0.36527400  |
| C | 6.12259000  | 0.30958600  | 1.74830100  |
| H | 4.83695800  | 1.48068500  | 0.48506800  |
| H | 6.44555000  | 1.22991700  | -0.17821900 |
| C | 6.65066700  | 1.48120500  | 2.57021200  |
| H | 5.29750700  | -0.17887200 | 2.28530500  |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| H          | 6.90648200  | -0.44974100 | 1.63695000  |
| H          | 6.99561500  | 1.15863300  | 3.55567700  |
| H          | 7.49096300  | 1.96455300  | 2.06245600  |
| H          | 5.87300800  | 2.23781600  | 2.71658000  |
| cis-ts-24' |             |             |             |
| C          | 1.96049400  | -1.68646300 | -0.57911900 |
| C          | 1.86999600  | -0.95758300 | -1.80470900 |
| C          | 0.61457700  | -1.24029900 | -2.41465000 |
| C          | -0.06556000 | -2.19992300 | -1.60713500 |
| C          | 0.74416500  | -2.45780700 | -0.47109700 |
| Sc         | 0.14601400  | -0.09333700 | -0.30614400 |
| C          | 3.83644400  | -3.71736200 | 0.74015200  |
| C          | 4.98352900  | -1.02626300 | -0.04065000 |
| C          | 3.00632900  | -1.18951800 | 2.29499200  |
| H          | 3.08545500  | -4.27322800 | 1.30616700  |
| H          | 3.92892200  | -4.17804800 | -0.24793900 |
| H          | 4.79449800  | -3.83806600 | 1.25591100  |
| H          | 4.93133800  | 0.06585700  | -0.01839900 |
| H          | 5.81384900  | -1.32279200 | 0.60914300  |
| H          | 5.23496900  | -1.33743700 | -1.05846600 |
| H          | 3.83746300  | -1.34578500 | 2.99023400  |
| H          | 2.80515600  | -0.11515700 | 2.23605000  |
| H          | 2.12272500  | -1.67330200 | 2.72595300  |
| Si         | 3.43474900  | -1.88409600 | 0.59895100  |
| C          | 0.44722100  | -3.48375700 | 0.59067200  |
| H          | 0.88335200  | -4.44845100 | 0.31050700  |
| H          | 0.86889700  | -3.20275000 | 1.55938900  |
| H          | -0.62535200 | -3.63765200 | 0.72624200  |
| C          | -1.33648300 | -2.89350500 | -2.00749200 |
| H          | -2.09614800 | -2.19411900 | -2.37086100 |
| H          | -1.13065900 | -3.59345800 | -2.82431500 |
| H          | -1.77043400 | -3.46824500 | -1.18720500 |
| C          | 0.11805200  | -0.71365200 | -3.73327000 |
| H          | 0.50975600  | 0.28377800  | -3.95016100 |
| H          | 0.43090100  | -1.36902700 | -4.55299600 |
| H          | -0.97412500 | -0.66165400 | -3.76051600 |
| C          | 2.92188100  | -0.07328500 | -2.41633400 |
| H          | 3.51833500  | 0.43793300  | -1.65971900 |
| H          | 3.60871600  | -0.66979300 | -3.02575600 |
| H          | 2.48299200  | 0.68250900  | -3.07494500 |
| C          | -2.11561400 | 2.00352300  | 3.27404800  |
| C          | -0.97859900 | 1.09693200  | 2.77936900  |
| H          | -1.73026700 | 2.99891600  | 3.51483600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.90708300 | 2.12266400  | 2.52763100  |
| H | -2.56381700 | 1.58781600  | 4.18056000  |
| C | -1.47175700 | -0.34265600 | 2.60208700  |
| C | 0.17857500  | 1.13600000  | 3.78741900  |
| H | -0.61323500 | -0.98285700 | 2.31156100  |
| H | -1.82462300 | -0.73672500 | 3.56256300  |
| H | -0.18901300 | 0.82590300  | 4.76970100  |
| H | 0.98591100  | 0.46557100  | 3.48603200  |
| H | 0.58802700  | 2.14620500  | 3.87907900  |
| C | -0.49480600 | 1.64590500  | 1.43567100  |
| H | -0.97937400 | 2.57333800  | 1.12444700  |
| N | 0.73517000  | 1.39634900  | 0.99402700  |
| C | 1.32525300  | 2.23732100  | -0.06208400 |
| C | 0.61254700  | 3.55090700  | -0.39322000 |
| C | 2.79969500  | 2.46192900  | 0.28935600  |
| H | 1.33899100  | 1.64810600  | -1.03140400 |
| C | 1.37187800  | 4.32449400  | -1.47625600 |
| H | 0.56420600  | 4.15516100  | 0.52252600  |
| H | -0.41782500 | 3.36774300  | -0.71999800 |
| C | 3.54177800  | 3.27266100  | -0.77311000 |
| H | 2.81623900  | 2.99436600  | 1.24957600  |
| H | 3.27390100  | 1.48908500  | 0.46206900  |
| C | 2.81955800  | 4.58816700  | -1.06295700 |
| H | 0.84888000  | 5.26278300  | -1.67945200 |
| H | 1.36058400  | 3.74748300  | -2.41220700 |
| H | 4.56702300  | 3.45581600  | -0.43932100 |
| H | 3.60998700  | 2.69178300  | -1.70239300 |
| H | 3.34080300  | 5.14196700  | -1.84845100 |
| H | 2.83021600  | 5.21799200  | -0.16426800 |
| C | -2.56084100 | -0.40435100 | 1.52437300  |
| C | -2.03084700 | 0.37212900  | 0.30488900  |
| H | -3.44518000 | 0.10542000  | 1.92678800  |
| H | -2.14258600 | -0.24039900 | -0.62197800 |
| H | -2.58683500 | 1.28615900  | 0.08284600  |
| C | -2.96596000 | -1.85578000 | 1.22616200  |
| C | -4.39433900 | -2.08507700 | 0.71468700  |
| H | -2.84157400 | -2.44652000 | 2.14262800  |
| H | -2.25518900 | -2.27107900 | 0.49947500  |
| C | -4.76163300 | -1.40119000 | -0.60957200 |
| H | -4.52627800 | -3.16729300 | 0.60848800  |
| H | -5.10478100 | -1.76907400 | 1.49023400  |
| H | -3.88435000 | -1.38512500 | -1.27078500 |
| H | -5.50994700 | -2.00705400 | -1.13356300 |
| C | -5.32234500 | 0.01441500  | -0.46372500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.44407000 | 0.74307500  | -1.79936600 |
| H | -4.69729500 | 0.61081200  | 0.21182700  |
| H | -6.30939600 | -0.04389300 | 0.01360700  |
| C | -6.04903600 | 2.13660000  | -1.65827700 |
| H | -4.44679300 | 0.81608300  | -2.25682500 |
| H | -6.05147500 | 0.14053400  | -2.48600600 |
| H | -6.12973200 | 2.64142200  | -2.62408300 |
| H | -7.05130400 | 2.08208700  | -1.22298800 |
| H | -5.43689000 | 2.76313200  | -1.00067300 |

trans-ts-24'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.35578600 | 2.26462000  | 0.00198200  |
| C  | -0.83110300 | 1.85942200  | -1.28745900 |
| C  | 0.25533100  | 1.29142200  | -2.01235900 |
| C  | 1.42564100  | 1.38737100  | -1.20764700 |
| C  | 1.05196700  | 1.96841000  | 0.03408200  |
| Sc | -0.13657200 | -0.14037000 | -0.06979400 |
| C  | -0.31068400 | 4.54659600  | 2.06565900  |
| C  | -2.98673400 | 3.73229200  | 0.87068400  |
| C  | -1.56182400 | 1.82246700  | 2.80629900  |
| H  | 0.56620000  | 4.24203900  | 2.64201400  |
| H  | 0.02719700  | 5.18367200  | 1.24268300  |
| H  | -0.94171500 | 5.15491000  | 2.72128500  |
| H  | -3.71608300 | 2.94153900  | 0.67497900  |
| H  | -3.38935800 | 4.35337700  | 1.67766100  |
| H  | -2.91128600 | 4.35824500  | -0.02278400 |
| H  | -2.06117900 | 2.28797300  | 3.66211900  |
| H  | -2.18888400 | 0.98904900  | 2.46592000  |
| H  | -0.61042500 | 1.41275100  | 3.16697000  |
| Si | -1.30774700 | 3.08675900  | 1.42221300  |
| C  | 1.99020000  | 2.25001400  | 1.18002300  |
| H  | 2.29509200  | 3.30131100  | 1.18184500  |
| H  | 1.52506500  | 2.04498600  | 2.14995500  |
| H  | 2.90051000  | 1.64740800  | 1.11507600  |
| C  | 2.80586400  | 0.98526700  | -1.65203900 |
| H  | 2.93885200  | -0.10253500 | -1.71883700 |
| H  | 3.01763900  | 1.39554200  | -2.64356100 |
| H  | 3.56947200  | 1.36708200  | -0.97089600 |
| C  | 0.20555000  | 0.76009200  | -3.41867300 |
| H  | -0.70751800 | 0.18798700  | -3.60933900 |
| H  | 0.23381100  | 1.57924700  | -4.14502700 |
| H  | 1.05726200  | 0.10710500  | -3.62692900 |
| C  | -2.18533500 | 2.12592100  | -1.88520600 |
| H  | -2.99861300 | 1.97724500  | -1.17404000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.23783200 | 3.16398200  | -2.23020000 |
| H | -2.37055200 | 1.49032700  | -2.75511000 |
| C | -0.14924800 | -4.23143300 | 1.51183100  |
| C | -0.57302300 | -2.76031500 | 1.58083600  |
| H | -1.03259000 | -4.86681200 | 1.39859700  |
| H | 0.52540500  | -4.44822300 | 0.68288500  |
| H | 0.35338300  | -4.51857300 | 2.43962900  |
| C | 0.62157900  | -1.83972100 | 1.87496200  |
| C | -1.62515900 | -2.60988900 | 2.69246600  |
| H | 0.22262100  | -0.83296700 | 2.14196400  |
| H | 1.12671400  | -2.14034400 | 2.79790300  |
| H | -1.20983400 | -2.96216600 | 3.64110800  |
| H | -1.93821900 | -1.56889800 | 2.80187200  |
| H | -2.51161100 | -3.20988200 | 2.46547400  |
| C | -1.22877100 | -2.33320400 | 0.25326700  |
| H | -1.53697000 | -3.15820100 | -0.39186800 |
| N | -1.90386500 | -1.18405600 | 0.20858300  |
| C | -3.05719000 | -0.99401800 | -0.69957700 |
| C | -3.66680100 | -2.27922100 | -1.26056000 |
| C | -4.09974400 | -0.20299600 | 0.09562100  |
| H | -2.74650400 | -0.37839700 | -1.56097500 |
| C | -4.90992300 | -1.96052000 | -2.09986900 |
| H | -3.94069000 | -2.93806400 | -0.42351000 |
| H | -2.94263900 | -2.81838600 | -1.88167100 |
| C | -5.33524700 | 0.11553300  | -0.74453000 |
| H | -4.38439300 | -0.80735200 | 0.96834300  |
| H | -3.63208800 | 0.70840000  | 0.48797300  |
| C | -5.94778700 | -1.16978900 | -1.30239300 |
| H | -5.34094000 | -2.89235300 | -2.47682100 |
| H | -4.60739400 | -1.37506500 | -2.97848000 |
| H | -6.06474700 | 0.66364900  | -0.14102700 |
| H | -5.05270700 | 0.77329900  | -1.57852300 |
| H | -6.81281300 | -0.94012700 | -1.93116600 |
| H | -6.31097500 | -1.78685200 | -0.46999900 |
| C | 1.62003400  | -1.77823700 | 0.67819800  |
| C | 0.82764000  | -2.07273600 | -0.61155200 |
| H | 2.04183500  | -0.75025700 | 0.63268000  |
| H | 1.23887100  | -1.57551700 | -1.50658500 |
| H | 0.77679300  | -3.13207800 | -0.84750500 |
| C | 2.85724500  | -2.68151000 | 0.88304900  |
| C | 4.01252000  | -2.35722300 | -0.06607000 |
| H | 2.54533900  | -3.72318100 | 0.76147300  |
| H | 3.20613900  | -2.57309400 | 1.91769700  |
| C | 4.79524700  | -1.11509900 | 0.35876700  |

|         |             |             |             |
|---------|-------------|-------------|-------------|
| H       | 4.69723300  | -3.21122000 | -0.10135100 |
| H       | 3.62920700  | -2.23513800 | -1.08877800 |
| H       | 4.10762100  | -0.27664100 | 0.54169500  |
| H       | 5.28285200  | -1.31564400 | 1.32177800  |
| C       | 5.84200200  | -0.67294200 | -0.65886400 |
| C       | 6.59709700  | 0.58137700  | -0.22492000 |
| H       | 5.35720800  | -0.48800000 | -1.62825000 |
| H       | 6.55566600  | -1.49046900 | -0.82661200 |
| C       | 7.62696500  | 1.03305000  | -1.25574400 |
| H       | 5.87626900  | 1.39059200  | -0.04181100 |
| H       | 7.09028900  | 0.39006600  | 0.73600500  |
| H       | 8.15383700  | 1.93294300  | -0.92968000 |
| H       | 8.37268600  | 0.25107800  | -1.42797500 |
| H       | 7.14789000  | 1.25214600  | -2.21523800 |
| cis-25' |             |             |             |
| C       | -2.13001700 | -1.86568900 | -0.02284400 |
| C       | -2.18311400 | -1.97269700 | 1.41163400  |
| C       | -0.98367200 | -2.58187300 | 1.86540800  |
| C       | -0.16825200 | -2.86105400 | 0.72507500  |
| C       | -0.88211600 | -2.44437700 | -0.43292800 |
| Sc      | -0.43953300 | -0.41917100 | 0.77613900  |
| C       | -4.31625500 | -2.87980600 | -1.87872100 |
| C       | -4.78814800 | -0.26008000 | -0.39143500 |
| C       | -2.69811500 | -0.36070000 | -2.65262600 |
| H       | -3.60355100 | -3.55546500 | -2.35991100 |
| H       | -4.79836000 | -3.42568500 | -1.06213600 |
| H       | -5.08545900 | -2.62269100 | -2.61362500 |
| H       | -4.37607300 | 0.62229800  | 0.10673000  |
| H       | -5.48581800 | 0.09492400  | -1.15752500 |
| H       | -5.36624900 | -0.82900400 | 0.34153000  |
| H       | -3.43428400 | 0.31548800  | -3.09927900 |
| H       | -1.84939200 | 0.24447300  | -2.31371800 |
| H       | -2.34200100 | -1.02951400 | -3.44147300 |
| Si      | -3.48343400 | -1.32463100 | -1.23177600 |
| C       | -0.42865000 | -2.63203400 | -1.85877200 |
| H       | -1.21277100 | -3.12415300 | -2.44243700 |
| H       | -0.19625900 | -1.68790000 | -2.36325300 |
| H       | 0.45901500  | -3.26548200 | -1.90746300 |
| C       | 1.15960100  | -3.56861000 | 0.75958300  |
| H       | 1.76046000  | -3.27001500 | 1.62378200  |
| H       | 1.01368600  | -4.65162000 | 0.82824900  |
| H       | 1.75180600  | -3.36996700 | -0.13743700 |
| C       | -0.64330900 | -2.95421500 | 3.28217400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.06357600 | -2.25491300 | 4.00894700  |
| H | -1.04109400 | -3.94607500 | 3.52020700  |
| H | 0.43744500  | -2.99687600 | 3.43973300  |
| C | -3.34086800 | -1.58151800 | 2.29345800  |
| H | -3.71507100 | -0.57873500 | 2.07146900  |
| H | -4.17543000 | -2.27651000 | 2.15340200  |
| H | -3.06405300 | -1.61654900 | 3.34928300  |
| C | 2.46321000  | 3.39686300  | -1.85277100 |
| C | 1.33446700  | 2.35566600  | -1.84215500 |
| H | 2.13940200  | 4.31063600  | -1.34358700 |
| H | 3.36531400  | 3.04129900  | -1.34453300 |
| H | 2.73604300  | 3.66008300  | -2.87922700 |
| C | 1.75765000  | 1.09378500  | -2.60449700 |
| C | 0.07836900  | 2.97957400  | -2.43295900 |
| H | 0.88222800  | 0.43541900  | -2.72799900 |
| H | 2.14907800  | 1.31146700  | -3.60359200 |
| H | 0.25981700  | 3.25566400  | -3.47652600 |
| H | -0.76488800 | 2.28414300  | -2.40417600 |
| H | -0.20049400 | 3.89250200  | -1.89613900 |
| C | 1.18140200  | 1.83100500  | -0.37705200 |
| H | 1.50604700  | 2.61696000  | 0.31701100  |
| N | -0.12965700 | 1.33729500  | 0.01816700  |
| C | -1.12979100 | 2.11074500  | 0.73282600  |
| C | -0.58496300 | 3.19989200  | 1.66544300  |
| C | -2.30971300 | 2.64408300  | -0.09331500 |
| H | -1.64931500 | 1.35663900  | 1.42343000  |
| C | -1.68874000 | 3.77432600  | 2.55831900  |
| H | -0.16767600 | 4.00183100  | 1.04138900  |
| H | 0.23916300  | 2.80580600  | 2.27309500  |
| C | -3.41298100 | 3.18350700  | 0.81902500  |
| H | -1.94810300 | 3.45223600  | -0.73682900 |
| H | -2.67814000 | 1.84909900  | -0.75163300 |
| C | -2.87009800 | 4.28455500  | 1.73139700  |
| H | -1.27794500 | 4.57591800  | 3.17873400  |
| H | -2.04100700 | 2.99270600  | 3.24617900  |
| H | -4.24697100 | 3.55361800  | 0.21569300  |
| H | -3.81193900 | 2.36816200  | 1.44137200  |
| H | -3.65820500 | 4.65681100  | 2.39210200  |
| H | -2.54162200 | 5.13232800  | 1.11632700  |
| C | 2.78327000  | 0.40001300  | -1.70394800 |
| C | 2.16685800  | 0.61655500  | -0.30223800 |
| H | 3.73260600  | 0.94567400  | -1.76345400 |
| H | 1.61581000  | -0.33432600 | -0.09552900 |
| H | 2.89659200  | 0.71088500  | 0.50712600  |



|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.03722300 | -1.05896500 | -2.09327200 |
| C | 4.31792000 | -1.70930400 | -1.56029800 |
| H | 3.05564100 | -1.11895800 | -3.18823300 |
| H | 2.16585700 | -1.65247200 | -1.77677700 |
| C | 4.49875100 | -1.67342000 | -0.03377100 |
| H | 4.32712500 | -2.74736400 | -1.90866300 |
| H | 5.18475200 | -1.22704400 | -2.03016000 |
| H | 3.51558900 | -1.65125900 | 0.45988000  |
| H | 4.97202600 | -2.60246900 | 0.30459200  |
| C | 5.35197600 | -0.50348200 | 0.45975400  |
| C | 5.38863300 | -0.38481500 | 1.98071700  |
| H | 4.99557500 | 0.44278800  | 0.02997700  |
| H | 6.37399300 | -0.63197600 | 0.08034700  |
| C | 6.28974200 | 0.74903600  | 2.46100900  |
| H | 4.36611000 | -0.22814300 | 2.35516300  |
| H | 5.72660000 | -1.33711100 | 2.40794400  |
| H | 6.29914400 | 0.82324300  | 3.55107000  |
| H | 7.31940800 | 0.59301800  | 2.12609100  |
| H | 5.95368000 | 1.71071700  | 2.05990300  |

trans-25'

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -1.04383000 | 2.30569700 | -0.54143600 |
| C  | -1.17692200 | 1.72573100 | -1.84858600 |
| C  | 0.11917200  | 1.53544600 | -2.40030000 |
| C  | 1.07514900  | 2.03024400 | -1.46124200 |
| C  | 0.36895200  | 2.49705800 | -0.32042100 |
| Sc | -0.13700800 | 0.12066600 | -0.42669900 |
| C  | -2.77705000 | 4.76144200 | -0.20197300 |
| C  | -4.04000400 | 1.99651300 | 0.28312400  |
| C  | -2.08037000 | 3.15343800 | 2.30538100  |
| H  | -1.88593100 | 5.38497800 | -0.08027500 |
| H  | -3.02702400 | 4.73722400 | -1.26685100 |
| H  | -3.60325700 | 5.24430100 | 0.32879600  |
| H  | -3.86652200 | 0.92986500 | 0.46088200  |
| H  | -4.76686500 | 2.33684800 | 1.02832200  |
| H  | -4.50220000 | 2.10907300 | -0.70037000 |
| H  | -2.98803500 | 3.48979600 | 2.81801700  |
| H  | -1.79548900 | 2.19577600 | 2.75208500  |
| H  | -1.29608300 | 3.88444600 | 2.51640600  |
| Si | -2.47670600 | 3.03166400 | 0.46823300  |
| C  | 0.99714400  | 3.14176100 | 0.88738800  |
| H  | 0.83696500  | 4.22519100 | 0.87160300  |
| H  | 0.57623000  | 2.76616400 | 1.82357300  |
| H  | 2.07557900  | 2.96867800 | 0.91678200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.55624300  | 2.09958400  | -1.71648600 |
| H | 2.97860900  | 1.13643300  | -2.02148000 |
| H | 2.76286500  | 2.80939600  | -2.52388800 |
| H | 3.10528900  | 2.43618200  | -0.83603800 |
| C | 0.44061100  | 0.98816600  | -3.76494700 |
| H | -0.18816900 | 0.13292200  | -4.02959800 |
| H | 0.28500000  | 1.75408300  | -4.53151000 |
| H | 1.48435800  | 0.67154800  | -3.82998800 |
| C | -2.46375400 | 1.38119600  | -2.55613200 |
| H | -3.08470800 | 0.67749200  | -1.99144000 |
| H | -3.06355500 | 2.28279600  | -2.71719000 |
| H | -2.26237300 | 0.94250900  | -3.53556900 |
| C | -0.56429600 | -1.89994000 | 4.04342800  |
| C | -0.88530400 | -1.25293300 | 2.68812900  |
| H | -1.07645600 | -2.86283600 | 4.13591200  |
| H | 0.50314300  | -2.06942800 | 4.20047900  |
| H | -0.91435800 | -1.25520100 | 4.85474600  |
| C | 0.04621400  | -0.04660100 | 2.43149200  |
| C | -2.36054400 | -0.86618300 | 2.67567700  |
| H | -0.47270900 | 0.68339500  | 1.77279400  |
| H | 0.25215200  | 0.53568100  | 3.33668400  |
| H | -2.57805200 | -0.16340400 | 3.48677300  |
| H | -2.64451400 | -0.39827500 | 1.73008900  |
| H | -2.99141400 | -1.74936400 | 2.82284500  |
| C | -0.46662200 | -2.17913300 | 1.51197900  |
| H | -0.87976400 | -3.18881100 | 1.62439000  |
| N | -0.84179900 | -1.56186100 | 0.24210000  |
| C | -1.57540200 | -2.29992100 | -0.77837700 |
| C | -0.88820500 | -3.60190800 | -1.21466900 |
| C | -3.04354700 | -2.54862100 | -0.40779800 |
| H | -1.59752000 | -1.63325100 | -1.67952300 |
| C | -1.65752800 | -4.30209400 | -2.33753400 |
| H | -0.82934300 | -4.27034100 | -0.34508300 |
| H | 0.14283200  | -3.38759300 | -1.52202200 |
| C | -3.80135800 | -3.25698400 | -1.53267400 |
| H | -3.06781200 | -3.16365800 | 0.50348700  |
| H | -3.51714300 | -1.59151400 | -0.16014300 |
| C | -3.10952700 | -4.56062600 | -1.93288700 |
| H | -1.15747300 | -5.23845300 | -2.60184000 |
| H | -1.64120000 | -3.67049400 | -3.23681700 |
| H | -4.83397500 | -3.44579900 | -1.22483800 |
| H | -3.84857300 | -2.59248800 | -2.40714600 |
| H | -3.65081200 | -5.04332900 | -2.75183400 |
| H | -3.12951500 | -5.25598200 | -1.08319400 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.35530400 | -0.61952600 | 1.81264500  |
| C | 1.07214000 | -2.13064700 | 1.59202700  |
| H | 1.59339300 | -0.11461200 | 0.84141400  |
| H | 1.53518800 | -2.52635400 | 0.68372700  |
| H | 1.46353800 | -2.70281500 | 2.43843900  |
| C | 2.61116500 | -0.32646800 | 2.63782600  |
| C | 3.89656500 | -0.86877300 | 2.00840500  |
| H | 2.46763000 | -0.75827100 | 3.63576900  |
| H | 2.70091700 | 0.75966700  | 2.77207700  |
| C | 4.16467500 | -0.31917400 | 0.60683600  |
| H | 4.73680600 | -0.60418500 | 2.65992400  |
| H | 3.86667000 | -1.96510800 | 1.97486400  |
| H | 3.43954000 | -0.73681200 | -0.11063000 |
| H | 4.00449900 | 0.76963900  | 0.60974700  |
| C | 5.57046100 | -0.61473800 | 0.09114300  |
| C | 5.80933800 | -0.07573100 | -1.31724000 |
| H | 5.74560100 | -1.69873300 | 0.10471800  |
| H | 6.30464500 | -0.17500200 | 0.77859900  |
| C | 7.22877800 | -0.33214000 | -1.81516500 |
| H | 5.08788100 | -0.53550100 | -2.00685100 |
| H | 5.60273400 | 1.00285200  | -1.32778800 |
| H | 7.37866200 | 0.06706600  | -2.82110600 |
| H | 7.96235400 | 0.13878800  | -1.15396500 |
| H | 7.44552800 | -1.40423500 | -1.84193300 |

#### Configurational Search

cis-ts-10-2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.38070400 | -1.07620500 | -2.09006100 |
| C  | -2.61015400 | -1.21593600 | -1.40856900 |
| C  | -2.45436000 | -2.24494600 | -0.43900400 |
| C  | -1.13965400 | -2.76811200 | -0.55623200 |
| C  | -0.44147300 | -2.04296100 | -1.58116000 |
| Sc | -0.87047400 | -0.46193200 | 0.30997700  |
| C  | -0.65294300 | -3.94547600 | 0.24821500  |
| H  | -1.39075000 | -4.75311400 | 0.22048000  |
| H  | 0.28239200  | -4.34011700 | -0.14532100 |
| H  | -0.48457800 | -3.69904400 | 1.30416800  |
| C  | -3.55122700 | -2.77733300 | 0.43940500  |
| H  | -4.19450100 | -1.97205300 | 0.80889500  |
| H  | -4.18544100 | -3.47380500 | -0.11999400 |
| H  | -3.15514300 | -3.31848000 | 1.30377200  |
| C  | -3.91416000 | -0.62123500 | -1.84891700 |
| H  | -3.78637700 | 0.35694200  | -2.31456300 |
| H  | -4.36579500 | -1.28625500 | -2.59483500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.62507400 | -0.50781600 | -1.02852000 |
| N | 0.53301400  | 1.01286200  | -0.90784400 |
| H | 1.13847400  | 0.35191800  | -1.40155500 |
| C | 1.32571600  | 2.27165100  | -0.66514800 |
| C | 2.80790600  | 1.99965000  | -0.96090100 |
| C | 0.83154200  | 3.37660600  | -1.61364800 |
| C | 1.17484500  | 2.76011800  | 0.78063200  |
| H | 2.91348000  | 1.64897400  | -1.99685100 |
| H | 3.17178900  | 1.20162900  | -0.30202500 |
| C | 3.63888100  | 3.27376400  | -0.75006500 |
| H | -0.23376600 | 3.57671300  | -1.42345600 |
| H | 0.92349800  | 3.02987200  | -2.65294200 |
| C | 1.65331000  | 4.65913100  | -1.40470500 |
| H | 1.48216100  | 1.96262000  | 1.47132900  |
| H | 0.12357000  | 2.99259300  | 0.98359400  |
| C | 2.01288100  | 4.03049400  | 0.99969700  |
| H | 4.68929900  | 3.05087000  | -0.96454700 |
| C | 3.13240800  | 4.36839500  | -1.70033900 |
| C | 3.49051900  | 3.73900400  | 0.70499600  |
| H | 1.28332900  | 5.43328900  | -2.08441700 |
| C | 1.50553400  | 5.12764400  | 0.05069400  |
| H | 1.89712500  | 4.35792500  | 2.03828000  |
| H | 3.25559400  | 4.04983400  | -2.74254200 |
| H | 3.72389100  | 5.28129400  | -1.56654500 |
| H | 3.87220600  | 2.96862400  | 1.38782600  |
| H | 4.08863500  | 4.64223300  | 0.87163400  |
| H | 2.07964700  | 6.04834500  | 0.20472500  |
| H | 0.45564500  | 5.35789900  | 0.26927400  |
| C | -0.59047800 | 0.06935500  | 4.61430500  |
| C | -0.56803500 | -1.05554900 | 3.56068500  |
| H | 0.11135000  | -0.15564500 | 5.42258900  |
| H | -0.32334100 | 1.04604100  | 4.20691500  |
| H | -1.59200400 | 0.13832200  | 5.04980100  |
| C | -1.62061200 | -0.92158900 | 2.46579000  |
| C | -0.74859500 | -2.39581700 | 4.31299800  |
| H | -1.58354200 | -1.87028600 | 1.89520500  |
| H | -2.62862000 | -0.90400300 | 2.88571400  |
| H | -0.16916200 | 1.24259700  | -1.61407400 |
| H | -1.71968700 | -2.39474200 | 4.81589700  |
| H | -0.72084600 | -3.24726500 | 3.62610100  |
| H | 0.02753800  | -2.53594800 | 5.07238300  |
| C | 0.78656300  | -1.09740900 | 2.92701400  |
| H | 1.63065400  | -1.29943700 | 3.59624100  |
| N | 0.97327000  | -0.95279300 | 1.66940300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.35360500  | -1.13919800 | 1.16300600  |
| C  | 3.42786700  | -0.34178400 | 1.91145700  |
| C  | 2.70783300  | -2.62912400 | 1.15803600  |
| H  | 2.33748300  | -0.79303200 | 0.12225400  |
| C  | 4.79684800  | -0.56045800 | 1.25773800  |
| H  | 3.48726300  | -0.67944800 | 2.95307400  |
| H  | 3.16852700  | 0.72208100  | 1.93383000  |
| C  | 4.08079200  | -2.86482800 | 0.52551500  |
| H  | 2.71131600  | -2.98797600 | 2.19721700  |
| H  | 1.92415800  | -3.18112900 | 0.63251200  |
| C  | 5.16190700  | -2.04621400 | 1.23395100  |
| H  | 5.55579300  | 0.01471400  | 1.79580200  |
| H  | 4.78072900  | -0.17666600 | 0.22808300  |
| H  | 4.32269900  | -3.93182000 | 0.55528300  |
| H  | 4.04462500  | -2.58152600 | -0.53567200 |
| H  | 6.12866300  | -2.19069200 | 0.74370600  |
| H  | 5.27017200  | -2.40724900 | 2.26514500  |
| C  | -1.73666500 | 1.22919900  | 1.94057400  |
| C  | -2.19600100 | 1.58882700  | 0.67930600  |
| H  | -0.69900000 | 1.44616300  | 2.18729700  |
| H  | -2.40373000 | 1.23562500  | 2.79492700  |
| H  | -1.52902000 | 2.13957700  | 0.02128300  |
| C  | -3.62845200 | 1.66111100  | 0.36701700  |
| C  | -4.58653500 | 0.97558600  | 1.12898200  |
| C  | -4.07395100 | 2.45581400  | -0.69851900 |
| C  | -5.94142600 | 1.07475100  | 0.82594900  |
| H  | -4.27135800 | 0.34780400  | 1.95794700  |
| C  | -5.42647200 | 2.55445800  | -1.00118800 |
| H  | -3.34354400 | 3.00361100  | -1.29101200 |
| C  | -6.36831700 | 1.85983500  | -0.24275400 |
| H  | -6.66624200 | 0.53303300  | 1.42559400  |
| H  | -5.74801600 | 3.17671000  | -1.83030200 |
| H  | -7.42420000 | 1.93471700  | -0.47919900 |
| C  | -1.20765900 | -0.17095500 | -3.28172500 |
| H  | -1.68934900 | 0.80243300  | -3.12604600 |
| H  | -0.15641100 | 0.00439900  | -3.52923100 |
| H  | -1.67785400 | -0.60883600 | -4.16882200 |
| Si | 1.03942200  | -2.58905700 | -2.63331600 |
| C  | 0.37964900  | -2.92302300 | -4.36714600 |
| H  | 1.15532500  | -3.41647100 | -4.96211700 |
| H  | -0.48746900 | -3.58938000 | -4.32809600 |
| H  | 0.08440500  | -2.01483300 | -4.89747200 |
| C  | 1.84843200  | -4.20437600 | -2.10084500 |
| H  | 1.13052000  | -5.02968100 | -2.11940700 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 2.61732400 | -4.42760300 | -2.84912200 |
| H | 2.34041700 | -4.19190000 | -1.12688500 |
| C | 2.40346400 | -1.28525800 | -2.81452600 |
| H | 2.06177900 | -0.38117800 | -3.33104100 |
| H | 2.88338500 | -0.98916200 | -1.87633100 |
| H | 3.18824700 | -1.72156500 | -3.44291700 |

