

## Supporting Information

# Theoretical Investigations toward the Tandem Reactions of N-aziridinyl Imine Compounds Forming Triquinanes via Trimethylenemethane Diyls: Mechanisms and Stereoselectivity

Yan Qiao, Ke-Li Han\*

*State Key Laboratory of Molecular Reaction Dynamics*

*Dalian Institute of Chemical Physics of CAS*

*NO.457, Zhongshan Road, Dalian 116023, P. R. China*

*klhan@dicp.ac.cn*

## Supporting Information

### Table of Contents

|                                                                                                                                                                                                                 |    |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| <b>Table 1.</b> The ZPE, $\delta G$ , E, and E+ZPE (stationary points) at the UB3LYP/6-31G(d) level in gas phase and E at UB3LYP/6-31++G (2d, 2p) level in solvent toluene using IEFPCM model (unit: a.u.)..... | S2 |
| Cartesian Coordinates of all stationary points at UB3LYP/6-31G(d) level.....                                                                                                                                    | S3 |

**Table 1.** The ZPE,  $\delta G$ , E, E+ZPE, and G of SP (stationary points) at the UB3LYP/6-31G (d) level, and E at UB3LYP/6-31++G (2d,2p) level (unit: a.u.)

| SP                  | ZPE      | $\delta G$ | E              | E+ZPE        | E(UB3LYP/B2)   |
|---------------------|----------|------------|----------------|--------------|----------------|
| <b>R</b>            | 0.529876 | 0.460305   | -1382.17333074 | -1381.643455 | -1382.31231232 |
| <b>Phenylethene</b> | 0.133731 | 0.102255   | -309.648259110 | -309.514528  | -309.681804643 |
| <b>TS1</b>          | 0.526136 | 0.455493   | -1382.12751164 | -1381.601376 | -1382.26773838 |
| <b>M1</b>           | 0.390147 | 0.329500   | -1072.51810255 | -1072.127956 | -1072.62888598 |
| <b>TS2a</b>         | 0.390430 | 0.334122   | -1072.48777829 | -1072.097348 | -1072.59754787 |
| <b>TS2b</b>         | 0.389259 | 0.330586   | -1072.47806778 | -1072.088809 | -1072.58931511 |
| <b>M2a</b>          | 0.395950 | 0.340849   | -1072.56189441 | -1072.165944 | -1072.67064305 |
| <b>M2b</b>          | 0.396343 | 0.341202   | -1072.56372631 | -1072.167384 | -1072.67163093 |
| <b>TS3a</b>         | 0.389742 | 0.333057   | -1072.52002480 | -1072.130283 | -1072.63157898 |
| <b>TS3b</b>         | 0.388684 | 0.331785   | -1072.50641004 | -1072.117726 | -1072.61680805 |
| <b>M3S</b>          | 0.378300 | 0.322896   | -963.03125879  | -962.652959  | -963.135147145 |
| <b>M3T</b>          | 0.379570 | 0.322457   | -963.04739546  | -962.667825  | -963.150574478 |
| <b>TS4S1</b>        | 0.380417 | 0.327270   | -963.00466922  | -962.624252  | -963.11077344  |
| <b>TS4S2</b>        | 0.379784 | 0.327110   | -962.99824324  | -962.618459  | -963.10516662  |
| <b>TS4T1</b>        | 0.379592 | 0.325024   | -963.03044585  | -962.650853  | -963.133076944 |
| <b>M4T1</b>         | 0.381028 | 0.324882   | -963.05183320  | -962.670806  | -963.152965738 |
| <b>TS5T1</b>        | 0.381870 | 0.328559   | -963.00072252  | -962.618852  | -963.101788454 |
| <b>TS5T2</b>        | 0.381981 | 0.328891   | -962.99991598  | -962.617935  | -963.100393902 |
| <b>TS4T2</b>        | 0.380442 | 0.328118   | -963.01363500  | -962.633193  | -963.11467823  |
| <b>M4T2</b>         | 0.382332 | 0.329925   | -963.04490970  | -962.662578  | -963.14463925  |
| <b>TS5T3</b>        | 0.382486 | 0.331059   | -962.98948040  | -962.606995  | -963.08936355  |
| <b>TS5T4</b>        | 0.383455 | 0.332078   | -962.98720819  | -962.603753  | -963.08522617  |
| <b>TS4T3</b>        | 0.380652 | 0.327845   | -963.01359861  | -962.632947  | -963.11342858  |
| <b>M4T3</b>         | 0.382409 | 0.329425   | -963.04094745  | -962.658538  | -963.138733    |
| <b>TS5T5</b>        | 0.381472 | 0.329677   | -962.96653476  | -962.585063  | -963.06562585  |
| <b>P1</b>           | 0.389780 | 0.338535   | -963.15454941  | -962.764769  | -963.252276468 |
| <b>P2</b>           | 0.389664 | 0.341402   | -963.15398171  | -962.764318  | -963.251706326 |
| <b>P3</b>           | 0.390656 | 0.341402   | -963.14186096  | -962.751205  | -963.238124792 |
| <b>P4</b>           | 0.390584 | 0.341340   | -963.11807133  | -962.727487  | -963.21399996  |
| <b>P5</b>           | 0.390546 | 0.341211   | -963.13908051  | -962.748534  | -963.234406713 |
| <b>N2</b>           | 0.005599 | -0.012851  | -109.52412901  | -109.518530  | -109.532852422 |
| <b>R'</b>           | 0.557796 | 0.485638   | -1421.49127924 | -1420.933483 | -1421.63378063 |
| <b>TS1'</b>         | 0.554372 | 0.482817   | -1421.44544936 | -1420.891077 | -1421.58931462 |
| <b>M1'</b>          | 0.418398 | 0.355838   | -1111.83585654 | -1111.417458 | -1111.94988900 |
| <b>TS2a'</b>        | 0.418220 | 0.359923   | -1111.80710610 | -1111.388886 | -1111.92033241 |
| <b>M2a'</b>         | 0.423616 | 0.366777   | -1111.88193474 | -1111.458318 | -1111.99449689 |
| <b>TS3a'</b>        | 0.417790 | 0.359438   | -1111.84398028 | -1111.426191 | -1111.95934386 |
| <b>M3S'</b>         | 0.406431 | 0.347813   | -1002.35265688 | -1001.946225 | -1002.44957208 |
| <b>M3T'</b>         | 0.407616 | 0.348295   | -1002.36750525 | -1001.959889 | -1002.47423795 |
| <b>TS4S1'</b>       | 0.407964 | 0.352726   | -1002.33061942 | -1001.922655 | -1002.44191784 |

|               |          |          |                |              |                |
|---------------|----------|----------|----------------|--------------|----------------|
| <b>TS4T1'</b> | 0.407430 | 0.350216 | -1002.35022300 | -1001.942793 | -1002.45639027 |
| <b>M4T1'</b>  | 0.409086 | 0.351454 | -1002.37176402 | -1001.962678 | -1002.47641999 |
| <b>TS5T1'</b> | 0.410035 | 0.354173 | -1002.32202073 | -1001.911986 | -1002.42710558 |
| <b>TS5T2'</b> | 0.410201 | 0.355902 | -1002.31542461 | -1001.905224 | -1002.41990399 |
| <b>P1'</b>    | 0.417533 | 0.364015 | -1002.47512525 | -1002.057592 | -1002.57633812 |
| <b>P2'</b>    | 0.417535 | 0.364864 | -1002.46746728 | -1002.049932 | -1002.56948177 |

**Cartesian Coordinates of all stationary points at UB3LYP/6-31G(d) level**

**R**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.36311300 | -3.00136000 | 2.58791100  |
| C | -2.25600400 | -2.05822500 | 2.28496300  |
| C | -0.97773800 | 0.77085800  | -0.86359100 |
| C | -0.26439700 | 1.75904300  | -0.38192700 |
| C | 2.56142600  | 0.40106800  | 0.46063200  |
| C | 0.45740100  | 2.74134100  | 0.09925100  |
| C | 1.97088300  | 2.83570100  | 0.05707500  |
| C | 2.68438900  | 1.58378600  | -0.46384700 |
| H | -0.83907700 | -3.00475400 | 3.53996400  |
| H | -1.11962600 | -3.80697300 | 1.89773500  |
| H | 2.33577900  | 3.07473900  | 1.06755900  |
| H | 3.75072400  | 1.80912700  | -0.60837100 |
| C | -3.04357400 | -2.02995100 | 0.99932300  |
| C | -1.34013700 | -0.46457800 | -0.06991700 |
| C | -2.87009000 | -0.75145200 | 0.10769600  |
| H | -4.10531000 | -2.14972500 | 1.24216200  |
| H | -2.75820300 | -2.89380300 | 0.38623400  |
| H | -0.91407800 | -1.34286200 | -0.56739700 |
| H | -0.89615800 | -0.40447300 | 0.92601200  |
| H | -1.31133200 | 0.79941300  | -1.89948600 |
| H | -2.47489100 | -1.26328500 | 2.99306000  |
| H | 2.20799500  | 0.57873300  | 1.47811300  |
| H | 2.30182300  | 1.28959200  | -1.44952500 |
| H | 2.25053400  | 3.69891500  | -0.56392500 |
| C | -3.48542300 | 0.48983200  | 0.76061400  |
| C | -3.47947000 | -1.05582500 | -1.28501400 |
| O | -3.59244900 | 0.66643400  | 1.95715600  |
| O | -3.83083100 | 1.40613800  | -0.16621600 |
| O | -4.81561000 | -1.22421600 | -1.44558600 |
| O | -2.78397200 | -1.20784200 | -2.26237800 |
| C | -5.83422900 | -1.18501100 | -0.43038500 |
| H | -5.96379500 | -2.20008100 | -0.03724500 |
| H | -5.55754600 | -0.53009200 | 0.39817400  |
| C | -7.11182600 | -0.69763000 | -1.09328500 |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| H          | -7.38215300 | -1.34811900 | -1.93045500 |
| H          | -7.93444700 | -0.69890000 | -0.36961300 |
| H          | -6.98136700 | 0.31937800  | -1.47548000 |
| C          | -4.20751200 | 2.72283400  | 0.31421100  |
| H          | -3.95085600 | 3.38749000  | -0.51354600 |
| H          | -3.58682600 | 2.96422600  | 1.18016500  |
| C          | -5.68665000 | 2.80175900  | 0.65760900  |
| H          | -5.92532200 | 2.14532400  | 1.49902600  |
| H          | -5.94281700 | 3.82872800  | 0.94268300  |
| H          | -6.30521300 | 2.52362400  | -0.20208300 |
| N          | 3.22287200  | -1.05755400 | -1.14116300 |
| N          | 2.82613500  | -0.82434300 | 0.19580100  |
| C          | 4.68656300  | -0.95861600 | -1.47970300 |
| H          | 4.82165200  | -0.59550600 | -2.49735500 |
| C          | 3.99343400  | -2.27550100 | -1.32251400 |
| H          | 3.74321400  | -2.86384400 | -2.20377800 |
| H          | 4.21405500  | -2.85360800 | -0.42725200 |
| C          | 5.73678500  | -0.46352700 | -0.54400900 |
| C          | 6.71695700  | 0.40192900  | -1.05651400 |
| C          | 5.80975600  | -0.82068600 | 0.81313500  |
| C          | 7.74499900  | 0.88752200  | -0.24911600 |
| H          | 6.67502000  | 0.69044800  | -2.10449000 |
| C          | 6.83537000  | -0.33110400 | 1.62123200  |
| H          | 5.05425100  | -1.47022700 | 1.24128700  |
| C          | 7.80776000  | 0.52248200  | 1.09604200  |
| H          | 8.49504800  | 1.55066500  | -0.67221400 |
| H          | 6.87320500  | -0.61933700 | 2.66858500  |
| H          | 8.60582200  | 0.89973800  | 1.72984200  |
| H          | -0.05362000 | 3.58647800  | 0.56609800  |
| <b>TS1</b> |             |             |             |
| C          | 0.59837600  | -3.01114500 | 0.50377100  |
| C          | -0.49706900 | -2.33412400 | 0.85478000  |
| C          | -1.17719100 | 1.61331800  | -1.00859800 |
| C          | -0.65417900 | 2.59578800  | -0.31625800 |
| C          | 2.70135100  | 2.23946500  | -0.22353400 |
| C          | -0.13137200 | 3.58213800  | 0.36928300  |
| C          | 1.19937300  | 4.25533400  | 0.08937900  |
| C          | 2.13502300  | 3.49147700  | -0.85596000 |
| H          | 1.43358600  | -3.14072200 | 1.18666200  |
| H          | 0.69937600  | -3.47324600 | -0.47689100 |
| H          | 1.71073100  | 4.42896800  | 1.04762000  |
| H          | 2.96065900  | 4.16025100  | -1.14751200 |
| C          | -1.70660800 | -2.17859900 | -0.03235200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.92311900 | 0.15094400  | -0.71760000 |
| C | -2.17163100 | -0.70994000 | -0.32439800 |
| H | -2.53812900 | -2.72591400 | 0.42560000  |
| H | -1.50380800 | -2.65718000 | -0.99842600 |
| H | -0.49361200 | -0.31890400 | -1.60991000 |
| H | -0.19224100 | 0.06245500  | 0.08939100  |
| H | -1.81098600 | 1.83350900  | -1.86587000 |
| H | -0.57364500 | -1.89138200 | 1.84478700  |
| H | 2.80339300  | 2.17694400  | 0.85667500  |
| H | 1.60966900  | 3.22762200  | -1.78197300 |
| H | 1.00665400  | 5.25689300  | -0.32244700 |
| C | -2.78904600 | -0.05539300 | 0.91454600  |
| C | -3.14239900 | -0.74967400 | -1.53266900 |
| O | -2.48153700 | -0.31659000 | 2.05994400  |
| O | -3.66947300 | 0.90488400  | 0.57239600  |
| O | -4.36817900 | -1.31915600 | -1.43215900 |
| O | -2.81906200 | -0.32440200 | -2.61769600 |
| C | -4.93133800 | -1.99332800 | -0.29229800 |
| H | -4.63957300 | -3.04891500 | -0.33998100 |
| H | -4.56293600 | -1.57762400 | 0.64784000  |
| C | -6.44088400 | -1.84768100 | -0.38648900 |
| H | -6.80661200 | -2.25237100 | -1.33487100 |
| H | -6.92235100 | -2.39054600 | 0.43435400  |
| H | -6.72910700 | -0.79367600 | -0.32774700 |
| C | -4.16357000 | 1.76017400  | 1.63631400  |
| H | -4.40622300 | 2.69643700  | 1.12910600  |
| H | -3.35119700 | 1.93072000  | 2.34644300  |
| C | -5.38193800 | 1.16402000  | 2.32337900  |
| H | -5.12060400 | 0.23883800  | 2.84467900  |
| H | -5.77096000 | 1.87386400  | 3.06244700  |
| H | -6.17738200 | 0.95648300  | 1.60004000  |
| N | 3.34551300  | 0.81490700  | -2.03528300 |
| N | 3.11757000  | 1.23175700  | -0.90662300 |
| C | 4.51332200  | -1.24843500 | -1.64479600 |
| H | 5.31708600  | -1.31478500 | -2.37427600 |
| C | 3.22432000  | -0.95758600 | -2.12280400 |
| H | 3.04367500  | -1.09796800 | -3.18416000 |
| H | 2.35279100  | -1.17404300 | -1.50944500 |
| C | 4.89979000  | -1.20912300 | -0.26613900 |
| C | 6.26862100  | -1.33678300 | 0.08600900  |
| C | 3.97191100  | -0.98169000 | 0.78090100  |
| C | 6.68444700  | -1.24734100 | 1.40418700  |
| H | 6.99762300  | -1.50256300 | -0.70387000 |
| C | 4.40089400  | -0.88258800 | 2.10621700  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | 2.91155100  | -0.92787000 | 0.56514300 |
| C | 5.75078700  | -1.01316400 | 2.42548200 |
| H | 7.73882400  | -1.35196800 | 1.64677300 |
| H | 3.67032800  | -0.71238100 | 2.89314200 |
| H | 6.07928500  | -0.94119100 | 3.45877200 |
| H | -0.69866900 | 3.98934600  | 1.20924100 |

**M1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.78404400  | -1.17473200 | 3.58054700  |
| C | -0.03579400 | -0.46196500 | 2.80649300  |
| C | 1.37178400  | 0.51807100  | 0.18590500  |
| C | 2.57248700  | 0.29043500  | 0.65653400  |
| C | 4.29439500  | -0.81165700 | -1.88047900 |
| C | 3.74287500  | 0.03252500  | 1.18233500  |
| C | 5.06489900  | -0.10685000 | 0.45770200  |
| C | 5.04661600  | 0.19885300  | -1.05082600 |
| H | 1.42575500  | -0.69996100 | 4.31820400  |
| H | 0.84496900  | -2.25933100 | 3.51086500  |
| H | 5.45432800  | -1.12332900 | 0.62146000  |
| H | 6.08921000  | 0.25303400  | -1.39707800 |
| C | -1.00816400 | -1.07611600 | 1.83209400  |
| C | 0.42364600  | -0.56902600 | -0.27694600 |
| C | -1.00389200 | -0.53597100 | 0.36738200  |
| H | -2.01488500 | -0.94338300 | 2.24436000  |
| H | -0.82718500 | -2.15693900 | 1.78092500  |
| H | 0.29867600  | -0.49004700 | -1.36014900 |
| H | 0.85899500  | -1.55138200 | -0.07988900 |
| H | 1.04369700  | 1.55265600  | 0.06873100  |
| H | -0.07849400 | 0.61908100  | 2.90784300  |
| H | 4.61050300  | 1.19060100  | -1.21606100 |
| H | 5.79413600  | 0.56259500  | 0.93753000  |
| C | -1.51903200 | 0.90601900  | 0.28939400  |
| C | -1.88661900 | -1.49610100 | -0.48735700 |
| O | -1.71981100 | 1.63951300  | 1.23672100  |
| O | -1.67548800 | 1.27865500  | -0.99681500 |
| O | -3.23516100 | -1.53744600 | -0.34201800 |
| O | -1.39465800 | -2.25620400 | -1.28619900 |
| C | -4.04279700 | -0.87965800 | 0.65430200  |
| H | -4.05790100 | -1.50817900 | 1.55242000  |
| H | -3.63743200 | 0.09584700  | 0.92723100  |
| C | -5.44047100 | -0.74222400 | 0.07387300  |
| H | -5.83614000 | -1.72176300 | -0.21055000 |
| H | -6.11107800 | -0.29644300 | 0.81684000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.42937300 | -0.10346300 | -0.81467800 |
| C | -2.06177700 | 2.65369200  | -1.25416100 |
| H | -1.63967500 | 2.86724900  | -2.23855500 |
| H | -1.58887500 | 3.29458600  | -0.50636500 |
| C | -3.57343300 | 2.81726300  | -1.24814300 |
| H | -3.98154900 | 2.63092100  | -0.25047500 |
| H | -3.83471900 | 3.84181900  | -1.53664900 |
| H | -4.04160300 | 2.13051500  | -1.96076400 |
| N | 2.43297800  | -0.11639700 | -3.29977400 |
| N | 3.30666400  | -0.45745100 | -2.63439300 |
| H | 4.53922200  | -1.86750400 | -1.88784600 |
| H | 3.78871200  | -0.09504900 | 2.26710000  |

