

Electronic Supplementary Information

**Mechanistic insight into the self-coupling of 5-hydroxymethyl furfural to C₁₂ fuel
intermediate catalyzed by ionic liquids**

Jingjing Li,^{*a} Binfen Wang,^a Yefan Dou^a and Yiying Yang^b

^aCollege of Arts and Sciences, Shanxi Agricultural University, Taigu Shanxi, 030801,
P. R. China

^bKey Lab of Colloid and Interface Chemistry, Ministry of Education, Institute of
Theoretical Chemistry, Shandong University, Jinan, 250100, P. R. China

E-mail: jjljsxau@qq.com

Contents

| | |
|---|----|
| 1. Additional Computational Results..... | S3 |
| 2. Cartesian Coordinates of All the Structures..... | S6 |

1. Additional Computational Results

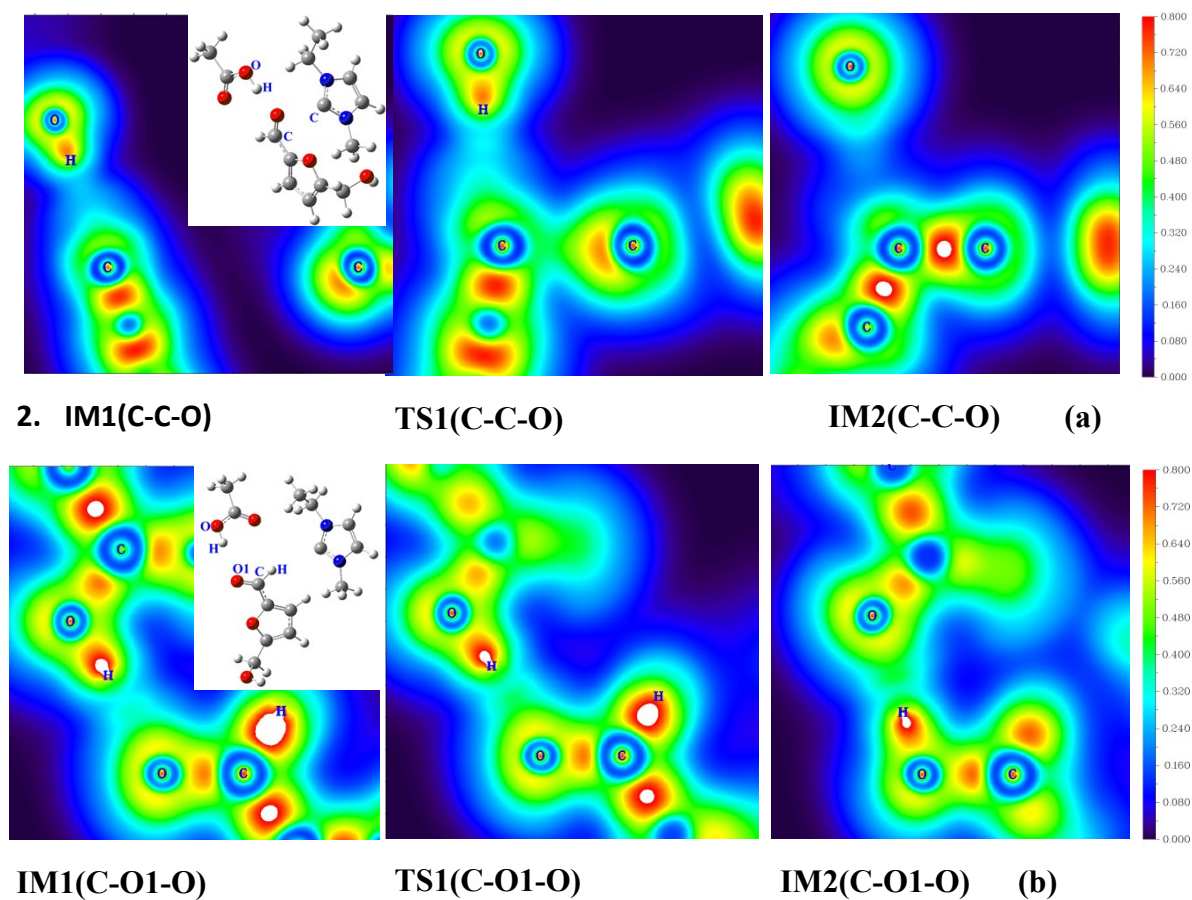


Fig. S1 Localized orbital locator (LOL) profiles of **IM1**, **TS1** and **IM2** along (a) the C-C-O plane and (b) C-O1-O plane.

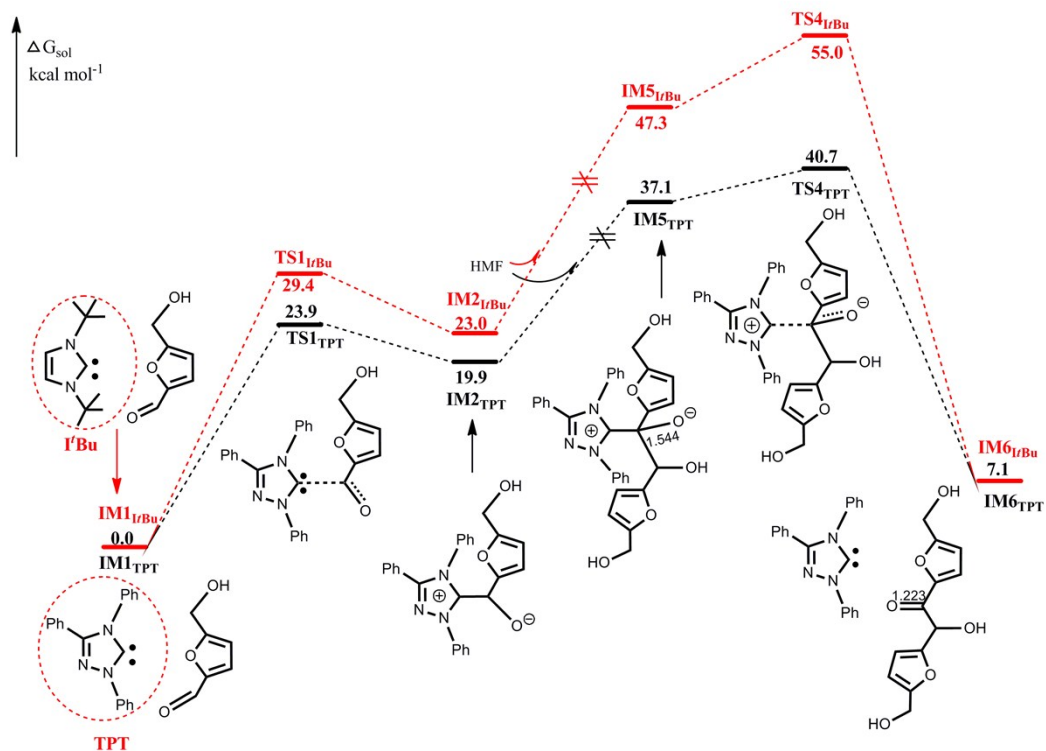


Fig. S2 Calculated free energy profiles with schematic structures for the first nucleophilic attack and last rate-determining step catalyzed by TPT (black line) and tBu (red line). The symbol \times denotes the pathway for the conversion from IM2_{TPT} (IM2_{tBu}) to IM5_{TPT} (IM5_{tBu}) has been omitted.

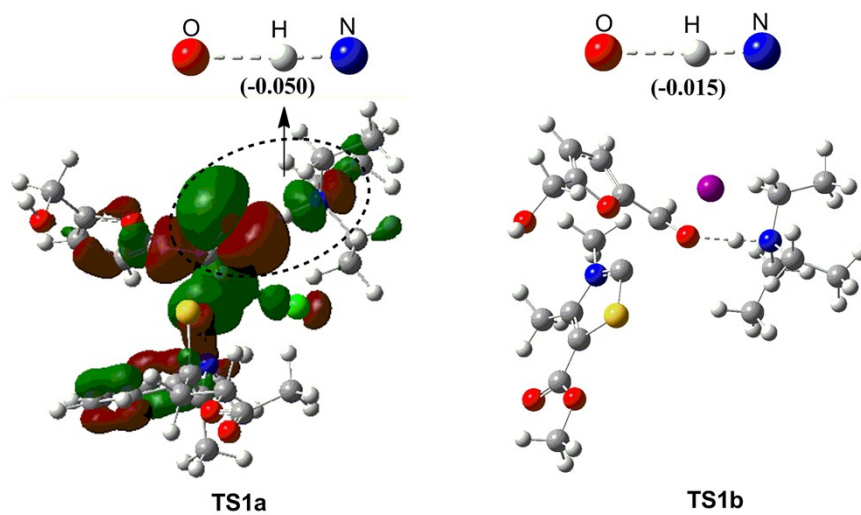


Fig. S3 Molecular orbital involving in 3c-4e bonding in **TS1a** and M-CBO (in brackets) of **TS1a** and **TS1b** (the molecular orbital of such a 3c-4e bond is absent in **TS1b**).

2. Cartesian Coordinates of All the Structures

IM1

| | | | |
|---|--------------|--------------|--------------|
| O | 1. 67768600 | 3. 76711700 | -1. 34525100 |
| H | 2. 33686800 | 3. 42238200 | -0. 72737900 |
| C | -0. 08743900 | 3. 48975400 | 0. 31105300 |
| C | -0. 10837200 | 3. 35275700 | 1. 67681500 |
| H | 0. 44036300 | 3. 95737800 | 2. 38198000 |
| C | -0. 98010200 | 2. 27336600 | 1. 95771500 |
| C | -2. 34525000 | 0. 74851300 | 0. 44161900 |
| H | -2. 72894300 | 0. 21555400 | 1. 32435000 |
| C | -1. 43802300 | 1. 81621600 | 0. 74277400 |
| O | -0. 89205700 | 2. 56433500 | -0. 26698100 |
| O | -2. 69769900 | 0. 42119300 | -0. 69281100 |
| C | 0. 65202300 | 4. 42067700 | -0. 58880000 |
| H | 1. 06303300 | 5. 23303100 | 0. 01826600 |
| H | -1. 24552900 | 1. 86998800 | 2. 92331700 |
| H | -0. 03125800 | 4. 85143800 | -1. 32347700 |
| C | 3. 78481600 | -2. 66186700 | -0. 90104900 |
| C | 4. 45490000 | -2. 86012100 | 0. 26114500 |
| C | 2. 90270500 | -1. 22483200 | 0. 64296000 |
| N | 2. 84895600 | -1. 66766500 | -0. 64617200 |
| H | 3. 88837500 | -3. 13854900 | -1. 86217600 |
| H | 5. 25222000 | -3. 54193100 | 0. 50889400 |
| N | 3. 90338600 | -1. 97848800 | 1. 18148900 |
| C | 1. 92351800 | -1. 14443600 | -1. 65718500 |
| C | 2. 60776400 | -0. 25073400 | -2. 68775200 |
| H | 1. 15545000 | -0. 58968300 | -1. 11860000 |
| H | 1. 44082700 | -1. 99390300 | -2. 14775000 |
| H | 3. 07575600 | 0. 61295200 | -2. 20784100 |
| H | 1. 86755600 | 0. 11761200 | -3. 40363500 |
| C | 4. 34943700 | -1. 88003200 | 2. 56615700 |
| H | 3. 72111900 | -1. 15458600 | 3. 07917800 |
| H | 4. 25955600 | -2. 84777900 | 3. 06481800 |
| H | 5. 39012500 | -1. 55045100 | 2. 61090400 |
| H | 3. 37539900 | -0. 79425800 | -3. 24561300 |
| H | -3. 79931100 | -0. 85609500 | -0. 87401200 |
| C | -5. 89415300 | -3. 22899100 | -0. 18674600 |
| H | -5. 38515800 | -4. 04179100 | -0. 71192500 |
| H | -6. 71160000 | -2. 88724300 | -0. 82682100 |
| H | -6. 29222100 | -3. 59530800 | 0. 75769300 |
| C | -4. 92900300 | -2. 10339300 | 0. 05797400 |
| O | -4. 43741300 | -1. 59475800 | -1. 07649200 |
| O | -4. 61251100 | -1. 68875600 | 1. 15809900 |

TS1

| | | | |
|---|-------------|-------------|-------------|
| O | -4.92055800 | -0.08802800 | -1.04147700 |
| H | -5.11918200 | 0.43312900 | -0.25204800 |
| C | -3.33681400 | -1.44031200 | 0.24508900 |
| C | -3.15325400 | -1.67373600 | 1.57864800 |
| H | -3.92753700 | -1.91332200 | 2.29172300 |
| C | -1.75273800 | -1.54822400 | 1.82586500 |
| C | 0.23123800 | -1.05583500 | 0.24729600 |
| H | 0.91804700 | -1.13416100 | 1.09515800 |
| C | -1.17515800 | -1.24336000 | 0.62452300 |
| O | -2.13108500 | -1.18411800 | -0.34684900 |
| O | 0.63036000 | -1.29346600 | -0.91754400 |
| C | -4.54783200 | -1.41068500 | -0.61837600 |
| H | -5.36912500 | -1.89133800 | -0.07723000 |
| H | -1.23730300 | -1.67241600 | 2.76598800 |
| H | -4.37194300 | -1.97072900 | -1.53914600 |
| C | 0.90546700 | 3.34620000 | -0.12052200 |
| C | 1.20262000 | 3.23081100 | 1.19721900 |
| C | 0.40170600 | 1.22443400 | 0.50293300 |
| N | 0.41930900 | 2.10950900 | -0.52475100 |
| H | 0.99996000 | 4.18246900 | -0.79359500 |
| H | 1.60758500 | 3.94385600 | 1.89656400 |
| N | 0.88813500 | 1.92702300 | 1.55732100 |
| C | -0.04599200 | 1.81588100 | -1.88859100 |
| C | -1.38697100 | 2.47185600 | -2.20298800 |
| H | -0.11099900 | 0.73253300 | -1.97042300 |
| H | 0.72341900 | 2.16137800 | -2.58353500 |
| H | -2.16316600 | 2.12343500 | -1.51706600 |
| H | -1.69135300 | 2.21226200 | -3.22080500 |
| C | 1.05257200 | 1.40266800 | 2.90975600 |
| H | 0.83589200 | 0.33737000 | 2.90414800 |
| H | 2.07864400 | 1.55695800 | 3.24798400 |
| H | 0.36718200 | 1.90479400 | 3.59583500 |
| H | -1.32682800 | 3.56168500 | -2.13645900 |
| H | 2.18127800 | -1.38722700 | -1.17943000 |
| C | 5.40816500 | -1.79681000 | -0.87195500 |
| H | 5.72256000 | -0.90916300 | -1.42716900 |
| H | 5.51484500 | -2.65532700 | -1.54066600 |
| H | 6.04622600 | -1.93115900 | -0.00015900 |
| C | 3.96907700 | -1.65624900 | -0.45174300 |
| O | 3.15105600 | -1.46165400 | -1.48127400 |
| O | 3.58737300 | -1.71530700 | 0.70582100 |

IM2

| | | | |
|---|-------------|-------------|-------------|
| O | -4.94811800 | -0.27495900 | 0.34423900 |
| H | -4.99248000 | -0.57162300 | 1.26309800 |
| C | -2.96821000 | -1.66370400 | -0.02746200 |
| C | -2.42775300 | -2.70536100 | 0.66640600 |
| H | -2.96770500 | -3.55705600 | 1.05169400 |
| C | -1.02398600 | -2.44530100 | 0.77485900 |
| C | 0.45753000 | -0.49661100 | -0.12713200 |
| C | -0.80071600 | -1.26306300 | 0.13650000 |
| O | -1.97853000 | -0.77170400 | -0.35610000 |
| O | 0.83220900 | -0.55459400 | -1.48733200 |
| C | -4.35964000 | -1.33260300 | -0.43399700 |
| H | -4.96337000 | -2.24328200 | -0.36804900 |
| H | -0.27534000 | -3.05863100 | 1.25263500 |
| H | -4.38397100 | -0.98072900 | -1.46713800 |
| C | 0.01500100 | 3.13048600 | 0.49906300 |
| C | 0.60913000 | 2.73070400 | 1.65179300 |
| C | 0.36064700 | 0.94158200 | 0.35641300 |
| N | -0.13887400 | 2.00921100 | -0.29419200 |
| H | -0.30523200 | 4.10514000 | 0.17351600 |
| H | 0.90686100 | 3.28536700 | 2.52509100 |
| N | 0.82057600 | 1.37100100 | 1.54740400 |
| C | -0.74923300 | 2.04426200 | -1.64472300 |
| C | -2.18885000 | 2.54033900 | -1.60994800 |
| H | -0.67804500 | 1.04107900 | -2.05151800 |
| H | -0.12272400 | 2.69825600 | -2.25485100 |
| H | -2.81525100 | 1.89193600 | -0.99433300 |
| H | -2.58505700 | 2.53333500 | -2.62867500 |
| C | 1.44425700 | 0.54191500 | 2.58749800 |
| H | 2.24876800 | -0.04978500 | 2.14921400 |
| H | 1.85110100 | 1.21015700 | 3.34374200 |
| H | 0.69763700 | -0.10991200 | 3.04214400 |
| H | -2.25964000 | 3.56276500 | -1.23100700 |
| H | 1.84520500 | -0.62273500 | -1.51818500 |
| C | 5.57816100 | -1.07106700 | -0.63574900 |
| H | 5.96602700 | -0.08331600 | -0.90437000 |
| H | 5.85347100 | -1.75500600 | -1.44353800 |
| H | 6.04827500 | -1.39770700 | 0.29273500 |
| C | 4.05719600 | -1.00296500 | -0.50373000 |
| O | 3.42191500 | -0.71420300 | -1.56932900 |
| O | 3.53485300 | -1.22050700 | 0.61549000 |
| H | 1.23971500 | -0.96368800 | 0.48080800 |

TS2

| | | | |
|---|------------|-------------|-------------|
| O | 4.89579100 | -0.98526000 | -1.17378200 |
|---|------------|-------------|-------------|

| | | | |
|---|-------------|-------------|-------------|
| H | 4.73447200 | -1.88186200 | -1.49633200 |
| C | 3.00366400 | -1.25721900 | 0.36236300 |
| C | 2.35844000 | -2.36477400 | 0.82672600 |
| H | 2.83029800 | -3.25436100 | 1.21765100 |
| C | 0.95609900 | -2.12227400 | 0.66960000 |
| C | -0.30028100 | -0.00414300 | -0.24382400 |
| C | 0.82389300 | -0.86651300 | 0.13220700 |
| O | 2.07933700 | -0.33210400 | -0.05161600 |
| O | -0.28320300 | 0.34056300 | -1.63247900 |
| C | 4.44008300 | -0.92025900 | 0.19254500 |
| H | 5.03022200 | -1.59141700 | 0.82563000 |
| H | 0.14883800 | -2.79853400 | 0.90532700 |
| H | 4.63671500 | 0.10656100 | 0.50829900 |
| C | -3.80303600 | -0.81788300 | 0.45561600 |
| C | -3.27995000 | -0.80810000 | 1.70034900 |
| C | -1.60494900 | -0.38792700 | 0.25354500 |
| N | -2.76987000 | -0.56169400 | -0.43845200 |
| H | -4.81178200 | -0.97788100 | 0.11491900 |
| H | -3.73977700 | -0.95221800 | 2.66301600 |
| N | -1.92647600 | -0.53230900 | 1.57575600 |
| C | -2.96717800 | -0.64537000 | -1.89870400 |
| C | -2.51524000 | -1.98091900 | -2.47877500 |
| H | -2.42868600 | 0.17493400 | -2.36289300 |
| H | -4.03634800 | -0.49780400 | -2.05896500 |
| H | -1.44194200 | -2.12571800 | -2.34023900 |
| H | -2.72312700 | -1.99636800 | -3.55256700 |
| C | -1.03077000 | -0.34572000 | 2.71127800 |
| H | -0.35797400 | 0.48909900 | 2.51745100 |
| H | -1.63655600 | -0.11872800 | 3.58747000 |
| H | -0.43917900 | -1.24299300 | 2.89877900 |
| H | -3.04719100 | -2.81702700 | -2.01604800 |
| H | -0.13069600 | 1.30597400 | -1.68229600 |
| C | 0.60592300 | 4.71503100 | 0.35596400 |
| H | -0.08124400 | 4.99706600 | 1.15687900 |
| H | 0.54520600 | 5.43399700 | -0.45982400 |
| H | 1.61764500 | 4.72717200 | 0.77226800 |
| C | 0.29366600 | 3.32616200 | -0.13620400 |
| O | 0.15731800 | 3.06565100 | -1.33357000 |
| O | 0.19320100 | 2.42963900 | 0.81648800 |
| H | -0.01620800 | 1.40966200 | 0.42390300 |