cis-ts-10-3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.60856600 | 0.15197200  | -2.55836200 |
| C  | -0.99721600 | 1.45536600  | -2.13461000 |
| C  | -2.22414300 | 1.33343700  | -1.43120200 |
| C  | -2.59507600 | -0.05056600 | -1.39233300 |
| C  | -1.57910000 | -0.77045000 | -2.10654400 |
| Sc | -0.58385400 | 0.16678500  | -0.00722100 |
| C  | -3.04809000 | 2.47393900  | -0.89673400 |
| H  | -2.49935100 | 3.41784700  | -0.91833200 |
| H  | -3.95633300 | 2.59618100  | -1.49809400 |
| H  | -3.36062200 | 2.30677500  | 0.13832900  |
| C  | -0.29451300 | 2.71311600  | -2.55723500 |
| H  | 0.76818100  | 2.70515200  | -2.28793300 |
| H  | -0.35010200 | 2.82279400  | -3.64595600 |
| H  | -0.74313600 | 3.59841400  | -2.10762700 |
| N  | 1.70865700  | -0.34424100 | -0.49633600 |
| H  | 1.72500300  | -1.28587800 | -0.10115100 |
| C  | 3.11032300  | 0.16894400  | -0.32022300 |
| C  | 4.09334800  | -0.90054900 | -0.83461800 |
| C  | 3.32185600  | 1.45162600  | -1.13464800 |
| C  | 3.39617500  | 0.43668000  | 1.16174900  |
| H  | 3.87974000  | -1.11102000 | -1.89250200 |
| H  | 3.94040000  | -1.83545300 | -0.27563300 |
| C  | 5.54366400  | -0.42324600 | -0.66976600 |
| H  | 2.62629900  | 2.23504000  | -0.81346600 |
| H  | 3.12340000  | 1.24992300  | -2.19640500 |
| C  | 4.76941500  | 1.94340500  | -0.95806100 |
| H  | 3.22607000  | -0.48191800 | 1.74357600  |
| H  | 2.71636300  | 1.20570800  | 1.54234900  |
| C  | 4.84781400  | 0.91498600  | 1.33186800  |
| H  | 6.22075200  | -1.19892500 | -1.04190600 |
| C  | 5.74079500  | 0.87125800  | -1.47121300 |
| C  | 5.81671500  | -0.15831200 | 0.81761700  |
| H  | 4.89968700  | 2.86729300  | -1.53084400 |
| C  | 5.03772100  | 2.21209000  | 0.53040000  |
| H  | 5.03422000  | 1.10633500  | 2.39350500  |
| H  | 5.56875100  | 0.68552800  | -2.53838300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 6.77323600  | 1.22304900  | -1.36452400 |
| H | 5.69663600  | -1.08397800 | 1.39437700  |
| H | 6.85096500  | 0.17758500  | 0.95357400  |
| H | 6.05942700  | 2.58577800  | 0.66171200  |
| H | 4.35656500  | 2.98725400  | 0.90340600  |
| C | -0.84321200 | -0.87594900 | 4.15674700  |
| C | -1.64481200 | -1.12487500 | 2.86219900  |
| H | -0.85005000 | -1.76964100 | 4.78752400  |
| H | 0.19835100  | -0.60878900 | 3.96550800  |
| H | -1.31307300 | -0.06458500 | 4.72104300  |
| C | -1.77839500 | 0.11306400  | 1.98512200  |
| C | -3.03727600 | -1.65552400 | 3.27224700  |
| H | -2.45084500 | -0.16090500 | 1.14282100  |
| H | -2.32697400 | 0.89881800  | 2.50852900  |
| H | 1.60462300  | -0.50463100 | -1.50035900 |
| H | -3.53245700 | -0.90331000 | 3.89279800  |
| H | -3.66764200 | -1.84541900 | 2.39919000  |
| H | -2.95890600 | -2.57920900 | 3.85528500  |
| C | -0.94192500 | -2.20180800 | 2.09772600  |
| H | -0.86343900 | -3.17674700 | 2.59469500  |
| N | -0.44524800 | -2.02508600 | 0.93139600  |
| C | 0.24907200  | -3.18725600 | 0.31965400  |
| C | 1.56226300  | -3.50849500 | 1.05026800  |
| C | -0.60315900 | -4.46075700 | 0.24141600  |
| H | 0.48612600  | -2.89443100 | -0.71346700 |
| C | 2.34223300  | -4.58396100 | 0.29030300  |
| H | 1.31759600  | -3.86897300 | 2.05827400  |
| H | 2.17550000  | -2.60932100 | 1.19460600  |
| C | 0.15302800  | -5.54290400 | -0.53521400 |
| H | -0.80714600 | -4.82689000 | 1.25539500  |
| H | -1.57106200 | -4.24963700 | -0.22206800 |
| C | 1.50192800  | -5.85124300 | 0.11870900  |
| H | 3.27391200  | -4.80822400 | 0.81752700  |
| H | 2.62265900  | -4.19313600 | -0.69808600 |
| H | -0.45827400 | -6.44755100 | -0.59331300 |
| H | 0.31132000  | -5.19992100 | -1.56682100 |
| H | 2.05041200  | -6.58975000 | -0.47270000 |
| H | 1.32764600  | -6.29948100 | 1.10550800  |
| C | 0.05978600  | 1.32114400  | 2.07155000  |
| C | 0.25259000  | 2.21731300  | 1.02648300  |
| H | 0.76402000  | 0.49129700  | 2.16911300  |
| H | -0.35772200 | 1.64492100  | 3.01825500  |
| H | 1.11314900  | 2.07931700  | 0.37806000  |
| C | -0.41041800 | 3.52693300  | 0.97340300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.54606000 | 3.82195100  | 1.74362200  |
| C  | 0.10977100  | 4.54214900  | 0.15604000  |
| C  | -2.15289300 | 5.07163900  | 1.67409500  |
| H  | -1.97506700 | 3.06242900  | 2.39095800  |
| C  | -0.49945600 | 5.78875600  | 0.08126500  |
| H  | 1.00671900  | 4.34542700  | -0.42629500 |
| C  | -1.64085600 | 6.05865500  | 0.83528700  |
| H  | -3.03483300 | 5.27358800  | 2.27376200  |
| H  | -0.07842600 | 6.55455800  | -0.56253800 |
| H  | -2.11843800 | 7.03079000  | 0.77658300  |
| C  | 0.52610400  | -0.13212000 | -3.50223200 |
| H  | 1.31721100  | 0.61942100  | -3.41931400 |
| H  | 0.97071500  | -1.12292400 | -3.35313000 |
| H  | 0.17197400  | -0.10513800 | -4.53843300 |
| C  | -1.60902000 | -2.22584600 | -2.48401900 |
| H  | -1.88971700 | -2.86266400 | -1.64525500 |
| H  | -2.33963800 | -2.39895800 | -3.28272900 |
| H  | -0.63960500 | -2.56586300 | -2.85892800 |
| Si | -4.28386400 | -0.76121700 | -0.93592100 |
| C  | -5.32452300 | -0.77196800 | -2.50336400 |
| H  | -6.31737300 | -1.18912700 | -2.30785700 |
| H  | -5.45310900 | 0.24346600  | -2.89001700 |
| H  | -4.85364800 | -1.37296000 | -3.28724700 |
| C  | -5.19295700 | 0.25299700  | 0.36875000  |
| H  | -5.51909400 | 1.21911700  | -0.02478000 |
| H  | -6.09076200 | -0.30243600 | 0.66132700  |
| H  | -4.60871900 | 0.43425800  | 1.27603900  |
| C  | -4.11675600 | -2.53289700 | -0.29483800 |
| H  | -4.04174100 | -3.25123000 | -1.11640400 |
| H  | -3.23620400 | -2.65739000 | 0.34494100  |
| H  | -5.00001900 | -2.79797700 | 0.29519700  |

cis-ts-10-4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.94411500  | -0.42304300 | -2.41190900 |
| C  | 2.16068800  | -0.67541200 | -1.73746500 |
| C  | 2.66566300  | 0.56366600  | -1.22340800 |
| C  | 1.74666600  | 1.58546400  | -1.63957400 |
| C  | 0.68797300  | 0.98120200  | -2.36466500 |
| Sc | 0.57393500  | 0.17533500  | 0.01671100  |
| C  | 2.88724400  | -1.98962600 | -1.78505400 |
| H  | 2.21913100  | -2.79911600 | -2.08445900 |
| H  | 3.69021900  | -1.93019900 | -2.53016900 |
| H  | 3.33593700  | -2.26780400 | -0.83026700 |
| N  | -1.70680500 | -0.29245800 | -0.66099500 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.06310200 | 0.66413700  | -0.60861800 |
| C | -2.88521500 | -1.17274000 | -0.34110900 |
| C | -4.15013000 | -0.54759600 | -0.96038900 |
| C | -2.68654300 | -2.56170600 | -0.96611000 |
| C | -3.07667700 | -1.31045700 | 1.17459400  |
| H | -4.00095500 | -0.43413600 | -2.04383100 |
| H | -4.30575400 | 0.45756100  | -0.54349500 |
| C | -5.37954500 | -1.42124300 | -0.67313000 |
| H | -1.77967200 | -3.03771700 | -0.57553400 |
| H | -2.55962200 | -2.45693000 | -2.05278100 |
| C | -3.90786700 | -3.44816700 | -0.66508700 |
| H | -3.19605800 | -0.31907200 | 1.63277500  |
| H | -2.19394900 | -1.78012100 | 1.62051900  |
| C | -4.31076800 | -2.18144000 | 1.46497900  |
| H | -6.26330300 | -0.95328200 | -1.11892200 |
| C | -5.16319600 | -2.81427900 | -1.28009300 |
| C | -5.56027700 | -1.53891300 | 0.84734400  |
| H | -3.73995300 | -4.43790600 | -1.10173400 |
| C | -4.08740200 | -3.57358400 | 0.85527600  |
| H | -4.43475400 | -2.26840200 | 2.54938900  |
| H | -5.05448200 | -2.73952400 | -2.36890600 |
| H | -6.03531700 | -3.44765900 | -1.08192200 |
| H | -5.72809400 | -0.54612300 | 1.28386500  |
| H | -6.44310500 | -2.14735100 | 1.07363600  |
| H | -4.94534500 | -4.21911300 | 1.07508700  |
| H | -3.20251100 | -4.04227700 | 1.30364900  |
| C | 0.33590700  | 1.38133400  | 4.17685300  |
| C | 0.91965300  | 1.87634000  | 2.84007500  |
| H | -0.04870300 | 2.22454700  | 4.75794700  |
| H | -0.47803900 | 0.66537000  | 4.05154400  |
| H | 1.12776300  | 0.90544100  | 4.76337600  |
| C | 1.59231400  | 0.78757400  | 2.00910100  |
| C | 1.92723800  | 3.00715200  | 3.16066300  |
| H | 2.09770900  | 1.30582800  | 1.16551000  |
| H | 2.41542000  | 0.32317700  | 2.55737900  |
| H | -1.53034100 | -0.43227600 | -1.65787500 |
| H | 2.75207300  | 2.59606100  | 3.74981700  |
| H | 2.34352100  | 3.43971800  | 2.24553300  |
| H | 1.45771900  | 3.80686800  | 3.74315500  |
| C | -0.16572600 | 2.51279200  | 2.02982800  |
| H | -0.67391100 | 3.37246600  | 2.48316700  |
| N | -0.46315500 | 2.13207900  | 0.84536100  |
| C | -1.49331100 | 2.91526300  | 0.12238200  |
| C | -2.89036600 | 2.73279200  | 0.72785800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.17362100 | 4.41067300  | 0.00702800  |
| H  | -1.50497300 | 2.52130900  | -0.90245100 |
| C  | -3.93948900 | 3.39699800  | -0.16666200 |
| H  | -2.90658700 | 3.19104600  | 1.72576800  |
| H  | -3.11348700 | 1.67026000  | 0.87502300  |
| C  | -2.21098400 | 5.09014400  | -0.89216600 |
| H  | -1.20438000 | 4.87200800  | 1.00255100  |
| H  | -0.16283600 | 4.55018700  | -0.38525400 |
| C  | -3.63053100 | 4.88350200  | -0.35928600 |
| H  | -4.93634500 | 3.26045000  | 0.26254100  |
| H  | -3.94254300 | 2.89584000  | -1.14614300 |
| H  | -1.98451400 | 6.15667500  | -0.97468900 |
| H  | -2.13690200 | 4.67145600  | -1.90541300 |
| H  | -4.35897800 | 5.33533000  | -1.03830900 |
| H  | -3.73164500 | 5.39705600  | 0.60554000  |
| C  | 0.38115100  | -1.05198100 | 2.15935600  |
| C  | 0.45935300  | -1.97378100 | 1.12027500  |
| H  | -0.56976800 | -0.53584400 | 2.29950000  |
| H  | 0.94568500  | -1.18562000 | 3.07529600  |
| H  | -0.43633700 | -2.15630300 | 0.53534500  |
| C  | 1.52698800  | -2.97159600 | 1.00008200  |
| C  | 2.74290200  | -2.85516000 | 1.68906500  |
| C  | 1.33813500  | -4.09129100 | 0.17605400  |
| C  | 3.74111100  | -3.81538000 | 1.54004100  |
| H  | 2.92088000  | -1.99990200 | 2.33639600  |
| C  | 2.33157200  | -5.05054800 | 0.03104500  |
| H  | 0.39771400  | -4.20250200 | -0.35989600 |
| C  | 3.54386900  | -4.91379700 | 0.70738700  |
| H  | 4.67998900  | -3.69824600 | 2.07254100  |
| H  | 2.16177000  | -5.90761800 | -0.61309700 |
| H  | 4.32304500  | -5.65903900 | 0.58991800  |
| C  | 0.14736400  | -1.44362200 | -3.17791700 |
| H  | -0.07452400 | -2.33261300 | -2.57691600 |
| H  | -0.79952300 | -1.03146300 | -3.54476400 |
| H  | 0.70078300  | -1.77950300 | -4.06101300 |
| C  | -0.40855300 | 1.68032900  | -3.12416600 |
| H  | -0.45419200 | 2.74490000  | -2.88426000 |
| H  | -0.23153800 | 1.59662300  | -4.20144400 |
| H  | -1.40742300 | 1.26331000  | -2.94154700 |
| C  | 1.93229300  | 3.06165800  | -1.41180000 |
| H  | 1.88180300  | 3.33397000  | -0.35055800 |
| H  | 2.90768100  | 3.38956000  | -1.78511800 |
| H  | 1.17357100  | 3.64313000  | -1.94006800 |
| Si | 4.44612000  | 0.88301100  | -0.67065700 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 5.38821000 | 1.36570100  | -2.22883500 |
| H | 6.44559600 | 1.53788400  | -2.00449600 |
| H | 5.32579200 | 0.57047600  | -2.97805000 |
| H | 4.98658500 | 2.27891200  | -2.67863300 |
| C | 4.61430400 | 2.27352600  | 0.59561900  |
| H | 5.68161200 | 2.50224200  | 0.69156100  |
| H | 4.10653100 | 3.19968500  | 0.31636200  |
| H | 4.25955700 | 1.96664100  | 1.58398200  |
| C | 5.25329400 | -0.62878400 | 0.10253800  |
| H | 4.63667700 | -1.05131800 | 0.90150300  |
| H | 5.45318500 | -1.42045600 | -0.62339400 |
| H | 6.21008900 | -0.32402000 | 0.53986300  |

cis-ts-10-5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.70640400 | -0.82405400 | -2.39271400 |
| C  | -1.92857100 | -1.01752200 | -1.67112300 |
| C  | -1.82961500 | -2.30837700 | -1.04735300 |
| C  | -0.57040200 | -2.87417000 | -1.37125100 |
| C  | 0.12909600  | -1.94983000 | -2.20041300 |
| Sc | -0.18373400 | -0.89074800 | 0.08017300  |
| N  | 1.11217100  | 1.01417600  | -0.57168700 |
| H  | 2.03081500  | 0.56433600  | -0.55753400 |
| C  | 1.36652100  | 2.44667300  | -0.18874600 |
| C  | 2.64839500  | 2.92784200  | -0.89531300 |
| C  | 0.19945800  | 3.32786100  | -0.65351800 |
| C  | 1.54113700  | 2.58496100  | 1.32709100  |
| H  | 2.52660500  | 2.81361600  | -1.98207300 |
| H  | 3.49455200  | 2.29425000  | -0.59101300 |
| C  | 2.94117200  | 4.39355600  | -0.54240800 |
| H  | -0.73653400 | 3.01008400  | -0.18050400 |
| H  | 0.07006200  | 3.22388600  | -1.74054300 |
| C  | 0.48055900  | 4.79712400  | -0.29114400 |
| H  | 2.35702100  | 1.93557000  | 1.67383100  |
| H  | 0.62394900  | 2.27203700  | 1.83631100  |
| C  | 1.83888900  | 4.05156800  | 1.68338100  |
| H  | 3.85643600  | 4.70869500  | -1.05389600 |
| C  | 1.76173600  | 5.26531100  | -0.99533000 |
| C  | 3.12167600  | 4.51304200  | 0.97719800  |
| H  | -0.36758100 | 5.40747200  | -0.61746300 |
| C  | 0.65590100  | 4.92003100  | 1.22983300  |
| H  | 1.96256000  | 4.13264300  | 2.76823300  |
| H  | 1.64076600  | 5.20222800  | -2.08361900 |
| H  | 1.95865200  | 6.31506900  | -0.74974700 |
| H  | 3.97324900  | 3.90321500  | 1.30414800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.34232100  | 5.55205100  | 1.24667900  |
| H | 0.83658600  | 5.96691800  | 1.49877600  |
| H | -0.26100100 | 4.60395000  | 1.74335200  |
| C | 1.15841500  | -1.93000100 | 4.06716000  |
| C | 0.92037200  | -2.62020200 | 2.70946500  |
| H | 2.04856700  | -2.34137100 | 4.55174900  |
| H | 1.29632300  | -0.85055200 | 3.97961100  |
| H | 0.30334200  | -2.11841100 | 4.72362400  |
| C | -0.37004400 | -2.20043500 | 2.01477600  |
| C | 0.92814300  | -4.14803600 | 2.94979200  |
| H | -0.48673400 | -2.87245200 | 1.14313200  |
| H | -1.23814600 | -2.42141900 | 2.63824500  |
| H | 0.87113900  | 1.04221500  | -1.56444700 |
| H | 0.10319700  | -4.40732600 | 3.61899900  |
| H | 0.79441000  | -4.69597400 | 2.01202600  |
| H | 1.86238200  | -4.47698200 | 3.41718000  |
| C | 2.07864900  | -2.31738000 | 1.81343400  |
| H | 3.06142000  | -2.66429400 | 2.15500700  |
| N | 1.95825300  | -1.71806700 | 0.68926900  |
| C | 3.19797100  | -1.53941900 | -0.10501700 |
| C | 4.15119100  | -0.52434600 | 0.53738500  |
| C | 3.94684200  | -2.84793700 | -0.38699600 |
| H | 2.87954200  | -1.14811600 | -1.08011800 |
| C | 5.33203500  | -0.24224900 | -0.39493300 |
| H | 4.51621900  | -0.93536700 | 1.48801400  |
| H | 3.62238800  | 0.40344100  | 0.78781400  |
| C | 5.11205100  | -2.57522700 | -1.34276800 |
| H | 4.34213900  | -3.25796800 | 0.55067600  |
| H | 3.26164700  | -3.59590800 | -0.79918600 |
| C | 6.06890800  | -1.53401400 | -0.75709400 |
| H | 6.01374600  | 0.47249500  | 0.07484800  |
| H | 4.95816300  | 0.23225600  | -1.31345500 |
| H | 5.64293200  | -3.50739100 | -1.55393700 |
| H | 4.71329200  | -2.21239600 | -2.30025100 |
| H | 6.87594800  | -1.32195500 | -1.46388100 |
| H | 6.53639300  | -1.94567600 | 0.14685200  |
| C | -0.66382100 | -0.04346100 | 2.33819500  |
| C | -1.51481300 | 0.63187800  | 1.47172000  |
| H | 0.39896900  | 0.21025000  | 2.32043700  |
| H | -1.01349000 | -0.37643300 | 3.30901500  |
| H | -1.10034600 | 1.41406400  | 0.84169200  |
| C | -2.97041500 | 0.65104500  | 1.68166000  |
| C | -3.63184600 | -0.37275500 | 2.37813500  |
| C | -3.72558200 | 1.75795100  | 1.26489500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.99465400 | -0.28774900 | 2.65043600  |
| H  | -3.07765000 | -1.24739700 | 2.70764600  |
| C  | -5.08706500 | 1.84047500  | 1.53315200  |
| H  | -3.22903200 | 2.57501200  | 0.74839100  |
| C  | -5.72995900 | 0.81790500  | 2.22974600  |
| H  | -5.48436700 | -1.09228800 | 3.18992900  |
| H  | -5.64655700 | 2.71148200  | 1.20621200  |
| H  | -6.79182400 | 0.88196500  | 2.44111800  |
| C  | -0.40923900 | 0.30233400  | -3.34549300 |
| H  | -0.82008700 | 1.25591300  | -3.00083100 |
| H  | 0.66613400  | 0.42775500  | -3.51566900 |
| H  | -0.84789400 | 0.09991800  | -4.32827600 |
| C  | 1.40569500  | -2.24208200 | -2.93834500 |
| H  | 2.03736700  | -2.95118600 | -2.39788700 |
| H  | 1.17704000  | -2.69338600 | -3.91038700 |
| H  | 1.99652800  | -1.34240600 | -3.13850000 |
| C  | -0.05075500 | -4.23286500 | -0.99198900 |
| H  | -0.70573000 | -4.73204400 | -0.27381900 |
| H  | 0.01463200  | -4.87723900 | -1.87489600 |
| H  | 0.95226100  | -4.17901000 | -0.55168800 |
| C  | -2.89958000 | -2.97585800 | -0.22488200 |
| H  | -3.44758100 | -2.25093900 | 0.38199000  |
| H  | -3.62397000 | -3.48436200 | -0.87050800 |
| H  | -2.48234400 | -3.73046500 | 0.44798600  |
| Si | -3.50540300 | -0.06370300 | -2.09687700 |
| C  | -3.90935300 | -0.52905900 | -3.88113800 |
| H  | -4.84577900 | -0.05253400 | -4.19010400 |
| H  | -3.13197400 | -0.21920700 | -4.58505300 |
| H  | -4.03804400 | -1.61201500 | -3.97397300 |
| C  | -4.99509600 | -0.57479400 | -1.07641200 |
| H  | -5.26919400 | -1.61335800 | -1.28452300 |
| H  | -4.85780900 | -0.45620100 | -0.00086000 |
| H  | -5.84035500 | 0.05541000  | -1.37478400 |
| C  | -3.21972000 | 1.80517300  | -2.02431100 |
| H  | -2.42590500 | 2.06924500  | -1.31970900 |
| H  | -2.94433800 | 2.19534700  | -3.00905100 |
| H  | -4.13160100 | 2.31857000  | -1.70435600 |

trans-ts-10-2

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.77744700 | -1.38345800 | -2.11441100 |
| C | 1.96355100 | -2.66886000 | -1.55378900 |
| C | 2.83717900 | -2.53800700 | -0.44362000 |
| C | 3.22600400 | -1.17870500 | -0.34148500 |
| C | 2.57324900 | -0.43154300 | -1.37930200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Sc | 0.76276900  | -1.18228700 | 0.15994000  |
| C  | 4.27155200  | -0.73235100 | 0.64693800  |
| H  | 5.14499300  | -1.38933700 | 0.58159800  |
| H  | 4.61106000  | 0.28274300  | 0.45497400  |
| H  | 3.92092100  | -0.77394900 | 1.68655000  |
| C  | 3.41960900  | -3.66413000 | 0.35945500  |
| H  | 2.78300700  | -4.55367000 | 0.34736600  |
| H  | 4.38858900  | -3.96141700 | -0.05767100 |
| H  | 3.59077900  | -3.38344300 | 1.40297100  |
| C  | 1.50882500  | -3.97149600 | -2.14721500 |
| H  | 0.73008600  | -3.82635100 | -2.90028900 |
| H  | 2.35285600  | -4.46040500 | -2.64476100 |
| H  | 1.12654100  | -4.67429500 | -1.39986900 |
| N  | -0.78077600 | 0.19216700  | -1.07605300 |
| H  | -0.15371600 | 0.68947900  | -1.71398500 |
| C  | -1.99128200 | 1.07327700  | -0.88169300 |
| C  | -1.57100300 | 2.54493800  | -0.78886400 |
| C  | -2.92736500 | 0.93244800  | -2.09483700 |
| C  | -2.73247700 | 0.67232100  | 0.39547400  |
| H  | -1.03784000 | 2.83562900  | -1.70383600 |
| H  | -0.89126600 | 2.68610800  | 0.05319700  |
| C  | -2.80681400 | 3.44230700  | -0.59890200 |
| H  | -3.22607900 | -0.11543400 | -2.20429600 |
| H  | -2.38568300 | 1.22633300  | -3.00575600 |
| C  | -4.17498500 | 1.81064100  | -1.90914200 |
| H  | -2.04676000 | 0.76705700  | 1.25180400  |
| H  | -3.04249400 | -0.37520400 | 0.33115400  |
| C  | -3.97110200 | 1.56496900  | 0.58353100  |
| H  | -2.47399700 | 4.48342500  | -0.52264300 |
| C  | -3.74678000 | 3.27990700  | -1.80036500 |
| C  | -3.54170600 | 3.03492900  | 0.68585100  |
| H  | -4.83663200 | 1.67760500  | -2.77171300 |
| C  | -4.90368900 | 1.38764000  | -0.62445900 |
| H  | -4.49186800 | 1.26132400  | 1.49824000  |
| H  | -3.24186100 | 3.59663300  | -2.72125900 |
| H  | -4.62778100 | 3.91993300  | -1.67389600 |
| H  | -2.89240200 | 3.18481400  | 1.55808200  |
| H  | -4.42148100 | 3.67359900  | 0.82764200  |
| H  | -5.80549100 | 1.99701100  | -0.49159600 |
| H  | -5.21969300 | 0.34027900  | -0.69804600 |
| C  | -0.95375800 | -1.69218700 | 3.66742700  |
| C  | 0.52736900  | -1.40977300 | 3.36417000  |
| H  | -1.29903300 | -1.09492100 | 4.51689300  |
| H  | -1.58355500 | -1.45683000 | 2.80400600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.08682200 | -2.74797800 | 3.92627700  |
| C | 1.09288900  | -2.26732800 | 2.22773400  |
| C | 1.35508200  | -1.62989800 | 4.64715300  |
| H | 2.07910500  | -1.85000800 | 1.95346300  |
| H | 1.32360500  | -3.25975000 | 2.61624800  |
| H | -1.11529900 | -0.60625700 | -1.62605200 |
| H | 1.26013400  | -2.67120900 | 4.96637100  |
| H | 2.41502700  | -1.42083700 | 4.47182700  |
| H | 1.00425600  | -0.99116600 | 5.46438500  |
| C | 0.63313300  | 0.04061300  | 3.00688600  |
| H | 0.52454300  | 0.75659400  | 3.82804800  |
| N | 0.85074200  | 0.43748200  | 1.81316200  |
| C | 1.06367300  | 1.87974400  | 1.57056300  |
| C | 0.16373100  | 2.82152700  | 2.37525200  |
| C | 2.53549300  | 2.22544500  | 1.80627400  |
| H | 0.86100500  | 2.02482100  | 0.50385200  |
| C | 0.42350100  | 4.27448700  | 1.96226300  |
| H | 0.38830400  | 2.73352700  | 3.44477600  |
| H | -0.88893200 | 2.54846300  | 2.24176700  |
| C | 2.81700500  | 3.68299000  | 1.43178300  |
| H | 2.76868100  | 2.05485000  | 2.86708000  |
| H | 3.15843300  | 1.54296200  | 1.22367100  |
| C | 1.89237200  | 4.64264400  | 2.18210000  |
| H | -0.23034200 | 4.93963400  | 2.53360100  |
| H | 0.16684200  | 4.41203600  | 0.90242400  |
| H | 3.86605300  | 3.91988400  | 1.63535200  |
| H | 2.67072400  | 3.81044100  | 0.35003900  |
| H | 2.07731200  | 5.67205600  | 1.86232600  |
| H | 2.11723500  | 4.59670600  | 3.25568200  |
| C | -0.14824000 | -3.47611200 | 0.90578800  |
| C | -0.88097400 | -2.96708300 | -0.16842600 |
| H | -0.67017400 | -3.77734700 | 1.80846600  |
| H | 0.73688100  | -4.06607400 | 0.69327300  |
| H | -0.48121100 | -3.14369200 | -1.16263600 |
| C | -2.34162400 | -2.77218600 | -0.14052300 |
| C | -3.12203700 | -2.86267400 | 1.02346100  |
| C | -3.01281200 | -2.56215900 | -1.35531900 |
| C | -4.50283500 | -2.70097400 | 0.97618700  |
| H | -2.65621900 | -3.07497700 | 1.97887500  |
| C | -4.39456800 | -2.41098200 | -1.40587800 |
| H | -2.43978400 | -2.54146100 | -2.28172400 |
| C | -5.14925200 | -2.46527700 | -0.23585800 |
| H | -5.07897300 | -2.77166500 | 1.89342200  |
| H | -4.88252800 | -2.25171700 | -2.36296400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -6.22656300 | -2.34387200 | -0.27056300 |
| C  | 0.99995700  | -1.13625000 | -3.38223800 |
| H  | 1.56317700  | -1.48467400 | -4.25471300 |
| H  | 0.04278100  | -1.67163600 | -3.39341800 |
| H  | 0.78781800  | -0.07573900 | -3.54375600 |
| Si | 3.13118200  | 1.19563500  | -2.17571000 |
| C  | 3.73229800  | 0.76587900  | -3.90924700 |
| H  | 4.23904100  | 1.63176600  | -4.34759700 |
| H  | 4.44864900  | -0.06064100 | -3.87508400 |
| H  | 2.92033400  | 0.48213300  | -4.58285000 |
| C  | 1.75939500  | 2.48246100  | -2.35465100 |
| H  | 2.19135900  | 3.37867200  | -2.81366900 |
| H  | 0.95183400  | 2.15211400  | -3.01798000 |
| H  | 1.32059800  | 2.78843300  | -1.40093600 |
| C  | 4.60013200  | 2.01143200  | -1.32278900 |
| H  | 4.42409900  | 2.34883800  | -0.29959600 |
| H  | 5.47231800  | 1.35113400  | -1.32729600 |
| H  | 4.86018900  | 2.89549200  | -1.91549500 |

