

Supporting Information

Insights into Gold-Catalyzed Formations of Aza-Heterocycles Using Benzofuroxans as Nitrene Transfer Reagents: Mechanism and Origins of Chemoselectivity

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Fig. S1 Potential energy surface in MeCN solvent for the transformation of **5** to **P**. The solvent-corrected relative free energies are given in kcal mol⁻¹.

Fig. S2 Potential energy surface in MeCN solvent for the other pathway of nucleophilic attacks on α -imino gold carbene **5**. The solvent-corrected relative free energies are given in kcal mol⁻¹.

Cartesian coordinates and electronic energies for all of the calculated structure

A1

SCF done: -490.829084

| | | | |
|---|-------------|-------------|-------------|
| C | 0.23003900 | -0.93663000 | 0.00005700 |
| C | -0.17523500 | 0.42967700 | -0.00003400 |
| C | 0.73970900 | 1.51110100 | 0.00005700 |
| C | 2.06875900 | 1.17729200 | -0.00000700 |
| C | 2.50312000 | -0.19569700 | -0.00005200 |
| C | 1.62520200 | -1.24640000 | -0.00000500 |
| H | 0.38374600 | 2.53526000 | 0.00026700 |
| H | 2.82033700 | 1.96055500 | -0.00007500 |
| H | 3.57083500 | -0.39503300 | -0.00012100 |
| H | 1.95342200 | -2.27992500 | 0.00013200 |
| O | -1.92085200 | -0.94930100 | -0.00002900 |
| N | -0.81287900 | -1.75536600 | 0.00003200 |
| N | -1.51857800 | 0.44222700 | -0.00002000 |
| O | -2.37386000 | 1.31618500 | -0.00001900 |

A2

SCF done: -911.293127

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|---|-------------|-------------|-------------|
| C | -5.14874900 | 1.07798900 | -0.95058000 |
| C | -3.90477900 | 0.45859900 | -1.03999000 |
| C | -3.29275700 | -0.08166900 | 0.10999700 |
| C | -3.96781300 | 0.01100900 | 1.34392700 |
| C | -5.21809800 | 0.61999100 | 1.41996400 |
| C | -5.81263800 | 1.15950500 | 0.27645200 |
| H | -5.60578200 | 1.49236700 | -1.84535200 |
| H | -3.39303300 | 0.38353900 | -1.99459300 |
| H | -3.50240300 | -0.40028600 | 2.23468400 |
| H | -5.72807700 | 0.67853900 | 2.37795700 |
| H | -6.78586600 | 1.63824400 | 0.34063900 |
| C | -2.01448800 | -0.70564800 | 0.01937000 |
| C | -0.92814700 | -1.23786300 | -0.10264400 |
| S | 1.40032600 | -1.20855500 | -1.36980000 |
| O | 2.52487400 | -2.16177200 | -1.34575300 |
| O | 0.61312700 | -0.91936700 | -2.57674100 |
| C | 1.95137400 | 0.35263900 | -0.68131600 |
| C | 3.12020500 | 0.39531500 | 0.07873900 |
| C | 1.20726000 | 1.50938400 | -0.93322800 |
| C | 3.53926200 | 1.61749600 | 0.60274100 |
| H | 3.69232900 | -0.51031500 | 0.24462900 |
| C | 1.63984800 | 2.71767600 | -0.39468600 |
| H | 0.31763900 | 1.45849200 | -1.55054800 |
| C | 2.80790700 | 2.79227600 | 0.38102100 |

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|---|-------------|-------------|-------------|
| H | 4.45311900 | 1.65919700 | 1.18984800 |
| H | 1.06611500 | 3.62099300 | -0.58737000 |
| C | 3.25837700 | 4.11246400 | 0.95994600 |
| H | 4.23713900 | 4.02672100 | 1.44135400 |
| H | 3.32936500 | 4.88376400 | 0.18395300 |
| H | 2.54689300 | 4.47738500 | 1.71154200 |
| N | 0.26344100 | -1.84992400 | -0.21246300 |
| C | 0.73322200 | -2.75799100 | 0.86291000 |
| H | -0.10748300 | -3.43510700 | 1.05712900 |
| H | 1.55280800 | -3.34807100 | 0.44978000 |
| C | 1.14876700 | -2.04865800 | 2.12374800 |
| C | 2.30572000 | -2.26415600 | 2.75031600 |
| H | 0.42727500 | -1.33916100 | 2.52837600 |
| H | 2.55759100 | -1.75392800 | 3.67610400 |
| H | 3.04222800 | -2.96704800 | 2.36573100 |

a

SCF done: -1748.065031

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|---|-------------|-------------|-------------|
| C | -1.11188300 | -3.35886900 | -1.35297800 |
| C | 0.21921700 | -2.95741300 | -1.29551300 |
| C | 0.91595100 | -2.94764400 | -0.06281500 |
| C | 0.24720600 | -3.38987200 | 1.10767200 |
| C | -1.08298100 | -3.77837700 | 1.05735500 |
| C | -1.80706900 | -3.73677700 | -0.16821100 |
| H | -1.62267100 | -3.40586600 | -2.31043300 |
| H | 0.74027900 | -2.65335900 | -2.19710100 |
| H | 0.78762800 | -3.40612000 | 2.04813900 |
| H | -1.58226300 | -4.12527600 | 1.95726900 |
| H | -2.77872400 | -4.22078600 | -0.23904600 |
| C | 2.23882800 | -2.45986700 | -0.01337600 |
| C | 3.35825800 | -1.97845200 | -0.01654300 |
| S | 4.90031600 | -0.34512000 | -1.41836400 |
| O | 5.87003600 | -1.03384500 | -2.28486300 |
| O | 3.56678200 | 0.06873500 | -1.88789300 |
| C | 5.71842500 | 1.02068800 | -0.60670300 |
| C | 7.07821200 | 1.23251100 | -0.84156100 |
| C | 4.97723400 | 1.87892900 | 0.21212400 |
| C | 7.70372800 | 2.31952400 | -0.23204900 |
| H | 7.62728000 | 0.56203600 | -1.49382200 |
| C | 5.62317900 | 2.95445200 | 0.81243200 |
| H | 3.91836300 | 1.70530400 | 0.37481200 |
| C | 6.99210600 | 3.19492600 | 0.60016100 |
| H | 8.76217900 | 2.48984300 | -0.40903500 |
| H | 5.05847100 | 3.62305400 | 1.45703000 |

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|----|-------------|-------------|-------------|
| C | 7.67114100 | 4.38479200 | 1.23256000 |
| H | 8.74062300 | 4.20576700 | 1.37849400 |
| H | 7.57232300 | 5.27225200 | 0.59374500 |
| H | 7.22831200 | 4.63095100 | 2.20287600 |
| N | 4.56078700 | -1.40701500 | -0.03325000 |
| C | 5.72479000 | -2.07161000 | 0.62117700 |
| H | 5.97673200 | -2.99061800 | 0.08118800 |
| H | 6.56577300 | -1.37784400 | 0.51670300 |
| Au | -2.47318100 | -1.50643300 | -0.00204500 |
| P | -3.06080000 | 0.74198500 | 0.06621200 |
| C | -4.18140600 | 1.16398000 | -1.32471900 |
| C | -3.97149200 | 2.30082500 | -2.11815000 |
| C | -5.27658000 | 0.32291900 | -1.58588400 |
| C | -4.85404000 | 2.59264400 | -3.16059400 |
| H | -3.12456500 | 2.95290600 | -1.93133700 |
| C | -6.15555000 | 0.62405700 | -2.62444700 |
| H | -5.44254600 | -0.56408200 | -0.97909500 |
| C | -5.94363200 | 1.75830100 | -3.41389500 |
| H | -4.68553500 | 3.47206000 | -3.77507700 |
| H | -7.00094700 | -0.02855500 | -2.82126300 |
| H | -6.62557000 | 1.98754400 | -4.22746600 |
| C | -3.91061000 | 1.22594100 | 1.61802000 |
| C | -3.45197400 | 0.70037400 | 2.83685500 |
| C | -4.98448300 | 2.12847700 | 1.60813500 |
| C | -4.05749300 | 1.08160700 | 4.03277800 |
| H | -2.62448500 | -0.00473800 | 2.85026700 |
| C | -5.58810400 | 2.50317000 | 2.81041400 |
| H | -5.35357800 | 2.53189400 | 0.67051500 |
| C | -5.12635300 | 1.98238900 | 4.02028400 |
| H | -3.70054800 | 0.67121100 | 4.97277700 |
| H | -6.42167500 | 3.19913900 | 2.79819100 |
| H | -5.60147800 | 2.27278500 | 4.95272400 |
| C | -1.55558500 | 1.78474800 | -0.08659200 |
| C | -1.51608400 | 3.07617000 | 0.46355700 |
| C | -0.44035100 | 1.29187900 | -0.78263600 |
| C | -0.37491200 | 3.86338000 | 0.30398900 |
| H | -2.36563000 | 3.46388400 | 1.01754100 |
| C | 0.70073900 | 2.08025700 | -0.93541400 |
| H | -0.45655200 | 0.29025000 | -1.20298800 |
| C | 0.72993500 | 3.36799200 | -0.39359800 |
| H | -0.34935700 | 4.86245000 | 0.72932700 |
| H | 1.56188500 | 1.68043600 | -1.46370500 |
| H | 1.61571500 | 3.98562400 | -0.51303400 |
| C | 5.44917100 | -2.34356900 | 2.07194500 |

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|---|-------------|--------------|-------------|
| H | 5. 21765800 | -1. 47258700 | 2. 68347000 |
| C | 5. 50309100 | -3. 55928600 | 2. 61545700 |
| H | 5. 73230000 | -4. 44227000 | 2. 02285500 |
| H | 5. 33500300 | -3. 71609200 | 3. 67705600 |

b

SCF done: -1327. 603731

| | | | |
|----|--------------|--------------|--------------|
| Au | -0. 44433800 | -0. 47560000 | -0. 00699400 |
| P | 1. 78240800 | 0. 03110500 | 0. 00209700 |
| C | 2. 74543700 | -1. 23319800 | -0. 91054400 |
| C | 3. 97859100 | -1. 69324700 | -0. 42558000 |
| C | 2. 24635100 | -1. 72243500 | -2. 12921200 |
| C | 4. 70347100 | -2. 63559400 | -1. 15772300 |
| H | 4. 37047300 | -1. 32649300 | 0. 51765000 |
| C | 2. 97823900 | -2. 65987900 | -2. 85551700 |
| H | 1. 28967600 | -1. 37247300 | -2. 50918400 |
| C | 4. 20593900 | -3. 11862700 | -2. 36921000 |
| H | 5. 65579500 | -2. 99279900 | -0. 77727800 |
| H | 2. 58793000 | -3. 03637900 | -3. 79631100 |
| H | 4. 77135400 | -3. 85463100 | -2. 93315300 |
| C | 2. 09200000 | 1. 65418700 | -0. 79009900 |
| C | 1. 23610700 | 2. 72953400 | -0. 49896200 |
| C | 3. 18108700 | 1. 84203800 | -1. 65384200 |
| C | 1. 47257700 | 3. 98073200 | -1. 06521600 |
| H | 0. 38830400 | 2. 59013700 | 0. 16716100 |
| C | 3. 40806400 | 3. 09791700 | -2. 22028000 |
| H | 3. 84503300 | 1. 01659800 | -1. 88952200 |
| C | 2. 55710000 | 4. 16506300 | -1. 92774600 |
| H | 0. 80785000 | 4. 80889700 | -0. 83835200 |
| H | 4. 24973200 | 3. 23886500 | -2. 89182100 |
| H | 2. 73564600 | 5. 13923400 | -2. 37336100 |
| C | 2. 43420400 | 0. 10890000 | 1. 71308500 |
| C | 3. 34168500 | 1. 10796800 | 2. 09526100 |
| C | 2. 03761600 | -0. 86896700 | 2. 64036100 |
| C | 3. 84672200 | 1. 12428900 | 3. 39685500 |
| H | 3. 64846700 | 1. 87144200 | 1. 38763800 |
| C | 2. 54978200 | -0. 84764800 | 3. 93626900 |
| H | 1. 33186500 | -1. 64365700 | 2. 35102500 |
| C | 3. 45269400 | 0. 14992000 | 4. 31554800 |
| H | 4. 54596600 | 1. 90123900 | 3. 69118800 |
| H | 2. 24031700 | -1. 60475400 | 4. 65054100 |
| H | 3. 84534800 | 0. 16862800 | 5. 32794900 |
| C | -5. 35712600 | 0. 92633500 | -0. 00332800 |
| C | -4. 82365000 | -0. 40402000 | -0. 00147500 |

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|---|-------------|-------------|-------------|
| C | -5.63819200 | -1.56369500 | 0.00857700 |
| C | -6.98880700 | -1.33315400 | 0.01653700 |
| C | -7.54851300 | -0.00336300 | 0.01479800 |
| C | -6.77142500 | 1.12216200 | 0.00514300 |
| H | -5.20378600 | -2.55624000 | 0.00971100 |
| H | -7.67127000 | -2.17705700 | 0.02445800 |
| H | -8.62935800 | 0.09496200 | 0.02145300 |
| H | -7.18543200 | 2.12379300 | 0.00374500 |
| O | -3.21721600 | 1.11604700 | -0.01798000 |
| N | -4.38456100 | 1.82714300 | -0.01292600 |
| N | -3.50066400 | -0.25441500 | -0.01054200 |
| O | -2.54533900 | -1.09653700 | -0.01457000 |

c

SCF done: -1748.065772

| | | | |
|---|-------------|-------------|-------------|
| C | -6.48832800 | 4.79211900 | 0.91537200 |
| C | -5.62338000 | 3.71465300 | 1.08891300 |
| C | -5.36219500 | 2.83320500 | 0.02057700 |
| C | -5.98869900 | 3.05935900 | -1.22144200 |
| C | -6.85194900 | 4.13927400 | -1.38745900 |
| C | -7.10337900 | 5.00712300 | -0.32111200 |
| H | -6.68554000 | 5.46432300 | 1.74554200 |
| H | -5.14624800 | 3.53882800 | 2.04811800 |
| H | -5.79190700 | 2.37935600 | -2.04471600 |
| H | -7.33114000 | 4.30441600 | -2.34827900 |
| H | -7.77832800 | 5.84807700 | -0.45288200 |
| C | -4.47733700 | 1.72483500 | 0.19485500 |
| C | -3.73283200 | 0.77923600 | 0.36482700 |
| S | -3.48073000 | -1.66706700 | 1.44466100 |
| O | -2.35184300 | -2.61792500 | 1.35812500 |
| O | -3.99169400 | -1.17953500 | 2.73477600 |
| C | -4.84047200 | -2.22945500 | 0.44064300 |
| C | -4.58740300 | -3.09058800 | -0.63067300 |
| C | -6.13690600 | -1.82926300 | 0.76889000 |
| C | -5.66060700 | -3.54321400 | -1.39108300 |
| H | -3.57349300 | -3.40798500 | -0.84916200 |
| C | -7.19551600 | -2.29353100 | -0.00903600 |
| H | -6.30777500 | -1.17537700 | 1.61650400 |
| C | -6.97805700 | -3.15486900 | -1.09435400 |
| H | -5.47673800 | -4.21633900 | -2.22435000 |
| H | -8.20835000 | -1.98544000 | 0.23555400 |
| C | -8.13528700 | -3.68184200 | -1.90685800 |
| H | -7.85856400 | -3.82006900 | -2.95704300 |
| H | -8.46344400 | -4.65772300 | -1.52568500 |

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|----|-------------|-------------|-------------|
| H | -8.99627100 | -3.00799000 | -1.86392300 |
| N | -2.89156200 | -0.27077000 | 0.49666800 |
| C | -1.45014800 | 0.01218100 | 0.62430600 |
| H | -1.27027100 | 0.85931000 | 1.29704500 |
| H | -0.98213500 | -0.88308700 | 1.04210900 |
| Au | 1.47747000 | 0.51609000 | -0.55597900 |
| P | 3.70656000 | -0.00921500 | -0.03466200 |
| C | 4.68202100 | 1.51424200 | 0.26305900 |
| C | 5.98695100 | 1.64903000 | -0.23308200 |
| C | 4.11141000 | 2.55014900 | 1.02171000 |
| C | 6.71200000 | 2.81285400 | 0.03087400 |
| H | 6.43483900 | 0.85647300 | -0.82382800 |
| C | 4.84364700 | 3.70632300 | 1.28465000 |
| H | 3.10012300 | 2.45250100 | 1.40939700 |
| C | 6.14329400 | 3.83919300 | 0.78705100 |
| H | 7.72096600 | 2.91558200 | -0.35723500 |
| H | 4.39911900 | 4.50430700 | 1.87182500 |
| H | 6.71003400 | 4.74374400 | 0.98696300 |
| C | 3.79176900 | -1.03995100 | 1.47881700 |
| C | 2.85511800 | -2.07272300 | 1.65168200 |
| C | 4.78269600 | -0.82545100 | 2.44820400 |
| C | 2.91221700 | -2.88386100 | 2.78347200 |
| H | 2.08494500 | -2.24617300 | 0.90383700 |
| C | 4.83177900 | -1.64136100 | 3.58026400 |
| H | 5.50687100 | -0.02622500 | 2.32651700 |
| C | 3.89947100 | -2.66677000 | 3.74912700 |
| H | 2.18357400 | -3.67817700 | 2.91433400 |
| H | 5.59755700 | -1.47091700 | 4.33110800 |
| H | 3.93831300 | -3.29466800 | 4.63432500 |
| C | 4.51009900 | -0.93553200 | -1.39674600 |
| C | 5.37857700 | -2.00468900 | -1.13110100 |
| C | 4.26704100 | -0.54518000 | -2.72415400 |
| C | 5.99771300 | -2.67413300 | -2.18845700 |
| H | 5.56799800 | -2.31788200 | -0.10934200 |
| C | 4.89265100 | -1.21569300 | -3.77364700 |
| H | 3.59430700 | 0.28211700 | -2.93788000 |
| C | 5.75628200 | -2.28189200 | -3.50630100 |
| H | 6.66648600 | -3.50377900 | -1.97962300 |
| H | 4.70221200 | -0.91060600 | -4.79827100 |
| H | 6.23730700 | -2.80790900 | -4.32563600 |
| C | -0.91538700 | 0.28697300 | -0.76040000 |
| H | -1.00752100 | -0.53511000 | -1.46966700 |
| C | -0.53527100 | 1.52412000 | -1.21286200 |
| H | -0.59955900 | 2.39891400 | -0.56878300 |