IM3

| | | | |
|---|-------------|-------------|------------|
| O | -4.99869400 | -0.59885100 | 1.26461700 |
| H | -4.91247800 | -1.51323500 | 1.56554100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -3.16184200 | -1.02196400 | -0.30621600 |
| C | -2.64252100 | -2.18502200 | -0.79281100 |
| H | -3.21113000 | -3.01482800 | -1.18687800 |
| C | -1.22212200 | -2.09972600 | -0.64629400 |
| C | 0.26268100 | -0.15864600 | 0.27961600 |
| C | -0.94610400 | -0.86895500 | -0.09663400 |
| O | -2.13891100 | -0.20650400 | 0.11118600 |
| O | 0.26281900 | 0.29487400 | 1.62888900 |
| C | -4.55336600 | -0.54521500 | -0.10677200 |
| H | -5.21559700 | -1.13862700 | -0.74641600 |
| H | -0.49882800 | -2.86234600 | -0.88956700 |
| H | -4.65200600 | 0.50374200 | -0.39428900 |
| C | 3.72395400 | -1.00808900 | -0.48820000 |
| C | 3.16065200 | -1.09737400 | -1.70978200 |
| C | 1.52247500 | -0.56655400 | -0.24245100 |
| N | 2.72097300 | -0.68519800 | 0.42244500 |
| H | 4.74452700 | -1.14237300 | -0.17235300 |
| H | 3.59099700 | -1.31388700 | -2.67255800 |
| N | 1.80529300 | -0.82100200 | -1.56709400 |
| C | 2.95981400 | -0.69391400 | 1.87551100 |
| C | 2.49760300 | -1.98094300 | 2.55133400 |
| H | 2.45987700 | 0.16462600 | 2.31476100 |
| H | 4.03656300 | -0.56438300 | 1.99717200 |
| H | 1.41621000 | -2.10380800 | 2.46441500 |
| H | 2.74799500 | -1.94096100 | 3.61562500 |
| C | 0.89718700 | -0.65874200 | -2.69174400 |
| H | 0.28063900 | 0.23007800 | -2.54733600 |
| H | 1.49242800 | -0.53420600 | -3.59558100 |
| H | 0.23950800 | -1.52216600 | -2.80653800 |
| H | 2.98882700 | -2.85688800 | 2.11815400 |
| H | 0.26771300 | 1.26988600 | 1.61669700 |
| C | -0.00879600 | 4.78979000 | -0.44664400 |
| H | 0.70437600 | 4.96314500 | -1.25611700 |
| H | 0.17675700 | 5.48520100 | 0.36975700 |
| H | -1.01123700 | 4.95698200 | -0.85047800 |
| C | 0.10184100 | 3.37536100 | 0.04086200 |
| O | 0.29628000 | 3.07003000 | 1.21000000 |
| O | -0.03851000 | 2.47402700 | -0.92611200 |
| H | 0.05840600 | 1.52880500 | -0.55876900 |

IM4

| | | | |
|---|-------------|-------------|-------------|
| O | -5.56689100 | -2.38758900 | -0.98191200 |
| H | -6.13128400 | -1.69787100 | -0.60799500 |
| C | -3.82941900 | -1.64131500 | 0.58580200 |

| | | | |
|---|-------------|-------------|-------------|
| C | -3.90167600 | -0.94152700 | 1.75490100 |
| H | -4.58324300 | -1.14412000 | 2.56858200 |
| C | -2.94523300 | 0.11557300 | 1.67461200 |
| C | -1.28582300 | 0.72506000 | -0.23547900 |
| C | -2.30976900 | -0.00760900 | 0.45253400 |
| O | -2.85594000 | -1.08555400 | -0.21465400 |
| O | -1.45204900 | 0.86494200 | -1.62195900 |
| C | -4.61394300 | -2.77199000 | 0.03484000 |
| H | -5.12523900 | -3.27321300 | 0.86403000 |
| H | -2.77519300 | 0.89323000 | 2.40207200 |
| H | -3.96499100 | -3.50143100 | -0.45539300 |
| C | 1.16780300 | 3.17738000 | 0.81526700 |
| C | 1.15723000 | 2.36204300 | 1.88792400 |
| C | -0.33670500 | 1.53710500 | 0.39331000 |
| N | 0.25897500 | 2.68055000 | -0.11728600 |
| H | 1.73685400 | 4.07046700 | 0.61893700 |
| H | 1.73102100 | 2.38825100 | 2.79858100 |
| N | 0.24058000 | 1.34118500 | 1.63854800 |
| C | -0.18006800 | 3.46812800 | -1.27654500 |
| C | -1.49269300 | 4.21099200 | -1.03786300 |
| H | -0.27348000 | 2.80502700 | -2.13322400 |
| H | 0.62594300 | 4.17611700 | -1.47854400 |
| H | -2.31231500 | 3.51366000 | -0.85071900 |
| H | -1.74577900 | 4.79855800 | -1.92539900 |
| C | 0.19103800 | 0.11209900 | 2.41117700 |
| H | 0.18231500 | -0.74633300 | 1.73469000 |
| H | 1.08266500 | 0.06242200 | 3.03605500 |
| H | -0.69785400 | 0.06067300 | 3.04404500 |
| H | -1.41331200 | 4.89414500 | -0.18722900 |
| H | -0.90075100 | 0.19943700 | -2.07329200 |
| C | 0.99208700 | -1.51766000 | -1.69444700 |
| O | 0.37930300 | -1.00205300 | -2.62985100 |
| C | 2.37051900 | -1.22584100 | -1.39079600 |
| C | 3.31085700 | -0.39889500 | -1.95854000 |
| O | 2.92413600 | -1.87805500 | -0.31447400 |
| C | 4.49188600 | -0.54822700 | -1.19072900 |
| H | 3.15723300 | 0.23332400 | -2.81920400 |
| C | 4.20669000 | -1.45534600 | -0.20167000 |
| H | 5.43833600 | -0.05113500 | -1.33746400 |
| C | 5.02255700 | -2.02038100 | 0.90379900 |
| H | 4.94007700 | -3.11340600 | 0.90080900 |
| H | 6.06910100 | -1.75156900 | 0.72945600 |
| O | 4.55545000 | -1.48800400 | 2.15340700 |
| H | 4.98999700 | -1.97940900 | 2.86292500 |

| | | | |
|------------|--------------|--------------|--------------|
| H | 0. 50891500 | -2. 25598900 | -1. 03358500 |
| TS3 | | | |
| O | 4. 48256900 | 1. 89640600 | -0. 76809900 |
| H | 4. 81521700 | 1. 37966000 | -1. 51420300 |
| C | 3. 64780100 | -0. 19042500 | 0. 21267500 |
| C | 3. 96924400 | -1. 50553300 | 0. 05172800 |
| H | 4. 96919100 | -1. 91362000 | 0. 04192300 |
| C | 2. 73971500 | -2. 22121900 | -0. 09553300 |
| C | 0. 28139500 | -1. 43223600 | -0. 21759700 |
| C | 1. 73272000 | -1. 29615600 | -0. 00799700 |
| O | 2. 28023500 | -0. 04940400 | 0. 16133300 |
| O | -0. 02808800 | -2. 62797500 | -0. 84920500 |
| C | 4. 46344900 | 1. 03774300 | 0. 38874000 |
| H | 5. 48090100 | 0. 73735100 | 0. 66098400 |
| H | 2. 60925700 | -3. 28144300 | -0. 24057400 |
| H | 4. 06526000 | 1. 65797300 | 1. 19489800 |
| C | -2. 65651600 | -0. 78679300 | 1. 85036700 |
| C | -1. 70244800 | -0. 24737900 | 2. 63829800 |
| C | -0. 68387300 | -1. 08557800 | 0. 81906300 |
| N | -2. 03117100 | -1. 29868100 | 0. 72774200 |
| H | -3. 72348300 | -0. 84967000 | 1. 97841900 |
| H | -1. 76792100 | 0. 25631300 | 3. 58706800 |
| N | -0. 48453300 | -0. 44352400 | 2. 00749500 |
| C | -2. 80047300 | -2. 02380200 | -0. 30660100 |
| C | -3. 02768100 | -3. 48757900 | 0. 05533700 |
| H | -2. 28352900 | -1. 92466300 | -1. 25372100 |
| H | -3. 75296100 | -1. 49786100 | -0. 38761400 |
| H | -2. 07824800 | -4. 01907000 | 0. 13624600 |
| H | -3. 62356600 | -3. 96285900 | -0. 72924700 |
| C | 0. 77384500 | -0. 03967500 | 2. 63958500 |
| H | 1. 17405200 | 0. 85413900 | 2. 16557800 |
| H | 0. 55731200 | 0. 16918200 | 3. 68565800 |
| H | 1. 50184500 | -0. 84650500 | 2. 58736400 |
| H | -3. 57247900 | -3. 58492800 | 0. 99846800 |
| H | -0. 15822000 | -2. 35623600 | -1. 81264600 |
| C | -0. 03316000 | -0. 19903800 | -1. 96242000 |
| O | -0. 35569900 | -1. 11696000 | -2. 79913100 |
| C | -1. 00922500 | 0. 84991900 | -1. 62694800 |
| C | -2. 31036000 | 1. 07379600 | -1. 98771600 |
| O | -0. 57115800 | 1. 88437700 | -0. 84054300 |
| C | -2. 69404100 | 2. 31058200 | -1. 38223300 |
| H | -2. 90810200 | 0. 44046300 | -2. 62349800 |
| C | -1. 60810900 | 2. 76685100 | -0. 69400200 |

| | | | |
|---|-------------|------------|-------------|
| H | -3.65021100 | 2.80723200 | -1.45310200 |
| C | -1.35829600 | 3.99336000 | 0.09974500 |
| H | -0.41975900 | 4.45994700 | -0.22154800 |
| H | -2.17580400 | 4.69669000 | -0.08979900 |
| O | -1.28612300 | 3.66958100 | 1.50324100 |
| H | -0.96636500 | 4.45453100 | 1.96707400 |
| H | 0.99973600 | 0.16957000 | -1.93210400 |

IM5

| | | | |
|---|-------------|-------------|-------------|
| O | 4.98905100 | 1.37978900 | -1.00995500 |
| H | 5.43807300 | 0.61022300 | -1.38479100 |
| C | 3.63944700 | -0.12526100 | 0.37520800 |
| C | 3.79202600 | -1.41899900 | 0.77940300 |
| H | 4.69227100 | -1.85081100 | 1.19115000 |
| C | 2.54505000 | -2.07817000 | 0.53607900 |
| C | 0.26877500 | -1.28123600 | -0.49561900 |
| C | 1.70415100 | -1.14457900 | 0.00494700 |
| O | 2.36544300 | 0.04968700 | -0.10312600 |
| O | 0.07026500 | -2.51581300 | -0.99832600 |
| C | 4.56195400 | 1.03908500 | 0.32148200 |
| H | 5.42460800 | 0.82403500 | 0.96098800 |
| H | 2.30200100 | -3.11212000 | 0.72077700 |
| H | 4.07227200 | 1.93798900 | 0.70193800 |
| C | -2.65029600 | -1.11693400 | 1.81631400 |
| C | -1.78559000 | -0.33972000 | 2.50808500 |
| C | -0.75234200 | -1.01546400 | 0.64287100 |
| N | -2.00536800 | -1.52600700 | 0.66635500 |
| H | -3.66433000 | -1.40891500 | 2.02923100 |
| H | -1.89108400 | 0.18123500 | 3.44390200 |
| N | -0.61647700 | -0.28026700 | 1.77329000 |
| C | -2.69400700 | -2.38553200 | -0.32563100 |
| C | -2.69628900 | -3.85044300 | 0.09087300 |
| H | -2.19885600 | -2.25531200 | -1.27937500 |
| H | -3.71147500 | -1.99600800 | -0.39476700 |
| H | -1.67412500 | -4.22629400 | 0.15279500 |
| H | -3.23650300 | -4.43457600 | -0.65953300 |
| C | 0.54141200 | 0.49892900 | 2.23072900 |
| H | 0.83064900 | 1.22466500 | 1.47621000 |
| H | 0.23829800 | 1.02384700 | 3.13399100 |
| H | 1.37500000 | -0.16180600 | 2.46301000 |
| H | -3.19395200 | -3.99491500 | 1.05382000 |
| H | -0.23696800 | -1.90321200 | -2.41049600 |
| C | 0.02549600 | -0.18448800 | -1.74532000 |
| O | -0.34593200 | -0.98373700 | -2.83185800 |

| | | | |
|---|-------------|------------|-------------|
| C | -0.99137000 | 0.88210300 | -1.51062800 |
| C | -2.25503600 | 1.09788600 | -1.97579300 |
| O | -0.61886500 | 1.91883200 | -0.69628600 |
| C | -2.69142800 | 2.34026500 | -1.40778100 |
| H | -2.79695600 | 0.45912400 | -2.65418500 |
| C | -1.67026500 | 2.80492100 | -0.63734800 |
| H | -3.64095300 | 2.83158800 | -1.55980400 |
| C | -1.49247600 | 4.02570100 | 0.18177200 |
| H | -0.51709100 | 4.48057100 | -0.02693300 |
| H | -2.27307900 | 4.74134900 | -0.09610100 |
| O | -1.58701400 | 3.69987200 | 1.58510300 |
| H | -1.35224500 | 4.49343000 | 2.08409200 |
| H | 0.98850600 | 0.30239500 | -1.92570800 |

TS4

| | | | |
|---|-------------|-------------|-------------|
| O | 4.48771300 | -2.05454200 | -0.62069200 |
| H | 4.42311800 | -2.93085700 | -1.02345000 |
| C | 2.25471800 | -2.34499900 | 0.34131500 |
| C | 1.47123100 | -3.43662400 | 0.58619600 |
| H | 1.79431700 | -4.35414100 | 1.05473600 |
| C | 0.16636000 | -3.12573100 | 0.09661300 |
| C | -0.78188100 | -1.03682900 | -1.11410400 |
| C | 0.23613800 | -1.85835400 | -0.40913700 |
| O | 1.50566100 | -1.37538300 | -0.26801000 |
| O | -1.76483000 | -1.64396500 | -1.59811900 |
| C | 3.69429500 | -2.05787700 | 0.57898800 |
| H | 4.07767800 | -2.79235100 | 1.29481800 |
| H | -0.71006700 | -3.75386700 | 0.11060900 |
| H | 3.81976100 | -1.06279000 | 1.01011200 |
| C | -3.31599100 | 0.54233500 | 2.07812700 |
| C | -2.16785000 | 0.54327000 | 2.79653500 |
| C | -1.62897100 | 0.01183500 | 0.65772200 |
| N | -2.96744500 | 0.21650300 | 0.77413500 |
| H | -4.33096300 | 0.75848600 | 2.36802900 |
| H | -1.98219400 | 0.75509400 | 3.83656600 |
| N | -1.14960200 | 0.21996700 | 1.91135600 |
| C | -3.95940600 | 0.14129600 | -0.30992700 |
| C | -4.81994900 | -1.11538500 | -0.23390900 |
| H | -3.41529700 | 0.18085300 | -1.24849900 |
| H | -4.58039700 | 1.03784700 | -0.24103600 |
| H | -4.20334800 | -2.01203900 | -0.32199000 |
| H | -5.54186300 | -1.11248600 | -1.05575100 |
| C | 0.24860200 | 0.09967700 | 2.32096700 |
| H | 0.89580000 | 0.35062300 | 1.48658700 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.43601100 | 0.79749000 | 3.13673900 |
| H | 0.46152700 | -0.91529900 | 2.66323400 |
| H | -5.37990100 | -1.16217800 | 0.70421900 |
| H | -1.87590800 | -0.32451500 | -2.86341800 |
| C | -0.25638700 | 0.16547300 | -2.00438000 |
| O | -1.28532200 | 0.45453800 | -2.93303700 |
| C | 0.16677300 | 1.45321500 | -1.37431400 |
| C | -0.43888500 | 2.67198300 | -1.28626500 |
| O | 1.42615300 | 1.52579600 | -0.85370400 |
| C | 0.50156400 | 3.54616000 | -0.65119200 |
| H | -1.42804700 | 2.91509400 | -1.63852400 |
| C | 1.62045400 | 2.80977100 | -0.40544700 |
| H | 0.36742100 | 4.59096000 | -0.41390200 |
| C | 2.93442800 | 3.12920600 | 0.19981700 |
| H | 3.74134400 | 2.72578700 | -0.42242000 |
| H | 3.03936000 | 4.21852100 | 0.23760800 |
| O | 3.01883600 | 2.57045100 | 1.52779100 |
| H | 3.93804100 | 2.64390800 | 1.81630800 |
| H | 0.61579200 | -0.25513300 | -2.52846900 |

IM6

| | | | |
|---|-------------|-------------|-------------|
| O | 3.04714800 | -2.47101300 | 3.32675500 |
| H | 3.18783000 | -3.42228400 | 3.22714600 |
| C | 1.51012400 | -2.42522300 | 1.43461700 |
| C | 0.80828600 | -3.38801300 | 0.75539500 |
| H | 0.21742300 | -4.17247500 | 1.20232500 |
| C | 1.01300400 | -3.14341100 | -0.62625400 |
| C | 2.37928400 | -1.32711600 | -1.84260900 |
| C | 1.82900100 | -2.04248500 | -0.70818900 |
| O | 2.13226600 | -1.59943200 | 0.55516000 |
| O | 2.21027500 | -1.70544500 | -2.99569900 |
| C | 1.71649800 | -2.16630200 | 2.88766500 |
| H | 0.97331600 | -2.74035200 | 3.44920400 |
| H | 0.61280900 | -3.69738500 | -1.46102400 |
| H | 1.56843000 | -1.10681200 | 3.10462200 |
| C | -4.82834000 | 1.29533900 | -0.46847900 |
| C | -4.08967200 | 1.75026800 | 0.57362100 |
| C | -3.95170900 | -0.53256100 | 0.59061300 |
| N | -4.72981900 | -0.09006700 | -0.43951800 |
| H | -5.39599500 | 1.82811100 | -1.21396400 |
| H | -3.88736600 | 2.75388500 | 0.91116400 |
| N | -3.56876200 | 0.62569300 | 1.19989300 |
| C | -5.40652800 | -0.97203300 | -1.39655100 |
| C | -6.91100900 | -1.07086200 | -1.15831600 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.93833300 | -1.95152700 | -1.30150800 |
| H | -5.20266300 | -0.60029300 | -2.40424200 |
| H | -7.12452400 | -1.46162400 | -0.15984900 |
| H | -7.35576600 | -1.74833500 | -1.89292000 |
| C | -2.70851200 | 0.69166300 | 2.37558400 |
| H | -1.80388500 | 1.26273400 | 2.15544300 |
| H | -3.23555700 | 1.16611300 | 3.20673800 |
| H | -2.43281200 | -0.32171800 | 2.65947200 |
| H | -7.39894200 | -0.09763700 | -1.25979200 |
| H | 3.49600800 | -0.16109500 | -3.49909600 |
| C | 3.19512100 | -0.04581300 | -1.59150000 |
| O | 3.95505400 | 0.26298500 | -2.75445100 |
| C | 2.28498300 | 1.07573300 | -1.18833500 |
| C | 1.03088800 | 1.45649800 | -1.56445500 |
| O | 2.79539600 | 1.97987600 | -0.29952600 |
| C | 0.75078400 | 2.67220400 | -0.86427800 |
| H | 0.38539700 | 0.93651500 | -2.25589700 |
| C | 1.84960100 | 2.95167500 | -0.10778500 |
| H | -0.15257800 | 3.26102300 | -0.91194000 |
| C | 2.17720600 | 4.04679300 | 0.83679800 |
| H | 3.19362000 | 4.41019100 | 0.64786900 |
| H | 1.47791400 | 4.87148000 | 0.66497700 |
| O | 2.06926900 | 3.56613700 | 2.19086500 |
| H | 2.43813100 | 4.24378400 | 2.77254800 |
| H | 3.89829700 | -0.22467700 | -0.77399800 |