trans-ts-10-3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.24388000  | -1.33859300 | -2.48732100 |
| C  | 1.78320100  | -2.46793900 | -1.81426700 |
| C  | 2.82185500  | -2.01801400 | -0.96781600 |
| C  | 2.96323700  | -0.59672100 | -1.11799900 |
| C  | 1.96577400  | -0.18944300 | -2.06394300 |
| Sc | 0.75557600  | -0.93758000 | -0.02785500 |
| C  | 3.72103200  | -2.92936400 | -0.17934700 |
| H  | 3.20045000  | -3.83649200 | 0.14189300  |
| H  | 4.56910800  | -3.25523800 | -0.79028800 |
| H  | 4.12501200  | -2.44203400 | 0.71352200  |
| C  | 1.45540800  | -3.90319000 | -2.11119600 |
| H  | 0.48155200  | -4.00709900 | -2.59804000 |
| H  | 2.20402300  | -4.32247800 | -2.79183800 |
| H  | 1.45133700  | -4.52961900 | -1.21347200 |
| N  | -1.26351900 | -0.18341000 | -1.11747200 |
| H  | -0.90238400 | 0.09324600  | -2.03205800 |
| C  | -2.52844000 | 0.60411900  | -0.92868000 |
| C  | -2.27002900 | 2.08629100  | -1.21237900 |
| C  | -3.58837100 | 0.10852100  | -1.92925400 |
| C  | -3.04919500 | 0.43519800  | 0.50006200  |
| H  | -1.87670400 | 2.20588600  | -2.23315800 |
| H  | -1.51929900 | 2.46607500  | -0.51959500 |
| C  | -3.56904900 | 2.89415700  | -1.04400100 |
| H  | -3.77297400 | -0.95854000 | -1.76485100 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.20105000 | 0.22785900  | -2.95149700 |
| C | -4.89488900 | 0.89719800  | -1.75518700 |
| H | -2.27943200 | 0.77653400  | 1.20843200  |
| H | -3.24143200 | -0.62330800 | 0.70190100  |
| C | -4.34863100 | 1.23962700  | 0.67423000  |
| H | -3.35512500 | 3.95069600  | -1.24015100 |
| C | -4.62786600 | 2.38306700  | -2.02953700 |
| C | -4.08472200 | 2.72610800  | 0.39364000  |
| H | -5.63990700 | 0.51550800  | -2.46117000 |
| C | -5.40068900 | 0.71468500  | -0.31544400 |
| H | -4.71145400 | 1.11080900  | 1.69969100  |
| H | -4.28256700 | 2.52109200  | -3.06150800 |
| H | -5.55320600 | 2.95943500  | -1.91470300 |
| H | -3.35427700 | 3.12759000  | 1.10756100  |
| H | -5.00938700 | 3.30052200  | 0.52414900  |
| H | -6.34383700 | 1.25667800  | -0.17954800 |
| H | -5.59722700 | -0.34651600 | -0.11872500 |
| C | -0.14050500 | -0.93642900 | 3.74924800  |
| C | 1.20663300  | -0.53980500 | 3.11940700  |
| H | -0.43743100 | -0.22366500 | 4.52511400  |
| H | -0.92731400 | -0.96455800 | 2.98852500  |
| H | -0.05976800 | -1.92336100 | 4.21722100  |
| C | 1.68930600  | -1.52492900 | 2.04704400  |
| C | 2.26510300  | -0.40583100 | 4.23219000  |
| H | 2.50426600  | -1.03574300 | 1.48040200  |
| H | 2.17384500  | -2.37108000 | 2.53465600  |
| H | -1.57586800 | -1.14984700 | -1.25640300 |
| H | 2.39362500  | -1.37167200 | 4.72776300  |
| H | 3.23211000  | -0.09928500 | 3.82290400  |
| H | 1.95798300  | 0.32526600  | 4.98725500  |
| C | 0.99656400  | 0.81362700  | 2.51180000  |
| H | 0.97042800  | 1.66415800  | 3.20212800  |
| N | 0.84730900  | 0.98561200  | 1.25570300  |
| C | 0.72546700  | 2.37044500  | 0.74688300  |
| C | -0.25820900 | 3.25101300  | 1.52375200  |
| C | 2.09632000  | 3.04637100  | 0.69534300  |
| H | 0.37336900  | 2.27547800  | -0.28682200 |
| C | -0.38971000 | 4.61773800  | 0.84335300  |
| H | 0.11354700  | 3.41121500  | 2.54310600  |
| H | -1.22917700 | 2.75200000  | 1.61084600  |
| C | 1.98837900  | 4.41365400  | 0.01783300  |
| H | 2.47500800  | 3.16150400  | 1.72124100  |
| H | 2.80095100  | 2.40161300  | 0.16588900  |
| C | 0.97339500  | 5.30665300  | 0.73527000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.09221000 | 5.24085900  | 1.40451900  |
| H  | -0.81305900 | 4.49071800  | -0.16256200 |
| H  | 2.97196700  | 4.89228800  | -0.01006000 |
| H  | 1.67404400  | 4.27133000  | -1.02623900 |
| H  | 0.87388200  | 6.26266000  | 0.21357100  |
| H  | 1.34362900  | 5.53060900  | 1.74426100  |
| C  | 0.42631800  | -3.13629300 | 1.29796900  |
| C  | -0.56818300 | -2.98117600 | 0.32955000  |
| H  | 0.14180100  | -3.27873400 | 2.33563700  |
| H  | 1.33485200  | -3.65836500 | 1.01756500  |
| H  | -0.33497500 | -3.33787300 | -0.66819700 |
| C  | -2.01152600 | -2.95227300 | 0.62827500  |
| C  | -2.54374600 | -2.86951300 | 1.92554200  |
| C  | -2.91902800 | -3.09164900 | -0.43509000 |
| C  | -3.91825400 | -2.87227500 | 2.13937800  |
| H  | -1.88395400 | -2.82272300 | 2.78422500  |
| C  | -4.29376200 | -3.10453900 | -0.22157000 |
| H  | -2.53407200 | -3.21445900 | -1.44768100 |
| C  | -4.80414900 | -2.97728400 | 1.06845500  |
| H  | -4.29955500 | -2.80334800 | 3.15331300  |
| H  | -4.96800900 | -3.21526800 | -1.06581300 |
| H  | -5.87533600 | -2.98201500 | 1.23871400  |
| C  | 0.23329400  | -1.40526500 | -3.60077000 |
| H  | 0.68061300  | -1.87548400 | -4.48261800 |
| H  | -0.65478000 | -1.99569700 | -3.34528500 |
| H  | -0.09838200 | -0.41071000 | -3.91445900 |
| C  | 1.74889600  | 1.20002700  | -2.60377400 |
| H  | 2.14587200  | 1.95854900  | -1.92711100 |
| H  | 2.24817200  | 1.32831700  | -3.57050200 |
| H  | 0.68765000  | 1.42681500  | -2.76431500 |
| Si | 4.55466600  | 0.29925000  | -0.60905300 |
| C  | 6.01368900  | -0.78551700 | -1.11644400 |
| H  | 6.92207300  | -0.17452400 | -1.13147500 |
| H  | 6.18854900  | -1.61425600 | -0.42677700 |
| H  | 5.87315000  | -1.19914400 | -2.11979300 |
| C  | 4.80900300  | 1.90187600  | -1.57408500 |
| H  | 4.73485000  | 1.70566400  | -2.64870000 |
| H  | 4.14333800  | 2.73373800  | -1.33691200 |
| H  | 5.83258800  | 2.23756000  | -1.37548400 |
| C  | 4.69205100  | 0.58572300  | 1.25286400  |
| H  | 4.83878400  | -0.36486500 | 1.77744200  |
| H  | 5.56717600  | 1.21020500  | 1.46206600  |
| H  | 3.81649600  | 1.07943500  | 1.68247300  |

trans-ts-4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.51242800  | -0.66677300 | -2.54062400 |
| C  | 2.54348200  | -1.30462000 | -1.80942900 |
| C  | 3.27863900  | -0.31617000 | -1.08575800 |
| C  | 2.69672000  | 0.95098700  | -1.41867900 |
| C  | 1.60337000  | 0.73705400  | -2.29759900 |
| Sc | 0.96025300  | -0.25655000 | -0.10753200 |
| C  | 2.89770100  | -2.76129900 | -1.93610500 |
| H  | 2.13614700  | -3.30625600 | -2.50055800 |
| H  | 3.84461000  | -2.87448500 | -2.47510600 |
| H  | 3.01556300  | -3.25984700 | -0.96972000 |
| N  | -1.21848500 | -0.54622000 | -1.12311400 |
| H  | -1.02946800 | -0.24629100 | -2.08066700 |
| C  | -2.68701800 | -0.32330600 | -0.90668800 |
| C  | -3.06024400 | 1.10727800  | -1.29896500 |
| C  | -3.49595500 | -1.28356900 | -1.79855100 |
| C  | -3.03603800 | -0.57526800 | 0.56059000  |
| H  | -2.81069200 | 1.27697200  | -2.35722000 |
| H  | -2.47885500 | 1.81170200  | -0.70501300 |
| C  | -4.56452100 | 1.34386300  | -1.07106600 |
| H  | -3.22849600 | -2.31916300 | -1.55795600 |
| H  | -3.23497900 | -1.10468700 | -2.85188700 |
| C  | -5.00230300 | -1.06747600 | -1.57764000 |
| H  | -2.43711100 | 0.09329500  | 1.19718000  |
| H  | -2.77743400 | -1.60376800 | 0.82747400  |
| C  | -4.53958700 | -0.34731000 | 0.78373900  |
| H  | -4.80532700 | 2.37898800  | -1.33776200 |
| C  | -5.36884700 | 0.37570700  | -1.94939700 |
| C  | -4.90973200 | 1.09316000  | 0.40578700  |
| H  | -5.56006500 | -1.76707700 | -2.20914600 |
| C  | -5.33075600 | -1.32517400 | -0.09897400 |
| H  | -4.77428800 | -0.53059500 | 1.83792300  |
| H  | -5.15474000 | 0.55882100  | -3.00952900 |
| H  | -6.44213400 | 0.54068900  | -1.79998500 |
| H  | -4.38066400 | 1.80749600  | 1.04846600  |
| H  | -5.98223700 | 1.25676900  | 0.56378900  |
| H  | -6.40584300 | -1.19643300 | 0.07259500  |
| H  | -5.07402800 | -2.35775200 | 0.16896100  |
| C  | 0.40149700  | -0.18635700 | 3.82199500  |
| C  | 1.36893100  | 0.64267000  | 2.96100700  |
| H  | -0.07389300 | 0.43612100  | 4.58632800  |
| H  | -0.38433900 | -0.63301300 | 3.20642500  |
| H  | 0.94768800  | -0.98521800 | 4.33458000  |
| C  | 2.13464100  | -0.18630300 | 1.92616200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.36878900  | 1.36833700  | 3.88629300  |
| H | 2.64655900  | 0.52243600  | 1.24911300  |
| H | 2.95350600  | -0.69902200 | 2.43280600  |
| H | -1.11046100 | -1.56496900 | -1.15754100 |
| H | 2.96314100  | 0.62957300  | 4.43039900  |
| H | 3.05088700  | 2.00147600  | 3.30981100  |
| H | 1.85068900  | 1.99416400  | 4.62036900  |
| C | 0.56009500  | 1.69918600  | 2.27501200  |
| H | 0.19884200  | 2.51960700  | 2.90508300  |
| N | 0.30610900  | 1.68115400  | 1.02337800  |
| C | -0.42751300 | 2.84406800  | 0.46473400  |
| C | -1.71564200 | 3.17859900  | 1.22516400  |
| C | 0.46129300  | 4.09145100  | 0.40238700  |
| H | -0.68409000 | 2.56802300  | -0.56522500 |
| C | -2.47771700 | 4.29663000  | 0.50752000  |
| H | -1.46647800 | 3.52683800  | 2.23493800  |
| H | -2.33090600 | 2.28195700  | 1.34157400  |
| C | -0.27808800 | 5.23362900  | -0.30171400 |
| H | 0.71856800  | 4.39020200  | 1.42835700  |
| H | 1.39751100  | 3.86194300  | -0.10928800 |
| C | -1.60762700 | 5.54982000  | 0.38637200  |
| H | -3.40281200 | 4.51891800  | 1.04784700  |
| H | -2.77027100 | 3.95888400  | -0.49653300 |
| H | 0.35965100  | 6.12160000  | -0.33022800 |
| H | -0.46750500 | 4.94600300  | -1.34535300 |
| H | -2.14125600 | 6.33081200  | -0.16268600 |
| H | -1.40783400 | 5.94633300  | 1.39051000  |
| C | 1.65483400  | -2.23259500 | 1.38123700  |
| C | 0.64480100  | -2.59567500 | 0.48542000  |
| H | 1.51597200  | -2.40293300 | 2.44438300  |
| H | 2.68170200  | -2.33380600 | 1.04781200  |
| H | 0.96371900  | -2.90846200 | -0.50552700 |
| C | -0.66222000 | -3.13766900 | 0.89632700  |
| C | -1.13723100 | -3.11524600 | 2.21769500  |
| C | -1.45944400 | -3.77722900 | -0.06785700 |
| C | -2.37219400 | -3.66517300 | 2.54562600  |
| H | -0.53275500 | -2.68286900 | 3.00673600  |
| C | -2.69195300 | -4.33272400 | 0.26022700  |
| H | -1.09066000 | -3.86312000 | -1.08989900 |
| C | -3.16481200 | -4.26655800 | 1.56924300  |
| H | -2.71377900 | -3.63095800 | 3.57539100  |
| H | -3.28145900 | -4.82308100 | -0.50882900 |
| H | -4.12659300 | -4.69586400 | 1.82867100  |
| C | 0.62061600  | -1.34064900 | -3.54903300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.20515200  | -1.65148700 | -4.42089400 |
| H  | 0.13430900  | -2.24091000 | -3.15570900 |
| H  | -0.15861800 | -0.66889200 | -3.92277900 |
| C  | 0.76200800  | 1.79379200  | -2.96098600 |
| H  | 0.86249800  | 2.76150500  | -2.46260900 |
| H  | 1.05927700  | 1.92840100  | -4.00640700 |
| H  | -0.30617500 | 1.54576300  | -2.96517500 |
| C  | 3.26630000  | 2.28920300  | -1.03233900 |
| H  | 3.27771200  | 2.45707600  | 0.05119900  |
| H  | 4.29951000  | 2.37123300  | -1.38397600 |
| H  | 2.71236100  | 3.10462600  | -1.49937600 |
| Si | 4.99884200  | -0.56191100 | -0.33258400 |
| C  | 6.19005700  | -0.60649300 | -1.78916600 |
| H  | 6.10962600  | 0.30762200  | -2.38533700 |
| H  | 7.22348300  | -0.69455100 | -1.43956700 |
| H  | 5.98407200  | -1.45479000 | -2.44884100 |
| C  | 5.52344100  | 0.83163600  | 0.82732300  |
| H  | 6.46418700  | 0.52412600  | 1.29744900  |
| H  | 5.71022000  | 1.77423700  | 0.30887000  |
| H  | 4.80523700  | 1.01662800  | 1.63183600  |
| C  | 5.21277300  | -2.15253800 | 0.66122500  |
| H  | 4.71616900  | -2.10974800 | 1.63572800  |
| H  | 4.89215800  | -3.05887300 | 0.14255800  |
| H  | 6.28519800  | -2.25752800 | 0.86057900  |

trans-ts-10-5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.05836900  | 0.25929000  | -2.04436200 |
| C  | 3.12733400  | 0.11310400  | -1.10707500 |
| C  | 3.26422300  | 1.37446100  | -0.44801900 |
| C  | 2.29595500  | 2.27411800  | -0.96472600 |
| C  | 1.53442400  | 1.57747900  | -1.94631400 |
| Sc | 1.01232900  | 0.48146100  | 0.22266800  |
| N  | -0.60192800 | -0.86142100 | -0.95984900 |
| H  | -0.38050400 | -0.62745000 | -1.92844900 |
| C  | -2.04831700 | -1.25828500 | -0.95520100 |
| C  | -2.87406800 | -0.19435300 | -1.68409100 |
| C  | -2.22825700 | -2.59161200 | -1.70507600 |
| C  | -2.54113600 | -1.41685100 | 0.48425400  |
| H  | -2.51065900 | -0.09342200 | -2.71832000 |
| H  | -2.74559800 | 0.77247700  | -1.19375100 |
| C  | -4.36165100 | -0.58829900 | -1.68787900 |
| H  | -1.62491800 | -3.36721200 | -1.22045800 |
| H  | -1.86705100 | -2.47923000 | -2.73753500 |
| C  | -3.70903500 | -3.00400800 | -1.70032400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.37519600 | -0.47680500 | 1.03032500  |
| H | -1.95956300 | -2.19701000 | 0.98703100  |
| C | -4.02895300 | -1.80500900 | 0.48357700  |
| H | -4.93393800 | 0.19330800  | -2.19985600 |
| C | -4.53482100 | -1.92736000 | -2.41783400 |
| C | -4.85694200 | -0.73288600 | -0.24066700 |
| H | -3.81433000 | -3.96191800 | -2.22053800 |
| C | -4.18698400 | -3.14757600 | -0.24692400 |
| H | -4.37173200 | -1.90576800 | 1.51899300  |
| H | -4.21020800 | -1.83592800 | -3.46164200 |
| H | -5.59384000 | -2.21011500 | -2.42908800 |
| H | -4.78673500 | 0.22818000  | 0.28266900  |
| H | -5.91538400 | -1.01829500 | -0.24124000 |
| H | -5.23686300 | -3.46261400 | -0.22908300 |
| H | -3.60068800 | -3.92011200 | 0.26668500  |
| C | -0.27633000 | 0.68497200  | 3.88969700  |
| C | 0.44534500  | 1.79816500  | 3.10904200  |
| H | -1.12584800 | 1.08638000  | 4.45102200  |
| H | -0.64876900 | -0.08967900 | 3.21131200  |
| H | 0.41172600  | 0.22774800  | 4.60855800  |
| C | 1.68010700  | 1.30549400  | 2.34752700  |
| C | 0.84545700  | 2.92272600  | 4.08453200  |
| H | 1.98495900  | 2.10255800  | 1.64768900  |
| H | 2.51307900  | 1.23583900  | 3.04729000  |
| H | -0.08491200 | -1.72952700 | -0.78757400 |
| H | 1.53434800  | 2.52639500  | 4.83497100  |
| H | 1.34799000  | 3.73924300  | 3.55669600  |
| H | -0.02757000 | 3.32968000  | 4.60545700  |
| C | -0.55647800 | 2.36175000  | 2.15041700  |
| H | -1.31151500 | 3.03202400  | 2.57578300  |
| N | -0.55910000 | 2.08836200  | 0.90308100  |
| C | -1.59322500 | 2.75376100  | 0.07058700  |
| C | -3.01604800 | 2.56688500  | 0.60924000  |
| C | -1.30701200 | 4.24816200  | -0.11232500 |
| H | -1.52780200 | 2.28467000  | -0.91718400 |
| C | -4.03580500 | 3.15297400  | -0.37058700 |
| H | -3.12016900 | 3.08966000  | 1.56789400  |
| H | -3.20730200 | 1.50793300  | 0.80347600  |
| C | -2.32286700 | 4.86443500  | -1.07923300 |
| H | -1.37416900 | 4.74577000  | 0.86564600  |
| H | -0.28929900 | 4.39493800  | -0.47857600 |
| C | -3.76014200 | 4.64000700  | -0.60576200 |
| H | -5.04830800 | 3.00356300  | 0.01627000  |
| H | -3.97837700 | 2.61617400  | -1.32812600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.11891300 | 5.93274100  | -1.19435100 |
| H  | -2.19236900 | 4.40893800  | -2.07079300 |
| H  | -4.46626700 | 5.04656000  | -1.33517700 |
| H  | -3.92034000 | 5.18655100  | 0.33290100  |
| C  | 2.19543000  | -0.80120000 | 2.13123100  |
| C  | 1.61980000  | -1.67301400 | 1.20533100  |
| H  | 1.93081100  | -0.88883400 | 3.18023000  |
| H  | 3.21770800  | -0.48297600 | 1.95625000  |
| H  | 2.21144400  | -1.90840900 | 0.32292400  |
| C  | 0.60497900  | -2.68720900 | 1.54224300  |
| C  | -0.06534900 | -2.74845100 | 2.77544700  |
| C  | 0.33153800  | -3.70025000 | 0.60792000  |
| C  | -0.99590700 | -3.74892300 | 3.03757000  |
| H  | 0.14917500  | -2.02222100 | 3.55104300  |
| C  | -0.59322900 | -4.70568300 | 0.87217000  |
| H  | 0.87377800  | -3.71191300 | -0.33741600 |
| C  | -1.27657300 | -4.72781200 | 2.08564600  |
| H  | -1.49938500 | -3.76877100 | 3.99905200  |
| H  | -0.77617900 | -5.47504600 | 0.12784900  |
| H  | -2.00096000 | -5.50767300 | 2.29423700  |
| C  | 1.66836900  | -0.73546500 | -3.10674200 |
| H  | 2.46565700  | -0.82160300 | -3.85274500 |
| H  | 1.49329000  | -1.74210400 | -2.71255500 |
| H  | 0.77273400  | -0.41515000 | -3.64989900 |
| C  | 0.44676700  | 2.15038600  | -2.81485100 |
| H  | 0.12351900  | 3.13038800  | -2.45492200 |
| H  | 0.79487900  | 2.27530800  | -3.84548400 |
| H  | -0.44432200 | 1.51050200  | -2.85300300 |
| C  | 2.21961500  | 3.73669300  | -0.61912500 |
| H  | 1.79269900  | 3.92959400  | 0.37344900  |
| H  | 3.22023700  | 4.17774400  | -0.63382200 |
| H  | 1.62268300  | 4.28255900  | -1.35231100 |
| C  | 4.34661000  | 1.76364500  | 0.52251600  |
| H  | 5.32982600  | 1.72358400  | 0.04060300  |
| H  | 4.20063600  | 2.78319700  | 0.88753200  |
| H  | 4.39293300  | 1.11128300  | 1.39905100  |
| Si | 4.48607300  | -1.20370200 | -1.15974100 |
| C  | 5.81128100  | -0.50755200 | -2.30092100 |
| H  | 6.21872800  | 0.43116000  | -1.91364100 |
| H  | 6.63871400  | -1.21518300 | -2.41139600 |
| H  | 5.40020000  | -0.30762400 | -3.29536300 |
| C  | 5.25162000  | -1.58600300 | 0.51876500  |
| H  | 6.10075600  | -2.25574600 | 0.34317900  |
| H  | 5.63547000  | -0.70544600 | 1.03887700  |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 4.55663300 | -2.11374000 | 1.17874400  |
| C | 3.89313000 | -2.85146100 | -1.86009200 |
| H | 3.04318600 | -3.27322600 | -1.31420900 |
| H | 3.63032600 | -2.79262600 | -2.91858300 |
| H | 4.71777300 | -3.56618200 | -1.76636000 |

cis-ts-10'-2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.22835500  | -1.93364400 | 1.33599200  |
| C  | 1.01946300  | -1.77071100 | 2.05521800  |
| C  | 0.99954900  | -0.44665800 | 2.58602100  |
| C  | 2.19217000  | 0.20396300  | 2.18723100  |
| C  | 2.97167900  | -0.70355000 | 1.39886700  |
| Sc | 0.92181900  | -0.26845300 | 0.03572700  |
| C  | 2.61449800  | 1.56062100  | 2.68020000  |
| H  | 1.75196400  | 2.20687500  | 2.86927000  |
| H  | 3.16586600  | 1.47277900  | 3.62353500  |
| H  | 3.26659800  | 2.07550000  | 1.97085800  |
| C  | 0.05010800  | 0.02622800  | 3.65156000  |
| H  | -0.98093100 | -0.29433600 | 3.48074600  |
| H  | 0.35675000  | -0.38755700 | 4.61924500  |
| H  | 0.05004600  | 1.11398500  | 3.75642300  |
| C  | 0.02291700  | -2.83563300 | 2.41962600  |
| H  | 0.09137300  | -3.70729200 | 1.76652400  |
| H  | 0.19774900  | -3.17852200 | 3.44583100  |
| H  | -1.01011900 | -2.47204900 | 2.38528600  |
| C  | 0.74036700  | -0.03341500 | -3.98972300 |
| C  | 1.42934900  | -1.04502000 | -3.05477200 |
| H  | 0.23696500  | -0.54339100 | -4.81656300 |
| H  | -0.00364900 | 0.56622700  | -3.45562400 |
| H  | 1.48746800  | 0.64189700  | -4.41877100 |
| C  | 2.20925800  | -0.36628500 | -1.91927700 |
| C  | 2.39685800  | -1.91209500 | -3.89067300 |
| H  | 2.58923100  | -1.15426700 | -1.23766100 |
| H  | 3.11838500  | 0.02638600  | -2.36349200 |
| H  | 3.16379000  | -1.27367700 | -4.33710000 |
| H  | 2.89570400  | -2.65820800 | -3.26350900 |
| H  | 1.87325000  | -2.43142800 | -4.70023300 |
| C  | 0.36788100  | -1.96352400 | -2.53362100 |
| H  | -0.07895200 | -2.64826300 | -3.26419500 |
| N  | -0.01411300 | -1.96849100 | -1.31608300 |
| C  | -1.04563100 | -2.95974900 | -0.92132400 |
| C  | -2.28650400 | -2.99725700 | -1.82502700 |
| C  | -0.44438600 | -4.36819900 | -0.83180600 |
| H  | -1.37027100 | -2.67629800 | 0.08978000  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.32675600 | -3.95445400 | -1.23566400 |
| H | -2.00774700 | -3.35430400 | -2.82401700 |
| H | -2.71719800 | -2.00006800 | -1.95195900 |
| C | -1.46766800 | -5.35414700 | -0.26219000 |
| H | -0.14779700 | -4.67840300 | -1.84367700 |
| H | 0.46393600  | -4.35325900 | -0.22574900 |
| C | -2.75269800 | -5.36531800 | -1.09173200 |
| H | -4.21916800 | -3.96227400 | -1.86769100 |
| H | -3.63960300 | -3.58426300 | -0.24838800 |
| H | -1.02913800 | -6.35500800 | -0.21734900 |
| H | -1.70535100 | -5.06588100 | 0.77144200  |
| H | -3.49148500 | -6.03154300 | -0.63736900 |
| H | -2.53444800 | -5.76535100 | -2.09051300 |
| C | 1.92646000  | 1.73393000  | -1.37536000 |
| C | 1.04245900  | 1.98051600  | -0.30312500 |
| H | 1.54031100  | 1.86150300  | -2.38505200 |
| H | 1.45805700  | 2.40335200  | 0.60640300  |
| H | 0.03758100  | 2.31150800  | -0.54472300 |
| C | 3.37506700  | 2.13671900  | -1.19670300 |
| C | 3.64288000  | 3.62391900  | -1.51144300 |
| H | 4.04747900  | 1.55222400  | -1.82873700 |
| H | 3.65612800  | 1.93184200  | -0.15851400 |
| C | 2.87461200  | 4.64522200  | -0.66266700 |
| H | 4.72030800  | 3.76845300  | -1.37728500 |
| H | 3.44257800  | 3.80866700  | -2.57505400 |
| H | 2.72041100  | 4.23833700  | 0.34590000  |
| H | 3.49107600  | 5.54087300  | -0.52871500 |
| C | 1.52898800  | 5.06663800  | -1.26283100 |
| C | 0.57078600  | 5.65467800  | -0.23103500 |
| H | 1.04426100  | 4.20710700  | -1.74073800 |
| H | 1.70444600  | 5.79768100  | -2.06291600 |
| C | -0.77577300 | 6.04154900  | -0.83449000 |
| H | 0.41940900  | 4.91411700  | 0.56692900  |
| H | 1.03441900  | 6.52765700  | 0.24454700  |
| H | -1.45362300 | 6.45350800  | -0.08277500 |
| H | -0.65213000 | 6.79088900  | -1.62208300 |
| H | -1.26210900 | 5.16800300  | -1.28467900 |
| N | -1.41756000 | 0.24092400  | 0.10672100  |
| H | -1.87097200 | -0.62960800 | 0.39379100  |
| C | -1.97872700 | 0.59372200  | -1.23079500 |
| H | -1.41988300 | 1.45942900  | -1.60092500 |
| H | -1.75833600 | -0.23630200 | -1.90420300 |
| C | -1.77859300 | 1.27303400  | 1.12664500  |
| H | -0.96918000 | 1.31938300  | 1.85908300  |

|                           |             |             |             |
|---------------------------|-------------|-------------|-------------|
| H                         | -1.80438200 | 2.24390000  | 0.62225300  |
| C                         | -3.10794200 | 1.03269700  | 1.81037000  |
| C                         | -4.04444100 | 2.06262900  | 1.89718600  |
| C                         | -3.43187500 | -0.21732700 | 2.34490700  |
| C                         | -5.28378100 | 1.84586600  | 2.49225200  |
| H                         | -3.81361900 | 3.03379300  | 1.46761800  |
| C                         | -4.67151600 | -0.43986900 | 2.93685300  |
| H                         | -2.72048100 | -1.04077600 | 2.29283000  |
| C                         | -5.60280300 | 0.59296900  | 3.00886700  |
| H                         | -6.00635800 | 2.65413100  | 2.53905400  |
| H                         | -4.90791300 | -1.41791900 | 3.34334000  |
| H                         | -6.57161200 | 0.42211700  | 3.46624500  |
| C                         | -3.45462200 | 0.92287800  | -1.23381900 |
| C                         | -4.40817400 | -0.02754100 | -0.85410300 |
| C                         | -3.87834100 | 2.20756300  | -1.57037800 |
| C                         | -5.75505500 | 0.30749600  | -0.79631300 |
| H                         | -4.09979500 | -1.02973400 | -0.56197900 |
| C                         | -5.23041400 | 2.54470400  | -1.52501400 |
| H                         | -3.14461300 | 2.95542200  | -1.86362200 |
| C                         | -6.16908400 | 1.59665800  | -1.13309700 |
| H                         | -6.48232700 | -0.43354400 | -0.48108200 |
| H                         | -5.54561100 | 3.54876100  | -1.78920400 |
| H                         | -7.22107700 | 1.85819900  | -1.08716900 |
| C                         | 2.68778200  | -3.20741100 | 0.67205300  |
| H                         | 2.45799000  | -3.24298900 | -0.40078000 |
| H                         | 3.76768700  | -3.33453300 | 0.77042500  |
| H                         | 2.22110600  | -4.07932000 | 1.13794200  |
| Si                        | 4.84264700  | -0.65515300 | 1.11525000  |
| C                         | 5.58042500  | -1.85488000 | 2.37468200  |
| H                         | 6.67281100  | -1.84914300 | 2.29810300  |
| H                         | 5.31541200  | -1.53211900 | 3.38677900  |
| H                         | 5.24284100  | -2.88741000 | 2.25866200  |
| C                         | 5.67743900  | 0.98986100  | 1.50678500  |
| H                         | 5.49730400  | 1.29628800  | 2.54079200  |
| H                         | 6.75525900  | 0.82040900  | 1.40243100  |
| H                         | 5.41694400  | 1.82102100  | 0.84819700  |
| C                         | 5.35779900  | -1.18054200 | -0.62212700 |
| H                         | 4.84351800  | -2.08142900 | -0.97021100 |
| H                         | 5.18356600  | -0.38715900 | -1.35406100 |
| H                         | 6.43217100  | -1.39296900 | -0.61735600 |
| cis-ts-10 <sup>1</sup> -3 |             |             |             |
| C                         | 2.07631600  | -2.66667000 | 1.43608100  |
| C                         | 0.90460200  | -2.29251700 | 2.15153600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.06988500  | -0.95721200 | 2.59239500  |
| C  | 2.32889800  | -0.46406400 | 2.12686300  |
| C  | 2.94877300  | -1.54542000 | 1.41189900  |
| Sc | 1.06003600  | -0.88729500 | 0.02537900  |
| C  | 0.17361300  | -0.32507500 | 3.62372900  |
| H  | -0.88948200 | -0.45518200 | 3.40133700  |
| H  | 0.35381000  | -0.79526100 | 4.59764400  |
| H  | 0.35816100  | 0.74421400  | 3.74399400  |
| C  | -0.18680000 | -3.21397400 | 2.61640400  |
| H  | -0.26506400 | -4.10428100 | 1.98956200  |
| H  | 0.02126100  | -3.55451600 | 3.63763900  |
| H  | -1.16672100 | -2.72459900 | 2.64068700  |
| C  | 0.97495900  | -1.62321400 | -4.17456600 |
| C  | 1.29738400  | -2.42936800 | -2.90220500 |
| H  | 0.40550300  | -2.23537400 | -4.88040900 |
| H  | 0.38665100  | -0.72701400 | -3.95988500 |
| H  | 1.90128100  | -1.32028700 | -4.67073300 |
| C  | 2.16726600  | -1.67998100 | -1.89066100 |
| C  | 2.00234700  | -3.73862200 | -3.32494900 |
| H  | 2.27180600  | -2.35271900 | -1.01576500 |
| H  | 3.19022300  | -1.61555600 | -2.25759600 |
| H  | 2.93620000  | -3.49448100 | -3.83862700 |
| H  | 2.24100300  | -4.35733700 | -2.45388300 |
| H  | 1.38164200  | -4.32583500 | -4.00963400 |
| C  | 0.00018100  | -2.82099000 | -2.26502600 |
| H  | -0.65575700 | -3.47784100 | -2.85038200 |
| N  | -0.33238600 | -2.44014600 | -1.09261100 |
| C  | -1.61087300 | -2.93772900 | -0.54133900 |
| C  | -2.83097100 | -2.48707700 | -1.35205700 |
| C  | -1.63865500 | -4.46307200 | -0.39116700 |
| H  | -1.69025200 | -2.50866800 | 0.46782900  |
| C  | -4.11765400 | -2.88260900 | -0.62368900 |
| H  | -2.80267700 | -2.96595500 | -2.33957800 |
| H  | -2.80063100 | -1.40877900 | -1.53300200 |
| C  | -2.90996400 | -4.88427000 | 0.35056000  |
| H  | -1.62712400 | -4.92123200 | -1.38944900 |
| H  | -0.74205500 | -4.81264700 | 0.12917800  |
| C  | -4.16451800 | -4.39311100 | -0.37720800 |
| H  | -4.98744600 | -2.56093800 | -1.20404300 |
| H  | -4.16232700 | -2.34965600 | 0.33739900  |
| H  | -2.93373000 | -5.97210200 | 0.45888100  |
| H  | -2.88464000 | -4.46508600 | 1.36599400  |
| H  | -5.05941200 | -4.65497100 | 0.19416800  |
| H  | -4.24238200 | -4.90784600 | -1.34360100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.09614500  | 0.50884100  | -1.93287900 |
| C | 1.99620100  | 1.07224100  | -0.63838500 |
| H | 1.19476600  | 0.54360000  | -2.54621900 |
| H | 2.92279300  | 1.36076600  | -0.15171000 |
| H | 1.15261900  | 1.72116800  | -0.41516800 |
| C | 3.35798700  | 0.68713600  | -2.75306900 |
| C | 3.40175100  | 2.04849400  | -3.47550500 |
| H | 3.44613700  | -0.08827300 | -3.51776300 |
| H | 4.22946100  | 0.59582200  | -2.09062700 |
| C | 3.40331700  | 3.28585600  | -2.56654100 |
| H | 4.30771900  | 2.03680200  | -4.08943500 |
| H | 2.56074700  | 2.10715500  | -4.17989800 |
| H | 3.84877900  | 3.01997200  | -1.59874900 |
| H | 4.05566600  | 4.05477200  | -2.99446000 |
| C | 2.01905600  | 3.89882900  | -2.33406700 |
| C | 1.98047500  | 4.81352900  | -1.11261300 |
| H | 1.27636100  | 3.10086900  | -2.20467600 |
| H | 1.70978700  | 4.45567700  | -3.22831400 |
| C | 0.57395000  | 5.29610200  | -0.77373500 |
| H | 2.39592200  | 4.26861400  | -0.25375300 |
| H | 2.64349500  | 5.67102500  | -1.27950200 |
| H | 0.57432200  | 5.97962700  | 0.07889500  |
| H | 0.11620500  | 5.81496700  | -1.62260800 |
| H | -0.07320900 | 4.44747400  | -0.51826500 |
| N | -0.98610300 | 0.33548400  | -0.06648700 |
| H | -1.71338500 | -0.35028400 | 0.15116600  |
| C | -1.31235200 | 0.89167100  | -1.41315600 |
| H | -0.47809400 | 1.53625400  | -1.70584100 |
| H | -1.33550200 | 0.04940500  | -2.11444800 |
| C | -1.05688200 | 1.39174000  | 0.98966900  |
| H | -0.32622200 | 1.14174200  | 1.76192600  |
| H | -0.73038300 | 2.33545300  | 0.54025900  |
| C | -2.43229100 | 1.56357300  | 1.59358300  |
| C | -3.02341900 | 2.82467000  | 1.65329300  |
| C | -3.14219200 | 0.45829500  | 2.07260600  |
| C | -4.30981600 | 2.97772400  | 2.16248900  |
| H | -2.48828200 | 3.68664100  | 1.26321300  |
| C | -4.43145800 | 0.60698400  | 2.57597700  |
| H | -2.69627000 | -0.53708400 | 2.04673200  |
| C | -5.01896300 | 1.86929900  | 2.61834400  |
| H | -4.76398000 | 3.96290200  | 2.18841800  |
| H | -4.97407400 | -0.26046500 | 2.93798500  |
| H | -6.02439800 | 1.98780900  | 3.00814400  |
| C | -2.58287100 | 1.71212700  | -1.48384000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.83318500 | 1.17759600  | -1.15586400 |
| C  | -2.49773500 | 3.05637700  | -1.84516600 |
| C  | -4.96802600 | 1.97868000  | -1.17003600 |
| H  | -3.92672600 | 0.14176500  | -0.84002300 |
| C  | -3.63593500 | 3.86182200  | -1.86844700 |
| H  | -1.53079800 | 3.48046700  | -2.10758400 |
| C  | -4.87137100 | 3.32435100  | -1.52512900 |
| H  | -5.92839500 | 1.55583200  | -0.89377100 |
| H  | -3.55219800 | 4.90678900  | -2.14869500 |
| H  | -5.75846400 | 3.94900400  | -1.53152500 |
| C  | 2.32738400  | -4.04174100 | 0.87860100  |
| H  | 1.51841100  | -4.36863100 | 0.21413900  |
| H  | 3.25961500  | -4.08709000 | 0.31064100  |
| H  | 2.40326300  | -4.77667400 | 1.68666700  |
| C  | 4.29758200  | -1.50353500 | 0.74253400  |
| H  | 5.10596300  | -1.56689600 | 1.47812100  |
| H  | 4.42859900  | -2.33594900 | 0.04640800  |
| H  | 4.44241500  | -0.57551600 | 0.17906000  |
| Si | 3.11469400  | 1.13795300  | 2.74285500  |
| C  | 3.41001000  | 0.92981200  | 4.59156000  |
| H  | 3.86524200  | 1.83205100  | 5.01233500  |
| H  | 2.47982800  | 0.73837700  | 5.13423200  |
| H  | 4.08655100  | 0.09075000  | 4.78053300  |
| C  | 4.78730800  | 1.50954400  | 1.95559100  |
| H  | 5.16720900  | 2.42652300  | 2.41955300  |
| H  | 5.51665100  | 0.71894300  | 2.14991700  |
| H  | 4.75321200  | 1.68391100  | 0.87612900  |
| C  | 2.01964800  | 2.65814600  | 2.48396300  |
| H  | 1.70623700  | 2.78139400  | 1.44338500  |
| H  | 1.12368100  | 2.65513600  | 3.11147400  |
| H  | 2.59917200  | 3.54670500  | 2.75845100  |