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| H | -0.35451000 | 1.70357500 | -2.27022000 |
|---|-------------|------------|-------------|

d

SCF done: -1327.611285

| | | | |
|----|-------------|-------------|-------------|
| Au | 0.63618300 | -0.19660700 | 0.01284000 |
| P | -1.66071400 | 0.03697000 | 0.00461300 |
| C | -2.45280700 | -1.34333100 | -0.90567400 |
| C | -3.55662200 | -1.12215200 | -1.74278400 |
| C | -1.95645200 | -2.64608000 | -0.73272800 |
| C | -4.15665700 | -2.19894000 | -2.39838800 |
| H | -3.94322300 | -0.11859400 | -1.88927600 |
| C | -2.56317400 | -3.71588600 | -1.38845600 |
| H | -1.09995400 | -2.82548900 | -0.08735200 |
| C | -3.66214500 | -3.49263600 | -2.22273700 |
| H | -5.00874800 | -2.02386500 | -3.04842400 |
| H | -2.17503000 | -4.72092400 | -1.25293600 |
| H | -4.12956500 | -4.32664900 | -2.73787500 |
| C | -2.34902000 | 0.04945300 | 1.70387200 |
| C | -1.64715800 | 0.71190900 | 2.72417700 |
| C | -3.57693300 | -0.56684600 | 1.98858400 |
| C | -2.17239500 | 0.76052700 | 4.01446300 |
| H | -0.69295400 | 1.18772100 | 2.51154700 |
| C | -4.09482600 | -0.51633700 | 3.28391100 |
| H | -4.12329100 | -1.08863200 | 1.20928900 |
| C | -3.39537000 | 0.14501100 | 4.29518600 |
| H | -1.62510900 | 1.27198500 | 4.80066000 |
| H | -5.04334500 | -0.99814500 | 3.50160200 |
| H | -3.79979500 | 0.17741000 | 5.30256300 |
| C | -2.16153700 | 1.60103500 | -0.81317000 |
| C | -3.16329100 | 2.41953000 | -0.27206200 |
| C | -1.53888100 | 1.96382400 | -2.01943500 |
| C | -3.53524800 | 3.59137000 | -0.93464100 |
| H | -3.64902900 | 2.15014900 | 0.66021100 |
| C | -1.91957400 | 3.13197700 | -2.67725300 |
| H | -0.76277900 | 1.33282800 | -2.44610200 |
| C | -2.91621100 | 3.94796400 | -2.13366000 |
| H | -4.30927300 | 4.22417500 | -0.51069800 |
| H | -1.43731000 | 3.40685600 | -3.61065700 |
| H | -3.20795900 | 4.86085500 | -2.64451700 |
| C | 3.79123000 | 0.42255300 | 0.00702400 |
| C | 4.99938400 | -0.32390000 | 0.00825900 |
| C | 6.28362500 | 0.27085400 | 0.00442200 |
| C | 6.30751600 | 1.64179300 | -0.00080400 |
| C | 5.09581700 | 2.41303000 | -0.00250100 |

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|---|------------|-------------|-------------|
| C | 3.84662300 | 1.84156300 | 0.00115500 |
| H | 7.17759800 | -0.34203400 | 0.00569000 |
| H | 7.25820400 | 2.16409300 | -0.00386000 |
| H | 5.17806900 | 3.49560500 | -0.00691000 |
| H | 2.93739000 | 2.43254500 | -0.00062000 |
| O | 3.22970400 | -1.69710800 | 0.01607900 |
| N | 2.74266600 | -0.40328200 | 0.01198300 |
| N | 4.66989900 | -1.63502600 | 0.01375600 |
| O | 5.29342400 | -2.66939700 | 0.01683900 |

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SCF done: -913.179089

| | | | |
|----|-------------|-------------|-------------|
| Au | -1.91807600 | -0.02660300 | -0.00418800 |
| P | 0.36926300 | 0.00254900 | 0.00057500 |
| C | 0.98837600 | 1.47164700 | -0.89843700 |
| C | 2.03754900 | 1.36291900 | -1.82274400 |
| C | 0.41323700 | 2.72638300 | -0.63409700 |
| C | 2.50484300 | 2.50477700 | -2.47660300 |
| H | 2.48539500 | 0.39805500 | -2.03640000 |
| C | 0.88842800 | 3.86076800 | -1.28857300 |
| H | -0.39963900 | 2.81700900 | 0.08233200 |
| C | 1.93284100 | 3.75009100 | -2.21180100 |
| H | 3.31503100 | 2.41757400 | -3.19417300 |
| H | 0.44177600 | 4.82874500 | -1.08244400 |
| H | 2.29735200 | 4.63479600 | -2.72532300 |
| C | 1.01299500 | 0.06379200 | 1.71250300 |
| C | 0.43562300 | -0.76271400 | 2.69116900 |
| C | 2.09455300 | 0.89317200 | 2.04554800 |
| C | 0.93927800 | -0.75890200 | 3.99029900 |
| H | -0.40233100 | -1.40820900 | 2.43907900 |
| C | 2.59053700 | 0.89282700 | 3.35083000 |
| H | 2.54472600 | 1.53804700 | 1.29776100 |
| C | 2.01533500 | 0.07042200 | 4.32111500 |
| H | 0.49067400 | -1.39852200 | 4.74447300 |
| H | 3.42557800 | 1.53792300 | 3.60707300 |
| H | 2.40245400 | 0.07616700 | 5.33570300 |
| C | 1.03494500 | -1.49632400 | -0.81008500 |
| C | 2.15555300 | -2.15758300 | -0.28484300 |
| C | 0.43287700 | -1.96411500 | -1.99043100 |
| C | 2.66634100 | -3.27961100 | -0.93984200 |
| H | 2.62411200 | -1.80673800 | 0.62897600 |
| C | 0.95201900 | -3.08288700 | -2.63909600 |
| H | -0.43629000 | -1.45712700 | -2.40233600 |
| C | 2.06710700 | -3.74196000 | -2.11304200 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.53112500 | -3.79238100 | -0.52952700 |
| H | 0.48351100 | -3.44309400 | -3.55001300 |
| H | 2.46563600 | -4.61773900 | -2.61652000 |
| O | -4.14298300 | -0.07999500 | -0.03877700 |
| H | -4.55017100 | -0.53458800 | 0.71956300 |
| H | -4.56063100 | 0.79722400 | -0.09704800 |

Au⁺PPPh₃

SCF done: -836.722393

| | | | |
|----|-------------|-------------|-------------|
| Au | 0.00734100 | 0.00777900 | 2.06829400 |
| P | -0.00076100 | -0.00097800 | -0.23212200 |
| C | -0.71181700 | 1.56744900 | -0.82153800 |
| C | -1.93103100 | 2.01447100 | -0.28107100 |
| C | -0.06775500 | 2.31000000 | -1.82434100 |
| C | -2.50219000 | 3.19472700 | -0.74905100 |
| H | -2.42775800 | 1.44592100 | 0.50109900 |
| C | -0.64962900 | 3.49250300 | -2.28385300 |
| H | 0.87436600 | 1.97312700 | -2.24349200 |
| C | -1.86050500 | 3.93487400 | -1.74815400 |
| H | -3.44204100 | 3.54127400 | -0.33056300 |
| H | -0.15269200 | 4.06756000 | -3.05910400 |
| H | -2.30475800 | 4.85916800 | -2.10511600 |
| C | -1.00911000 | -1.40185300 | -0.80968900 |
| C | -1.97152500 | -1.21868900 | -1.81569900 |
| C | -0.79244900 | -2.67823700 | -0.26005700 |
| C | -2.70798900 | -2.31411300 | -2.26920200 |
| H | -2.14628300 | -0.23633400 | -2.24139500 |
| C | -1.53232700 | -3.76340600 | -0.72201900 |
| H | -0.05375600 | -2.82170500 | 0.52455000 |
| C | -2.49132100 | -3.58109400 | -1.72446600 |
| H | -3.45256700 | -2.17366400 | -3.04672600 |
| H | -1.36718600 | -4.74827700 | -0.29622800 |
| H | -3.07192700 | -4.42831300 | -2.07691700 |
| C | 1.71185300 | -0.17529500 | -0.82300900 |
| C | 2.02729600 | -1.10469100 | -1.82724800 |
| C | 2.71287000 | 0.65304700 | -0.28436400 |
| C | 3.34083400 | -1.19651200 | -2.28999800 |
| H | 1.26117300 | -1.74908200 | -2.24509400 |
| C | 4.01919100 | 0.55312000 | -0.75552200 |
| H | 2.47335200 | 1.36821500 | 0.49861100 |
| C | 4.33362300 | -0.37294600 | -1.75618700 |
| H | 3.58587700 | -1.91489000 | -3.06623900 |
| H | 4.79247700 | 1.19067900 | -0.33827400 |
| H | 5.35505900 | -0.45370500 | -2.11569200 |

1

SCF done: -1748.075854

| | | | |
|----|-------------|-------------|-------------|
| C | 1.42817000 | 5.46809700 | -0.69774800 |
| C | 0.63816900 | 4.34620700 | -0.92251900 |
| C | 0.09386600 | 3.63456000 | 0.17109000 |
| C | 0.36510200 | 4.06837600 | 1.48864700 |
| C | 1.15963900 | 5.18881600 | 1.70153200 |
| C | 1.68974700 | 5.88806400 | 0.61119100 |
| H | 1.84088000 | 6.01741800 | -1.53839700 |
| H | 0.42675900 | 4.00816600 | -1.93218100 |
| H | -0.05517900 | 3.51797200 | 2.32424800 |
| H | 1.36642900 | 5.52186200 | 2.71393000 |
| H | 2.30858100 | 6.76417900 | 0.78242200 |
| C | -0.74968300 | 2.51536300 | -0.05859700 |
| C | -1.48166300 | 1.51329600 | -0.25853600 |
| S | -3.00630000 | -0.52785900 | -1.12173500 |
| O | -3.28128600 | -0.40226400 | -2.56235200 |
| O | -1.85595500 | -1.31463800 | -0.61723100 |
| C | -4.49081500 | -1.04307000 | -0.27793000 |
| C | -5.66748300 | -1.19003900 | -1.01486200 |
| C | -4.43812900 | -1.34604600 | 1.08719100 |
| C | -6.81643900 | -1.63260300 | -0.36035400 |
| H | -5.67592900 | -0.97000300 | -2.07691800 |
| C | -5.59703600 | -1.78416700 | 1.71759900 |
| H | -3.50906100 | -1.24638300 | 1.63856000 |
| C | -6.80208200 | -1.93606400 | 1.00817700 |
| H | -7.73720300 | -1.74738800 | -0.92541200 |
| H | -5.56886100 | -2.01940700 | 2.77820500 |
| C | -8.04138200 | -2.44255000 | 1.70334400 |
| H | -8.94841500 | -2.17703000 | 1.15263800 |
| H | -8.01640800 | -3.53664800 | 1.78976500 |
| H | -8.12434300 | -2.03953400 | 2.71802200 |
| N | -2.76013900 | 1.08314200 | -0.46134200 |
| C | -3.75622800 | 2.10890700 | -0.89552700 |
| H | -3.45582000 | 2.53204200 | -1.86076100 |
| H | -4.70052000 | 1.57327100 | -1.03926700 |
| Au | 0.34348200 | 0.26884200 | -0.09796700 |
| P | 2.29080600 | -1.02249800 | 0.04871100 |
| C | 3.19662200 | -0.70190500 | 1.61693500 |
| C | 4.59507600 | -0.60329500 | 1.65093600 |
| C | 2.46246800 | -0.58452800 | 2.80831500 |
| C | 5.24920400 | -0.39256100 | 2.86693300 |
| H | 5.17275800 | -0.68534100 | 0.73571700 |
| C | 3.12194900 | -0.38002700 | 4.01916600 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1. 37744600 | -0. 65373500 | 2. 78866000 |
| C | 4. 51599700 | -0. 28217500 | 4. 04936600 |
| H | 6. 33231800 | -0. 31446500 | 2. 88693500 |
| H | 2. 54862500 | -0. 29281700 | 4. 93756800 |
| H | 5. 02823600 | -0. 11744800 | 4. 99286800 |
| C | 1. 95962300 | -2. 82686000 | -0. 00994900 |
| C | 0. 88795400 | -3. 30520400 | -0. 78061600 |
| C | 2. 78587200 | -3. 73222600 | 0. 67529300 |
| C | 0. 65504000 | -4. 67781500 | -0. 86999000 |
| H | 0. 22669000 | -2. 61480500 | -1. 29525700 |
| C | 2. 54370800 | -5. 10308400 | 0. 58162900 |
| H | 3. 60922000 | -3. 37176200 | 1. 28410200 |
| C | 1. 48100600 | -5. 57653800 | -0. 19133300 |
| H | -0. 17756300 | -5. 04205900 | -1. 46449000 |
| H | 3. 18368500 | -5. 79941000 | 1. 11566000 |
| H | 1. 29348000 | -6. 64428100 | -0. 25936700 |
| C | 3. 45369900 | -0. 63579300 | -1. 32217900 |
| C | 4. 15038100 | -1. 64607500 | -2. 00050300 |
| C | 3. 65480600 | 0. 70778000 | -1. 67972300 |
| C | 5. 03993100 | -1. 31216600 | -3. 02413800 |
| H | 3. 99828500 | -2. 68792300 | -1. 73808000 |
| C | 4. 54900100 | 1. 03387500 | -2. 69781700 |
| H | 3. 11324600 | 1. 49673200 | -1. 16343500 |
| C | 5. 24085500 | 0. 02406700 | -3. 37268100 |
| H | 5. 57273700 | -2. 09940000 | -3. 54937100 |
| H | 4. 70114100 | 2. 07449400 | -2. 96928700 |
| H | 5. 93141700 | 0. 27939500 | -4. 17116700 |
| C | -3. 92171600 | 3. 17575900 | 0. 14599600 |
| H | -4. 23806100 | 2. 83481300 | 1. 13083300 |
| C | -3. 73430700 | 4. 47420900 | -0. 09519000 |
| H | -3. 42606500 | 4. 83599500 | -1. 07378500 |
| H | -3. 90151600 | 5. 22587600 | 0. 67068900 |

TS1-2

SCF done: -1748.074743

| | | | |
|---|-------------|-------------|--------------|
| C | 1. 74804800 | 5. 59295400 | -1. 03557400 |
| C | 0. 79949200 | 4. 57533800 | -1. 05966200 |
| C | 0. 61214600 | 3. 76059300 | 0. 07765200 |
| C | 1. 39449600 | 3. 98189900 | 1. 23026200 |
| C | 2. 33894200 | 5. 00319100 | 1. 24347600 |
| C | 2. 51667400 | 5. 80768600 | 0. 11306200 |
| H | 1. 88849000 | 6. 22017900 | -1. 91063500 |
| H | 0. 19737300 | 4. 39917200 | -1. 94549000 |
| H | 1. 24652600 | 3. 35239900 | 2. 10204100 |

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|----|-------------|-------------|-------------|
| H | 2.93685200 | 5.17479800 | 2.13334700 |
| H | 3.25531400 | 6.60387100 | 0.12754900 |
| C | -0.39223700 | 2.74213200 | 0.05990100 |
| C | -1.33673700 | 1.95379900 | -0.14420900 |
| S | -3.08750400 | 0.36687100 | -1.38945500 |
| O | -3.75466500 | 1.10650900 | -2.47207100 |
| O | -1.85900100 | -0.42208400 | -1.62041500 |
| C | -4.28913300 | -0.62514300 | -0.52227500 |
| C | -5.63732700 | -0.50223400 | -0.86357400 |
| C | -3.85833500 | -1.54084300 | 0.44444500 |
| C | -6.57064000 | -1.30269200 | -0.20568900 |
| H | -5.94242500 | 0.19778100 | -1.63388600 |
| C | -4.80784800 | -2.32653300 | 1.08739800 |
| H | -2.80347800 | -1.64137500 | 0.67799100 |
| C | -6.17567100 | -2.22261000 | 0.77534600 |
| H | -7.62195300 | -1.21257200 | -0.46409700 |
| H | -4.48552400 | -3.03899300 | 1.84222800 |
| C | -7.18646500 | -3.10440300 | 1.46557800 |
| H | -8.20374500 | -2.72173900 | 1.34430000 |
| H | -7.16313700 | -4.11987200 | 1.04953600 |
| H | -6.97684500 | -3.18926100 | 2.53718000 |
| N | -2.62384400 | 1.54074700 | -0.14215700 |
| C | -3.66411200 | 2.56978500 | 0.18101200 |
| H | -3.65081300 | 3.36147400 | -0.57603900 |
| H | -4.62573000 | 2.04989900 | 0.11307300 |
| Au | 0.43049600 | 0.48975400 | -0.01410500 |
| P | 2.00424300 | -1.23392000 | 0.04509200 |
| C | 3.05048800 | -1.16567400 | 1.55393300 |
| C | 4.41470900 | -1.48972200 | 1.50801800 |
| C | 2.46106500 | -0.81007500 | 2.77792600 |
| C | 5.17668600 | -1.46136500 | 2.67781900 |
| H | 4.88329300 | -1.75678700 | 0.56602800 |
| C | 3.22670100 | -0.78885700 | 3.94280000 |
| H | 1.40663100 | -0.54868500 | 2.81966700 |
| C | 4.58531600 | -1.11284700 | 3.89341200 |
| H | 6.23311800 | -1.70976400 | 2.63612100 |
| H | 2.76494700 | -0.51416900 | 4.88672400 |
| H | 5.18203100 | -1.08952200 | 4.80062300 |
| C | 1.21092200 | -2.88951500 | 0.01117800 |
| C | 0.09597800 | -3.09116700 | -0.81990700 |
| C | 1.72030500 | -3.95458900 | 0.76946100 |
| C | -0.49276500 | -4.35354900 | -0.89488200 |
| H | -0.31662000 | -2.27098800 | -1.40004500 |
| C | 1.12049500 | -5.21285400 | 0.69090600 |

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|---|-------------|-------------|-------------|
| H | 2.57607600 | -3.80578700 | 1.42014100 |
| C | 0.01735700 | -5.41385400 | -0.14105500 |
| H | -1.35236700 | -4.50574000 | -1.54108300 |
| H | 1.51714900 | -6.03424500 | 1.28046100 |
| H | -0.44565700 | -6.39469900 | -0.20029900 |
| C | 3.13539200 | -1.14140700 | -1.39854200 |
| C | 3.54716700 | -2.29595200 | -2.08008600 |
| C | 3.60937000 | 0.11596500 | -1.80774900 |
| C | 4.42736900 | -2.18956000 | -3.15891500 |
| H | 3.18034800 | -3.27170500 | -1.77809800 |
| C | 4.49132000 | 0.21354000 | -2.88249600 |
| H | 3.28939200 | 1.01628800 | -1.28875600 |
| C | 4.89934900 | -0.93877500 | -3.56015700 |
| H | 4.73980500 | -3.08584500 | -3.68663400 |
| H | 4.85377400 | 1.18828500 | -3.19544400 |
| H | 5.58042500 | -0.86018400 | -4.40249200 |
| C | -3.47101000 | 3.12147600 | 1.56267500 |
| H | -3.50065000 | 2.39596600 | 2.37439400 |
| C | -3.30803900 | 4.42003300 | 1.81828500 |
| H | -3.28266900 | 5.16195400 | 1.02306400 |
| H | -3.21330000 | 4.79253800 | 2.83405200 |