IM1_{DBU}

| | | | |
|---|-------------|-------------|-------------|
| C | -3.18359200 | -4.28570700 | 0.86680100 |
| C | -3.95822400 | -4.72524500 | -0.15506500 |
| C | -3.43987900 | -2.53972900 | -0.58766700 |
| N | -2.88085200 | -2.96059000 | 0.58355000 |
| H | -2.81973400 | -4.79501500 | 1.74427100 |
| H | -4.40153400 | -5.69010400 | -0.34050100 |
| N | -4.10046400 | -3.65068300 | -1.02343200 |
| C | -2.07379600 | -2.11279400 | 1.46803400 |
| C | -2.84577800 | -1.62553300 | 2.69123700 |
| H | -1.73184300 | -1.26852700 | 0.87006000 |
| H | -1.19297500 | -2.68343700 | 1.77159200 |
| H | -3.71327800 | -1.02899500 | 2.39592300 |
| H | -2.19647100 | -1.00230400 | 3.31294400 |
| C | -4.86243900 | -3.72486000 | -2.26392400 |
| H | -4.43558100 | -4.47826900 | -2.93022200 |
| H | -5.90411000 | -3.98105000 | -2.05644500 |
| H | -4.82522600 | -2.75373900 | -2.75335900 |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.19416800 | -2.46205900 | 3.30318900 |
| Cl | 2.59089000 | -4.04102500 | 1.65273700 |
| C | 5.72287300 | 2.66539400 | 0.03574200 |
| C | 6.33509600 | 1.31138200 | -0.34001200 |
| C | 5.69337200 | 0.11589100 | 0.37181000 |
| C | 4.21846200 | 2.79696400 | -0.22523900 |
| C | 3.34179400 | 1.78300400 | 0.54085500 |
| C | 3.29813300 | 0.41207900 | -0.08027600 |
| H | 6.24584200 | 3.45712100 | -0.51052000 |
| H | 7.39735300 | 1.32012700 | -0.07461000 |
| H | 5.55250200 | 0.32664400 | 1.43568300 |
| H | 4.00695400 | 2.72258900 | -1.29778000 |
| H | 3.69503400 | 1.68865000 | 1.57310200 |
| C | 4.38536800 | -1.62853900 | -0.88900000 |
| H | 4.32614000 | -2.40890700 | -0.12361600 |
| C | 1.92914500 | -1.33793000 | -1.14254100 |
| H | 1.67671700 | -2.07177700 | -0.37118300 |
| H | 6.34630100 | -0.75328900 | 0.30746800 |
| H | 6.28310500 | 1.15050800 | -1.42295300 |
| H | 5.90960600 | 2.85040500 | 1.10108800 |
| H | 3.89809600 | 3.79619300 | 0.08332700 |
| H | 2.31704200 | 2.15089000 | 0.59400200 |
| N | 4.40335500 | -0.31067400 | -0.21272400 |
| N | 2.12656800 | -0.02563600 | -0.51818600 |
| H | 5.33311800 | -1.73044600 | -1.41970700 |
| H | 1.09103000 | -1.25373100 | -1.83511000 |
| C | 3.21328500 | -1.73918400 | -1.85493600 |
| H | 3.37641500 | -1.09468300 | -2.72412600 |
| H | 3.13818500 | -2.76935900 | -2.20692400 |
| H | 1.31778900 | 0.59162800 | -0.42068200 |
| O | -3.59375400 | 5.48892500 | 1.95742900 |
| H | -4.36548600 | 4.98317500 | 2.24303000 |
| C | -3.49323200 | 4.25419200 | -0.14324400 |
| C | -4.39068000 | 3.48751600 | -0.84365800 |
| H | -5.41698500 | 3.74660900 | -1.05279300 |
| C | -3.70106000 | 2.30971900 | -1.22329500 |
| C | -1.30837000 | 1.52871800 | -0.82088800 |
| H | -1.53594500 | 0.60879900 | -1.38344600 |
| C | -2.42304200 | 2.43191600 | -0.72912800 |
| O | -2.29491100 | 3.62435800 | -0.06908000 |
| O | -0.19635500 | 1.72140900 | -0.33628300 |
| C | -3.62088500 | 5.57950400 | 0.52782300 |
| H | -4.54133000 | 6.05654600 | 0.17707600 |
| H | -4.08200300 | 1.46875700 | -1.78279100 |

| | | | |
|--------------------------|-------------|-------------|-------------|
| H | -2.77908300 | 6.21945900 | 0.25592100 |
| TS1_{DBU} | | | |
| C | -1.69096400 | 3.06387800 | 1.34322500 |
| C | -1.71332200 | 2.64398700 | 2.63198900 |
| C | -1.89666400 | 0.80618900 | 1.31421400 |
| N | -1.80184000 | 1.92570500 | 0.55543300 |
| H | -1.59688700 | 4.05261500 | 0.92516500 |
| H | -1.64791500 | 3.19461300 | 3.55600200 |
| N | -1.84132700 | 1.26095600 | 2.59158800 |
| C | -1.86274700 | 1.94757100 | -0.91419700 |
| C | -3.20396300 | 2.45272100 | -1.43771100 |
| H | -1.66799700 | 0.93046400 | -1.24932200 |
| H | -1.05109900 | 2.58634700 | -1.26937100 |
| H | -4.02577800 | 1.81603600 | -1.10030200 |
| H | -3.19396900 | 2.44340100 | -2.53123900 |
| C | -1.88452800 | 0.41776500 | 3.78156800 |
| H | -0.92779800 | 0.45153400 | 4.30783300 |
| H | -2.67455700 | 0.75999100 | 4.45281400 |
| H | -2.09612000 | -0.60585600 | 3.48101100 |
| H | -3.39915000 | 3.47815300 | -1.11278400 |
| Cl | 1.38689400 | 5.62173900 | -1.01722300 |
| C | 4.97292300 | -3.43695100 | 0.65553400 |
| C | 5.88893500 | -2.24509200 | 0.35630400 |
| C | 5.51019900 | -1.47051500 | -0.91029000 |
| C | 3.48809500 | -3.09348600 | 0.81926000 |
| C | 2.83691400 | -2.44147500 | -0.42024000 |
| C | 3.12765900 | -0.96987800 | -0.56477300 |
| H | 5.32175400 | -3.93533800 | 1.56565400 |
| H | 6.91181100 | -2.61247700 | 0.22364400 |
| H | 5.28720600 | -2.15740800 | -1.73156800 |
| H | 3.34006700 | -2.44680500 | 1.69114000 |
| H | 3.16596400 | -2.95936000 | -1.32725400 |
| C | 4.68597800 | 0.90648700 | -0.79440100 |
| H | 4.77569300 | 1.19977800 | -1.84542600 |
| C | 2.24103000 | 1.32281100 | -0.58023800 |
| H | 2.08945700 | 1.63485800 | -1.61786900 |
| H | 6.34766500 | -0.85396000 | -1.23406700 |
| H | 5.91150600 | -1.55120200 | 1.20436500 |
| H | 5.07471200 | -4.16867400 | -0.15579500 |
| H | 2.93849600 | -4.01675900 | 1.02371200 |
| H | 1.75369500 | -2.55306300 | -0.36962600 |
| N | 4.37523100 | -0.53957500 | -0.73283800 |
| N | 2.10643900 | -0.13380700 | -0.48334900 |

| | | | |
|---|-------------|-------------|-------------|
| H | 5.65874100 | 1.04877500 | -0.32178500 |
| H | 1.45233500 | 1.77271500 | 0.02203700 |
| C | 3.62049800 | 1.73017400 | -0.08573800 |
| H | 3.68650900 | 1.57167900 | 0.99470100 |
| H | 3.78837000 | 2.79011300 | -0.28032700 |
| H | 1.15634800 | -0.52595200 | -0.36871400 |
| O | -5.89068600 | -1.03204200 | -2.32814900 |
| H | -6.44413600 | -0.83015400 | -1.56309200 |
| C | -4.43091200 | -2.35041200 | -0.87011400 |
| C | -4.60968400 | -2.93550600 | 0.35121000 |
| H | -5.45646400 | -3.53589500 | 0.64808700 |
| C | -3.46241800 | -2.60311800 | 1.13431800 |
| C | -1.32670800 | -1.25581800 | 0.57075900 |
| H | -0.96913100 | -1.45047900 | 1.59026100 |
| C | -2.66154200 | -1.83433100 | 0.33628600 |
| O | -3.23771900 | -1.68278000 | -0.88896000 |
| O | -0.52028700 | -1.07101200 | -0.36745000 |
| C | -5.26780700 | -2.30719500 | -2.09878800 |
| H | -6.02046300 | -3.10005600 | -2.03111200 |
| H | -3.25492800 | -2.89684800 | 2.15208800 |
| H | -4.65695800 | -2.49346000 | -2.98449300 |

IM2_{DBU}

| | | | |
|----|-------------|-------------|-------------|
| C | 3.03683500 | -1.99252300 | 0.72036000 |
| C | 2.54693000 | -1.83879300 | 1.97649600 |
| C | 1.48471700 | -0.40077800 | 0.65444500 |
| N | 2.37240600 | -1.08790900 | -0.08789900 |
| H | 3.77858500 | -2.68359200 | 0.33744300 |
| H | 2.78646200 | -2.34769000 | 2.89440500 |
| N | 1.58436300 | -0.85012800 | 1.92165400 |
| C | 2.64699400 | -0.95132400 | -1.53937700 |
| C | 4.06544200 | -0.46587300 | -1.80955200 |
| H | 1.90093200 | -0.27280500 | -1.93996600 |
| H | 2.48237200 | -1.93714000 | -1.97817400 |
| H | 4.23989800 | 0.51399200 | -1.36140000 |
| H | 4.20529100 | -0.37946700 | -2.89034100 |
| C | 0.80452900 | -0.38765500 | 3.07311800 |
| H | -0.26029000 | -0.53312100 | 2.88980700 |
| H | 1.10133700 | -0.97891000 | 3.93674300 |
| H | 1.00960200 | 0.66470000 | 3.26966000 |
| H | 4.81258200 | -1.16718300 | -1.43169600 |
| Cl | 5.24488600 | -4.70334400 | -0.09257500 |
| C | -5.74580500 | 1.76537200 | 0.64939200 |
| C | -6.40128600 | 0.38253900 | 0.56723100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -6.01720300 | -0.41395700 | -0.68645700 |
| C | -4.21322500 | 1.76500600 | 0.58994200 |
| C | -3.61564600 | 1.15866300 | -0.69777300 |
| C | -3.52957900 | -0.35354300 | -0.71504100 |
| H | -6.06687600 | 2.26031500 | 1.57226800 |
| H | -7.48959900 | 0.50950100 | 0.56571700 |
| H | -6.07926800 | 0.22551700 | -1.57289700 |
| H | -3.80078200 | 1.24394900 | 1.46241200 |
| H | -4.19358300 | 1.50079600 | -1.56419400 |
| C | -4.69269300 | -2.52015500 | -0.49247100 |
| H | -4.95794700 | -2.97007700 | -1.45702200 |
| C | -2.24411100 | -2.34995700 | -0.84968600 |
| H | -2.31219500 | -2.67848400 | -1.89577800 |
| H | -6.73486400 | -1.22137000 | -0.83865200 |
| H | -6.15540200 | -0.21396500 | 1.45391800 |
| H | -6.12459500 | 2.38049200 | -0.17714500 |
| H | -3.86823800 | 2.80146800 | 0.65966900 |
| H | -2.59995200 | 1.52584000 | -0.84062200 |
| N | -4.69400500 | -1.05338300 | -0.62233400 |
| N | -2.34348900 | -0.88949300 | -0.79184700 |
| H | -5.47278700 | -2.79575500 | 0.22231800 |
| H | -1.25257100 | -2.64355000 | -0.49557500 |
| C | -3.33553300 | -3.02576500 | -0.02574700 |
| H | -3.19242300 | -2.79073100 | 1.03413800 |
| H | -3.29215300 | -4.11265600 | -0.13149700 |
| H | -0.92734500 | -0.06848600 | -0.95477600 |
| O | 4.97301700 | 3.71558100 | -0.43599300 |
| H | 5.01613400 | 4.04515000 | 0.47052700 |
| C | 2.53082300 | 3.62922700 | -0.29405200 |
| C | 1.64166600 | 4.20168200 | 0.56618900 |
| H | 1.64611400 | 5.23180100 | 0.88881800 |
| C | 0.71496000 | 3.17744900 | 0.94285300 |
| C | 0.50039300 | 0.67624600 | 0.21547200 |
| H | -0.29513300 | 0.67000000 | 0.96955900 |
| C | 1.10082600 | 2.04942400 | 0.28349100 |
| O | 2.20848200 | 2.30772700 | -0.47120400 |
| O | -0.03420600 | 0.41422700 | -1.05984000 |
| C | 3.72773300 | 4.15057800 | -1.00680400 |
| H | 3.66950200 | 5.24392500 | -1.02357300 |
| H | -0.13168100 | 3.26984800 | 1.60585400 |
| H | 3.74193900 | 3.79545700 | -2.03906900 |

IM1a

| | | | |
|---|-------------|-------------|------------|
| C | -3.59524900 | -2.88317600 | 2.47924200 |
|---|-------------|-------------|------------|

| | | | |
|----|-------------|-------------|-------------|
| C | -3.16972100 | -3.59203400 | 1.39097100 |
| H | -3.07418300 | -4.66357000 | 1.32159500 |
| C | -2.87927100 | -2.62784500 | 0.38951600 |
| C | -3.02571100 | -0.08218200 | 0.37225500 |
| H | -2.67429600 | -0.04322600 | -0.67113500 |
| C | -3.14999600 | -1.39893300 | 0.94124700 |
| O | -3.59212300 | -1.55815600 | 2.23029500 |
| O | -3.29981300 | 0.95818500 | 0.97272100 |
| H | -2.50803100 | -2.80140900 | -0.60884100 |
| C | 1.01526900 | -0.17194300 | 0.31495300 |
| C | 2.90208800 | -0.76000300 | -1.01934400 |
| N | 1.51824900 | -0.48836500 | -0.89450400 |
| C | 5.00001800 | -0.85162100 | 0.48136700 |
| C | 5.73439300 | 0.47867500 | 0.65276000 |
| H | 5.48838700 | -1.41846700 | -0.31522500 |
| H | 5.12332300 | -1.43461400 | 1.39865900 |
| H | 5.67363200 | 1.06686600 | -0.26789900 |
| C | 0.60172000 | -0.57703300 | -2.04663400 |
| H | -0.21513600 | 0.12707500 | -1.87889900 |
| H | 1.12797000 | -0.22264400 | -2.93619700 |
| H | 5.28996700 | 1.05680500 | 1.46782500 |
| O | 7.10536300 | 0.16287200 | 0.95349700 |
| C | 8.03539700 | 1.13037100 | 1.18676200 |
| O | 9.16482100 | 0.79643500 | 1.42480900 |
| C | 0.03796000 | -1.96319800 | -2.30120300 |
| C | -1.02436700 | -2.07573100 | -3.20941700 |
| C | 0.52239700 | -3.11712800 | -1.68130700 |
| C | -1.57331800 | -3.32188400 | -3.50066700 |
| H | -1.43612600 | -1.17547800 | -3.65523900 |
| C | -0.02948900 | -4.36595900 | -1.97492400 |
| H | 1.32302100 | -3.05000100 | -0.95370300 |
| C | -1.07526200 | -4.47387200 | -2.88830400 |
| H | -2.39785800 | -3.39179000 | -4.20176200 |
| H | 0.35986000 | -5.25227900 | -1.48552900 |
| H | -1.50255900 | -5.44378300 | -3.11814200 |
| Cl | -2.30436900 | 1.40773800 | -2.70890000 |
| N | -3.08516300 | 3.55220400 | 0.05053800 |
| C | -3.41192900 | 4.06407200 | 1.43610100 |
| H | -4.46552700 | 3.83177500 | 1.59740300 |
| H | -2.84447100 | 3.43808200 | 2.12470400 |
| C | -4.18461500 | 3.73221800 | -0.98112400 |
| H | -3.88254500 | 3.07937600 | -1.80537800 |
| H | -5.08297300 | 3.30946900 | -0.52640900 |
| C | -1.72654600 | 3.95553400 | -0.47536800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.66977500 | 3.50720900 | -1.47030700 |
| H | -1.71206900 | 5.04250300 | -0.55693800 |
| C | -3.12783600 | 5.53707800 | 1.70489000 |
| H | -3.67649200 | 6.20641900 | 1.04311900 |
| H | -3.43843600 | 5.75768200 | 2.72934200 |
| H | -2.06517200 | 5.77308700 | 1.63070700 |
| C | -4.43556800 | 5.15185600 | -1.46882100 |
| H | -5.16783000 | 5.09573800 | -2.27801700 |
| H | -4.84844200 | 5.81014900 | -0.70222800 |
| H | -3.53735500 | 5.61136200 | -1.88516900 |
| C | -0.58446000 | 3.43466300 | 0.38606000 |
| H | 0.35669800 | 3.72626400 | -0.08631500 |
| H | -0.58371400 | 3.84519400 | 1.39910600 |
| H | -0.59042100 | 2.34383300 | 0.44553500 |
| C | 7.58244000 | 2.57396500 | 1.13113600 |
| H | 7.17817900 | 2.82386000 | 0.14689300 |
| H | 6.80032900 | 2.77113000 | 1.86875500 |
| H | 8.44114600 | 3.20798000 | 1.33891100 |
| C | 3.54373800 | -0.66441400 | 0.17270400 |
| S | 2.35817100 | -0.22641000 | 1.40351600 |
| C | 3.50128500 | -1.08356300 | -2.35455700 |
| H | 2.97877300 | -1.91089800 | -2.84121300 |
| H | 3.46070200 | -0.22363800 | -3.03080700 |
| H | 4.54832900 | -1.36636000 | -2.24364700 |
| H | -3.05264100 | 2.51314400 | 0.18506600 |
| C | -4.06022200 | -3.30317500 | 3.88601200 |
| H | -3.41631100 | -2.86546600 | 4.61996700 |
| H | -5.06333500 | -2.96662500 | 4.04538200 |
| O | -4.01192800 | -4.72793200 | 3.99841500 |
| H | -4.30212100 | -4.99023800 | 4.87510400 |