cis-ts-10'-4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.96157000  | -1.83968100 | 1.27337500  |
| C  | 1.81661500  | -1.56068100 | 2.06420600  |
| C  | 1.84688900  | -0.17348500 | 2.44057600  |
| C  | 3.04418800  | 0.37512100  | 1.87216200  |
| C  | 3.71342900  | -0.63582700 | 1.15035000  |
| Sc | 1.50964200  | -0.26585400 | -0.02817400 |
| C  | 0.81656900  | -2.58945500 | 2.52389800  |
| H  | 0.80407800  | -3.46166400 | 1.86397600  |
| H  | 1.06143500  | -2.94824000 | 3.52997000  |
| H  | -0.19951200 | -2.18603300 | 2.57202900  |
| C  | 1.62917800  | -0.38753700 | -4.25701000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.27034700  | -1.17827600 | -3.10051300 |
| H | 1.36122800  | -1.05687300 | -5.07980100 |
| H | 0.72311200  | 0.14129900  | -3.94919100 |
| H | 2.34295600  | 0.34592500  | -4.64374000 |
| C | 2.80264400  | -0.29927600 | -1.96645700 |
| C | 3.42103900  | -2.03083200 | -3.68190400 |
| H | 3.18932800  | -1.00714500 | -1.20536000 |
| H | 3.70713300  | 0.21388300  | -2.28658600 |
| H | 4.16573800  | -1.36946600 | -4.13318700 |
| H | 3.91439900  | -2.61542900 | -2.89878400 |
| H | 3.06227900  | -2.71734100 | -4.45580500 |
| C | 1.24207800  | -2.12967900 | -2.56781400 |
| H | 0.87982300  | -2.89804900 | -3.26181400 |
| N | 0.80198800  | -2.07030800 | -1.36987900 |
| C | -0.20504600 | -3.07243100 | -0.95073400 |
| C | -1.42994000 | -3.11815700 | -1.87169400 |
| C | 0.38150300  | -4.47935100 | -0.80172800 |
| H | -0.53816600 | -2.76580000 | 0.05165600  |
| C | -2.50215400 | -4.03139500 | -1.27452600 |
| H | -1.13345700 | -3.51289800 | -2.85160300 |
| H | -1.81950900 | -2.11086500 | -2.04925300 |
| C | -0.67462400 | -5.42247800 | -0.21602100 |
| H | 0.70044800  | -4.83690500 | -1.79040700 |
| H | 1.27013800  | -4.45181100 | -0.16702400 |
| C | -1.94811300 | -5.44327900 | -1.06491200 |
| H | -3.37834800 | -4.05296500 | -1.92915000 |
| H | -2.83664300 | -3.61949500 | -0.31060700 |
| H | -0.25870300 | -6.42955400 | -0.12448900 |
| H | -0.92205200 | -5.08906300 | 0.80196700  |
| H | -2.70301500 | -6.08135500 | -0.59679800 |
| H | -1.72122700 | -5.88469000 | -2.04412000 |
| C | 1.88602100  | 1.71468000  | -1.69345000 |
| C | 1.50528600  | 1.98521800  | -0.36526100 |
| H | 1.08540500  | 1.48057800  | -2.39588000 |
| H | 2.19230700  | 2.54843300  | 0.25668900  |
| H | 0.45352800  | 2.14360000  | -0.14042200 |
| C | 3.01989000  | 2.48784800  | -2.33185400 |
| C | 2.55424300  | 3.85962800  | -2.86424100 |
| H | 3.45125100  | 1.94449800  | -3.17613000 |
| H | 3.81603600  | 2.63021000  | -1.58907500 |
| C | 1.95441800  | 4.81511700  | -1.82260100 |
| H | 3.43258900  | 4.31839900  | -3.32918400 |
| H | 1.83161400  | 3.70060400  | -3.67610900 |
| H | 2.39555500  | 4.60143800  | -0.84086800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.24263400  | 5.84421300  | -2.06246400 |
| C | 0.42580500  | 4.75387400  | -1.71704200 |
| C | -0.09601400 | 5.30691400  | -0.39343400 |
| H | 0.08244600  | 3.71696900  | -1.83060100 |
| H | -0.01972400 | 5.30907000  | -2.55305800 |
| C | -1.60941400 | 5.18187900  | -0.24922000 |
| H | 0.39582300  | 4.77066900  | 0.43012500  |
| H | 0.20454100  | 6.35733600  | -0.29679900 |
| H | -1.96467500 | 5.62397600  | 0.68499200  |
| H | -2.12818400 | 5.67830600  | -1.07574900 |
| H | -1.91392200 | 4.12819400  | -0.25479400 |
| N | -0.92022300 | 0.00492900  | -0.13655700 |
| H | -1.29181100 | -0.94580300 | -0.08480100 |
| C | -1.37078300 | 0.57005800  | -1.43839000 |
| H | -0.88886900 | 1.54612200  | -1.55226900 |
| H | -0.96571500 | -0.08444800 | -2.22031200 |
| C | -1.47080500 | 0.73833500  | 1.04054800  |
| H | -0.79658100 | 0.53458100  | 1.87488100  |
| H | -1.41162600 | 1.81133700  | 0.83030000  |
| C | -2.87920200 | 0.35974400  | 1.43639100  |
| C | -3.89791500 | 1.31116200  | 1.46184600  |
| C | -3.17524900 | -0.96357500 | 1.77703100  |
| C | -5.19948700 | 0.94042800  | 1.78737100  |
| H | -3.67742300 | 2.34083500  | 1.19196100  |
| C | -4.47672600 | -1.33902600 | 2.09598700  |
| H | -2.38459900 | -1.71465800 | 1.79547100  |
| C | -5.49298000 | -0.38581800 | 2.09560000  |
| H | -5.98762800 | 1.68639200  | 1.78754300  |
| H | -4.69545900 | -2.37045200 | 2.35318700  |
| H | -6.50908800 | -0.67499100 | 2.34263800  |
| C | -2.86239800 | 0.76412500  | -1.61796300 |
| C | -3.77770800 | -0.27995700 | -1.44806100 |
| C | -3.34056400 | 2.02902500  | -1.95908500 |
| C | -5.14070400 | -0.05460900 | -1.59135300 |
| H | -3.43941000 | -1.26807100 | -1.14861800 |
| C | -4.70756200 | 2.25748100  | -2.11203000 |
| H | -2.63761000 | 2.84645600  | -2.10316600 |
| C | -5.60966800 | 1.21676100  | -1.92267300 |
| H | -5.84006700 | -0.86923000 | -1.43445500 |
| H | -5.06274000 | 3.24897900  | -2.37305700 |
| H | -6.67497000 | 1.39209300  | -2.03080300 |
| C | 3.41647700  | -3.17271600 | 0.74289700  |
| H | 3.28893200  | -3.27506300 | -0.34295700 |
| H | 4.47903600  | -3.31786800 | 0.95911300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 2.87697000  | -3.99344300 | 1.22063000  |
| C  | 5.04945100  | -0.49841600 | 0.47660100  |
| H  | 5.86115700  | -0.57515500 | 1.20821300  |
| H  | 5.20718600  | -1.28068400 | -0.27206300 |
| H  | 5.15349900  | 0.46835700  | -0.02694000 |
| C  | 3.63248100  | 1.73302700  | 2.13516400  |
| H  | 4.39126800  | 1.66529800  | 2.92313700  |
| H  | 4.13030200  | 2.13877700  | 1.24853600  |
| H  | 2.88180000  | 2.45789000  | 2.46064200  |
| Si | 0.94598700  | 0.70730100  | 3.84812500  |
| C  | 2.17938600  | 0.89981900  | 5.25689700  |
| H  | 1.69984600  | 1.38339700  | 6.11412700  |
| H  | 2.55263700  | -0.07550800 | 5.58315800  |
| H  | 3.03811900  | 1.51055400  | 4.96518400  |
| C  | 0.34020100  | 2.42620600  | 3.30998600  |
| H  | -0.74289400 | 2.51725000  | 3.44580900  |
| H  | 0.81492800  | 3.20655700  | 3.91276300  |
| H  | 0.56491500  | 2.63485000  | 2.25897400  |
| C  | -0.51350000 | -0.27598500 | 4.52305600  |
| H  | -1.32486300 | -0.43764400 | 3.80656800  |
| H  | -0.19796000 | -1.24823300 | 4.91167500  |
| H  | -0.93353200 | 0.29080000  | 5.36150400  |

cis-ts-10'-5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.77193400 | -3.21394800 | -1.00943700 |
| C  | 0.28145900  | -2.44186800 | -1.60191100 |
| C  | -0.36603300 | -1.47188400 | -2.44730900 |
| C  | -1.76792200 | -1.64795600 | -2.36866300 |
| C  | -2.02087400 | -2.72627500 | -1.47397200 |
| Sc | -0.99860100 | -0.90219800 | -0.05473400 |
| C  | -2.35612800 | -0.13679400 | 3.71524400  |
| C  | -1.87686600 | -1.43024100 | 3.03019400  |
| H  | -1.95090200 | -0.06475900 | 4.72891000  |
| H  | -2.04169200 | 0.75350900  | 3.16050500  |
| H  | -3.44809100 | -0.13597900 | 3.79123800  |
| C  | -2.46103600 | -1.64809800 | 1.62765800  |
| C  | -2.24685100 | -2.63014500 | 3.93003800  |
| H  | -1.94838100 | -2.52968100 | 1.19264400  |
| H  | -3.48882600 | -1.98370000 | 1.74421400  |
| H  | -3.33352700 | -2.68115700 | 4.03877600  |
| H  | -1.90160600 | -3.57066800 | 3.48896500  |
| H  | -1.80886100 | -2.53220600 | 4.92881700  |
| C  | -0.38264700 | -1.37042800 | 2.98418200  |
| H  | 0.13439900  | -1.43873300 | 3.94752700  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.27338800  | -1.25223100 | 1.89655900  |
| C | 1.75308900  | -1.30650500 | 1.96065200  |
| C | 2.42339300  | -0.57011000 | 3.12716900  |
| C | 2.17038300  | -2.77900000 | 1.95183800  |
| H | 2.11304900  | -0.85268800 | 1.02679400  |
| C | 3.94632700  | -0.70190900 | 3.00742600  |
| H | 2.11859200  | -1.01372300 | 4.08232500  |
| H | 2.13383800  | 0.48642100  | 3.14959200  |
| C | 3.68891600  | -2.94778400 | 1.89561200  |
| H | 1.77351700  | -3.24610000 | 2.86500100  |
| H | 1.68634100  | -3.26607000 | 1.10282100  |
| C | 4.37459100  | -2.17035500 | 3.02025600  |
| H | 4.42446100  | -0.15240500 | 3.82284900  |
| H | 4.28205700  | -0.23378400 | 2.07127800  |
| H | 3.94041300  | -4.01156500 | 1.95324300  |
| H | 4.05833300  | -2.59072300 | 0.92578700  |
| H | 5.46135700  | -2.24975100 | 2.92701400  |
| H | 4.10345100  | -2.61419900 | 3.98718500  |
| C | -3.39961600 | 0.04857200  | 0.60875600  |
| C | -2.58031200 | 0.72386000  | -0.31853100 |
| H | -3.46195100 | 0.46786600  | 1.60871300  |
| H | -2.88468300 | 0.73408400  | -1.36085700 |
| H | -2.08422500 | 1.62616300  | 0.02797900  |
| C | -4.70631700 | -0.55104800 | 0.13339000  |
| C | -5.86554000 | 0.46173200  | 0.24105200  |
| H | -4.98827200 | -1.44018900 | 0.70252200  |
| H | -4.60228600 | -0.85892000 | -0.91171700 |
| C | -5.69411400 | 1.74355700  | -0.58649800 |
| H | -6.76815200 | -0.06928200 | -0.07730700 |
| H | -6.02154000 | 0.72213500  | 1.29647900  |
| H | -5.09659300 | 1.51643100  | -1.47984900 |
| H | -6.67089400 | 2.07407300  | -0.95615300 |
| C | -5.05066800 | 2.90377500  | 0.17868500  |
| C | -4.52483300 | 4.00254100  | -0.74027200 |
| H | -4.22211800 | 2.53686000  | 0.79635300  |
| H | -5.78508000 | 3.32504500  | 0.87779400  |
| C | -3.85801400 | 5.14205400  | 0.02472300  |
| H | -3.80530900 | 3.55799800  | -1.44192700 |
| H | -5.34760000 | 4.39296500  | -1.35176100 |
| H | -3.49220600 | 5.92139800  | -0.64842500 |
| H | -4.55761000 | 5.60523300  | 0.72704700  |
| H | -3.00477000 | 4.77195100  | 0.60559600  |
| N | 0.42648500  | 1.02981100  | -0.09555000 |
| H | 1.35993900  | 0.62378100  | -0.20069300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.41077200  | 1.78690800  | 1.18806900  |
| H | -0.58893200 | 2.22150100  | 1.29532200  |
| H | 0.52906600  | 1.06527800  | 1.99698700  |
| C | 0.23699900  | 1.95348500  | -1.25556000 |
| H | -0.22708400 | 1.37997700  | -2.06089800 |
| H | -0.48481100 | 2.71899200  | -0.95374900 |
| C | 1.51070500  | 2.61519200  | -1.73764200 |
| C | 1.59716600  | 4.00153800  | -1.85597000 |
| C | 2.62972800  | 1.84178000  | -2.05109200 |
| C | 2.78330400  | 4.60274200  | -2.26970200 |
| H | 0.74022500  | 4.61676400  | -1.59493800 |
| C | 3.81784700  | 2.43631100  | -2.46167600 |
| H | 2.58607300  | 0.76067400  | -1.95321300 |
| C | 3.89692600  | 3.82259400  | -2.57094000 |
| H | 2.84015600  | 5.68380800  | -2.34468800 |
| H | 4.67865900  | 1.81782700  | -2.69615600 |
| H | 4.82206600  | 4.29263800  | -2.88787400 |
| C | 1.44619700  | 2.87989100  | 1.30412500  |
| C | 2.80604800  | 2.57620500  | 1.19591000  |
| C | 1.05802300  | 4.20385200  | 1.49674300  |
| C | 3.76041800  | 3.58389000  | 1.25072900  |
| H | 3.12230600  | 1.54560100  | 1.03262000  |
| C | 2.01312400  | 5.21669500  | 1.56736900  |
| H | 0.00103500  | 4.44696100  | 1.57906800  |
| C | 3.36300100  | 4.90841000  | 1.43664600  |
| H | 4.81257000  | 3.34030900  | 1.14643700  |
| H | 1.70049100  | 6.24530800  | 1.71440800  |
| H | 4.10759300  | 5.69645100  | 1.48026800  |
| C | -0.66055300 | -4.44915800 | -0.15542800 |
| H | -1.51782700 | -4.54547100 | 0.51932800  |
| H | -0.65425600 | -5.34720300 | -0.78432000 |
| H | 0.24641000  | -4.46907300 | 0.44953500  |
| C | -3.34397600 | -3.38852500 | -1.20465500 |
| H | -3.31677100 | -4.42861400 | -1.54606300 |
| H | -3.60662000 | -3.40771400 | -0.14078300 |
| H | -4.15556700 | -2.89209600 | -1.73952200 |
| C | -2.76575300 | -0.96045800 | -3.25596800 |
| H | -2.84440300 | -1.48618400 | -4.21408600 |
| H | -3.76680500 | -0.93079400 | -2.81916600 |
| H | -2.47114100 | 0.06971400  | -3.47749100 |
| C | 0.29781100  | -0.62957700 | -3.50284600 |
| H | 1.32212400  | -0.35315900 | -3.24108700 |
| H | 0.33977700  | -1.18887600 | -4.44395800 |
| H | -0.25340600 | 0.28912400  | -3.71828900 |

|    |            |             |             |
|----|------------|-------------|-------------|
| Si | 2.04245600 | -3.03799500 | -1.96502300 |
| C  | 2.10829400 | -3.43708200 | -3.80885400 |
| H  | 2.12712100 | -2.54317000 | -4.43649500 |
| H  | 3.01416400 | -4.01255400 | -4.02587100 |
| H  | 1.24705800 | -4.04396600 | -4.10550500 |
| C  | 3.40248400 | -1.75948900 | -1.63729300 |
| H  | 4.36095600 | -2.27556100 | -1.51531700 |
| H  | 3.50888600 | -1.09118900 | -2.49814700 |
| H  | 3.24716300 | -1.14438200 | -0.74490500 |
| C  | 2.48129300 | -4.67014500 | -1.12799900 |
| H  | 2.58859800 | -4.65001600 | -0.04279600 |
| H  | 1.75224000 | -5.44366700 | -1.38641700 |
| H  | 3.44557200 | -4.98263400 | -1.54434900 |

trans-ts-10<sup>1</sup>-2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.98708300 | -1.40629500 | -1.12816200 |
| C  | -1.83680300 | -1.86218500 | -1.81461000 |
| C  | -1.33932600 | -0.78333500 | -2.60330400 |
| C  | -2.19190400 | 0.32768300  | -2.41722600 |
| C  | -3.21298800 | -0.02696800 | -1.47281000 |
| Sc | -1.16023500 | -0.03607300 | -0.13398200 |
| C  | -2.10778100 | 1.57558900  | -3.25132500 |
| H  | -1.07014600 | 1.85283700  | -3.46161500 |
| H  | -2.60322500 | 1.41631700  | -4.21603100 |
| H  | -2.58980200 | 2.42888700  | -2.77572300 |
| C  | -0.29782500 | -0.93153300 | -3.67757400 |
| H  | 0.58666100  | -1.48276300 | -3.34591100 |
| H  | -0.71977900 | -1.48486200 | -4.52470300 |
| H  | 0.03760700  | 0.03433000  | -4.06248200 |
| C  | -1.36411700 | -3.27965900 | -1.98226900 |
| H  | -1.70031200 | -3.93756100 | -1.17976900 |
| H  | -1.75729400 | -3.68406100 | -2.92229500 |
| H  | -0.27273900 | -3.35260700 | -2.04520800 |
| C  | -0.90488500 | 0.46991100  | 4.04828100  |
| C  | -1.85198500 | -0.24385800 | 3.06535300  |
| H  | -0.59886200 | -0.21298400 | 4.84750600  |
| H  | -0.00613500 | 0.84169100  | 3.54911800  |
| H  | -1.41632500 | 1.31389300  | 4.51794200  |
| C  | -2.29895800 | 0.62241900  | 1.87115400  |
| C  | -3.10720700 | -0.69240200 | 3.85066000  |
| H  | -2.99234400 | 0.00996500  | 1.25928400  |
| H  | -2.96131800 | 1.38140400  | 2.28587700  |
| H  | -3.63518700 | 0.18986500  | 4.22231100  |
| H  | -3.79415000 | -1.25783300 | 3.21271900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.83966100 | -1.31535300 | 4.71041000  |
| C | -1.15276100 | -1.49109100 | 2.63256100  |
| H | -0.95901300 | -2.23247800 | 3.41785800  |
| N | -0.78848500 | -1.70842500 | 1.42997200  |
| C | -0.11629800 | -2.99498700 | 1.13584400  |
| C | 1.20770300  | -3.17006700 | 1.88873300  |
| C | -1.02626600 | -4.19885800 | 1.40574300  |
| H | 0.10675600  | -2.97813900 | 0.06147000  |
| C | 1.90861500  | -4.45109100 | 1.43090700  |
| H | 1.00939500  | -3.22619800 | 2.96722200  |
| H | 1.85770700  | -2.30463400 | 1.73544200  |
| C | -0.34093900 | -5.49328600 | 0.95792300  |
| H | -1.23308000 | -4.25082700 | 2.48316600  |
| H | -1.98993600 | -4.06047400 | 0.90606400  |
| C | 1.01256600  | -5.67144500 | 1.64893000  |
| H | 2.85557500  | -4.56569500 | 1.96633900  |
| H | 2.15630200  | -4.36064800 | 0.36281800  |
| H | -0.99291600 | -6.34645300 | 1.16473800  |
| H | -0.18984800 | -5.46437200 | -0.12978400 |
| H | 1.50717700  | -6.57550500 | 1.28286700  |
| H | 0.85319200  | -5.80909500 | 2.72638000  |
| C | -1.50963100 | 2.39058100  | 0.89217200  |
| C | -0.75369000 | 2.20047000  | -0.28696800 |
| H | -2.55825000 | 2.64203400  | 0.72705300  |
| H | -1.21922100 | 2.48230500  | -1.22369600 |
| H | 0.31187700  | 2.40522100  | -0.22933800 |
| C | -0.91119900 | 3.09866200  | 2.08628800  |
| C | -0.93421400 | 4.62898600  | 1.90029500  |
| H | 0.11880800  | 2.76161400  | 2.25019400  |
| H | -1.47263400 | 2.86878200  | 2.99386500  |
| C | -0.08020900 | 5.19934800  | 0.76517400  |
| H | -1.97520100 | 4.94707400  | 1.76254700  |
| H | -0.60165500 | 5.07041600  | 2.84757300  |
| H | -0.46670600 | 4.86314900  | -0.20413300 |
| H | -0.18894600 | 6.29084300  | 0.77623600  |
| C | 1.40648900  | 4.85885300  | 0.85395100  |
| C | 2.22965000  | 5.53615600  | -0.24067600 |
| H | 1.54650800  | 3.77115000  | 0.77618000  |
| H | 1.79735000  | 5.14379400  | 1.84117800  |
| C | 3.68263000  | 5.06985600  | -0.26727900 |
| H | 1.76231700  | 5.33709600  | -1.21383600 |
| H | 2.18809100  | 6.62249900  | -0.09848100 |
| H | 4.26850500  | 5.62129100  | -1.00670900 |
| H | 4.15815500  | 5.20997500  | 0.70983600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.74685800  | 4.00461800  | -0.51811800 |
| N  | 1.20046600  | -0.19199500 | -0.15905200 |
| H  | 1.41210500  | -1.19161800 | -0.19622200 |
| C  | 1.81485400  | 0.32841600  | 1.10020800  |
| H  | 1.42510200  | 1.34012000  | 1.25245500  |
| H  | 1.43583600  | -0.28636200 | 1.92181600  |
| C  | 1.81284900  | 0.42707400  | -1.37296500 |
| H  | 1.04034100  | 0.49196600  | -2.14437700 |
| H  | 2.09783300  | 1.45302000  | -1.12029100 |
| C  | 3.02175100  | -0.31991900 | -1.89070400 |
| C  | 4.19951800  | 0.36694400  | -2.18223700 |
| C  | 2.98853800  | -1.70776000 | -2.05823300 |
| C  | 5.32900800  | -0.32002800 | -2.61765100 |
| H  | 4.24289800  | 1.44265800  | -2.03239400 |
| C  | 4.11726300  | -2.39854900 | -2.48884500 |
| H  | 2.07926600  | -2.26952300 | -1.84009100 |
| C  | 5.29243100  | -1.70420500 | -2.76664700 |
| H  | 6.24344600  | 0.22568300  | -2.82593400 |
| H  | 4.07861200  | -3.47637700 | -2.60935600 |
| H  | 6.17523300  | -2.24083400 | -3.09795900 |
| C  | 3.32728000  | 0.38291600  | 1.10243200  |
| C  | 4.10768600  | -0.77163900 | 0.98020500  |
| C  | 3.96423900  | 1.62107400  | 1.17649800  |
| C  | 5.49209900  | -0.68293000 | 0.90646600  |
| H  | 3.63792900  | -1.74825300 | 0.89245300  |
| C  | 5.35348100  | 1.71486200  | 1.10605000  |
| H  | 3.36958400  | 2.52502000  | 1.28711400  |
| C  | 6.11851800  | 0.56236000  | 0.96397400  |
| H  | 6.08342900  | -1.58549200 | 0.79215600  |
| H  | 5.83057500  | 2.68858000  | 1.15777900  |
| H  | 7.19949400  | 0.63003800  | 0.89891300  |
| C  | -3.86875500 | -2.26076000 | -0.25329900 |
| H  | -3.69447800 | -2.10815700 | 0.82024800  |
| H  | -4.92594800 | -2.05670100 | -0.44415300 |
| H  | -3.70539600 | -3.32106300 | -0.46151500 |
| Si | -4.83446600 | 0.89389500  | -1.16648200 |
| C  | -5.49748500 | 0.71418700  | 0.59422600  |
| H  | -6.56104100 | 0.97654400  | 0.57693800  |
| H  | -5.41269600 | -0.29253700 | 1.01107900  |
| H  | -5.00454700 | 1.40947400  | 1.28008400  |
| C  | -6.09027800 | 0.16141400  | -2.36424900 |
| H  | -7.05530900 | 0.67003100  | -2.27407900 |
| H  | -5.74187900 | 0.27249400  | -3.39576200 |
| H  | -6.25258500 | -0.90497900 | -2.18049400 |

|                             |             |             |             |
|-----------------------------|-------------|-------------|-------------|
| C                           | -4.72422800 | 2.74994300  | -1.49021000 |
| H                           | -3.86230100 | 3.22521100  | -1.00974800 |
| H                           | -4.69164300 | 2.98283600  | -2.55756100 |
| H                           | -5.62651600 | 3.21652100  | -1.08022100 |
| trans-ts-10 <sup>1</sup> -3 |             |             |             |
| C                           | 2.84802500  | -2.12122100 | 0.92918400  |
| C                           | 1.73297100  | -2.05383600 | 1.80982800  |
| C                           | 1.68928600  | -0.74569700 | 2.35982600  |
| C                           | 2.76932300  | 0.02028700  | 1.82103000  |
| C                           | 3.47878500  | -0.84852200 | 0.92915500  |
| Sc                          | 1.28108200  | -0.47431800 | -0.14692700 |
| C                           | 0.81693200  | -0.37985700 | 3.53122700  |
| H                           | -0.20020600 | -0.77306600 | 3.43863500  |
| H                           | 1.23786500  | -0.80419100 | 4.45053200  |
| H                           | 0.74377400  | 0.69925600  | 3.67600000  |
| C                           | 0.91707800  | -3.20591600 | 2.32601600  |
| H                           | 0.94394800  | -4.06787300 | 1.65726900  |
| H                           | 1.30917700  | -3.53209800 | 3.29631800  |
| H                           | -0.13238400 | -2.93688800 | 2.48708600  |
| C                           | 0.72675600  | -0.69417000 | -4.27642300 |
| C                           | 1.58802700  | -1.43940000 | -3.23895500 |
| H                           | 0.17904300  | -1.40789400 | -4.90053900 |
| H                           | 0.00487400  | -0.02772400 | -3.79788300 |
| H                           | 1.36195900  | -0.10160700 | -4.93933300 |
| C                           | 2.34625200  | -0.52508900 | -2.25101100 |
| C                           | 2.60912400  | -2.31021900 | -4.00687300 |
| H                           | 2.90964500  | -1.19981400 | -1.57506600 |
| H                           | 3.14477100  | -0.05024400 | -2.82199200 |
| H                           | 3.27126900  | -1.66305700 | -4.58833500 |
| H                           | 3.22442200  | -2.90131300 | -3.32125800 |
| H                           | 2.10791100  | -2.99333000 | -4.70078600 |
| C                           | 0.66260300  | -2.37935200 | -2.53324700 |
| H                           | 0.23292900  | -3.18349800 | -3.14392800 |
| N                           | 0.36180500  | -2.26994900 | -1.29884500 |
| C                           | -0.56964200 | -3.26772000 | -0.72367000 |
| C                           | -1.95865000 | -3.23965900 | -1.37023900 |
| C                           | -0.01274900 | -4.69458100 | -0.77829500 |
| H                           | -0.68715400 | -3.00051100 | 0.33467900  |
| C                           | -2.90441600 | -4.16575200 | -0.60229800 |
| H                           | -1.88148900 | -3.57277300 | -2.41383300 |
| H                           | -2.35644500 | -2.22236800 | -1.39730500 |
| C                           | -0.94207000 | -5.64943400 | -0.02302400 |
| H                           | 0.05749600  | -5.00873100 | -1.82842000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.00108800  | -4.72151800 | -0.36883900 |
| C | -2.36721400 | -5.59824500 | -0.57959400 |
| H | -3.90186700 | -4.13343600 | -1.05023400 |
| H | -3.00416900 | -3.79225700 | 0.42773700  |
| H | -0.54688700 | -6.66770000 | -0.07631800 |
| H | -0.95626600 | -5.36994500 | 1.03943000  |
| H | -3.02586800 | -6.24071900 | 0.01147300  |
| H | -2.36887100 | -5.99528000 | -1.60292200 |
| C | 2.07822300  | 1.55595800  | -1.64770100 |
| C | 1.36773000  | 1.79771400  | -0.45873000 |
| H | 3.16507400  | 1.57241600  | -1.55304000 |
| H | 1.92527800  | 2.12351300  | 0.40747100  |
| H | 0.37031600  | 2.21759800  | -0.54424300 |
| C | 1.58253300  | 2.13306800  | -2.95323300 |
| C | 1.97921300  | 3.61775700  | -3.08678900 |
| H | 0.49335900  | 2.03257400  | -3.01771800 |
| H | 2.00800400  | 1.60017400  | -3.80550800 |
| C | 1.41218600  | 4.58141300  | -2.04107400 |
| H | 3.07415100  | 3.68572900  | -3.07725000 |
| H | 1.66015900  | 3.94525600  | -4.08358000 |
| H | 1.80379600  | 4.32849800  | -1.04857600 |
| H | 1.78699700  | 5.58677700  | -2.26892500 |
| C | -0.11354000 | 4.63766200  | -1.97734600 |
| C | -0.61595300 | 5.59688500  | -0.89922100 |
| H | -0.52364500 | 3.63761800  | -1.77428000 |
| H | -0.51637900 | 4.93476600  | -2.95552100 |
| C | -2.13385800 | 5.57452000  | -0.74132400 |
| H | -0.14358100 | 5.33585700  | 0.05748600  |
| H | -0.27992000 | 6.61266400  | -1.13909500 |
| H | -2.47518400 | 6.32669700  | -0.02593300 |
| H | -2.63110300 | 5.77029400  | -1.69741600 |
| H | -2.47572100 | 4.59670500  | -0.38297400 |
| N | -1.03051400 | -0.03999100 | 0.08614400  |
| H | -1.46205900 | -0.92864700 | 0.35246300  |
| C | -1.66348800 | 0.37288200  | -1.20159300 |
| H | -1.09646800 | 1.22966500  | -1.58036700 |
| H | -1.51281500 | -0.44543000 | -1.91160500 |
| C | -1.31758600 | 0.92887000  | 1.18831500  |
| H | -0.45788300 | 0.92720100  | 1.86522600  |
| H | -1.38096300 | 1.92963200  | 0.74875100  |
| C | -2.58787700 | 0.62231700  | 1.94927900  |
| C | -3.55413700 | 1.60854900  | 2.14498700  |
| C | -2.82110200 | -0.66344500 | 2.44590000  |
| C | -4.74141500 | 1.31032400  | 2.80757600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -3.39117000 | 2.60595800  | 1.74454000  |
| C  | -4.00916700 | -0.96663900 | 3.10359400  |
| H  | -2.07332700 | -1.44640400 | 2.31529900  |
| C  | -4.97461800 | 0.02198700  | 3.28228100  |
| H  | -5.49215300 | 2.08260400  | 2.93916600  |
| H  | -4.17875000 | -1.97004800 | 3.48055100  |
| H  | -5.90336700 | -0.21125100 | 3.79212700  |
| C  | -3.12213500 | 0.75978000  | -1.09909100 |
| C  | -4.09775500 | -0.14876100 | -0.67547400 |
| C  | -3.50074400 | 2.07061100  | -1.38638900 |
| C  | -5.41742700 | 0.25623700  | -0.51982500 |
| H  | -3.82860100 | -1.17040700 | -0.41727100 |
| C  | -4.82442900 | 2.48059700  | -1.23466400 |
| H  | -2.75128200 | 2.78070000  | -1.72908500 |
| C  | -5.78337000 | 1.57420300  | -0.79520600 |
| H  | -6.16041000 | -0.45344200 | -0.17101800 |
| H  | -5.09865900 | 3.50731800  | -1.45591500 |
| H  | -6.81339900 | 1.89012200  | -0.66692700 |
| C  | 3.34143200  | -3.34609000 | 0.20616500  |
| H  | 3.04550100  | -3.37727300 | -0.85060700 |
| H  | 4.43237100  | -3.40322200 | 0.24107000  |
| H  | 2.95821100  | -4.25365400 | 0.67926800  |
| C  | 4.74904800  | -0.53379400 | 0.18161700  |
| H  | 4.69121600  | 0.40581900  | -0.37592400 |
| H  | 5.59527800  | -0.44767800 | 0.87225400  |
| H  | 4.98997400  | -1.32556400 | -0.53293500 |
| Si | 3.39136300  | 1.65801100  | 2.52428400  |
| C  | 4.36525300  | 1.25707800  | 4.08313800  |
| H  | 5.21129500  | 0.60140900  | 3.85574600  |
| H  | 4.75609200  | 2.16929500  | 4.54465500  |
| H  | 3.73369100  | 0.74899600  | 4.81845900  |
| C  | 4.52934400  | 2.56701600  | 1.32332300  |
| H  | 4.76010900  | 3.54745600  | 1.75391800  |
| H  | 5.47662300  | 2.04304300  | 1.17508500  |
| H  | 4.07552400  | 2.74225500  | 0.34197000  |
| C  | 1.97480400  | 2.83413700  | 2.97678600  |
| H  | 1.09582300  | 2.73267200  | 2.33191900  |
| H  | 1.65272900  | 2.68619600  | 4.01160400  |
| H  | 2.32635900  | 3.86750300  | 2.89128300  |