2

SCF done: -1748.090121

| | | | |
|---|-------------|-------------|-------------|
| C | 0.86048200 | 5.13990400 | 0.28855800 |
| C | 0.55535100 | 3.78052900 | 0.32989700 |
| C | 1.55034900 | 2.83213200 | 0.62499800 |
| C | 2.86128600 | 3.28471600 | 0.87990600 |
| C | 3.16252200 | 4.64136900 | 0.83977200 |
| C | 2.16232400 | 5.57384400 | 0.54369000 |
| H | 0.08065200 | 5.85968100 | 0.05834400 |
| H | -0.45834400 | 3.44507300 | 0.13109300 |
| H | 3.64146900 | 2.56390700 | 1.11126500 |
| H | 4.17625900 | 4.97528500 | 1.04101500 |
| H | 2.39901700 | 6.63335100 | 0.51377100 |
| C | 1.23447600 | 1.40188000 | 0.66614400 |
| C | 1.97611700 | 0.37935000 | 0.90483000 |
| S | 3.18041700 | -1.61529300 | -0.49482900 |
| O | 3.06601900 | -3.02945400 | -0.10969700 |
| O | 2.38285600 | -0.97181700 | -1.54414200 |
| C | 4.88707600 | -1.14551100 | -0.63111200 |
| C | 5.87140200 | -2.00075000 | -0.12714000 |
| C | 5.21001300 | 0.06234800 | -1.26042400 |
| C | 7.20603600 | -1.62251100 | -0.24871300 |

| | | | |
|----|-------------|-------------|-------------|
| H | 5.59853300 | -2.94615000 | 0.32868500 |
| C | 6.55064200 | 0.41658700 | -1.36601600 |
| H | 4.43108200 | 0.69718800 | -1.66925100 |
| C | 7.56808200 | -0.41488200 | -0.86590300 |
| H | 7.98030900 | -2.28085500 | 0.13506300 |
| H | 6.81550900 | 1.35014400 | -1.85485900 |
| C | 9.01796500 | -0.03124500 | -1.02182300 |
| H | 9.64414600 | -0.50523000 | -0.26034200 |
| H | 9.39596500 | -0.34864000 | -2.00246000 |
| H | 9.15507300 | 1.05269800 | -0.95665900 |
| N | 2.62812300 | -0.70570900 | 1.05822100 |
| C | 2.77847800 | -1.41633300 | 2.37568000 |
| H | 3.44925200 | -2.25798000 | 2.20083100 |
| H | 3.27059700 | -0.71021400 | 3.05188400 |
| Au | -0.68772900 | 0.57153100 | 0.26568800 |
| P | -2.83190900 | -0.25446000 | -0.23051800 |
| C | -3.90936400 | -0.35157800 | 1.25574300 |
| C | -4.85980200 | -1.37257000 | 1.40691300 |
| C | -3.78894600 | 0.63656900 | 2.24626900 |
| C | -5.68162000 | -1.39815700 | 2.53524800 |
| H | -4.95569900 | -2.14724400 | 0.65248000 |
| C | -4.61585200 | 0.60777900 | 3.36873600 |
| H | -3.04889500 | 1.42610600 | 2.14124900 |
| C | -5.56194300 | -0.41002000 | 3.51454000 |
| H | -6.41338500 | -2.19274700 | 2.64839400 |
| H | -4.51744300 | 1.37546500 | 4.13071200 |
| H | -6.20156400 | -0.43494100 | 4.39203600 |
| C | -3.69350000 | 0.81943800 | -1.44902300 |
| C | -2.96659200 | 1.29174100 | -2.55489800 |
| C | -5.04536500 | 1.16387900 | -1.30837000 |
| C | -3.58974900 | 2.09254100 | -3.51064400 |
| H | -1.91709700 | 1.03141400 | -2.66995900 |
| C | -5.66169400 | 1.97134500 | -2.26708200 |
| H | -5.61545800 | 0.81005500 | -0.45533500 |
| C | -4.93732400 | 2.43477700 | -3.36638400 |
| H | -3.02283200 | 2.45275900 | -4.36414300 |
| H | -6.70828100 | 2.23766400 | -2.15149900 |
| H | -5.41992800 | 3.06379500 | -4.10878000 |
| C | -2.76971000 | -1.93871000 | -0.96208400 |
| C | -3.66610600 | -2.33371300 | -1.96669400 |
| C | -1.81065800 | -2.84877400 | -0.48885300 |
| C | -3.60455000 | -3.62840000 | -2.48532900 |
| H | -4.40279700 | -1.63438700 | -2.34988300 |
| C | -1.75651000 | -4.14082300 | -1.00999000 |

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|---|-------------|-------------|-------------|
| H | -1.10428600 | -2.54847300 | 0.28121900 |
| C | -2.65229300 | -4.53132400 | -2.00863000 |
| H | -4.29840500 | -3.92782600 | -3.26540400 |
| H | -1.00875000 | -4.83816200 | -0.64389700 |
| H | -2.60365200 | -5.53586400 | -2.41881300 |
| C | 1.45905900 | -1.88397800 | 2.92218200 |
| H | 0.76946400 | -1.10503700 | 3.24398400 |
| C | 1.13267500 | -3.17116500 | 3.04699100 |
| H | 1.80511000 | -3.96679400 | 2.73513900 |
| H | 0.18251100 | -3.47496300 | 3.47707400 |

3

SCF done: -2238.929610

| | | | |
|---|-------------|-------------|-------------|
| C | -0.48555800 | 4.22841900 | -2.61283900 |
| C | -0.02154000 | 3.00484600 | -2.13363800 |
| C | -0.92221500 | 1.96556200 | -1.84038500 |
| C | -2.30102000 | 2.18535100 | -2.03312700 |
| C | -2.76212700 | 3.41175100 | -2.50112000 |
| C | -1.85443800 | 4.43537000 | -2.79471700 |
| H | 0.22157200 | 5.02044700 | -2.84116800 |
| H | 1.04363000 | 2.84462900 | -1.99210500 |
| H | -3.00781200 | 1.39702400 | -1.79488900 |
| H | -3.82859900 | 3.57503300 | -2.62774900 |
| H | -2.21608500 | 5.39133800 | -3.16227500 |
| C | -0.43729500 | 0.67684200 | -1.34585400 |
| C | -1.00363600 | -0.46282600 | -1.17163900 |
| S | -1.84432800 | -2.14493000 | 0.78015600 |
| O | -0.81262500 | -3.14450700 | 1.11127600 |
| O | -1.95252300 | -0.84981700 | 1.46202500 |
| C | -3.41991900 | -2.93884300 | 0.59662900 |
| C | -3.48129700 | -4.33410300 | 0.67625800 |
| C | -4.56252900 | -2.15257900 | 0.40773500 |
| C | -4.72354200 | -4.95097200 | 0.55072100 |
| H | -2.58140800 | -4.91454400 | 0.84775500 |
| C | -5.78789100 | -2.79848000 | 0.28250000 |
| H | -4.50243500 | -1.06848900 | 0.36430600 |
| C | -5.89206900 | -4.19882300 | 0.35192900 |
| H | -4.78717500 | -6.03358100 | 0.61563200 |
| H | -6.68370200 | -2.20187200 | 0.13294600 |
| C | -7.23709100 | -4.87193500 | 0.24304900 |
| H | -7.78521800 | -4.79292400 | 1.19079100 |
| H | -7.85697400 | -4.40235300 | -0.52783200 |
| H | -7.13877500 | -5.93522800 | 0.00646400 |
| N | -1.41874100 | -1.65405900 | -0.97131200 |

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|----|-------------|-------------|-------------|
| C | -1.29386500 | -2.74737400 | -1.99359900 |
| H | -0.26348900 | -2.70582600 | -2.36408700 |
| H | -1.42347900 | -3.69463900 | -1.46638900 |
| Au | 1.53293900 | 0.31332000 | -0.60553200 |
| P | 3.67908200 | -0.08746000 | 0.26253800 |
| C | 3.59926600 | -0.94013500 | 1.88794500 |
| C | 4.57171000 | -0.71788000 | 2.87552200 |
| C | 2.55318800 | -1.84409800 | 2.13363000 |
| C | 4.49829800 | -1.39954900 | 4.09121500 |
| H | 5.37776700 | -0.01153600 | 2.70186900 |
| C | 2.48718300 | -2.52252500 | 3.35032800 |
| H | 1.78472900 | -2.01969500 | 1.38578300 |
| C | 3.45848100 | -2.30122100 | 4.32942300 |
| H | 5.25181000 | -1.22145000 | 4.85295000 |
| H | 1.67043500 | -3.21499500 | 3.53086400 |
| H | 3.40250100 | -2.82573800 | 5.27899300 |
| C | 4.68182200 | -1.14435900 | -0.85965600 |
| C | 4.62382100 | -0.90043500 | -2.24197600 |
| C | 5.50387100 | -2.16984400 | -0.37058000 |
| C | 5.38701000 | -1.66737700 | -3.12101300 |
| H | 3.98261700 | -0.11285700 | -2.63040300 |
| C | 6.26100800 | -2.93856600 | -1.25729500 |
| H | 5.55091100 | -2.37390600 | 0.69437200 |
| C | 6.20486600 | -2.68860400 | -2.62943100 |
| H | 5.33870000 | -1.47196200 | -4.18831700 |
| H | 6.89308400 | -3.73379300 | -0.87290100 |
| H | 6.79411900 | -3.28983600 | -3.31576600 |
| C | 4.63107400 | 1.46346600 | 0.52151300 |
| C | 5.99731700 | 1.55084900 | 0.21733600 |
| C | 3.96556700 | 2.57886000 | 1.05669100 |
| C | 6.68824300 | 2.74203000 | 0.45011800 |
| H | 6.52065900 | 0.69846400 | -0.20415200 |
| C | 4.66239800 | 3.76335100 | 1.29054700 |
| H | 2.90550700 | 2.52080900 | 1.29198000 |
| C | 6.02394600 | 3.84647600 | 0.98594200 |
| H | 7.74552800 | 2.80491100 | 0.20963500 |
| H | 4.14212400 | 4.62185900 | 1.70524200 |
| H | 6.56422700 | 4.77192900 | 1.16301800 |
| C | -2.29315000 | -2.59263300 | -3.10387400 |
| C | -3.20961600 | -3.51223200 | -3.40420100 |
| H | -2.21683500 | -1.67665400 | -3.68841900 |
| H | -3.89529700 | -3.37845700 | -4.23563300 |
| H | -3.30448900 | -4.43614800 | -2.83812800 |
| C | -4.45996300 | 2.13025600 | 1.40872600 |

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|---|-------------|------------|-------------|
| C | -4.93033000 | 3.43271900 | 1.06996500 |
| C | -4.80954900 | 4.55091500 | 1.93205400 |
| C | -4.20137400 | 4.31671100 | 3.13703000 |
| C | -3.70791700 | 3.01174300 | 3.49527200 |
| C | -3.81897300 | 1.92544900 | 2.66882300 |
| H | -5.18646500 | 5.52268600 | 1.63407300 |
| H | -4.08119500 | 5.13011900 | 3.84539500 |
| H | -3.22735600 | 2.89513000 | 4.46215400 |
| H | -3.43225300 | 0.94687500 | 2.92940400 |
| O | -5.32958900 | 1.97005400 | -0.56004100 |
| N | -4.70033600 | 1.26036200 | 0.43590300 |
| N | -5.46458100 | 3.35347900 | -0.15982900 |
| O | -5.97493800 | 4.14699200 | -0.93650600 |

Ts3-4

SCF done:-2238.907295

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|---|------------|-------------|-------------|
| C | 0.59646200 | -4.92285000 | 0.72803300 |
| C | 0.45124400 | -3.53656200 | 0.75990400 |
| C | 0.82953100 | -2.75487300 | -0.34605500 |
| C | 1.31893000 | -3.39793700 | -1.49657400 |
| C | 1.44417100 | -4.78762800 | -1.52933400 |
| C | 1.09064400 | -5.55376000 | -0.41653300 |
| H | 0.31148700 | -5.51230100 | 1.59505800 |
| H | 0.04992800 | -3.04930200 | 1.64431100 |
| H | 1.58195100 | -2.80894200 | -2.36972600 |
| H | 1.81407800 | -5.27085100 | -2.42938100 |
| H | 1.18739500 | -6.63517100 | -0.44531600 |
| C | 0.65194200 | -1.29042900 | -0.31187900 |
| C | 1.56757000 | -0.35039200 | -0.38782300 |
| S | 1.86722900 | 1.94394200 | 0.93361600 |
| O | 0.70229700 | 2.84980600 | 0.93963800 |
| O | 2.09858000 | 0.95141100 | 1.99803800 |
| C | 3.33621800 | 2.91806700 | 0.66133200 |
| C | 3.20448200 | 4.27868900 | 0.37885000 |
| C | 4.59276200 | 2.31594500 | 0.78246900 |
| C | 4.35789500 | 5.04029700 | 0.19666900 |
| H | 2.22064600 | 4.73102900 | 0.32178300 |
| C | 5.72860600 | 3.09486800 | 0.59417800 |
| H | 4.67677500 | 1.26387100 | 1.03108600 |
| C | 5.63264400 | 4.46517300 | 0.29418200 |
| H | 4.26412800 | 6.10173100 | -0.01555300 |
| H | 6.70958400 | 2.63705500 | 0.69045100 |
| C | 6.87666600 | 5.28968600 | 0.07425600 |
| H | 7.65679100 | 5.03614300 | 0.79979800 |

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|----|-------------|-------------|-------------|
| H | 7.29251400 | 5.10723200 | -0.92516500 |
| H | 6.66911200 | 6.36044700 | 0.15503500 |
| N | 1.71809500 | 0.96222800 | -0.53210100 |
| C | 1.47906900 | 1.65057000 | -1.83410700 |
| H | 0.62032000 | 1.14382700 | -2.29069700 |
| H | 1.16614300 | 2.67267400 | -1.60559100 |
| Au | -1.30178100 | -0.53544500 | -0.13087800 |
| P | -3.50551300 | 0.29033500 | 0.05969700 |
| C | -3.72341800 | 1.36732300 | 1.53316800 |
| C | -4.92686700 | 1.39181100 | 2.25480100 |
| C | -2.65666000 | 2.19119000 | 1.92873600 |
| C | -5.06060500 | 2.23684800 | 3.35772000 |
| H | -5.75367500 | 0.75099300 | 1.96470300 |
| C | -2.80065700 | 3.03564300 | 3.02961300 |
| H | -1.71447300 | 2.17789800 | 1.38773900 |
| C | -4.00007400 | 3.05867800 | 3.74527800 |
| H | -5.99292000 | 2.24906100 | 3.91496500 |
| H | -1.96991400 | 3.66753900 | 3.32965000 |
| H | -4.10688200 | 3.71188400 | 4.60670000 |
| C | -3.97293400 | 1.29498700 | -1.41065200 |
| C | -3.64131300 | 0.80835200 | -2.68629400 |
| C | -4.65284000 | 2.51512300 | -1.29094300 |
| C | -3.99465300 | 1.53014000 | -3.82536400 |
| H | -3.11029600 | -0.13518800 | -2.78791900 |
| C | -4.99859800 | 3.23675300 | -2.43598300 |
| H | -4.90908000 | 2.90452000 | -0.31076900 |
| C | -4.67195400 | 2.74660300 | -3.70123900 |
| H | -3.73833800 | 1.14560500 | -4.80842500 |
| H | -5.52354800 | 4.18239400 | -2.33578100 |
| H | -4.94218600 | 3.31070400 | -4.58931400 |
| C | -4.76192000 | -1.04684600 | 0.18794700 |
| C | -6.01837100 | -0.94131500 | -0.42698500 |
| C | -4.45404900 | -2.18972900 | 0.94326100 |
| C | -6.95436600 | -1.96741700 | -0.28269200 |
| H | -6.26527200 | -0.06687900 | -1.02102900 |
| C | -5.39452900 | -3.20884800 | 1.08761100 |
| H | -3.47952900 | -2.28243500 | 1.41599800 |
| C | -6.64489800 | -3.09930000 | 0.47359500 |
| H | -7.92416100 | -1.88127700 | -0.76420700 |
| H | -5.14904900 | -4.09027400 | 1.67292100 |
| H | -7.37441900 | -3.89683800 | 0.58116500 |
| C | 2.67515100 | 1.63413400 | -2.74524200 |
| C | 3.20953500 | 2.72994700 | -3.28373800 |
| H | 3.08275300 | 0.65283400 | -2.98360500 |

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|---|------------|-------------|-------------|
| H | 4.04894000 | 2.67478900 | -3.97082900 |
| H | 2.82354500 | 3.72372500 | -3.06727400 |
| C | 3.84082500 | -1.91657700 | 0.62734900 |
| C | 4.74225600 | -2.85008700 | 0.04839500 |
| C | 5.46494600 | -3.80531500 | 0.80245500 |
| C | 5.24853800 | -3.78431800 | 2.15615000 |
| C | 4.34378100 | -2.84486900 | 2.75833400 |
| C | 3.63701000 | -1.91602200 | 2.03431300 |
| H | 6.14406200 | -4.49633100 | 0.31658700 |
| H | 5.77289800 | -4.48688100 | 2.79538200 |
| H | 4.21972100 | -2.87382200 | 3.83667600 |
| H | 2.96587100 | -1.19618200 | 2.48707800 |
| O | 3.84501300 | -1.53808800 | -1.52765500 |
| N | 3.32628400 | -1.12208200 | -0.31847800 |
| N | 4.74647300 | -2.64393700 | -1.28558100 |
| O | 5.32084000 | -3.14427900 | -2.22630700 |

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SCF done: -2238.923159

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|---|-------------|-------------|-------------|
| C | 0.34433800 | -5.09069600 | 0.55229300 |
| C | 0.24562700 | -3.70080100 | 0.58751500 |
| C | 0.86325700 | -2.90966100 | -0.40011400 |
| C | 1.54746600 | -3.56037300 | -1.44553800 |
| C | 1.61848200 | -4.95293600 | -1.49353000 |
| C | 1.02717400 | -5.72316200 | -0.49032900 |
| H | -0.12681500 | -5.68247700 | 1.33223800 |
| H | -0.30707800 | -3.21510000 | 1.38770600 |
| H | 1.99395900 | -2.97190600 | -2.24252500 |
| H | 2.13184400 | -5.43612900 | -2.32039900 |
| H | 1.08426600 | -6.80707600 | -0.52817300 |
| C | 0.74927300 | -1.43334800 | -0.35667800 |
| C | 1.84757800 | -0.64129000 | -0.42933500 |
| S | 1.87191000 | 1.65940300 | 0.89904100 |
| O | 0.51680300 | 2.22158700 | 1.09704900 |
| O | 2.47593600 | 0.74611100 | 1.89515900 |
| C | 2.98691800 | 3.02413100 | 0.58555700 |
| C | 2.46802600 | 4.30609100 | 0.40400500 |
| C | 4.36620500 | 2.79217200 | 0.58004100 |
| C | 3.35060000 | 5.36680900 | 0.19583200 |
| H | 1.39624500 | 4.46751800 | 0.44043500 |
| C | 5.22795900 | 3.86240000 | 0.37154200 |
| H | 4.75258200 | 1.79335000 | 0.75278200 |
| C | 4.73668400 | 5.16527800 | 0.17235200 |
| H | 2.95291900 | 6.36845900 | 0.05780500 |