**TS2a**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.44662200 | -2.54839500 | -2.05996100 |
| C | -0.57006000 | -1.56477400 | -1.84537700 |
| C | -1.32408700 | 0.51700800  | 0.92684700  |
| C | -2.25152600 | 0.71176100  | -0.03938500 |
| C | -3.97880300 | -0.45231500 | 0.34477700  |
| C | -2.76996900 | 1.34034300  | -1.08597800 |
| C | -4.22887100 | 1.18723300  | -1.44548600 |
| C | -4.94958300 | 0.54717000  | -0.23679500 |
| H | -2.31502100 | -2.40754800 | -2.69882600 |
| H | -1.32178300 | -3.53755600 | -1.62247000 |
| H | -4.33859400 | 0.55368700  | -2.33957500 |
| H | -5.90433200 | 0.09640400  | -0.53484200 |
| C | 0.68477200  | -1.72455200 | -1.02876600 |
| C | -0.43222300 | -0.70060400 | 1.07934400  |
| C | 0.86644100  | -0.74022300 | 0.17227000  |
| H | 1.54001000  | -1.62300000 | -1.70569700 |
| H | 0.71723700  | -2.74289400 | -0.62149200 |
| H | -0.10585900 | -0.76976500 | 2.11577700  |
| H | -0.99450000 | -1.61460900 | 0.86297000  |
| H | -1.13254500 | 1.33824200  | 1.61413600  |
| H | -0.71922200 | -0.59172900 | -2.30383900 |
| H | -5.15969200 | 1.31630300  | 0.51382600  |
| H | -4.68765800 | 2.15086900  | -1.70159700 |
| C | 1.14930300  | 0.68710100  | -0.30511300 |
| C | 2.04107900  | -1.28788300 | 1.04009800  |
| O | 0.98295500  | 1.10298200  | -1.43438000 |
| O | 1.58644200  | 1.44661600  | 0.72027400  |
| O | 3.31815200  | -1.28297500 | 0.57776500  |
| O | 1.86002100  | -1.77550600 | 2.13006200  |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| C           | 3.79769900  | -0.87784600 | -0.71829300 |
| H           | 3.74713900  | -1.74473900 | -1.38766800 |
| H           | 3.18996500  | -0.07987000 | -1.14737500 |
| C           | 5.23709000  | -0.42373000 | -0.53951000 |
| H           | 5.83890700  | -1.22205600 | -0.09508100 |
| H           | 5.66944500  | -0.15919400 | -1.51092800 |
| H           | 5.28729400  | 0.45137900  | 0.11568900  |
| C           | 1.74943000  | 2.86613000  | 0.47216100  |
| H           | 1.58170500  | 3.32718100  | 1.44827600  |
| H           | 0.96942100  | 3.18848800  | -0.22136100 |
| C           | 3.13611400  | 3.18786500  | -0.06223600 |
| H           | 3.28399500  | 2.74839700  | -1.05290300 |
| H           | 3.25473300  | 4.27401700  | -0.15023000 |
| H           | 3.91096600  | 2.81347600  | 0.61477600  |
| N           | -3.11561000 | -0.37704900 | 2.57435400  |
| N           | -3.82138800 | -0.56216700 | 1.67435800  |
| H           | -3.86225500 | -1.40992800 | -0.16232700 |
| H           | -2.13203200 | 1.94427700  | -1.73158400 |
| <b>TS2b</b> |             |             |             |
| C           | -1.65759800 | 4.16030600  | -1.05909800 |
| C           | -1.76849000 | 2.83983200  | -1.21181500 |
| C           | 1.25887400  | 0.40308300  | 0.90504800  |
| C           | 2.37067500  | 0.28987600  | 0.14290300  |
| C           | 3.96231000  | 0.10420300  | 1.14060600  |
| C           | 2.86896300  | 0.37379100  | -1.11044400 |
| C           | 4.31811300  | 0.76978700  | -1.22873500 |
| C           | 4.80197500  | 1.00758000  | 0.22105600  |
| H           | -1.35195500 | 4.80467900  | -1.87927500 |
| H           | -1.87249800 | 4.65083500  | -0.11125300 |
| H           | 4.46903800  | 1.68217500  | -1.82269800 |
| H           | 4.58083800  | 2.03575000  | 0.52392500  |
| C           | -2.23459000 | 1.90610300  | -0.12399400 |
| C           | 0.15659500  | 1.37791400  | 0.59422900  |
| C           | -1.25029200 | 0.75039000  | 0.27096400  |
| H           | -3.19613800 | 1.47144700  | -0.42405200 |
| H           | -2.42720000 | 2.48548600  | 0.78723100  |
| H           | -0.01554000 | 2.04880600  | 1.44564900  |
| H           | 0.44493000  | 1.98872400  | -0.26466500 |
| H           | 1.15024000  | -0.18532600 | 1.81255000  |
| H           | -1.54384400 | 2.37912900  | -2.17001600 |
| H           | 5.87834500  | 0.85040800  | 0.34331200  |
| H           | 4.90819800  | -0.01439500 | -1.72787700 |
| C           | -1.03505700 | -0.25900300 | -0.85751400 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.80932000 | 0.10480400  | 1.56396100  |
| O | -1.07815700 | -0.00240200 | -2.04389800 |
| O | -0.70287100 | -1.47011000 | -0.36506600 |
| O | -2.99467600 | -0.55640800 | 1.54655200  |
| O | -1.28848500 | 0.28056600  | 2.64089700  |
| C | -3.66351200 | -1.10929800 | 0.39828100  |
| H | -3.44900200 | -0.54054300 | -0.50973500 |
| H | -3.29118100 | -2.12830800 | 0.25500500  |
| C | -5.15419700 | -1.10343900 | 0.69349100  |
| H | -5.52375700 | -0.08007700 | 0.81445700  |
| H | -5.70080200 | -1.57614200 | -0.13007400 |
| H | -5.36480200 | -1.65590600 | 1.61414600  |
| C | -0.21280800 | -2.45989400 | -1.30778800 |
| H | 0.45921800  | -3.08107900 | -0.71201000 |
| H | 0.36243400  | -1.94506600 | -2.08016700 |
| C | -1.34182800 | -3.27599400 | -1.91701300 |
| H | -2.00076000 | -2.64143300 | -2.51635800 |
| H | -0.92251400 | -4.04840800 | -2.57209800 |
| H | -1.93195400 | -3.77501600 | -1.14104500 |
| N | 4.35062300  | -2.30000500 | 0.78326500  |
| N | 4.37504000  | -1.20120200 | 1.12598400  |
| H | 3.81318700  | 0.43821300  | 2.16520500  |
| H | 2.30050400  | 0.05108600  | -1.97760200 |

**M2a**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.49389500 | -2.83310500 | -1.72981300 |
| C | -0.64574300 | -1.80418700 | -1.66860300 |
| C | -1.47098500 | 0.37947200  | 1.08399500  |
| C | -2.43662000 | 0.43286000  | -0.05225400 |
| C | -3.67595600 | -0.28036900 | 0.41778700  |
| C | -2.68252900 | 1.18563100  | -1.12668700 |
| C | -4.13107500 | 1.04214500  | -1.56465600 |
| C | -4.82498200 | 0.45376500  | -0.29783900 |
| H | -2.39159400 | -2.79597700 | -2.34152000 |
| H | -1.31791600 | -3.75793800 | -1.18315500 |
| H | -4.23193800 | 0.36161000  | -2.42367200 |
| H | -5.67856800 | -0.18952700 | -0.53009000 |
| C | 0.64182100  | -1.82812500 | -0.88882400 |
| C | -0.44311800 | -0.76713200 | 1.20359200  |
| C | 0.80270100  | -0.76141000 | 0.24612100  |
| H | 1.46721600  | -1.71780400 | -1.59896100 |
| H | 0.75349100  | -2.81248000 | -0.41751400 |
| H | -0.07703000 | -0.75144700 | 2.23077400  |
| H | -0.96004800 | -1.72227700 | 1.06896500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.97322100 | 1.33491600  | 1.27224900  |
| H | -0.84561300 | -0.89809900 | -2.23237700 |
| H | -5.18202000 | 1.26976500  | 0.34096300  |
| H | -4.56712100 | 1.99921900  | -1.87680500 |
| C | 1.00327100  | 0.64761800  | -0.32252200 |
| C | 2.04637400  | -1.18788200 | 1.09607200  |
| O | 0.74862900  | 0.99418000  | -1.45858900 |
| O | 1.46951900  | 1.47936900  | 0.63170300  |
| O | 3.29531400  | -1.16241800 | 0.56833300  |
| O | 1.93971100  | -1.59540300 | 2.22713800  |
| C | 3.70335300  | -0.82625700 | -0.77199000 |
| H | 3.65207200  | -1.73469000 | -1.38299800 |
| H | 3.05104100  | -0.07522700 | -1.22116400 |
| C | 5.13371200  | -0.31959400 | -0.68774600 |
| H | 5.77970900  | -1.07173800 | -0.22546200 |
| H | 5.51297300  | -0.10277300 | -1.69252300 |
| H | 5.18609200  | 0.59479500  | -0.08901900 |
| C | 1.61527800  | 2.88386800  | 0.28718200  |
| H | 1.48878300  | 3.40281600  | 1.23969200  |
| H | 0.80490700  | 3.16179400  | -0.39064900 |
| C | 2.97533600  | 3.17166500  | -0.32734300 |
| H | 3.08128700  | 2.67143900  | -1.29425000 |
| H | 3.08389500  | 4.25019100  | -0.48897600 |
| H | 3.78072500  | 2.84309900  | 0.33729100  |
| N | -2.43643600 | 0.17090200  | 2.26598400  |
| N | -3.57613700 | -0.17087600 | 1.90590300  |
| H | -3.68340600 | -1.35838900 | 0.19427400  |
| H | -1.97274100 | 1.83892500  | -1.62578500 |

**M2b**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.42769000 | 4.01160600  | -1.57577500 |
| C | -1.53632000 | 2.68210200  | -1.59176400 |
| C | 1.21593700  | 0.63159400  | 1.22888400  |
| C | 2.35749500  | 0.23833200  | 0.67136400  |
| C | 3.48869500  | -0.61576100 | 1.19556500  |
| C | 2.98614000  | 0.41280600  | -0.69366200 |
| C | 4.35875400  | 1.06058600  | -0.32645000 |
| C | 4.71228700  | 0.33690500  | 1.00867100  |
| H | -1.03291700 | 4.56094900  | -2.42645500 |
| H | -1.73628300 | 4.60477900  | -0.71667300 |
| H | 4.24003300  | 2.13933400  | -0.18952900 |
| H | 4.77291300  | 1.03420200  | 1.84920400  |
| C | -2.12025100 | 1.87559300  | -0.45977900 |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| C           | 0.18357900  | 1.50019600  | 0.56102100  |
| C           | -1.17535500 | 0.80672500  | 0.19575300  |
| H           | -3.02812800 | 1.37477700  | -0.81719100 |
| H           | -2.43356400 | 2.55704300  | 0.34042200  |
| H           | -0.06639700 | 2.33436100  | 1.22585100  |
| H           | 0.58274200  | 1.92836900  | -0.36180600 |
| H           | 0.99349700  | 0.32301300  | 2.24745900  |
| H           | -1.21997700 | 2.11734100  | -2.46462100 |
| H           | 5.64878500  | -0.22564700 | 0.95856700  |
| H           | 5.09694700  | 0.89268800  | -1.11572500 |
| C           | -0.83700400 | -0.33954400 | -0.76395200 |
| C           | -1.86688100 | 0.34572200  | 1.50233100  |
| O           | -0.77720200 | -0.23091500 | -1.97236100 |
| O           | -0.52389100 | -1.46243700 | -0.09279900 |
| O           | -3.02117500 | -0.36111000 | 1.46094000  |
| O           | -1.47694900 | 0.71556500  | 2.58639100  |
| C           | -3.55073000 | -1.09671100 | 0.34058300  |
| H           | -3.28970300 | -0.62631500 | -0.61086700 |
| H           | -3.10797000 | -2.09677600 | 0.35882500  |
| C           | -5.05913700 | -1.15696500 | 0.51174400  |
| H           | -5.49689800 | -0.15430900 | 0.47544000  |
| H           | -5.50150800 | -1.75947800 | -0.28924000 |
| H           | -5.31805700 | -1.61099900 | 1.47289900  |
| C           | 0.07111400  | -2.55163400 | -0.85808300 |
| H           | 0.67755900  | -3.08410500 | -0.12316000 |
| H           | 0.72959000  | -2.12140400 | -1.61479600 |
| C           | -0.98372800 | -3.45092700 | -1.48040800 |
| H           | -1.58017800 | -2.90235700 | -2.21477200 |
| H           | -0.49153700 | -4.28430000 | -1.99467800 |
| H           | -1.64848800 | -3.87033200 | -0.71759600 |
| N           | 3.34739600  | -1.01737000 | -1.00596200 |
| N           | 3.63398300  | -1.60020600 | 0.06667300  |
| H           | 3.39905200  | -1.11165100 | 2.16104700  |
| H           | 2.43313100  | 0.87129100  | -1.51120900 |
| <b>TS3a</b> |             |             |             |
| C           | -1.69084500 | -2.46198500 | -1.70268600 |
| C           | -0.69331000 | -1.57544500 | -1.63963300 |
| C           | -1.41222800 | 0.79976200  | 0.40869000  |
| C           | -2.66785300 | 0.46281900  | -0.15800400 |
| C           | -3.60240200 | -0.53969200 | 0.38260700  |
| C           | -3.36714700 | 1.18678700  | -1.08185700 |
| C           | -4.78675600 | 0.76217400  | -1.26102100 |
| C           | -4.94025700 | -0.43675400 | -0.29367600 |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| H           | -2.51561700 | -2.34512600 | -2.40075800 |
| H           | -1.71140200 | -3.35058300 | -1.07396200 |
| H           | -4.99824900 | 0.47488500  | -2.30105900 |
| H           | -5.20027900 | -1.35686900 | -0.83379300 |
| C           | 0.50973700  | -1.73716000 | -0.75112200 |
| C           | -0.44092200 | -0.13889300 | 1.06903800  |
| C           | 0.82619800  | -0.56564900 | 0.22706800  |
| H           | 1.38020800  | -1.89988800 | -1.39682300 |
| H           | 0.38693700  | -2.64437700 | -0.14656900 |
| H           | -0.05882500 | 0.33089700  | 1.97893300  |
| H           | -0.93251700 | -1.06123500 | 1.39196900  |
| H           | -1.01409100 | 1.77059900  | 0.12012900  |
| H           | -0.69062600 | -0.70805000 | -2.29379300 |
| H           | -5.74482100 | -0.27170700 | 0.43625400  |
| H           | -5.46985900 | 1.59633100  | -1.04035000 |
| C           | 1.32363400  | 0.67513700  | -0.51761300 |
| C           | 1.88830500  | -1.08308700 | 1.24369700  |
| O           | 1.28247600  | 0.84594900  | -1.71992300 |
| O           | 1.77944600  | 1.59524400  | 0.35738400  |
| O           | 3.17164300  | -1.32553000 | 0.86746500  |
| O           | 1.60001600  | -1.31921400 | 2.39203600  |
| C           | 3.72398300  | -1.30031100 | -0.46249000 |
| H           | 3.53572500  | -2.27308500 | -0.93210400 |
| H           | 3.26177800  | -0.52842300 | -1.07991200 |
| C           | 5.21725400  | -1.05656200 | -0.31962100 |
| H           | 5.67293500  | -1.82515900 | 0.31173900  |
| H           | 5.69656800  | -1.08374000 | -1.30454700 |
| H           | 5.40786500  | -0.07948900 | 0.13498000  |
| C           | 2.20339800  | 2.87563100  | -0.17599800 |
| H           | 2.01868100  | 3.57807000  | 0.63982500  |
| H           | 1.56658800  | 3.12806200  | -1.02708500 |
| C           | 3.67211600  | 2.85392300  | -0.56918100 |
| H           | 3.84090500  | 2.17389000  | -1.40928500 |
| H           | 3.98797700  | 3.85785000  | -0.87520500 |
| H           | 4.29506000  | 2.54062200  | 0.27486300  |
| N           | -2.66419800 | 0.95940100  | 2.36707400  |
| N           | -3.58805700 | 0.29364300  | 2.22798500  |
| H           | -3.25708700 | -1.50366600 | 0.74214200  |
| H           | -2.93814700 | 2.01313300  | -1.64588800 |
| <b>TS3b</b> |             |             |             |
| C           | -1.50707600 | 4.06223500  | -1.53367000 |
| C           | -1.69916900 | 2.74251500  | -1.56136000 |
| C           | 1.20378300  | 0.55920900  | 0.99735200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.48036600  | 0.41225500  | 0.51105700  |
| C | 3.47592600  | -0.14231100 | 1.43696000  |
| C | 3.11053600  | 0.80185700  | -0.68079500 |
| C | 4.60990400  | 0.92726300  | -0.44246600 |
| C | 4.79156900  | 0.48633300  | 1.05540100  |
| H | -1.17158100 | 4.60717700  | -2.41198400 |
| H | -1.68503700 | 4.65167200  | -0.63597800 |
| H | 4.97253700  | 1.95487500  | -0.58580900 |
| H | 4.96368100  | 1.36692200  | 1.69740600  |
| C | -2.20255700 | 1.94359900  | -0.38637500 |
| C | 0.16966200  | 1.45777400  | 0.40399800  |
| C | -1.23946400 | 0.82796800  | 0.14547900  |
| H | -3.15829100 | 1.47957500  | -0.65723900 |
| H | -2.40479100 | 2.62098800  | 0.45186900  |
| H | 0.00701600  | 2.28442000  | 1.10933800  |
| H | 0.53463600  | 1.89509300  | -0.52798300 |
| H | 0.93518000  | 0.05702600  | 1.92154500  |
| H | -1.51701100 | 2.18201900  | -2.47477900 |
| H | 5.64532000  | -0.18084400 | 1.22135200  |
| H | 5.19956900  | 0.30107700  | -1.12713100 |
| C | -1.05539400 | -0.30120000 | -0.87877400 |
| C | -1.82455200 | 0.35176100  | 1.50245200  |
| O | -1.40219200 | -0.25400700 | -2.04052900 |
| O | -0.39766900 | -1.33489500 | -0.32414000 |
| O | -2.95191400 | -0.38922900 | 1.55379000  |
| O | -1.35489700 | 0.73598000  | 2.54995800  |
| C | -3.56821100 | -1.10419600 | 0.45977600  |
| H | -3.55381800 | -0.51196600 | -0.45785000 |
| H | -2.99976900 | -2.02335900 | 0.28946300  |
| C | -4.99443300 | -1.41198300 | 0.88117300  |
| H | -5.55957200 | -0.48890600 | 1.04314900  |
| H | -5.49455100 | -1.99415000 | 0.09960400  |
| H | -5.00542800 | -1.99125100 | 1.80915500  |
| C | 0.06237000  | -2.39580700 | -1.21459500 |
| H | 0.96164400  | -2.77373400 | -0.72789400 |
| H | 0.33521500  | -1.94319000 | -2.16959800 |
| C | -0.99012300 | -3.47740800 | -1.38817300 |
| H | -1.87668900 | -3.08513200 | -1.89489600 |
| H | -0.57894800 | -4.28779700 | -2.00079700 |
| H | -1.28403100 | -3.90064400 | -0.42169300 |
| N | 3.52119600  | -1.67124900 | -0.83816100 |
| N | 3.73519600  | -1.96171000 | 0.23996400  |
| H | 3.24338500  | -0.47521400 | 2.44244900  |
| H | 2.61113600  | 1.18408500  | -1.56159200 |