trans-ts-10<sup>1</sup>-4

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -3.61557300 | -1.34296300 | 0.66607600 |
| C | -3.20340900 | -0.16558000 | 1.33064300 |
| C | -2.18050300 | -0.50550300 | 2.28046600 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.00149200 | -1.92195200 | 2.19916500  |
| C  | -2.86378600 | -2.43455400 | 1.19536100  |
| Sc | -1.22617400 | -0.97575600 | -0.01309200 |
| C  | -3.90216300 | 1.16568300  | 1.23215400  |
| H  | -4.75728700 | 1.10611300  | 0.55588800  |
| H  | -4.29493900 | 1.45728100  | 2.21182700  |
| H  | -3.25809600 | 1.98518300  | 0.89879900  |
| C  | -0.35652900 | -1.57479000 | -4.06273200 |
| C  | -1.64702700 | -1.54196400 | -3.21931600 |
| H  | -0.46771600 | -0.94714900 | -4.95288700 |
| H  | 0.50322200  | -1.21271600 | -3.49240500 |
| H  | -0.14989700 | -2.59305400 | -4.40017800 |
| C  | -1.60473400 | -2.37642800 | -1.92665300 |
| C  | -2.81273000 | -2.03734200 | -4.10442800 |
| H  | -2.58073500 | -2.22413000 | -1.43190300 |
| H  | -1.64325600 | -3.42566900 | -2.22146100 |
| H  | -2.63476500 | -3.07854500 | -4.38617200 |
| H  | -3.76610600 | -1.98495200 | -3.56923800 |
| H  | -2.89609400 | -1.44721000 | -5.02333400 |
| C  | -1.89045800 | -0.09553400 | -2.93903300 |
| H  | -2.15035000 | 0.51693000  | -3.81035700 |
| N  | -1.78204900 | 0.43966700  | -1.78486400 |
| C  | -2.03800900 | 1.89863500  | -1.70446000 |
| C  | -1.14002100 | 2.73603300  | -2.62522000 |
| C  | -3.50925700 | 2.22041800  | -1.99046500 |
| H  | -1.82100000 | 2.18949300  | -0.66620600 |
| C  | -1.39990100 | 4.22784400  | -2.39161600 |
| H  | -1.36761100 | 2.49884000  | -3.67211800 |
| H  | -0.08456400 | 2.49660100  | -2.46581500 |
| C  | -3.78795300 | 3.70714000  | -1.76329600 |
| H  | -3.72193400 | 1.96369500  | -3.03736300 |
| H  | -4.15654000 | 1.59748600  | -1.37007300 |
| C  | -2.87089300 | 4.57588500  | -2.62700300 |
| H  | -0.75036500 | 4.81977500  | -3.04278500 |
| H  | -1.12950400 | 4.48781200  | -1.35824600 |
| H  | -4.83810300 | 3.92347400  | -1.97842700 |
| H  | -3.62669800 | 3.94515800  | -0.70250200 |
| H  | -3.04729800 | 5.63521700  | -2.42019900 |
| H  | -3.11368400 | 4.41259500  | -3.68514500 |
| C  | 0.07015600  | -3.18718900 | -0.75360000 |
| C  | 0.55588300  | -2.38986200 | 0.29791000  |
| H  | -0.61633800 | -3.98386500 | -0.46500100 |
| H  | 0.39179000  | -2.72562000 | 1.31572100  |
| H  | 1.50051600  | -1.88077300 | 0.12305400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.97615700  | -3.55401900 | -1.90425800 |
| C | 1.97433100  | -4.65230900 | -1.48806000 |
| H | 1.52539900  | -2.67134500 | -2.24727900 |
| H | 0.39448900  | -3.92584300 | -2.75080300 |
| C | 3.12387500  | -4.22114600 | -0.57200700 |
| H | 1.42233200  | -5.47700000 | -1.02040600 |
| H | 2.40674900  | -5.05787000 | -2.41049900 |
| H | 2.74418200  | -3.92842900 | 0.41426100  |
| H | 3.76143900  | -5.09802200 | -0.40461100 |
| C | 3.98820100  | -3.09697700 | -1.14393500 |
| C | 5.28788300  | -2.88531700 | -0.37079800 |
| H | 3.42997600  | -2.14756000 | -1.15457900 |
| H | 4.22654900  | -3.31711900 | -2.19440800 |
| C | 6.14045700  | -1.76759300 | -0.96385500 |
| H | 5.05424100  | -2.66621600 | 0.68042500  |
| H | 5.85832000  | -3.82173300 | -0.36387300 |
| H | 7.07104400  | -1.62817100 | -0.40667300 |
| H | 6.40242800  | -1.99027100 | -2.00276900 |
| H | 5.59853400  | -0.81551600 | -0.95070200 |
| N | 0.44227700  | 0.65252900  | 0.36997800  |
| H | -0.03292100 | 1.55398600  | 0.41620400  |
| C | 1.35907300  | 0.70852700  | -0.79697600 |
| H | 2.04789600  | -0.13689800 | -0.73192800 |
| H | 0.74749000  | 0.55418500  | -1.69604800 |
| C | 1.11683100  | 0.45353300  | 1.70244200  |
| H | 0.54115600  | 1.03710900  | 2.41949900  |
| H | 1.00617200  | -0.59919300 | 1.97481500  |
| C | 2.57015000  | 0.84548000  | 1.79787700  |
| C | 3.57475200  | -0.09859800 | 1.57753700  |
| C | 2.92717700  | 2.16072400  | 2.10640800  |
| C | 4.91702900  | 0.27103700  | 1.64432100  |
| H | 3.30788000  | -1.13343100 | 1.36395300  |
| C | 4.26398600  | 2.53646100  | 2.15858500  |
| H | 2.14685200  | 2.89694000  | 2.28661300  |
| C | 5.26153300  | 1.59058000  | 1.92300500  |
| H | 5.69194100  | -0.47237700 | 1.48640600  |
| H | 4.52887600  | 3.56392700  | 2.38544200  |
| H | 6.30625300  | 1.88013900  | 1.96976600  |
| C | 2.16481900  | 1.98512000  | -0.93326000 |
| C | 1.60624900  | 3.24057100  | -0.68496600 |
| C | 3.50276300  | 1.90693800  | -1.31864400 |
| C | 2.36979900  | 4.39677600  | -0.81536500 |
| H | 0.56751500  | 3.33408200  | -0.37014200 |
| C | 4.27074000  | 3.06011000  | -1.45016600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.95217700  | 0.93179000  | -1.49085700 |
| C  | 3.70655900  | 4.30779700  | -1.19609200 |
| H  | 1.92057800  | 5.36474400  | -0.61697200 |
| H  | 5.31438600  | 2.98230600  | -1.73697900 |
| H  | 4.30582500  | 5.20724000  | -1.29075900 |
| C  | -4.72296800 | -1.44123700 | -0.34803900 |
| H  | -4.61169500 | -0.71007700 | -1.15683100 |
| H  | -4.76069700 | -2.43570500 | -0.80125900 |
| H  | -5.69591800 | -1.26412100 | 0.12228000  |
| C  | -3.06472600 | -3.88063700 | 0.83501300  |
| H  | -2.24919200 | -4.50647100 | 1.20572700  |
| H  | -3.99163900 | -4.26257100 | 1.27563600  |
| H  | -3.13637400 | -4.03494700 | -0.24733200 |
| C  | -1.17582700 | -2.75010600 | 3.14438400  |
| H  | -1.71763000 | -2.90423800 | 4.08463500  |
| H  | -0.95391400 | -3.74036600 | 2.73767400  |
| H  | -0.22709500 | -2.26633300 | 3.39330100  |
| Si | -1.78521500 | 0.61399600  | 3.74307300  |
| C  | -3.28796700 | 0.60192600  | 4.88022100  |
| H  | -3.10933500 | 1.24203500  | 5.75051200  |
| H  | -4.19985100 | 0.95018600  | 4.38831400  |
| H  | -3.47126800 | -0.41411500 | 5.24385500  |
| C  | -1.48126800 | 2.39077500  | 3.13686600  |
| H  | -2.38775500 | 2.99340300  | 3.24912800  |
| H  | -0.68821300 | 2.87415200  | 3.71675600  |
| H  | -1.19866500 | 2.43679500  | 2.07811400  |
| C  | -0.34805000 | 0.02988700  | 4.81898100  |
| H  | -0.62764400 | -0.87569200 | 5.36488800  |
| H  | 0.58996300  | -0.16895600 | 4.29562700  |
| H  | -0.15133100 | 0.80748400  | 5.56549700  |

trans-ts-10<sup>-5</sup>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.16093500  | -1.61157100 | -0.97645700 |
| C  | 2.55774300  | -0.64563200 | -1.85271200 |
| C  | 1.51387700  | -1.34278100 | -2.55942100 |
| C  | 1.48068700  | -2.68548500 | -2.11881300 |
| C  | 2.49182200  | -2.85119000 | -1.13779200 |
| Sc | 0.85178700  | -1.21901600 | -0.10999700 |
| C  | -0.18454400 | -1.78203400 | 3.85110300  |
| C  | 1.14446500  | -1.90967600 | 3.07942700  |
| H  | -0.03901500 | -1.18510000 | 4.75737300  |
| H  | -0.95777500 | -1.30021400 | 3.24577200  |
| H  | -0.54303000 | -2.76625100 | 4.15958200  |
| C  | 1.07992800  | -2.68158500 | 1.75084600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.17610100  | -2.58600300 | 4.00861100  |
| H | 2.07361500  | -2.55145400 | 1.28401100  |
| H | 1.05786000  | -3.74787000 | 1.97757500  |
| H | 1.83880500  | -3.59858600 | 4.24599600  |
| H | 3.15658400  | -2.65629800 | 3.52705300  |
| H | 2.28841700  | -2.03679900 | 4.94944200  |
| C | 1.60318100  | -0.50444400 | 2.85486300  |
| H | 1.91012000  | 0.04264700  | 3.75353700  |
| N | 1.61946800  | 0.06383800  | 1.71180700  |
| C | 2.09446200  | 1.47008600  | 1.66775200  |
| C | 1.41062900  | 2.40118600  | 2.67839800  |
| C | 3.61351300  | 1.53314900  | 1.85249000  |
| H | 1.86847500  | 1.82861500  | 0.65457100  |
| C | 1.91127400  | 3.83873500  | 2.50140200  |
| H | 1.65796500  | 2.08032800  | 3.69760100  |
| H | 0.32198900  | 2.35400400  | 2.57814800  |
| C | 4.12247600  | 2.96737100  | 1.68703600  |
| H | 3.85483600  | 1.17065900  | 2.86159700  |
| H | 4.09682500  | 0.85504100  | 1.14640400  |
| C | 3.42944500  | 3.91624800  | 2.66515800  |
| H | 1.40515900  | 4.49125600  | 3.21871700  |
| H | 1.64029800  | 4.20343600  | 1.50129800  |
| H | 5.20808000  | 2.99188500  | 1.82105200  |
| H | 3.92274000  | 3.30403200  | 0.65976900  |
| H | 3.77603500  | 4.94167400  | 2.50818000  |
| H | 3.69946700  | 3.64081700  | 3.69284000  |
| C | -0.67551200 | -3.26316700 | 0.55974600  |
| C | -1.13269400 | -2.32075200 | -0.37853700 |
| H | -0.06562600 | -4.07451200 | 0.15827600  |
| H | -1.05094700 | -2.55516600 | -1.43569500 |
| H | -1.99611700 | -1.72181000 | -0.09551500 |
| C | -1.56696400 | -3.69547400 | 1.70041100  |
| C | -2.61588100 | -4.71860700 | 1.21821700  |
| H | -2.07336100 | -2.82601000 | 2.12856100  |
| H | -0.98462600 | -4.16209100 | 2.49861400  |
| C | -3.67088000 | -4.20418900 | 0.23502100  |
| H | -2.09530300 | -5.57611400 | 0.77412900  |
| H | -3.12379700 | -5.09845600 | 2.11287600  |
| H | -3.19761300 | -3.91941100 | -0.71179000 |
| H | -4.34719200 | -5.03511400 | 0.00016600  |
| C | -4.50249300 | -3.03270400 | 0.75433500  |
| C | -5.55192400 | -2.56267400 | -0.25011600 |
| H | -3.85326600 | -2.17955700 | 0.99893000  |
| H | -4.99383700 | -3.31696400 | 1.69533000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -6.34543300 | -1.36059100 | 0.25344000  |
| H | -5.05344000 | -2.31170200 | -1.19675800 |
| H | -6.23407600 | -3.39044400 | -0.47770900 |
| H | -7.08375400 | -1.02804000 | -0.48140400 |
| H | -6.87874700 | -1.60439600 | 1.17730500  |
| H | -5.68059900 | -0.51551200 | 0.47027900  |
| N | -0.55072200 | 0.68252100  | -0.48859300 |
| H | 0.08449800  | 1.47311300  | -0.60948000 |
| C | -1.37122400 | 0.94845000  | 0.72344400  |
| H | -2.24199700 | 0.28658100  | 0.69327500  |
| H | -0.77634000 | 0.65381900  | 1.59644500  |
| C | -1.36518100 | 0.59248300  | -1.74974000 |
| H | -0.69260000 | 0.85531000  | -2.56574900 |
| H | -1.64740200 | -0.45303000 | -1.88494200 |
| C | -2.60974200 | 1.44315600  | -1.81634000 |
| C | -3.85323900 | 0.88558200  | -1.51592800 |
| C | -2.53595000 | 2.79351600  | -2.16543500 |
| C | -5.00534100 | 1.66958500  | -1.53927000 |
| H | -3.92244100 | -0.17180700 | -1.26218300 |
| C | -3.68060900 | 3.58185900  | -2.18088800 |
| H | -1.57105300 | 3.23404800  | -2.40800400 |
| C | -4.91729600 | 3.02003900  | -1.86387600 |
| H | -5.96770800 | 1.22421000  | -1.30749500 |
| H | -3.61108900 | 4.63293400  | -2.44116900 |
| H | -5.81174400 | 3.63414000  | -1.87871900 |
| C | -1.84082000 | 2.38036800  | 0.89480800  |
| C | -0.99592900 | 3.46100800  | 0.63393700  |
| C | -3.13753800 | 2.63362200  | 1.34100800  |
| C | -1.43606400 | 4.76921600  | 0.80742500  |
| H | 0.01898500  | 3.29591900  | 0.27484400  |
| C | -3.58351300 | 3.94109700  | 1.51472900  |
| H | -3.81340300 | 1.80209400  | 1.52563500  |
| C | -2.73531000 | 5.01209600  | 1.24655800  |
| H | -0.76534000 | 5.59614400  | 0.59630900  |
| H | -4.60027100 | 4.12202800  | 1.84809700  |
| H | -3.08565700 | 6.03061000  | 1.37604200  |
| C | 4.37345400  | -1.46320900 | -0.09508400 |
| H | 4.14300800  | -1.58400600 | 0.97208700  |
| H | 5.11658600  | -2.22625200 | -0.34872000 |
| H | 4.84875200  | -0.49276700 | -0.22351100 |
| C | 2.89067200  | -4.16011800 | -0.51885900 |
| H | 2.02304900  | -4.78576600 | -0.28348100 |
| H | 3.52065400  | -4.73068800 | -1.21015000 |
| H | 3.46086900  | -4.02063000 | 0.40386400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.67229300  | -3.79788300 | -2.72089500 |
| H  | 1.29554500  | -4.38605900 | -3.40333700 |
| H  | 0.28355100  | -4.49128500 | -1.96763600 |
| H  | -0.17421900 | -3.42063800 | -3.30024700 |
| C  | 0.75154800  | -0.86647600 | -3.76734200 |
| H  | 0.76466400  | 0.21998200  | -3.87229800 |
| H  | 1.20529100  | -1.28015500 | -4.67523700 |
| H  | -0.29404800 | -1.18982500 | -3.75531900 |
| Si | 3.23762800  | 1.00667800  | -2.47399200 |
| C  | 4.87966700  | 1.52115600  | -1.71049300 |
| H  | 5.66330000  | 0.78509800  | -1.91266100 |
| H  | 5.17901800  | 2.45792100  | -2.19379300 |
| H  | 4.84782200  | 1.70792600  | -0.63568500 |
| C  | 3.58446900  | 0.83450700  | -4.31929600 |
| H  | 2.68230400  | 0.79787300  | -4.93340800 |
| H  | 4.18014600  | 1.68963600  | -4.65547600 |
| H  | 4.16296900  | -0.07346600 | -4.51577600 |
| C  | 2.02446000  | 2.44186200  | -2.23192600 |
| H  | 1.01690000  | 2.21555300  | -2.59777300 |
| H  | 1.95770700  | 2.75665800  | -1.18422400 |
| H  | 2.38086200  | 3.30878700  | -2.79856900 |
| 4' |             |             |             |
| C  | -1.85751500 | 0.57416300  | 0.27537800  |
| C  | -1.45087000 | 1.64987600  | -0.58631900 |
| C  | -0.26193100 | 2.22860000  | -0.06673300 |
| C  | 0.07550400  | 1.53187000  | 1.13355400  |
| C  | -0.89990700 | 0.52333200  | 1.34520800  |
| Sc | 0.21844700  | -0.08996200 | -0.68187000 |
| C  | -4.53720200 | -0.06291800 | -1.22727400 |
| C  | -2.78377300 | -2.32316500 | -0.17808800 |
| C  | -4.31678500 | -0.49953100 | 1.78502400  |
| H  | -4.83189900 | 0.98821100  | -1.17220000 |
| H  | -4.12047100 | -0.25174200 | -2.22051300 |
| H  | -5.44592100 | -0.66706800 | -1.13469800 |
| H  | -2.21707300 | -2.74229800 | 0.65978300  |
| H  | -3.64343900 | -2.97902800 | -0.34947600 |
| H  | -2.15751600 | -2.38266900 | -1.08034200 |
| H  | -5.21082500 | -1.12673000 | 1.71116500  |
| H  | -3.72779900 | -0.85573900 | 2.63337400  |
| H  | -4.64140900 | 0.52187600  | 2.00412300  |
| Si | -3.37325100 | -0.55512000 | 0.16270100  |
| C  | -0.91256500 | -0.39580200 | 2.53840100  |
| H  | 0.10315100  | -0.60903100 | 2.88842800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.44834900 | 0.06792800  | 3.37381400  |
| H  | -1.40732200 | -1.34757400 | 2.32454100  |
| C  | 1.19444100  | 1.87333200  | 2.07533300  |
| H  | 1.90478700  | 2.56352900  | 1.61638900  |
| H  | 0.79362600  | 2.35295100  | 2.97456100  |
| H  | 1.75322300  | 0.98816000  | 2.39558100  |
| C  | 0.49793700  | 3.39936200  | -0.62089600 |
| H  | 0.31414500  | 3.53570800  | -1.68819500 |
| H  | 0.20863500  | 4.32404700  | -0.11116700 |
| H  | 1.57616300  | 3.27205900  | -0.48446700 |
| C  | -2.14197000 | 2.09662000  | -1.84769700 |
| H  | -2.45416600 | 1.25540600  | -2.47227900 |
| H  | -3.04223700 | 2.67268600  | -1.61269100 |
| H  | -1.49228600 | 2.73467800  | -2.44954600 |
| C  | 4.25146900  | 0.81750300  | 0.74834700  |
| C  | 4.02983400  | -0.36380800 | 1.46968700  |
| C  | 3.12358200  | -1.29401700 | 0.99703700  |
| C  | 2.43385300  | -1.06579300 | -0.20720300 |
| C  | 2.64968300  | 0.12395000  | -0.97019900 |
| C  | 3.56979100  | 1.05604400  | -0.42751100 |
| H  | 4.96141300  | 1.55054600  | 1.11676200  |
| H  | 4.56601300  | -0.55297100 | 2.39272700  |
| H  | 2.95973500  | -2.21032800 | 1.55248500  |
| H  | 3.75299900  | 1.96914200  | -0.98618300 |
| N  | 1.43675900  | -2.00456700 | -0.70772900 |
| C  | 1.90884200  | -2.78245200 | -1.87604000 |
| H  | 2.62757800  | -3.54035900 | -1.54546100 |
| H  | 1.05686600  | -3.27360100 | -2.35072800 |
| H  | 2.39862700  | -2.12583900 | -2.59278100 |
| C  | 0.88485700  | -2.92175800 | 0.30977500  |
| H  | 0.52999100  | -2.35696300 | 1.17947100  |
| H  | 0.04848900  | -3.46406100 | -0.13439700 |
| H  | 1.63109000  | -3.64950100 | 0.64725800  |
| C  | 1.79709200  | 0.47311800  | -2.11412300 |
| H  | 1.72286700  | -0.26790700 | -2.91332300 |
| H  | 1.98593600  | 1.46815500  | -2.51042000 |
| 5' |             |             |             |
| C  | -0.19199400 | 1.65108700  | 1.23476900  |
| C  | 0.17115900  | 0.70549200  | 2.26192800  |
| C  | -0.99295700 | -0.00104800 | 2.65543300  |
| C  | -2.09459000 | 0.49925100  | 1.91289200  |
| C  | -1.61295600 | 1.49809300  | 1.03245100  |
| Sc | -0.57655600 | -0.56464100 | 0.24503700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.35679200  | 3.51292300  | 1.54717700  |
| C  | 0.91185700  | 3.44026000  | -1.16407800 |
| C  | -0.38337800 | 4.68467300  | 1.27103500  |
| H  | 2.23192600  | 3.58470700  | 2.63197700  |
| H  | 3.12765800  | 2.76957600  | 1.33634700  |
| H  | 2.73584100  | 4.48072600  | 1.20035000  |
| H  | -0.05024200 | 3.58498200  | -1.66612200 |
| H  | 1.50113400  | 4.34708400  | -1.34162800 |
| H  | 1.43210200  | 2.61429200  | -1.65612100 |
| H  | 0.19427800  | 5.61345500  | 1.22006000  |
| H  | -1.27345900 | 4.81564400  | 0.65101400  |
| H  | -0.70749500 | 4.54716800  | 2.30706900  |
| Si | 0.69138600  | 3.24345300  | 0.70353800  |
| C  | -2.50493700 | 2.33249900  | 0.15137300  |
| H  | -3.34770600 | 1.74681100  | -0.22585200 |
| H  | -2.91465900 | 3.17895500  | 0.71301800  |
| H  | -1.97291100 | 2.73824600  | -0.71474700 |
| C  | -3.52284200 | 0.14293400  | 2.19110500  |
| H  | -3.66830800 | -0.93967900 | 2.25978000  |
| H  | -3.82559700 | 0.57312700  | 3.15277600  |
| H  | -4.19664800 | 0.52914700  | 1.42537900  |
| C  | -1.12949600 | -1.00249900 | 3.76704400  |
| H  | -0.16684900 | -1.24082900 | 4.22394500  |
| H  | -1.77820100 | -0.60021100 | 4.55252800  |
| H  | -1.58398800 | -1.93889000 | 3.42365300  |
| C  | 1.50272800  | 0.52571000  | 2.94622800  |
| H  | 2.17966000  | 1.34870500  | 2.72612500  |
| H  | 1.36578700  | 0.50134900  | 4.03136900  |
| H  | 2.01236400  | -0.40312600 | 2.66251200  |
| C  | -5.19583600 | -0.27961400 | -1.41423400 |
| C  | -4.61284800 | 0.47202300  | -2.43394900 |
| C  | -3.24740800 | 0.37183800  | -2.66643200 |
| C  | -2.46220000 | -0.47230100 | -1.87697200 |
| C  | -3.02832200 | -1.25524500 | -0.84483100 |
| C  | -4.41361600 | -1.12491500 | -0.64042400 |
| H  | -6.26299000 | -0.21259200 | -1.22974900 |
| H  | -5.21712200 | 1.12978700  | -3.04872700 |
| H  | -2.80525900 | 0.96171900  | -3.45992200 |
| H  | -4.87401000 | -1.71689100 | 0.14519200  |
| N  | -1.01758600 | -0.60119800 | -2.08248500 |
| C  | -0.72941400 | -1.85807900 | -2.81972700 |
| H  | -1.04702900 | -1.75107200 | -3.86386100 |
| H  | 0.34053600  | -2.07147400 | -2.78471800 |
| H  | -1.27309100 | -2.68997900 | -2.37669900 |



|       |             |             |             |
|-------|-------------|-------------|-------------|
| C     | -0.43592300 | 0.52321500  | -2.83940800 |
| H     | -0.66228900 | 1.46791500  | -2.34007000 |
| H     | 0.64487000  | 0.39315500  | -2.89527700 |
| H     | -0.81760100 | 0.55581400  | -3.86585200 |
| C     | -2.16962000 | -2.08980900 | 0.04103400  |
| H     | -1.72335200 | -2.94738500 | -0.47794600 |
| H     | -2.73283200 | -2.47393400 | 0.89520400  |
| C     | 2.81281900  | -4.16870400 | 1.68788900  |
| C     | 1.64536200  | -3.52618100 | 0.92286900  |
| H     | 3.59606200  | -4.50766000 | 1.00321900  |
| H     | 3.25442100  | -3.46470500 | 2.40015800  |
| H     | 2.45255800  | -5.03672100 | 2.24582700  |
| C     | 0.57261200  | -3.08079400 | 1.91079700  |
| C     | 1.07547600  | -4.53271000 | -0.09373100 |
| H     | -0.33630300 | -2.71581200 | 1.41423500  |
| H     | 0.24773700  | -3.93148600 | 2.51784100  |
| H     | 0.95492500  | -2.31203100 | 2.58683700  |
| H     | 0.71662600  | -5.41886000 | 0.43726600  |
| H     | 0.23729500  | -4.09716000 | -0.64677500 |
| H     | 1.83824900  | -4.85140400 | -0.81063600 |
| C     | 2.20208700  | -2.36931700 | 0.13961800  |
| H     | 3.21122800  | -2.53408200 | -0.25758300 |
| N     | 1.61257200  | -1.26032500 | -0.09916600 |
| C     | 2.39023200  | -0.24463600 | -0.86418300 |
| C     | 3.54081200  | 0.31906500  | -0.02336000 |
| C     | 2.92368000  | -0.74567000 | -2.21221900 |
| H     | 1.69217400  | 0.58446500  | -1.05250800 |
| C     | 4.26366400  | 1.44298500  | -0.77078600 |
| H     | 4.24615200  | -0.49509200 | 0.19366700  |
| H     | 3.14985600  | 0.67119300  | 0.93380100  |
| C     | 3.61189400  | 0.39608600  | -2.96577000 |
| H     | 3.65645700  | -1.54395800 | -2.04459500 |
| H     | 2.12005500  | -1.17831000 | -2.81459900 |
| C     | 4.75997800  | 0.97901500  | -2.14060300 |
| H     | 5.09537200  | 1.80947500  | -0.16130000 |
| H     | 3.57526000  | 2.28853400  | -0.90273300 |
| H     | 3.97433000  | 0.03210100  | -3.93097800 |
| H     | 2.87990300  | 1.18820400  | -3.18064500 |
| H     | 5.22599800  | 1.81157200  | -2.67479400 |
| H     | 5.53360300  | 0.21146700  | -2.00808200 |
| ts-6' |             |             |             |
| C     | -0.16083600 | 1.79615000  | 0.99351700  |
| C     | 0.05747200  | 1.02207500  | 2.18897100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.17998200 | 0.48154500  | 2.61127200  |
| C  | -2.18662100 | 0.91050800  | 1.70253900  |
| C  | -1.57125700 | 1.71571900  | 0.71448500  |
| Sc | -0.58159900 | -0.53938700 | 0.40245500  |
| C  | 2.62159100  | 3.24997600  | 1.14737400  |
| C  | 1.21583600  | 3.23308100  | -1.53388900 |
| C  | 0.04222000  | 4.80347700  | 0.78223700  |
| H  | 2.55480600  | 3.35932900  | 2.23307500  |
| H  | 3.23597000  | 2.37273300  | 0.92806400  |
| H  | 3.15174200  | 4.12590000  | 0.75777300  |
| H  | 0.29521700  | 3.35073400  | -2.11275700 |
| H  | 1.83468500  | 4.11305000  | -1.74309900 |
| H  | 1.75707800  | 2.36214300  | -1.91511400 |
| H  | 0.69558400  | 5.65868800  | 0.58126800  |
| H  | -0.87596900 | 4.94442800  | 0.20573900  |
| H  | -0.21864900 | 4.81907400  | 1.84466000  |
| Si | 0.92480900  | 3.20192300  | 0.33339200  |
| C  | -2.33784500 | 2.50169000  | -0.31407300 |
| H  | -3.19308900 | 1.93985900  | -0.69949700 |
| H  | -2.72514400 | 3.42423200  | 0.13292400  |
| H  | -1.71713900 | 2.79308900  | -1.16633200 |
| C  | -3.65674300 | 0.70640700  | 1.91999900  |
| H  | -3.90412900 | -0.33847800 | 2.13390500  |
| H  | -3.98259900 | 1.29564800  | 2.78453800  |
| H  | -4.24368000 | 1.02443300  | 1.05767800  |
| C  | -1.45567200 | -0.30738600 | 3.85838200  |
| H  | -0.53743800 | -0.67028100 | 4.32577800  |
| H  | -1.97130800 | 0.32015900  | 4.59331400  |
| H  | -2.09926200 | -1.17138800 | 3.66029400  |
| C  | 1.34736100  | 0.84069700  | 2.94030700  |
| H  | 2.20909700  | 0.99280100  | 2.29394800  |
| H  | 1.42184700  | 1.55748900  | 3.76579400  |
| H  | 1.42949500  | -0.16029800 | 3.37735300  |
| C  | -5.17316500 | -0.10210200 | -1.72746000 |
| C  | -4.43339500 | 0.46603900  | -2.76193600 |
| C  | -3.06300700 | 0.24642600  | -2.82972100 |
| C  | -2.43173700 | -0.54055900 | -1.86524500 |
| C  | -3.16120500 | -1.14844900 | -0.82875100 |
| C  | -4.54037500 | -0.89941800 | -0.78203600 |
| H  | -6.24267200 | 0.06697700  | -1.66292400 |
| H  | -4.91738200 | 1.08082700  | -3.51279700 |
| H  | -2.49287600 | 0.70021200  | -3.63175400 |
| H  | -5.12111400 | -1.35438400 | 0.01535800  |
| N  | -0.99217400 | -0.77276100 | -1.88995300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.69751700 | -2.08541800 | -2.51313600 |
| H | -0.91475800 | -2.04335400 | -3.58709000 |
| H | 0.35530700  | -2.33542700 | -2.36298700 |
| H | -1.31865400 | -2.85878500 | -2.06311300 |
| C | -0.24827000 | 0.27941000  | -2.60545000 |
| H | -0.55326600 | 1.25889400  | -2.23584900 |
| H | 0.81774100  | 0.14654200  | -2.42065900 |
| H | -0.41306900 | 0.23075800  | -3.68819200 |
| C | -2.52360300 | -2.06596300 | 0.18392600  |
| H | -2.39670100 | -3.06587500 | -0.25450000 |
| H | -3.21284400 | -2.19486600 | 1.02521400  |
| C | 1.80260600  | -3.91603800 | 2.32124300  |
| C | 0.96422700  | -3.28245700 | 1.19295600  |
| H | 2.61832200  | -4.52815200 | 1.92174400  |
| H | 2.23149500  | -3.14805100 | 2.97278000  |
| H | 1.16050100  | -4.55887100 | 2.92909500  |
| C | -0.17959400 | -2.44484600 | 1.76872300  |
| C | 0.44974700  | -4.40622600 | 0.27488700  |
| H | -1.36167600 | -2.18144000 | 0.90864800  |
| H | -0.83715700 | -3.10032700 | 2.35520500  |
| H | 0.24104300  | -1.74414500 | 2.49985800  |
| H | -0.17589400 | -5.08715300 | 0.85934300  |
| H | -0.15166900 | -4.01072000 | -0.54731300 |
| H | 1.27464300  | -4.98618000 | -0.15054100 |
| C | 1.89369800  | -2.41221800 | 0.40063000  |
| H | 2.87382400  | -2.84630700 | 0.16744200  |
| N | 1.61548700  | -1.22052800 | 0.02362000  |
| C | 2.69318200  | -0.46894600 | -0.67515400 |
| C | 3.92970000  | -0.27119100 | 0.21149700  |
| C | 3.11825900  | -1.12051300 | -1.99966200 |
| H | 2.27675700  | 0.52533300  | -0.88387900 |
| C | 4.96061400  | 0.60918600  | -0.50070200 |
| H | 4.37892200  | -1.25028200 | 0.42491100  |
| H | 3.63991200  | 0.16058400  | 1.17367500  |
| C | 4.15235800  | -0.25208300 | -2.72210200 |
| H | 3.56023800  | -2.10274500 | -1.78661400 |
| H | 2.25384600  | -1.29959800 | -2.64648200 |
| C | 5.37552800  | -0.00025300 | -1.83982000 |
| H | 5.83017300  | 0.75344800  | 0.14674200  |
| H | 4.52795500  | 1.60312100  | -0.67849200 |
| H | 4.44423100  | -0.73496100 | -3.65894100 |
| H | 3.69240500  | 0.70902700  | -2.99079700 |
| H | 6.08306900  | 0.65722300  | -2.35278300 |
| H | 5.89383500  | -0.95133400 | -1.66116300 |

cis-13''