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|----|-------------|-------------|-------------|
| H | 6.30135000 | 3.69092800 | 0.37097700 |
| C | 5.68852700 | 6.31221000 | -0.06373400 |
| H | 6.49240900 | 6.32068600 | 0.68082600 |
| H | 6.16327400 | 6.23081400 | -1.04976300 |
| H | 5.17489800 | 7.27667100 | -0.02025100 |
| N | 1.92908200 | 0.76444400 | -0.59071900 |
| C | 1.23455100 | 1.41827200 | -1.73648100 |
| H | 0.14816800 | 1.39913500 | -1.57876800 |
| H | 1.55388800 | 2.46463700 | -1.73743000 |
| Au | -1.15118600 | -0.63174100 | -0.16239000 |
| P | -3.34428400 | 0.24269800 | 0.09445100 |
| C | -3.65769400 | 0.82277400 | 1.81286900 |
| C | -4.89044500 | 0.62167100 | 2.45127500 |
| C | -2.62238700 | 1.49144900 | 2.48922900 |
| C | -5.08674000 | 1.08883800 | 3.75232800 |
| H | -5.69310000 | 0.09904700 | 1.94076300 |
| C | -2.83057200 | 1.96009500 | 3.78654700 |
| H | -1.65983700 | 1.64994600 | 2.00964900 |
| C | -4.05954100 | 1.75831400 | 4.41991200 |
| H | -6.04248300 | 0.92691200 | 4.24257700 |
| H | -2.02752600 | 2.47753700 | 4.30357700 |
| H | -4.21510000 | 2.11893100 | 5.43283400 |
| C | -3.64561400 | 1.68806600 | -1.00826300 |
| C | -3.22737200 | 1.60324200 | -2.34671200 |
| C | -4.28572800 | 2.85029700 | -0.55677000 |
| C | -3.45506400 | 2.66466800 | -3.22144500 |
| H | -2.72927800 | 0.70521200 | -2.70474000 |
| C | -4.50639000 | 3.91298600 | -1.43644700 |
| H | -4.60825900 | 2.92957000 | 0.47652700 |
| C | -4.09341500 | 3.82197600 | -2.76641000 |
| H | -3.13219300 | 2.58985200 | -4.25596700 |
| H | -5.00188300 | 4.81121500 | -1.07913000 |
| H | -4.26679700 | 4.65021100 | -3.44757500 |
| C | -4.66620700 | -0.97243900 | -0.31102100 |
| C | -5.90518200 | -0.56473000 | -0.82962700 |
| C | -4.42962500 | -2.33668300 | -0.08008000 |
| C | -6.89411000 | -1.51079700 | -1.10376900 |
| H | -6.09602100 | 0.48573300 | -1.02730900 |
| C | -5.42265800 | -3.27756400 | -0.35286000 |
| H | -3.46753500 | -2.66350400 | 0.30602300 |
| C | -6.65518900 | -2.86586400 | -0.86483700 |
| H | -7.84940000 | -1.18814100 | -1.50774300 |
| H | -5.23052800 | -4.33151000 | -0.17351600 |
| H | -7.42554000 | -3.59990300 | -1.08317900 |

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| C | 1. 59259900 | 0. 78017500 | -3. 05076700 |
| C | 2. 28677900 | 1. 39618900 | -4. 00789700 |
| H | 1. 21854300 | -0. 22853300 | -3. 21741900 |
| H | 2. 49500400 | 0. 91542800 | -4. 95967900 |
| H | 2. 66616500 | 2. 40807300 | -3. 88207100 |
| C | 3. 77522700 | -1. 90331200 | 0. 68200300 |
| C | 5. 03601900 | -2. 35054700 | 0. 21177300 |
| C | 5. 94523300 | -3. 08875000 | 1. 00532400 |
| C | 5. 53304400 | -3. 35662400 | 2. 28564000 |
| C | 4. 26449000 | -2. 89878600 | 2. 77561400 |
| C | 3. 37576200 | -2. 17990000 | 2. 01043700 |
| H | 6. 89927400 | -3. 40883500 | 0. 60330600 |
| H | 6. 17815400 | -3. 91938700 | 2. 95182500 |
| H | 4. 00064000 | -3. 12643400 | 3. 80374400 |
| H | 2. 43400800 | -1. 80762200 | 2. 38919400 |
| O | 3. 99676500 | -1. 21798600 | -1. 43089600 |
| N | 3. 15637400 | -1. 23747500 | -0. 30150600 |
| N | 5. 18305800 | -1. 93066800 | -1. 06873800 |
| O | 6. 06703000 | -2. 02343600 | -1. 88502600 |

TS4-5

SCF done: -2238.918353

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|---|--------------|--------------|--------------|
| C | 0. 37128100 | -5. 12003500 | 0. 13608500 |
| C | 0. 22984900 | -3. 74171900 | 0. 26340300 |
| C | 0. 97271400 | -2. 86001000 | -0. 55180400 |
| C | 1. 82394500 | -3. 41500200 | -1. 53365800 |
| C | 1. 92860400 | -4. 79611500 | -1. 68597100 |
| C | 1. 21499900 | -5. 65278600 | -0. 84408600 |
| H | -0. 19135100 | -5. 78222500 | 0. 78785300 |
| H | -0. 44403900 | -3. 32931000 | 1. 00918600 |
| H | 2. 36646900 | -2. 75721800 | -2. 20507700 |
| H | 2. 56460700 | -5. 20462600 | -2. 46622000 |
| H | 1. 30256300 | -6. 72902800 | -0. 96093500 |
| C | 0. 80910500 | -1. 40872400 | -0. 41450800 |
| C | 1. 90122900 | -0. 55887600 | -0. 41505700 |
| S | 1. 74253600 | 1. 80388300 | 0. 81364000 |
| O | 0. 38439200 | 2. 39074000 | 0. 89078000 |
| O | 2. 26110700 | 0. 93493800 | 1. 89254900 |
| C | 2. 89408200 | 3. 13920900 | 0. 50840700 |
| C | 2. 40607300 | 4. 42363600 | 0. 26586600 |
| C | 4. 26724300 | 2. 88132000 | 0. 56136600 |
| C | 3. 31552700 | 5. 46111900 | 0. 05986200 |
| H | 1. 33672700 | 4. 60296600 | 0. 24885600 |
| C | 5. 15631000 | 3. 92995200 | 0. 35408900 |

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|----|-------------|-------------|-------------|
| H | 4.62777900 | 1.87898700 | 0.76650400 |
| C | 4.69794200 | 5.23501500 | 0.10205600 |
| H | 2.94244500 | 6.46364800 | -0.13135500 |
| H | 6.22543100 | 3.73800400 | 0.39211800 |
| C | 5.67651000 | 6.36780500 | -0.08874300 |
| H | 6.56618900 | 6.04063800 | -0.63679300 |
| H | 5.22507200 | 7.20195300 | -0.63397600 |
| H | 6.01655300 | 6.75425600 | 0.88091500 |
| N | 1.86386200 | 0.84338000 | -0.62453200 |
| C | 1.18655700 | 1.41476500 | -1.82129200 |
| H | 0.09710400 | 1.40238000 | -1.68737900 |
| H | 1.50012600 | 2.46141700 | -1.88308800 |
| Au | -1.10103200 | -0.64834500 | -0.17463200 |
| P | -3.30051100 | 0.21444800 | 0.11158000 |
| C | -3.60244900 | 0.76669900 | 1.84070500 |
| C | -4.80710200 | 0.49566300 | 2.50585900 |
| C | -2.58593200 | 1.48179200 | 2.49839900 |
| C | -4.99402500 | 0.93776900 | 3.81712400 |
| H | -5.59546900 | -0.05966500 | 2.00798200 |
| C | -2.78564600 | 1.92478600 | 3.80587500 |
| H | -1.64705300 | 1.69914900 | 1.99528800 |
| C | -3.98599500 | 1.65179500 | 4.46722400 |
| H | -5.92792200 | 0.72219700 | 4.32831100 |
| H | -1.99839100 | 2.47910000 | 4.30873500 |
| H | -4.13426700 | 1.99315900 | 5.48785100 |
| C | -3.60433400 | 1.67435100 | -0.96943000 |
| C | -3.19850900 | 1.60523300 | -2.31258400 |
| C | -4.23644900 | 2.83230800 | -0.49656400 |
| C | -3.42990600 | 2.67896400 | -3.17109900 |
| H | -2.70783300 | 0.70987500 | -2.68733800 |
| C | -4.46092200 | 3.90719600 | -1.36023300 |
| H | -4.54909400 | 2.89902100 | 0.54060300 |
| C | -4.05980000 | 3.83237800 | -2.69482300 |
| H | -3.11667500 | 2.61677900 | -4.20938100 |
| H | -4.94992700 | 4.80234000 | -0.98673200 |
| H | -4.23594300 | 4.67027600 | -3.36329400 |
| C | -4.62186000 | -0.99634200 | -0.30652100 |
| C | -5.86390500 | -0.57960700 | -0.81047400 |
| C | -4.38504300 | -2.36418500 | -0.09893500 |
| C | -6.85448200 | -1.52073400 | -1.09513400 |
| H | -6.05595000 | 0.47420200 | -0.98782000 |
| C | -5.37973400 | -3.30029900 | -0.38174100 |
| H | -3.42167500 | -2.69732000 | 0.27835800 |
| C | -6.61469600 | -2.87971600 | -0.88046300 |

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|---|-------------|-------------|-------------|
| H | -7.81198900 | -1.19106400 | -1.48793100 |
| H | -5.18764800 | -4.35713500 | -0.22024100 |
| H | -7.38647700 | -3.60977000 | -1.10681200 |
| C | 1.57397700 | 0.69697300 | -3.08611200 |
| C | 2.32931500 | 1.23757400 | -4.04248600 |
| H | 1.17209700 | -0.30647000 | -3.21848700 |
| H | 2.56107900 | 0.70003400 | -4.95771200 |
| H | 2.73951500 | 2.24108100 | -3.95160900 |
| C | 3.64382000 | -1.85478400 | 0.84775200 |
| C | 4.85371400 | -2.46659800 | 0.45560600 |
| C | 5.60938400 | -3.31396000 | 1.28952700 |
| C | 5.10309500 | -3.53631100 | 2.54863000 |
| C | 3.88685900 | -2.91794200 | 2.96507200 |
| C | 3.14749400 | -2.08352800 | 2.15075500 |
| H | 6.53464900 | -3.75152400 | 0.93269400 |
| H | 5.63362600 | -4.18136700 | 3.24047600 |
| H | 3.52983300 | -3.10722900 | 3.97301700 |
| H | 2.24567000 | -1.58578600 | 2.48175700 |
| O | 4.22929800 | -1.25339000 | -1.32814300 |
| N | 3.16146200 | -1.02825500 | -0.10191900 |
| N | 5.17140300 | -2.07485700 | -0.82287800 |
| O | 6.15429300 | -2.34695900 | -1.48277700 |

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SCF done: -2238.963844

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|---|-------------|-------------|-------------|
| C | 0.08121400 | -4.48278800 | -2.71229500 |
| C | -0.17076600 | -3.32882100 | -1.99377000 |
| C | 0.89667900 | -2.45556400 | -1.61420900 |
| C | 2.23159500 | -2.80990800 | -1.99016100 |
| C | 2.47157000 | -3.96894200 | -2.70815100 |
| C | 1.40158100 | -4.80107600 | -3.07058200 |
| H | -0.73300300 | -5.14004100 | -2.99994600 |
| H | -1.18452900 | -3.06448600 | -1.70879200 |
| H | 3.06113800 | -2.17922000 | -1.68610300 |
| H | 3.48584900 | -4.23413600 | -2.98891000 |
| H | 1.59717000 | -5.70786600 | -3.63653500 |
| C | 0.61243300 | -1.26006600 | -0.91486000 |
| C | 1.71106300 | -0.35698400 | -0.46508400 |
| S | 1.93955100 | 2.31841600 | -0.00425200 |
| O | 1.46917100 | 3.42523300 | -0.85465200 |
| O | 1.27640700 | 1.97945900 | 1.27047900 |
| C | 3.69337400 | 2.49517300 | 0.26799200 |
| C | 4.45689200 | 3.16374300 | -0.69203900 |
| C | 4.26000600 | 2.01636500 | 1.45092900 |

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|----|-------------|-------------|-------------|
| C | 5.81995900 | 3.33044300 | -0.46294500 |
| H | 3.99245100 | 3.54304800 | -1.59511100 |
| C | 5.62377300 | 2.20059200 | 1.65976400 |
| H | 3.64224200 | 1.51478700 | 2.18594800 |
| C | 6.42478700 | 2.85557200 | 0.71112000 |
| H | 6.42390900 | 3.84463900 | -1.20577100 |
| H | 6.07539700 | 1.83083300 | 2.57645000 |
| C | 7.89676300 | 3.07106700 | 0.96295800 |
| H | 8.32413400 | 2.25909400 | 1.55961300 |
| H | 8.45811200 | 3.14093800 | 0.02620400 |
| H | 8.06325100 | 4.00532300 | 1.51518400 |
| N | 1.72072800 | 0.90738100 | -1.04016400 |
| C | 1.34318200 | 1.12667100 | -2.45622600 |
| H | 0.78482800 | 0.23375600 | -2.76953200 |
| H | 0.65444500 | 1.97097900 | -2.51339300 |
| Au | -1.23977600 | -0.54978800 | -0.37350200 |
| P | -3.33191400 | 0.38917900 | 0.28552900 |
| C | -3.22751500 | 1.20964900 | 1.92487000 |
| C | -4.32193000 | 1.22627000 | 2.80382500 |
| C | -2.02998200 | 1.85001700 | 2.28519500 |
| C | -4.21733900 | 1.88326600 | 4.03054700 |
| H | -5.24807000 | 0.72666600 | 2.53683600 |
| C | -1.93674900 | 2.50692200 | 3.51256000 |
| H | -1.16729300 | 1.84213300 | 1.62429800 |
| C | -3.02730500 | 2.52345500 | 4.38510000 |
| H | -5.06543700 | 1.89231600 | 4.70906100 |
| H | -1.00719300 | 2.99868200 | 3.78305800 |
| H | -2.94971400 | 3.03125700 | 5.34223300 |
| C | -3.88542200 | 1.65645000 | -0.92742600 |
| C | -3.80514100 | 1.35512500 | -2.29754400 |
| C | -4.38169100 | 2.90217000 | -0.51919800 |
| C | -4.22591500 | 2.28665300 | -3.24501400 |
| H | -3.41800900 | 0.39226500 | -2.62296500 |
| C | -4.79608800 | 3.83347100 | -1.47416100 |
| H | -4.44029800 | 3.14889900 | 0.53589500 |
| C | -4.71975500 | 3.52807000 | -2.83374100 |
| H | -4.16393000 | 2.04673400 | -4.30253800 |
| H | -5.17606900 | 4.79856000 | -1.15217300 |
| H | -5.04088500 | 4.25614000 | -3.57294200 |
| C | -4.67711200 | -0.86033700 | 0.38942300 |
| C | -5.98842300 | -0.56551700 | -0.01185900 |
| C | -4.38043500 | -2.13095500 | 0.90908100 |
| C | -6.98918900 | -1.53189400 | 0.10968200 |
| H | -6.22860000 | 0.41062700 | -0.42148400 |

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|---|-------------|-------------|-------------|
| C | -5.38477800 | -3.09021600 | 1.03202000 |
| H | -3.36606700 | -2.36798300 | 1.22148800 |
| C | -6.68983100 | -2.79182900 | 0.63095100 |
| H | -8.00213300 | -1.29823900 | -0.20485300 |
| H | -5.14893000 | -4.07013300 | 1.43700600 |
| H | -7.47060300 | -3.54129900 | 0.72241700 |
| C | 2.53157600 | 1.33668100 | -3.35529300 |
| C | 2.65082200 | 2.37395600 | -4.18558600 |
| H | 3.30816900 | 0.57336900 | -3.31034800 |
| H | 3.50597700 | 2.47855700 | -4.84725700 |
| H | 1.89545000 | 3.15507100 | -4.23473300 |
| C | 2.50613600 | -1.74189900 | 1.32165800 |
| C | 3.66824000 | -2.52364600 | 1.51953900 |
| C | 3.71381600 | -3.54622000 | 2.47157400 |
| C | 2.59898300 | -3.82024200 | 3.25327100 |
| C | 1.44435900 | -3.04699100 | 3.09121300 |
| C | 1.40143000 | -2.02205700 | 2.15142600 |
| H | 4.63300500 | -4.10959900 | 2.57719700 |
| H | 2.63224900 | -4.61934500 | 3.98628100 |
| H | 0.57220500 | -3.23559800 | 3.71087100 |
| H | 0.52640200 | -1.38487000 | 2.07296200 |
| O | 4.77639600 | -1.71118300 | -0.35528600 |
| N | 2.51826700 | -0.62602500 | 0.49467400 |
| N | 4.87998400 | -2.29563600 | 0.72996200 |
| O | 5.94309000 | -2.70800700 | 1.18739600 |

TS5-6

SCF done: -2238.938167

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|---|-------------|-------------|-------------|
| C | 0.43273400 | 3.62554900 | 3.14370000 |
| C | 0.14822900 | 2.77696500 | 2.08073800 |
| C | 1.13872700 | 1.92566100 | 1.53934500 |
| C | 2.42737000 | 1.95837300 | 2.12244700 |
| C | 2.70374200 | 2.79415100 | 3.20167000 |
| C | 1.71143600 | 3.63381400 | 3.71290500 |
| H | -0.34329700 | 4.27408800 | 3.53949300 |
| H | -0.84879800 | 2.76297000 | 1.64896500 |
| H | 3.21420300 | 1.31620500 | 1.73823700 |
| H | 3.69571000 | 2.79018800 | 3.64353800 |
| H | 1.92952200 | 4.28637500 | 4.55314400 |
| C | 0.80311800 | 1.01918400 | 0.42281100 |
| C | 1.90674700 | 0.08477700 | -0.04327100 |
| S | 2.73905600 | -2.45893000 | -0.68228200 |
| O | 2.18303900 | -3.70626500 | -0.13115300 |
| O | 2.49767300 | -2.02525100 | -2.06153500 |