TS1a

| | | | |
|---|-------------|-------------|-------------|
| C | -1.56507600 | -2.15200200 | 3.51820400 |
| C | -2.23697800 | -2.99903100 | 2.68549900 |
| H | -2.57084100 | -3.99546300 | 2.92985200 |
| C | -2.39748700 | -2.30928500 | 1.44630600 |
| C | -1.69712400 | 0.06865200 | 0.69986600 |
| H | -2.15240700 | -0.10445700 | -0.28209600 |
| C | -1.81301200 | -1.08502100 | 1.61138400 |
| O | -1.30972500 | -0.97585200 | 2.87444600 |
| O | -1.63106400 | 1.24198000 | 1.16593400 |
| H | -2.87292200 | -2.66707700 | 0.54670600 |
| C | 0.26152900 | -0.40585700 | -0.06059800 |
| C | 2.09841800 | -1.10434900 | -1.34571300 |

| | | | |
|----|-------------|-------------|-------------|
| N | 0.70206800 | -0.94277700 | -1.20335200 |
| C | 4.24949400 | -0.64668300 | 0.00852200 |
| C | 4.86006900 | 0.73761500 | -0.21842300 |
| H | 4.75696500 | -1.36230900 | -0.64242400 |
| H | 4.46287500 | -0.95601200 | 1.03540500 |
| H | 4.70272700 | 1.05790900 | -1.25297400 |
| C | -0.25861100 | -1.33722500 | -2.26162900 |
| H | -1.04706400 | -0.57782500 | -2.30083800 |
| H | 0.26751800 | -1.28357300 | -3.21638400 |
| H | 4.39897600 | 1.47157600 | 0.44888900 |
| O | 6.26452500 | 0.61833000 | 0.05919000 |
| C | 7.11053600 | 1.68598800 | -0.01495400 |
| O | 8.27574000 | 1.51000500 | 0.21548300 |
| C | -0.86759700 | -2.71275300 | -2.07553900 |
| C | -2.13724300 | -2.93907400 | -2.62148500 |
| C | -0.21335800 | -3.75869800 | -1.41958700 |
| C | -2.72808000 | -4.19733800 | -2.52656500 |
| H | -2.66458100 | -2.11520900 | -3.09243800 |
| C | -0.80936800 | -5.01572500 | -1.32064300 |
| H | 0.75540800 | -3.59726100 | -0.95932700 |
| C | -2.06580300 | -5.24054500 | -1.87932700 |
| H | -3.71343800 | -4.35830800 | -2.94997700 |
| H | -0.29260700 | -5.81584000 | -0.80212200 |
| H | -2.52930700 | -6.21795500 | -1.80308200 |
| Cl | -2.97661700 | 0.78093400 | -2.64506800 |
| N | -2.72823600 | 3.37662500 | 0.08448400 |
| C | -2.52378300 | 4.27843300 | 1.27649000 |
| H | -3.22263000 | 3.92867000 | 2.03787800 |
| H | -1.52237800 | 4.05899200 | 1.64931600 |
| C | -4.16140300 | 2.95453800 | -0.16082200 |
| H | -4.08897100 | 2.15627400 | -0.90599300 |
| H | -4.50099800 | 2.51516700 | 0.77967800 |
| C | -2.03531400 | 3.81755700 | -1.17823600 |
| H | -2.30377200 | 3.06753400 | -1.92830400 |
| H | -2.44341500 | 4.78441000 | -1.47561500 |
| C | -2.68037300 | 5.77732400 | 1.04027100 |
| H | -3.66785200 | 6.04833500 | 0.66805300 |
| H | -2.53382800 | 6.28915800 | 1.99500900 |
| H | -1.93394500 | 6.16634100 | 0.34557100 |
| C | -5.12266800 | 4.03669700 | -0.63391400 |
| H | -6.07315700 | 3.55290800 | -0.87185100 |
| H | -5.32461200 | 4.79916700 | 0.12112100 |
| H | -4.77800200 | 4.52334200 | -1.54831400 |
| C | -0.52065300 | 3.87508400 | -1.02167500 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.08193500 | 4.10650900 | -1.99510300 |
| H | -0.18829200 | 4.64125900 | -0.31636400 |
| H | -0.12811400 | 2.90948600 | -0.69716000 |
| C | 6.51973000 | 3.03022900 | -0.38226000 |
| H | 6.03585800 | 2.99683200 | -1.36170300 |
| H | 5.76814100 | 3.34263000 | 0.34734600 |
| H | 7.32483600 | 3.76083100 | -0.40351400 |
| C | 2.77072000 | -0.67132200 | -0.24696800 |
| S | 1.61725700 | -0.06950100 | 0.93574400 |
| C | 2.68086300 | -1.67747000 | -2.60156400 |
| H | 2.22188300 | -2.63534000 | -2.85838100 |
| H | 2.54284300 | -1.00366600 | -3.45280000 |
| H | 3.75161200 | -1.84075100 | -2.48021800 |
| H | -2.25082500 | 2.45952200 | 0.38999200 |
| C | -1.09425000 | -2.27609800 | 4.91866700 |
| H | -1.33897600 | -1.35827100 | 5.46729900 |
| H | -1.62394200 | -3.11371900 | 5.38736900 |
| O | 0.32473600 | -2.50134300 | 4.93760000 |
| H | 0.63595600 | -2.38143100 | 5.84075600 |

IM2a

| | | | |
|---|-------------|-------------|-------------|
| C | -3.16923800 | -1.82701300 | 2.11792000 |
| C | -4.04835100 | -1.67410400 | 1.08820800 |
| H | -5.00590900 | -2.16245200 | 0.99546800 |
| C | -3.44779000 | -0.76165900 | 0.16359500 |
| C | -1.18457100 | 0.53155400 | 0.24260500 |
| H | -1.46599900 | 0.84592700 | -0.78825000 |
| C | -2.24424900 | -0.41986800 | 0.69851400 |
| O | -2.05681400 | -1.06241700 | 1.89352700 |
| O | -1.03003700 | 1.63295700 | 1.11750000 |
| H | -3.82933300 | -0.40691400 | -0.78195000 |
| C | 0.16786100 | -0.12652300 | 0.14953700 |
| C | 1.92408600 | -1.45827400 | -0.51579000 |
| N | 0.57847700 | -1.08421600 | -0.68072500 |
| C | 3.96100300 | -0.82467000 | 0.93792000 |
| C | 4.85125400 | 0.20588100 | 0.23742900 |
| H | 4.36578200 | -1.82227900 | 0.75626200 |
| H | 4.02087600 | -0.65987700 | 2.01688700 |
| H | 4.85267200 | 0.03509300 | -0.84361300 |
| C | -0.27838500 | -1.67299400 | -1.74629500 |
| H | -1.13215700 | -1.00283100 | -1.89465800 |
| H | 0.28971100 | -1.59909800 | -2.67457400 |
| H | 4.48548400 | 1.21914700 | 0.42926900 |
| O | 6.16830900 | 0.03249400 | 0.77550000 |

| | | | |
|----|-------------|-------------|-------------|
| C | 7.21865100 | 0.82422700 | 0.39687300 |
| O | 8.29391400 | 0.61036700 | 0.88330700 |
| C | -0.68878900 | -3.10675500 | -1.48583900 |
| C | -0.91825200 | -3.93708100 | -2.58887600 |
| C | -0.90472300 | -3.61134700 | -0.20158100 |
| C | -1.35563300 | -5.24687700 | -2.40969000 |
| H | -0.76450500 | -3.55280400 | -3.59219800 |
| C | -1.33927500 | -4.92399800 | -0.02186100 |
| H | -0.75287600 | -2.99004400 | 0.67274800 |
| C | -1.56392100 | -5.74562200 | -1.12411800 |
| H | -1.53277400 | -5.87660100 | -3.27439900 |
| H | -1.51689100 | -5.28374200 | 0.98461700 |
| H | -1.90446200 | -6.76543400 | -0.98449800 |
| Cl | -2.01692500 | 1.03166400 | -2.91416200 |
| N | -1.96550000 | 3.95259300 | 0.00589700 |
| C | -1.82774600 | 4.86252500 | 1.16393500 |
| H | -2.56148300 | 4.53626600 | 1.90675100 |
| H | -0.84528400 | 4.67957500 | 1.61253500 |
| C | -3.35707600 | 3.57031300 | -0.33494600 |
| H | -3.27810500 | 2.77613100 | -1.08249300 |
| H | -3.79342200 | 3.12437600 | 0.56545600 |
| C | -1.17363900 | 4.32550200 | -1.18574400 |
| H | -1.38688300 | 3.57255700 | -1.94903000 |
| H | -1.49148000 | 5.29705700 | -1.59001300 |
| C | -1.96998700 | 6.37488400 | 0.92949900 |
| H | -2.94815300 | 6.65121500 | 0.53526700 |
| H | -1.83372000 | 6.89589400 | 1.88223700 |
| H | -1.21140600 | 6.75387000 | 0.24044300 |
| C | -4.30302000 | 4.65523400 | -0.87017000 |
| H | -5.23557500 | 4.18164900 | -1.19070700 |
| H | -4.55686000 | 5.40271400 | -0.11531600 |
| H | -3.88515300 | 5.16760300 | -1.73993100 |
| C | 0.33219800 | 4.35886500 | -0.92510400 |
| H | 0.85649900 | 4.54768200 | -1.86566000 |
| H | 0.62278500 | 5.14387000 | -0.22121700 |
| H | 0.68266800 | 3.40195800 | -0.52995000 |
| C | 6.94715300 | 1.91923700 | -0.61035500 |
| H | 6.54944200 | 1.51236100 | -1.54347800 |
| H | 6.21845500 | 2.63727300 | -0.22505100 |
| H | 7.88309900 | 2.43431500 | -0.81293700 |
| C | 2.53312600 | -0.75730200 | 0.47792100 |
| S | 1.41922000 | 0.38832400 | 1.19320600 |
| C | 2.53527300 | -2.49432200 | -1.40471400 |
| H | 1.97319700 | -3.42953100 | -1.37110500 |

| | | | |
|---|-------------|-------------|-------------|
| H | 2.56222100 | -2.15816200 | -2.44555700 |
| H | 3.55932600 | -2.69674200 | -1.09370400 |
| H | -1.35616400 | 2.47333200 | 0.65887600 |
| C | -3.19424600 | -2.63119600 | 3.36271500 |
| H | -2.93010400 | -1.99656500 | 4.21729300 |
| H | -4.21286200 | -3.00681300 | 3.50990100 |
| O | -2.26166700 | -3.72306500 | 3.25667600 |
| H | -2.12121400 | -4.08445300 | 4.13792500 |

IM5a

| | | | |
|---|-------------|-------------|-------------|
| C | -4.51402100 | -0.47879800 | -1.09367500 |
| C | -4.44885400 | -0.75443600 | -2.42502500 |
| H | -5.26071800 | -0.65423800 | -3.12898900 |
| C | -3.12051800 | -1.21774400 | -2.69200000 |
| C | -1.05033900 | -1.65445200 | -1.16629600 |
| C | -2.45941200 | -1.19501900 | -1.50352600 |
| O | -3.29691600 | -0.74285400 | -0.51518300 |
| O | -0.48474100 | -2.26758200 | -2.21803500 |
| H | -2.69828200 | -1.55711700 | -3.62263300 |
| C | -0.11185300 | -0.46923100 | -0.84979000 |
| C | 1.08678700 | 1.33426100 | -0.05477500 |
| N | -0.07179500 | 0.53678000 | 0.02813700 |
| C | 3.24680700 | 1.47988700 | -1.44628400 |
| C | 4.40369600 | 0.72021100 | -0.79268900 |
| H | 3.31617800 | 2.53329100 | -1.16735200 |
| H | 3.37287800 | 1.43743600 | -2.53184000 |
| H | 4.31648500 | 0.75609300 | 0.29779300 |
| C | -1.13662200 | 0.81941000 | 1.01773000 |
| H | -1.80144200 | -0.03978200 | 1.02759500 |
| H | -0.66009500 | 0.87675900 | 1.99634000 |
| H | 4.39758100 | -0.32640000 | -1.10919000 |
| O | 5.61194800 | 1.37317300 | -1.21364400 |
| C | 6.84700800 | 0.87916800 | -0.90832100 |
| O | 7.81277200 | 1.50749100 | -1.24627700 |
| C | -1.92250900 | 2.08055100 | 0.71357800 |
| C | -2.37640200 | 2.86702400 | 1.77682200 |
| C | -2.25438400 | 2.45153600 | -0.59231700 |
| C | -3.14911200 | 4.00291700 | 1.54194600 |
| H | -2.12175300 | 2.59059700 | 2.79519400 |
| C | -3.01890900 | 3.59234800 | -0.82877100 |
| H | -1.92409700 | 1.84832600 | -1.43051200 |
| C | -3.46933500 | 4.37093900 | 0.23635700 |
| H | -3.49284500 | 4.60306700 | 2.37704900 |
| H | -3.26668900 | 3.86871600 | -1.84736100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.06378300 | 5.25814400 | 0.05016800 |
| C | 6.91727200 | -0.44151600 | -0.17265800 |
| H | 6.36326400 | -0.40838700 | 0.76873100 |
| H | 6.49238600 | -1.24653800 | -0.77842000 |
| H | 7.96257500 | -0.66221400 | 0.02968600 |
| C | 1.90838600 | 0.92141500 | -1.05695300 |
| S | 1.24472800 | -0.47979500 | -1.88299200 |
| C | 1.31654500 | 2.43995400 | 0.92658400 |
| H | 0.51734900 | 3.18360100 | 0.89644700 |
| H | 1.38186000 | 2.04062100 | 1.94292900 |
| H | 2.25591200 | 2.94393400 | 0.70156400 |
| C | -1.11665500 | -2.72422700 | 0.09043000 |
| O | -1.18212600 | -3.97177600 | -0.53351500 |
| C | 0.05555600 | -2.65915200 | 1.01732800 |
| C | 1.27668400 | -3.26337400 | 1.03069800 |
| O | -0.05561400 | -1.82427600 | 2.10119200 |
| C | 1.96620300 | -2.76285800 | 2.18180500 |
| H | 1.62136600 | -3.98732700 | 0.31119600 |
| C | 1.12202000 | -1.89202300 | 2.80187300 |
| H | 2.95712900 | -3.02887700 | 2.51746600 |
| H | -2.02737400 | -2.53429900 | 0.66657400 |
| H | -0.85783000 | -3.76174000 | -1.45105100 |
| C | -5.58980200 | 0.04089400 | -0.21705300 |
| H | -6.40764300 | 0.38888100 | -0.85923100 |
| H | -5.21759300 | 0.89747100 | 0.35976700 |
| O | -6.04187900 | -0.99224900 | 0.67121900 |
| H | -6.63480400 | -0.59555600 | 1.31772000 |
| C | 1.21133300 | -1.10632300 | 4.05134600 |
| H | 2.13023500 | -1.39338700 | 4.57292100 |
| H | 0.35675600 | -1.33182200 | 4.70131100 |
| O | 1.22196300 | 0.31135200 | 3.75610900 |
| H | 1.17924000 | 0.78561400 | 4.59393300 |

TS4a

| | | | |
|---|-------------|-------------|-------------|
| C | -4.38064900 | -0.33572600 | -1.36380600 |
| C | -4.26235400 | -0.61591400 | -2.69205200 |
| H | -4.98261600 | -0.36508400 | -3.45545000 |
| C | -3.02629200 | -1.31566000 | -2.85961300 |
| C | -1.20952300 | -2.07357500 | -1.16473600 |
| C | -2.47115800 | -1.41550800 | -1.61968700 |
| O | -3.28695800 | -0.81975900 | -0.69524100 |
| O | -0.50037100 | -2.62978400 | -2.03757000 |
| H | -2.59789200 | -1.71346100 | -3.76467500 |
| C | -0.11298700 | -0.43016600 | -0.65040000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1. 13381400 | 1. 42283400 | 0. 05902300 |
| N | -0. 01857200 | 0. 61648700 | 0. 17717200 |
| C | 3. 25681000 | 1. 54355500 | -1. 39659800 |
| C | 4. 43946000 | 0. 74229400 | -0. 84908200 |
| H | 3. 35923300 | 2. 58216100 | -1. 07507900 |
| H | 3. 31661700 | 1. 54938700 | -2. 48857900 |
| H | 4. 41995100 | 0. 73526000 | 0. 24506600 |
| C | -1. 08412700 | 0. 91050700 | 1. 15743400 |
| H | -1. 75042200 | 0. 05005100 | 1. 14222600 |
| H | -0. 62917000 | 0. 95815200 | 2. 14782600 |
| H | 4. 39836000 | -0. 29031500 | -1. 20652600 |
| O | 5. 63054600 | 1. 39429200 | -1. 32033100 |
| C | 6. 87480500 | 0. 88988100 | -1. 08031800 |
| O | 7. 82805600 | 1. 50938900 | -1. 46748600 |
| C | -1. 86635500 | 2. 17384100 | 0. 85094400 |
| C | -2. 38596200 | 2. 92456600 | 1. 91037400 |
| C | -2. 13066800 | 2. 58338500 | -0. 45914000 |
| C | -3. 15626500 | 4. 06054200 | 1. 66828600 |
| H | -2. 18466100 | 2. 61938700 | 2. 93254200 |
| C | -2. 89208600 | 3. 72540100 | -0. 70264200 |
| H | -1. 74334200 | 2. 01112900 | -1. 29425100 |
| C | -3. 40882200 | 4. 46658900 | 0. 35890700 |
| H | -3. 55070100 | 4. 63181000 | 2. 50126900 |
| H | -3. 08399100 | 4. 03313600 | -1. 72443500 |
| H | -4. 00040600 | 5. 35465600 | 0. 16755400 |
| C | 6. 97168600 | -0. 43016800 | -0. 34650300 |
| H | 6. 47478700 | -0. 38554100 | 0. 62572000 |
| H | 6. 50029000 | -1. 23126800 | -0. 92206000 |
| H | 8. 02422300 | -0. 66405100 | -0. 20512800 |
| C | 1. 93431600 | 0. 99037500 | -0. 95010800 |
| S | 1. 24471400 | -0. 43798000 | -1. 70057100 |
| C | 1. 38325400 | 2. 54273500 | 1. 01932800 |
| H | 0. 58579600 | 3. 28862700 | 0. 99212000 |
| H | 1. 45746800 | 2. 15512800 | 2. 03992400 |
| H | 2. 32196400 | 3. 04197300 | 0. 77999700 |
| C | -1. 32230400 | -2. 83586000 | 0. 20893800 |
| O | -1. 65237700 | -4. 17752300 | -0. 12803600 |
| C | -0. 08130100 | -2. 77050800 | 1. 04431800 |
| C | 1. 16013300 | -3. 32226100 | 0. 94508000 |
| O | -0. 14710000 | -1. 98684700 | 2. 16706500 |
| C | 1. 91128800 | -2. 83700200 | 2. 06184800 |
| H | 1. 49323800 | -3. 98569000 | 0. 16400000 |
| C | 1. 07991500 | -2. 02597500 | 2. 77488500 |
| H | 2. 93564700 | -3. 06858600 | 2. 31133600 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.14899500 | -2.43508300 | 0.79783100 |
| H | -1.19599900 | -4.35173400 | -0.96636000 |
| C | -5.41505500 | 0.36298200 | -0.56400500 |
| H | -6.08345200 | 0.88656900 | -1.25795400 |
| H | -4.93714100 | 1.10939600 | 0.08245800 |
| O | -6.14462200 | -0.58641100 | 0.22755600 |
| H | -6.67388500 | -0.10097200 | 0.86853000 |
| C | 1.23769300 | -1.27425300 | 4.03923800 |
| H | 2.18812100 | -1.56874200 | 4.49646500 |
| H | 0.42505300 | -1.52774800 | 4.73099200 |
| O | 1.22314200 | 0.15090100 | 3.78698800 |
| H | 1.21038000 | 0.59822300 | 4.64053900 |