### M3S

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.08807700 | -2.07811800 | -1.74530500 |
| C | -1.03142700 | -1.26206300 | -1.65942100 |
| C | -1.64316700 | 0.79261100  | 0.44338600  |
| C | -3.04019400 | 0.55479100  | 0.35126500  |
| C | -3.80418700 | -0.62382200 | 0.74081800  |
| C | -3.93896300 | 1.46620900  | -0.17827400 |
| C | -5.34729900 | 0.97665200  | -0.18841200 |
| C | -5.27044000 | -0.43146000 | 0.46910100  |
| H | -2.93869700 | -1.84514100 | -2.37966800 |
| H | -2.13866500 | -3.01292800 | -1.18879200 |
| H | -5.75532400 | 0.92831500  | -1.20841500 |
| H | -5.69231600 | -1.20823900 | -0.19046400 |
| C | 0.19813300  | -1.57459200 | -0.84607800 |
| C | -0.64728700 | -0.11165600 | 1.11510200  |
| C | 0.59412100  | -0.52192600 | 0.23510500  |
| H | 1.03987500  | -1.70355200 | -1.53641100 |
| H | 0.05228800  | -2.53395300 | -0.33221400 |
| H | -0.23743400 | 0.35631900  | 2.02211800  |
| H | -1.12469500 | -1.04014500 | 1.44420800  |
| H | -1.29387600 | 1.77419000  | 0.12306900  |
| H | -1.00150600 | -0.34157100 | -2.23770400 |
| H | -3.39530900 | -1.49354200 | 1.24176900  |
| H | -5.88300400 | -0.47646500 | 1.38634400  |
| H | -6.02347400 | 1.64823300  | 0.35896800  |
| C | 1.14700100  | 0.75861300  | -0.40195900 |
| C | 1.63542600  | -1.16875500 | 1.19475300  |
| O | 1.14837600  | 1.01793900  | -1.58979400 |
| O | 1.60571400  | 1.59913600  | 0.55007900  |
| O | 2.90220900  | -1.44198000 | 0.78822500  |
| O | 1.34487400  | -1.47099200 | 2.32894800  |
| C | 3.43578000  | -1.36186700 | -0.54882600 |
| H | 3.19558300  | -2.29659500 | -1.06996700 |
| H | 2.99791600  | -0.53510600 | -1.11106600 |
| C | 4.94010900  | -1.19089100 | -0.41763800 |
| H | 5.37154800  | -2.01254100 | 0.16247600  |
| H | 5.40328700  | -1.18286000 | -1.41087700 |
| H | 5.17969200  | -0.24912400 | 0.08684800  |
| C | 2.08571800  | 2.89789400  | 0.11690900  |
| H | 1.90946900  | 3.54721300  | 0.97823800  |
| H | 1.47396200  | 3.23280800  | -0.72475600 |
| C | 3.55994100  | 2.85037700  | -0.25266900 |
| H | 3.71962100  | 2.22137500  | -1.13378500 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 3.91563900  | 3.86071900 | -0.48608100 |
| H | 4.15635500  | 2.45939500 | 0.57862800  |
| H | -3.65144600 | 2.43838700 | -0.55926700 |

**M3T**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.61236700  | -2.52930500 | 2.04705300  |
| C | 0.65324100  | -1.61618100 | 1.88566500  |
| C | 1.74548300  | 0.49419400  | 0.03570400  |
| C | 3.14271700  | 0.45874600  | -0.17506700 |
| C | 3.83801600  | -0.27318300 | -1.17028300 |
| C | 4.08915400  | 1.17394200  | 0.60271900  |
| C | 5.49394700  | 0.92124000  | 0.13205400  |
| C | 5.32309600  | -0.05585800 | -1.07212900 |
| H | 2.37316400  | -2.42616500 | 2.81594000  |
| H | 1.67941500  | -3.41210600 | 1.41379400  |
| H | 6.12004100  | 0.48435600  | 0.92462200  |
| H | 5.86392100  | -1.00044000 | -0.91130100 |
| C | -0.45783700 | -1.73928100 | 0.87591600  |
| C | 0.75134400  | -0.21838800 | -0.83087700 |
| C | -0.61096900 | -0.57051500 | -0.14989500 |
| H | -1.40064500 | -1.85104400 | 1.42237000  |
| H | -0.31214500 | -2.66036900 | 0.29800800  |
| H | 0.51857000  | 0.38480400  | -1.71867100 |
| H | 1.17252700  | -1.15230000 | -1.21713300 |
| H | 1.38058400  | 1.13804600  | 0.83197900  |
| H | 0.60869300  | -0.75116800 | 2.54217000  |
| H | 3.37811200  | -0.90754500 | -1.91940600 |
| H | 5.73538300  | 0.36548000  | -2.00118200 |
| H | 6.00197700  | 1.85069200  | -0.16628400 |
| C | -1.13697600 | 0.70784100  | 0.51193600  |
| C | -1.56454500 | -1.04921800 | -1.28383500 |
| O | -1.18514000 | 0.91548300  | 1.70824700  |
| O | -1.49208100 | 1.61134500  | -0.42348100 |
| O | -2.88356600 | -1.26427800 | -1.05108500 |
| O | -1.15626900 | -1.27907900 | -2.39709200 |
| C | -3.58656900 | -1.18679400 | 0.20439300  |
| H | -3.50901600 | -2.16123500 | 0.70028600  |
| H | -3.15645900 | -0.43250000 | 0.86565500  |
| C | -5.03608100 | -0.86130400 | -0.11582100 |
| H | -5.45856600 | -1.61324100 | -0.78889700 |
| H | -5.62824800 | -0.84469100 | 0.80583500  |
| H | -5.11423500 | 0.11724100  | -0.59949900 |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.89522200 | 2.92774700 | 0.03684500  |
| H | -1.62679100 | 3.59066000 | -0.78871000 |
| H | -1.30360300 | 3.18452800 | 0.91849500  |
| C | -3.38531300 | 2.98222400 | 0.33366800  |
| H | -3.63781100 | 2.33629600 | 1.17957100  |
| H | -3.67246900 | 4.00806700 | 0.59135400  |
| H | -3.96820400 | 2.67273300 | -0.53993200 |
| H | 3.83714200  | 1.81668700 | 1.43994600  |

**TS4T1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.08521500  | -1.80448800 | 1.99778300  |
| C | 1.09738500  | -0.88703300 | 1.67382200  |
| C | 1.70628700  | 0.44287300  | 0.13525900  |
| C | 3.13342700  | 0.38264000  | -0.13752400 |
| C | 3.78734100  | -0.49700700 | -1.01459900 |
| C | 4.08679000  | 1.19684400  | 0.49646300  |
| C | 5.48128400  | 0.87359300  | 0.03446900  |
| C | 5.27635600  | -0.27691400 | -0.99829100 |
| H | 2.90086200  | -1.54220500 | 2.66469400  |
| H | 2.15917900  | -2.76186100 | 1.48737500  |
| H | 6.12893400  | 0.56283100  | 0.86785500  |
| H | 5.81944900  | -1.18848200 | -0.70806200 |
| C | -0.17793900 | -1.36829400 | 0.99488000  |
| C | 0.70364800  | -0.03780300 | -0.88090300 |
| C | -0.61648100 | -0.43434900 | -0.16396600 |
| H | -0.96712700 | -1.45958500 | 1.74643300  |
| H | -0.00585400 | -2.36758300 | 0.57602000  |
| H | 0.49968100  | 0.71640700  | -1.65099400 |
| H | 1.06689300  | -0.92440000 | -1.40638700 |
| H | 1.40966300  | 1.34494900  | 0.67012600  |
| H | 0.95431200  | -0.05895000 | 2.36374100  |
| H | 3.30651400  | -1.24479300 | -1.63517600 |
| H | 5.66091600  | -0.00753900 | -1.99317400 |
| H | 5.97760200  | 1.74527000  | -0.41735500 |
| C | -1.26657600 | 0.84933200  | 0.36461400  |
| C | -1.53860600 | -1.15160300 | -1.18035000 |
| O | -1.26740600 | 1.20970000  | 1.52500700  |
| O | -1.79673600 | 1.56540400  | -0.64708700 |
| O | -2.79982600 | -1.51430700 | -0.83475500 |
| O | -1.16715400 | -1.41627700 | -2.29890100 |
| C | -3.36234900 | -1.47909700 | 0.49152700  |
| H | -2.99823100 | -2.34967400 | 1.04901200  |
| H | -3.06188900 | -0.57782100 | 1.03091600  |
| C | -4.87238100 | -1.53313400 | 0.33333300  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.16954500 | -2.43077600 | -0.21706300 |
| H | -5.35129400 | -1.55229200 | 1.31848300  |
| H | -5.23456600 | -0.65741800 | -0.21416800 |
| C | -2.37154000 | 2.85734800  | -0.32050500 |
| H | -2.26315200 | 3.43612000  | -1.24046600 |
| H | -1.77398800 | 3.31450500  | 0.47155700  |
| C | -3.83040000 | 2.72780500  | 0.08808100  |
| H | -3.92393200 | 2.17066700  | 1.02479000  |
| H | -4.26120400 | 3.72404300  | 0.24010800  |
| H | -4.40830200 | 2.21911300  | -0.69032100 |
| H | 3.85530400  | 1.96902600  | 1.22338400  |

#### M4T1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.88357600 | -2.41656400 | -0.61379400 |
| C | -1.37057200 | -1.17173900 | -1.25488000 |
| C | -1.74701800 | 0.15782500  | -0.49767200 |
| C | -3.19749100 | 0.32858000  | -0.12076900 |
| C | -3.82651200 | -0.16444100 | 1.02298500  |
| C | -4.12018500 | 1.02106900  | -0.90605500 |
| C | -5.49066900 | 1.00522500  | -0.28283200 |
| C | -5.28637400 | 0.20833500  | 1.04202600  |
| H | -2.93989900 | -2.66074900 | -0.65690300 |
| H | -1.25378100 | -3.02305100 | 0.03039200  |
| H | -6.23325600 | 0.52501500  | -0.93717300 |
| H | -5.93437600 | -0.67885800 | 1.09148200  |
| C | 0.17603500  | -1.09988600 | -1.26595000 |
| C | -0.74124800 | 0.16023900  | 0.66109700  |
| C | 0.60711000  | -0.30852700 | 0.01785600  |
| H | 0.52513800  | -0.55215200 | -2.14503000 |
| H | 0.61515800  | -2.10133000 | -1.29859200 |
| H | -0.65063600 | 1.13231700  | 1.15448600  |
| H | -1.01471300 | -0.56622000 | 1.42922400  |
| H | -1.48251700 | 0.97407500  | -1.18365100 |
| H | -1.76733300 | -1.10835200 | -2.27845100 |
| H | -3.34992000 | -0.74043100 | 1.80817000  |
| H | -5.54119500 | 0.81148100  | 1.92589700  |
| H | -5.86973400 | 2.02081000  | -0.09776800 |
| C | 1.37313700  | 0.97117400  | -0.34039600 |
| C | 1.40100000  | -1.18496800 | 1.01149700  |
| O | 1.35040700  | 1.52018100  | -1.42337900 |
| O | 2.01396200  | 1.46248200  | 0.73904500  |
| O | 2.63061600  | -1.64526100 | 0.66585900  |
| O | 0.96633500  | -1.50676600 | 2.09174600  |
| C | 3.25558500  | -1.50330200 | -0.62340500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.93371600  | -2.33883600 | -1.25606300 |
| H | 2.95879000  | -0.57546300 | -1.11780300 |
| C | 4.75854900  | -1.54081400 | -0.40356400 |
| H | 5.04972400  | -2.46684200 | 0.10120300  |
| H | 5.27941400  | -1.48874800 | -1.36602700 |
| H | 5.07937800  | -0.69626200 | 0.21405700  |
| C | 2.65876700  | 2.75523000  | 0.59749800  |
| H | 2.66138200  | 3.16107400  | 1.61159600  |
| H | 2.03912200  | 3.38425500  | -0.04593400 |
| C | 4.06966400  | 2.62123200  | 0.04704500  |
| H | 4.05259900  | 2.23489500  | -0.97598900 |
| H | 4.55428800  | 3.60421900  | 0.03243500  |
| H | 4.67041100  | 1.95344000  | 0.67313100  |
| H | -3.88953500 | 1.51861400  | -1.84298300 |

# **TS5T1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.59934500 | -1.10513900 | -1.50994100 |
| C | -1.38031900 | -0.25641400 | -1.23462500 |
| C | -1.64918000 | 0.71106100  | 0.01680600  |
| C | -3.07955800 | 0.50390700  | 0.41092100  |
| C | -3.59007800 | -0.79100200 | 0.35312600  |
| C | -4.19990100 | 1.46982900  | 0.21387700  |
| C | -5.44330600 | 0.69137100  | -0.12524100 |
| C | -5.10727400 | -0.77371700 | 0.29304400  |
| H | -3.32646300 | -0.71538800 | -2.21960000 |
| H | -2.47959100 | -2.18681400 | -1.56061500 |
| H | -5.66037300 | 0.72520000  | -1.20647000 |
| H | -5.50910800 | -1.52094200 | -0.40089400 |
| C | -0.10842500 | -1.06035200 | -0.87072800 |
| C | -0.59548200 | 0.29778900  | 1.06665600  |
| C | 0.60644900  | -0.27013500 | 0.25837200  |
| H | 0.52811600  | -1.21928500 | -1.74328400 |
| H | -0.38484500 | -2.04537800 | -0.47238000 |
| H | -0.29707500 | 1.11178400  | 1.73237700  |
| H | -0.97285400 | -0.50834400 | 1.70130800  |
| H | -1.48410700 | 1.75121700  | -0.28453700 |
| H | -1.15710900 | 0.37510700  | -2.10061900 |
| H | -3.08035400 | -1.66676100 | 0.75144500  |
| H | -5.53372900 | -1.00169700 | 1.28087200  |
| H | -6.33814900 | 1.08083400  | 0.37499600  |
| C | 1.40155500  | 0.91210900  | -0.30510600 |
| C | 1.48588700  | -1.15127200 | 1.17359500  |
| O | 1.35698900  | 1.30432900  | -1.45407800 |
| O | 2.12816700  | 1.50270000  | 0.66533400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.63129100  | -1.70358200 | 0.69702600  |
| O | 1.19053100  | -1.37768600 | 2.32275100  |
| C | 3.02987600  | -1.74664100 | -0.68688800 |
| H | 2.44332800  | -2.51899300 | -1.19764500 |
| H | 2.84625500  | -0.79237200 | -1.18659000 |
| C | 4.50972900  | -2.08956500 | -0.71033900 |
| H | 4.69282800  | -3.03997400 | -0.20016900 |
| H | 4.85760000  | -2.17549800 | -1.74564700 |
| H | 5.09407800  | -1.31148200 | -0.20934900 |
| C | 2.88084300  | 2.68953100  | 0.30522300  |
| H | 2.95718400  | 3.24921600  | 1.24018200  |
| H | 2.30018400  | 3.26545300  | -0.41911300 |
| C | 4.25279800  | 2.32947700  | -0.24268200 |
| H | 4.16323400  | 1.79816100  | -1.19465700 |
| H | 4.83378600  | 3.24265400  | -0.41535800 |
| H | 4.80153500  | 1.70196400  | 0.46710500  |
| H | -4.23581200 | 2.43022100  | 0.72395500  |