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|----|-------------|-------------|-------------|
| C | 4.46184400 | -2.36382800 | -0.25175600 |
| C | 4.94689800 | -3.21199000 | 0.75084400 |
| C | 5.30359700 | -1.49344800 | -0.95061600 |
| C | 6.30095500 | -3.15931000 | 1.06914500 |
| H | 4.28396800 | -3.91028900 | 1.24958200 |
| C | 6.65249700 | -1.45994700 | -0.61037500 |
| H | 4.90920200 | -0.84982400 | -1.72502500 |
| C | 7.17306600 | -2.28686500 | 0.39820500 |
| H | 6.68982200 | -3.81421500 | 1.84412000 |
| H | 7.30927800 | -0.77621500 | -1.14079100 |
| C | 8.64452100 | -2.26081200 | 0.72947200 |
| H | 8.83558800 | -2.61899900 | 1.74556600 |
| H | 9.20614000 | -2.90703700 | 0.04227600 |
| H | 9.05795300 | -1.25162000 | 0.63512400 |
| N | 1.91262900 | -1.20999900 | 0.34633300 |
| C | 1.38873300 | -1.67304700 | 1.66019100 |
| H | 2.17383100 | -2.31109500 | 2.08317200 |
| H | 1.30898100 | -0.79660900 | 2.30803600 |
| Au | -1.17273000 | 0.35755100 | 0.16667200 |
| P | -3.42094400 | -0.32317000 | -0.21913900 |
| C | -3.55711900 | -1.62082800 | -1.51313000 |
| C | -4.72954700 | -1.77297400 | -2.27108200 |
| C | -2.46999100 | -2.48020500 | -1.73811700 |
| C | -4.81119600 | -2.77897800 | -3.23438200 |
| H | -5.57140900 | -1.10442800 | -2.11742700 |
| C | -2.55799700 | -3.48465600 | -2.70255400 |
| H | -1.55516400 | -2.36235900 | -1.16397200 |
| C | -3.72786200 | -3.63450300 | -3.45035200 |
| H | -5.71934900 | -2.89040500 | -3.81961300 |
| H | -1.71077700 | -4.14219800 | -2.87351500 |
| H | -3.79357100 | -4.41298800 | -4.20491300 |
| C | -4.21429500 | -0.98144700 | 1.30586800 |
| C | -4.06022600 | -0.26040300 | 2.50237000 |
| C | -4.95104400 | -2.17389900 | 1.30890300 |
| C | -4.64537500 | -0.72157500 | 3.68059900 |
| H | -3.48385600 | 0.66171600 | 2.51237600 |
| C | -5.52665000 | -2.63671500 | 2.49509700 |
| H | -5.07535600 | -2.74333900 | 0.39354000 |
| C | -5.37695800 | -1.91296000 | 3.67894900 |
| H | -4.52581000 | -0.15567400 | 4.60004300 |
| H | -6.09359200 | -3.56311100 | 2.48983600 |
| H | -5.82671500 | -2.27542300 | 4.59872800 |
| C | -4.48431700 | 1.06941800 | -0.79069800 |
| C | -5.75445200 | 1.31198800 | -0.24980800 |

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|---|-------------|-------------|-------------|
| C | -4.00138700 | 1.89602800 | -1.81916200 |
| C | -6.52912400 | 2.37027200 | -0.73204800 |
| H | -6.14025200 | 0.68237100 | 0.54541100 |
| C | -4.78165200 | 2.94512600 | -2.30182200 |
| H | -3.01984700 | 1.71035200 | -2.24914900 |
| C | -6.04605600 | 3.18580700 | -1.75584400 |
| H | -7.51157400 | 2.55301900 | -0.30648200 |
| H | -4.40468100 | 3.57493800 | -3.10265200 |
| H | -6.65161300 | 4.00649500 | -2.12925900 |
| C | 0.08814000 | -2.43301100 | 1.62526400 |
| C | -0.89898300 | -2.22110900 | 2.49846100 |
| H | 0.02808800 | -3.23813300 | 0.89865500 |
| H | -1.79549400 | -2.83357800 | 2.50206900 |
| H | -0.84611200 | -1.43789900 | 3.25207100 |
| C | 2.54678000 | 1.78223500 | -1.27029700 |
| C | 3.47525700 | 2.83881600 | -1.47110400 |
| C | 3.03461700 | 4.14788200 | -1.51216700 |
| C | 1.65460900 | 4.47114200 | -1.47317100 |
| C | 0.71872600 | 3.46541400 | -1.42554200 |
| C | 1.13807500 | 2.10472700 | -1.32713700 |
| H | 3.78119000 | 4.93318700 | -1.56341300 |
| H | 1.35628800 | 5.51215300 | -1.53804400 |
| H | -0.34220600 | 3.68941300 | -1.48813000 |
| H | 0.50687500 | 1.36789800 | -1.81353100 |
| O | 5.29793200 | 1.52062200 | -1.98796700 |
| N | 2.86974200 | 0.54968300 | -0.82898900 |
| N | 4.92406700 | 2.59695400 | -1.53158300 |
| O | 5.65955100 | 3.50497000 | -1.15024700 |

6

SCF done: -2238.968616

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|---|-------------|------------|-------------|
| C | -0.35324500 | 5.09980000 | 1.12706600 |
| C | -0.36706500 | 3.81167700 | 0.58619800 |
| C | 0.81235600 | 3.05752400 | 0.48901500 |
| C | 2.01283700 | 3.64415200 | 0.93287800 |
| C | 2.02623200 | 4.92666600 | 1.48249400 |
| C | 0.84156900 | 5.65935100 | 1.58230000 |
| H | -1.27938600 | 5.66355000 | 1.19420800 |
| H | -1.30370900 | 3.38525500 | 0.23656000 |
| H | 2.94535800 | 3.08968700 | 0.85245800 |
| H | 2.96342700 | 5.35331500 | 1.82843100 |
| H | 0.85075400 | 6.65828500 | 2.00805900 |
| C | 0.85141400 | 1.70507900 | -0.18525000 |
| C | 1.69985200 | 0.60683700 | 0.29372500 |

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|----|-------------|-------------|-------------|
| S | 2.55453200 | -1.54596400 | 1.80463100 |
| O | 2.44548900 | -1.65781200 | 3.26839400 |
| O | 1.78113000 | -2.40594700 | 0.89881200 |
| C | 4.27548500 | -1.51153200 | 1.35884400 |
| C | 5.20005900 | -1.07950900 | 2.31559700 |
| C | 4.67640000 | -2.01178200 | 0.11756000 |
| C | 6.55451600 | -1.12894800 | 1.99993700 |
| H | 4.86890800 | -0.73276500 | 3.28817300 |
| C | 6.03755900 | -2.05785300 | -0.16851800 |
| H | 3.94186300 | -2.34268700 | -0.60512000 |
| C | 6.99562200 | -1.62009200 | 0.76025500 |
| H | 7.28266000 | -0.79444400 | 2.73374800 |
| H | 6.35954400 | -2.44483700 | -1.13149400 |
| C | 8.46812800 | -1.70909200 | 0.44560200 |
| H | 9.04816900 | -0.98191700 | 1.02177800 |
| H | 8.85470800 | -2.70663900 | 0.69212100 |
| H | 8.66153000 | -1.54089500 | -0.61854400 |
| N | 1.90991100 | 0.16243000 | 1.54329500 |
| C | 1.33359800 | 0.79652800 | 2.75652500 |
| H | 2.03075200 | 0.57610300 | 3.56801000 |
| H | 1.33169500 | 1.87420300 | 2.59715800 |
| Au | -1.06586400 | 0.56630600 | -0.10829100 |
| P | -3.06886800 | -0.67901200 | -0.17953900 |
| C | -2.74901000 | -2.47982100 | -0.33923600 |
| C | -3.73699600 | -3.34055400 | -0.84663400 |
| C | -1.50890500 | -3.00182700 | 0.05999500 |
| C | -3.48380300 | -4.70830200 | -0.94426200 |
| H | -4.69470500 | -2.94521800 | -1.17192600 |
| C | -1.26336700 | -4.37200900 | -0.04083200 |
| H | -0.72503200 | -2.35311000 | 0.43885800 |
| C | -2.24860700 | -5.22464200 | -0.54179100 |
| H | -4.24909000 | -5.36954500 | -1.34021200 |
| H | -0.29712700 | -4.76155000 | 0.26476200 |
| H | -2.05394200 | -6.28998300 | -0.62575400 |
| C | -4.06792100 | -0.42466500 | 1.34424800 |
| C | -4.44304900 | 0.88526100 | 1.69008200 |
| C | -4.42967900 | -1.49048800 | 2.17888100 |
| C | -5.18185500 | 1.12022700 | 2.84820300 |
| H | -4.16255100 | 1.72031100 | 1.05252400 |
| C | -5.16210700 | -1.24732700 | 3.34404200 |
| H | -4.14474500 | -2.50609000 | 1.92464100 |
| C | -5.54007600 | 0.05338400 | 3.67887000 |
| H | -5.47557600 | 2.13408600 | 3.10457400 |
| H | -5.43858600 | -2.07846900 | 3.98618200 |

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|---|-------------|-------------|-------------|
| H | -6.11209900 | 0.23793100 | 4.58352000 |
| C | -4.15341800 | -0.21075100 | -1.59071300 |
| C | -5.54876400 | -0.14434700 | -1.46180600 |
| C | -3.56151100 | 0.04465200 | -2.83827400 |
| C | -6.33816300 | 0.17435300 | -2.56910500 |
| H | -6.02011100 | -0.33541400 | -0.50304600 |
| C | -4.35480200 | 0.35709500 | -3.94105700 |
| H | -2.48095100 | -0.00773100 | -2.94748700 |
| C | -5.74428500 | 0.42495500 | -3.80692800 |
| H | -7.41764600 | 0.22637100 | -2.46116900 |
| H | -3.88960300 | 0.55074300 | -4.90330200 |
| H | -6.36124400 | 0.67408300 | -4.66537100 |
| C | -0.04223800 | 0.30038700 | 3.12383100 |
| C | -1.07301800 | 1.11532300 | 3.36219200 |
| H | -0.14083200 | -0.77325600 | 3.26857300 |
| H | -2.03207000 | 0.73302300 | 3.69833400 |
| H | -0.98964800 | 2.19375000 | 3.24555300 |
| C | 2.21828300 | 0.63094000 | -1.81514700 |
| C | 2.93451500 | 0.52374600 | -3.06193700 |
| C | 3.06285200 | 1.64327600 | -3.83556000 |
| C | 2.44526600 | 2.90075200 | -3.48662900 |
| C | 1.60479000 | 2.99284100 | -2.42817800 |
| C | 1.22259700 | 1.74557600 | -1.69329400 |
| H | 3.68934900 | 1.57763300 | -4.71932400 |
| H | 2.66563500 | 3.76786400 | -4.10064100 |
| H | 1.10700900 | 3.92308500 | -2.17211500 |
| H | 0.34479200 | 1.39095300 | -2.27921500 |
| O | 3.33655900 | -1.73561200 | -2.87036900 |
| N | 2.39167900 | -0.05077400 | -0.71919600 |
| N | 3.65307500 | -0.69727300 | -3.44644400 |
| O | 4.49573300 | -0.60375400 | -4.33586100 |

TS6-7

SCF done: -2729.790619

| | | | |
|---|-------------|-------------|------------|
| C | -0.35603000 | -1.82232400 | 5.10890800 |
| C | -0.36535300 | -1.25788800 | 3.83002000 |
| C | 0.82741300 | -1.05843300 | 3.12014500 |
| C | 2.03567700 | -1.42757400 | 3.74160100 |
| C | 2.04644800 | -2.00215000 | 5.01256200 |
| C | 0.84811200 | -2.20190600 | 5.70225500 |
| H | -1.29416700 | -1.96915700 | 5.63704000 |
| H | -1.31135600 | -0.97839500 | 3.37373300 |
| H | 2.97763100 | -1.26538200 | 3.22186100 |
| H | 2.99162300 | -2.28926000 | 5.46479800 |

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|----|-------------|-------------|-------------|
| H | 0.85445900 | -2.64701400 | 6.69291000 |
| C | 0.87506300 | -0.36121300 | 1.77097100 |
| C | 1.80445500 | -0.81930700 | 0.69190000 |
| S | 2.48238700 | -2.28141600 | -1.52141300 |
| O | 2.21748200 | -3.71456100 | -1.74470000 |
| O | 1.78994400 | -1.24035500 | -2.29662900 |
| C | 4.24565000 | -2.02372500 | -1.54575300 |
| C | 5.07935800 | -3.12342800 | -1.31797900 |
| C | 4.75997200 | -0.76643600 | -1.86957800 |
| C | 6.45751100 | -2.94217500 | -1.39258000 |
| H | 4.65845900 | -4.10035700 | -1.10800400 |
| C | 6.14177400 | -0.61358400 | -1.94276700 |
| H | 4.09551000 | 0.06976200 | -2.04078500 |
| C | 7.01041900 | -1.69056200 | -1.70675600 |
| H | 7.11463300 | -3.78944900 | -1.21563800 |
| H | 6.54966000 | 0.36329300 | -2.18832600 |
| C | 8.50466700 | -1.51494800 | -1.82222200 |
| H | 9.04406500 | -2.23597000 | -1.20017500 |
| H | 8.83336600 | -1.66662900 | -2.85879800 |
| H | 8.81358700 | -0.50680600 | -1.52824800 |
| N | 1.95040500 | -2.07523500 | 0.19075600 |
| C | 1.45381200 | -3.30062300 | 0.85992500 |
| H | 2.12178100 | -4.10358100 | 0.53811600 |
| H | 1.59102300 | -3.16852000 | 1.93350400 |
| Au | -1.02134500 | -0.54080300 | 0.64058500 |
| P | -3.01436800 | -0.63398300 | -0.63160400 |
| C | -2.72589500 | -0.05137500 | -2.35283100 |
| C | -3.75300900 | 0.53358900 | -3.11151800 |
| C | -1.45233800 | -0.22010800 | -2.92044100 |
| C | -3.50515100 | 0.94048800 | -4.42261400 |
| H | -4.73958300 | 0.67826000 | -2.68221400 |
| C | -1.21404400 | 0.18561900 | -4.23463000 |
| H | -0.63849100 | -0.65852600 | -2.35000800 |
| C | -2.23773300 | 0.76646000 | -4.98533800 |
| H | -4.30283600 | 1.39443000 | -5.00383400 |
| H | -0.22401400 | 0.05132100 | -4.65947100 |
| H | -2.04889200 | 1.08709200 | -6.00595000 |
| C | -3.73933700 | -2.32274800 | -0.76209300 |
| C | -4.19734900 | -2.95138200 | 0.40857900 |
| C | -3.82276500 | -2.99881400 | -1.98662500 |
| C | -4.74318500 | -4.23258900 | 0.34845400 |
| H | -4.13526700 | -2.43774700 | 1.36480800 |
| C | -4.36040100 | -4.28782900 | -2.03853300 |
| H | -3.47389600 | -2.52522700 | -2.89841400 |

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|---|-------------|-------------|-------------|
| C | -4.82275100 | -4.90427800 | -0.87581800 |
| H | -5.10528500 | -4.70740000 | 1.25601500 |
| H | -4.41998400 | -4.80499200 | -2.99173800 |
| H | -5.24447200 | -5.90420300 | -0.92031200 |
| C | -4.36502700 | 0.41004200 | 0.06353500 |
| C | -5.71740300 | 0.09049700 | -0.13708600 |
| C | -4.03114700 | 1.56872500 | 0.78202400 |
| C | -6.71726100 | 0.92342700 | 0.36804300 |
| H | -5.99102700 | -0.81002900 | -0.67802700 |
| C | -5.03450300 | 2.39830300 | 1.28339500 |
| H | -2.98609900 | 1.81682700 | 0.94821700 |
| C | -6.37816700 | 2.07719600 | 1.07751600 |
| H | -7.76082400 | 0.66713100 | 0.20981600 |
| H | -4.76838900 | 3.29151400 | 1.84194200 |
| H | -7.15852900 | 2.72058900 | 1.47368000 |
| C | 0.03233700 | -3.68727500 | 0.54058200 |
| C | -0.84170900 | -4.08041500 | 1.47021900 |
| H | -0.22627300 | -3.72836400 | -0.51522000 |
| H | -1.83103300 | -4.43565200 | 1.19959200 |
| H | -0.59597200 | -4.07072900 | 2.52976300 |
| C | 2.35160600 | 1.26171200 | 0.88668400 |
| C | 3.05305200 | 2.50098600 | 0.88451000 |
| C | 2.91238900 | 3.37066800 | 1.95312100 |
| C | 2.04385700 | 3.09346800 | 3.03522300 |
| C | 1.28090000 | 1.94299500 | 3.03318600 |
| C | 1.29269400 | 1.09537100 | 1.87507300 |
| H | 3.51232300 | 4.27400800 | 1.95076600 |
| H | 2.00532300 | 3.78234500 | 3.87255900 |
| H | 0.61898900 | 1.70415600 | 3.86136400 |
| H | 0.40103100 | 1.91416300 | 1.19397700 |
| O | 3.86478600 | 2.32102400 | -1.26839900 |
| N | 2.55231300 | 0.16776100 | 0.14670200 |
| N | 4.00317200 | 2.86204700 | -0.17298700 |
| O | 4.85136100 | 3.71397700 | 0.09158700 |
| C | -0.36470900 | 4.10049000 | 0.39500700 |
| C | -0.17601300 | 4.60063400 | -0.91813100 |
| C | -0.16459600 | 5.97780900 | -1.23859300 |
| C | -0.35983200 | 6.83769600 | -0.18719600 |
| C | -0.56062600 | 6.35216600 | 1.14733000 |
| C | -0.56696700 | 5.01341100 | 1.46254500 |
| H | -0.01233200 | 6.30818500 | -2.25968500 |
| H | -0.36759500 | 7.90848300 | -0.36063900 |
| H | -0.71563600 | 7.07880400 | 1.93913700 |
| H | -0.71796500 | 4.65920900 | 2.47520400 |

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| O | -0.12810900 | 2.36219300 | -0.91971600 |
| N | -0.34924000 | 2.75446200 | 0.39006000 |
| N | -0.00867300 | 3.53603100 | -1.73990600 |
| O | 0.17091300 | 3.40549700 | -2.92596600 |