IM6a

| | | | |
|---|-------------|-------------|-------------|
| C | 3.12398600 | -2.26927700 | -1.92377100 |
| C | 4.00316800 | -2.36956600 | -2.97167600 |
| H | 4.02531300 | -3.16518100 | -3.69936000 |
| C | 4.86818100 | -1.25082000 | -2.88895100 |
| C | 5.02259600 | 0.67192100 | -1.20007400 |
| C | 4.46930700 | -0.52933600 | -1.79171900 |
| O | 3.39189900 | -1.14985000 | -1.20236600 |
| O | 6.01632900 | 1.21389800 | -1.66393700 |
| H | 5.69480100 | -0.99490300 | -3.53227600 |
| C | -1.17382100 | -1.43711100 | -0.91843600 |
| C | -2.52061200 | -0.36121300 | 0.72755900 |
| N | -1.25298100 | -0.64153800 | 0.16621900 |
| C | -4.99827000 | -0.91694000 | 0.27505400 |
| C | -5.69209400 | 0.07134300 | -0.66352000 |
| H | -5.20869300 | -0.62568800 | 1.30694800 |
| H | -5.44678800 | -1.90419400 | 0.13323700 |
| H | -5.28777100 | 1.07792300 | -0.51872600 |
| C | -0.01230700 | -0.10773500 | 0.75510900 |
| H | 0.72744400 | -0.14138800 | -0.04597400 |
| H | -0.15906300 | 0.94037800 | 1.01721000 |
| H | -5.53761400 | -0.22131600 | -1.70587000 |
| O | -7.09179100 | 0.04671300 | -0.33540700 |
| C | -8.00895600 | 0.77981600 | -1.02785400 |
| O | -9.15824100 | 0.73609000 | -0.68114200 |
| C | 0.49535400 | -0.88329400 | 1.95851600 |
| C | 1.35373600 | -0.24192400 | 2.85960900 |
| C | 0.18113700 | -2.22993800 | 2.16742500 |
| C | 1.89277500 | -0.93460100 | 3.94128400 |
| H | 1.60212700 | 0.80326000 | 2.70758300 |
| C | 0.71809600 | -2.92175700 | 3.25504600 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.48792900 | -2.74199500 | 1.48550900 |
| C | 1.57680400 | -2.27805900 | 4.14292600 |
| H | 2.55931500 | -0.42409300 | 4.62757000 |
| H | 0.46502500 | -3.96568600 | 3.40269500 |
| H | 1.99546200 | -2.81727500 | 4.98493800 |
| C | -7.51665100 | 1.60133800 | -2.20021700 |
| H | -6.75296000 | 2.31949200 | -1.89121900 |
| H | -7.07614700 | 0.96199800 | -2.96973600 |
| H | -8.36528200 | 2.13542100 | -2.62103300 |
| C | -3.51730000 | -0.97585200 | 0.04221200 |
| S | -2.79934800 | -1.88590500 | -1.28726900 |
| C | -2.64154200 | 0.52688100 | 1.92733200 |
| H | -2.06547900 | 0.13505900 | 2.77035200 |
| H | -2.27077500 | 1.53365300 | 1.71379200 |
| H | -3.68308000 | 0.60585900 | 2.23926800 |
| C | 4.37186300 | 1.29772600 | 0.05086200 |
| O | 5.34566100 | 2.05639800 | 0.74677700 |
| C | 3.19859200 | 2.14772800 | -0.34748400 |
| C | 2.72235300 | 2.62355700 | -1.53224000 |
| O | 2.45204400 | 2.64679700 | 0.68354300 |
| C | 1.61323000 | 3.47071300 | -1.21311900 |
| H | 3.11650900 | 2.40726900 | -2.51236700 |
| C | 1.49308300 | 3.45944800 | 0.14309800 |
| H | 0.99271000 | 4.02203700 | -1.90228900 |
| H | 4.02994800 | 0.50832400 | 0.72649200 |
| H | 5.99081100 | 2.33627800 | 0.07728100 |
| C | 2.00200100 | -3.14184000 | -1.46640500 |
| H | 1.89928900 | -3.95512000 | -2.18776600 |
| H | 1.05920800 | -2.58013500 | -1.45354900 |
| O | 2.25990500 | -3.74376600 | -0.19623100 |
| H | 1.93731900 | -3.15883700 | 0.49906800 |
| C | 0.60062300 | 4.17557800 | 1.08594000 |
| H | 0.03113600 | 4.92225400 | 0.52277400 |
| H | 1.20506100 | 4.69560500 | 1.83773800 |
| O | -0.29550300 | 3.25270400 | 1.73764600 |
| H | -0.54388500 | 3.62365500 | 2.59037500 |

IM1b

| | | | |
|---|-------------|------------|-------------|
| C | -1.47337300 | 4.12235500 | -0.69097800 |
| C | -1.60892700 | 3.55580100 | -1.92946900 |
| H | -2.28989000 | 3.88050500 | -2.69797100 |
| C | -0.67978900 | 2.48380100 | -1.96712400 |
| C | 0.99352800 | 1.59648400 | -0.27033000 |
| H | 1.29050100 | 0.80479600 | -0.97689800 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.03938600 | 2.46850600 | -0.75174500 |
| O | -0.52933600 | 3.48547500 | 0.03454700 |
| O | 1.55045000 | 1.70515800 | 0.82592900 |
| H | -0.48535700 | 1.80107100 | -2.78014200 |
| N | 3.58797000 | 0.11439600 | 1.75249400 |
| C | 3.57268200 | 0.74892800 | 3.12573400 |
| H | 3.95931900 | 1.76010400 | 2.98972100 |
| H | 2.52078600 | 0.84682300 | 3.39567400 |
| C | 4.77108100 | 0.49272900 | 0.88068500 |
| H | 4.49928300 | 0.14014700 | -0.11923900 |
| H | 4.78270600 | 1.58445500 | 0.86139000 |
| C | 3.30769300 | -1.37100800 | 1.73372700 |
| H | 3.38026900 | -1.66275600 | 0.68253100 |
| H | 4.10095400 | -1.86456200 | 2.29525200 |
| C | 4.33151800 | 0.01550900 | 4.22553300 |
| H | 5.39183600 | -0.10493700 | 4.00598300 |
| H | 4.24824400 | 0.60527600 | 5.14198600 |
| H | 3.90789900 | -0.96824500 | 4.43344900 |
| C | 6.12682600 | -0.06231400 | 1.29188100 |
| H | 6.83939700 | 0.19826400 | 0.50568600 |
| H | 6.50265500 | 0.35854200 | 2.22630500 |
| H | 6.12245100 | -1.15106000 | 1.36710200 |
| C | 1.92791600 | -1.71529800 | 2.27703200 |
| H | 1.78856200 | -2.79531400 | 2.18687100 |
| H | 1.80628300 | -1.45606600 | 3.33194200 |
| H | 1.13243600 | -1.23708000 | 1.69945200 |
| H | 2.77805900 | 0.57978800 | 1.27028500 |
| C | -2.15645100 | 5.26699400 | -0.02313200 |
| H | -2.68382600 | 4.89910700 | 0.86819800 |
| H | -1.40057900 | 5.99030100 | 0.31350800 |
| O | -3.05355200 | 5.84426600 | -0.96049900 |
| H | -3.56107900 | 6.53253300 | -0.52144400 |
| C | -1.35615700 | -1.03371900 | 0.42789100 |
| C | -3.11859700 | -2.28901900 | -0.55414000 |
| N | -1.76435000 | -1.93444600 | -0.49890600 |
| C | -5.28792800 | -1.72498500 | 0.64356400 |
| C | -0.78320600 | -2.53214200 | -1.42221100 |
| H | 0.17973900 | -2.05116000 | -1.26718800 |
| H | -0.69052200 | -3.60382700 | -1.23414100 |
| C | -3.84463100 | -1.62258300 | 0.39262600 |
| S | -2.75906000 | -0.57956400 | 1.30853000 |
| C | -3.60384600 | -3.28172900 | -1.56060700 |
| H | -3.42654200 | -2.92169800 | -2.57879500 |
| H | -3.07258800 | -4.23247300 | -1.45575100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.66889000 | -3.45288600 | -1.42903000 |
| H | -1.09115800 | -2.37530000 | -2.45682600 |
| O | -5.66000500 | -0.91387600 | 1.66002800 |
| C | -7.05778500 | -0.92940300 | 1.99880800 |
| H | -7.36438900 | -1.92934000 | 2.30880500 |
| H | -7.66093500 | -0.61805700 | 1.14487000 |
| H | -7.16286500 | -0.22442000 | 2.82041300 |
| O | -6.07158800 | -2.42914600 | 0.04285100 |
| I | 2.97532300 | -1.16957800 | -2.18552700 |

TS1b

| | | | |
|---|-------------|-------------|-------------|
| C | -1.60937700 | 4.10719700 | 0.07395000 |
| C | -1.09450400 | 4.25513600 | -1.18161900 |
| H | -1.31232100 | 5.06124200 | -1.86481200 |
| C | -0.22505800 | 3.14411800 | -1.39721000 |
| C | 0.46124100 | 1.17228500 | 0.11429000 |
| H | 1.07742800 | 0.78440700 | -0.70570500 |
| C | -0.26956500 | 2.39617400 | -0.25286600 |
| O | -1.10375300 | 2.97970200 | 0.65297800 |
| O | 0.76685400 | 0.92960700 | 1.31369000 |
| H | 0.37432700 | 2.92663300 | -2.26785100 |
| C | -1.15261100 | -0.21169400 | -0.37976800 |
| C | -2.84644300 | -1.44643600 | -1.43017900 |
| N | -1.65243300 | -0.72063900 | -1.51880500 |
| C | -4.49641700 | -2.18630900 | 0.36124500 |
| C | -0.96428800 | -0.49931600 | -2.80561400 |
| H | 0.08144400 | -0.26384600 | -2.61030000 |
| H | -0.99666500 | -1.41013700 | -3.40067200 |
| N | 3.00783000 | -0.31072000 | 1.97117100 |
| C | 2.86049300 | -0.16454100 | 3.46605900 |
| H | 2.98809000 | 0.89869800 | 3.67565600 |
| H | 1.81923300 | -0.40331800 | 3.68713200 |
| C | 4.04832400 | 0.58721600 | 1.33609500 |
| H | 3.88032700 | 0.49233200 | 0.25905600 |
| H | 3.77752200 | 1.60302800 | 1.63149200 |
| C | 3.09780000 | -1.73066800 | 1.47420900 |
| H | 3.23125900 | -1.65384100 | 0.39140300 |
| H | 3.99023900 | -2.18812700 | 1.90255800 |
| C | 3.78672200 | -1.00824500 | 4.33565400 |
| H | 4.84212200 | -0.80483400 | 4.15746900 |
| H | 3.57602100 | -0.77268700 | 5.38205300 |
| H | 3.61593900 | -2.07795500 | 4.20390600 |
| C | 5.50464200 | 0.29272200 | 1.66660500 |
| H | 6.12254500 | 0.94246700 | 1.04219800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 5.76031200 | 0.49941900 | 2.70756200 |
| H | 5.78471200 | -0.73490700 | 1.42752200 |
| C | 1.84761800 | -2.54287100 | 1.78534700 |
| H | 1.94897300 | -3.52344500 | 1.31501000 |
| H | 1.69118500 | -2.70100200 | 2.85540600 |
| H | 0.95801800 | -2.06669600 | 1.36852500 |
| C | -3.28677700 | -1.51110500 | -0.13748400 |
| S | -2.18142600 | -0.63911800 | 0.91385900 |
| C | -3.47163800 | -2.03746300 | -2.65125900 |
| H | -3.61432300 | -1.27500000 | -3.42201400 |
| H | -2.83322300 | -2.81951500 | -3.07441500 |
| H | -4.43304100 | -2.47586900 | -2.39737200 |
| H | 2.08266800 | 0.09456300 | 1.60030000 |
| C | -2.56765500 | 4.90963300 | 0.87250200 |
| H | -2.19405300 | 5.00299400 | 1.89937900 |
| H | -2.63008800 | 5.91158300 | 0.43207300 |
| O | -3.85486200 | 4.27329900 | 0.86634700 |
| H | -4.39596800 | 4.68034500 | 1.55064100 |
| H | -1.44841300 | 0.31387800 | -3.35026400 |
| O | -4.60922600 | -2.04108300 | 1.69802100 |
| C | -5.76210700 | -2.65310900 | 2.30670300 |
| H | -5.75498900 | -3.73017900 | 2.13561100 |
| H | -6.67833300 | -2.22795400 | 1.89549700 |
| H | -5.67814800 | -2.43133700 | 3.36793400 |
| O | -5.29732900 | -2.79586400 | -0.31249800 |
| I | 3.00766700 | -0.64541800 | -2.31455700 |

IM2b

| | | | |
|---|-------------|-------------|-------------|
| C | 0.59700200 | 3.66302700 | -1.90297000 |
| C | -0.49421700 | 4.08359800 | -1.20317000 |
| H | -0.88951800 | 5.08734500 | -1.18950800 |
| C | -0.99116300 | 2.94752500 | -0.48876900 |
| C | -0.17470700 | 0.46790100 | -0.41556000 |
| H | -0.85465600 | 0.38105200 | 0.46334000 |
| C | -0.16985000 | 1.91136300 | -0.80984600 |
| O | 0.80723200 | 2.33123400 | -1.67267400 |
| O | -0.54872500 | -0.40030600 | -1.46453900 |
| H | -1.82392500 | 2.89490800 | 0.19600000 |
| C | 1.18325900 | 0.01298400 | 0.03427700 |
| C | 3.16295500 | -0.11449200 | 1.19285000 |
| N | 1.92828500 | 0.51289500 | 1.02765300 |
| C | 4.48834800 | -2.03666100 | 0.16365500 |
| C | 1.46790500 | 1.63852200 | 1.87391200 |
| H | 0.40800600 | 1.50044600 | 2.10542600 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2. 02685900 | 1. 62235600 | 2. 80422000 |
| N | -3. 06449500 | -1. 43238400 | -1. 31370100 |
| C | -3. 07961400 | -2. 03274800 | -2. 66632800 |
| H | -3. 06689400 | -1. 20138400 | -3. 37716700 |
| H | -2. 12802500 | -2. 55725600 | -2. 80173600 |
| C | -3. 90432900 | -0. 22252300 | -1. 14854600 |
| H | -3. 62952400 | 0. 20707200 | -0. 18077700 |
| H | -3. 58851900 | 0. 49110300 | -1. 91698000 |
| C | -3. 22821800 | -2. 39214900 | -0. 20034600 |
| H | -3. 20993300 | -1. 80671400 | 0. 72231400 |
| H | -4. 20540800 | -2. 89287100 | -0. 24473600 |
| C | -4. 21554100 | -3. 00233100 | -3. 02688100 |
| H | -5. 20028200 | -2. 53703000 | -2. 97859700 |
| H | -4. 06466800 | -3. 35948100 | -4. 05025800 |
| H | -4. 22644100 | -3. 87944100 | -2. 37547700 |
| C | -5. 43149800 | -0. 37537000 | -1. 19652200 |
| H | -5. 88893300 | 0. 58001000 | -0. 92326100 |
| H | -5. 79806500 | -0. 64261600 | -2. 18994700 |
| H | -5. 78955700 | -1. 12064100 | -0. 48250300 |
| C | -2. 12377500 | -3. 44571600 | -0. 13723900 |
| H | -2. 26377200 | -4. 06032200 | 0. 75556900 |
| H | -2. 12630300 | -4. 11397100 | -1. 00281500 |
| H | -1. 13887000 | -2. 97787000 | -0. 06883400 |
| C | 3. 32666200 | -1. 13354300 | 0. 29478500 |
| S | 1. 93382600 | -1. 29435600 | -0. 75340900 |
| C | 4. 11391600 | 0. 33774800 | 2. 25081800 |
| H | 4. 32620800 | 1. 40557700 | 2. 15201600 |
| H | 3. 69612400 | 0. 16605100 | 3. 24745500 |
| H | 5. 04189800 | -0. 22060700 | 2. 16436000 |
| H | -1. 48072300 | -0. 76895500 | -1. 31120600 |
| C | 1. 55420800 | 4. 35288600 | -2. 80053600 |
| H | 1. 68797300 | 3. 76690900 | -3. 71827700 |
| H | 1. 13156900 | 5. 32776300 | -3. 06872600 |
| O | 2. 81257800 | 4. 50999100 | -2. 12507800 |
| H | 3. 46242400 | 4. 81876600 | -2. 76498200 |
| H | 1. 63847900 | 2. 57873000 | 1. 34844000 |
| O | 4. 27535500 | -2. 93399500 | -0. 81636000 |
| C | 5. 33408600 | -3. 88657300 | -1. 05309700 |
| H | 5. 51603200 | -4. 47663700 | -0. 15475600 |
| H | 6. 24870100 | -3. 36783800 | -1. 34095200 |
| H | 4. 97573300 | -4. 51652400 | -1. 86312500 |
| O | 5. 49495400 | -1. 98965200 | 0. 83131700 |
| I | -2. 13202700 | 0. 45357200 | 2. 74562500 |

IM5b

| | | | |
|---|--------------|--------------|--------------|
| C | 4. 05156800 | -1. 50639000 | 0. 74918500 |
| C | 4. 07480500 | -2. 51069100 | -0. 16852000 |
| H | 4. 81473800 | -3. 29451600 | -0. 22484000 |
| C | 2. 95777500 | -2. 30752600 | -1. 04045000 |
| C | 1. 12568600 | -0. 45657200 | -1. 18825900 |
| C | 2. 32415300 | -1. 18802800 | -0. 59865600 |
| O | 2. 97674500 | -0. 68717700 | 0. 50050300 |
| O | 0. 72615800 | -1. 04351600 | -2. 32780600 |
| H | 2. 65736400 | -2. 88260900 | -1. 89917300 |
| C | 1. 53731400 | 1. 09197700 | -1. 51365800 |
| O | 2. 04466000 | 1. 04519300 | -2. 81600400 |
| C | 0. 39012100 | 2. 04885600 | -1. 41528700 |
| C | -0. 58248200 | 2. 45254400 | -2. 27845900 |
| O | 0. 21225600 | 2. 66642400 | -0. 20300300 |
| C | -1. 42247400 | 3. 35871100 | -1. 55284600 |
| H | -0. 67539100 | 2. 14196000 | -3. 30522700 |
| C | -0. 90413800 | 3. 45778200 | -0. 29832000 |
| H | -2. 29606200 | 3. 87632600 | -1. 91929300 |
| H | 2. 31986800 | 1. 41362400 | -0. 81899800 |
| H | 1. 63688700 | 0. 21473900 | -3. 17195700 |
| C | 4. 92261400 | -1. 16247100 | 1. 89744600 |
| H | 5. 58082100 | -2. 01866300 | 2. 08882700 |
| H | 4. 31074900 | -0. 99373200 | 2. 79410500 |
| O | 5. 68843200 | 0. 01346000 | 1. 59675600 |
| H | 6. 17945300 | 0. 26495800 | 2. 38646600 |
| C | -1. 26905100 | 4. 25121900 | 0. 89647500 |
| H | -2. 10310100 | 4. 90927700 | 0. 62839500 |
| H | -0. 42152200 | 4. 87226100 | 1. 21434800 |
| O | -1. 64439600 | 3. 37255800 | 1. 98350600 |
| H | -1. 87498100 | 3. 92346500 | 2. 74073700 |
| C | -0. 08978300 | -0. 55684100 | -0. 24284700 |
| C | -1. 66954700 | -0. 52234000 | 1. 43237100 |
| N | -0. 38092000 | -0. 18158700 | 1. 01312700 |
| C | -3. 71774800 | -1. 72797600 | 0. 53461300 |
| C | 0. 53475700 | 0. 55132300 | 1. 90739500 |
| H | 1. 47065100 | 0. 73212100 | 1. 39552600 |
| H | 0. 06938700 | 1. 49541400 | 2. 18437600 |
| C | -2. 34667100 | -1. 18748300 | 0. 44746000 |
| S | -1. 37370300 | -1. 36660400 | -1. 00791400 |
| C | -2. 13996100 | -0. 12790900 | 2. 79326800 |
| H | -1. 50056400 | -0. 55948800 | 3. 57145200 |
| H | -2. 11626800 | 0. 96167300 | 2. 89688400 |
| H | -3. 15636400 | -0. 48186800 | 2. 94046900 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.72554800 | -0.05780900 | 2.79126900 |
| O | -4.08882100 | -2.26994200 | -0.64218300 |
| C | -5.39949100 | -2.86817400 | -0.69004000 |
| H | -6.15837800 | -2.13267500 | -0.41835300 |
| H | -5.45305200 | -3.71605500 | -0.00473100 |
| H | -5.53059200 | -3.19561400 | -1.71895200 |
| O | -4.42730800 | -1.70651100 | 1.51550500 |