#### TS5T2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.62014600 | -0.63469400 | -1.81663000 |
| C | -1.35529000 | 0.06076800  | -1.37336200 |
| C | -1.62389700 | 0.92362500  | -0.05029800 |
| C | -3.08128900 | 0.75736900  | 0.27224900  |
| C | -3.67597800 | 0.06303200  | 1.45258800  |
| C | -3.96851300 | 0.66264800  | -0.79654400 |
| C | -5.28284700 | 0.04074600  | -0.35896800 |
| C | -4.93217300 | -0.63554100 | 1.00247500  |
| H | -2.91398900 | -0.56829600 | -2.86290200 |
| H | -2.84284300 | -1.60056900 | -1.36388700 |
| H | -5.68153900 | -0.66326800 | -1.09839000 |
| H | -4.76019600 | -1.71346800 | 0.84401000  |
| C | -0.18019500 | -0.88063600 | -1.00347400 |
| C | -0.63797400 | 0.38914600  | 1.00423700  |
| C | 0.54737500  | -0.21812700 | 0.19899500  |
| H | 0.47903700  | -1.05370800 | -1.85600100 |
| H | -0.56582300 | -1.85316500 | -0.67237500 |
| H | -0.30197300 | 1.14183900  | 1.72224200  |
| H | -1.09187800 | -0.42130200 | 1.58120600  |
| H | -1.38827000 | 1.97128500  | -0.28162900 |
| H | -1.01604700 | 0.73848900  | -2.16114700 |
| H | -3.55516000 | 0.43603300  | 2.46752900  |
| H | -5.74403700 | -0.56237300 | 1.73557800  |
| H | -6.04889900 | 0.81762600  | -0.21942900 |
| C | 1.45220600  | 0.93016500  | -0.26167400 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| C            | 1.32717100  | -1.21449900 | 1.08731100  |
| O            | 1.48817700  | 1.39079800  | -1.38528600 |
| O            | 2.17978300  | 1.40426900  | 0.77009700  |
| O            | 2.43898800  | -1.83207000 | 0.61023500  |
| O            | 0.98334000  | -1.47377600 | 2.21563400  |
| C            | 2.87491700  | -1.83581600 | -0.76291800 |
| H            | 2.24247800  | -2.52758200 | -1.33119400 |
| H            | 2.78707500  | -0.84424000 | -1.21395200 |
| C            | 4.32110500  | -2.30151700 | -0.76581000 |
| H            | 4.40803400  | -3.28943800 | -0.30374200 |
| H            | 4.69277400  | -2.36244600 | -1.79462700 |
| H            | 4.95251000  | -1.60336300 | -0.20742600 |
| C            | 3.04089600  | 2.54251300  | 0.51175100  |
| H            | 3.11558300  | 3.04444100  | 1.47911100  |
| H            | 2.54458700  | 3.20132100  | -0.20458900 |
| C            | 4.40496400  | 2.09919100  | 0.00693500  |
| H            | 4.31982100  | 1.62565700  | -0.97550800 |
| H            | 5.06463400  | 2.96907600  | -0.08988500 |
| H            | 4.86647200  | 1.39348600  | 0.70521700  |
| H            | -3.94665400 | 1.31995800  | -1.66482700 |
| <b>TS4T2</b> |             |             |             |
| C            | -1.69485900 | -0.61593500 | -2.21571200 |
| C            | -1.52911600 | -1.41052200 | -1.10263800 |
| C            | -1.58621100 | 1.03222600  | 1.28658100  |
| C            | -2.75100100 | 0.56633800  | 0.67112200  |
| C            | -3.01048800 | -0.83981000 | 0.39897600  |
| C            | -3.77943900 | 1.33869500  | 0.11787300  |
| C            | -4.80894700 | 0.48816300  | -0.57069300 |
| C            | -4.39900700 | -0.96615300 | -0.19919900 |
| H            | -2.53018700 | -0.80093500 | -2.88645600 |
| H            | -1.09145200 | 0.26343400  | -2.39656700 |
| H            | -4.78045200 | 0.64586600  | -1.66022900 |
| H            | -4.43362100 | -1.64231300 | -1.06270800 |
| C            | -0.23033300 | -1.55042100 | -0.29025600 |
| C            | -0.47986400 | 0.11738800  | 1.71856300  |
| C            | 0.44094200  | -0.41419100 | 0.55958900  |
| H            | 0.52122900  | -1.94442000 | -0.98356900 |
| H            | -0.39900800 | -2.35537200 | 0.43571200  |
| H            | 0.16368900  | 0.62195200  | 2.44001000  |
| H            | -0.87599200 | -0.76737900 | 2.22867000  |
| H            | -1.45175800 | 2.10300200  | 1.42114400  |
| H            | -2.05220600 | -2.36731900 | -1.13572100 |
| H            | -2.66403500 | -1.60470900 | 1.09001900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.09127900 | -1.38283100 | 0.54621500  |
| H | -5.83672700 | 0.72448400  | -0.26049900 |
| C | 0.92325400  | 0.79823700  | -0.24718100 |
| C | 1.64105400  | -1.12657800 | 1.26983400  |
| O | 0.80428200  | 0.97249400  | -1.44119700 |
| O | 1.51492300  | 1.69394000  | 0.57538600  |
| O | 2.73059100  | -1.53534900 | 0.57374300  |
| O | 1.58060200  | -1.43607300 | 2.43579900  |
| C | 3.14203300  | -1.09932400 | -0.73991600 |
| H | 2.30604700  | -1.10553000 | -1.44163300 |
| H | 3.52162700  | -0.07524600 | -0.66364000 |
| C | 4.23785800  | -2.05030000 | -1.18949400 |
| H | 3.85461600  | -3.07252500 | -1.26738200 |
| H | 4.61603200  | -1.74458000 | -2.17115000 |
| H | 5.06871500  | -2.04693900 | -0.47759300 |
| C | 1.90648300  | 2.96656100  | -0.00100200 |
| H | 1.86456400  | 3.66093200  | 0.84151100  |
| H | 1.16103400  | 3.25352300  | -0.74643600 |
| C | 3.30036300  | 2.91671600  | -0.60628000 |
| H | 3.32394700  | 2.25373400  | -1.47559700 |
| H | 3.59331100  | 3.92027400  | -0.93577100 |
| H | 4.03414000  | 2.57193300  | 0.12975300  |
| H | -3.80175200 | 2.42433800  | 0.12105700  |

#### M4T2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.02208600 | -1.31309600 | 2.11711900  |
| C | -1.75750500 | 0.06070000  | 1.58894100  |
| C | -1.70606500 | -1.35656800 | -1.16873500 |
| C | -2.74406100 | -0.54805900 | -0.73458500 |
| C | -2.66308900 | 0.46249900  | 0.40886600  |
| C | -4.02599300 | -0.50754000 | -1.27554200 |
| C | -4.92028700 | 0.45390100  | -0.54422200 |
| C | -4.14871600 | 0.69569500  | 0.77454000  |
| H | -2.75104900 | -1.97363300 | 1.66111900  |
| H | -1.48381900 | -1.67039400 | 2.99014600  |
| H | -5.93439100 | 0.06593500  | -0.38050100 |
| H | -4.45761300 | -0.04792500 | 1.52029400  |
| C | -0.25334900 | 0.33476100  | 1.30019300  |
| C | -0.34716000 | -1.54740800 | -0.55276400 |
| C | 0.41438300  | -0.31051700 | 0.03894700  |
| H | 0.31973500  | 0.01209100  | 2.17436300  |
| H | -0.14493300 | 1.42245900  | 1.22972600  |
| H | -0.41133500 | -2.28618100 | 0.26225300  |
| H | 0.30207000  | -1.98364900 | -1.31716000 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| H            | -1.90408600 | -1.99538900 | -2.02740400 |
| H            | -1.97928700 | 0.77273900  | 2.40669700  |
| H            | -2.26217600 | 1.40204800  | -0.00501200 |
| H            | -4.32411700 | 1.68766300  | 1.20529300  |
| H            | -5.04121500 | 1.39448300  | -1.10905600 |
| C            | 1.78252200  | -0.91104900 | 0.43975400  |
| C            | 0.60469200  | 0.73561000  | -1.09081700 |
| O            | 2.09171700  | -1.26726800 | 1.55627400  |
| O            | 2.57079100  | -1.07427400 | -0.64418100 |
| O            | 1.26572700  | 1.89751300  | -0.81890800 |
| O            | 0.11631300  | 0.61113400  | -2.18625300 |
| C            | 2.28158300  | 2.06156200  | 0.18818000  |
| H            | 2.02423500  | 1.53497900  | 1.11126100  |
| H            | 3.21522700  | 1.63963800  | -0.19934700 |
| C            | 2.42381900  | 3.55197000  | 0.44673200  |
| H            | 1.49477000  | 3.96718000  | 0.85049400  |
| H            | 3.22782200  | 3.73198100  | 1.16886500  |
| H            | 2.66217300  | 4.08121900  | -0.48071800 |
| C            | 3.80957300  | -1.80970400 | -0.45915300 |
| H            | 4.00303500  | -2.25004200 | -1.43994500 |
| H            | 3.63369900  | -2.60441600 | 0.26945700  |
| C            | 4.94909700  | -0.90352800 | -0.02164200 |
| H            | 4.74966300  | -0.47688900 | 0.96535000  |
| H            | 5.87653500  | -1.48460100 | 0.03864800  |
| H            | 5.10290600  | -0.09201900 | -0.74056000 |
| H            | -4.33838500 | -1.07951200 | -2.14459000 |
| <b>TS5T3</b> |             |             |             |
| C            | -2.10345300 | -1.48277400 | 1.62794000  |
| C            | -1.74971400 | -0.01087300 | 1.53785300  |
| C            | -1.80973000 | -1.67355800 | -0.46851300 |
| C            | -2.61433100 | -0.56837400 | -0.69021700 |
| C            | -2.49982100 | 0.57993400  | 0.30210600  |
| C            | -4.01806100 | -0.60634900 | -1.21346400 |
| C            | -4.77260200 | 0.56727200  | -0.68212100 |
| C            | -3.98143500 | 0.97085000  | 0.58423000  |
| H            | -3.15149700 | -1.73323700 | 1.77918200  |
| H            | -1.41533500 | -2.14054300 | 2.15814500  |
| H            | -5.83227700 | 0.36154400  | -0.47734500 |
| H            | -4.35227900 | 0.39519000  | 1.44127700  |
| C            | -0.22357700 | 0.17048400  | 1.43935500  |
| C            | -0.28422400 | -1.67163800 | -0.39941200 |
| C            | 0.43535700  | -0.39329400 | 0.14479300  |
| H            | 0.24843200  | -0.32653100 | 2.29264900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.00624700  | 1.23685100  | 1.52935600  |
| H | 0.03341000  | -2.52984500 | 0.20510800  |
| H | 0.08989700  | -1.84096000 | -1.41505800 |
| H | -2.17169900 | -2.62635900 | -0.86357300 |
| H | -2.07009300 | 0.52726800  | 2.44515600  |
| H | -1.96696700 | 1.45806200  | -0.08744200 |
| H | -4.09025000 | 2.03126700  | 0.83532500  |
| H | -4.76375300 | 1.39765900  | -1.41470600 |
| C | 1.86444200  | -0.88652500 | 0.45768800  |
| C | 0.48543900  | 0.66962900  | -0.98699100 |
| O | 2.28790000  | -1.17109200 | 1.55742800  |
| O | 2.56913500  | -1.04561400 | -0.68286700 |
| O | 1.04511000  | 1.88661000  | -0.72727000 |
| O | -0.02993800 | 0.50495800  | -2.06459000 |
| C | 2.14410500  | 2.11510100  | 0.17555900  |
| H | 2.02492500  | 1.55583100  | 1.10747900  |
| H | 3.06250500  | 1.77351500  | -0.31476000 |
| C | 2.19768900  | 3.60809000  | 0.45080900  |
| H | 1.28581800  | 3.94324300  | 0.95551500  |
| H | 3.05513400  | 3.84029200  | 1.09194000  |
| H | 2.29866300  | 4.16709200  | -0.48427000 |
| C | 3.87034600  | -1.68149300 | -0.57509400 |
| H | 4.01505400  | -2.15205500 | -1.55023700 |
| H | 3.81563500  | -2.45182700 | 0.19756000  |
| C | 4.96950900  | -0.67551500 | -0.27342100 |
| H | 4.81917600  | -0.21922100 | 0.70901100  |
| H | 5.94085400  | -1.18330900 | -0.26937300 |
| H | 5.00007500  | 0.11103000  | -1.03462100 |
| H | -4.31896900 | -1.17965600 | -2.08453400 |

**TS5T4**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.07880100 | 0.03549200  | -1.71562100 |
| C | -1.90096600 | -1.12611500 | -0.74188800 |
| C | -1.58163400 | 1.08955900  | 1.47238700  |
| C | -2.73536500 | 0.60018200  | 0.69387400  |
| C | -2.93175900 | -0.88172800 | 0.42402400  |
| C | -3.32858300 | 1.20512800  | -0.40769600 |
| C | -4.61006900 | 0.46067700  | -0.77046500 |
| C | -4.37812700 | -0.94053200 | -0.12472100 |
| H | -2.74650800 | -0.12430900 | -2.55896300 |
| H | -1.21716100 | 0.65082400  | -1.94264600 |
| H | -4.79098900 | 0.41238200  | -1.84906300 |
| H | -4.51655300 | -1.76016500 | -0.83977600 |
| C | -0.43978500 | -1.38875800 | -0.28187200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.42339900 | 0.19787300  | 1.79377600  |
| C | 0.37788900  | -0.36867000 | 0.57818400  |
| H | 0.13091600  | -1.60844600 | -1.18709400 |
| H | -0.46292900 | -2.31786700 | 0.30428700  |
| H | 0.27619800  | 0.71894200  | 2.44719800  |
| H | -0.76923300 | -0.67689100 | 2.36769600  |
| H | -1.72445700 | 1.95580400  | 2.11622000  |
| H | -2.18473800 | -2.06425000 | -1.24283400 |
| H | -2.76700400 | -1.56036500 | 1.26775900  |
| H | -5.08043400 | -1.10672400 | 0.69879500  |
| H | -5.48078100 | 0.96422800  | -0.32900400 |
| C | 0.95653900  | 0.80675500  | -0.23146700 |
| C | 1.58824100  | -1.15062900 | 1.19740300  |
| O | 0.94376600  | 0.92078000  | -1.44200300 |
| O | 1.54078700  | 1.70166700  | 0.58676200  |
| O | 2.65357200  | -1.52101600 | 0.44243300  |
| O | 1.62880200  | -1.40738600 | 2.37677300  |
| C | 2.69687400  | -1.76318300 | -0.98401200 |
| H | 2.16639100  | -2.70054500 | -1.18734700 |
| H | 2.21695500  | -0.95788600 | -1.54035700 |
| C | 4.16431600  | -1.88616600 | -1.35676400 |
| H | 4.64528700  | -2.68277100 | -0.78127600 |
| H | 4.25784500  | -2.11863500 | -2.42336300 |
| H | 4.69393000  | -0.94883600 | -1.15854700 |
| C | 2.16465300  | 2.85746100  | -0.02816500 |
| H | 2.11569400  | 3.62782600  | 0.74480100  |
| H | 1.56343200  | 3.16397800  | -0.88699100 |
| C | 3.60115400  | 2.56036100  | -0.42920200 |
| H | 3.63448200  | 1.80741800  | -1.22187700 |
| H | 4.07638100  | 3.47367000  | -0.80512100 |
| H | 4.17767700  | 2.19904300  | 0.42823600  |
| H | -3.19688800 | 2.25498700  | -0.65910700 |

**TS4T3**

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.61324000 | 2.28765000  | 1.23048000  |
| C | 1.97962100 | 0.94299400  | 1.27352300  |
| C | 1.37151900 | 0.30890500  | -1.67573700 |
| C | 2.63349500 | -0.14273800 | -1.16505900 |
| C | 3.14502900 | -1.42184800 | -1.14585000 |
| C | 3.40291900 | 0.71716200  | -0.27694000 |
| C | 4.63518400 | -0.05870100 | 0.17165800  |
| C | 4.36824800 | -1.52701700 | -0.27230600 |
| H | 0.74620400 | 2.64571200  | 0.68883100  |
| H | 2.30156600 | 3.04920600  | 1.58702200  |



|             |             |             |             |
|-------------|-------------|-------------|-------------|
| H           | 4.82845000  | 0.02525600  | 1.24830200  |
| H           | 4.17756600  | -2.18449800 | 0.58997600  |
| C           | 0.97286300  | -0.21496600 | 1.20106200  |
| C           | 0.15163800  | -0.46747500 | -1.30843300 |
| C           | -0.23878400 | -0.22721200 | 0.21064200  |
| H           | 0.53906600  | -0.29598800 | 2.20391700  |
| H           | 1.51306600  | -1.15174000 | 1.03896000  |
| H           | -0.71335300 | -0.22127500 | -1.92804700 |
| H           | 0.35128000  | -1.54026800 | -1.41810100 |
| H           | 1.24604900  | 1.37493700  | -1.85242500 |
| H           | 2.74473900  | 0.70839300  | 2.01675700  |
| H           | 2.70955500  | -2.27482200 | -1.65764000 |
| H           | 5.23004300  | -1.96467700 | -0.79519000 |
| H           | 5.52576600  | 0.34243100  | -0.33160000 |
| C           | -1.12750300 | 1.00319700  | 0.44733200  |
| C           | -1.11816400 | -1.43772900 | 0.59357000  |
| O           | -1.64231800 | 1.23425200  | 1.52056500  |
| O           | -1.27834400 | 1.78177300  | -0.64492300 |
| O           | -2.31121300 | -1.37334300 | -0.03543800 |
| O           | -0.78162000 | -2.35902800 | 1.30174100  |
| C           | -3.22179500 | -2.47167800 | 0.21295100  |
| H           | -2.74924400 | -3.40038200 | -0.12275000 |
| H           | -3.38514900 | -2.55178200 | 1.29187300  |
| C           | -4.50494200 | -2.17798700 | -0.54050500 |
| H           | -4.31783000 | -2.09209000 | -1.61575700 |
| H           | -5.22338100 | -2.98910000 | -0.37941900 |
| H           | -4.95655800 | -1.24366300 | -0.19225200 |
| C           | -2.15959700 | 2.92598200  | -0.50527500 |
| H           | -1.80088100 | 3.63404500  | -1.25614500 |
| H           | -2.02639800 | 3.35104800  | 0.49221800  |
| C           | -3.60750600 | 2.53161400  | -0.75176000 |
| H           | -3.94444600 | 1.81936000  | 0.00646500  |
| H           | -4.24832600 | 3.41942600  | -0.70122300 |
| H           | -3.72429100 | 2.07721000  | -1.74094400 |
| H           | 3.51167500  | 1.77310500  | -0.50450100 |
| <b>M4T3</b> |             |             |             |
| C           | -1.49227300 | 2.19192700  | -1.21925600 |
| C           | -2.03219800 | 0.79793100  | -1.24777000 |
| C           | -1.37009700 | 0.32267400  | 1.65618600  |
| C           | -2.67776700 | -0.04729900 | 1.12133400  |
| C           | -3.54146900 | -0.97383000 | 1.56546000  |
| C           | -3.15840000 | 0.56410900  | -0.19735600 |
| C           | -4.25733700 | -0.43504100 | -0.64173200 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| C            | -4.73820500 | -1.12691200 | 0.65631400  |
| H            | -0.71334500 | 2.49081700  | -1.91238300 |
| H            | -1.98436200 | 2.97061300  | -0.64439000 |
| H            | -3.80971300 | -1.18774500 | -1.30333700 |
| H            | -5.02544700 | -2.17401500 | 0.49682200  |
| C            | -0.92089200 | -0.30265700 | -1.28518300 |
| C            | -0.20672200 | -0.52409200 | 1.25069500  |
| C            | 0.24067500  | -0.28545100 | -0.24342100 |
| H            | -0.44059200 | -0.25104500 | -2.26671900 |
| H            | -1.39277600 | -1.28899700 | -1.23247900 |
| H            | 0.66114300  | -0.35887600 | 1.89400200  |
| H            | -0.49344200 | -1.58080000 | 1.32824100  |
| H            | -1.17296200 | 1.36546400  | 1.89947500  |
| H            | -2.52662300 | 0.67498500  | -2.23165100 |
| H            | -3.42350300 | -1.53106400 | 2.49124800  |
| H            | -5.62257800 | -0.62534100 | 1.07979400  |
| H            | -5.06470500 | 0.05097400  | -1.20053900 |
| C            | 1.09195000  | 0.98034000  | -0.44098600 |
| C            | 1.17315100  | -1.46749100 | -0.58582800 |
| O            | 1.58813500  | 1.26929100  | -1.51170700 |
| O            | 1.25387000  | 1.70411600  | 0.68271400  |
| O            | 2.35306600  | -1.34924800 | 0.06005200  |
| O            | 0.88349400  | -2.41217100 | -1.28457400 |
| C            | 3.30418400  | -2.42065000 | -0.15110400 |
| H            | 2.85134200  | -3.36050900 | 0.18034000  |
| H            | 3.50075700  | -2.50578700 | -1.22418600 |
| C            | 4.55561700  | -2.07997200 | 0.63525300  |
| H            | 4.33492100  | -1.99021900 | 1.70379800  |
| H            | 5.30298700  | -2.86988900 | 0.50292300  |
| H            | 4.98819900  | -1.13521900 | 0.29095800  |
| C            | 2.08191400  | 2.88835000  | 0.57674000  |
| H            | 1.72249700  | 3.53965900  | 1.37715000  |
| H            | 1.89464000  | 3.36149300  | -0.38989800 |
| C            | 3.55358100  | 2.54599500  | 0.75098500  |
| H            | 3.89224900  | 1.89189800  | -0.05709600 |
| H            | 4.15357300  | 3.46310100  | 0.72881000  |
| H            | 3.72569700  | 2.04390200  | 1.70855400  |
| H            | -3.62074400 | 1.54312100  | 0.00671300  |
| <b>TS5T5</b> |             |             |             |
| C            | -1.89275400 | -2.12437400 | 1.53244900  |
| C            | -1.75038700 | -0.62509200 | 1.72862400  |
| C            | -1.83236200 | -1.82941800 | -0.62566600 |
| C            | -2.75098900 | -0.79426100 | -0.50206500 |