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SCF done: -2729.891073

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|----|-------------|-------------|-------------|
| C | -0.51601800 | -5.36375600 | -0.17152800 |
| C | -0.52168200 | -4.00786700 | 0.16088200 |
| C | 0.64516400 | -3.23272800 | 0.05860800 |
| C | 1.82318300 | -3.86403700 | -0.37784700 |
| C | 1.82572100 | -5.21558100 | -0.72343400 |
| C | 0.65646300 | -5.97165400 | -0.62167000 |
| H | -1.43089700 | -5.94258200 | -0.08125800 |
| H | -1.44208900 | -3.54594200 | 0.50887100 |
| H | 2.74725200 | -3.29641500 | -0.44519800 |
| H | 2.74737700 | -5.68032900 | -1.06226500 |
| H | 0.66079100 | -7.02493400 | -0.88607600 |
| C | 0.67749300 | -1.79165800 | 0.50915000 |
| C | 1.58641500 | -0.81455800 | -0.07782700 |
| S | 3.45848400 | 0.24489600 | -1.78965100 |
| O | 3.45758700 | 0.24248700 | -3.25698300 |
| O | 3.39142900 | 1.49275300 | -1.00338500 |
| C | 4.80617000 | -0.75330300 | -1.18354800 |
| C | 5.28721100 | -1.78881900 | -1.99344700 |
| C | 5.39118800 | -0.46088200 | 0.05266300 |
| C | 6.35559500 | -2.55434900 | -1.53703600 |
| H | 4.85014500 | -1.97384100 | -2.96883500 |
| C | 6.45994700 | -1.24269600 | 0.48560100 |
| H | 5.03161000 | 0.36356300 | 0.65795400 |
| C | 6.95913300 | -2.29646800 | -0.29483100 |
| H | 6.73813400 | -3.35698200 | -2.16164000 |
| H | 6.92161600 | -1.02109900 | 1.44390400 |
| C | 8.14230300 | -3.10813100 | 0.17050800 |
| H | 8.11130500 | -4.12783100 | -0.22544400 |
| H | 9.08045000 | -2.65293900 | -0.17286500 |
| H | 8.18745500 | -3.16295100 | 1.26247900 |
| N | 2.00701900 | -0.69993900 | -1.37467800 |
| C | 1.22872200 | -1.25353000 | -2.51888200 |
| H | 1.95762500 | -1.52621200 | -3.28505900 |
| H | 0.74434100 | -2.17129600 | -2.18455300 |
| Au | -1.28973600 | -0.74898500 | 0.13853400 |
| P | -3.47998900 | 0.08428000 | -0.05318400 |
| C | -3.59886200 | 1.88525500 | -0.39145200 |

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|---|-------------|-------------|-------------|
| C | -4.60499100 | 2.67065700 | 0.19294100 |
| C | -2.68980500 | 2.46922400 | -1.28746200 |
| C | -4.70223700 | 4.02590400 | -0.12701200 |
| H | -5.30678700 | 2.23110700 | 0.89467700 |
| C | -2.79680900 | 3.82295200 | -1.60549600 |
| H | -1.89511100 | 1.87852900 | -1.73178300 |
| C | -3.80220700 | 4.60119600 | -1.02670400 |
| H | -5.48099500 | 4.63029600 | 0.32909400 |
| H | -2.08322500 | 4.26022500 | -2.29697700 |
| H | -3.88159800 | 5.65650800 | -1.27206100 |
| C | -4.40971700 | -0.76178000 | -1.39863500 |
| C | -4.20060000 | -2.13378200 | -1.61523000 |
| C | -5.33670800 | -0.07076300 | -2.19275000 |
| C | -4.91599800 | -2.80554100 | -2.60571300 |
| H | -3.47680000 | -2.67580700 | -1.01201200 |
| C | -6.04701200 | -0.74797300 | -3.18658000 |
| H | -5.50285700 | 0.99084100 | -2.04062300 |
| C | -5.83941100 | -2.11262800 | -3.39343800 |
| H | -4.74912300 | -3.86675500 | -2.76640400 |
| H | -6.76117800 | -0.20569500 | -3.79938700 |
| H | -6.39213100 | -2.63513100 | -4.16880400 |
| C | -4.42085500 | -0.22262400 | 1.49934600 |
| C | -5.75351600 | -0.65913100 | 1.48172900 |
| C | -3.78419300 | 0.01257000 | 2.72936800 |
| C | -6.43904900 | -0.85710400 | 2.68254200 |
| H | -6.25585500 | -0.84760800 | 0.53830600 |
| C | -4.47670500 | -0.17957300 | 3.92398900 |
| H | -2.74955000 | 0.34586400 | 2.75269300 |
| C | -5.80385500 | -0.61732000 | 3.90196500 |
| H | -7.46976400 | -1.19898300 | 2.66183100 |
| H | -3.97922600 | 0.00773200 | 4.87120500 |
| H | -6.33992200 | -0.77304200 | 4.83371700 |
| C | 0.23217100 | -0.27169600 | -3.07761400 |
| C | -1.02618500 | -0.60551600 | -3.37361900 |
| H | 0.59996900 | 0.73175600 | -3.28287400 |
| H | -1.70566000 | 0.10405500 | -3.83693100 |
| H | -1.41819500 | -1.60351200 | -3.19007700 |
| C | 1.62357700 | -0.39607800 | 2.14123900 |
| C | 1.87011600 | 0.13460000 | 3.41152300 |
| C | 1.30597100 | -0.48573600 | 4.52833600 |
| C | 0.52050700 | -1.62939200 | 4.36622700 |
| C | 0.25372900 | -2.15126200 | 3.09596200 |
| C | 0.78912800 | -1.51586600 | 1.97396400 |
| H | 1.50520600 | -0.06998200 | 5.50838800 |

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|---|-------------|-------------|-------------|
| H | 0.11179800 | -2.11947400 | 5.24392900 |
| H | -0.36073300 | -3.03910300 | 2.98384400 |
| H | 2.53827700 | 0.88967000 | 0.73073600 |
| O | 3.33563100 | 1.71257100 | 2.58843800 |
| N | 2.07694500 | -0.00274600 | 0.89345400 |
| N | 2.72271800 | 1.30057400 | 3.58635400 |
| O | 2.79699200 | 1.80956400 | 4.69869400 |
| C | 1.89892100 | 4.06777500 | 0.41417300 |
| C | 1.72343200 | 4.43308900 | -0.95394800 |
| C | 2.37100200 | 5.54596400 | -1.54678200 |
| C | 3.19326900 | 6.26832000 | -0.72328000 |
| C | 3.39417600 | 5.90924600 | 0.65781100 |
| C | 2.77566800 | 4.83551500 | 1.23937100 |
| H | 2.21191800 | 5.78902300 | -2.59106100 |
| H | 3.71834200 | 7.13371000 | -1.11497000 |
| H | 4.07046100 | 6.51776600 | 1.25059100 |
| H | 2.94381400 | 4.54627300 | 2.27030200 |
| O | 0.52931800 | 2.63535600 | -0.43051200 |
| N | 1.18266800 | 2.99484500 | 0.72457500 |
| N | 0.88102000 | 3.54054300 | -1.49126000 |
| O | 0.38963000 | 3.36539200 | -2.60616100 |

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SCF done: -2238.965246

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|---|-------------|-------------|-------------|
| C | -0.06599000 | 4.64375500 | -2.36508500 |
| C | 0.18091700 | 3.43640000 | -1.74080400 |
| C | -0.89153800 | 2.54056300 | -1.42896700 |
| C | -2.22608100 | 2.93039100 | -1.77278800 |
| C | -2.45995200 | 4.14415500 | -2.39743700 |
| C | -1.38651900 | 4.99567300 | -2.69473200 |
| H | 0.75062700 | 5.31848900 | -2.60071100 |
| H | 1.19348800 | 3.14532100 | -1.47836100 |
| H | -3.05684400 | 2.28069000 | -1.52188500 |
| H | -3.47306900 | 4.43600100 | -2.65476600 |
| H | -1.57804400 | 5.94599000 | -3.18581600 |
| C | -0.61355800 | 1.29417800 | -0.82785500 |
| C | -1.71596000 | 0.36157400 | -0.45123900 |
| S | -1.89874200 | -2.35173100 | -0.27706400 |
| O | -1.41803800 | -3.35618700 | -1.24286600 |
| O | -1.21994800 | -2.12295800 | 1.01337200 |
| C | -3.64030400 | -2.61882400 | 0.00601900 |
| C | -4.38487600 | -3.27621200 | -0.97688900 |
| C | -4.21347700 | -2.22748000 | 1.21800900 |
| C | -5.73542000 | -3.51979100 | -0.74126400 |

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|----|-------------|-------------|-------------|
| H | -3.91276400 | -3.60237700 | -1.89676300 |
| C | -5.56424500 | -2.48622900 | 1.43195500 |
| H | -3.60954100 | -1.74084900 | 1.97422600 |
| C | -6.34776600 | -3.12634100 | 0.45860300 |
| H | -6.32133800 | -4.03422800 | -1.49808100 |
| H | -6.01823100 | -2.19165800 | 2.37436300 |
| C | -7.81796100 | -3.37098900 | 0.69282300 |
| H | -8.02806100 | -3.56809200 | 1.74888300 |
| H | -8.40793300 | -2.49185900 | 0.40208100 |
| H | -8.18279300 | -4.21931700 | 0.10587400 |
| N | -1.74320900 | -0.83660000 | -1.16069200 |
| C | -1.44039400 | -0.86514600 | -2.59995600 |
| H | -0.57513500 | -0.21054700 | -2.78832500 |
| H | -1.09522200 | -1.87489300 | -2.83986200 |
| Au | 1.23918100 | 0.53560900 | -0.35352900 |
| P | 3.34270700 | -0.43385100 | 0.21936900 |
| C | 3.24676200 | -1.40631100 | 1.77291900 |
| C | 4.33756400 | -1.47987300 | 2.65359200 |
| C | 2.06367200 | -2.10610800 | 2.06306400 |
| C | 4.24391000 | -2.25143200 | 3.81260000 |
| H | 5.25242400 | -0.93564600 | 2.44003700 |
| C | 1.98131600 | -2.87715600 | 3.22300200 |
| H | 1.20424900 | -2.05507000 | 1.39989700 |
| C | 3.06806100 | -2.94999900 | 4.09745500 |
| H | 5.08920400 | -2.30444600 | 4.49260000 |
| H | 1.06292300 | -3.41414400 | 3.44056000 |
| H | 2.99840600 | -3.54749800 | 5.00195500 |
| C | 3.93848300 | -1.56476000 | -1.10223900 |
| C | 3.80920000 | -1.16286100 | -2.44230600 |
| C | 4.51967100 | -2.80517300 | -0.80340500 |
| C | 4.26477700 | -1.98900600 | -3.46842500 |
| H | 3.35536400 | -0.20424500 | -2.68296300 |
| C | 4.96841900 | -3.63073500 | -1.83651300 |
| H | 4.61728800 | -3.13035300 | 0.22732500 |
| C | 4.84283600 | -3.22510900 | -3.16607400 |
| H | 4.16357700 | -1.67174000 | -4.50226700 |
| H | 5.41347200 | -4.59255200 | -1.59930500 |
| H | 5.19067000 | -3.87166300 | -3.96643900 |
| C | 4.65301600 | 0.83425300 | 0.46489000 |
| C | 5.95199000 | 0.66445400 | -0.03495900 |
| C | 4.33617300 | 1.99313500 | 1.19298600 |
| C | 6.92132400 | 1.64380800 | 0.19447500 |
| H | 6.20781300 | -0.22417900 | -0.60332500 |
| C | 5.30946600 | 2.96394400 | 1.42391100 |

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|---|-------------|-------------|-------------|
| H | 3.33079900 | 2.13318600 | 1.58356900 |
| C | 6.60289200 | 2.79093500 | 0.92286700 |
| H | 7.92510900 | 1.50728200 | -0.19716400 |
| H | 5.05866300 | 3.85576300 | 1.99106900 |
| H | 7.35928200 | 3.55023200 | 1.09903800 |
| C | -2.59100900 | -0.47306700 | -3.49096500 |
| C | -3.83162600 | -0.17674500 | -3.09928000 |
| H | -2.33778300 | -0.45779900 | -4.55145700 |
| H | -4.59677700 | 0.08243000 | -3.82512200 |
| H | -4.13446600 | -0.19337800 | -2.05632300 |
| C | -2.47760600 | 1.56645700 | 1.47058500 |
| C | -3.62659200 | 2.34051400 | 1.75577400 |
| C | -3.64809600 | 3.26763200 | 2.80184400 |
| C | -2.52188300 | 3.45048200 | 3.59360400 |
| C | -1.38050700 | 2.68019700 | 3.34596400 |
| C | -1.36170900 | 1.74977100 | 2.31184400 |
| H | -4.55821000 | 3.83008700 | 2.97139900 |
| H | -2.53648600 | 4.17606100 | 4.40001200 |
| H | -0.50002800 | 2.79615500 | 3.97165200 |
| H | -0.49619300 | 1.11233100 | 2.16220200 |
| O | -4.76687300 | 1.72478400 | -0.17374300 |
| N | -2.51173900 | 0.53653700 | 0.53757300 |
| N | -4.85025200 | 2.20444400 | 0.96373700 |
| O | -5.90243500 | 2.58443800 | 1.47117600 |

TS8-9

SCF done:-2238.947685

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|---|-------------|-------------|-------------|
| C | -0.13393200 | 4.59112100 | -1.91021500 |
| C | 0.10709000 | 3.22771200 | -1.75834900 |
| C | -0.95707700 | 2.31455400 | -1.60397700 |
| C | -2.27746400 | 2.81692900 | -1.62224900 |
| C | -2.51312800 | 4.18078800 | -1.75937800 |
| C | -1.44505200 | 5.07208400 | -1.90729800 |
| H | 0.69999700 | 5.27644000 | -2.02862300 |
| H | 1.12986000 | 2.86078000 | -1.76472700 |
| H | -3.11785000 | 2.13886900 | -1.51072600 |
| H | -3.53431500 | 4.55026900 | -1.75907900 |
| H | -1.63521700 | 6.13517900 | -2.02277200 |
| C | -0.67213300 | 0.86832800 | -1.44612600 |
| C | -1.62828300 | -0.06703300 | -0.74943100 |
| S | -2.20023600 | -2.73544000 | -0.30627300 |
| O | -2.02080400 | -3.84998100 | -1.25475700 |
| O | -1.45194200 | -2.68185300 | 0.96348200 |
| C | -3.92946800 | -2.44854400 | -0.01963200 |

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|----|-------------|-------------|-------------|
| C | -4.82540300 | -2.61177700 | -1.07761400 |
| C | -4.36002000 | -2.09387800 | 1.26073200 |
| C | -6.17501900 | -2.35597700 | -0.85153300 |
| H | -4.47529300 | -2.93092600 | -2.05353700 |
| C | -5.71498800 | -1.86104000 | 1.46631100 |
| H | -3.64163500 | -1.99430200 | 2.06597700 |
| C | -6.63788000 | -1.95758600 | 0.41174400 |
| H | -6.88121300 | -2.46254600 | -1.67019200 |
| H | -6.06234400 | -1.57635000 | 2.45559800 |
| C | -8.08454700 | -1.59908400 | 0.63376100 |
| H | -8.45850200 | -2.00294000 | 1.58070800 |
| H | -8.18937200 | -0.50744500 | 0.67915100 |
| H | -8.72347200 | -1.96680100 | -0.17430600 |
| N | -1.68262400 | -1.35475900 | -1.30189500 |
| C | -0.70107400 | -1.69905000 | -2.33755400 |
| H | 0.22435900 | -2.10455100 | -1.91009400 |
| H | -1.12545900 | -2.46928300 | -2.98905200 |
| Au | 1.28104200 | 0.34741000 | -0.70820800 |
| P | 3.29017500 | -0.31379600 | 0.33965800 |
| C | 2.93350400 | -1.18553600 | 1.91495100 |
| C | 3.84592000 | -1.16106800 | 2.98215800 |
| C | 1.73569700 | -1.90899800 | 2.03812300 |
| C | 3.56020200 | -1.85919900 | 4.15592800 |
| H | 4.76994500 | -0.59667600 | 2.90184500 |
| C | 1.45888200 | -2.60637800 | 3.21415700 |
| H | 1.00878100 | -1.93554200 | 1.23122400 |
| C | 2.36952200 | -2.58156000 | 4.27265800 |
| H | 4.26720600 | -1.83548900 | 4.98008200 |
| H | 0.52765300 | -3.15859900 | 3.29461000 |
| H | 2.15104900 | -3.12058300 | 5.19005200 |
| C | 4.23743400 | -1.47112400 | -0.73145400 |
| C | 4.52416700 | -1.08060800 | -2.05117800 |
| C | 4.66410300 | -2.72420200 | -0.27142200 |
| C | 5.23724800 | -1.93125100 | -2.89370100 |
| H | 4.19872900 | -0.10899900 | -2.41634700 |
| C | 5.37202300 | -3.57526700 | -1.12407800 |
| H | 4.44611700 | -3.03895600 | 0.74387200 |
| C | 5.65956000 | -3.18166000 | -2.43133500 |
| H | 5.46169000 | -1.62077300 | -3.91011000 |
| H | 5.69770600 | -4.54603500 | -0.76220400 |
| H | 6.21019200 | -3.84624800 | -3.09062000 |
| C | 4.41501000 | 1.08613700 | 0.72557200 |
| C | 5.80910300 | 0.95211100 | 0.64041100 |
| C | 3.85934600 | 2.30536600 | 1.14616400 |

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|---|-------------|-------------|-------------|
| C | 6.63445100 | 2.02666400 | 0.97776800 |
| H | 6.25019300 | 0.01783200 | 0.30733500 |
| C | 4.68917400 | 3.37322600 | 1.48507300 |
| H | 2.77978800 | 2.41888200 | 1.20952000 |
| C | 6.07720000 | 3.23498400 | 1.40017200 |
| H | 7.71278500 | 1.91796600 | 0.90796000 |
| H | 4.25336500 | 4.31345500 | 1.81028800 |
| H | 6.72255400 | 4.06919300 | 1.65940400 |
| C | -0.40399900 | -0.45065000 | -3.11782300 |
| C | -1.38556300 | 0.43076300 | -3.47469500 |
| H | 0.60266900 | -0.32093600 | -3.50282300 |
| H | -1.15612500 | 1.30103900 | -4.07861200 |
| H | -2.42903400 | 0.25014800 | -3.23837100 |
| C | -2.42158800 | 1.26683900 | 1.12006500 |
| C | -3.67958400 | 1.84983500 | 1.41124900 |
| C | -3.82870800 | 2.83443000 | 2.39213200 |
| C | -2.72327800 | 3.27822800 | 3.10520100 |
| C | -1.47119600 | 2.70761200 | 2.84757600 |
| C | -1.32521200 | 1.71618900 | 1.88414000 |
| H | -4.81875200 | 3.23574600 | 2.57319100 |
| H | -2.83558800 | 4.05060800 | 3.85872600 |
| H | -0.60159400 | 3.03086700 | 3.41302900 |
| H | -0.36207500 | 1.24020700 | 1.72677100 |
| O | -4.76315400 | 0.99865100 | -0.45696900 |
| N | -2.31758300 | 0.16312800 | 0.29843200 |
| N | -4.88349800 | 1.44153400 | 0.69110600 |
| O | -5.96438700 | 1.56833100 | 1.26715100 |