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.88867400 | -0.83743800 | -0.83571700 |
| C  | -2.25319700 | -2.11930000 | -0.85329500 |
| C  | -1.20258800 | -2.10229300 | -1.80769400 |
| C  | -1.20517900 | -0.82709000 | -2.44478500 |
| C  | -2.24132000 | -0.05610900 | -1.86167900 |
| Sc | -0.51183400 | -0.36557000 | -0.14616700 |
| C  | -5.83105800 | -0.97455100 | -1.45397600 |
| C  | -5.10474800 | -1.16592600 | 1.49357800  |
| C  | -4.77465000 | 1.46978800  | 0.11420300  |
| H  | -5.61726900 | -0.53552200 | -2.43287400 |
| H  | -5.78813800 | -2.06318700 | -1.55969500 |
| H  | -6.85313100 | -0.70084700 | -1.17478100 |
| H  | -4.55763400 | -0.76459600 | 2.35175900  |
| H  | -6.15574200 | -0.88900900 | 1.63720600  |
| H  | -5.06092600 | -2.25681900 | 1.53098300  |
| H  | -5.64838800 | 1.65091900  | 0.74877200  |
| H  | -3.90613200 | 1.90349300  | 0.62323400  |
| H  | -4.92649500 | 2.01774400  | -0.81865000 |
| Si | -4.60282100 | -0.39079800 | -0.15567400 |
| C  | -2.74301600 | 1.23857400  | -2.44236000 |
| H  | -2.06764600 | 1.60322400  | -3.21948800 |
| H  | -3.71863100 | 1.07228300  | -2.91393800 |
| H  | -2.87200200 | 2.02943600  | -1.70377100 |
| C  | -0.34486300 | -0.41543700 | -3.60779100 |
| H  | 0.47234400  | -1.12499600 | -3.75655900 |
| H  | -0.93261800 | -0.39492000 | -4.53165300 |
| H  | 0.09119600  | 0.57875000  | -3.46586700 |
| C  | -0.37934000 | -3.29601600 | -2.20186900 |
| H  | -0.40769800 | -4.07063300 | -1.43068100 |
| H  | -0.77454000 | -3.74005600 | -3.12205800 |
| H  | 0.66739200  | -3.04162600 | -2.38059200 |
| C  | -2.73663900 | -3.39303900 | -0.21210700 |
| H  | -3.52276200 | -3.21787400 | 0.52047500  |
| H  | -3.15330400 | -4.04350600 | -0.98882800 |
| H  | -1.94178500 | -3.96564300 | 0.27765500  |
| C  | 3.04356200  | 3.88230800  | -0.67424800 |
| C  | 2.96384800  | 2.42812100  | -1.17508200 |
| H  | 2.06738600  | 4.35555100  | -0.54832100 |
| H  | 3.55953900  | 3.93038600  | 0.29164000  |
| H  | 3.61162200  | 4.49167200  | -1.38376600 |
| C  | 4.41572000  | 1.88054200  | -1.18946800 |
| C  | 2.36724900  | 2.41348800  | -2.58473500 |
| H  | 4.54247800  | 1.16319000  | -2.00815000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.14940800  | 2.67801900  | -1.33857600 |
| H | 2.87352500  | 3.16814400  | -3.19611300 |
| H | 2.51210300  | 1.45566700  | -3.08803900 |
| H | 1.30047000  | 2.64236000  | -2.59148100 |
| C | 2.24592600  | 1.51418200  | -0.07214600 |
| H | 2.32150700  | 2.12367100  | 0.83580300  |
| N | 0.83261000  | 1.12466000  | -0.17749300 |
| C | -0.12901400 | 2.18117100  | 0.19475100  |
| C | 0.20337700  | 2.95031400  | 1.48905700  |
| C | -0.51545700 | 3.19197500  | -0.89916700 |
| H | -1.11676500 | 1.66389300  | 0.40695200  |
| C | -0.95800000 | 3.83973000  | 1.94311700  |
| H | 1.05745100  | 3.60595100  | 1.28928100  |
| H | 0.53305200  | 2.25673500  | 2.27281300  |
| C | -1.66744000 | 4.09849200  | -0.45437800 |
| H | 0.35134400  | 3.81711300  | -1.12468400 |
| H | -0.76008500 | 2.65569800  | -1.81885800 |
| C | -1.32926100 | 4.83462300  | 0.84237900  |
| H | -0.68017100 | 4.36673400  | 2.86086600  |
| H | -1.84107400 | 3.22950000  | 2.18416600  |
| H | -1.90481500 | 4.80886500  | -1.25218100 |
| H | -2.57444300 | 3.50030600  | -0.28769400 |
| H | -2.17277000 | 5.45511500  | 1.15844500  |
| H | -0.48159200 | 5.51040200  | 0.66784700  |
| C | 4.58397800  | 1.15440500  | 0.14436700  |
| C | 3.25153300  | 0.38538300  | 0.26538300  |
| H | 4.67388500  | 1.87052800  | 0.96970300  |
| H | 5.45725200  | 0.49872800  | 0.17203000  |
| H | 3.07854700  | 0.05841200  | 1.29894000  |
| C | 3.34168100  | -0.85048800 | -0.60632300 |
| C | 4.14859600  | -1.90102700 | -0.14605200 |
| C | 2.74718100  | -0.98434100 | -1.86304400 |
| C | 4.34609200  | -3.04917700 | -0.90293200 |
| H | 4.63858300  | -1.79925100 | 0.81955200  |
| C | 2.97004800  | -2.12295100 | -2.64278600 |
| H | 2.10623200  | -0.19282500 | -2.23622100 |
| C | 3.75774800  | -3.16328800 | -2.16341400 |
| H | 4.97499800  | -3.84771500 | -0.52186700 |
| H | 2.52859500  | -2.19293700 | -3.63333400 |
| H | 3.92662300  | -4.04747400 | -2.76901000 |
| C | 2.86833200  | -1.51756300 | 3.91147200  |
| C | 2.03189200  | -0.55456200 | 4.46257500  |
| C | 0.78646000  | -0.30031200 | 3.89104300  |
| C | 0.39354400  | -0.98242800 | 2.74187100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.25550900  | -1.91577400 | 2.13962700  |
| C | 2.47304700  | -2.19336500 | 2.76009700  |
| H | 3.82482700  | -1.74084200 | 4.37120100  |
| H | 2.32921200  | -0.01297700 | 5.35387200  |
| H | 0.12968200  | 0.42369100  | 4.35834300  |
| H | 3.12503900  | -2.94039400 | 2.31742200  |
| N | -0.93452400 | -0.81599700 | 2.15669100  |
| C | -1.75516000 | -2.00726100 | 2.51437600  |
| H | -1.89827000 | -2.02812500 | 3.60084000  |
| H | -2.72020900 | -1.92612500 | 2.01829700  |
| H | -1.26621300 | -2.93180500 | 2.21777500  |
| C | -1.68441100 | 0.34753800  | 2.67928000  |
| H | -1.08888400 | 1.25238400  | 2.61070100  |
| H | -2.59660500 | 0.46257800  | 2.08677200  |
| H | -1.97635700 | 0.19159600  | 3.72447000  |
| C | 0.93319000  | -2.55294900 | 0.81077400  |
| H | -0.11351200 | -2.83798400 | 0.67954800  |
| H | 1.52529000  | -3.45664100 | 0.64565800  |
| H | 1.26143000  | -1.90860200 | -0.02815800 |

trans-13''

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 3.17876800 | -0.55629500 | -0.88805000 |
| C  | 2.63441000 | -0.16949600 | -2.15365900 |
| C  | 1.62778200 | -1.10271100 | -2.51512300 |
| C  | 1.58332700 | -2.12001300 | -1.52194000 |
| C  | 2.52237600 | -1.78445800 | -0.51392200 |
| Sc | 0.80410800 | -0.02819300 | -0.40350700 |
| C  | 6.12708600 | -1.07879200 | -0.21201000 |
| C  | 5.30198900 | 1.78586100  | -0.40944700 |
| C  | 4.19021800 | 0.09084800  | 1.91866900  |
| H  | 5.91545400 | -2.11963700 | 0.04280300  |
| H  | 6.42079500 | -1.04633100 | -1.26577000 |
| H  | 6.98638800 | -0.75542700 | 0.38418200  |
| H  | 4.58833500 | 2.60786000  | -0.31899000 |
| H  | 6.13679000 | 2.01544600  | 0.26260100  |
| H  | 5.70484900 | 1.78849100  | -1.42621600 |
| H  | 4.68753500 | 0.90991800  | 2.44805400  |
| H  | 3.10739000 | 0.21040200  | 2.06074000  |
| H  | 4.47950000 | -0.84341600 | 2.40837200  |
| Si | 4.67137800 | 0.07625100  | 0.08248300  |
| C  | 2.88894200 | -2.65649800 | 0.66166600  |
| H  | 2.46584500 | -3.65587800 | 0.54635100  |
| H  | 3.97369900 | -2.77151400 | 0.73143800  |
| H  | 2.54268600 | -2.26332900 | 1.62266400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.83635100  | -3.41107800 | -1.68780900 |
| H | -0.15586500 | -3.26012100 | -2.12269100 |
| H | 1.38930900  | -4.06421300 | -2.37283600 |
| H | 0.71395200  | -3.94545300 | -0.74596000 |
| C | 0.85913600  | -1.12439300 | -3.80661900 |
| H | 0.88197200  | -0.15279700 | -4.30717900 |
| H | 1.28855700  | -1.85778100 | -4.49777600 |
| H | -0.18998700 | -1.40169300 | -3.65505400 |
| C | 3.17315300  | 0.85464700  | -3.11655000 |
| H | 3.88716700  | 1.53041000  | -2.64726200 |
| H | 3.69969400  | 0.33695800  | -3.92565400 |
| H | 2.39077300  | 1.45802000  | -3.58796900 |
| C | -2.68431400 | -3.24818500 | 2.54222300  |
| C | -1.73517200 | -3.11687000 | 1.34310000  |
| H | -2.42734700 | -2.53693300 | 3.33521600  |
| H | -3.72425100 | -3.05823500 | 2.25376900  |
| H | -2.62956300 | -4.25640400 | 2.96524700  |
| C | -2.26455800 | -4.01470000 | 0.20096000  |
| C | -0.32914400 | -3.55738100 | 1.74931000  |
| H | -1.44108200 | -4.30748800 | -0.45865700 |
| H | -2.71055300 | -4.93532800 | 0.59107900  |
| H | -0.22376400 | -4.64030500 | 1.61956900  |
| H | 0.41905400  | -3.05521800 | 1.13536200  |
| H | -0.10510800 | -3.33520600 | 2.79517500  |
| C | -1.85198500 | -1.63306200 | 0.76150800  |
| H | -2.58646900 | -1.14269600 | 1.40562000  |
| N | -0.66932600 | -0.76920600 | 0.71743500  |
| C | -0.44245000 | 0.05477400  | 1.91586000  |
| C | -1.63768100 | 0.92699900  | 2.34545400  |
| C | 0.12995000  | -0.67361300 | 3.14243900  |
| H | 0.35922600  | 0.78863300  | 1.64231800  |
| C | -1.26919700 | 1.89748000  | 3.47162000  |
| H | -2.42465100 | 0.26574100  | 2.73061700  |
| H | -2.04950000 | 1.44954200  | 1.47494800  |
| C | 0.50506000  | 0.30307100  | 4.25992900  |
| H | -0.62855400 | -1.37147300 | 3.51725800  |
| H | 0.99636000  | -1.27468900 | 2.84608700  |
| C | -0.69493600 | 1.15334500  | 4.67678700  |
| H | -2.15234000 | 2.47837600  | 3.75622400  |
| H | -0.52809900 | 2.62377700  | 3.11262100  |
| H | 0.90306200  | -0.25069500 | 5.11555300  |
| H | 1.31584900  | 0.96265200  | 3.91381100  |
| H | -0.40870600 | 1.85983800  | 5.46168400  |
| H | -1.46778700 | 0.49904700  | 5.10162200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.24115000 | -3.14165000 | -0.56931800 |
| C | -2.51808300 | -1.78588300 | -0.62882100 |
| H | -4.18417300 | -3.02265800 | -0.02237000 |
| H | -3.48857800 | -3.51825600 | -1.56582400 |
| H | -1.71286800 | -1.88379700 | -1.37547000 |
| C | -3.47516900 | -0.70244700 | -1.08493300 |
| C | -3.64559800 | -0.48286500 | -2.45809000 |
| C | -4.32892800 | -0.02976400 | -0.20431700 |
| C | -4.63516000 | 0.37012300  | -2.94016600 |
| H | -3.00605800 | -1.01433900 | -3.16132800 |
| C | -5.32141000 | 0.82534400  | -0.68036100 |
| H | -4.24481700 | -0.18665600 | 0.86707600  |
| C | -5.48276500 | 1.02654700  | -2.04877000 |
| H | -4.75274000 | 0.51171700  | -4.00999200 |
| H | -5.97738800 | 1.32768300  | 0.02378000  |
| H | -6.26199900 | 1.68503300  | -2.41816200 |
| C | -2.95734200 | 3.68123300  | -0.16374000 |
| C | -2.05357700 | 4.24404200  | 0.73098400  |
| C | -0.72043700 | 3.84291400  | 0.71930500  |
| C | -0.29262400 | 2.85799200  | -0.17001600 |
| C | -1.19168300 | 2.30279000  | -1.09565300 |
| C | -2.51968700 | 2.72748200  | -1.07619800 |
| H | -3.99886000 | 3.98477800  | -0.16005800 |
| H | -2.37747200 | 5.00007400  | 1.43824400  |
| H | -0.02609100 | 4.30096100  | 1.41375600  |
| H | -3.21896500 | 2.29053200  | -1.78257800 |
| N | 1.09604700  | 2.40602800  | -0.21154700 |
| C | 1.77261300  | 3.11940600  | -1.32936300 |
| H | 1.76010400  | 4.19665800  | -1.12754900 |
| H | 2.80166600  | 2.77360600  | -1.40234000 |
| H | 1.26179400  | 2.94541600  | -2.27472900 |
| C | 1.86912200  | 2.74475700  | 1.00600100  |
| H | 1.34674100  | 2.43130000  | 1.90957500  |
| H | 2.83396500  | 2.23793200  | 0.95546600  |
| H | 2.05532300  | 3.82295200  | 1.06871400  |
| C | -0.79219500 | 1.23046700  | -2.07996400 |
| H | 0.26687200  | 1.24126700  | -2.36673000 |
| H | -1.34354700 | 1.32528400  | -3.01828300 |
| H | -1.09634100 | 0.23465900  | -1.70836000 |

cis-ts-14'

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.77110000 | -1.40994300 | 0.13125200  |
| C | 2.35916600 | -1.95392400 | -1.13363200 |
| C | 1.17332700 | -2.71075300 | -0.94679900 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.88097100  | -2.72017900 | 0.45048900  |
| C  | 1.84170900  | -1.91521200 | 1.10520700  |
| Sc | 0.54143000  | -0.38709000 | -0.36475200 |
| C  | 5.27106700  | -2.08041200 | 1.70571200  |
| C  | 5.64114500  | -0.44164000 | -0.80686500 |
| C  | 4.37774600  | 0.85949400  | 1.62124500  |
| H  | 4.75864500  | -2.21712900 | 2.66105200  |
| H  | 5.27291800  | -3.04132700 | 1.18202300  |
| H  | 6.31053000  | -1.81278800 | 1.92104500  |
| H  | 5.28933800  | 0.29821700  | -1.53179800 |
| H  | 6.57727400  | -0.05841700 | -0.38582100 |
| H  | 5.87834600  | -1.36402000 | -1.34357500 |
| H  | 5.35088100  | 1.04179900  | 2.08979900  |
| H  | 4.16727200  | 1.71536300  | 0.97255300  |
| H  | 3.62894400  | 0.84664800  | 2.41838700  |
| Si | 4.47524700  | -0.74835700 | 0.64157300  |
| C  | 1.95223400  | -1.81801000 | 2.60253700  |
| H  | 0.97561900  | -1.68644700 | 3.07432100  |
| H  | 2.38294300  | -2.74395700 | 3.00100200  |
| H  | 2.59555200  | -0.99527700 | 2.92090800  |
| C  | -0.02246500 | -3.70327400 | 1.13486000  |
| H  | -0.83257500 | -4.03074000 | 0.48653700  |
| H  | 0.56690000  | -4.59194900 | 1.38979500  |
| H  | -0.44604300 | -3.32730100 | 2.06749600  |
| C  | 0.45569900  | -3.50956600 | -1.99863600 |
| H  | 0.60689500  | -3.08819100 | -2.99636600 |
| H  | 0.82282000  | -4.54169700 | -2.01890000 |
| H  | -0.62124200 | -3.54104400 | -1.81254300 |
| C  | 3.17736800  | -2.02864300 | -2.39341100 |
| H  | 3.89312900  | -1.21288500 | -2.48219600 |
| H  | 3.75558300  | -2.95995500 | -2.37499200 |
| H  | 2.55982200  | -2.05428800 | -3.29387200 |
| C  | -2.86338700 | 1.17456500  | 3.77406700  |
| C  | -2.68469900 | 0.01597000  | 2.77755600  |
| H  | -1.99597400 | 1.83832600  | 3.81617900  |
| H  | -3.73048700 | 1.78892200  | 3.50993000  |
| H  | -3.02838500 | 0.78031900  | 4.78163300  |
| C  | -4.06275900 | -0.66936900 | 2.62816900  |
| C  | -1.61854000 | -0.93855000 | 3.29907600  |
| H  | -3.94269800 | -1.72660900 | 2.36558800  |
| H  | -4.63604000 | -0.62697000 | 3.55896300  |
| H  | -2.00893300 | -1.51494400 | 4.14406200  |
| H  | -1.29783600 | -1.63467400 | 2.52181300  |
| H  | -0.73190500 | -0.39917200 | 3.64497900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.40521900 | 0.58874200  | 1.32508800  |
| H | -2.61903000 | 1.65432000  | 1.42405000  |
| N | -1.04104000 | 0.50543700  | 0.74193600  |
| C | -0.19020800 | 1.70207700  | 1.02660900  |
| C | -0.85760700 | 3.07009700  | 0.79560100  |
| C | 0.53139000  | 1.67080200  | 2.38174600  |
| H | 0.64315000  | 1.69515700  | 0.27925100  |
| C | 0.14334300  | 4.21959100  | 0.93296700  |
| H | -1.62237400 | 3.22166100  | 1.56605800  |
| H | -1.35754800 | 3.08614900  | -0.17903600 |
| C | 1.50342100  | 2.84701700  | 2.52714100  |
| H | -0.20915700 | 1.71106900  | 3.18488000  |
| H | 1.06423400  | 0.71668500  | 2.49359600  |
| C | 0.80888100  | 4.18996400  | 2.30790900  |
| H | -0.37480200 | 5.16893300  | 0.76812800  |
| H | 0.90990500  | 4.14602000  | 0.14956500  |
| H | 1.98085900  | 2.80669200  | 3.51109600  |
| H | 2.30910600  | 2.74422900  | 1.78823000  |
| H | 1.52909300  | 5.00732500  | 2.40538700  |
| H | 0.04586900  | 4.34000700  | 3.08282700  |
| C | -4.73377600 | 0.07278900  | 1.47313500  |
| C | -3.60174100 | 0.14634200  | 0.42395100  |
| H | -5.02647900 | 1.08317900  | 1.78068400  |
| H | -5.62183800 | -0.43049000 | 1.08499800  |
| H | -3.79023800 | 0.95246000  | -0.29664800 |
| C | -3.60858000 | -1.14983700 | -0.35868600 |
| C | -4.46435300 | -1.21083300 | -1.46781100 |
| C | -2.90244600 | -2.29892400 | -0.00554900 |
| C | -4.60647700 | -2.37572300 | -2.21131700 |
| H | -5.02864800 | -0.32354600 | -1.74695300 |
| C | -3.06583300 | -3.47998400 | -0.73470300 |
| H | -2.23900100 | -2.27753200 | 0.85363800  |
| C | -3.90588100 | -3.52258200 | -1.84208700 |
| H | -5.26962300 | -2.39277100 | -3.07012100 |
| H | -2.54931800 | -4.38533200 | -0.43162800 |
| H | -4.02245600 | -4.44348700 | -2.40342100 |
| C | -2.08541700 | 3.56527500  | -2.87602700 |
| C | -0.85198100 | 4.20025600  | -2.77209700 |
| C | 0.29140600  | 3.45357800  | -2.49166000 |
| C | 0.18870800  | 2.08056400  | -2.28851900 |
| C | -1.04794100 | 1.42178800  | -2.38502700 |
| C | -2.17832700 | 2.18905000  | -2.68290500 |
| H | -2.97631700 | 4.13957300  | -3.10677200 |
| H | -0.77041800 | 5.27195500  | -2.91611700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.24938300  | 3.95745200  | -2.42438000 |
| H | -3.14145800 | 1.69145100  | -2.76126300 |
| N | 1.35446200  | 1.23082200  | -2.03723500 |
| C | 1.75314100  | 0.67135100  | -3.36138300 |
| H | 1.83922800  | 1.49036700  | -4.08346200 |
| H | 2.71572700  | 0.17748400  | -3.27198900 |
| H | 1.00937000  | -0.03930700 | -3.72403600 |
| C | 2.52793100  | 1.96712400  | -1.52077900 |
| H | 2.26509900  | 2.55438800  | -0.63874500 |
| H | 3.29520900  | 1.23795600  | -1.25305400 |
| H | 2.94557100  | 2.64063100  | -2.27774500 |
| C | -1.16335400 | -0.01367000 | -1.98721200 |
| H | -0.47424200 | -0.67525500 | -2.53628100 |
| H | -2.15564900 | -0.41747200 | -2.17271500 |
| H | -1.26451300 | 0.26986900  | -0.57643800 |

trans-ts-14'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.29114800  | -0.65450200 | -0.80474400 |
| C  | 2.75326700  | -0.36482200 | -2.10090500 |
| C  | 1.73146000  | -1.30659300 | -2.38424100 |
| C  | 1.67885100  | -2.24327700 | -1.31326000 |
| C  | 2.62277000  | -1.84340300 | -0.33592700 |
| Sc | 0.95019000  | -0.04413200 | -0.39302500 |
| C  | 6.22822500  | -1.08222100 | 0.01525200  |
| C  | 5.36788500  | 1.73729100  | -0.51897500 |
| C  | 4.21231900  | 0.27622700  | 1.94880300  |
| H  | 6.03132900  | -2.08121900 | 0.41078500  |
| H  | 6.53370400  | -1.18906300 | -1.03007800 |
| H  | 7.07502200  | -0.66422500 | 0.56937600  |
| H  | 4.62077800  | 2.53222800  | -0.57850000 |
| H  | 6.15035900  | 2.08548500  | 0.16446900  |
| H  | 5.83082000  | 1.62581900  | -1.50348500 |
| H  | 4.62254500  | 1.19215600  | 2.38600800  |
| H  | 3.11928700  | 0.31619200  | 2.05378800  |
| H  | 4.56071900  | -0.56440400 | 2.55613700  |
| Si | 4.75381100  | 0.07922800  | 0.13937300  |
| C  | 2.96306300  | -2.59736500 | 0.92604500  |
| H  | 2.56474100  | -3.61296400 | 0.88890000  |
| H  | 4.04624800  | -2.67780500 | 1.04564700  |
| H  | 2.57163800  | -2.12824300 | 1.83561800  |
| C  | 0.89607100  | -3.52096800 | -1.39310700 |
| H  | -0.15375100 | -3.34178600 | -1.64079800 |
| H  | 1.31031300  | -4.14797400 | -2.19058900 |
| H  | 0.93175800  | -4.09420900 | -0.46678000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.94477300  | -1.42404900 | -3.65805600 |
| H | 0.99542400  | -0.50677600 | -4.24986300 |
| H | 1.33486200  | -2.23886600 | -4.27808200 |
| H | -0.11170400 | -1.63935200 | -3.46177000 |
| C | 3.30718700  | 0.57130000  | -3.14085400 |
| H | 4.00858500  | 1.29102700  | -2.72071200 |
| H | 3.85301600  | -0.01726300 | -3.88611600 |
| H | 2.52892800  | 1.12068700  | -3.67840300 |
| C | -2.58909500 | -3.05981300 | 2.78479300  |
| C | -1.68480600 | -2.98696700 | 1.54545200  |
| H | -2.33998900 | -2.28100900 | 3.51388000  |
| H | -3.64469500 | -2.93688300 | 2.51818400  |
| H | -2.47627700 | -4.02939800 | 3.27980600  |
| C | -2.20113000 | -4.01202700 | 0.50916500  |
| C | -0.24598100 | -3.31524000 | 1.93853100  |
| H | -1.38259600 | -4.33046900 | -0.14396900 |
| H | -2.59089400 | -4.90967100 | 0.99953600  |
| H | -0.10007900 | -4.40115400 | 1.94171700  |
| H | 0.45321800  | -2.87452000 | 1.22811400  |
| H | 0.01255600  | -2.95228500 | 2.93560500  |
| C | -1.90496300 | -1.57600100 | 0.83969100  |
| H | -2.63762000 | -1.06170300 | 1.46450400  |
| N | -0.76341400 | -0.64965100 | 0.67490000  |
| C | -0.57582900 | 0.32192500  | 1.78720000  |
| C | -1.80750900 | 1.17344800  | 2.13934100  |
| C | 0.03906200  | -0.27780400 | 3.05770100  |
| H | 0.17745300  | 1.06433600  | 1.43520400  |
| C | -1.46601300 | 2.25292200  | 3.17067500  |
| H | -2.56832600 | 0.52028900  | 2.58501200  |
| H | -2.23869200 | 1.61316800  | 1.23380400  |
| C | 0.36365100  | 0.80238500  | 4.09380000  |
| H | -0.67236900 | -0.99100300 | 3.48908000  |
| H | 0.94279100  | -0.84283800 | 2.79338100  |
| C | -0.87031400 | 1.63738900  | 4.43597100  |
| H | -2.36647000 | 2.82946200  | 3.40308300  |
| H | -0.74904100 | 2.96330700  | 2.73777000  |
| H | 0.77796200  | 0.33477400  | 4.99172100  |
| H | 1.14896400  | 1.46379600  | 3.69811300  |
| H | -0.61256200 | 2.41790700  | 5.15784900  |
| H | -1.62001100 | 0.99372200  | 4.91499800  |
| C | -3.24498400 | -3.26262700 | -0.30456500 |
| C | -2.60278600 | -1.88114400 | -0.51042000 |
| H | -4.17696400 | -3.14484400 | 0.26076900  |
| H | -3.49823500 | -3.74003900 | -1.25487600 |