|           |             |             |             |
|-----------|-------------|-------------|-------------|
| C         | -2.80766900 | -0.02091700 | 0.77915400  |
| C         | -3.75207800 | -0.15571900 | -1.38241100 |
| C         | -3.90011400 | 1.28215500  | -0.94318600 |
| C         | -2.97760400 | 1.44131400  | 0.31795800  |
| H         | -2.87986200 | -2.54149700 | 1.72714700  |
| H         | -1.07164300 | -2.76126500 | 1.85977100  |
| H         | -4.94892700 | 1.50366100  | -0.68612700 |
| H         | -3.42882200 | 2.08933400  | 1.07736200  |
| C         | -0.29929600 | -0.16171300 | 1.51534700  |
| C         | -0.29813400 | -1.72683300 | -0.57746700 |
| C         | 0.33824900  | -0.48787400 | 0.12988600  |
| H         | 0.32467400  | -0.63812900 | 2.27779400  |
| H         | -0.25090700 | 0.91650700  | 1.69663500  |
| H         | 0.12012600  | -2.64205000 | -0.14137300 |
| H         | 0.03829500  | -1.69127700 | -1.61928700 |
| H         | -2.09079400 | -2.59595800 | -1.36774200 |
| H         | -2.02144400 | 1.88561000  | 0.02681000  |
| H         | -3.62993200 | 2.00193700  | -1.73161600 |
| C         | 1.81472400  | -0.90091000 | 0.31562500  |
| C         | 0.24845400  | 0.72622900  | -0.83471900 |
| O         | 2.31395400  | -1.29497300 | 1.34783600  |
| O         | 2.47128300  | -0.84770000 | -0.86318800 |
| O         | 0.74668100  | 1.93035800  | -0.43087700 |
| O         | -0.32522900 | 0.68560800  | -1.89509700 |
| C         | 1.85041700  | 2.10838600  | 0.47885900  |
| H         | 1.76893600  | 1.44752800  | 1.34597200  |
| H         | 2.77445900  | 1.86333500  | -0.05587400 |
| C         | 1.84348400  | 3.56407600  | 0.91292500  |
| H         | 0.92454900  | 3.80256900  | 1.45799800  |
| H         | 2.69814700  | 3.76264600  | 1.56889500  |
| H         | 1.90934200  | 4.22476300  | 0.04330200  |
| C         | 3.81594700  | -1.39511500 | -0.89788600 |
| H         | 3.94711000  | -1.70449200 | -1.93727100 |
| H         | 3.84806000  | -2.27364600 | -0.24920300 |
| C         | 4.85925900  | -0.36890400 | -0.48616900 |
| H         | 4.72471800  | -0.07709000 | 0.55906400  |
| H         | 5.86095600  | -0.80053400 | -0.59444400 |
| H         | 4.80311300  | 0.52276800  | -1.11934700 |
| H         | -4.33410300 | -0.62363600 | -2.16832300 |
| H         | -2.01171300 | -0.34523500 | 2.76364800  |
| H         | -3.78274800 | -0.29837100 | 1.22926300  |
| <b>P1</b> |             |             |             |
| C         | -2.67524000 | -0.89460200 | -1.58912900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34922800 | -0.12626100 | -1.31974900 |
| C | -1.64409200 | 0.88767300  | -0.14500800 |
| C | -3.07162000 | 0.59446400  | 0.22504800  |
| C | -3.47206900 | -0.77995500 | -0.27285200 |
| C | -4.10317500 | 1.26947700  | 0.73637900  |
| C | -5.36826000 | 0.42982600  | 0.71452900  |
| C | -5.01615100 | -0.71360700 | -0.28456400 |
| H | -3.23305300 | -0.39364100 | -2.39064400 |
| H | -2.49812000 | -1.92726100 | -1.91304200 |
| H | -6.25164900 | 1.00114200  | 0.40144700  |
| H | -5.35957600 | -0.43343400 | -1.28854800 |
| C | -0.17897500 | -1.00993200 | -0.82501600 |
| C | -0.61688200 | 0.54775200  | 0.96568000  |
| C | 0.56239200  | -0.17399300 | 0.25108700  |
| H | 0.46765700  | -1.31548500 | -1.65010600 |
| H | -0.56291000 | -1.91968200 | -0.34482100 |
| H | -0.28538600 | 1.42076900  | 1.53314900  |
| H | -1.03790900 | -0.15584900 | 1.68845100  |
| H | -1.51609900 | 1.92469300  | -0.47339400 |
| H | -1.02180000 | 0.41087600  | -2.21270800 |
| H | -3.12559100 | -1.55634900 | 0.42988100  |
| H | -5.49671400 | -1.66340100 | -0.02811400 |
| H | -5.59922400 | 0.03168200  | 1.71490000  |
| C | 1.46120000  | 0.88966300  | -0.39050900 |
| C | 1.35201900  | -1.02502600 | 1.27288500  |
| O | 1.49643300  | 1.15953800  | -1.57442800 |
| O | 2.18461100  | 1.53063500  | 0.54958200  |
| O | 2.46263700  | -1.70277200 | 0.88664900  |
| O | 1.01511300  | -1.11461400 | 2.42939600  |
| C | 2.88939600  | -1.91253700 | -0.47377100 |
| H | 2.25738700  | -2.68641000 | -0.92423200 |
| H | 2.79102900  | -1.00143800 | -1.06864000 |
| C | 4.33856500  | -2.36510500 | -0.41656200 |
| H | 4.43523900  | -3.26938000 | 0.19169000  |
| H | 4.70331700  | -2.58198300 | -1.42657500 |
| H | 4.96930800  | -1.58570100 | 0.02230900  |
| C | 3.03759800  | 2.61736900  | 0.10654000  |
| H | 3.11578800  | 3.26700000  | 0.98119100  |
| H | 2.53213100  | 3.15129200  | -0.70152200 |
| C | 4.40128600  | 2.10715300  | -0.33227700 |
| H | 4.31357900  | 1.48468200  | -1.22750500 |
| H | 5.05476000  | 2.95452200  | -0.56925500 |
| H | 4.87160200  | 1.52261000  | 0.46503300  |
| H | -4.07470200 | 2.28431400  | 1.12519400  |

**P2**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.68625300 | -1.19436800 | -1.32586400 |
| C | -1.37953300 | -0.35312000 | -1.29700300 |
| C | -1.61545600 | 0.77817700  | -0.22557100 |
| C | -3.08535800 | 0.68232800  | 0.08441700  |
| C | -3.89333100 | 1.01938900  | 1.09244300  |
| C | -3.78574300 | -0.18284100 | -0.94623100 |
| C | -5.06939400 | -0.62935000 | -0.21339600 |
| C | -5.28932000 | 0.45901600  | 0.88011600  |
| H | -2.84656400 | -1.68729900 | -2.29153700 |
| H | -2.64147900 | -1.98019100 | -0.55880900 |
| H | -4.89129100 | -1.59693300 | 0.27318500  |
| H | -5.72490500 | 0.04577100  | 1.79869400  |
| C | -0.09301000 | -1.10135300 | -0.86661600 |
| C | -0.64248600 | 0.45472700  | 0.92314800  |
| C | 0.57737900  | -0.22419400 | 0.23206300  |
| H | 0.57552700  | -1.27841400 | -1.71080300 |
| H | -0.34564600 | -2.07509000 | -0.42889400 |
| H | -0.34659400 | 1.32301500  | 1.51767700  |
| H | -1.08206500 | -0.27115700 | 1.61209700  |
| H | -1.36409500 | 1.75490500  | -0.65914100 |
| H | -1.22120200 | 0.10500700  | -2.27790700 |
| H | -3.62181500 | 1.61097100  | 1.96300400  |
| H | -5.98456600 | 1.24058300  | 0.53507700  |
| H | -5.93384900 | -0.74866200 | -0.87476400 |
| C | 1.43015300  | 0.88258600  | -0.39901200 |
| C | 1.38483800  | -1.03244900 | 1.27241500  |
| O | 1.42364900  | 1.18436700  | -1.57554600 |
| O | 2.15284500  | 1.52493600  | 0.54079900  |
| O | 2.51791600  | -1.68319200 | 0.90413800  |
| O | 1.03965300  | -1.11745900 | 2.42670400  |
| C | 2.98509700  | -1.85293700 | -0.44772200 |
| H | 2.38014900  | -2.62486400 | -0.93670400 |
| H | 2.88820600  | -0.92806000 | -1.02221400 |
| C | 4.44018300  | -2.28141100 | -0.36138700 |
| H | 4.53608300  | -3.19977900 | 0.22549700  |
| H | 4.83697100  | -2.46505000 | -1.36590600 |
| H | 5.04397400  | -1.50322200 | 0.11578500  |
| C | 2.95045000  | 2.65723900  | 0.10853000  |
| H | 3.02959900  | 3.28196400  | 1.00103900  |
| H | 2.40120400  | 3.19582300  | -0.66726500 |
| C | 4.31892600  | 2.21462800  | -0.38529500 |
| H | 4.22847800  | 1.61906000  | -1.29834600 |

|           |             |             |             |
|-----------|-------------|-------------|-------------|
| H         | 4.93295100  | 3.09386900  | -0.61136400 |
| H         | 4.83397000  | 1.62293400  | 0.37845100  |
| H         | -4.03840500 | 0.41919000  | -1.83583600 |
| <b>P3</b> |             |             |             |
| C         | -2.02554200 | -1.65299300 | 1.40069300  |
| C         | -1.75393300 | -0.14198400 | 1.59455900  |
| C         | -1.81163600 | -1.79530400 | -0.13261200 |
| C         | -2.67573900 | -0.64210800 | -0.56852900 |
| C         | -2.50051300 | 0.52023100  | 0.39997700  |
| C         | -3.80392700 | -0.52758200 | -1.27357100 |
| C         | -4.54477400 | 0.74320300  | -0.88661600 |
| C         | -3.94306300 | 1.05917200  | 0.51449500  |
| H         | -3.05744100 | -1.90923900 | 1.66590400  |
| H         | -1.35213600 | -2.28606400 | 1.99222000  |
| H         | -5.63266900 | 0.60378700  | -0.85810500 |
| H         | -4.49650200 | 0.49658900  | 1.27846700  |
| C         | -0.23243300 | 0.09223000  | 1.49052900  |
| C         | -0.29844100 | -1.68800600 | -0.42472300 |
| C         | 0.41762000  | -0.41307100 | 0.15612100  |
| H         | 0.27065800  | -0.42580800 | 2.31299600  |
| H         | -0.02920300 | 1.16094600  | 1.61540600  |
| H         | 0.16688700  | -2.57485000 | 0.02459100  |
| H         | -0.10696800 | -1.72120300 | -1.49838400 |
| H         | -2.16654100 | -2.75394200 | -0.52664900 |
| H         | -2.09383700 | 0.22674000  | 2.56953700  |
| H         | -1.88096100 | 1.31560900  | -0.03615900 |
| H         | -3.99301100 | 2.12193800  | 0.77850400  |
| H         | -4.35174800 | 1.56550300  | -1.59316600 |
| C         | 1.86053300  | -0.88545200 | 0.41755900  |
| C         | 0.41666300  | 0.69465900  | -0.93320300 |
| O         | 2.31580600  | -1.20864600 | 1.49384300  |
| O         | 2.53983600  | -0.98094800 | -0.74569700 |
| O         | 0.99728200  | 1.89648500  | -0.66199800 |
| O         | -0.15566700 | 0.57423700  | -1.98880800 |
| C         | 2.08629800  | 2.11300400  | 0.25588000  |
| H         | 1.97930700  | 1.50926300  | 1.16063300  |
| H         | 3.01406100  | 1.81772800  | -0.24624500 |
| C         | 2.10017200  | 3.59289500  | 0.59916000  |
| H         | 1.17870100  | 3.88096500  | 1.11537200  |
| H         | 2.94979500  | 3.81734300  | 1.25338400  |
| H         | 2.18906100  | 4.19702200  | -0.30868800 |
| C         | 3.85487600  | -1.59483300 | -0.69896700 |
| H         | 3.97946500  | -2.02762800 | -1.69421300 |

|           |             |             |             |
|-----------|-------------|-------------|-------------|
| H         | 3.83835400  | -2.39285300 | 0.04683100  |
| C         | 4.94338700  | -0.57840900 | -0.39341800 |
| H         | 4.81406600  | -0.16122300 | 0.60925200  |
| H         | 5.92413400  | -1.06589300 | -0.43683200 |
| H         | 4.93555100  | 0.23580700  | -1.12557600 |
| H         | -4.19436600 | -1.25346900 | -1.98179900 |
| <b>P4</b> |             |             |             |
| C         | -2.36108300 | 0.35782200  | -1.61292800 |
| C         | -1.97829900 | -0.97622400 | -0.85367000 |
| C         | -1.52540300 | 1.08998100  | 1.30478600  |
| C         | -2.58034500 | 0.60575000  | 0.65039700  |
| C         | -2.85059400 | -0.87185000 | 0.41507000  |
| C         | -3.26938100 | 1.13359000  | -0.58916200 |
| C         | -4.65913200 | 0.46973400  | -0.56011800 |
| C         | -4.35699700 | -0.93079800 | 0.06235500  |
| H         | -2.89890100 | 0.14562600  | -2.54543500 |
| H         | -1.47173700 | 0.94054500  | -1.85849600 |
| H         | -5.10625200 | 0.40394200  | -1.55815600 |
| H         | -4.57391800 | -1.75463900 | -0.62755200 |
| C         | -0.47467200 | -1.22633400 | -0.51328300 |
| C         | -0.46196000 | 0.13822500  | 1.78688400  |
| C         | 0.35051800  | -0.37690100 | 0.53451100  |
| H         | 0.07410400  | -1.20147800 | -1.45763800 |
| H         | -0.43223400 | -2.26451400 | -0.15652100 |
| H         | 0.24070800  | 0.60093400  | 2.48066300  |
| H         | -0.87712400 | -0.73323700 | 2.29690600  |
| H         | -1.28132400 | 2.15092700  | 1.24885400  |
| H         | -2.26584800 | -1.84360900 | -1.46456900 |
| H         | -2.56168600 | -1.56419300 | 1.20846800  |
| H         | -4.95558000 | -1.09960700 | 0.96392100  |
| H         | -5.34945700 | 1.03999400  | 0.07186900  |
| C         | 0.99009600  | 0.85745700  | -0.12678400 |
| C         | 1.47657500  | -1.29808500 | 1.10543700  |
| O         | 0.81747100  | 1.22786900  | -1.27100300 |
| O         | 1.78618300  | 1.50310800  | 0.74952700  |
| O         | 2.51779300  | -1.71143400 | 0.33750000  |
| O         | 1.46009500  | -1.66897100 | 2.25468600  |
| C         | 2.64042200  | -1.64259000 | -1.09867300 |
| H         | 2.03064000  | -2.44039200 | -1.53750200 |
| H         | 2.28766500  | -0.68613000 | -1.48779900 |
| C         | 4.11037400  | -1.84998300 | -1.42272300 |
| H         | 4.46306400  | -2.80472600 | -1.02131000 |
| H         | 4.25577000  | -1.85184200 | -2.50868500 |

|           |             |             |             |
|-----------|-------------|-------------|-------------|
| H         | 4.71837300  | -1.04874700 | -0.99110600 |
| C         | 2.44683700  | 2.70966500  | 0.29008200  |
| H         | 2.58890600  | 3.29752500  | 1.19978100  |
| H         | 1.77391800  | 3.24097300  | -0.38683900 |
| C         | 3.77441000  | 2.39210300  | -0.38005700 |
| H         | 3.61777000  | 1.83037600  | -1.30551000 |
| H         | 4.29428000  | 3.32381500  | -0.63079300 |
| H         | 4.41647700  | 1.80841200  | 0.28742200  |
| H         | -3.26815700 | 2.21607800  | -0.73840200 |
| <b>P5</b> |             |             |             |
| C         | -2.01483600 | -2.19139300 | 1.01900600  |
| C         | -1.90990300 | -0.77609300 | 1.63478900  |
| C         | -1.93618000 | -1.85871200 | -0.49229500 |
| C         | -2.76977300 | -0.59818900 | -0.58155000 |
| C         | -3.15924200 | 0.26542700  | -1.52053900 |
| C         | -3.00648800 | -0.05370900 | 0.81553300  |
| C         | -3.12854100 | 1.46223300  | 0.57116600  |
| C         | -3.69207000 | 1.53877300  | -0.88151100 |
| H         | -2.14084900 | 1.93918800  | 0.58989500  |
| H         | -3.36011300 | 2.43959800  | -1.41124300 |
| C         | -0.47158600 | -0.24495600 | 1.45511900  |
| C         | -0.45696900 | -1.57143800 | -0.83594000 |
| C         | 0.21461700  | -0.45453500 | 0.05695700  |
| H         | 0.15744300  | -0.75405000 | 2.19130800  |
| H         | -0.45838300 | 0.81621900  | 1.71576800  |
| H         | 0.09319600  | -2.51194700 | -0.70468100 |
| H         | -0.34832100 | -1.26679800 | -1.87772100 |
| H         | -4.79383700 | 1.56388500  | -0.87921800 |
| H         | -3.76010700 | 1.97654500  | 1.30402300  |
| C         | 1.65374500  | -0.97860600 | 0.26217300  |
| C         | 0.29045100  | 0.86751800  | -0.76491400 |
| O         | 2.07363800  | -1.52030800 | 1.26359400  |
| O         | 2.37487100  | -0.82920300 | -0.86705800 |
| O         | 0.80060100  | 1.99037400  | -0.18640700 |
| O         | -0.10941600 | 0.96960300  | -1.89798600 |
| C         | 1.59040200  | 2.07955200  | 1.01528800  |
| H         | 0.95252700  | 2.49154400  | 1.80552600  |
| H         | 1.94147000  | 1.10040200  | 1.34642200  |
| C         | 2.76034700  | 3.00887300  | 0.73247900  |
| H         | 2.40107200  | 3.98465300  | 0.39210100  |
| H         | 3.35286100  | 3.15300600  | 1.64317200  |
| H         | 3.40820700  | 2.59069600  | -0.04399000 |
| C         | 3.69895600  | -1.42313000 | -0.89378200 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.87103900  | -1.63689200 | -1.95109600 |
| H | 3.67165000  | -2.35917200 | -0.33116000 |
| C | 4.75013900  | -0.47529400 | -0.33898000 |
| H | 4.57539000  | -0.28004700 | 0.72286900  |
| H | 5.74412200  | -0.92507100 | -0.44419300 |
| H | 4.74576400  | 0.47437100  | -0.88378500 |
| H | -3.97304100 | -0.42722000 | 1.19816700  |
| H | -3.06841300 | 0.13933700  | -2.59514000 |
| H | -1.21805100 | -2.86886700 | 1.34840400  |
| H | -2.97736500 | -2.65122000 | 1.27376200  |
| H | -2.28419800 | -2.67666800 | -1.13381600 |
| H | -2.12802800 | -0.77313900 | 2.70948000  |