TS4b

| | | | |
|---|-------------|-------------|-------------|
| C | 3.88826300 | -1.71719900 | 0.72104700 |
| C | 3.90287800 | -2.68276900 | -0.24015400 |
| H | 4.52588500 | -3.56383500 | -0.23878100 |
| C | 2.96016400 | -2.28688600 | -1.23919600 |
| C | 1.42837800 | -0.20405500 | -1.47121400 |
| C | 2.43093200 | -1.10367600 | -0.82102500 |
| O | 2.98674900 | -0.74318300 | 0.37825200 |
| O | 0.94348400 | -0.58388700 | -2.56428100 |
| H | 2.70450400 | -2.78933400 | -2.15726000 |
| C | 1.73509000 | 1.33138400 | -1.35688200 |
| O | 2.51450600 | 1.65520100 | -2.50296500 |
| C | 0.50118700 | 2.17464200 | -1.26197700 |
| C | -0.52920700 | 2.45399500 | -2.10799700 |
| O | 0.29754500 | 2.81080700 | -0.06483800 |
| C | -1.43280400 | 3.29559400 | -1.38524000 |
| H | -0.63440900 | 2.08534200 | -3.11503300 |
| C | -0.89316400 | 3.48247000 | -0.14816300 |
| H | -2.36532600 | 3.70874900 | -1.73814900 |
| H | 2.35300700 | 1.53508800 | -0.48112400 |
| H | 2.16025800 | 1.10806100 | -3.22080900 |
| C | 4.63417200 | -1.54509200 | 1.99049300 |
| H | 5.11212900 | -2.50137300 | 2.23400000 |
| H | 3.93624200 | -1.29410900 | 2.80068100 |
| O | 5.61284500 | -0.50658700 | 1.84459600 |
| H | 5.99959900 | -0.33035400 | 2.70863800 |
| C | -1.31460100 | 4.25878800 | 1.03879800 |
| H | -2.18421500 | 4.86402200 | 0.76233300 |
| H | -0.50759300 | 4.93092300 | 1.35602700 |
| O | -1.64697800 | 3.36490500 | 2.12619500 |
| H | -1.81234400 | 3.90196000 | 2.90876300 |
| C | -0.11182100 | -0.42271300 | -0.15999900 |
| C | -1.80324000 | -0.63396800 | 1.43945100 |
| N | -0.51403000 | -0.20886700 | 1.10468900 |
| C | -3.75765800 | -1.82042900 | 0.33099100 |
| C | 0.34934300 | 0.46945700 | 2.08715400 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1. 33513600 | 0. 57941300 | 1. 64855200 |
| H | -0. 06934000 | 1. 44678900 | 2. 32622700 |
| C | -2. 40489500 | -1. 23692200 | 0. 37005000 |
| S | -1. 34506200 | -1. 22541600 | -1. 02755200 |
| C | -2. 35380200 | -0. 37526500 | 2. 80295100 |
| H | -1. 76136300 | -0. 88361700 | 3. 57030400 |
| H | -2. 33318200 | 0. 69778200 | 3. 01546600 |
| H | -3. 37786600 | -0. 73433700 | 2. 85934400 |
| H | 0. 42264200 | -0. 14269100 | 2. 98717400 |
| O | -4. 03060700 | -2. 31601000 | -0. 89270600 |
| C | -5. 32774600 | -2. 91868400 | -1. 06057400 |
| H | -6. 11336100 | -2. 18706700 | -0. 86795400 |
| H | -5. 44478700 | -3. 76266800 | -0. 37967400 |
| H | -5. 35733800 | -3. 25192500 | -2. 09523400 |
| O | -4. 53727900 | -1. 86376400 | 1. 25742800 |

IM6b

| | | | |
|---|--------------|--------------|--------------|
| C | 2. 32136300 | -2. 86476700 | -0. 67551800 |
| C | 3. 46384000 | -3. 58225000 | -0. 92336200 |
| H | 3. 50729200 | -4. 55335300 | -1. 39027600 |
| C | 4. 54643500 | -2. 81070700 | -0. 43197700 |
| C | 4. 61594900 | -0. 52586600 | 0. 74104100 |
| C | 4. 00121000 | -1. 66445500 | 0. 08948700 |
| O | 2. 63534500 | -1. 69563400 | -0. 06331000 |
| O | 5. 82162700 | -0. 46767900 | 0. 94011600 |
| H | 5. 59765100 | -3. 05056800 | -0. 44055800 |
| C | 3. 73963200 | 0. 65720500 | 1. 20049700 |
| O | 4. 44780400 | 1. 41630500 | 2. 16387700 |
| C | 3. 33669000 | 1. 48895200 | 0. 01867200 |
| C | 3. 85054800 | 1. 67121400 | -1. 22999900 |
| O | 2. 26850400 | 2. 32118200 | 0. 20502000 |
| C | 3. 05037900 | 2. 67887900 | -1. 85429200 |
| H | 4. 69957600 | 1. 15685500 | -1. 65155700 |
| C | 2. 10597200 | 3. 04550600 | -0. 94428200 |
| H | 3. 16301300 | 3. 08023300 | -2. 84936400 |
| H | 2. 83442700 | 0. 27269200 | 1. 68000600 |
| H | 5. 38727700 | 1. 21516100 | 2. 01971100 |
| C | 0. 87824600 | -3. 15025200 | -0. 93547600 |
| H | 0. 83009300 | -4. 06765600 | -1. 53657200 |
| H | 0. 45572300 | -2. 33791200 | -1. 54332600 |
| O | 0. 16135000 | -3. 29775100 | 0. 27076200 |
| H | -0. 64442000 | -2. 72096300 | 0. 22419200 |
| C | 1. 02801500 | 4. 06163200 | -0. 96816400 |
| H | 1. 18373200 | 4. 69639000 | -1. 84671700 |

| | | | |
|---|-------------|-------------|-------------|
| H | 1.08834100 | 4.68830300 | -0.06972800 |
| O | -0.26187700 | 3.42130900 | -1.03007700 |
| H | -0.92960900 | 4.11264300 | -1.09547100 |
| C | -2.07171100 | -1.46533100 | 0.13001900 |
| C | -3.16807000 | 0.56911000 | 0.62305200 |
| N | -1.99178200 | -0.18511200 | 0.55110400 |
| C | -5.65276400 | 0.27120600 | 0.16796300 |
| C | -0.68634400 | 0.40114400 | 0.90529100 |
| H | 0.05983000 | -0.38188900 | 0.80663700 |
| H | -0.45029600 | 1.23033500 | 0.23797100 |
| C | -4.25014700 | -0.16815300 | 0.23244100 |
| S | -3.71800900 | -1.78643600 | -0.20744700 |
| C | -3.12591100 | 1.98814800 | 1.08717800 |
| H | -2.78099500 | 2.04472000 | 2.12472600 |
| H | -2.42523800 | 2.56639500 | 0.47870500 |
| H | -4.11731100 | 2.42885900 | 1.02454800 |
| H | -0.70267400 | 0.75745000 | 1.93664600 |
| O | -6.44837700 | -0.72735800 | -0.26850800 |
| C | -7.85144300 | -0.42142400 | -0.37455800 |
| H | -8.00969100 | 0.39717100 | -1.07766200 |
| H | -8.25422100 | -0.14314500 | 0.60001800 |
| H | -8.31772200 | -1.33465900 | -0.73649100 |
| O | -6.06631400 | 1.37249600 | 0.45935800 |

IM1_{TPT}

| | | | |
|---|-------------|-------------|-------------|
| O | -1.99297600 | 1.85829300 | -1.32412400 |
| H | -1.18089800 | 1.51404600 | -0.87981400 |
| C | -3.63549300 | 1.28716600 | 0.38787200 |
| C | -3.56226900 | 0.82042100 | 1.67576800 |
| H | -2.89828700 | 1.18574300 | 2.44372900 |
| C | -4.51747900 | -0.22245600 | 1.78113300 |
| C | -6.15477000 | -1.22314900 | 0.09445100 |
| H | -6.49500900 | -1.91819600 | 0.88513600 |
| C | -5.11595900 | -0.32808800 | 0.54795300 |
| O | -4.57826100 | 0.59875000 | -0.30381500 |
| O | -6.64139300 | -1.25265200 | -1.02499300 |
| C | -2.88809200 | 2.35767900 | -0.34099500 |
| H | -2.36991600 | 2.96921200 | 0.40632400 |
| H | -4.74530700 | -0.82638800 | 2.64676000 |
| H | -3.60321500 | 3.00300400 | -0.85945600 |
| C | 2.40925000 | -0.48689600 | -0.01491200 |
| C | 0.59763600 | 0.85654900 | -0.22039900 |
| N | 1.02593700 | -0.44437100 | -0.17609000 |
| N | 1.75637900 | 1.52870000 | -0.07176200 |

| | | | |
|---|--------------|--------------|--------------|
| N | 2. 87588300 | 0. 72995700 | 0. 04949300 |
| C | 3. 26678100 | -1. 68057500 | 0. 07255900 |
| C | 3. 04842900 | -2. 80823900 | -0. 73071600 |
| C | 4. 35752400 | -1. 66590900 | 0. 95475400 |
| C | 3. 90676500 | -3. 90187700 | -0. 64750900 |
| H | 2. 22351900 | -2. 82891300 | -1. 43160000 |
| C | 5. 21022500 | -2. 76283100 | 1. 03407200 |
| H | 4. 52899300 | -0. 79629900 | 1. 57783000 |
| C | 4. 98590300 | -3. 88465900 | 0. 23545400 |
| H | 3. 73255600 | -4. 76662300 | -1. 27782400 |
| H | 6. 04741300 | -2. 74263100 | 1. 72285300 |
| H | 5. 65015500 | -4. 73941000 | 0. 29898500 |
| C | 1. 92124700 | 2. 94896200 | -0. 05087500 |
| C | 3. 05488200 | 3. 51720200 | -0. 63245500 |
| C | 0. 95428000 | 3. 74951600 | 0. 55634500 |
| C | 3. 21380700 | 4. 90085800 | -0. 60793100 |
| H | 3. 79678200 | 2. 88279500 | -1. 10005400 |
| C | 1. 11888900 | 5. 13281100 | 0. 56464200 |
| H | 0. 09106100 | 3. 29248500 | 1. 02206900 |
| C | 2. 24748200 | 5. 71267000 | -0. 01414300 |
| H | 4. 09342000 | 5. 34359200 | -1. 06152100 |
| H | 0. 36717400 | 5. 75581500 | 1. 03613000 |
| H | 2. 37454700 | 6. 78919200 | -0. 00033800 |
| C | -1. 47235300 | -2. 90776700 | -1. 41718600 |
| C | -1. 61857400 | -3. 72853600 | -0. 29906700 |
| C | -0. 88969400 | -3. 46282600 | 0. 86021300 |
| C | -0. 01590300 | -2. 37828300 | 0. 90574200 |
| C | 0. 12879500 | -1. 57077900 | -0. 22070600 |
| C | -0. 59314200 | -1. 82694700 | -1. 38391000 |
| H | -2. 04033700 | -3. 10725800 | -2. 31871800 |
| H | -2. 30146100 | -4. 57019100 | -0. 33004800 |
| H | -1. 00515300 | -4. 09398000 | 1. 73407800 |
| H | 0. 54561600 | -2. 15736700 | 1. 80591500 |
| H | -0. 46698900 | -1. 18786100 | -2. 24938800 |

TS1_{TPT}

| | | | |
|---|--------------|--------------|--------------|
| O | -2. 37985000 | -3. 65560900 | -2. 67267600 |
| H | -2. 73153900 | -2. 95759100 | -3. 23948700 |
| C | -3. 37809300 | -2. 53061300 | -0. 73706700 |
| C | -4. 35497700 | -1. 58289700 | -0. 64332300 |
| H | -5. 30405700 | -1. 59855300 | -1. 15832900 |
| C | -3. 87424600 | -0. 59038300 | 0. 26984300 |
| C | -1. 68292200 | -0. 41343400 | 1. 67191300 |
| H | -2. 08673900 | 0. 56747100 | 1. 98953700 |

| | | | |
|---|-------------|-------------|-------------|
| C | -2.63485000 | -0.99993000 | 0.67087200 |
| O | -2.32531900 | -2.18354600 | 0.06875700 |
| O | -1.09823700 | -1.14652000 | 2.51064600 |
| C | -3.25594700 | -3.77839100 | -1.53452300 |
| H | -4.25726700 | -4.08596400 | -1.85382000 |
| H | -4.38319700 | 0.30421700 | 0.59517000 |
| H | -2.82937900 | -4.58115400 | -0.93008800 |
| C | 1.67643000 | 1.09417700 | -0.21230200 |
| C | -0.34253400 | 0.45255800 | 0.51657000 |
| N | 0.94232100 | 0.04060500 | 0.33083300 |
| N | -0.32861400 | 1.72030400 | 0.09222900 |
| N | 0.90518900 | 2.13750400 | -0.36449000 |
| C | 3.10526100 | 1.09695400 | -0.57069900 |
| C | 3.72268500 | -0.00017900 | -1.18674900 |
| C | 3.85296400 | 2.25854900 | -0.32506700 |
| C | 5.06674900 | 0.06624100 | -1.54530000 |
| H | 3.15787300 | -0.89783000 | -1.40125700 |
| C | 5.19600200 | 2.31684000 | -0.68420300 |
| H | 3.37965500 | 3.10822100 | 0.15198700 |
| C | 5.80712500 | 1.22050900 | -1.29299500 |
| H | 5.53346200 | -0.78585600 | -2.02637300 |
| H | 5.76546600 | 3.21761200 | -0.48461000 |
| H | 6.85438800 | 1.26606300 | -1.57050500 |
| C | -1.42636600 | 2.65132300 | 0.06421700 |
| C | -2.10258500 | 2.86709800 | -1.13338600 |
| C | -1.76470500 | 3.34359000 | 1.22411400 |
| C | -3.14715000 | 3.78890200 | -1.16498000 |
| H | -1.81270900 | 2.31953900 | -2.02247300 |
| C | -2.81361700 | 4.26067200 | 1.18331900 |
| H | -1.21307700 | 3.16843800 | 2.14013300 |
| C | -3.50330200 | 4.48321900 | -0.00851900 |
| H | -3.68068400 | 3.96359500 | -2.09224600 |
| H | -3.08616300 | 4.80343900 | 2.08115700 |
| H | -4.31659500 | 5.19979200 | -0.03665500 |
| C | 1.61326200 | -3.62050000 | 0.29480100 |
| C | 2.49740100 | -3.73889200 | 1.36651600 |
| C | 2.85839500 | -2.60977900 | 2.10231900 |
| C | 2.33801200 | -1.36167600 | 1.76925500 |
| C | 1.45968700 | -1.25878300 | 0.69429900 |
| C | 1.09189700 | -2.37476200 | -0.04908400 |
| H | 1.32792000 | -4.49606100 | -0.27714800 |
| H | 2.90162900 | -4.70970900 | 1.63082900 |
| H | 3.53913000 | -2.69961300 | 2.94115200 |
| H | 2.60221800 | -0.48025800 | 2.34113100 |

| | | | |
|--------------------------|-------------|-------------|-------------|
| H | 0.40718400 | -2.27177000 | -0.88098300 |
| IM2_{TPT} | | | |
| O | 1.69511300 | 3.97217700 | -2.66520800 |
| H | 2.30410600 | 3.47070600 | -3.22183700 |
| C | 2.77700800 | 3.02176000 | -0.67791800 |
| C | 3.98656900 | 2.42577300 | -0.47309300 |
| H | 4.93871900 | 2.78506100 | -0.83516700 |
| C | 3.73814400 | 1.25729400 | 0.31730900 |
| C | 1.55409000 | 0.29357300 | 1.42465200 |
| H | 2.27276100 | -0.53314100 | 1.64499600 |
| C | 2.39239300 | 1.21534100 | 0.54555000 |
| O | 1.79743700 | 2.28685100 | -0.05994900 |
| O | 0.97981000 | 0.84475200 | 2.48733900 |
| C | 2.36433200 | 4.24266900 | -1.41760400 |
| H | 3.25166300 | 4.86200500 | -1.58506600 |
| H | 4.46365700 | 0.54648300 | 0.68305100 |
| H | 1.65112500 | 4.82510900 | -0.83143800 |
| C | -1.42504200 | -1.21355300 | -0.26279100 |
| C | 0.49152400 | -0.45853300 | 0.55854500 |
| N | -0.81361500 | -0.13162500 | 0.36345600 |
| N | 0.61983800 | -1.68954000 | 0.05474400 |
| N | -0.55859800 | -2.17230700 | -0.45753000 |
| C | -2.84353900 | -1.33227200 | -0.64342400 |
| C | -3.53399700 | -0.29759000 | -1.28911100 |
| C | -3.49811400 | -2.54641500 | -0.38771700 |
| C | -4.86199600 | -0.47779400 | -1.66648800 |
| H | -3.03887500 | 0.63871200 | -1.51110200 |
| C | -4.82664600 | -2.71744800 | -0.76512600 |
| H | -2.96718900 | -3.34681400 | 0.11351100 |
| C | -5.51189300 | -1.68362600 | -1.40338600 |
| H | -5.38711000 | 0.32578500 | -2.17038700 |
| H | -5.32699300 | -3.65660500 | -0.55678500 |
| H | -6.54766700 | -1.81717400 | -1.69517100 |
| C | 1.79636400 | -2.52178200 | 0.01653800 |
| C | 2.70590900 | -2.37606000 | -1.02760200 |
| C | 1.96657800 | -3.48511800 | 1.00827500 |
| C | 3.82253100 | -3.20944600 | -1.06665500 |
| H | 2.54149800 | -1.62815300 | -1.79465900 |
| C | 3.08663500 | -4.31156200 | 0.95891300 |
| H | 1.23748200 | -3.57813000 | 1.80513700 |
| C | 4.01357600 | -4.17274700 | -0.07549400 |
| H | 4.53984700 | -3.10625800 | -1.87327000 |
| H | 3.23379000 | -5.06117500 | 1.72842200 |

| | | | |
|---|-------------|-------------|-------------|
| H | 4.88428300 | -4.81787500 | -0.11015100 |
| C | -2.09903600 | 3.36440000 | 0.48813200 |
| C | -2.91741800 | 3.30365400 | 1.61465800 |
| C | -3.02588200 | 2.11370200 | 2.33589900 |
| C | -2.31499500 | 0.98608000 | 1.93614300 |
| C | -1.49802500 | 1.06567400 | 0.81238700 |
| C | -1.38724900 | 2.23864800 | 0.07609000 |
| H | -2.01360400 | 4.28609100 | -0.07602800 |
| H | -3.47047500 | 4.18104100 | 1.93091500 |
| H | -3.65828800 | 2.06357600 | 3.21482700 |
| H | -2.38137600 | 0.06114900 | 2.49536900 |
| H | -0.75055100 | 2.27594800 | -0.79740700 |