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SCF done: -2239.012161

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|---|-------------|-------------|-------------|
| C | 1.48069500 | 2.64166100 | -2.64859300 |
| C | 0.46212600 | 1.65705400 | -2.70163800 |
| C | -0.81606200 | 1.91094300 | -2.13413500 |
| C | -1.03689600 | 3.15151700 | -1.53503400 |
| C | -0.02008600 | 4.11482900 | -1.46116100 |
| C | 1.23786300 | 3.86672900 | -2.00065900 |
| H | 2.40641400 | 2.49033400 | -3.19777600 |
| H | 0.59443900 | 0.78209400 | -3.33455500 |
| H | -2.01872700 | 3.37340100 | -1.13073600 |
| H | -0.22746000 | 5.07118400 | -0.99037300 |
| H | 2.01481100 | 4.62393500 | -1.96676100 |
| C | -1.90216600 | 0.88546300 | -2.23435900 |
| C | -2.19761300 | -0.03636600 | -1.06389400 |
| S | -3.08144400 | -2.63829300 | -0.64810400 |

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|----|-------------|-------------|-------------|
| O | -3.43611700 | -3.61519500 | -1.69172400 |
| O | -2.03377800 | -2.91979000 | 0.34860800 |
| C | -4.55486400 | -2.05304900 | 0.16352000 |
| C | -5.75220200 | -2.03833100 | -0.55613800 |
| C | -4.49303100 | -1.61256200 | 1.48756700 |
| C | -6.89423200 | -1.52942100 | 0.05597900 |
| H | -5.78905300 | -2.42619600 | -1.56854300 |
| C | -5.64970800 | -1.11708700 | 2.08190700 |
| H | -3.55535700 | -1.65322300 | 2.02838500 |
| C | -6.85898300 | -1.04436800 | 1.37224000 |
| H | -7.82893200 | -1.50583700 | -0.49738800 |
| H | -5.61272400 | -0.76671100 | 3.10992300 |
| C | -8.07904600 | -0.42394600 | 2.00409800 |
| H | -8.17341200 | -0.70480800 | 3.05838700 |
| H | -8.00393000 | 0.67038000 | 1.96178100 |
| H | -8.99708000 | -0.71677700 | 1.48621800 |
| N | -2.56193400 | -1.26538400 | -1.59426700 |
| C | -2.42650700 | -1.38261000 | -3.05728800 |
| H | -1.60773500 | -2.06268500 | -3.31655700 |
| H | -3.34584600 | -1.77926500 | -3.49473400 |
| Au | 1.92451500 | 0.78465700 | -0.97420600 |
| P | 3.20717800 | -0.54142900 | 0.44937100 |
| C | 2.25121400 | -1.30190200 | 1.81245900 |
| C | 2.77578800 | -1.35362400 | 3.11410100 |
| C | 1.00178200 | -1.88297800 | 1.53607300 |
| C | 2.05321000 | -1.98665900 | 4.12631700 |
| H | 3.73894000 | -0.90716100 | 3.33869600 |
| C | 0.28969300 | -2.51857800 | 2.55280000 |
| H | 0.57202900 | -1.84808800 | 0.53869900 |
| C | 0.81505200 | -2.56937600 | 3.84667900 |
| H | 2.46079100 | -2.02391800 | 5.13232900 |
| H | -0.67204900 | -2.96101000 | 2.31771800 |
| H | 0.25754200 | -3.06124800 | 4.63862300 |
| C | 3.98677000 | -1.89892500 | -0.50859400 |
| C | 4.58868900 | -1.60634200 | -1.74435300 |
| C | 4.01138300 | -3.21134100 | -0.01533200 |
| C | 5.21061800 | -2.61720500 | -2.47418500 |
| H | 4.57658600 | -0.59079900 | -2.13298800 |
| C | 4.63223400 | -4.22001600 | -0.75563500 |
| H | 3.54740000 | -3.44945800 | 0.93594100 |
| C | 5.23019100 | -3.92574400 | -1.98158500 |
| H | 5.67549700 | -2.38580600 | -3.42798400 |
| H | 4.64441200 | -5.23564500 | -0.37159100 |
| H | 5.70927000 | -4.71369600 | -2.55519800 |

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|---|-------------|-------------|-------------|
| C | 4.56023100 | 0.45137300 | 1.19173700 |
| C | 5.83953900 | -0.09620600 | 1.37133700 |
| C | 4.29683300 | 1.76332800 | 1.61795300 |
| C | 6.84243300 | 0.66511100 | 1.97480200 |
| H | 6.05517800 | -1.10703100 | 1.04000300 |
| C | 5.30201000 | 2.51551600 | 2.22369900 |
| H | 3.30929800 | 2.19532100 | 1.47520800 |
| C | 6.57557900 | 1.96746000 | 2.40085500 |
| H | 7.83209600 | 0.23877800 | 2.10913900 |
| H | 5.09416600 | 3.52987800 | 2.55129700 |
| H | 7.35937900 | 2.55722500 | 2.86699200 |
| C | -2.12620200 | 0.04274500 | -3.48476900 |
| C | -3.11485300 | 1.10993900 | -3.13205100 |
| H | -1.50051900 | 0.18387900 | -4.36082800 |
| H | -3.09972400 | 2.01440800 | -3.73365700 |
| H | -4.08978800 | 0.84175700 | -2.73853100 |
| C | -2.00203300 | 1.29344400 | 0.94783400 |
| C | -3.06279100 | 2.16347200 | 1.31059300 |
| C | -2.89317500 | 3.19483200 | 2.24243600 |
| C | -1.65512900 | 3.41364900 | 2.82820600 |
| C | -0.59455000 | 2.55633900 | 2.50798800 |
| C | -0.77223000 | 1.51268000 | 1.60945700 |
| H | -3.75126500 | 3.80992300 | 2.48704600 |
| H | -1.52247400 | 4.22338900 | 3.53810200 |
| H | 0.37368900 | 2.69041900 | 2.98316600 |
| H | 0.03180700 | 0.81119500 | 1.41416300 |
| O | -4.50669200 | 1.57321100 | -0.40106100 |
| N | -2.15914100 | 0.14354800 | 0.19835900 |
| N | -4.40349300 | 2.01517200 | 0.74663400 |
| O | -5.35796200 | 2.35877700 | 1.44358600 |

TSS-10

SCF done: -2238.957366

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|---|-------------|------------|-------------|
| C | -0.09791100 | 4.85595900 | -1.92596200 |
| C | 0.12248800 | 3.58391200 | -1.42822800 |
| C | -0.95750800 | 2.66239600 | -1.26618700 |
| C | -2.27052100 | 3.08376000 | -1.64500700 |
| C | -2.47909100 | 4.35720700 | -2.14563500 |
| C | -1.39836500 | 5.24171100 | -2.28588900 |
| H | 0.72742900 | 5.55114000 | -2.04117200 |
| H | 1.12205600 | 3.26770800 | -1.14584600 |
| H | -3.10595700 | 2.40095000 | -1.53573300 |
| H | -3.47777000 | 4.67103500 | -2.43255000 |
| H | -1.57048300 | 6.23887700 | -2.68191400 |

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|----|-------------|-------------|-------------|
| C | -0.69865100 | 1.36704000 | -0.75084000 |
| C | -1.80451300 | 0.42534500 | -0.42696100 |
| S | -1.68449900 | -2.23477400 | 0.10224100 |
| O | -0.80951100 | -3.20282700 | -0.58520700 |
| O | -1.33596700 | -1.69752500 | 1.43192900 |
| C | -3.34865200 | -2.88516300 | 0.10678300 |
| C | -3.62082800 | -4.02196100 | -0.65693300 |
| C | -4.33522500 | -2.27686400 | 0.89016200 |
| C | -4.91392300 | -4.54473500 | -0.64386700 |
| H | -2.83188800 | -4.49529900 | -1.23064100 |
| C | -5.61562000 | -2.81761100 | 0.88735400 |
| H | -4.09962200 | -1.39927900 | 1.47985200 |
| C | -5.92864400 | -3.95430900 | 0.12074200 |
| H | -5.13324100 | -5.43122200 | -1.23252400 |
| H | -6.38896600 | -2.35235100 | 1.49304600 |
| C | -7.32868300 | -4.51685500 | 0.12812500 |
| H | -8.04039900 | -3.80283600 | -0.30439400 |
| H | -7.39306200 | -5.44495000 | -0.44672300 |
| H | -7.66504700 | -4.72645400 | 1.15015100 |
| N | -1.72076500 | -0.85612200 | -0.98089900 |
| C | -1.48424500 | -1.17896500 | -2.41872100 |
| H | -0.50652600 | -1.65892400 | -2.51674400 |
| H | -2.24484300 | -1.91453100 | -2.70188900 |
| Au | 1.15132400 | 0.58106200 | -0.31161400 |
| P | 3.25522500 | -0.41295600 | 0.22179700 |
| C | 3.24096200 | -1.23582900 | 1.86318600 |
| C | 4.39853200 | -1.29688800 | 2.65568800 |
| C | 2.05160800 | -1.83115900 | 2.31486000 |
| C | 4.36424400 | -1.95397000 | 3.88616400 |
| H | 5.31965000 | -0.83109100 | 2.31901500 |
| C | 2.02819700 | -2.48731300 | 3.54602700 |
| H | 1.14290700 | -1.78769800 | 1.72130300 |
| C | 3.18126500 | -2.54899000 | 4.33158000 |
| H | 5.26127100 | -1.99775900 | 4.49705000 |
| H | 1.10425800 | -2.94360300 | 3.88851000 |
| H | 3.15824400 | -3.05644700 | 5.29177300 |
| C | 3.71841800 | -1.68010700 | -1.02725100 |
| C | 3.53972600 | -1.37998600 | -2.38830500 |
| C | 4.24192700 | -2.92591500 | -0.65514400 |
| C | 3.89104700 | -2.31236000 | -3.36304200 |
| H | 3.13070000 | -0.41713300 | -2.68601800 |
| C | 4.58564500 | -3.85822000 | -1.63656200 |
| H | 4.37588300 | -3.17232000 | 0.39311700 |
| C | 4.41223200 | -3.55376100 | -2.98742800 |

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|---|-------------|-------------|-------------|
| H | 3.75337200 | -2.07307800 | -4.41355400 |
| H | 4.98660700 | -4.82354800 | -1.34187200 |
| H | 4.67888200 | -4.28263100 | -3.74722600 |
| C | 4.62350100 | 0.81702900 | 0.25886600 |
| C | 5.87950700 | 0.54461200 | -0.30151300 |
| C | 4.39895300 | 2.05220700 | 0.88935100 |
| C | 6.89748500 | 1.49852200 | -0.22969700 |
| H | 6.06414300 | -0.40449500 | -0.79469700 |
| C | 5.42059800 | 2.99771600 | 0.96323500 |
| H | 3.42792000 | 2.27084800 | 1.32809600 |
| C | 6.67065900 | 2.72241600 | 0.40150700 |
| H | 7.86752000 | 1.28203900 | -0.66765300 |
| H | 5.24136700 | 3.94902000 | 1.45605900 |
| H | 7.46466900 | 3.46157400 | 0.45519700 |
| C | -1.57896900 | 0.00597200 | -3.34031800 |
| C | -2.63406800 | 0.25076600 | -4.11994000 |
| H | -0.70291500 | 0.64927400 | -3.40269500 |
| H | -2.64969500 | 1.08921300 | -4.81077900 |
| H | -3.51769000 | -0.38324300 | -4.10427800 |
| C | -2.74900400 | 1.70817400 | 1.36124400 |
| C | -3.93252000 | 2.45736600 | 1.55222000 |
| C | -4.03780800 | 3.42048700 | 2.55926800 |
| C | -2.96472600 | 3.65813600 | 3.40889000 |
| C | -1.79130700 | 2.91188400 | 3.25450300 |
| C | -1.68619200 | 1.94941700 | 2.25558300 |
| H | -4.96858000 | 3.96668300 | 2.65260200 |
| H | -3.04453300 | 4.40934300 | 4.18752300 |
| H | -0.95214700 | 3.07316000 | 3.92522200 |
| H | -0.80085100 | 1.32703100 | 2.17854400 |
| O | -4.93079600 | 1.66573700 | -0.38674300 |
| N | -2.69734400 | 0.64216800 | 0.47241000 |
| N | -5.09524600 | 2.25771800 | 0.68784900 |
| O | -6.17751600 | 2.69274400 | 1.07371500 |

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SCF done:-2238.964066

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|---|-------------|------------|-------------|
| C | -0.08286100 | 4.58057500 | -2.54053500 |
| C | 0.13359600 | 3.39647500 | -1.85940900 |
| C | -0.95721500 | 2.53659600 | -1.52316500 |
| C | -2.27780400 | 2.93518400 | -1.90112500 |
| C | -2.48327800 | 4.12378300 | -2.58140800 |
| C | -1.39039800 | 4.94226300 | -2.90344600 |
| H | 0.75006000 | 5.22830500 | -2.79441500 |
| H | 1.13724000 | 3.09942700 | -1.57096000 |

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|----|-------------|-------------|-------------|
| H | -3.12577900 | 2.31496000 | -1.62800500 |
| H | -3.48810100 | 4.42248500 | -2.86268300 |
| H | -1.55817300 | 5.87244700 | -3.43955000 |
| C | -0.71093400 | 1.31632300 | -0.84816100 |
| C | -1.83838100 | 0.42515900 | -0.45520700 |
| S | -1.93551100 | -2.29261200 | -0.21388000 |
| O | -1.31014200 | -3.27148200 | -1.12281300 |
| O | -1.35794000 | -1.96571000 | 1.10360200 |
| C | -3.66188100 | -2.71322200 | -0.03825700 |
| C | -4.21419900 | -3.64545400 | -0.92008900 |
| C | -4.41779700 | -2.14522800 | 0.99188900 |
| C | -5.55664900 | -3.99157600 | -0.77567300 |
| H | -3.59903300 | -4.10675700 | -1.68456100 |
| C | -5.75393400 | -2.50909500 | 1.11709500 |
| H | -3.96426900 | -1.43698000 | 1.67431100 |
| C | -6.34762800 | -3.42883000 | 0.23553700 |
| H | -5.99247300 | -4.71977600 | -1.45418500 |
| H | -6.34904200 | -2.07586400 | 1.91668400 |
| C | -7.80594100 | -3.78981800 | 0.37410500 |
| H | -8.44377700 | -2.98753700 | -0.01885100 |
| H | -8.04837900 | -4.70427800 | -0.17491400 |
| H | -8.08236800 | -3.93684800 | 1.42365000 |
| N | -1.87895800 | -0.80168700 | -1.12712900 |
| C | -1.78770600 | -0.88938300 | -2.60412300 |
| H | -2.35842000 | -1.77730100 | -2.89414900 |
| H | -2.31669400 | -0.02775300 | -3.02431700 |
| Au | 1.11646700 | 0.54473300 | -0.31583200 |
| P | 3.19074600 | -0.42648100 | 0.34892800 |
| C | 3.06654500 | -1.27443000 | 1.97356500 |
| C | 4.14029500 | -1.28630700 | 2.87739900 |
| C | 1.87196600 | -1.93986400 | 2.29629400 |
| C | 4.01852100 | -1.96309000 | 4.09193900 |
| H | 5.06388000 | -0.76778000 | 2.63945900 |
| C | 1.76179900 | -2.61671400 | 3.51134900 |
| H | 1.02576600 | -1.93361100 | 1.61450500 |
| C | 2.83189600 | -2.62829600 | 4.40911700 |
| H | 4.85077100 | -1.96802700 | 4.78986200 |
| H | 0.83500100 | -3.12807900 | 3.75379700 |
| H | 2.74059800 | -3.15163000 | 5.35663800 |
| C | 3.75769600 | -1.67855600 | -0.87439200 |
| C | 3.67600300 | -1.36635500 | -2.24192400 |
| C | 4.26995800 | -2.92114200 | -0.47644600 |
| C | 4.11221300 | -2.28364900 | -3.19657300 |
| H | 3.27339700 | -0.40702300 | -2.55854200 |

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|---|-------------|-------------|-------------|
| C | 4.69884100 | -3.83846900 | -1.43856400 |
| H | 4.32964300 | -3.17653300 | 0.57655900 |
| C | 4.62188800 | -3.52197300 | -2.79550900 |
| H | 4.05106600 | -2.03547700 | -4.25235600 |
| H | 5.09097300 | -4.80122800 | -1.12422800 |
| H | 4.95470900 | -4.23884000 | -3.54044700 |
| C | 4.54283000 | 0.81299200 | 0.49076400 |
| C | 5.86016400 | 0.51245400 | 0.11402300 |
| C | 4.24472300 | 2.08155100 | 1.01469200 |
| C | 6.86507600 | 1.47041300 | 0.26434100 |
| H | 6.10200100 | -0.46189800 | -0.29892200 |
| C | 5.25318100 | 3.03245500 | 1.16660900 |
| H | 3.22565300 | 2.32353100 | 1.30715800 |
| C | 6.56409200 | 2.72810900 | 0.79015400 |
| H | 7.88258600 | 1.23204700 | -0.03141800 |
| H | 5.01580200 | 4.01068600 | 1.57484600 |
| H | 7.34813900 | 3.47107100 | 0.90410300 |
| C | -0.38769100 | -0.98539600 | -3.15240300 |
| C | 0.07510500 | -0.20467100 | -4.13203200 |
| H | 0.22496000 | -1.78180500 | -2.73578100 |
| H | 1.07080000 | -0.33985200 | -4.54489900 |
| H | -0.52975300 | 0.58438100 | -4.57499000 |
| C | -2.59684600 | 1.71298800 | 1.40330900 |
| C | -3.71915100 | 2.54176200 | 1.63245900 |
| C | -3.72202800 | 3.51166600 | 2.63893200 |
| C | -2.60505300 | 3.67950200 | 3.44735200 |
| C | -1.49202600 | 2.85424900 | 3.25549700 |
| C | -1.49059300 | 1.88317800 | 2.25876000 |
| H | -4.61058600 | 4.11815400 | 2.76505100 |
| H | -2.60569400 | 4.43710300 | 4.22390400 |
| H | -0.62028500 | 2.95901100 | 3.89517000 |
| H | -0.64978600 | 1.20572700 | 2.15209700 |
| O | -4.85054900 | 1.85602900 | -0.27800700 |
| N | -2.64991300 | 0.64451400 | 0.51041200 |
| N | -4.93080200 | 2.42240100 | 0.81885000 |
| O | -5.96949100 | 2.89829400 | 1.27020700 |

TS10-11

SCF done: -2238.939402

| | | | |
|---|-------------|------------|-------------|
| C | 0.12958400 | 4.86222300 | -1.40785000 |
| C | 0.27764700 | 3.48139600 | -1.31689500 |
| C | -0.83682800 | 2.62146000 | -1.42214200 |
| C | -2.10578100 | 3.20076100 | -1.65113900 |
| C | -2.25214800 | 4.58133400 | -1.73514400 |