**N<sub>2</sub>**

|   |            |            |             |
|---|------------|------------|-------------|
| N | 0.00000000 | 0.00000000 | 0.55275100  |
| N | 0.00000000 | 0.00000000 | -0.55275100 |

**Phenylethene**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.36239900  | 1.32953100  | -0.00001100 |
| C | 2.26538100  | 0.26173400  | 0.00002800  |
| C | 1.78076000  | -1.04624400 | 0.00003100  |
| C | 0.40638600  | -1.28132800 | -0.00000100 |
| C | -0.51525500 | -0.22030800 | -0.00003300 |
| C | -0.00871600 | 1.09247000  | -0.00004500 |
| H | 1.73057200  | 2.35226100  | -0.00002700 |
| H | 3.33553000  | 0.45031400  | 0.00005100  |
| H | 2.47181000  | -1.88513600 | 0.00005200  |
| H | 0.03483600  | -2.30377900 | 0.00000500  |
| H | -0.69373300 | 1.93543300  | -0.00008900 |
| C | -1.95473800 | -0.52923000 | -0.00004700 |
| C | -2.97748100 | 0.33495600  | 0.00006700  |
| H | -2.18616800 | -1.59464400 | -0.00015000 |
| H | -4.00453900 | -0.01697000 | 0.00003900  |
| H | -2.84073100 | 1.41303800  | 0.00019800  |

**R'**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.16789500 | -2.77679600 | 2.87650100  |
| C | -2.11981800 | -1.94142700 | 2.45891600  |
| C | -0.89354200 | 0.74182100  | -0.84193900 |
| C | -0.22684200 | 1.79182600  | -0.42837400 |
| C | 2.56255900  | 0.53248400  | 0.62099900  |
| C | 0.46259400  | 2.83383900  | -0.02462700 |
| C | 1.98227700  | 2.88854100  | -0.10649900 |
| C | 2.67142600  | 1.56792800  | -0.46712800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.70113400 | -2.66586000 | 3.85164900  |
| H | -0.81482500 | -3.60277900 | 2.26187200  |
| H | 2.36889200  | 3.25216900  | 0.85872100  |
| H | 3.73631100  | 1.75858800  | -0.66537500 |
| C | -2.83242600 | -2.07255100 | 1.13640400  |
| C | -1.20356800 | -0.45393600 | 0.03141600  |
| C | -2.71269300 | -0.85259400 | 0.15829300  |
| H | -3.89272600 | -2.26493500 | 1.33456400  |
| H | -2.44317500 | -2.95037900 | 0.60626700  |
| H | -0.68182300 | -1.32833800 | -0.37368100 |
| H | -0.81802800 | -0.28357400 | 1.03875000  |
| H | -1.21110400 | 0.67647200  | -1.88151900 |
| H | -2.44584200 | -1.12218900 | 3.09447300  |
| H | 2.33913100  | 0.87816600  | 1.63255700  |
| H | 2.25854900  | 1.14457900  | -1.39037700 |
| H | 2.26409200  | 3.65950800  | -0.83912600 |
| C | -3.46100900 | 0.37647800  | 0.68293500  |
| C | -3.22283400 | -1.30869600 | -1.23328000 |
| O | -3.64900500 | 0.63093500  | 1.85522300  |
| O | -3.83141300 | 1.18915400  | -0.32807100 |
| O | -4.53145900 | -1.60065600 | -1.44182200 |
| O | -2.46882000 | -1.47335900 | -2.16391200 |
| C | -5.60114000 | -1.57880700 | -0.48049900 |
| H | -5.65864600 | -2.56666700 | -0.00871700 |
| H | -5.43036900 | -0.83578200 | 0.30111700  |
| C | -6.88081800 | -1.27204800 | -1.24071700 |
| H | -7.04333800 | -2.01113900 | -2.03088000 |
| H | -7.73788300 | -1.29481500 | -0.55855800 |
| H | -6.82478400 | -0.28139700 | -1.70215800 |
| C | -4.36058800 | 2.49133200  | 0.03069400  |
| H | -4.11742600 | 3.12037900  | -0.82850000 |
| H | -3.82295400 | 2.85229900  | 0.91067300  |
| C | -5.85947700 | 2.44550900  | 0.28305000  |
| H | -6.08719900 | 1.82801700  | 1.15639600  |
| H | -6.23116000 | 3.45866500  | 0.47505200  |
| H | -6.39167400 | 2.04726200  | -0.58707000 |
| N | 2.92720900  | -1.19426500 | -0.80373200 |
| N | 2.70328200  | -0.73653900 | 0.51462000  |
| C | 4.34314600  | -1.27208000 | -1.30673300 |
| H | 4.38218400  | -1.07315400 | -2.37656700 |
| C | 3.58437300  | -2.48773300 | -0.87521100 |
| H | 3.19159000  | -3.17493100 | -1.62271300 |
| H | 3.87073200  | -2.94433300 | 0.07010800  |
| C | 5.52846300  | -0.74001400 | -0.57480700 |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| C           | 6.49981100  | -0.04636600 | -1.31485100 |
| C           | 5.73715600  | -0.90476800 | 0.80515200  |
| C           | 7.64898400  | 0.45669800  | -0.70585800 |
| H           | 6.35414100  | 0.09194300  | -2.38391200 |
| C           | 6.88445200  | -0.39772200 | 1.41445800  |
| H           | 4.99431700  | -1.41789600 | 1.40606300  |
| C           | 7.84590300  | 0.28277400  | 0.66441700  |
| H           | 8.38848100  | 0.98392800  | -1.30293400 |
| H           | 7.02643500  | -0.53592700 | 2.48321200  |
| H           | 8.73898300  | 0.67413100  | 1.14418800  |
| C           | -0.20932600 | 4.07425300  | 0.52950700  |
| H           | -1.29836500 | 3.97836900  | 0.52667400  |
| H           | 0.11638300  | 4.26826700  | 1.56067500  |
| H           | 0.05934700  | 4.96073500  | -0.06180200 |
| <b>TS1'</b> |             |             |             |
| C           | 0.67590600  | -2.95028600 | 1.17438100  |
| C           | -0.46538100 | -2.27343700 | 1.31827600  |
| C           | -1.11734600 | 1.36208700  | -1.10565900 |
| C           | -0.62987400 | 2.43887200  | -0.53803500 |
| C           | 2.69253100  | 2.09031100  | -0.51194000 |
| C           | -0.14062500 | 3.52292200  | 0.01715900  |
| C           | 1.19422900  | 4.13030000  | -0.39145600 |
| C           | 2.09568900  | 3.25541800  | -1.27027400 |
| H           | 1.44375900  | -2.94634800 | 1.94318100  |
| H           | 0.88444100  | -3.54560700 | 0.28691300  |
| H           | 1.74065800  | 4.41007900  | 0.52267200  |
| H           | 2.90706000  | 3.88328000  | -1.67185400 |
| C           | -1.58697200 | -2.29721800 | 0.31088000  |
| C           | -0.83519200 | -0.04411200 | -0.62327100 |
| C           | -2.07909500 | -0.90473400 | -0.21542400 |
| H           | -2.43675600 | -2.82442800 | 0.75910700  |
| H           | -1.27224700 | -2.88548300 | -0.56003300 |
| H           | -0.32715700 | -0.59883200 | -1.42079000 |
| H           | -0.16163800 | -0.00460400 | 0.23570200  |
| H           | -1.73387400 | 1.45102000  | -1.99904900 |
| H           | -0.64990100 | -1.69506700 | 2.22001000  |
| H           | 2.82064200  | 2.15262100  | 0.56554600  |
| H           | 1.53687600  | 2.88033100  | -2.13616100 |
| H           | 0.99518100  | 5.08054300  | -0.90962400 |
| C           | -2.82586200 | -0.12114900 | 0.86773200  |
| C           | -2.94096000 | -1.15448200 | -1.48000300 |
| O           | -2.59779500 | -0.19625600 | 2.05799800  |
| O           | -3.72700900 | 0.72376400  | 0.32815400  |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| O          | -4.14140100 | -1.77966600 | -1.40187700 |
| O          | -2.54680100 | -0.85537500 | -2.58342800 |
| C          | -4.78347600 | -2.30816600 | -0.22774900 |
| H          | -4.45650700 | -3.34620000 | -0.09639900 |
| H          | -4.51429600 | -1.74694200 | 0.66921400  |
| C          | -6.28246000 | -2.24244700 | -0.46834600 |
| H          | -6.55005100 | -2.79411000 | -1.37444700 |
| H          | -6.81860300 | -2.68199800 | 0.38001500  |
| H          | -6.60590600 | -1.20403700 | -0.58923800 |
| C          | -4.35553600 | 1.67884900  | 1.22204100  |
| H          | -4.62363200 | 2.51226900  | 0.56909500  |
| H          | -3.61126700 | 2.01075800  | 1.94974800  |
| C          | -5.57803900 | 1.09453300  | 1.91237600  |
| H          | -5.29394300 | 0.27554600  | 2.57902600  |
| H          | -6.06544000 | 1.87050400  | 2.51384000  |
| H          | -6.30398100 | 0.72682300  | 1.17972800  |
| N          | 3.31197700  | 0.47432400  | -2.16453600 |
| N          | 3.10547700  | 1.01538200  | -1.08554400 |
| C          | 4.50899800  | -1.52357000 | -1.57161400 |
| H          | 5.29594500  | -1.66590300 | -2.30850800 |
| C          | 3.20660300  | -1.29733100 | -2.04792300 |
| H          | 3.00196000  | -1.55826700 | -3.08172400 |
| H          | 2.35168400  | -1.44888100 | -1.39320700 |
| C          | 4.92766500  | -1.32726900 | -0.21601500 |
| C          | 6.30567400  | -1.40655000 | 0.11382700  |
| C          | 4.02348300  | -0.99057200 | 0.82213700  |
| C          | 6.75279100  | -1.16786000 | 1.40289600  |
| H          | 7.01666600  | -1.65537700 | -0.67066800 |
| C          | 4.48388800  | -0.74080100 | 2.11669100  |
| H          | 2.95739100  | -0.96918500 | 0.62979200  |
| C          | 5.84222300  | -0.82641000 | 2.41475600  |
| H          | 7.81368000  | -1.23822800 | 1.62890800  |
| H          | 3.77106500  | -0.48807100 | 2.89773700  |
| H          | 6.19501900  | -0.63712200 | 3.42495600  |
| C          | -0.89909100 | 4.27956500  | 1.08980600  |
| H          | -1.86805500 | 3.81973700  | 1.30126200  |
| H          | -0.32305800 | 4.31430500  | 2.02460100  |
| H          | -1.07248400 | 5.32039900  | 0.78295200  |
| <b>M1'</b> |             |             |             |
| C          | 0.43240700  | 3.94179000  | -0.44138200 |
| C          | -0.29548900 | 2.86390300  | -0.73827200 |
| C          | 1.34643900  | 0.24163000  | -0.58735100 |
| C          | 2.61031900  | 0.56935800  | -0.47949500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.94320300  | -1.97962400 | 1.05477200  |
| C | 3.85713800  | 0.95944100  | -0.35527500 |
| C | 5.02515700  | 0.01409900  | -0.13068700 |
| C | 4.71771200  | -1.49348400 | -0.14516000 |
| H | 0.99864200  | 4.47268600  | -1.20226000 |
| H | 0.48718300  | 4.33964000  | 0.57042400  |
| H | 5.51434500  | 0.27847500  | 0.82003900  |
| H | 5.67577000  | -2.03104100 | -0.20512500 |
| C | -1.17355300 | 2.15177400  | 0.25915700  |
| C | 0.40756900  | 0.10848500  | 0.59785000  |
| C | -1.05928600 | 0.59891200  | 0.36059000  |
| H | -2.21290400 | 2.40293100  | 0.01755700  |
| H | -0.97712100 | 2.55730900  | 1.25954500  |
| H | 0.34775500  | -0.94496700 | 0.88747500  |
| H | 0.81139100  | 0.64763000  | 1.45780500  |
| H | 0.95296000  | -0.00383000 | -1.57579600 |
| H | -0.33939700 | 2.50127800  | -1.76149300 |
| H | 4.16098600  | -1.74473100 | -1.05490900 |
| H | 5.77950700  | 0.21764000  | -0.90635700 |
| C | -1.56823900 | -0.10504000 | -0.90268800 |
| C | -1.86805300 | 0.15795800  | 1.61802600  |
| O | -1.76484100 | 0.42506100  | -1.97860100 |
| O | -1.71044500 | -1.42557700 | -0.67726600 |
| O | -3.22257400 | 0.23754600  | 1.65036200  |
| O | -1.31495700 | -0.22849800 | 2.61931500  |
| C | -4.10533100 | 0.77837400  | 0.64909600  |
| H | -4.20990600 | 1.85449900  | 0.83076500  |
| H | -3.71184000 | 0.64043600  | -0.35942500 |
| C | -5.44407400 | 0.07644000  | 0.80681200  |
| H | -5.82765000 | 0.20643400  | 1.82313400  |
| H | -6.17123300 | 0.49507500  | 0.10221100  |
| H | -5.34368700 | -0.99542200 | 0.61053300  |
| C | -2.04118200 | -2.27042900 | -1.80999400 |
| H | -1.60461700 | -3.23773900 | -1.55254800 |
| H | -1.54646500 | -1.87077600 | -2.69836600 |
| C | -3.54471400 | -2.37092900 | -2.01151400 |
| H | -3.96519200 | -1.40332300 | -2.30050800 |
| H | -3.76213700 | -3.08892400 | -2.81056400 |
| H | -4.03725200 | -2.71733300 | -1.09713300 |
| N | 1.87647900  | -3.24819800 | 0.76883700  |
| N | 2.84829000  | -2.65057800 | 0.91795600  |
| H | 4.26751800  | -1.80697400 | 2.07454800  |
| C | 4.22100600  | 2.42945700  | -0.44998000 |
| H | 3.33206900  | 3.05070800  | -0.58431500 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| H            | 4.73961300  | 2.75990200  | 0.46062500  |
| H            | 4.90463700  | 2.61089600  | -1.29091400 |
| <b>TS2a'</b> |             |             |             |
| C            | 1.30575500  | -2.02723000 | 2.57873600  |
| C            | 0.44249600  | -1.10385700 | 2.15097400  |
| C            | 1.24403600  | 0.23629700  | -0.95717900 |
| C            | 2.29926600  | 0.47751500  | -0.14385400 |
| C            | 3.88627100  | -0.86213200 | -0.57221100 |
| C            | 2.97813800  | 1.22230500  | 0.72537000  |
| C            | 4.46532900  | 0.98944200  | 0.90452200  |
| C            | 4.98115800  | 0.13257700  | -0.26898900 |
| H            | 2.18999000  | -1.75947700 | 3.15152900  |
| H            | 1.15550300  | -3.08815800 | 2.38576200  |
| H            | 4.65018700  | 0.48202800  | 1.86504000  |
| H            | 5.93949700  | -0.34367900 | -0.02639200 |
| C            | -0.82787700 | -1.42580400 | 1.41125400  |
| C            | 0.29554900  | -0.94622800 | -0.88786500 |
| C            | -1.00371600 | -0.77198400 | 0.00187200  |
| H            | -1.67073900 | -1.13071900 | 2.04563900  |
| H            | -0.89266600 | -2.51268500 | 1.27599800  |
| H            | -0.04069300 | -1.18468600 | -1.89581700 |
| H            | 0.81653600  | -1.83195500 | -0.51079800 |
| H            | 1.02186700  | 0.97287900  | -1.72777300 |
| H            | 0.61466200  | -0.05414100 | 2.37063100  |
| H            | 5.13551000  | 0.76733800  | -1.14788200 |
| H            | 5.01508000  | 1.93875500  | 0.95895000  |
| C            | -1.30070700 | 0.72479400  | 0.10798000  |
| C            | -2.16633700 | -1.53002100 | -0.71012700 |
| O            | -1.16067100 | 1.40622900  | 1.10494400  |
| O            | -1.71529200 | 1.20759800  | -1.08054100 |
| O            | -3.45014400 | -1.41321200 | -0.28115900 |
| O            | -1.96863200 | -2.27822800 | -1.63712300 |
| C            | -3.94175500 | -0.71213000 | 0.87661300  |
| H            | -3.86729700 | -1.38133800 | 1.74180600  |
| H            | -3.35736100 | 0.18484700  | 1.08819200  |
| C            | -5.39320200 | -0.35732600 | 0.59854400  |
| H            | -5.97298200 | -1.25826500 | 0.37673900  |
| H            | -5.83236000 | 0.13470800  | 1.47352200  |
| H            | -5.46795100 | 0.31996700  | -0.25780400 |
| C            | -1.91630300 | 2.64046400  | -1.18531700 |
| H            | -1.75003200 | 2.85425500  | -2.24352800 |
| H            | -1.15261800 | 3.14379000  | -0.58792800 |
| C            | -3.31624100 | 3.04458700  | -0.75046600 |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| H           | -3.46118200 | 2.85682900  | 0.31714900  |
| H           | -3.46372000 | 4.11551600  | -0.93147800 |
| H           | -4.07408100 | 2.49431900  | -1.31764400 |
| N           | 2.77521900  | -1.00867200 | -2.68840500 |
| N           | 3.55878900  | -1.13376500 | -1.84511000 |
| H           | 3.78763500  | -1.73295300 | 0.07501400  |
| C           | 2.33035600  | 2.26782700  | 1.60267500  |
| H           | 1.24945300  | 2.30760500  | 1.45113300  |
| H           | 2.52339500  | 2.06641900  | 2.66653700  |
| H           | 2.75093900  | 3.26219300  | 1.39385200  |
| <b>M2a'</b> |             |             |             |
| C           | -1.41442400 | -2.57195200 | -2.01260000 |
| C           | -0.56242300 | -1.56211800 | -1.82597700 |
| C           | -1.37284500 | 0.30648300  | 1.04487600  |
| C           | -2.51608700 | 0.21180500  | 0.08824200  |
| C           | -3.57782800 | -0.58429100 | 0.79854900  |
| C           | -3.01831800 | 0.91762800  | -0.93437000 |
| C           | -4.49859400 | 0.59259700  | -1.10813000 |
| C           | -4.90636000 | -0.02526400 | 0.25796300  |
| H           | -2.32508000 | -2.44937500 | -2.59285900 |
| H           | -1.23172300 | -3.56261700 | -1.60000000 |
| H           | -4.65619000 | -0.12020900 | -1.93212200 |
| H           | -5.69593700 | -0.77800700 | 0.17682000  |
| C           | 0.73742500  | -1.69469500 | -1.08172400 |
| C           | -0.29279700 | -0.80061600 | 1.13111700  |
| C           | 0.94143600  | -0.76799200 | 0.16275700  |
| H           | 1.55212900  | -1.51485700 | -1.79063300 |
| H           | 0.83866100  | -2.72943600 | -0.73143300 |
| H           | 0.09499300  | -0.75922900 | 2.14994400  |
| H           | -0.77193300 | -1.77898900 | 1.02441900  |
| H           | -0.90486200 | 1.29473000  | 1.07400100  |
| H           | -0.76560300 | -0.58886500 | -2.26305600 |
| H           | -5.26383700 | 0.76135900  | 0.93234500  |
| H           | -5.08456100 | 1.48649100  | -1.36009600 |
| C           | 1.21439000  | 0.68249200  | -0.24143200 |
| C           | 2.15409900  | -1.35510700 | 0.95947700  |
| O           | 1.00123600  | 1.16104200  | -1.33843600 |
| O           | 1.68520100  | 1.38297100  | 0.80863100  |
| O           | 3.40926900  | -1.32747000 | 0.44616400  |
| O           | 2.01235400  | -1.89241700 | 2.03074800  |
| C           | 3.84433500  | -0.85876200 | -0.84482100 |
| H           | 3.74791400  | -1.68430200 | -1.55922800 |
| H           | 3.23689600  | -0.02523700 | -1.20169000 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| C            | 5.29926200  | -0.44408400 | -0.70023500 |
| H            | 5.90043600  | -1.27910600 | -0.32861800 |
| H            | 5.69713600  | -0.13210200 | -1.67223700 |
| H            | 5.39630700  | 0.38980900  | 0.00163600  |
| C            | 1.89993600  | 2.80922200  | 0.63091500  |
| H            | 1.74581300  | 3.22506200  | 1.62881200  |
| H            | 1.13611600  | 3.19588500  | -0.04750200 |
| C            | 3.29954600  | 3.10138500  | 0.11504900  |
| H            | 3.43493200  | 2.70649100  | -0.89620700 |
| H            | 3.45905700  | 4.18509000  | 0.08039800  |
| H            | 4.05649600  | 2.66511200  | 0.77462200  |
| N            | -2.13086300 | 0.15507600  | 2.38528900  |
| N            | -3.26583600 | -0.32808800 | 2.24118300  |
| H            | -3.50613700 | -1.67402300 | 0.66082000  |
| C            | -2.33998100 | 1.91655700  | -1.82033600 |
| H            | -1.28806300 | 2.05876400  | -1.56216700 |
| H            | -2.38123700 | 1.59921200  | -2.87213800 |
| H            | -2.85392800 | 2.88669500  | -1.77192200 |
| <b>TS3a'</b> |             |             |             |
| C            | -1.49189800 | -2.20013200 | -2.17709900 |
| C            | -0.54725900 | -1.29208600 | -1.91863300 |
| C            | -1.29773000 | 0.45141900  | 0.69651700  |
| C            | -2.55448500 | 0.22062100  | 0.08007000  |
| C            | -3.43126700 | -0.90889400 | 0.41124400  |
| C            | -3.30055600 | 1.11640000  | -0.65029600 |
| C            | -4.72351400 | 0.67417500  | -0.84429800 |
| C            | -4.79446200 | -0.72333800 | -0.19168300 |
| H            | -2.35538300 | -1.96669700 | -2.79445500 |
| H            | -1.43130200 | -3.21752500 | -1.79452200 |
| H            | -4.99273000 | 0.64319000  | -1.90948500 |
| H            | -5.02502300 | -1.49750800 | -0.93571900 |
| C            | 0.70249400  | -1.59074200 | -1.13679900 |
| C            | -0.26933200 | -0.58462400 | 1.06144600  |
| C            | 0.98965800  | -0.69805900 | 0.10991800  |
| H            | 1.55162600  | -1.51508900 | -1.82578700 |
| H            | 0.66515300  | -2.63112000 | -0.79044300 |
| H            | 0.12011900  | -0.36265800 | 2.05826500  |
| H            | -0.70991500 | -1.58384100 | 1.12675800  |
| H            | -0.93549500 | 1.47663900  | 0.67423200  |
| H            | -0.62503500 | -0.28907600 | -2.32837300 |
| H            | -5.58036700 | -0.78738400 | 0.57326500  |
| H            | -5.40924700 | 1.40354800  | -0.38675600 |
| C            | 1.38166300  | 0.72573200  | -0.28734800 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.11542400  | -1.39630500 | 0.92855700  |
| O | 1.23684700  | 1.22261600  | -1.38718100 |
| O | 1.86435700  | 1.39410400  | 0.78073600  |
| O | 3.39627900  | -1.44416500 | 0.47493500  |
| O | 1.88418300  | -1.95086800 | 1.97562900  |
| C | 3.89483800  | -1.02153800 | -0.80761500 |
| H | 3.74650500  | -1.83988300 | -1.52210200 |
| H | 3.36514200  | -0.14327900 | -1.18102900 |
| C | 5.37530500  | -0.72487700 | -0.63428300 |
| H | 5.89988500  | -1.60368800 | -0.24764500 |
| H | 5.81749500  | -0.44946500 | -1.59819700 |
| H | 5.52385100  | 0.10150300  | 0.06761600  |
| C | 2.17556600  | 2.80006300  | 0.60955400  |
| H | 2.02243500  | 3.22886700  | 1.60243200  |
| H | 1.45781000  | 3.23463400  | -0.09020000 |
| C | 3.60478100  | 3.00086600  | 0.13112200  |
| H | 3.73914100  | 2.59867100  | -0.87736200 |
| H | 3.83816500  | 4.07145900  | 0.10422200  |
| H | 4.31338400  | 2.51292200  | 0.80816900  |
| N | -2.46305100 | 0.10273400  | 2.65368900  |
| N | -3.38212400 | -0.53264700 | 2.38625400  |
| H | -3.03729800 | -1.91317100 | 0.53400600  |
| C | -2.82135700 | 2.40509300  | -1.23253200 |
| H | -1.75497400 | 2.56647300  | -1.06328400 |
| H | -3.00302400 | 2.42830400  | -2.31557500 |
| H | -3.38523200 | 3.24743800  | -0.80765300 |