IM5_{TPT}

| | | | |
|---|-------------|-------------|-------------|
| O | -4.90252400 | -2.64965800 | -1.68956300 |
| H | -4.65834900 | -3.38857700 | -2.26116900 |
| C | -2.82655400 | -1.55486500 | -2.39648000 |
| C | -2.02743800 | -1.74327600 | -3.48633900 |
| H | -2.36317600 | -1.82753100 | -4.50938100 |
| C | -0.68359800 | -1.82130200 | -3.00415700 |
| C | 0.35785000 | -1.79021900 | -0.60765000 |
| C | -0.74664100 | -1.66664600 | -1.65014200 |
| O | -2.04887300 | -1.50538100 | -1.26871300 |
| O | 1.31864200 | -2.61945100 | -1.03129000 |
| C | -4.29995300 | -1.45883600 | -2.23085900 |
| H | -4.73914900 | -1.21485300 | -3.20438400 |
| H | 0.21320100 | -1.99570100 | -3.57623400 |
| H | -4.55981600 | -0.66351800 | -1.53039700 |
| C | 1.58459100 | 1.73431000 | -0.08873200 |
| C | 1.02286200 | -0.40328100 | -0.32962200 |
| N | 2.33256900 | -0.26046100 | -0.08650000 |
| N | 0.52519400 | 0.86756200 | -0.33205200 |
| H | 1.25712400 | -3.41383600 | 0.36792900 |
| C | -0.26925900 | -2.43376000 | 0.79676500 |
| O | 0.71057500 | -3.34855500 | 1.21385600 |
| C | -0.63583100 | -1.53059300 | 1.92836400 |
| C | 0.08348000 | -0.81448700 | 2.84417200 |
| O | -1.96668400 | -1.44282300 | 2.23446400 |
| C | -0.86000900 | -0.25107200 | 3.75916600 |
| H | 1.15712800 | -0.72020400 | 2.87891700 |
| C | -2.09549800 | -0.65714600 | 3.34925200 |
| H | -0.64983900 | 0.36917600 | 4.61781400 |
| C | -3.46093900 | -0.42922300 | 3.87849400 |
| H | -4.03434200 | -1.36189400 | 3.83767900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.37795900 | -0.12037300 | 4.92591500 |
| O | -4.13127800 | 0.59276500 | 3.10982000 |
| H | -5.06367400 | 0.57834400 | 3.35954300 |
| H | -1.18280300 | -2.95008800 | 0.48445400 |
| C | 3.42152400 | -1.21638100 | -0.02097900 |
| C | 4.28268800 | -1.29671900 | -1.11086300 |
| C | 3.66854000 | -1.91047200 | 1.15614700 |
| C | 5.39554500 | -2.12852800 | -1.03184800 |
| H | 4.07189100 | -0.72882700 | -2.00908300 |
| C | 4.78631000 | -2.74124000 | 1.22451000 |
| H | 2.99345900 | -1.82259800 | 1.99625400 |
| C | 5.64684800 | -2.85451500 | 0.13379800 |
| H | 6.06535600 | -2.20946400 | -1.88041700 |
| H | 4.98226900 | -3.29739000 | 2.13420900 |
| H | 6.51417900 | -3.50256500 | 0.19244900 |
| C | -0.81572300 | 1.30859800 | -0.67118500 |
| C | -1.06740100 | 1.72236300 | -1.97706800 |
| C | -1.78968000 | 1.38608200 | 0.31684700 |
| C | -2.32765200 | 2.22335800 | -2.29470600 |
| H | -0.29090300 | 1.65573800 | -2.72919800 |
| C | -3.04738300 | 1.88738000 | -0.01159200 |
| H | -1.56886400 | 1.07409600 | 1.32835400 |
| C | -3.31567000 | 2.30825200 | -1.31311400 |
| H | -2.53374800 | 2.54773900 | -3.30817100 |
| H | -3.80908300 | 1.93935000 | 0.75677100 |
| H | -4.29463800 | 2.70100800 | -1.56464500 |
| C | 1.54946100 | 3.20642200 | -0.06384600 |
| C | 0.57435800 | 3.92442600 | 0.64030300 |
| C | 2.57017100 | 3.89758200 | -0.73323200 |
| C | 0.61888800 | 5.31590100 | 0.66449600 |
| H | -0.20487700 | 3.40522900 | 1.18174200 |
| C | 2.60644600 | 5.28827500 | -0.70599700 |
| H | 3.32553700 | 3.34239200 | -1.27615300 |
| C | 1.62994200 | 6.00012100 | -0.00945700 |
| H | -0.13582900 | 5.86465200 | 1.21621200 |
| H | 3.39568400 | 5.81457700 | -1.23066900 |
| H | 1.65815300 | 7.08390800 | 0.01019500 |
| N | 2.68689300 | 1.05332400 | 0.06372200 |

TS4_{TPT}

| | | | |
|---|------------|-------------|------------|
| O | 5.17542500 | -0.63415600 | 2.34650100 |
| H | 5.10120900 | -1.12964200 | 3.17186800 |
| C | 2.80700300 | -0.05338600 | 2.57339300 |
| C | 1.97755600 | -0.07095500 | 3.65805300 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2. 20538400 | 0. 32962400 | 4. 63462000 |
| C | 0. 77671700 | -0. 72595600 | 3. 24766500 |
| C | 0. 09173900 | -1. 88437700 | 1. 02375300 |
| C | 0. 94951400 | -1. 05961000 | 1. 93476300 |
| O | 2. 18269300 | -0. 65321500 | 1. 51379500 |
| O | -0. 76984400 | -2. 61007800 | 1. 60193200 |
| C | 4. 20068800 | 0. 42545200 | 2. 37956300 |
| H | 4. 43389500 | 1. 13711900 | 3. 17904000 |
| H | -0. 09393600 | -0. 94411700 | 3. 84521700 |
| H | 4. 30190500 | 0. 93897600 | 1. 42270200 |
| C | -2. 15189800 | 1. 42560100 | -0. 20892300 |
| C | -1. 00424100 | -0. 48099200 | 0. 11034500 |
| N | -2. 32434500 | -0. 68448400 | -0. 02795800 |
| N | -0. 88760600 | 0. 87888500 | -0. 00769300 |
| H | -0. 57009400 | -3. 80498400 | 0. 26738500 |
| C | 0. 89186900 | -2. 66831500 | -0. 11415900 |
| O | 0. 07789700 | -3. 77130100 | -0. 47135000 |
| C | 1. 34332900 | -1. 98686200 | -1. 36563200 |
| C | 0. 72941400 | -1. 70981500 | -2. 55408300 |
| O | 2. 67457800 | -1. 69386500 | -1. 46500900 |
| C | 1. 74209600 | -1. 21001500 | -3. 43121200 |
| H | -0. 31008500 | -1. 87166500 | -2. 78863800 |
| C | 2. 90919700 | -1. 21438500 | -2. 72621300 |
| H | 1. 62356900 | -0. 89687600 | -4. 45785700 |
| C | 4. 30193500 | -0. 84836100 | -3. 07883300 |
| H | 4. 99575300 | -1. 56808900 | -2. 63084800 |
| H | 4. 40657000 | -0. 89985600 | -4. 16787000 |
| O | 4. 60909200 | 0. 48383500 | -2. 61519200 |
| H | 5. 56395100 | 0. 60378400 | -2. 69074700 |
| H | 1. 79682600 | -3. 01979500 | 0. 40114900 |
| C | -3. 08672200 | -1. 90625900 | -0. 00810700 |
| C | -4. 04022500 | -2. 07556900 | 0. 99318600 |
| C | -2. 92785400 | -2. 84477700 | -1. 02041900 |
| C | -4. 83123900 | -3. 22034800 | 0. 99029100 |
| H | -4. 15004300 | -1. 32461900 | 1. 76612500 |
| C | -3. 72209500 | -3. 99093400 | -1. 01301400 |
| H | -2. 19332800 | -2. 68590100 | -1. 79789200 |
| C | -4. 67107500 | -4. 18090200 | -0. 01012300 |
| H | -5. 56937300 | -3. 36374800 | 1. 77120100 |
| H | -3. 60028900 | -4. 73033800 | -1. 79637800 |
| H | -5. 28778000 | -5. 07275000 | -0. 00923800 |
| C | 0. 32112500 | 1. 65918900 | 0. 12352300 |
| C | 0. 46804700 | 2. 49558200 | 1. 22798400 |
| C | 1. 28198400 | 1. 61574600 | -0. 88090500 |

| | | | |
|---|--------------|-------------|--------------|
| C | 1. 59356500 | 3. 31190100 | 1. 31612800 |
| H | -0. 28799300 | 2. 51205200 | 2. 00326000 |
| C | 2. 40921200 | 2. 42839000 | -0. 78020900 |
| H | 1. 14676900 | 0. 95963800 | -1. 73069800 |
| C | 2. 56120200 | 3. 28222300 | 0. 31179900 |
| H | 1. 71251000 | 3. 96842900 | 2. 17053900 |
| H | 3. 16801400 | 2. 37669400 | -1. 55149900 |
| H | 3. 43581700 | 3. 91935100 | 0. 38405800 |
| C | -2. 49667100 | 2. 84827000 | -0. 37838800 |
| C | -1. 74730700 | 3. 70148200 | -1. 19955200 |
| C | -3. 64476100 | 3. 33922400 | 0. 26019200 |
| C | -2. 14006900 | 5. 02637000 | -1. 37089900 |
| H | -0. 87052800 | 3. 33246900 | -1. 71593100 |
| C | -4. 02939900 | 4. 66564500 | 0. 08708000 |
| H | -4. 22828800 | 2. 68210700 | 0. 89356800 |
| C | -3. 27753000 | 5. 51270700 | -0. 72703500 |
| H | -1. 55768500 | 5. 67729700 | -2. 01313800 |
| H | -4. 91557700 | 5. 03695200 | 0. 58938000 |
| H | -3. 57756200 | 6. 54607500 | -0. 86096600 |
| N | -3. 04361600 | 0. 47506400 | -0. 22062000 |

IM6_{TPT}

| | | | |
|---|--------------|--------------|--------------|
| O | -5. 06377900 | -1. 24975600 | 3. 62406600 |
| H | -5. 23627700 | -0. 56595400 | 4. 28391600 |
| C | -3. 43067400 | 0. 16881800 | 2. 49901800 |
| C | -2. 78214400 | 1. 31255200 | 2. 88900400 |
| H | -2. 28597100 | 1. 46746300 | 3. 83459200 |
| C | -2. 89118900 | 2. 22956700 | 1. 81340500 |
| C | -4. 02502700 | 2. 01332500 | -0. 49203100 |
| C | -3. 59892100 | 1. 58814700 | 0. 82731100 |
| O | -3. 92802900 | 0. 32354100 | 1. 24596500 |
| O | -3. 83194500 | 3. 15064100 | -0. 90426700 |
| C | -3. 70071900 | -1. 12078300 | 3. 19479400 |
| H | -3. 01072800 | -1. 20961100 | 4. 03942500 |
| H | -2. 49870700 | 3. 23285200 | 1. 76030400 |
| H | -3. 52362400 | -1. 95815100 | 2. 51770200 |
| C | 3. 64555700 | -0. 12118300 | -0. 11119800 |
| C | 1. 95574200 | 1. 06817200 | 0. 82714700 |
| N | 2. 84165200 | 1. 82326300 | 0. 14326600 |
| N | 2. 48147600 | -0. 18554200 | 0. 65368600 |
| H | -4. 96176300 | 2. 57414600 | -2. 50519600 |
| C | -4. 73939900 | 1. 00254500 | -1. 40968200 |
| O | -5. 40044800 | 1. 70860900 | -2. 45238800 |
| C | -3. 75725800 | -0. 00425000 | -1. 93134400 |

| | | | |
|---|-------------|-------------|-------------|
| C | -2.47723400 | 0.08057900 | -2.39429100 |
| O | -4.20771600 | -1.28821000 | -2.05035400 |
| C | -2.11726200 | -1.23432900 | -2.82717100 |
| H | -1.86532700 | 0.96915500 | -2.42707100 |
| C | -3.19774200 | -2.03268400 | -2.59622300 |
| H | -1.17556400 | -1.54920500 | -3.25053700 |
| C | -3.45135400 | -3.47733600 | -2.81354600 |
| H | -4.43521500 | -3.61757100 | -3.27564300 |
| H | -2.69063900 | -3.86068500 | -3.50184900 |
| O | -3.39259800 | -4.17518600 | -1.55429300 |
| H | -3.74461600 | -5.06279600 | -1.69511100 |
| H | -5.49819600 | 0.46800700 | -0.83206800 |
| C | 2.80310800 | 3.24299100 | -0.01600300 |
| C | 3.98839800 | 3.94195300 | -0.25152900 |
| C | 1.58485700 | 3.92107100 | 0.06074900 |
| C | 3.94951500 | 5.32601100 | -0.40758300 |
| H | 4.92682900 | 3.40700000 | -0.30982900 |
| C | 1.56146100 | 5.30569700 | -0.08756100 |
| H | 0.66924800 | 3.37057900 | 0.22977300 |
| C | 2.73970400 | 6.01394300 | -0.32430800 |
| H | 4.87209700 | 5.86568200 | -0.59026500 |
| H | 0.61364500 | 5.82904000 | -0.02861600 |
| H | 2.71425800 | 7.09096200 | -0.44557700 |
| C | 1.92580200 | -1.36024800 | 1.27335800 |
| C | 2.64765500 | -2.02280700 | 2.26435400 |
| C | 0.66687100 | -1.81176900 | 0.88306900 |
| C | 2.10358100 | -3.15768200 | 2.86325800 |
| H | 3.62012700 | -1.65153900 | 2.56586700 |
| C | 0.12784400 | -2.94428000 | 1.49073400 |
| H | 0.11839600 | -1.28382000 | 0.11251500 |
| C | 0.84530700 | -3.62013100 | 2.47781800 |
| H | 2.66173700 | -3.67458900 | 3.63568900 |
| H | -0.85098400 | -3.29784000 | 1.18717400 |
| H | 0.42420600 | -4.50245800 | 2.94676300 |
| C | 4.50663300 | -1.24020400 | -0.52975500 |
| C | 3.97324900 | -2.46907900 | -0.94246300 |
| C | 5.89658400 | -1.05191000 | -0.55849900 |
| C | 4.81826300 | -3.48992600 | -1.37094700 |
| H | 2.90211500 | -2.62616700 | -0.94630500 |
| C | 6.73562900 | -2.07681100 | -0.98537900 |
| H | 6.31386700 | -0.10415800 | -0.24054400 |
| C | 6.19948400 | -3.29933900 | -1.39086600 |
| H | 4.39446300 | -4.43395700 | -1.69450800 |
| H | 7.80847000 | -1.92060800 | -0.99865900 |

| | | | |
|---|------------|-------------|-------------|
| H | 6.85409000 | -4.09774800 | -1.72233400 |
| N | 3.88291100 | 1.11958600 | -0.43427600 |

IM1_{1fBu}

| | | | |
|---|-------------|-------------|-------------|
| O | 4.89155400 | 1.98376600 | -1.07376900 |
| H | 4.43511500 | 1.80015000 | -1.90484800 |
| C | 4.92643700 | -0.39595700 | -0.53185900 |
| C | 4.77879500 | -1.53562000 | -1.27947800 |
| H | 5.26177300 | -1.74129100 | -2.22231200 |
| C | 3.87751900 | -2.36896800 | -0.56690400 |
| C | 2.65053000 | -2.05893400 | 1.65617300 |
| H | 2.19155400 | -3.05459200 | 1.51138200 |
| C | 3.53298800 | -1.68288600 | 0.57233200 |
| O | 4.17612400 | -0.47616600 | 0.59675700 |
| O | 2.40797500 | -1.38707200 | 2.64484600 |
| C | 5.71129900 | 0.85108300 | -0.75493800 |
| H | 6.44436400 | 0.65934600 | -1.54498500 |
| H | 3.52102500 | -3.34893100 | -0.84661500 |
| H | 6.25131800 | 1.12467800 | 0.15356000 |
| C | -3.22635300 | 1.74180600 | 0.88339100 |
| C | -4.16938900 | 0.78800000 | 0.70686200 |
| C | -2.31762300 | 0.13361300 | -0.45950000 |
| N | -2.10698400 | 1.32903400 | 0.16612400 |
| H | -3.26884900 | 2.65661200 | 1.44964500 |
| H | -5.17327000 | 0.73119300 | 1.09216300 |
| N | -3.60047200 | -0.18237900 | -0.11353700 |
| C | -0.83973200 | 2.12540000 | 0.13793200 |
| C | -4.34263200 | -1.41502500 | -0.52304300 |
| C | -5.62337900 | -0.99238000 | -1.26386600 |
| H | -5.37956800 | -0.39737700 | -2.14844000 |
| H | -6.17369300 | -1.87942500 | -1.58824600 |
| H | -6.28708200 | -0.40274900 | -0.62677600 |
| C | -3.48390300 | -2.27904400 | -1.44996600 |
| H | -2.56360200 | -2.60532800 | -0.96357400 |
| H | -4.06146200 | -3.16628100 | -1.72422000 |
| H | -3.21629700 | -1.74956200 | -2.36573700 |
| C | -4.69232900 | -2.21424600 | 0.74468300 |
| H | -3.78398300 | -2.50135500 | 1.28146400 |
| H | -5.32422800 | -1.63723900 | 1.42451700 |
| H | -5.23458600 | -3.12465600 | 0.47537900 |
| C | 0.20138900 | 1.45299300 | -0.76074200 |
| H | -0.14831400 | 1.36412700 | -1.79081600 |
| H | 1.10583000 | 2.06758100 | -0.75543700 |
| H | 0.46545000 | 0.45777700 | -0.40066500 |

| | | | |
|---|-------------|------------|-------------|
| C | -0.29337900 | 2.21861800 | 1.57296000 |
| H | 0.64112300 | 2.78560700 | 1.58158700 |
| H | -0.99733300 | 2.72214700 | 2.24047000 |
| H | -0.09254800 | 1.22175200 | 1.97411000 |
| C | -1.15493600 | 3.52790200 | -0.41056700 |
| H | -0.23667000 | 4.11836400 | -0.46727500 |
| H | -1.58306400 | 3.46298800 | -1.41485800 |
| H | -1.85785800 | 4.06751500 | 0.22893800 |