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|----|-------------|-------------|-------------|
| C | -1.13638300 | 5.41690400 | -1.61620900 |
| H | 0.99941300 | 5.50610200 | -1.31772100 |
| H | 1.26478900 | 3.05535500 | -1.15941800 |
| H | -2.98413500 | 2.56839500 | -1.73442300 |
| H | -3.23752300 | 5.00802500 | -1.89787500 |
| H | -1.25317600 | 6.49430400 | -1.68950800 |
| C | -0.65122500 | 1.14849000 | -1.37597400 |
| C | -1.78663000 | 0.29575100 | -0.84926400 |
| S | -2.01112700 | -2.44960200 | -0.40375100 |
| O | -1.58182700 | -3.51479700 | -1.32895500 |
| O | -1.26363300 | -2.10993800 | 0.81734000 |
| C | -3.73837300 | -2.66642900 | -0.03176600 |
| C | -4.50431100 | -3.48854400 | -0.86377800 |
| C | -4.28857900 | -2.05181300 | 1.09809700 |
| C | -5.85225500 | -3.67178900 | -0.56521100 |
| H | -4.04910400 | -3.99523700 | -1.70748400 |
| C | -5.63541700 | -2.25452600 | 1.37626900 |
| H | -3.67093500 | -1.43741300 | 1.74095500 |
| C | -6.44110300 | -3.05557100 | 0.54909000 |
| H | -6.45398400 | -4.31355300 | -1.20264200 |
| H | -6.07156400 | -1.78493900 | 2.25378700 |
| C | -7.90715100 | -3.23674900 | 0.85252100 |
| H | -8.47544500 | -2.34509500 | 0.55782600 |
| H | -8.32768600 | -4.09093400 | 0.31426200 |
| H | -8.07689800 | -3.38799100 | 1.92384400 |
| N | -1.90012200 | -1.00909000 | -1.41902900 |
| C | -2.03984300 | -1.14154600 | -2.87684400 |
| H | -2.14695200 | -2.19601200 | -3.12948600 |
| H | -2.87792300 | -0.55585700 | -3.26627100 |
| Au | 1.16220200 | 0.36953800 | -0.55170900 |
| C | 3.95735100 | -1.67285900 | -0.83460800 |
| C | 4.11921300 | -1.28836000 | -2.17708700 |
| C | 4.36145600 | -2.95157000 | -0.42866200 |
| C | 4.68647800 | -2.16974000 | -3.09548000 |
| H | 3.81123700 | -0.29638000 | -2.50035900 |
| C | 4.92124900 | -3.83410000 | -1.35626000 |
| H | 4.23910700 | -3.26203400 | 0.60380200 |
| C | 5.08527600 | -3.44607700 | -2.68619200 |
| H | 4.81644300 | -1.86290500 | -4.12944300 |
| H | 5.22938500 | -4.82469400 | -1.03482600 |
| H | 5.52209100 | -4.13448000 | -3.40379700 |
| C | 4.43509800 | 0.85885300 | 0.59051800 |
| C | 5.79955500 | 0.65544600 | 0.33546000 |
| C | 4.00088300 | 2.09967700 | 1.08471900 |

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|---|-------------|-------------|-------------|
| C | 6.71546100 | 1.68212200 | 0.57494800 |
| H | 6.14739900 | -0.29716900 | -0.05186800 |
| C | 4.92064500 | 3.11945200 | 1.32638900 |
| H | 2.94474800 | 2.26625700 | 1.28300900 |
| C | 6.27862000 | 2.91215900 | 1.06994100 |
| H | 7.77008300 | 1.51873600 | 0.37314000 |
| H | 4.57774900 | 4.07591400 | 1.71049500 |
| H | 6.99368600 | 3.70885600 | 1.25336600 |
| C | -0.69791600 | -0.59603600 | -3.19257500 |
| C | -0.50656900 | 0.78408400 | -3.23419200 |
| H | 0.14180500 | -1.27730400 | -3.07129200 |
| H | 0.48153700 | 1.16688400 | -3.46700200 |
| H | -1.33059300 | 1.37511300 | -3.62705000 |
| C | -2.53553900 | 1.56464300 | 1.05781100 |
| C | -3.68604300 | 2.34050000 | 1.33420200 |
| C | -3.71709600 | 3.25822100 | 2.38778900 |
| C | -2.60259400 | 3.42420700 | 3.19912400 |
| C | -1.46329400 | 2.64650600 | 2.96288500 |
| C | -1.43253800 | 1.72938000 | 1.91825700 |
| H | -4.62620500 | 3.82476100 | 2.54848300 |
| H | -2.62411500 | 4.14238000 | 4.01205800 |
| H | -0.59279800 | 2.74920000 | 3.60475300 |
| H | -0.56379700 | 1.09658800 | 1.76751300 |
| O | -4.80583400 | 1.71614300 | -0.60275600 |
| N | -2.56811300 | 0.53236100 | 0.13127600 |
| N | -4.89918700 | 2.21043500 | 0.52670700 |
| O | -5.95596500 | 2.60306200 | 1.01896400 |
| C | 3.00132700 | -1.33427800 | 1.94545300 |
| C | 4.02783200 | -1.32357100 | 2.90351900 |
| C | 1.81004300 | -2.03109300 | 2.20533100 |
| C | 3.86236500 | -2.00878400 | 4.10757700 |
| H | 4.94826500 | -0.77929500 | 2.71618800 |
| C | 1.65583100 | -2.71697500 | 3.41096400 |
| H | 1.00079700 | -2.04022100 | 1.48092500 |
| C | 2.67861200 | -2.70594700 | 4.36175700 |
| H | 4.65771500 | -1.99515900 | 4.84715200 |
| H | 0.73128600 | -3.25259800 | 3.60506100 |
| H | 2.55286200 | -3.23580800 | 5.30168500 |
| P | 3.19233700 | -0.47377700 | 0.33437700 |

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SCF done: -2238.980117

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|---|------------|------------|-------------|
| C | 0.60149000 | 4.78110500 | -1.67759300 |
| C | 0.58640300 | 3.38715900 | -1.60803200 |

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|----|-------------|-------------|-------------|
| C | -0.62280000 | 2.67746000 | -1.52913000 |
| C | -1.82093600 | 3.41235500 | -1.54449600 |
| C | -1.80641600 | 4.80664900 | -1.60523300 |
| C | -0.59571900 | 5.49779400 | -1.67002700 |
| H | 1.55137000 | 5.30502900 | -1.73964100 |
| H | 1.52793500 | 2.84362600 | -1.62391600 |
| H | -2.77656900 | 2.89727000 | -1.50176200 |
| H | -2.74637700 | 5.35177500 | -1.60830000 |
| H | -0.58563000 | 6.58275100 | -1.72093400 |
| C | -0.64301600 | 1.15987500 | -1.56638900 |
| C | -1.73222000 | 0.47286300 | -0.83251300 |
| S | -2.01117800 | -2.47514300 | -0.65325900 |
| O | -1.71923500 | -3.38834900 | -1.76668600 |
| O | -1.09650800 | -2.22421500 | 0.46216500 |
| C | -3.68465200 | -2.66377700 | -0.12098700 |
| C | -4.53809400 | -3.47325000 | -0.88172800 |
| C | -4.10442700 | -2.05344300 | 1.06817100 |
| C | -5.84669900 | -3.65016600 | -0.44309700 |
| H | -4.17710800 | -3.97124700 | -1.77487800 |
| C | -5.41649700 | -2.24884000 | 1.47957200 |
| H | -3.42166200 | -1.44124000 | 1.64357800 |
| C | -6.30985400 | -3.03847200 | 0.73285100 |
| H | -6.51718600 | -4.28108100 | -1.01926800 |
| H | -5.75742700 | -1.78159700 | 2.39905800 |
| C | -7.73674300 | -3.20977900 | 1.18504300 |
| H | -8.32277200 | -2.31203100 | 0.94917700 |
| H | -8.21749400 | -4.05954000 | 0.69282600 |
| H | -7.79611300 | -3.35812500 | 2.26827000 |
| N | -2.03048300 | -0.80387200 | -1.57512900 |
| C | -2.93069800 | -0.66627900 | -2.75451500 |
| H | -3.50775900 | -1.56007000 | -2.97216900 |
| H | -3.47842700 | 0.27166200 | -2.78128700 |
| Au | 1.12012800 | 0.28337900 | -0.61123600 |
| C | 3.78952600 | -1.99610400 | -0.57184900 |
| C | 3.74168800 | -1.98627000 | -1.97580900 |
| C | 4.34903100 | -3.09689100 | 0.09261700 |
| C | 4.25586700 | -3.05861900 | -2.70307200 |
| H | 3.30647600 | -1.13815100 | -2.49894900 |
| C | 4.85624300 | -4.17163400 | -0.64135600 |
| H | 4.38730800 | -3.12043200 | 1.17700100 |
| C | 4.81160600 | -4.15399100 | -2.03611600 |
| H | 4.21894500 | -3.04186200 | -3.78855200 |
| H | 5.28537400 | -5.02229700 | -0.11989800 |
| H | 5.20618700 | -4.99202100 | -2.60334700 |

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|---|-------------|-------------|-------------|
| C | 4.44884300 | 0.73704600 | 0.30511900 |
| C | 5.78339900 | 0.41359900 | 0.01929700 |
| C | 4.10515300 | 2.06880500 | 0.59091300 |
| C | 6.76018900 | 1.41178000 | 0.02273000 |
| H | 6.06077900 | -0.61051400 | -0.20966500 |
| C | 5.08602600 | 3.05975100 | 0.59939700 |
| H | 3.07175900 | 2.33069200 | 0.80477300 |
| C | 6.41419000 | 2.73257700 | 0.31325400 |
| H | 7.79102000 | 1.15481100 | -0.20326700 |
| H | 4.81271900 | 4.08702900 | 0.82273600 |
| H | 7.17626900 | 3.50650900 | 0.31312000 |
| C | -1.46047700 | -0.70015000 | -2.95738500 |
| C | -0.69826600 | 0.61362100 | -3.03227100 |
| H | -1.02815800 | -1.62540700 | -3.32463100 |
| H | 0.29005300 | 0.47280900 | -3.47170600 |
| H | -1.24330700 | 1.31514800 | -3.67666400 |
| C | -2.43813400 | 1.67684000 | 1.10452800 |
| C | -3.61114900 | 2.40681200 | 1.40076000 |
| C | -3.65288000 | 3.34204500 | 2.43705500 |
| C | -2.51677900 | 3.57613600 | 3.20202500 |
| C | -1.34885400 | 2.85332100 | 2.93593900 |
| C | -1.31130500 | 1.91396000 | 1.90986600 |
| H | -4.57996400 | 3.87233900 | 2.61906900 |
| H | -2.54179900 | 4.31131600 | 3.99954900 |
| H | -0.45891500 | 3.02012100 | 3.53603200 |
| H | -0.41214500 | 1.33433600 | 1.72643300 |
| O | -4.73288500 | 1.80964800 | -0.54480400 |
| N | -2.47035700 | 0.63207200 | 0.18353500 |
| N | -4.83332200 | 2.21519900 | 0.61962900 |
| O | -5.90378400 | 2.47417400 | 1.16669000 |
| C | 2.94747700 | -1.05755800 | 2.09734000 |
| C | 3.96286700 | -0.82747200 | 3.03814900 |
| C | 1.77025000 | -1.71564700 | 2.49062400 |
| C | 3.80141300 | -1.25508900 | 4.35736000 |
| H | 4.87420900 | -0.31480800 | 2.74660300 |
| C | 1.61981200 | -2.14493200 | 3.80932600 |
| H | 0.97554000 | -1.89417100 | 1.77154700 |
| C | 2.63265700 | -1.91408700 | 4.74368400 |
| H | 4.58992200 | -1.07186500 | 5.08157000 |
| H | 0.70873300 | -2.65599200 | 4.10716600 |
| H | 2.51017500 | -2.24475400 | 5.77112700 |
| P | 3.12573700 | -0.54221300 | 0.34064600 |

P1

SCF done:-1402.245581

| | | | |
|---|-------------|-------------|-------------|
| C | 4.99333100 | -1.15685700 | 0.44078700 |
| C | 3.67956400 | -1.58133400 | 0.24432700 |
| C | 2.85644400 | -0.94682100 | -0.69799400 |
| C | 3.37874500 | 0.11789900 | -1.44296800 |
| C | 4.69387000 | 0.54326300 | -1.24934800 |
| C | 5.50371200 | -0.09208100 | -0.30638200 |
| H | 5.62004800 | -1.65964500 | 1.17260800 |
| H | 3.28609900 | -2.41355300 | 0.82323900 |
| H | 2.74470400 | 0.61793900 | -2.16971000 |
| H | 5.08442200 | 1.37192700 | -1.83381400 |
| H | 6.52836200 | 0.23732500 | -0.15635200 |
| C | 1.44553800 | -1.40919800 | -0.89771700 |
| C | 0.38790200 | -1.08878500 | 0.13324700 |
| S | -1.98611400 | -2.17547500 | 1.08026500 |
| O | -2.64768000 | -3.39912900 | 0.58511100 |
| O | -1.65601000 | -1.99702600 | 2.50113700 |
| C | -2.86830600 | -0.74032400 | 0.48699000 |
| C | -3.53616200 | -0.81433300 | -0.73630600 |
| C | -2.85731200 | 0.43358900 | 1.24120100 |
| C | -4.15819600 | 0.32906600 | -1.23071000 |
| H | -3.56656500 | -1.74903900 | -1.28634500 |
| C | -3.49487200 | 1.56213500 | 0.73346000 |
| H | -2.34435800 | 0.45413500 | 2.19522700 |
| C | -4.12616500 | 1.53738200 | -0.51921800 |
| H | -4.66683400 | 0.28721100 | -2.19035300 |
| H | -3.48076900 | 2.48572500 | 1.30637100 |
| C | -4.70796600 | 2.79882200 | -1.10622700 |
| H | -5.19203100 | 3.41540600 | -0.34104200 |
| H | -3.90451300 | 3.39860700 | -1.55307300 |
| H | -5.44157500 | 2.58164100 | -1.88905000 |
| N | -0.52121900 | -2.14217400 | 0.14683600 |
| C | -0.09780100 | -3.32295200 | -0.62750800 |
| H | 0.19569000 | -4.13990800 | 0.04225300 |
| H | -0.91954700 | -3.67727200 | -1.25477100 |
| C | 1.08744900 | -2.79932100 | -1.41887300 |
| C | 0.86296800 | -1.60159200 | -2.28968500 |
| H | 1.88051600 | -3.49636500 | -1.67026300 |
| H | 1.55468200 | -1.45458700 | -3.11404100 |
| H | -0.14761500 | -1.24979300 | -2.47409100 |
| C | 0.96717700 | 1.09520300 | 0.91584900 |
| C | 0.64499300 | 2.25261300 | 0.16340300 |
| C | 1.28734500 | 3.47892300 | 0.38059400 |
| C | 2.28871600 | 3.58401400 | 1.33254000 |
| C | 2.62296100 | 2.45652700 | 2.09595100 |

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|---|-------------|-------------|-------------|
| C | 1.96371000 | 1.25167100 | 1.90479900 |
| H | 0.98252600 | 4.32891000 | -0.21801500 |
| H | 2.79854100 | 4.52979500 | 1.48622800 |
| H | 3.39818500 | 2.52392700 | 2.85443700 |
| H | 2.19856900 | 0.38734500 | 2.51666000 |
| O | -0.60835200 | 1.17568200 | -1.46485500 |
| N | 0.23231600 | -0.07600600 | 0.89101400 |
| N | -0.38285800 | 2.23373900 | -0.87346100 |
| O | -0.96723800 | 3.29471100 | -1.11918600 |

P2

SCF done: -1402.273274

| | | | |
|---|-------------|-------------|-------------|
| C | 0.48155500 | 4.74164900 | -0.19167600 |
| C | -0.36279800 | 3.63602300 | -0.08795600 |
| C | 0.13754500 | 2.32821700 | -0.22924400 |
| C | 1.51243200 | 2.16520400 | -0.47682200 |
| C | 2.35641400 | 3.27178200 | -0.57091700 |
| C | 1.84554900 | 4.56425100 | -0.43200900 |
| H | 0.07363200 | 5.74246300 | -0.07640800 |
| H | -1.41874000 | 3.78039700 | 0.12284100 |
| H | 1.91453500 | 1.16612700 | -0.61185500 |
| H | 3.41552800 | 3.12243000 | -0.76425300 |
| H | 2.50404400 | 5.42495700 | -0.51086200 |
| C | -0.76873500 | 1.16836400 | -0.13218900 |
| C | -0.60232900 | 0.01027500 | 0.61247400 |
| S | 1.20480400 | -1.82813400 | 1.42162300 |
| O | 1.95943500 | -1.97256400 | 2.68012400 |
| O | 0.19607300 | -2.81729100 | 0.98950800 |
| C | 2.37536100 | -1.63835000 | 0.07510800 |
| C | 3.67662900 | -1.21444000 | 0.35401100 |
| C | 1.96939200 | -1.91040900 | -1.23370400 |
| C | 4.57285700 | -1.04706900 | -0.69981000 |
| H | 3.98083800 | -1.03466300 | 1.37961300 |
| C | 2.88016300 | -1.73279500 | -2.27325800 |
| H | 0.96365500 | -2.26631000 | -1.42821700 |
| C | 4.19197700 | -1.30102600 | -2.02610800 |
| H | 5.58818400 | -0.72133800 | -0.48768800 |
| H | 2.56852600 | -1.94118400 | -3.29367100 |
| C | 5.18003600 | -1.14852500 | -3.15783500 |
| H | 5.95873200 | -0.41829700 | -2.91543500 |
| H | 5.68094600 | -2.10214900 | -3.37092300 |
| H | 4.68589400 | -0.82809300 | -4.08091100 |
| N | 0.39903400 | -0.32065700 | 1.53719600 |
| C | 0.72206500 | 0.61417100 | 2.64616900 |

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|---|-------------|-------------|-------------|
| H | 1.63749700 | 0.23894100 | 3.10853100 |
| H | 0.93112400 | 1.60164100 | 2.22525500 |
| C | -0.38785600 | 0.68340600 | 3.65875500 |
| C | -1.06519800 | 1.79729300 | 3.93710700 |
| H | -0.61883900 | -0.24968400 | 4.17145600 |
| H | -1.85237800 | 1.81683800 | 4.68582200 |
| H | -0.85202400 | 2.73523100 | 3.42807800 |
| C | -2.57258900 | -0.24497000 | -0.43311900 |
| C | -3.79325300 | -0.68592800 | -0.97341200 |
| C | -4.48504500 | 0.13214200 | -1.86484400 |
| C | -3.95935000 | 1.37643200 | -2.23163900 |
| C | -2.74531800 | 1.82696700 | -1.71214600 |
| C | -2.04144500 | 1.02727400 | -0.80169000 |
| H | -5.42860100 | -0.22166900 | -2.26151400 |
| H | -4.50752700 | 1.99556400 | -2.93486800 |
| H | -2.34311300 | 2.78814600 | -2.01778500 |
| H | -1.77943800 | -1.76647700 | 0.79394900 |
| O | -3.68955000 | -2.66971900 | 0.18639400 |
| N | -1.69994800 | -0.82279900 | 0.43673400 |
| N | -4.34179000 | -1.97868400 | -0.61037700 |
| O | -5.41455300 | -2.32509800 | -1.10396400 |