### **M3T'**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.23325900  | -2.51044500 | 2.32513200  |
| C | 0.34827900  | -1.54856900 | 2.05814000  |
| C | 1.58845100  | 0.21317900  | -0.07512700 |
| C | 2.96263600  | 0.11897100  | -0.39164800 |
| C | 3.51911600  | -0.69522000 | -1.40952000 |
| C | 4.01338700  | 0.83187200  | 0.25860500  |
| C | 5.34497300  | 0.47684100  | -0.35624800 |
| C | 5.01334500  | -0.55288400 | -1.47448000 |
| H | 2.00905900  | -2.37912000 | 3.07456800  |
| H | 1.22116400  | -3.46460400 | 1.80155700  |
| H | 6.03593400  | 0.06038300  | 0.39348500  |
| H | 5.52294200  | -1.51412600 | -1.30992300 |
| C | -0.78297400 | -1.70201700 | 1.07489100  |
| C | 0.52087800  | -0.52738300 | -0.82560600 |
| C | -0.85158500 | -0.66638400 | -0.09347400 |
| H | -1.72389600 | -1.66130600 | 1.63453300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.72454200 | -2.69867200 | 0.62015600  |
| H | 0.32307300  | -0.03797600 | -1.78826400 |
| H | 0.85620200  | -1.53882200 | -1.08048400 |
| H | 1.29117900  | 0.90776100  | 0.70457500  |
| H | 0.38085500  | -0.61077800 | 2.60663400  |
| H | 2.95259500  | -1.33789200 | -2.07347000 |
| H | 5.34867300  | -0.20668500 | -2.46348600 |
| H | 5.85269900  | 1.36818400  | -0.75760800 |
| C | -1.25094900 | 0.72863900  | 0.39905100  |
| C | -1.86426000 | -1.20358100 | -1.14783400 |
| O | -1.25614200 | 1.09329100  | 1.55840300  |
| O | -1.54448700 | 1.53098300  | -0.64358200 |
| O | -3.19266600 | -1.26798100 | -0.88039600 |
| O | -1.49801500 | -1.61476900 | -2.22280700 |
| C | -3.86305300 | -0.96280200 | 0.35781700  |
| H | -3.86231700 | -1.86614000 | 0.97880000  |
| H | -3.35619400 | -0.16929100 | 0.90962700  |
| C | -5.28434300 | -0.55470300 | 0.00735400  |
| H | -5.78193000 | -1.34705400 | -0.55967900 |
| H | -5.85631100 | -0.36809200 | 0.92303700  |
| H | -5.28683400 | 0.35669200  | -0.59843800 |
| C | -1.81517700 | 2.92796400  | -0.35760400 |
| H | -1.50718100 | 3.44889300  | -1.26688600 |
| H | -1.18180900 | 3.24179600  | 0.47522700  |
| C | -3.28664200 | 3.16037400  | -0.05352500 |
| H | -3.57728800 | 2.65696200  | 0.87309800  |
| H | -3.47226200 | 4.23349400  | 0.06978600  |
| H | -3.91602000 | 2.79611500  | -0.87201900 |
| C | 3.90610400  | 1.79928800  | 1.38930000  |
| H | 2.87504700  | 1.94486000  | 1.72582400  |
| H | 4.49201200  | 1.46650200  | 2.26059300  |
| H | 4.30695200  | 2.78787700  | 1.11446800  |

**M3S'**

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.63753200 | -2.42484200 | 1.91113500  |
| C | 0.71562200 | -1.47931900 | 1.71890800  |
| C | 1.52458800 | 0.49545100  | -0.54319400 |
| C | 2.86055500 | 0.18490000  | -0.45425900 |
| C | 3.52049000 | -1.05266400 | -0.80238100 |
| C | 3.89020000 | 1.07539000  | 0.02835600  |
| C | 5.24259600 | 0.42712200  | -0.00324200 |
| C | 4.99622300 | -0.99533000 | -0.56873100 |
| H | 2.49255300 | -2.26366900 | 2.56219200  |
| H | 1.57276000 | -3.39838500 | 1.42824900  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| H             | 5.69777200  | 0.39587600  | 0.99986400  |
| H             | 5.33200800  | -1.77748400 | 0.12960400  |
| C             | -0.52336700 | -1.68217000 | 0.88656700  |
| C             | 0.45627000  | -0.37586000 | -1.13300700 |
| C             | -0.80630100 | -0.62856400 | -0.22804300 |
| H             | -1.38195800 | -1.70762600 | 1.56691600  |
| H             | -0.47015800 | -2.66587800 | 0.40334300  |
| H             | 0.08095100  | 0.07101400  | -2.06112500 |
| H             | 0.84955500  | -1.35693300 | -1.41157200 |
| H             | 1.22479500  | 1.49882700  | -0.24714900 |
| H             | 0.80265200  | -0.52098100 | 2.22311800  |
| H             | 3.02028700  | -1.93054600 | -1.19352400 |
| H             | 5.56495200  | -1.16965300 | -1.49580000 |
| H             | 5.95133100  | 0.99885000  | -0.62378900 |
| C             | -1.23055800 | 0.71844700  | 0.36517500  |
| C             | -1.91366000 | -1.20544900 | -1.15940200 |
| O             | -1.18528800 | 1.02283100  | 1.54014100  |
| O             | -1.62970400 | 1.55887400  | -0.61312000 |
| O             | -3.19939000 | -1.33276100 | -0.74022900 |
| O             | -1.66254100 | -1.58241000 | -2.27921600 |
| C             | -3.71839900 | -1.14790000 | 0.59159700  |
| H             | -3.56849900 | -2.07882000 | 1.15089300  |
| H             | -3.20333100 | -0.34493600 | 1.12122800  |
| C             | -5.20006200 | -0.84006400 | 0.45149500  |
| H             | -5.70934900 | -1.64121200 | -0.09242100 |
| H             | -5.65744200 | -0.74456900 | 1.44255400  |
| H             | -5.35001400 | 0.09668000  | -0.09421000 |
| C             | -1.98424900 | 2.91143500  | -0.22893500 |
| H             | -1.75084100 | 3.50962100  | -1.11280100 |
| H             | -1.34302900 | 3.21907400  | 0.60027200  |
| C             | -3.45566600 | 3.01599700  | 0.14002900  |
| H             | -3.67190300 | 2.44044200  | 1.04486500  |
| H             | -3.71503500 | 4.06330500  | 0.33298600  |
| H             | -4.08800700 | 2.65035900  | -0.67553400 |
| C             | 3.65450300  | 2.46798300  | 0.50343400  |
| H             | 3.23536700  | 3.10152400  | -0.29415400 |
| H             | 2.92485000  | 2.49471700  | 1.32722300  |
| H             | 4.57719800  | 2.94075900  | 0.85514500  |
| <b>TS4S1'</b> |             |             |             |
| C             | -1.82557300 | -2.42302300 | -1.46814600 |
| C             | -0.82770300 | -1.52869700 | -1.46670200 |
| C             | -1.48214100 | 0.60157400  | 0.60207600  |
| C             | -2.78100900 | 0.21388200  | 0.39315800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.46827000 | -1.04066100 | 0.60975300  |
| C | -3.89949500 | 1.05727800  | 0.08513200  |
| C | -5.10764600 | 0.32738500  | -0.39344000 |
| C | -4.82270100 | -1.12869200 | -0.00118700 |
| H | -2.69720200 | -2.30396500 | -2.10634100 |
| H | -1.78297600 | -3.33266100 | -0.87187300 |
| H | -5.26787700 | 0.47654900  | -1.47613300 |
| H | -4.86822100 | -1.82712000 | -0.85400300 |
| C | 0.45053600  | -1.71516000 | -0.69529400 |
| C | -0.41341800 | -0.24167000 | 1.23688800  |
| C | 0.81834400  | -0.58849300 | 0.31516900  |
| H | 1.26449900  | -1.82345200 | -1.42134800 |
| H | 0.39493100  | -2.65564100 | -0.13266000 |
| H | -0.00450500 | 0.24884700  | 2.12628600  |
| H | -0.81250400 | -1.19980400 | 1.58552800  |
| H | -1.24545200 | 1.65299200  | 0.45238300  |
| H | -0.88209300 | -0.64548000 | -2.09535000 |
| H | -3.08089000 | -1.82619700 | 1.25137800  |
| H | -5.57640600 | -1.49064300 | 0.71367800  |
| H | -6.02220100 | 0.69917700  | 0.09032900  |
| C | 1.22930100  | 0.69511700  | -0.40808200 |
| C | 1.95886600  | -1.11129900 | 1.23396400  |
| O | 1.17596300  | 0.88717300  | -1.60665400 |
| O | 1.64277800  | 1.62570700  | 0.47998100  |
| O | 3.22876700  | -1.27867300 | 0.77281400  |
| O | 1.75575300  | -1.40437800 | 2.38827600  |
| C | 3.67533900  | -1.24240700 | -0.59642300 |
| H | 3.47922100  | -2.22208100 | -1.04863200 |
| H | 3.14513200  | -0.48632800 | -1.17730700 |
| C | 5.16764200  | -0.95556400 | -0.56871000 |
| H | 5.69326800  | -1.70808000 | 0.02685000  |
| H | 5.57105500  | -0.97126300 | -1.58739000 |
| H | 5.36353800  | 0.02840300  | -0.13110500 |
| C | 1.99951600  | 2.92851900  | -0.04146900 |
| H | 1.79691900  | 3.61311400  | 0.78571800  |
| H | 1.33931800  | 3.16359200  | -0.87964600 |
| C | 3.46179000  | 2.97977300  | -0.45733500 |
| H | 3.64696200  | 2.31537000  | -1.30630100 |
| H | 3.72688600  | 3.99990000  | -0.75851500 |
| H | 4.11202800  | 2.68653500  | 0.37333800  |
| C | -3.85062600 | 2.53667300  | 0.20185000  |
| H | -3.35818800 | 2.82549200  | 1.13993700  |
| H | -3.22043500 | 2.95129400  | -0.60237700 |
| H | -4.83740300 | 3.00560200  | 0.14100900  |