TS1₁₇Bu

| | | | |
|---|-------------|-------------|-------------|
| O | 5.08332400 | 0.41601400 | -0.20974400 |
| H | 4.92809300 | 0.46213400 | -1.16144300 |
| C | 3.38759100 | -1.35548000 | -0.09537300 |
| C | 2.87288500 | -2.20061300 | -1.03595300 |
| H | 3.44072100 | -2.75419000 | -1.76911700 |
| C | 1.45694300 | -2.21540900 | -0.83928800 |
| C | -0.07336800 | -1.06683500 | 0.95382200 |
| H | -0.77836100 | -1.87227400 | 0.71253500 |
| C | 1.19606000 | -1.36860900 | 0.20240700 |
| O | 2.36971800 | -0.84895000 | 0.66657000 |
| O | -0.00804900 | -0.64378100 | 2.14522500 |
| C | 4.77463300 | -0.92369600 | 0.21951800 |
| H | 5.46931100 | -1.63981100 | -0.23264500 |
| H | 0.72643700 | -2.78264500 | -1.39558300 |
| H | 4.94130300 | -0.92401600 | 1.29871000 |
| C | -2.14463400 | 2.28139700 | -0.04065500 |
| C | -3.12096500 | 1.34835800 | -0.05415500 |
| C | -1.14176700 | 0.25896300 | -0.03075100 |
| N | -0.93253000 | 1.61000000 | -0.04459900 |
| H | -2.23001400 | 3.35172000 | -0.04960500 |
| H | -4.18580100 | 1.48285000 | -0.07262100 |
| N | -2.50174700 | 0.10702300 | -0.06798000 |
| C | 0.39731500 | 2.32257200 | -0.13973300 |
| C | -3.28307400 | -1.18477300 | -0.16816700 |
| C | -4.70129400 | -0.88002800 | -0.68253100 |
| H | -4.68271100 | -0.34776500 | -1.63667000 |
| H | -5.21557000 | -1.83055000 | -0.83904800 |
| H | -5.29305000 | -0.30705100 | 0.03423800 |
| C | -2.61148700 | -2.10807400 | -1.19611100 |
| H | -1.59852000 | -2.39280600 | -0.91811100 |
| H | -3.20108000 | -3.02333400 | -1.29098200 |
| H | -2.57390000 | -1.62333700 | -2.17529400 |
| C | -3.40278800 | -1.82901500 | 1.22344600 |
| H | -2.43782800 | -2.09448400 | 1.65348900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.90249000 | -1.14560500 | 1.91503600 |
| H | -4.00450100 | -2.73889700 | 1.15136900 |
| C | 1.20227600 | 1.69404600 | -1.28582700 |
| H | 0.67519800 | 1.82333100 | -2.23558600 |
| H | 2.17212700 | 2.19131900 | -1.36168200 |
| H | 1.37370400 | 0.63130300 | -1.13557800 |
| C | 1.12056800 | 2.23962100 | 1.21123300 |
| H | 2.10277300 | 2.71272300 | 1.12599900 |
| H | 0.54908200 | 2.77699000 | 1.97414200 |
| H | 1.24740800 | 1.21392200 | 1.55070800 |
| C | 0.16435900 | 3.80198300 | -0.48431100 |
| H | 1.14155300 | 4.27418600 | -0.60548200 |
| H | -0.38488600 | 3.92599500 | -1.42105700 |
| H | -0.35851100 | 4.33841600 | 0.31048000 |

IM2_{ttBu}

| | | | |
|---|-------------|-------------|-------------|
| O | 5.11489100 | 0.09704500 | 0.04020100 |
| H | 5.04084000 | 0.28927200 | -0.90390300 |
| C | 3.23015200 | -1.46179500 | -0.17635500 |
| C | 2.67373800 | -2.12027000 | -1.23365600 |
| H | 3.21335900 | -2.64766700 | -2.00663100 |
| C | 1.25533900 | -1.99092000 | -1.09346600 |
| C | -0.25146700 | -0.87352700 | 0.78197100 |
| H | -0.87373200 | -1.75294200 | 0.54823400 |
| C | 1.03441200 | -1.24620200 | 0.03302000 |
| O | 2.23364300 | -0.92999200 | 0.60158600 |
| O | -0.12140400 | -0.64142400 | 2.09570700 |
| C | 4.63547100 | -1.24501900 | 0.25455300 |
| H | 5.27158800 | -1.96615100 | -0.26949700 |
| H | 0.49721400 | -2.40187600 | -1.74298000 |
| H | 4.73883300 | -1.41686200 | 1.32800200 |
| C | -1.92557500 | 2.24064400 | -0.52853500 |
| C | -2.93532800 | 1.34635200 | -0.54832000 |
| C | -1.08600400 | 0.26994300 | 0.10323700 |
| N | -0.77845700 | 1.58263900 | -0.12136400 |
| H | -1.94691600 | 3.28389700 | -0.77605200 |
| H | -3.96392800 | 1.49575800 | -0.81242400 |
| N | -2.41996400 | 0.12433300 | -0.15699500 |
| C | 0.56407100 | 2.30575000 | -0.03646800 |
| C | -3.29653900 | -1.12078600 | -0.03096200 |
| C | -4.73845600 | -0.75561700 | -0.42203900 |
| H | -4.81989100 | -0.43936800 | -1.46455000 |
| H | -5.34601900 | -1.65404900 | -0.30043900 |
| H | -5.16199200 | 0.01583000 | 0.22413200 |

| | | | |
|---|-------------|-------------|-------------|
| C | -2.81604100 | -2.20131500 | -1.01552000 |
| H | -1.85432200 | -2.63461400 | -0.74538200 |
| H | -3.54880900 | -3.01164400 | -1.03160400 |
| H | -2.74184100 | -1.79102800 | -2.02609400 |
| C | -3.31150700 | -1.59252600 | 1.43270300 |
| H | -2.31859100 | -1.77358700 | 1.84153400 |
| H | -3.79397100 | -0.83946200 | 2.06184800 |
| H | -3.89565700 | -2.51407000 | 1.49839600 |
| C | 1.45164600 | 1.82675300 | -1.19453900 |
| H | 0.96220400 | 2.02304700 | -2.15275500 |
| H | 2.39352200 | 2.38011800 | -1.17304600 |
| H | 1.67954900 | 0.76558800 | -1.13901300 |
| C | 1.19007000 | 2.08309700 | 1.34562300 |
| H | 2.20565100 | 2.48699600 | 1.33744900 |
| H | 0.61422300 | 2.62268500 | 2.10355300 |
| H | 1.21390900 | 1.03616100 | 1.64057500 |
| C | 0.33766500 | 3.81630200 | -0.21190800 |
| H | 1.30428400 | 4.30508300 | -0.07422200 |
| H | -0.02091500 | 4.07910900 | -1.20981100 |
| H | -0.34656900 | 4.22075700 | 0.53721200 |

IM5_{1tBu}

| | | | |
|---|-------------|-------------|-------------|
| O | -5.82094400 | -0.92465400 | -1.72396700 |
| H | -6.07739000 | -0.00564400 | -1.57561100 |
| C | -4.19654600 | -0.61086400 | 0.08912700 |
| C | -4.12495600 | 0.19722200 | 1.18489100 |
| H | -4.92585300 | 0.38727700 | 1.88417500 |
| C | -2.79615300 | 0.72857700 | 1.21980200 |
| C | -0.80154600 | 0.56478300 | -0.51569700 |
| C | -2.13625000 | 0.20870000 | 0.14251800 |
| O | -2.98362300 | -0.60500800 | -0.55414200 |
| O | -1.00522500 | 1.68179300 | -1.23528900 |
| C | -5.28691100 | -1.43679300 | -0.48958400 |
| H | -6.07823900 | -1.53034100 | 0.26279500 |
| H | -2.39787400 | 1.42258200 | 1.94289300 |
| H | -4.92933900 | -2.44040100 | -0.73089000 |
| C | 1.99535500 | 1.56404700 | 1.77340400 |
| C | 1.76288000 | 0.32306800 | 2.23070600 |
| C | 0.29556800 | 0.72227000 | 0.59492800 |
| N | 1.08818600 | 1.83426500 | 0.76843600 |
| H | 2.74035500 | 2.25956300 | 2.10016500 |
| H | 2.26806100 | -0.20432100 | 3.01502600 |
| N | 0.71140200 | -0.21478200 | 1.51626600 |
| C | 0.18472800 | -1.57346800 | 2.05939300 |

| | | | |
|--------------------------|-------------|-------------|-------------|
| H | -1.12801700 | 0.80681600 | -2.57057400 |
| C | -0.35040000 | -0.59576400 | -1.63056100 |
| O | -0.92956400 | -0.14808300 | -2.82568400 |
| C | 1.12762500 | -0.75534800 | -1.84321500 |
| C | 1.98797800 | -0.18102800 | -2.73282800 |
| O | 1.80109000 | -1.69448700 | -1.10319700 |
| C | 3.26507300 | -0.79297400 | -2.52544300 |
| H | 1.73193800 | 0.56763700 | -3.46421400 |
| C | 3.10885700 | -1.70752400 | -1.52908900 |
| H | 4.18241800 | -0.59070500 | -3.05828700 |
| C | 4.03567300 | -2.67587400 | -0.89948000 |
| H | 3.54968700 | -3.65399800 | -0.80162200 |
| H | 4.90516700 | -2.78949900 | -1.55501800 |
| O | 4.44955900 | -2.20493400 | 0.40168900 |
| H | 5.02205800 | -2.88166500 | 0.78473400 |
| H | -0.77563900 | -1.55677400 | -1.34869300 |
| C | 1.07014900 | 3.26571600 | 0.16421400 |
| C | -0.29382400 | 3.90887000 | 0.44830500 |
| H | -0.48865500 | 3.92430200 | 1.52524900 |
| H | -0.26943500 | 4.94503200 | 0.09894100 |
| H | -1.08514600 | 3.37316200 | -0.06928200 |
| C | 2.13588700 | 4.12426600 | 0.87263800 |
| H | 3.15304300 | 3.75881300 | 0.71543800 |
| H | 2.07853000 | 5.11840400 | 0.42569800 |
| H | 1.95048300 | 4.23914300 | 1.94293900 |
| C | 1.44003100 | 3.22279200 | -1.32206000 |
| H | 2.43938600 | 2.79873700 | -1.45266700 |
| H | 0.71037800 | 2.64521200 | -1.88105900 |
| H | 1.45859600 | 4.24844100 | -1.70244300 |
| C | 1.40918800 | -2.42353500 | 2.46171500 |
| H | 1.88175700 | -2.08425200 | 3.38439000 |
| H | 1.06286200 | -3.44286900 | 2.64232400 |
| H | 2.15832300 | -2.44931900 | 1.66893400 |
| C | -0.66245200 | -1.25320700 | 3.30036100 |
| H | -1.57448500 | -0.71923200 | 3.03276600 |
| H | -0.94498400 | -2.19053500 | 3.78662200 |
| H | -0.10165200 | -0.65449800 | 4.02196000 |
| C | -0.62378600 | -2.41009800 | 1.07101400 |
| H | -1.53012300 | -1.92283200 | 0.73140300 |
| H | -0.02115300 | -2.72171300 | 0.22050800 |
| H | -0.92952400 | -3.31293400 | 1.60484600 |
| TS4_tBu | | | |
| O | -4.16567300 | 3.13753400 | -1.55538300 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.78711700 | 3.73917600 | -2.20904500 |
| C | -1.97037300 | 3.06390600 | -0.46892600 |
| C | -0.88916700 | 3.89657800 | -0.48539900 |
| H | -0.91594900 | 4.96922400 | -0.36334100 |
| C | 0.26047100 | 3.07810100 | -0.70364400 |
| C | 0.55852500 | 0.53803800 | -1.22011500 |
| C | -0.18505600 | 1.79046200 | -0.79811700 |
| O | -1.54648900 | 1.77301700 | -0.65805100 |
| O | 1.50241000 | 0.81796000 | -2.03548800 |
| C | -3.43109800 | 3.30070800 | -0.32902000 |
| H | -3.57652600 | 4.30761700 | 0.07714700 |
| H | 1.28505000 | 3.39932000 | -0.80013400 |
| H | -3.87505300 | 2.58645800 | 0.36743500 |
| C | 3.33036100 | 0.52964700 | 1.62772700 |
| C | 2.27625900 | 0.79638700 | 2.42125100 |
| C | 1.46435800 | 0.03179800 | 0.45361200 |
| N | 2.84252900 | 0.02390800 | 0.43595000 |
| H | 4.37808800 | 0.63662800 | 1.83446700 |
| H | 2.25701000 | 1.17566000 | 3.42610700 |
| N | 1.13304600 | 0.45215900 | 1.72118600 |
| C | -0.17816000 | 0.42537200 | 2.49223600 |
| H | 0.94136900 | -0.37093700 | -3.13292200 |
| C | -0.41551700 | -0.60874600 | -1.83844700 |
| O | 0.21372800 | -1.03173100 | -3.04214300 |
| C | -0.83154700 | -1.82158200 | -1.07177300 |
| C | -0.20198000 | -2.94325400 | -0.61590100 |
| O | -2.18165600 | -1.95187800 | -0.87175000 |
| C | -1.21787700 | -3.80248000 | -0.09237700 |
| H | 0.85480900 | -3.14366400 | -0.66020800 |
| C | -2.40646000 | -3.15736000 | -0.26503000 |
| H | -1.08605500 | -4.77766200 | 0.35235800 |
| C | -3.80989100 | -3.53288900 | 0.02959600 |
| H | -4.44347600 | -3.30995700 | -0.83657800 |
| H | -3.84320000 | -4.61266000 | 0.21075000 |
| O | -4.29213800 | -2.81623900 | 1.18459600 |
| H | -5.24843500 | -2.93992800 | 1.22411800 |
| H | -1.34012200 | -0.07790500 | -2.08480100 |
| C | 3.84079600 | -0.55469900 | -0.56349100 |
| C | 4.41480100 | 0.57332200 | -1.43293900 |
| H | 4.86234000 | 1.34978600 | -0.80503700 |
| H | 5.20349300 | 0.16735200 | -2.07276300 |
| H | 3.64059900 | 1.02006200 | -2.05138300 |
| C | 4.99581900 | -1.20517000 | 0.23119000 |
| H | 4.62480800 | -1.90287300 | 0.98626600 |

| | | | |
|---|-------------|-------------|-------------|
| H | 5.60953800 | -1.76899900 | -0.47488600 |
| H | 5.65093100 | -0.47677100 | 0.71240300 |
| C | 3.19759400 | -1.66830600 | -1.38917600 |
| H | 2.94243900 | -2.51879200 | -0.75240100 |
| H | 2.31558700 | -1.33721800 | -1.92271000 |
| H | 3.92724200 | -2.01625800 | -2.12530800 |
| C | 0.07774100 | -0.31972200 | 3.82056900 |
| H | 0.73106900 | 0.22936000 | 4.50052500 |
| H | -0.87958800 | -0.45763700 | 4.32867100 |
| H | 0.50998700 | -1.30689900 | 3.63875600 |
| C | -0.61210700 | 1.86822400 | 2.78314700 |
| H | -0.83934100 | 2.41508000 | 1.86867800 |
| H | -1.51032700 | 1.85662600 | 3.40606900 |
| H | 0.16323700 | 2.41646200 | 3.32433400 |
| C | -1.26193200 | -0.34407900 | 1.74826700 |
| H | -1.52375400 | 0.10162500 | 0.79667900 |
| H | -0.97030000 | -1.38260500 | 1.59639500 |
| H | -2.16219800 | -0.33699200 | 2.36671000 |

IM6_{1tBu}

| | | | |
|---|-------------|-------------|-------------|
| O | 2.83434800 | -0.41215900 | 4.26186800 |
| H | 3.23817900 | -1.17549000 | 4.69422200 |
| C | 2.68119800 | -1.60657700 | 2.14133800 |
| C | 2.78285700 | -2.93401200 | 1.81086000 |
| H | 2.29176300 | -3.75092700 | 2.31672300 |
| C | 3.64798300 | -3.01002800 | 0.69006700 |
| C | 4.88612600 | -1.17081200 | -0.62569100 |
| C | 4.02153900 | -1.72082700 | 0.40104500 |
| O | 3.42844200 | -0.86027200 | 1.28958000 |
| O | 5.49483800 | -1.88382800 | -1.41409100 |
| C | 1.95882400 | -0.89410400 | 3.23292900 |
| H | 1.20095800 | -1.56853300 | 3.64305100 |
| H | 3.95898500 | -3.89397100 | 0.15543800 |
| H | 1.45354300 | -0.01220700 | 2.83586900 |
| C | -4.75007200 | -0.14595800 | -1.75902600 |
| C | -4.79933000 | 1.03791500 | -1.10603200 |
| C | -4.18679400 | -0.54916200 | 0.41664800 |
| N | -4.37500600 | -1.10052000 | -0.81774600 |
| H | -4.94571000 | -0.37226800 | -2.79340700 |
| H | -5.04715500 | 2.01878000 | -1.47425000 |
| N | -4.45215900 | 0.77488900 | 0.21610800 |
| C | -4.41940100 | 1.84458400 | 1.26161200 |
| H | 6.35459900 | -0.15477500 | -2.05138700 |
| C | 5.04261700 | 0.35780200 | -0.73438000 |

| | | | |
|---|-------------|-------------|-------------|
| O | 6.17633300 | 0.65276400 | -1.54075000 |
| C | 3.78260900 | 0.97067100 | -1.26823400 |
| C | 2.88713600 | 0.60104400 | -2.22796100 |
| O | 3.43371300 | 2.18638700 | -0.75387300 |
| C | 1.92485400 | 1.65605800 | -2.30905000 |
| H | 2.90814400 | -0.30995300 | -2.80655100 |
| C | 2.29610200 | 2.59584400 | -1.39434500 |
| H | 1.06288900 | 1.70744000 | -2.95668000 |
| C | 1.71506300 | 3.89945900 | -0.99265100 |
| H | 2.50256600 | 4.66068900 | -0.94525100 |
| H | 0.99045100 | 4.20139600 | -1.75627300 |
| O | 1.07566800 | 3.76984500 | 0.29113700 |
| H | 0.87179400 | 4.65834200 | 0.60798500 |
| H | 5.22154200 | 0.76828500 | 0.26339200 |
| C | -4.21444700 | -2.54677600 | -1.16371300 |
| C | -3.77987900 | -3.34653100 | 0.06754800 |
| H | -4.51792100 | -3.28888800 | 0.86907000 |
| H | -3.67021900 | -4.39463000 | -0.22460000 |
| H | -2.82353300 | -2.99723900 | 0.46023500 |
| C | -5.56566600 | -3.07829000 | -1.67276400 |
| H | -5.89829000 | -2.54320300 | -2.56575900 |
| H | -5.47753000 | -4.13702500 | -1.93063800 |
| H | -6.33584900 | -2.97574600 | -0.90327100 |
| C | -3.14144100 | -2.67095400 | -2.25961400 |
| H | -3.43712000 | -2.15531200 | -3.17677900 |
| H | -2.19154000 | -2.25040600 | -1.91830800 |
| H | -2.98171100 | -3.72414800 | -2.50548000 |
| C | -3.46993700 | 2.95968600 | 0.79037300 |
| H | -3.81547700 | 3.41939000 | -0.13885700 |
| H | -3.41481500 | 3.74463100 | 1.54901400 |
| H | -2.46242800 | 2.56757400 | 0.62753800 |
| C | -5.84540300 | 2.39464000 | 1.43751900 |
| H | -6.53007700 | 1.59996200 | 1.74600800 |
| H | -5.85282700 | 3.17268100 | 2.20555900 |
| H | -6.22388900 | 2.83419600 | 0.51088900 |
| C | -3.92059100 | 1.28069900 | 2.59519600 |
| H | -4.57409000 | 0.49426800 | 2.97470800 |
| H | -2.91117700 | 0.87395500 | 2.51263600 |
| H | -3.90430700 | 2.09443100 | 3.32560400 |