|         |             |             |             |
|---------|-------------|-------------|-------------|
| H       | -1.81994900 | -1.98981900 | -1.27807100 |
| C       | -3.62172100 | -0.87786300 | -1.01409300 |
| C       | -3.84132400 | -0.77538700 | -2.39402200 |
| C       | -4.44996500 | -0.14198600 | -0.16181900 |
| C       | -4.84206500 | 0.04238900  | -2.90967000 |
| H       | -3.21887700 | -1.35804100 | -3.07151800 |
| C       | -5.45312700 | 0.68103500  | -0.67275700 |
| H       | -4.33538700 | -0.21250300 | 0.91567700  |
| C       | -5.65338600 | 0.77821000  | -2.04636900 |
| H       | -4.99185600 | 0.10162000  | -3.98293500 |
| H       | -6.08295900 | 1.24353700  | 0.00923900  |
| H       | -6.43600200 | 1.41683500  | -2.44228100 |
| C       | -2.92152200 | 3.71326700  | -0.59119100 |
| C       | -2.00715800 | 4.44059700  | 0.16358500  |
| C       | -0.68002700 | 4.02059300  | 0.24139700  |
| C       | -0.28165000 | 2.85744000  | -0.41112500 |
| C       | -1.19609200 | 2.10647700  | -1.17078700 |
| C       | -2.51523900 | 2.55873200  | -1.25417400 |
| H       | -3.95501300 | 4.03676000  | -0.66044700 |
| H       | -2.31534400 | 5.33793300  | 0.68901000  |
| H       | 0.02561800  | 4.60322900  | 0.82339400  |
| H       | -3.23071500 | 1.98066500  | -1.83212800 |
| N       | 1.10854400  | 2.38619900  | -0.38950100 |
| C       | 1.76641000  | 2.91965000  | -1.61269600 |
| H       | 1.73018900  | 4.01486400  | -1.59647900 |
| H       | 2.80353200  | 2.58992200  | -1.63592600 |
| H       | 1.24964300  | 2.56830800  | -2.50623500 |
| C       | 1.88828400  | 2.88869800  | 0.76721300  |
| H       | 1.35391900  | 2.71165700  | 1.70205500  |
| H       | 2.84782400  | 2.36759700  | 0.79795900  |
| H       | 2.08734900  | 3.96216500  | 0.67476100  |
| C       | -0.79892500 | 0.77900100  | -1.73353100 |
| H       | 0.07362500  | 0.85269300  | -2.40240700 |
| H       | -1.59068000 | 0.33880800  | -2.33778900 |
| H       | -0.97380100 | 0.00164000  | -0.53416500 |
| cis-15' |             |             |             |
| C       | 2.81505900  | -1.08222900 | 0.67228600  |
| C       | 2.45864200  | -2.19478000 | -0.16287600 |
| C       | 1.32631900  | -2.84058300 | 0.38598600  |
| C       | 0.99103100  | -2.18079400 | 1.60285300  |
| C       | 1.89603800  | -1.10443000 | 1.77968400  |
| Sc      | 0.56596300  | -0.56617500 | -0.29604800 |
| C       | 5.38310600  | -0.87868400 | 2.25776700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.59524800  | -0.42004500 | -0.72263900 |
| C  | 4.31091600  | 1.69866600  | 1.00813100  |
| H  | 4.88748700  | -0.63709400 | 3.20167600  |
| H  | 5.45360600  | -1.96813900 | 2.18283900  |
| H  | 6.40032800  | -0.47648200 | 2.30235500  |
| H  | 5.15944400  | -0.13429000 | -1.68508900 |
| H  | 6.47673200  | 0.21262500  | -0.56862700 |
| H  | 5.94653400  | -1.45245400 | -0.79994100 |
| H  | 5.27788900  | 2.07700900  | 1.35772300  |
| H  | 4.08363800  | 2.22008900  | 0.07382500  |
| H  | 3.56230800  | 1.99328300  | 1.74777100  |
| Si | 4.47066200  | -0.16940100 | 0.77172500  |
| C  | 2.02566000  | -0.32726400 | 3.06219900  |
| H  | 1.05586300  | -0.07423200 | 3.49508500  |
| H  | 2.56036600  | -0.93113400 | 3.80442600  |
| H  | 2.58744400  | 0.59926800  | 2.93178200  |
| C  | 0.09254400  | -2.76377900 | 2.65728500  |
| H  | -0.84383100 | -3.14755100 | 2.24961300  |
| H  | 0.60497700  | -3.61195100 | 3.12649900  |
| H  | -0.14080200 | -2.05142300 | 3.45010100  |
| C  | 0.70284200  | -4.10811400 | -0.11926900 |
| H  | 1.05834000  | -4.35272000 | -1.12281400 |
| H  | 0.95772600  | -4.94906800 | 0.53577800  |
| H  | -0.38642800 | -4.03517000 | -0.16534000 |
| C  | 3.23463700  | -2.78075800 | -1.31004900 |
| H  | 4.00445300  | -2.10711900 | -1.67856300 |
| H  | 3.73755400  | -3.69406600 | -0.97220400 |
| H  | 2.59437700  | -3.06445600 | -2.15012800 |
| C  | -2.97454900 | 2.43908100  | 3.15160500  |
| C  | -2.71459100 | 1.04898800  | 2.54505000  |
| H  | -2.18169500 | 3.15584600  | 2.91918300  |
| H  | -3.91597500 | 2.85846000  | 2.78143100  |
| H  | -3.04678800 | 2.36386900  | 4.24088900  |
| C  | -4.01018300 | 0.21967100  | 2.74051800  |
| C  | -1.51778000 | 0.40835900  | 3.24425500  |
| H  | -3.77837600 | -0.84554200 | 2.83656100  |
| H  | -4.53638200 | 0.51800100  | 3.65195900  |
| H  | -1.83336200 | -0.05150400 | 4.18671400  |
| H  | -1.05103500 | -0.36300900 | 2.62698800  |
| H  | -0.75115000 | 1.14871900  | 3.48474800  |
| C  | -2.60031900 | 1.17073500  | 0.97643200  |
| H  | -2.88931600 | 2.20175600  | 0.75645400  |
| N  | -1.29230900 | 0.95965000  | 0.26021900  |
| C  | -0.44617400 | 2.19128700  | 0.14707500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.16391600 | 3.42318600  | -0.42055800 |
| C | 0.31481700  | 2.54676000  | 1.42053900  |
| H | 0.31618700  | 1.93136300  | -0.60910200 |
| C | -0.15924000 | 4.54032900  | -0.71293900 |
| H | -1.87897900 | 3.80518900  | 0.31751300  |
| H | -1.72699300 | 3.14618800  | -1.31929100 |
| C | 1.29693300  | 3.69490300  | 1.15568700  |
| H | -0.39321100 | 2.85427900  | 2.19547800  |
| H | 0.84891300  | 1.66828800  | 1.80635000  |
| C | 0.59802000  | 4.91717900  | 0.56114500  |
| H | -0.68298100 | 5.40812800  | -1.12338100 |
| H | 0.55135600  | 4.20789900  | -1.48345000 |
| H | 1.81298700  | 3.95599300  | 2.08466200  |
| H | 2.07236200  | 3.35446000  | 0.45735500  |
| H | 1.32905600  | 5.70430700  | 0.35615900  |
| H | -0.11282800 | 5.32290700  | 1.29269000  |
| C | -4.82739000 | 0.45925900  | 1.47236500  |
| C | -3.76654000 | 0.35425600  | 0.35575800  |
| H | -5.25971500 | 1.46638800  | 1.47704500  |
| H | -5.64118100 | -0.25568200 | 1.33436000  |
| H | -4.10368600 | 0.87361800  | -0.55014200 |
| C | -3.57034900 | -1.10077200 | -0.01735600 |
| C | -4.33060900 | -1.60330400 | -1.08139000 |
| C | -2.80954700 | -2.00497300 | 0.72772500  |
| C | -4.32870600 | -2.95674300 | -1.40078600 |
| H | -4.94417300 | -0.91714100 | -1.66124400 |
| C | -2.83347000 | -3.36916800 | 0.43463800  |
| H | -2.21161700 | -1.64547200 | 1.55917000  |
| C | -3.58242400 | -3.85009800 | -0.63427600 |
| H | -4.92384700 | -3.31577500 | -2.23424900 |
| H | -2.27457200 | -4.06681600 | 1.05051500  |
| H | -3.59371700 | -4.91089000 | -0.86103200 |
| C | -2.42401100 | 1.14835900  | -3.64897900 |
| C | -1.44407500 | 2.13136500  | -3.80707600 |
| C | -0.14468300 | 1.87598300  | -3.38927000 |
| C | 0.17619000  | 0.64731900  | -2.80380500 |
| C | -0.79190900 | -0.37608000 | -2.64572300 |
| C | -2.09763600 | -0.07658800 | -3.08551400 |
| H | -3.43948300 | 1.33392600  | -3.98434600 |
| H | -1.68788900 | 3.08829800  | -4.25589400 |
| H | 0.61605000  | 2.63754200  | -3.51982000 |
| H | -2.85150800 | -0.84897000 | -2.98542700 |
| N | 1.52077800  | 0.33734900  | -2.33490000 |
| C | 2.18038000  | -0.52907700 | -3.34789700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.23499000  | 0.01695200  | -4.29711200 |
| H | 3.18872900  | -0.76948200 | -3.01522100 |
| H | 1.61850600  | -1.44635300 | -3.50362500 |
| C | 2.40890800  | 1.50653300  | -2.17240000 |
| H | 1.97653600  | 2.25575500  | -1.50795300 |
| H | 3.34558500  | 1.15345000  | -1.74068700 |
| H | 2.62933600  | 1.97750000  | -3.13753300 |
| C | -0.47304300 | -1.62742100 | -1.91209600 |
| H | 0.26997800  | -2.26685400 | -2.39638600 |
| H | -1.36788500 | -2.21565600 | -1.69614100 |
| H | -1.62086800 | 0.79821900  | -0.69983400 |

trans-15'

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 3.26555600 | -0.79936100 | -0.01083000 |
| C  | 2.87766600 | -1.54799700 | -1.16933000 |
| C  | 1.91569400 | -2.51291600 | -0.79169000 |
| C  | 1.74151600 | -2.43894000 | 0.62008500  |
| C  | 2.56475500 | -1.38809500 | 1.10461600  |
| Sc | 0.85275700 | -0.29974200 | -0.36016500 |
| C  | 6.18610300 | -0.91668400 | 0.72735000  |
| C  | 5.44130300 | 1.27943700  | -1.20465800 |
| C  | 4.51465400 | 1.51492200  | 1.66351100  |
| H  | 5.91841700 | -1.54302000 | 1.58280600  |
| H  | 6.40922500 | -1.58103600 | -0.11359000 |
| H  | 7.10066500 | -0.37060000 | 0.97836600  |
| H  | 4.81478200 | 2.13130900  | -1.48119500 |
| H  | 6.40090800 | 1.69361300  | -0.87290600 |
| H  | 5.64882600 | 0.69291800  | -2.10281300 |
| H  | 5.17431500 | 2.37733500  | 1.52285400  |
| H  | 3.48577100 | 1.88867000  | 1.70351100  |
| H  | 4.74314600 | 1.08267500  | 2.64102500  |
| Si | 4.80329600 | 0.27182600  | 0.26305600  |
| C  | 2.82719900 | -1.08446600 | 2.55935300  |
| H  | 2.33392900 | -1.81189900 | 3.20587700  |
| H  | 3.89875700 | -1.14509000 | 2.77173100  |
| H  | 2.48995400 | -0.09019500 | 2.86805100  |
| C  | 1.02634000 | -3.50040900 | 1.41143700  |
| H  | 0.02068300 | -3.70492600 | 1.03057800  |
| H  | 1.58674000 | -4.43916100 | 1.33971100  |
| H  | 0.94105200 | -3.25184100 | 2.46977600  |
| C  | 1.31859800 | -3.55587300 | -1.68930100 |
| H  | 1.21856800 | -3.19367900 | -2.71593200 |
| H  | 1.94980300 | -4.45166900 | -1.71388800 |
| H  | 0.32668700 | -3.86280000 | -1.34457300 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.49049100  | -1.52628700 | -2.54246900 |
| H | 4.22746200  | -0.73237600 | -2.65351900 |
| H | 4.00514600  | -2.47708900 | -2.71865100 |
| H | 2.74834400  | -1.41834200 | -3.34032500 |
| C | -2.62932000 | -0.18574700 | 4.04094200  |
| C | -1.80491400 | -0.98359500 | 3.02334000  |
| H | -2.45273000 | 0.89199000  | 3.96727400  |
| H | -3.70149000 | -0.35810900 | 3.89466200  |
| H | -2.37506300 | -0.49578600 | 5.05911200  |
| C | -2.23612200 | -2.47939400 | 3.08516600  |
| C | -0.31799900 | -0.87697500 | 3.33976600  |
| H | -1.35511700 | -3.12047700 | 2.97243100  |
| H | -2.69299900 | -2.72244100 | 4.04853800  |
| H | -0.07633900 | -1.50606700 | 4.20365700  |
| H | 0.27434700  | -1.23114300 | 2.49453800  |
| H | 0.00304200  | 0.13764600  | 3.57834900  |
| C | -2.18338700 | -0.55701000 | 1.55912200  |
| H | -3.12810200 | -0.01111800 | 1.64111300  |
| N | -1.25642300 | 0.30006500  | 0.74823300  |
| C | -1.31784700 | 1.78022500  | 1.02396000  |
| C | -2.73891800 | 2.34832400  | 1.12661400  |
| C | -0.45499000 | 2.25365400  | 2.19290100  |
| H | -0.89443800 | 2.23030000  | 0.11960900  |
| C | -2.68787700 | 3.87884100  | 1.15844400  |
| H | -3.23052800 | 1.99770800  | 2.04241600  |
| H | -3.33283100 | 2.00202100  | 0.27070900  |
| C | -0.41393800 | 3.78662700  | 2.23281400  |
| H | -0.87041900 | 1.89524800  | 3.13930400  |
| H | 0.56436100  | 1.84313600  | 2.12042900  |
| C | -1.82492200 | 4.37008000  | 2.32100900  |
| H | -3.70220100 | 4.28048000  | 1.23515500  |
| H | -2.26919300 | 4.24362000  | 0.21067500  |
| H | 0.19569900  | 4.11556100  | 3.07923700  |
| H | 0.06948700  | 4.17017800  | 1.32291800  |
| H | -1.78105800 | 5.46294700  | 2.32975600  |
| H | -2.28408900 | 4.06079800  | 3.26953100  |
| C | -3.16511300 | -2.70292500 | 1.89670800  |
| C | -2.50340700 | -1.85631300 | 0.80238800  |
| H | -4.17100400 | -2.31042500 | 2.09198400  |
| H | -3.26791500 | -3.75173600 | 1.60800100  |
| H | -1.55208600 | -2.34482100 | 0.53387900  |
| C | -3.34082700 | -1.72650400 | -0.45088200 |
| C | -3.12136700 | -2.61210400 | -1.51130000 |
| C | -4.39739500 | -0.81496600 | -0.55775900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.92203100 | -2.58749700 | -2.64971700 |
| H | -2.31422100 | -3.33798200 | -1.43526600 |
| C | -5.19940300 | -0.78278200 | -1.69748100 |
| H | -4.61859400 | -0.12867200 | 0.25556600  |
| C | -4.96479000 | -1.66746500 | -2.74721800 |
| H | -3.73386400 | -3.28712500 | -3.45759200 |
| H | -6.01463700 | -0.06892200 | -1.75989700 |
| H | -5.59183800 | -1.64476900 | -3.63220200 |
| C | -2.74572400 | 2.04414300  | -2.74306400 |
| C | -1.97559300 | 3.18626600  | -2.51457400 |
| C | -0.62676900 | 3.05592500  | -2.20305600 |
| C | -0.05629000 | 1.78475300  | -2.11385100 |
| C | -0.79660000 | 0.61688700  | -2.40453700 |
| C | -2.16288300 | 0.78498400  | -2.69750800 |
| H | -3.80280600 | 2.13635700  | -2.97233600 |
| H | -2.42315500 | 4.17270000  | -2.57176300 |
| H | -0.03678500 | 3.94296000  | -1.99679100 |
| H | -2.76103700 | -0.09949400 | -2.90005800 |
| N | 1.32379400  | 1.57588300  | -1.68161400 |
| C | 2.20349500  | 1.42876000  | -2.86517400 |
| H | 2.26261100  | 2.38776300  | -3.39436800 |
| H | 3.19689000  | 1.12631200  | -2.53716900 |
| H | 1.79802500  | 0.67869100  | -3.54223200 |
| C | 1.86986900  | 2.65169800  | -0.83323300 |
| H | 1.21218800  | 2.83978600  | 0.01906000  |
| H | 2.84818300  | 2.33698400  | -0.46669600 |
| H | 1.99905500  | 3.58656400  | -1.39093000 |
| C | -0.17186300 | -0.72288100 | -2.25634200 |
| H | 0.64409300  | -0.89699600 | -2.96601000 |
| H | -0.90269100 | -1.52616100 | -2.36125500 |
| H | -1.69727300 | 0.23702100  | -0.17920400 |

cis-25''

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.66119100 | -1.36843300 | -1.04863200 |
| C  | 2.79596300 | -0.45524100 | -2.15398500 |
| C  | 1.66650100 | -0.58530400 | -2.99162200 |
| C  | 0.82097700 | -1.59542200 | -2.43288600 |
| C  | 1.45006200 | -2.10875500 | -1.27302600 |
| Sc | 0.84533300 | 0.19300700  | -0.70356900 |
| C  | 5.57026000 | -2.25948400 | -0.74939500 |
| C  | 4.48723400 | 0.01177200  | 1.03160800  |
| C  | 3.69990100 | -2.92910700 | 1.51349700  |
| H  | 5.33397900 | -3.17879200 | -1.29354600 |
| H  | 5.95238100 | -1.52965900 | -1.46722700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.37735300  | -2.48591300 | -0.04495700 |
| H  | 3.69824100  | 0.76239600  | 0.90251200  |
| H  | 4.63039500  | -0.12276800 | 2.10886000  |
| H  | 5.41310300  | 0.43470900  | 0.62909700  |
| H  | 4.61829700  | -3.05431600 | 2.09807200  |
| H  | 2.90710900  | -2.64634200 | 2.20890800  |
| H  | 3.45230800  | -3.90181100 | 1.07983600  |
| Si | 4.06286000  | -1.64091000 | 0.19470800  |
| C  | 0.99826100  | -3.33647200 | -0.53703300 |
| H  | 1.49792200  | -4.21640000 | -0.95852300 |
| H  | 1.23424400  | -3.29951600 | 0.52471900  |
| H  | -0.07760500 | -3.49777300 | -0.63940400 |
| C  | -0.42338400 | -2.10795800 | -3.10281900 |
| H  | -1.06300900 | -1.29388200 | -3.46223000 |
| H  | -0.16138700 | -2.71433500 | -3.97698400 |
| H  | -1.02214800 | -2.73474400 | -2.43850900 |
| C  | 1.46477700  | 0.00412200  | -4.36023700 |
| H  | 2.19283500  | 0.78576300  | -4.58421000 |
| H  | 1.58790500  | -0.77975900 | -5.11522800 |
| H  | 0.46122500  | 0.41993900  | -4.50658700 |
| C  | 4.03350600  | 0.34251100  | -2.46721400 |
| H  | 4.56768900  | 0.64963800  | -1.56395800 |
| H  | 4.72475800  | -0.27016900 | -3.05600700 |
| H  | 3.83050300  | 1.23622100  | -3.06093100 |
| C  | -1.86083600 | -1.62458600 | 3.87989200  |
| C  | -1.16011700 | -2.01989200 | 2.57377500  |
| H  | -1.38730300 | -0.74222200 | 4.32750600  |
| H  | -2.91815200 | -1.38929100 | 3.71513900  |
| H  | -1.80444400 | -2.44005000 | 4.60815100  |
| C  | -1.93845200 | -3.16974000 | 1.90169200  |
| C  | 0.26891100  | -2.48129700 | 2.88038100  |
| H  | -1.25322900 | -3.77163300 | 1.28873600  |
| H  | -2.38224800 | -3.84666000 | 2.64066200  |
| H  | 0.31386000  | -3.57318100 | 2.94776700  |
| H  | 0.94503100  | -2.15414200 | 2.09071200  |
| H  | 0.64540500  | -2.08741400 | 3.82750400  |
| C  | -1.30186600 | -0.81411400 | 1.53392200  |
| H  | -1.91737700 | -0.05845400 | 2.04095600  |
| N  | -0.11809500 | -0.13759900 | 1.00348800  |
| C  | 0.50507000  | 0.90405200  | 1.83191900  |
| C  | -0.46084000 | 1.94402900  | 2.42357800  |
| C  | 1.46923400  | 0.41936800  | 2.92530300  |
| H  | 1.15805000  | 1.49474300  | 1.13377400  |
| C  | 0.29009700  | 3.10280300  | 3.08790200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.06977600 | 1.44801200  | 3.19016500  |
| H | -1.14440000 | 2.30509200  | 1.64743200  |
| C | 2.22937400  | 1.58315000  | 3.56370600  |
| H | 0.87975900  | -0.08076800 | 3.70126200  |
| H | 2.15969900  | -0.32406100 | 2.50995800  |
| C | 1.25769000  | 2.60154500  | 4.15981300  |
| H | -0.42902800 | 3.81214700  | 3.51004100  |
| H | 0.85915200  | 3.65516200  | 2.32762700  |
| H | 2.91422000  | 1.20409600  | 4.32858300  |
| H | 2.85439400  | 2.07807500  | 2.80465000  |
| H | 1.80234000  | 3.44004700  | 4.60412900  |
| H | 0.68947900  | 2.12382500  | 4.96876600  |
| C | -2.97353900 | -2.53806700 | 0.97240800  |
| C | -2.16205400 | -1.37796300 | 0.38475100  |
| H | -3.80018400 | -2.13291200 | 1.57482100  |
| H | -1.49696100 | -1.78275300 | -0.39582200 |
| H | -2.78159000 | -0.59769500 | -0.07138200 |
| C | -3.52738100 | -3.55437800 | -0.03247600 |
| C | -4.86116800 | -3.22645100 | -0.70805000 |
| H | -3.64386600 | -4.51363200 | 0.48722500  |
| H | -2.76133300 | -3.72379500 | -0.80520400 |
| C | -4.90013400 | -1.90589200 | -1.49165600 |
| H | -5.10300800 | -4.05847400 | -1.37751000 |
| H | -5.65335600 | -3.21207200 | 0.05233600  |
| H | -3.89172200 | -1.66723600 | -1.86491000 |
| H | -5.52863200 | -2.02042500 | -2.38267900 |
| C | -5.44399200 | -0.73032000 | -0.67945800 |
| C | -5.38698700 | 0.59213400  | -1.43659000 |
| H | -4.89465400 | -0.63251200 | 0.26673400  |
| H | -6.48390000 | -0.94419500 | -0.39973300 |
| C | -5.88371300 | 1.77219300  | -0.60567700 |
| H | -4.34950700 | 0.76414900  | -1.76040600 |
| H | -5.97619300 | 0.51051300  | -2.35807900 |
| H | -5.83032200 | 2.71367900  | -1.16079300 |
| H | -6.92510100 | 1.62113700  | -0.30697100 |
| H | -5.29265900 | 1.88267400  | 0.31090200  |
| N | 1.21557500  | 2.53175400  | -1.28428200 |
| C | 2.41366600  | 3.04857400  | -0.57868200 |
| H | 2.30206900  | 2.96637000  | 0.50335000  |
| H | 3.27810500  | 2.46288800  | -0.89910900 |
| H | 2.60069700  | 4.09803500  | -0.83197000 |
| C | 1.39026100  | 2.89988800  | -2.71685800 |
| H | 1.46886100  | 3.98978500  | -2.80232700 |
| H | 2.30153600  | 2.44270300  | -3.09719000 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 0.54315800  | 2.57176900 | -3.31647000 |
| C | -0.04602000 | 3.10250200 | -0.81927600 |
| C | -1.23664100 | 2.44191600 | -1.16852800 |
| C | -0.09237700 | 4.28793400 | -0.08581100 |
| C | -2.44944400 | 2.98014600 | -0.73565700 |
| C | -1.31261200 | 4.80285200 | 0.34185000  |
| H | 0.81950200  | 4.81778200 | 0.16285200  |
| C | -2.49582900 | 4.14546300 | 0.02147500  |
| H | -3.37119900 | 2.47320600 | -1.00232500 |
| H | -1.33146300 | 5.71931200 | 0.92147500  |
| H | -3.45207700 | 4.53848000 | 0.34973200  |
| C | -1.26025500 | 1.16359600 | -1.97723900 |
| H | -1.46531900 | 0.28579700 | -1.34223000 |
| H | -2.07736100 | 1.17085000 | -2.70365900 |
| H | -0.36120300 | 0.99121000 | -2.58127600 |

trans-25''

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.10515400  | -2.65045400 | -0.62282900 |
| C  | -0.18107200 | -3.14094900 | 0.70026300  |
| C  | 0.75831400  | -2.59183500 | 1.60011900  |
| C  | 1.66019200  | -1.77245300 | 0.84889700  |
| C  | 1.28979500  | -1.84311400 | -0.51531800 |
| Sc | -0.53956100 | -0.64626900 | 0.53841100  |
| C  | -0.41159300 | -5.12593000 | -2.34114000 |
| C  | -2.64999300 | -3.04623300 | -1.98412300 |
| C  | -0.18961800 | -2.44937200 | -3.74785100 |
| H  | 0.66471500  | -5.30170300 | -2.42761300 |
| H  | -0.78179800 | -5.70222000 | -1.48894600 |
| H  | -0.88997900 | -5.51962300 | -3.24377500 |
| H  | -2.90663900 | -2.27001800 | -1.25315600 |
| H  | -3.09492100 | -2.74651100 | -2.93903300 |
| H  | -3.14078700 | -3.97306500 | -1.67079300 |
| H  | -0.76224900 | -2.86777800 | -4.58286800 |
| H  | -0.33960700 | -1.36648300 | -3.75289000 |
| H  | 0.86813000  | -2.64840700 | -3.94004700 |
| Si | -0.77483100 | -3.28785600 | -2.17026200 |
| C  | 2.07097800  | -1.26329000 | -1.65874600 |
| H  | 2.67555000  | -2.04424600 | -2.13377000 |
| H  | 1.41711000  | -0.83357900 | -2.41623300 |
| H  | 2.75905600  | -0.48138400 | -1.32532300 |
| C  | 2.87308600  | -1.10885300 | 1.43946400  |
| H  | 2.65571900  | -0.64496800 | 2.40871800  |
| H  | 3.66815000  | -1.84491700 | 1.60984800  |
| H  | 3.28247000  | -0.33744700 | 0.78324800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.97708500  | -2.96225100 | 3.04106600  |
| H | 0.17669600  | -3.59464200 | 3.42924200  |
| H | 1.91129500  | -3.52609800 | 3.13529600  |
| H | 1.07161700  | -2.09189900 | 3.70100100  |
| C | -1.17799300 | -4.22242800 | 1.02084200  |
| H | -2.04200600 | -4.19956000 | 0.35112600  |
| H | -0.70528400 | -5.20339500 | 0.90040300  |
| H | -1.54627700 | -4.18069000 | 2.04868900  |
| C | -0.70043600 | 3.64513900  | -2.87558400 |
| C | 0.40033200  | 2.72421700  | -2.33960400 |
| H | -1.61200200 | 3.11586100  | -3.16306300 |
| H | -0.96726600 | 4.40854400  | -2.13606000 |
| H | -0.33680400 | 4.16359800  | -3.76903300 |
| C | 1.66988500  | 3.56733600  | -2.10186200 |
| C | 0.69919600  | 1.62151300  | -3.35803100 |
| H | 2.15244100  | 3.85586100  | -3.04222000 |
| H | 1.39532500  | 4.49306500  | -1.57496400 |
| H | 0.78235400  | 2.05478100  | -4.36007600 |
| H | 1.63965500  | 1.11018700  | -3.14239900 |
| H | -0.09049800 | 0.86678100  | -3.37672700 |
| C | 0.13865000  | 2.17685100  | -0.88616500 |
| H | -0.37514000 | 3.00289800  | -0.36717700 |
| N | -0.62573700 | 0.94985400  | -0.64891900 |
| C | -2.06541800 | 0.94112900  | -0.91459700 |
| C | -2.82278900 | 2.20380900  | -0.47541200 |
| C | -2.49282700 | 0.50237000  | -2.32594500 |
| H | -2.49131000 | 0.12216700  | -0.26702400 |
| C | -4.33812600 | 2.03389000  | -0.60487600 |
| H | -2.51234300 | 3.03277100  | -1.11947500 |
| H | -2.53841000 | 2.47024400  | 0.54762700  |
| C | -4.01136400 | 0.34185300  | -2.43060000 |
| H | -2.15987900 | 1.24670600  | -3.05461100 |
| H | -1.98232100 | -0.43586900 | -2.57317600 |
| C | -4.73073900 | 1.62948900  | -2.02604800 |
| H | -4.83813200 | 2.96229900  | -0.31069600 |
| H | -4.68707400 | 1.26049900  | 0.09473100  |
| H | -4.28385500 | 0.04542300  | -3.44821700 |
| H | -4.34257900 | -0.47371600 | -1.76977800 |
| H | -5.81470200 | 1.50097500  | -2.10141700 |
| H | -4.45481700 | 2.43338400  | -2.72166000 |
| C | 2.56406400  | 2.71975900  | -1.19761700 |
| C | 1.55114500  | 2.05343200  | -0.24878000 |
| H | 3.03884800  | 1.94565000  | -1.81267200 |
| H | 1.80467900  | 1.00129400  | -0.06853100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.57139900  | 2.56412700  | 0.72301300  |
| C | 3.66351200  | 3.49731300  | -0.47611900 |
| C | 4.47584700  | 2.64867200  | 0.50662800  |
| H | 3.20139600  | 4.33376200  | 0.06567500  |
| H | 4.33819900  | 3.94056000  | -1.21975600 |
| C | 5.20358700  | 1.46902600  | -0.13463800 |
| H | 5.20817200  | 3.28623600  | 1.01647200  |
| H | 3.80975300  | 2.26412400  | 1.29384700  |
| H | 4.47781200  | 0.80712500  | -0.62836600 |
| H | 5.86645100  | 1.83038400  | -0.93232500 |
| C | 6.00735400  | 0.64664200  | 0.87019900  |
| C | 6.55431300  | -0.65026100 | 0.27902700  |
| H | 5.37206200  | 0.40638900  | 1.73580600  |
| H | 6.83489400  | 1.25226600  | 1.26258500  |
| C | 7.34176200  | -1.47306800 | 1.29427300  |
| H | 5.71554700  | -1.24477700 | -0.10959000 |
| H | 7.18876700  | -0.41563200 | -0.58449100 |
| H | 7.71954000  | -2.40031800 | 0.85647800  |
| H | 8.19841000  | -0.90761300 | 1.67361300  |
| H | 6.71413300  | -1.73722800 | 2.15212500  |
| N | -2.26105400 | -0.79338800 | 2.22622300  |
| C | -3.46169700 | -1.41519700 | 1.62125800  |
| H | -3.84693700 | -0.81133800 | 0.79893400  |
| H | -3.18715500 | -2.40418200 | 1.24655300  |
| H | -4.25845600 | -1.54306500 | 2.36291200  |
| C | -1.98175000 | -1.55582100 | 3.47389500  |
| H | -2.85236000 | -1.49515300 | 4.13666100  |
| H | -1.78877200 | -2.59635600 | 3.21953900  |
| H | -1.12133700 | -1.14823400 | 4.00170000  |
| C | -2.42646900 | 0.61624600  | 2.56816400  |
| C | -1.26591000 | 1.37535900  | 2.79617700  |
| C | -3.68563600 | 1.20197800  | 2.69225400  |
| C | -1.40476200 | 2.72840500  | 3.11029500  |
| C | -3.80120500 | 2.55354500  | 3.00335000  |
| H | -4.58455600 | 0.61575500  | 2.54182500  |
| C | -2.65943100 | 3.32151300  | 3.20657300  |
| H | -0.51053700 | 3.32052700  | 3.28458300  |
| H | -4.78588500 | 3.00012100  | 3.08831400  |
| H | -2.74301200 | 4.37527600  | 3.44808700  |
| C | 0.12407900  | 0.79110300  | 2.68346800  |
| H | 0.60422300  | 1.07894900  | 1.73562800  |
| H | 0.78847500  | 1.19207000  | 3.45309400  |
| H | 0.17156500  | -0.29666300 | 2.81454000  |

cis-ts-26'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.18565800  | -2.07448400 | -0.81540900 |
| C  | 2.41746900  | -1.42522700 | -2.07861600 |
| C  | 1.18697000  | -1.34092200 | -2.77334800 |
| C  | 0.18482400  | -1.98012000 | -1.97859100 |
| C  | 0.80092400  | -2.45984600 | -0.79622000 |
| Sc | 0.90628400  | -0.03392300 | -0.64463600 |
| C  | 4.34357300  | -4.16797900 | -0.32293200 |
| C  | 4.84107200  | -1.27505000 | 0.60916700  |
| C  | 2.85212400  | -3.03005800 | 2.09464600  |
| H  | 3.59651900  | -4.95534700 | -0.46282700 |
| H  | 4.81576400  | -3.97865400 | -1.29092800 |
| H  | 5.11200100  | -4.54740200 | 0.35768700  |
| H  | 4.42781300  | -0.35622100 | 1.04034900  |
| H  | 5.59891100  | -1.64086600 | 1.31034500  |
| H  | 5.35782800  | -1.02357600 | -0.32061200 |
| H  | 3.69432100  | -3.17890700 | 2.77870800  |
| H  | 2.23351300  | -2.22521300 | 2.50247600  |
| H  | 2.25945900  | -3.94782200 | 2.09675200  |
| Si | 3.53874800  | -2.62553500 | 0.38930900  |
| C  | 0.14916800  | -3.30630600 | 0.26175100  |
| H  | 0.69141300  | -4.24971600 | 0.37698500  |
| H  | 0.12787500  | -2.80778800 | 1.23513900  |
| H  | -0.87957900 | -3.55548500 | -0.00772200 |
| C  | -1.22355200 | -2.18533700 | -2.46295500 |
| H  | -1.78029100 | -1.24212400 | -2.53338900 |
| H  | -1.21432500 | -2.63269900 | -3.46212900 |
| H  | -1.78827700 | -2.85192200 | -1.80904800 |
| C  | 0.93873900  | -0.88298800 | -4.18314700 |
| H  | 1.79933500  | -0.37083300 | -4.61517900 |
| H  | 0.71830800  | -1.74845400 | -4.81742500 |
| H  | 0.07559900  | -0.21156500 | -4.25713300 |
| C  | 3.77284500  | -1.10966800 | -2.66054900 |
| H  | 4.28882900  | -0.26958000 | -2.18734600 |
| H  | 4.42886000  | -1.97956000 | -2.56013900 |
| H  | 3.69826800  | -0.89160900 | -3.72813700 |
| C  | -2.88007900 | -0.02737400 | 3.81982600  |
| C  | -1.95938200 | -0.86112400 | 2.91359100  |
| H  | -2.41274400 | 0.91540300  | 4.11941900  |
| H  | -3.82308400 | 0.21638100  | 3.32118400  |
| H  | -3.11658300 | -0.58570300 | 4.73081700  |
| C  | -2.72900600 | -2.12309000 | 2.47605700  |
| C  | -0.72106500 | -1.25568800 | 3.70931100  |
| H  | -2.02448300 | -2.91010000 | 2.17125100  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.33777100 | -2.52889800 | 3.29129000  |
| H | -1.00808600 | -1.97526800 | 4.48312400  |
| H | 0.03358700  | -1.73126000 | 3.07591200  |
| H | -0.26946500 | -0.39927300 | 4.21926900  |
| C | -1.73048400 | -0.07178600 | 1.55395900  |
| H | -2.22619700 | 0.90231500  | 1.67700900  |
| N | -0.36922700 | 0.19503800  | 1.01814500  |
| C | 0.50340300  | 1.22352400  | 1.66440100  |
| C | -0.22787800 | 2.25643200  | 2.52536900  |
| C | 1.72351600  | 0.61188100  | 2.37500900  |
| H | 0.92383200  | 1.84342900  | 0.84533200  |
| C | 0.74234300  | 3.29593300  | 3.08955800  |
| H | -0.72216900 | 1.73623500  | 3.35310200  |
| H | -1.00671600 | 2.74200000  | 1.92630200  |
| C | 2.64289500  | 1.65540600  | 3.01761400  |
| H | 1.39114700  | -0.09242300 | 3.13767300  |
| H | 2.30019300  | 0.00188900  | 1.65354400  |
| C | 1.85127000  | 2.62276600  | 3.89787800  |
| H | 0.19050100  | 4.00837100  | 3.70917900  |
| H | 1.18335500  | 3.87044200  | 2.26168500  |
| H | 3.41772300  | 1.14305400  | 3.59587800  |
| H | 3.16691100  | 2.23772200  | 2.24934500  |
| H | 2.52345700  | 3.37101400  | 4.32725000  |
| H | 1.40482800  | 2.07401700  | 4.73785400  |
| C | -3.55397500 | -1.70680200 | 1.25857600  |
| C | -2.51562000 | -0.87744700 | 0.49415800  |
| H | -4.37277200 | -1.05372500 | 1.59284700  |
| H | -1.81501800 | -1.57110300 | 0.01556100  |
| H | -2.93155500 | -0.23924200 | -0.28994800 |
| C | -4.15944100 | -2.90313000 | 0.51705900  |
| C | -5.35099800 | -2.62111000 | -0.40557000 |
| H | -4.48421200 | -3.63254600 | 1.26955600  |
| H | -3.36403500 | -3.40084400 | -0.05874000 |
| C | -5.06544000 | -1.65205000 | -1.56163500 |
| H | -5.69013300 | -3.58171200 | -0.80687700 |
| H | -6.18510500 | -2.23292500 | 0.19454400  |
| H | -4.01037700 | -1.74589700 | -1.85640600 |
| H | -5.64657500 | -1.93992400 | -2.44506800 |
| C | -5.37480800 | -0.18806800 | -1.24026400 |
| C | -4.78851300 | 0.77956600  | -2.26557000 |
| H | -4.99209300 | 0.06956200  | -0.24453400 |
| H | -6.46219500 | -0.05119800 | -1.18162800 |
| C | -4.92778000 | 2.23933600  | -1.84540500 |
| H | -3.72498900 | 0.53834000  | -2.41191700 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -5.26580200 | 0.61855400 | -3.23960200 |
| H | -4.47754500 | 2.91822000 | -2.57505700 |
| H | -5.98006300 | 2.51668600 | -1.73194000 |
| H | -4.44158800 | 2.40677100 | -0.87630700 |
| N | 1.92930800  | 1.94302100 | -1.46477200 |
| C | 3.22323400  | 2.03182800 | -0.74842800 |
| H | 3.05053800  | 2.34580000 | 0.28154900  |
| H | 3.70856800  | 1.04913600 | -0.74579700 |
| H | 3.90640700  | 2.74490400 | -1.22230300 |
| C | 2.18541500  | 1.93743500 | -2.92974100 |
| H | 2.61887800  | 2.89883400 | -3.22755300 |
| H | 2.87955000  | 1.13734800 | -3.18140100 |
| H | 1.24665000  | 1.79411600 | -3.46711500 |
| C | 1.03368100  | 3.07097200 | -1.18386200 |
| C | -0.34627700 | 2.81168900 | -1.21854100 |
| C | 1.52740700  | 4.34061100 | -0.90551100 |
| C | -1.21261000 | 3.87378700 | -0.94237700 |
| C | 0.64323600  | 5.38172700 | -0.62734000 |
| H | 2.59621500  | 4.52830200 | -0.89324000 |
| C | -0.72707500 | 5.14498800 | -0.64499600 |
| H | -2.28386800 | 3.69240600 | -0.95978400 |
| H | 1.02932500  | 6.36950600 | -0.40131100 |
| H | -1.42194000 | 5.94993800 | -0.43034700 |
| C | -0.85275500 | 1.41548600 | -1.42848800 |
| H | -0.75979100 | 0.79078000 | -0.12986800 |
| H | -1.94550300 | 1.40105200 | -1.44492300 |
| H | -0.54452100 | 1.00202900 | -2.40244700 |

trans-ts-26'