**TS4T1'**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.85484800  | -1.65388100 | 2.18556500  |
| C | 0.91075000  | -0.74966500 | 1.72275500  |
| C | 1.54169300  | 0.25461000  | -0.03894500 |
| C | 2.95103100  | 0.05728000  | -0.34029700 |
| C | 3.48210700  | -0.97688800 | -1.12582800 |
| C | 4.00060500  | 0.86285000  | 0.15628200  |
| C | 5.33227000  | 0.34402000  | -0.33236100 |
| C | 4.98141600  | -0.89546300 | -1.20327500 |
| H | 2.69826800  | -1.33001200 | 2.78786500  |
| H | 1.86523600  | -2.68685400 | 1.84587500  |
| H | 5.99374200  | 0.08177800  | 0.50804700  |
| H | 5.46077400  | -1.81115700 | -0.82662400 |
| C | -0.40818900 | -1.26562300 | 1.16405900  |
| C | 0.47586100  | -0.32192300 | -0.93431100 |
| C | -0.83715900 | -0.51828700 | -0.12632700 |
| H | -1.17715000 | -1.18450700 | 1.93747000  |
| H | -0.30136700 | -2.32943500 | 0.91837200  |
| H | 0.28483800  | 0.31053700  | -1.81029400 |
| H | 0.76616100  | -1.30154400 | -1.32032900 |
| H | 1.30798000  | 1.24721200  | 0.34266100  |
| H | 0.83179100  | 0.19118300  | 2.26189900  |
| H | 2.90615300  | -1.74491700 | -1.62911200 |
| H | 5.33276200  | -0.78218700 | -2.23960000 |
| H | 5.87649500  | 1.11069600  | -0.90550600 |
| C | -1.40383300 | 0.86985600  | 0.19078200  |
| C | -1.82616900 | -1.34738800 | -0.98197700 |
| O | -1.32658800 | 1.43046700  | 1.26615100  |
| O | -1.95537100 | 1.42286800  | -0.90831300 |
| O | -3.09145200 | -1.57842300 | -0.54915400 |
| O | -1.50484500 | -1.82092300 | -2.04581200 |
| C | -3.61401000 | -1.27401800 | 0.75832800  |
| H | -3.27329200 | -2.04360500 | 1.46040400  |
| H | -3.26044600 | -0.30409600 | 1.11644500  |
| C | -5.12893900 | -1.28347700 | 0.64255500  |
| H | -5.47998000 | -2.25119400 | 0.27205200  |
| H | -5.58033000 | -1.09989600 | 1.62377100  |
| H | -5.46813100 | -0.50601400 | -0.04904000 |
| C | -2.44672600 | 2.78381200  | -0.79487100 |
| H | -2.37255500 | 3.17734300  | -1.81108600 |
| H | -1.77676900 | 3.34227300  | -0.13693200 |
| C | -3.87937000 | 2.81809000  | -0.28678600 |
| H | -3.93574200 | 2.45161200  | 0.74226200  |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| H            | -4.25179600 | 3.84876800  | -0.30205000 |
| H            | -4.53136400 | 2.20839900  | -0.92073800 |
| C            | 3.91310800  | 2.06227200  | 1.04079300  |
| H            | 2.88211800  | 2.34264500  | 1.27783300  |
| H            | 4.43526600  | 1.89672000  | 1.99659200  |
| H            | 4.39762800  | 2.93726800  | 0.57993700  |
| <b>M4T1'</b> |             |             |             |
| C            | 1.67800300  | -2.44174400 | 0.67735700  |
| C            | 1.20534200  | -1.12515500 | 1.19552100  |
| C            | 1.56967400  | 0.09816600  | 0.27183700  |
| C            | 3.00344400  | 0.16984600  | -0.19681400 |
| C            | 3.47030600  | -0.23597900 | -1.44380600 |
| C            | 4.06340600  | 0.66016500  | 0.58403800  |
| C            | 5.35900400  | 0.57396000  | -0.18984500 |
| C            | 4.95692400  | -0.03148500 | -1.56485100 |
| H            | 2.72918100  | -2.70553600 | 0.73068000  |
| H            | 1.02936900  | -3.08253100 | 0.08712000  |
| H            | 6.10031400  | -0.04902400 | 0.33392100  |
| H            | 5.48395600  | -0.97503500 | -1.76872200 |
| C            | -0.33911300 | -1.02795900 | 1.26708400  |
| C            | 0.50180500  | -0.00210700 | -0.82456900 |
| C            | -0.81923500 | -0.35016800 | -0.06267700 |
| H            | -0.64279000 | -0.39973000 | 2.10832900  |
| H            | -0.78652200 | -2.01630000 | 1.40871500  |
| H            | 0.40794500  | 0.90652500  | -1.42623700 |
| H            | 0.71155700  | -0.82419300 | -1.51196700 |
| H            | 1.35786400  | 0.99611100  | 0.86882500  |
| H            | 1.64612900  | -0.95681400 | 2.18831800  |
| H            | 2.86230800  | -0.64591100 | -2.24196600 |
| H            | 5.21206800  | 0.63799900  | -2.39922700 |
| H            | 5.82899000  | 1.56388700  | -0.29540800 |
| C            | -1.52117700 | 0.98676700  | 0.20822400  |
| C            | -1.70078000 | -1.28702500 | -0.91743800 |
| O            | -1.42189600 | 1.63531700  | 1.23017500  |
| O            | -2.20396800 | 1.39626200  | -0.87973800 |
| O            | -2.92268400 | -1.66146200 | -0.45913200 |
| O            | -1.34307900 | -1.72932600 | -1.98316200 |
| C            | -3.46210500 | -1.37308200 | 0.84423300  |
| H            | -3.10266800 | -2.13556100 | 1.54502600  |
| H            | -3.13411700 | -0.39804900 | 1.21270600  |
| C            | -4.97605000 | -1.42131000 | 0.72436200  |
| H            | -5.30017700 | -2.39497700 | 0.34490800  |
| H            | -5.43526200 | -1.25808200 | 1.70560400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.33359400 | -0.64770100 | 0.03779700  |
| C | -2.80605000 | 2.71596600  | -0.82926300 |
| H | -2.84566800 | 3.02861000  | -1.87513500 |
| H | -2.14055100 | 3.38105400  | -0.27402400 |
| C | -4.19252400 | 2.67380900  | -0.20689200 |
| H | -4.13673300 | 2.38033900  | 0.84524100  |
| H | -4.65136300 | 3.66777900  | -0.25996900 |
| H | -4.83834000 | 1.96990800  | -0.74194900 |
| C | 4.01767000  | 1.20877600  | 1.97244500  |
| H | 2.99861100  | 1.27668300  | 2.36647300  |
| H | 4.60098700  | 0.58988600  | 2.67283500  |
| H | 4.46026700  | 2.21568600  | 2.01928200  |

**TS5T1'**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.25571500 | -1.57785500 | -1.46195600 |
| C | -1.11748700 | -0.60409900 | -1.25733400 |
| C | -1.47912400 | 0.42805600  | -0.08387600 |
| C | -2.90107600 | 0.14942900  | 0.29607400  |
| C | -3.30755400 | -1.17983200 | 0.35194700  |
| C | -4.08028700 | 1.01436800  | -0.03013000 |
| C | -5.26294100 | 0.10486300  | -0.27103100 |
| C | -4.81895600 | -1.29014000 | 0.26230300  |
| H | -2.99919700 | -1.32183700 | -2.21409900 |
| H | -2.04364500 | -2.64498900 | -1.40711800 |
| H | -5.51006500 | 0.03682600  | -1.34370100 |
| H | -5.13965500 | -2.11526800 | -0.38409500 |
| C | 0.22056200  | -1.25999300 | -0.83546800 |
| C | -0.42300800 | 0.16243700  | 1.00881300  |
| C | 0.84029100  | -0.34431000 | 0.25544400  |
| H | 0.88405100  | -1.40293000 | -1.69046900 |
| H | 0.03348200  | -2.24430800 | -0.38700700 |
| H | -0.20921700 | 1.03341800  | 1.63381100  |
| H | -0.74713700 | -0.63774200 | 1.67964800  |
| H | -1.37363900 | 1.45311000  | -0.45625900 |
| H | -0.95112600 | -0.02521800 | -2.17149200 |
| H | -2.74060100 | -1.97029200 | 0.84028600  |
| H | -5.25094900 | -1.48667600 | 1.25441100  |
| H | -6.17404800 | 0.47010600  | 0.22240000  |
| C | 1.53639000  | 0.86947600  | -0.36810900 |
| C | 1.77467300  | -1.08749700 | 1.23615300  |
| O | 1.46861900  | 1.19303100  | -1.53711200 |
| O | 2.19740000  | 1.57517600  | 0.57218200  |
| O | 2.97123300  | -1.56818800 | 0.81024600  |
| O | 1.47749800  | -1.26875200 | 2.39284100  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| C             | 3.40241300  | -1.64487800 | -0.56210700 |
| H             | 2.88380200  | -2.47876500 | -1.04884700 |
| H             | 3.16322500  | -0.72867900 | -1.10776800 |
| C             | 4.90293100  | -1.88158700 | -0.54102400 |
| H             | 5.14083100  | -2.79352900 | 0.01475400  |
| H             | 5.27966100  | -1.98726600 | -1.56432400 |
| H             | 5.41906500  | -1.04276900 | -0.06373000 |
| C             | 2.83583100  | 2.80857500  | 0.15293500  |
| H             | 2.84981900  | 3.42068400  | 1.05760300  |
| H             | 2.20819100  | 3.28716700  | -0.60245900 |
| C             | 4.24099400  | 2.55723000  | -0.37097800 |
| H             | 4.21281200  | 1.97262800  | -1.29513600 |
| H             | 4.73073900  | 3.51344600  | -0.58807500 |
| H             | 4.84317400  | 2.02413300  | 0.37189600  |
| C             | -4.21775400 | 2.41392200  | 0.46913400  |
| H             | -4.43661000 | 2.45061200  | 1.55498900  |
| H             | -3.29800100 | 2.99380200  | 0.32060800  |
| H             | -5.03406200 | 2.94520700  | -0.03582600 |
| <b>TS5T2'</b> |             |             |             |
| C             | 2.49494800  | -0.36220500 | 1.71418100  |
| C             | 1.22301700  | 0.23990200  | 1.16650700  |
| C             | 1.46247100  | 0.74002000  | -0.33789200 |
| C             | 2.88928400  | 0.38875900  | -0.65926700 |
| C             | 3.33135300  | -0.73908500 | -1.53070300 |
| C             | 3.84357800  | 0.58286600  | 0.35122000  |
| C             | 5.06250100  | -0.29469500 | 0.08636200  |
| C             | 4.56113500  | -1.36296900 | -0.92587400 |
| H             | 2.84464500  | -0.04254100 | 2.69405200  |
| H             | 2.66387400  | -1.42097600 | 1.51931000  |
| H             | 5.46740400  | -0.72549600 | 1.00987900  |
| H             | 4.32734800  | -2.30187400 | -0.39683500 |
| C             | 0.01120600  | -0.72086900 | 1.07757500  |
| C             | 0.38719400  | 0.03815800  | -1.18719000 |
| C             | -0.76729400 | -0.31420300 | -0.20363400 |
| H             | -0.60131300 | -0.67942000 | 1.98029800  |
| H             | 0.35702900  | -1.75464600 | 0.95034300  |
| H             | 0.03386200  | 0.62778800  | -2.03711400 |
| H             | 0.76776300  | -0.90485100 | -1.58852600 |
| H             | 1.30574500  | 1.82614000  | -0.36193300 |
| H             | 0.92896700  | 1.09961300  | 1.77368300  |
| H             | 3.15905000  | -0.73916000 | -2.60514300 |
| H             | 5.31595800  | -1.62136600 | -1.67819400 |
| H             | 5.86989000  | 0.30801100  | -0.35680600 |



|            |             |             |             |
|------------|-------------|-------------|-------------|
| C          | -1.60313500 | 0.94956800  | 0.02748400  |
| C          | -1.63176400 | -1.44943000 | -0.79930900 |
| O          | -1.55638900 | 1.65548500  | 1.01526700  |
| O          | -2.37314600 | 1.21185000  | -1.04816900 |
| O          | -2.73349500 | -1.89057500 | -0.13898700 |
| O          | -1.36312000 | -1.97588600 | -1.85257400 |
| C          | -3.09538800 | -1.55156900 | 1.21338200  |
| H          | -2.44799300 | -2.10698400 | 1.90147600  |
| H          | -2.96432400 | -0.48399600 | 1.40710700  |
| C          | -4.54847500 | -1.95620500 | 1.39590200  |
| H          | -4.67938500 | -3.02284200 | 1.19042800  |
| H          | -4.86624400 | -1.75646600 | 2.42519300  |
| H          | -5.19456500 | -1.39266300 | 0.71555600  |
| C          | -3.16182100 | 2.42876300  | -1.02263500 |
| H          | -3.27546300 | 2.69343100  | -2.07635700 |
| H          | -2.58943300 | 3.20577400  | -0.51053000 |
| C          | -4.51035700 | 2.20317400  | -0.35698400 |
| H          | -4.38633500 | 1.97335700  | 0.70530600  |
| H          | -5.11983300 | 3.11034600  | -0.44008000 |
| H          | -5.04929600 | 1.38181500  | -0.84026800 |
| C          | 4.04978800  | 1.86434100  | 1.13059200  |
| H          | 4.53156700  | 1.67842100  | 2.09750700  |
| H          | 4.70869900  | 2.53840700  | 0.56425500  |
| H          | 3.11212800  | 2.39726000  | 1.31479700  |
| <b>P1'</b> |             |             |             |
| C          | -2.33692200 | -1.44887100 | -1.54532000 |
| C          | -1.08306300 | -0.54814000 | -1.35278800 |
| C          | -1.49195900 | 0.58874900  | -0.33573200 |
| C          | -2.90663300 | 0.23894300  | 0.03625600  |
| C          | -3.18932400 | -1.21406700 | -0.28054600 |
| C          | -3.99607900 | 0.91045100  | 0.42943900  |
| C          | -5.19263100 | -0.03181400 | 0.48366400  |
| C          | -4.73201800 | -1.26221900 | -0.34818200 |
| H          | -2.89948100 | -1.11153500 | -2.42531000 |
| H          | -2.07069200 | -2.49945600 | -1.71347700 |
| H          | -6.10532200 | 0.42979700  | 0.08211000  |
| H          | -5.05290200 | -1.13515000 | -1.39000200 |
| C          | 0.13413400  | -1.26043400 | -0.71583700 |
| C          | -0.47639400 | 0.48663100  | 0.83161200  |
| C          | 0.77720900  | -0.22646600 | 0.24531000  |
| H          | 0.82666300  | -1.62707900 | -1.47596400 |
| H          | -0.19576400 | -2.12061600 | -0.11827200 |
| H          | -0.23094600 | 1.45152900  | 1.28212200  |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| H          | -0.86410500 | -0.14662600 | 1.63350300  |
| H          | -1.42767200 | 1.57791500  | -0.80301700 |
| H          | -0.76749500 | -0.11230400 | -2.30340400 |
| H          | -2.82065900 | -1.86465100 | 0.53083000  |
| H          | -5.15857400 | -2.20420800 | 0.01224100  |
| H          | -5.42582200 | -0.31198600 | 1.52335900  |
| C          | 1.60636700  | 0.81001500  | -0.52174800 |
| C          | 1.60297400  | -0.86258900 | 1.38725900  |
| O          | 1.65929000  | 0.91454500  | -1.73083300 |
| O          | 2.24301600  | 1.63532400  | 0.33409800  |
| O          | 2.77447000  | -1.49296600 | 1.11578200  |
| O          | 1.24253700  | -0.82250300 | 2.53941600  |
| C          | 3.25398800  | -1.84789200 | -0.19632000 |
| H          | 2.69190700  | -2.71882200 | -0.55256900 |
| H          | 3.10867000  | -1.03240300 | -0.90887700 |
| C          | 4.72928000  | -2.18087500 | -0.05218500 |
| H          | 4.87245200  | -2.99090200 | 0.66923300  |
| H          | 5.13742900  | -2.49688200 | -1.01854100 |
| H          | 5.29034700  | -1.30749000 | 0.29462900  |
| C          | 3.02049500  | 2.71816600  | -0.23754100 |
| H          | 3.00275500  | 3.49358900  | 0.53168700  |
| H          | 2.51042700  | 3.07996900  | -1.13328700 |
| C          | 4.44128600  | 2.27372000  | -0.54770700 |
| H          | 4.44796100  | 1.51814400  | -1.33877900 |
| H          | 5.03089400  | 3.13147000  | -0.89102800 |
| H          | 4.92232800  | 1.86060300  | 0.34476300  |
| C          | -4.11315700 | 2.36013500  | 0.79080800  |
| H          | -4.39367100 | 2.48687900  | 1.84621000  |
| H          | -3.17280800 | 2.89846100  | 0.63181400  |
| H          | -4.89574900 | 2.85589600  | 0.19968000  |
| <b>P2'</b> |             |             |             |
| C          | -2.53251400 | -0.94701700 | -1.38471700 |
| C          | -1.21608900 | -0.14596700 | -1.17219600 |
| C          | -1.43498500 | 0.72941900  | 0.12128100  |
| C          | -2.87687100 | 0.48815000  | 0.47634500  |
| C          | -3.60634200 | 0.48636900  | 1.59411200  |
| C          | -3.63353500 | -0.08524000 | -0.71569100 |
| C          | -4.82502600 | -0.80391200 | -0.02928000 |
| C          | -4.99050600 | -0.08360400 | 1.34158500  |
| H          | -2.72637700 | -1.15727900 | -2.44359500 |
| H          | -2.46664000 | -1.91339900 | -0.86717400 |
| H          | -4.56758600 | -1.85519800 | 0.14875800  |
| H          | -5.31275500 | -0.77109200 | 2.13394700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.05915300  | -0.98352900 | -0.91112000 |
| C | -0.38229200 | 0.24400600  | 1.13602600  |
| C | 0.79765900  | -0.28751100 | 0.26831400  |
| H | 0.68326200  | -1.06369100 | -1.80291700 |
| H | -0.20895900 | -1.99974000 | -0.59588100 |
| H | -0.05781800 | 1.01034200  | 1.84459400  |
| H | -0.76613400 | -0.59479500 | 1.72202000  |
| H | -1.25837500 | 1.78636300  | -0.11765100 |
| H | -1.03571900 | 0.50973900  | -2.02790900 |
| H | -3.27859900 | 0.82667400  | 2.57328700  |
| H | -5.75283000 | 0.70972600  | 1.29762400  |
| H | -5.74144400 | -0.78884500 | -0.62996100 |
| C | 1.60152100  | 0.92201600  | -0.22279500 |
| C | 1.67713000  | -1.24158100 | 1.10782300  |
| O | 1.52958300  | 1.40577700  | -1.33474600 |
| O | 2.36719300  | 1.42130300  | 0.76853600  |
| O | 2.79369600  | -1.79556400 | 0.56921300  |
| O | 1.40488700  | -1.52650800 | 2.24949100  |
| C | 3.17598100  | -1.73292300 | -0.81831000 |
| H | 2.55361500  | -2.43222600 | -1.38821000 |
| H | 3.02688500  | -0.73084400 | -1.22819000 |
| C | 4.64048800  | -2.13043300 | -0.89159300 |
| H | 4.78975300  | -3.12884200 | -0.46970000 |
| H | 4.97449900  | -2.13804400 | -1.93495600 |
| H | 5.26074800  | -1.42370400 | -0.33155900 |
| C | 3.12887300  | 2.62234200  | 0.48076900  |
| H | 3.24221500  | 3.10460900  | 1.45429800  |
| H | 2.53664800  | 3.26221000  | -0.17751600 |
| C | 4.47753000  | 2.28759200  | -0.13643200 |
| H | 4.35012600  | 1.83044700  | -1.12199600 |
| H | 5.06591000  | 3.20407500  | -0.25942700 |
| H | 5.03955200  | 1.60215300  | 0.50619500  |
| C | -4.12111600 | 1.02604800  | -1.67037200 |
| H | -4.63706500 | 0.59216100  | -2.53619400 |
| H | -4.81991700 | 1.70046900  | -1.16217000 |
| H | -3.29021600 | 1.63331000  | -2.04817500 |