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | 1.29614600  | 2.72794400 | -0.33664000 |
| C  | 1.40452900  | 2.92400900 | 1.08607600  |
| C  | 0.13524500  | 2.69737300 | 1.66872400  |
| C  | -0.78970400 | 2.40908100 | 0.61747000  |
| C  | -0.08745100 | 2.45515300 | -0.61163700 |
| Sc | 0.85571600  | 0.54717800 | 0.55323300  |
| C  | 2.81718500  | 4.97342800 | -1.74948500 |
| C  | 4.31443300  | 2.39185900 | -0.98773900 |
| C  | 2.31479800  | 2.38350800 | -3.28323900 |
| H  | 1.87246100  | 5.39867200 | -2.10159000 |
| H  | 3.07344200  | 5.46025200 | -0.80461700 |
| H  | 3.59366600  | 5.22624200 | -2.47840500 |
| H  | 4.27006900  | 1.30870700 | -0.82776200 |
| H  | 5.07165200  | 2.56908800 | -1.75889300 |
| H  | 4.67193400  | 2.86460600 | -0.06904000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.20681700  | 2.52066400  | -3.90403200 |
| H  | 2.09522900  | 1.31206700  | -3.25432600 |
| H  | 1.48461800  | 2.88841900  | -3.78298000 |
| Si | 2.66990400  | 3.10674200  | -1.58193700 |
| C  | -0.69232300 | 2.30203100  | -1.97788300 |
| H  | -0.56813200 | 3.22344900  | -2.55554200 |
| H  | -0.22460200 | 1.48702500  | -2.53639500 |
| H  | -1.76313400 | 2.09498700  | -1.91766400 |
| C  | -2.26924500 | 2.26873800  | 0.85147700  |
| H  | -2.51740500 | 1.39620000  | 1.46801800  |
| H  | -2.64565500 | 3.15361900  | 1.37554800  |
| H  | -2.82508800 | 2.18213900  | -0.08447400 |
| C  | -0.29664500 | 2.91766500  | 3.09080600  |
| H  | 0.54433300  | 3.05850400  | 3.77066700  |
| H  | -0.92054600 | 3.81611800  | 3.15072600  |
| H  | -0.90369800 | 2.08807600  | 3.47042000  |
| C  | 2.60381100  | 3.49316600  | 1.80114700  |
| H  | 3.47696600  | 2.83586500  | 1.81373600  |
| H  | 2.91695700  | 4.42091800  | 1.31264000  |
| H  | 2.36310000  | 3.74510900  | 2.83607600  |
| C  | -1.65748100 | -3.01573200 | -3.35192000 |
| C  | -1.21380200 | -1.58554900 | -2.99823400 |
| H  | -0.84559600 | -3.73098100 | -3.18423600 |
| H  | -2.50990200 | -3.34380200 | -2.75224700 |
| H  | -1.94318800 | -3.07630700 | -4.40646400 |
| C  | -2.34441300 | -0.58102900 | -3.32375700 |
| C  | 0.00632100  | -1.25477800 | -3.85171400 |
| H  | -1.89941800 | 0.38869200  | -3.57191000 |
| H  | -2.91203500 | -0.89974800 | -4.20574900 |
| H  | -0.30345400 | -1.17121800 | -4.89867900 |
| H  | 0.45855700  | -0.30203300 | -3.56031400 |
| H  | 0.76528100  | -2.04155100 | -3.80372200 |
| C  | -1.03922400 | -1.50838500 | -1.42880500 |
| H  | -1.12300100 | -2.53850200 | -1.06033500 |
| N  | 0.18082900  | -0.92794500 | -0.79577300 |
| C  | 1.45272500  | -1.70914100 | -0.76490300 |
| C  | 1.28752000  | -3.22627500 | -0.88768400 |
| C  | 2.54788500  | -1.16038500 | -1.69466900 |
| H  | 1.86816700  | -1.58627800 | 0.26025900  |
| C  | 2.62778300  | -3.94677500 | -0.73047200 |
| H  | 0.86340300  | -3.45382600 | -1.87358200 |
| H  | 0.57614100  | -3.57846300 | -0.13205800 |
| C  | 3.86754100  | -1.92597100 | -1.55830000 |
| H  | 2.21718000  | -1.20290700 | -2.73245500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.70725700  | -0.08927200 | -1.48110600 |
| C | 3.65071500  | -3.42825900 | -1.74067200 |
| H | 2.47772700  | -5.02359700 | -0.84963500 |
| H | 3.00364000  | -3.78989000 | 0.29104100  |
| H | 4.58623400  | -1.54189000 | -2.28833400 |
| H | 4.31038900  | -1.75615100 | -0.56766700 |
| H | 4.60006700  | -3.96094500 | -1.63479400 |
| H | 3.28530000  | -3.62250800 | -2.75805700 |
| C | -3.23110300 | -0.44028500 | -2.07792300 |
| C | -2.25721100 | -0.69752400 | -0.91569600 |
| H | -3.59459600 | 0.59333300  | -2.00910900 |
| H | -1.88082100 | 0.26149200  | -0.55219400 |
| H | -2.74396800 | -1.18418300 | -0.06521600 |
| C | -4.47915800 | -1.33638400 | -2.09758400 |
| C | -5.29804300 | -1.32879100 | -0.80188300 |
| H | -4.21005900 | -2.37010600 | -2.33737800 |
| H | -5.11376700 | -0.99076600 | -2.92367400 |
| C | -5.60407600 | 0.06472200  | -0.25627600 |
| H | -6.24071600 | -1.85933100 | -0.98302200 |
| H | -4.77987400 | -1.90555600 | -0.02411400 |
| H | -4.66684900 | 0.56144500  | 0.03209600  |
| H | -6.04811800 | 0.68405900  | -1.04849600 |
| C | -6.53253800 | 0.04003400  | 0.95513600  |
| C | -6.75881900 | 1.42196700  | 1.56403000  |
| H | -6.11179600 | -0.62775700 | 1.72033200  |
| H | -7.49884200 | -0.39583100 | 0.66810100  |
| C | -7.68356200 | 1.38633500  | 2.77754800  |
| H | -5.78841700 | 1.85066300  | 1.84929300  |
| H | -7.17554000 | 2.08935400  | 0.79946600  |
| H | -7.82739900 | 2.38202600  | 3.20441600  |
| H | -8.66755200 | 0.99253200  | 2.50517800  |
| H | -7.27395700 | 0.74027500  | 3.56053000  |
| N | 2.21092200  | -0.22284000 | 2.37584900  |
| C | 3.62810700  | -0.11231300 | 1.96183200  |
| H | 3.84852100  | -0.85636400 | 1.19408700  |
| H | 3.80567600  | 0.88728600  | 1.55637100  |
| H | 4.31227200  | -0.26028500 | 2.80440400  |
| C | 2.02482200  | 0.57842000  | 3.61491800  |
| H | 2.62616600  | 0.14645900  | 4.42276600  |
| H | 2.34374200  | 1.60470000  | 3.43612800  |
| H | 0.97600600  | 0.56738300  | 3.91440000  |
| C | 1.80514800  | -1.60174600 | 2.67114800  |
| C | 0.44976800  | -1.92232800 | 2.48029500  |
| C | 2.71480600  | -2.55301400 | 3.12104500  |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 0.04956900  | -3.23666400 | 2.73723800 |
| C | 2.29128400  | -3.85819200 | 3.36694600 |
| H | 3.75768200  | -2.29757200 | 3.27309700 |
| C | 0.95788500  | -4.19919000 | 3.17089800 |
| H | -0.99233400 | -3.50460200 | 2.58441400 |
| H | 3.00522900  | -4.59899400 | 3.70943100 |
| H | 0.62075100  | -5.21332600 | 3.35701300 |
| C | -0.49393300 | -0.91271200 | 1.89963500 |
| H | -0.26830300 | -1.01034000 | 0.47848400 |
| H | -1.51234000 | -1.30491100 | 1.85543900 |
| H | -0.56323000 | -0.00429900 | 2.51886700 |

cis-27'

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.50827400  | -1.83980200 | -0.24939500 |
| C  | 2.72250500  | -1.59257300 | -1.65102900 |
| C  | 1.57844200  | -2.01171000 | -2.36795700 |
| C  | 0.64534200  | -2.55122800 | -1.43576500 |
| C  | 1.22836800  | -2.48484400 | -0.14456000 |
| Sc | 0.83191500  | -0.14821400 | -0.83303300 |
| C  | 4.98356900  | -3.25134200 | 0.82514900  |
| C  | 4.90157500  | -0.16738800 | 0.83000700  |
| C  | 3.26746700  | -1.73289300 | 2.82351900  |
| H  | 4.41141800  | -4.16899800 | 0.99379500  |
| H  | 5.41816200  | -3.30848500 | -0.17658800 |
| H  | 5.80567600  | -3.22994400 | 1.54756200  |
| H  | 4.27005500  | 0.72817400  | 0.79687800  |
| H  | 5.56719600  | -0.06232900 | 1.69329300  |
| H  | 5.52831500  | -0.18076300 | -0.06481700 |
| H  | 4.15182500  | -1.71237000 | 3.47004800  |
| H  | 2.67437500  | -0.84525500 | 3.06049800  |
| H  | 2.68898700  | -2.62017300 | 3.09072400  |
| Si | 3.88085100  | -1.74252700 | 1.04341800  |
| C  | 0.69691700  | -3.20763200 | 1.06126100  |
| H  | 1.26083200  | -4.13707100 | 1.20414800  |
| H  | 0.78013200  | -2.63414500 | 1.98358800  |
| H  | -0.35078400 | -3.48616300 | 0.92687700  |
| C  | -0.65060900 | -3.19472500 | -1.83786200 |
| H  | -1.22311200 | -2.55342700 | -2.51637900 |
| H  | -0.46275200 | -4.13970400 | -2.35954500 |
| H  | -1.28568400 | -3.41630600 | -0.97800900 |
| C  | 1.40291800  | -2.09242100 | -3.85714600 |
| H  | 2.05961600  | -1.40986000 | -4.39940000 |
| H  | 1.63023400  | -3.10740800 | -4.20177500 |
| H  | 0.37214300  | -1.87979700 | -4.15561200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.03160900  | -1.19858900 | -2.28427800 |
| H | 4.40624400  | -0.22204800 | -1.97210000 |
| H | 4.80487800  | -1.92747600 | -2.01916700 |
| H | 3.96024800  | -1.20095400 | -3.37385400 |
| C | -2.41919600 | 0.27321600  | 4.09362500  |
| C | -1.57825700 | -0.44842400 | 3.02816600  |
| H | -2.15030400 | 1.32459600  | 4.21253700  |
| H | -3.48431700 | 0.23054300  | 3.84289700  |
| H | -2.28555600 | -0.21834300 | 5.06209800  |
| C | -2.20419300 | -1.85198200 | 2.83463300  |
| C | -0.12591800 | -0.55749200 | 3.48277800  |
| H | -1.43601600 | -2.57780900 | 2.54599100  |
| H | -2.65936000 | -2.21625900 | 3.76134100  |
| H | -0.01871300 | -1.35955700 | 4.22061800  |
| H | 0.52809200  | -0.78693600 | 2.63650600  |
| H | 0.23206600  | 0.36417100  | 3.95241600  |
| C | -1.77210300 | 0.23316500  | 1.62152600  |
| H | -2.50861300 | 1.03669700  | 1.75555300  |
| N | -0.62056100 | 0.83565000  | 0.85197200  |
| C | 0.05801500  | 2.08658700  | 1.34978100  |
| C | -0.64025800 | 2.84133500  | 2.47910200  |
| C | 1.52785500  | 1.83244300  | 1.69231600  |
| H | 0.05148700  | 2.76552000  | 0.48764600  |
| C | 0.09167300  | 4.15701500  | 2.76258500  |
| H | -0.63505800 | 2.23356600  | 3.38782800  |
| H | -1.68454000 | 3.03893300  | 2.21500200  |
| C | 2.25837500  | 3.14567900  | 1.98491400  |
| H | 1.61093300  | 1.16685500  | 2.55604800  |
| H | 2.03732000  | 1.30362500  | 0.86243000  |
| C | 1.55763500  | 3.90357000  | 3.11508200  |
| H | -0.41204300 | 4.68823600  | 3.57469300  |
| H | 0.03516600  | 4.80135700  | 1.87446900  |
| H | 3.30528100  | 2.94626600  | 2.23367400  |
| H | 2.25136000  | 3.78267000  | 1.08900000  |
| H | 2.07415400  | 4.84787300  | 3.30848200  |
| H | 1.61333200  | 3.31180900  | 4.03830900  |
| C | -3.20762600 | -1.72392400 | 1.68466100  |
| C | -2.40466400 | -0.84152900 | 0.72405900  |
| H | -4.08818000 | -1.16374300 | 2.03361300  |
| H | -1.60391400 | -1.45736200 | 0.28059200  |
| H | -2.97664100 | -0.40497100 | -0.10089700 |
| C | -3.66339100 | -3.08448600 | 1.15401200  |
| C | -4.91577800 | -3.10776100 | 0.27122300  |
| H | -3.84707700 | -3.73537000 | 2.01788600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.82519000 | -3.54181900 | 0.60730000  |
| C | -4.83529600 | -2.25987200 | -1.00809200 |
| H | -5.11147900 | -4.15261300 | 0.00955800  |
| H | -5.77891900 | -2.77964100 | 0.86579800  |
| H | -3.78656800 | -2.18710000 | -1.33467300 |
| H | -5.36339700 | -2.76487800 | -1.82470500 |
| C | -5.42775100 | -0.85700200 | -0.85387300 |
| C | -5.12155000 | 0.05298100  | -2.04041600 |
| H | -5.05868200 | -0.38848700 | 0.06861100  |
| H | -6.51474800 | -0.94018200 | -0.72567500 |
| C | -5.60831200 | 1.48438100  | -1.83405900 |
| H | -4.03574500 | 0.05174700  | -2.21834700 |
| H | -5.56943800 | -0.36854100 | -2.94839800 |
| H | -5.36855700 | 2.12053400  | -2.69080100 |
| H | -6.69223900 | 1.51202300  | -1.68904100 |
| H | -5.14789300 | 1.92716400  | -0.94258800 |
| N | 1.71237300  | 1.61636800  | -2.15846200 |
| C | 2.90972100  | 2.27992200  | -1.60131400 |
| H | 2.70157300  | 2.67782200  | -0.60882700 |
| H | 3.71619100  | 1.54972300  | -1.52987700 |
| H | 3.24546300  | 3.10099400  | -2.24518000 |
| C | 1.99287600  | 1.31733100  | -3.58557900 |
| H | 2.16549500  | 2.25649300  | -4.12446600 |
| H | 2.88626700  | 0.69572100  | -3.64961700 |
| H | 1.15299700  | 0.79754000  | -4.04170400 |
| C | 0.49602100  | 2.41592300  | -2.03946000 |
| C | -0.73544700 | 1.72418000  | -2.13249700 |
| C | 0.54077200  | 3.79379000  | -1.80443100 |
| C | -1.90148200 | 2.47242000  | -1.87264700 |
| C | -0.63214500 | 4.50164600  | -1.57375500 |
| H | 1.48987900  | 4.31651200  | -1.77220100 |
| C | -1.85630200 | 3.83089900  | -1.58811500 |
| H | -2.85992500 | 1.96028500  | -1.91432200 |
| H | -0.58995200 | 5.56742100  | -1.37867000 |
| H | -2.77779700 | 4.37238300  | -1.39963900 |
| C | -0.76629700 | 0.24716500  | -2.30647600 |
| H | -1.14627300 | 1.18191200  | 0.04623000  |
| H | -1.76795600 | -0.15658800 | -2.13654200 |
| H | -0.42491100 | -0.08870800 | -3.28800000 |

trans-27'

|   |            |            |             |
|---|------------|------------|-------------|
| C | 1.88112100 | 2.14498300 | -0.95578900 |
| C | 1.55301700 | 3.03638200 | 0.12488800  |
| C | 0.18557000 | 3.38699500 | 0.03510800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.36489100 | 2.72175400  | -1.09647700 |
| C  | 0.67982400  | 1.99125400  | -1.72304300 |
| Sc | 0.28601000  | 0.92250100  | 0.46897100  |
| C  | 4.20816800  | 3.42126000  | -2.38492400 |
| C  | 4.80824800  | 1.49818900  | -0.06544100 |
| C  | 3.83576600  | 0.43379800  | -2.76401600 |
| H  | 3.57639100  | 3.62430900  | -3.25534700 |
| H  | 4.14901600  | 4.28796900  | -1.72021400 |
| H  | 5.24245700  | 3.33274400  | -2.73192700 |
| H  | 4.35320000  | 0.87368600  | 0.71049500  |
| H  | 5.69813900  | 0.97303600  | -0.42770400 |
| H  | 5.14393200  | 2.42774600  | 0.40250200  |
| H  | 4.89800100  | 0.35478100  | -3.02056300 |
| H  | 3.52354800  | -0.53536100 | -2.36785400 |
| H  | 3.28943600  | 0.62331100  | -3.69144700 |
| Si | 3.65509700  | 1.84033800  | -1.52527600 |
| C  | 0.55261000  | 1.34787100  | -3.07669800 |
| H  | 0.94402900  | 2.02551700  | -3.84460800 |
| H  | 1.10492300  | 0.41168200  | -3.15874900 |
| H  | -0.49374600 | 1.15159800  | -3.32882100 |
| C  | -1.78121600 | 2.84017500  | -1.58454700 |
| H  | -2.46907200 | 3.05266200  | -0.76236700 |
| H  | -1.87867200 | 3.64538900  | -2.32047700 |
| H  | -2.12436400 | 1.91770700  | -2.06465300 |
| C  | -0.52965600 | 4.38482100  | 0.90029400  |
| H  | -0.27097900 | 4.28354300  | 1.95826900  |
| H  | -0.26691900 | 5.40420400  | 0.59860400  |
| H  | -1.61377700 | 4.28657900  | 0.81235800  |
| C  | 2.53362600  | 3.68965200  | 1.06131800  |
| H  | 3.19741200  | 2.97998900  | 1.55879400  |
| H  | 3.17717700  | 4.38225300  | 0.50665900  |
| H  | 2.02171200  | 4.28093100  | 1.82363800  |
| C  | -0.51797600 | -4.14056900 | -2.36120400 |
| C  | -0.26257500 | -2.62760300 | -2.26564000 |
| H  | 0.08010800  | -4.71422900 | -1.65101000 |
| H  | -1.56903400 | -4.38347700 | -2.18388100 |
| H  | -0.26481800 | -4.48806800 | -3.36760100 |
| C  | -1.24592200 | -1.89882300 | -3.23943400 |
| C  | 1.17943200  | -2.34171000 | -2.68414900 |
| H  | -0.70687300 | -1.11074600 | -3.77532700 |
| H  | -1.63122000 | -2.59129900 | -3.99525100 |
| H  | 1.26406800  | -2.37546900 | -3.77487200 |
| H  | 1.50457400  | -1.35282700 | -2.34907700 |
| H  | 1.87441100  | -3.08466800 | -2.28447400 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.65814100 | -2.07055700 | -0.84716000 |
| H | -1.22281200 | -2.86797000 | -0.34374900 |
| N | 0.33362800  | -1.53338100 | 0.17181400  |
| C | 1.52353200  | -2.30942400 | 0.66251300  |
| C | 1.41165500  | -3.83046700 | 0.59023000  |
| C | 2.87348800  | -1.82815700 | 0.13125600  |
| H | 1.53513800  | -2.07619100 | 1.73548000  |
| C | 2.54101200  | -4.46506300 | 1.40991500  |
| H | 1.50111500  | -4.16127400 | -0.44856100 |
| H | 0.43327900  | -4.15796200 | 0.96268600  |
| C | 4.00336800  | -2.45345100 | 0.95629300  |
| H | 3.00862200  | -2.11152800 | -0.91388800 |
| H | 2.93087300  | -0.73086900 | 0.16763000  |
| C | 3.91071100  | -3.98160400 | 0.92755200  |
| H | 2.47673200  | -5.55498800 | 1.34750400  |
| H | 2.40982400  | -4.19825900 | 2.46787200  |
| H | 4.97116700  | -2.11674100 | 0.57272200  |
| H | 3.93818400  | -2.10866200 | 1.99890100  |
| H | 4.70492700  | -4.42085200 | 1.53807500  |
| H | 4.07117500  | -4.32867700 | -0.10181800 |
| C | -2.36546600 | -1.26066200 | -2.40353200 |
| C | -1.60637200 | -0.89969800 | -1.12893300 |
| H | -2.72802900 | -0.34905300 | -2.89348300 |
| H | -0.99216800 | -0.01441600 | -1.37343400 |
| H | -2.24416200 | -0.65137100 | -0.27736100 |
| C | -3.57495200 | -2.17388400 | -2.15530200 |
| C | -4.53203000 | -1.66673600 | -1.07095700 |
| H | -3.24178800 | -3.18150300 | -1.88215600 |
| H | -4.11328300 | -2.27864500 | -3.10514700 |
| C | -4.95047500 | -0.20510400 | -1.22371600 |
| H | -5.42785900 | -2.29839400 | -1.06601700 |
| H | -4.06915200 | -1.80495600 | -0.08336400 |
| H | -4.06453700 | 0.44636800  | -1.19791000 |
| H | -5.40794200 | -0.05546400 | -2.21140100 |
| C | -5.91593000 | 0.25377300  | -0.13405900 |
| C | -6.27259200 | 1.73466500  | -0.23721100 |
| H | -5.46751300 | 0.06159300  | 0.85227000  |
| H | -6.83265100 | -0.34924700 | -0.17418900 |
| C | -7.22294000 | 2.18937700  | 0.86657600  |
| H | -5.34828200 | 2.32714500  | -0.19918600 |
| H | -6.72207500 | 1.92904900  | -1.21880700 |
| H | -7.46664300 | 3.25073300  | 0.77550600  |
| H | -8.15996700 | 1.62545100  | 0.82986200  |
| H | -6.77828700 | 2.02965500  | 1.85411000  |

|     |             |             |             |
|-----|-------------|-------------|-------------|
| N   | 0.82747200  | 0.96211100  | 2.75841100  |
| C   | 2.21894200  | 0.53137700  | 2.99990700  |
| H   | 2.46078100  | -0.35438500 | 2.40800400  |
| H   | 2.88570700  | 1.34452000  | 2.71144700  |
| H   | 2.39308000  | 0.30788200  | 4.05892700  |
| C   | 0.56266800  | 2.13298900  | 3.62931700  |
| H   | 0.75495800  | 1.85796400  | 4.67299100  |
| H   | 1.22718100  | 2.94997900  | 3.34399700  |
| H   | -0.47359600 | 2.45179600  | 3.54015400  |
| C   | -0.16857900 | -0.08387700 | 2.96265300  |
| C   | -1.43147100 | 0.10964000  | 2.33977800  |
| C   | 0.12365800  | -1.26244100 | 3.65791700  |
| C   | -2.34483100 | -0.96437100 | 2.41608800  |
| C   | -0.79820200 | -2.30049600 | 3.69870900  |
| H   | 1.08395800  | -1.38804800 | 4.14581500  |
| C   | -2.03645500 | -2.14942600 | 3.06657300  |
| H   | -3.31844400 | -0.83878200 | 1.94965100  |
| H   | -0.55613200 | -3.21649000 | 4.22604100  |
| H   | -2.76514000 | -2.95293600 | 3.10001600  |
| C   | -1.66774700 | 1.27579100  | 1.47146000  |
| H   | -0.27129700 | -1.56440700 | 0.99716900  |
| H   | -2.61763100 | 1.21782700  | 0.93483600  |
| H   | -1.58364300 | 2.24651000  | 1.96092000  |
| g'' |             |             |             |
| C   | -0.19282600 | -0.29655500 | -2.38555200 |
| C   | 1.23572300  | -0.25004500 | -2.54324700 |
| C   | 1.63993200  | 1.11267400  | -2.60830500 |
| C   | 0.47197500  | 1.92146700  | -2.51089600 |
| C   | -0.64470700 | 1.06555300  | -2.38470300 |
| Sc  | 0.72319300  | 0.75826200  | -0.32993900 |
| C   | -0.49490100 | -3.38288200 | -2.99739500 |
| C   | -2.62684900 | -1.96670600 | -1.28752900 |
| C   | -2.34022600 | -1.37323500 | -4.26118100 |
| H   | 0.02605600  | -3.36384000 | -3.95910400 |
| H   | 0.22167300  | -3.69260200 | -2.23459800 |
| H   | -1.26513000 | -4.15920400 | -3.06359000 |
| H   | -3.41991400 | -1.21243900 | -1.33505500 |
| H   | -3.10753900 | -2.94626500 | -1.38528300 |
| H   | -2.17716900 | -1.91824900 | -0.29065700 |
| H   | -2.93868900 | -2.24651400 | -4.54062500 |
| H   | -3.02133700 | -0.52609100 | -4.14658100 |
| H   | -1.66099800 | -1.15267300 | -5.09010300 |
| Si  | -1.37224000 | -1.74234500 | -2.68787200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.06143800 | 1.56115300  | -2.44824400 |
| H | -2.16355300 | 2.52584500  | -1.94501500 |
| H | -2.35565000 | 1.71421800  | -3.49303500 |
| H | -2.77910800 | 0.86438500  | -2.00687500 |
| C | 0.41022900  | 3.41522100  | -2.64589200 |
| H | 1.40031100  | 3.86726000  | -2.55200900 |
| H | 0.00866900  | 3.69430700  | -3.62624400 |
| H | -0.23698300 | 3.86805500  | -1.88661900 |
| C | 3.01711100  | 1.66945800  | -2.84497300 |
| H | 3.78762400  | 0.89784800  | -2.80896200 |
| H | 3.06920800  | 2.14077800  | -3.83185200 |
| H | 3.27697200  | 2.43455000  | -2.10452000 |
| C | 2.13979600  | -1.44044000 | -2.73858500 |
| H | 2.14694200  | -2.11972900 | -1.87824500 |
| H | 1.82581800  | -2.02080100 | -3.60969900 |
| H | 3.16910300  | -1.12758400 | -2.92448500 |
| C | 1.22576800  | 2.52188100  | 3.03291200  |
| C | 0.69702700  | 3.10861100  | 1.70630300  |
| H | 0.56527900  | 2.75121500  | 3.87620500  |
| H | 1.33407400  | 1.43301100  | 2.96149000  |
| H | 2.20812100  | 2.95451500  | 3.24670300  |
| C | 1.56256400  | 2.64679100  | 0.51774600  |
| C | 0.63265700  | 4.63977000  | 1.83418600  |
| H | 1.48121000  | 3.40000700  | -0.27826300 |
| H | 2.61421600  | 2.67028200  | 0.83235500  |
| H | 1.64545100  | 5.03151700  | 1.96000400  |
| H | 0.20656500  | 5.08948600  | 0.93180400  |
| H | 0.03399900  | 4.95516000  | 2.69648900  |
| C | -0.70544800 | 2.58405800  | 1.58823800  |
| H | -1.46872100 | 3.06557800  | 2.21292300  |
| N | -1.02257700 | 1.58309000  | 0.85402800  |
| C | -2.41086400 | 1.07489000  | 0.90978700  |
| C | -2.66334100 | 0.33157600  | 2.22448600  |
| C | -3.49592000 | 2.13829700  | 0.71050600  |
| H | -2.48819100 | 0.35270600  | 0.08867400  |
| C | -4.02941600 | -0.35640300 | 2.19525200  |
| H | -2.62453000 | 1.05731500  | 3.04949500  |
| H | -1.86537800 | -0.39247200 | 2.40262800  |
| C | -4.86660800 | 1.45645900  | 0.64635300  |
| H | -3.48914500 | 2.83858200  | 1.55535700  |
| H | -3.30542600 | 2.71889800  | -0.19541500 |
| C | -5.14600200 | 0.65323200  | 1.91920700  |
| H | -4.20490300 | -0.87499300 | 3.14292000  |
| H | -4.02456800 | -1.12331600 | 1.40759200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.64565200 | 2.20750200  | 0.48927700  |
| H | -4.89284200 | 0.78585500  | -0.22398000 |
| H | -6.10895200 | 0.14077700  | 1.83963700  |
| H | -5.22180100 | 1.34440300  | 2.76881000  |
| C | 5.02246000  | -1.80061600 | 1.10055500  |
| C | 4.01565600  | -0.63951600 | 1.16935500  |
| H | 5.05682300  | -2.35541900 | 2.04303500  |
| H | 4.76848600  | -2.49765900 | 0.29542100  |
| H | 6.02214400  | -1.40392700 | 0.90510500  |
| C | 4.02493600  | 0.12438600  | -0.14662700 |
| C | 4.37400400  | 0.28454300  | 2.34765900  |
| H | 3.34337300  | 0.97958400  | -0.12860900 |
| H | 5.02431300  | 0.52680700  | -0.33810500 |
| H | 3.75853100  | -0.53575800 | -0.97436500 |
| H | 5.39499100  | 0.65339100  | 2.21533400  |
| H | 3.69707500  | 1.14225600  | 2.39043200  |
| H | 4.32634500  | -0.24656000 | 3.30343700  |
| C | 2.67697600  | -1.25053700 | 1.47047400  |
| H | 2.72366000  | -2.05940100 | 2.20962500  |
| N | 1.54151700  | -0.94621100 | 0.96542600  |
| C | 0.39010500  | -1.80297900 | 1.37539400  |
| C | 0.53630400  | -3.18512800 | 0.72758400  |
| C | 0.19027000  | -1.90116400 | 2.89159600  |
| H | -0.51378500 | -1.32623900 | 0.95568900  |
| C | -0.60378700 | -4.13194800 | 1.10534500  |
| H | 1.49017800  | -3.61601200 | 1.06249100  |
| H | 0.60416700  | -3.05934700 | -0.35776500 |
| C | -0.98041700 | -2.83382000 | 3.22433800  |
| H | 1.09239000  | -2.31086700 | 3.36016100  |
| H | 0.03833700  | -0.89969200 | 3.31153400  |
| C | -0.76161600 | -4.22298400 | 2.62357300  |
| H | -0.40934600 | -5.11796800 | 0.67329100  |
| H | -1.54308100 | -3.77651600 | 0.66427500  |
| H | -1.09826000 | -2.89280300 | 4.30995900  |
| H | -1.91735200 | -2.42075500 | 2.82592500  |
| H | -1.59835400 | -4.87931400 | 2.87794500  |
| H | 0.14121100  | -4.67029900 | 3.06007100  |