

Supporting Information

Mechanistic investigation of the trimethylamine-N-oxide reduction catalysed by biomimetic molybdenum enzyme models

M. Fortino, T. Marino, N. Russo, E. Sicilia

Cartesian coordinates (Å) of all optimized structures

Tables S1-S5

The most relevant geometrical parameters of minima and transition states intercepted along the pathway for the Me_3NO reduction by the $[\text{Mo(IV)O}(\text{bdt})_2]^{2-}$ complex.

Figure S1

Me_3NO attack to the $[\text{Mo(IV)O}(\text{bdt})_2]^{2-}$ complex PESs for the examined singlet and the triplet electronic spin states.

Figure S2

M06-L optimized geometries for the Me_3NO cis-attack to the monooxomolybdenum(IV) $\text{E}_{(\text{carb})}$ complex in its *cis* and *trans* arrangements.

Figure S3

M06-L free energy profile for the Me_3NO trans-attack to the monooxomolybdenum(IV) $\text{E}_{(\text{carb})}$ complex in its *trans* arrangement. Energies are in kcal mol^{-1} and relative to reactants' asymptote

Figure S4

M06-L optimized geometries for the Me_3NO *trans*-attack to the monooxomolybdenum(IV) $\text{E}_{(\text{carb})}$ complex in its *cis* and *trans* arrangements.

Figure S5

M06-L optimized geometry of the transition state for the *cis* to *trans* interconversion of the initial monooxo(carb) complex.

Figure S6

M06-L optimized geometries for the Me_3NO cis-attack to the monooxomolybdenum(IV) $\text{E}_{(\text{acylam})}$ complex in its *cis* and *trans* arrangement

Figure S7

M06-L free energy profiles for the Me_3NO trans-attack to the monooxomolybdenum(IV) $\text{E}_{(\text{acylam})}$ complex in its *cis* and *trans* arrangements. Energies are in kcal mol^{-1} and relative to reactants' asymptote

Figure S8

M06-L optimized geometries for the Me_3NO *trans*-attack to the monooxomolybdenum(IV) $\text{E}_{(\text{acylam})}$ complex in its *cis* and *trans* arrangement

Figure S9

Table S1**E**

Mo	0.00003500	-0.00000600	0.73683200
S	-1.66518800	-1.61056200	-0.03008700
S	1.66501600	1.61049700	-0.03073600
S	-1.66525900	1.61058800	-0.02989900
S	1.66509500	-1.61052600	-0.03057600
O	0.00039800	-0.00001700	2.44881700
C	-5.54517600	-0.69889800	-0.84242700
H	-6.46350400	-1.25293500	-1.03918300
C	-5.54521300	0.69884500	-0.84232700
H	-6.46357000	1.25286300	-1.03900400
C	-3.15648900	0.70808300	-0.32318000
C	3.15641400	0.70808300	-0.32343800
C	-4.35726100	-1.38441900	-0.58795800
C	4.35735000	-1.38438700	-0.58770300
H	4.34251700	-2.47463700	-0.59011800
C	-4.35733100	1.38439400	-0.58777900
C	-3.15645700	-0.70808000	-0.32326300
C	4.35726800	1.38443300	-0.58787700
C	5.54524300	0.69891600	-0.84208000
H	6.46360300	1.25295900	-1.03866500
C	5.54528200	-0.69883100	-0.84200000
H	6.46367400	-1.25284500	-1.03851700
C	3.15645700	-0.70807500	-0.32333500
H	-4.34237800	-2.47466800	-0.59046900
H	-4.34250500	2.47464400	-0.59014700
H	4.34237100	2.47468200	-0.59042100

TS1

Mo	0.25056600	-0.12233600	-0.64179600
S	-1.11098500	-0.34913800	1.57505900
S	2.03303400	-1.72022800	-0.81694400
S	-1.38150000	-1.88960300	-1.23757600
S	1.82175700	1.01615000	0.87168700
O	0.38364800	0.79374200	-2.08971800
C	-5.00948800	-1.48510600	1.53212300
H	-5.86629200	-1.39868200	2.20155200
C	-5.13030600	-2.13972200	0.30264400
H	-6.08512900	-2.56496800	-0.00881100
C	-2.77481300	-1.68176800	-0.18572500
C	3.46680100	-0.99711200	-0.06817900
C	-3.77957500	-0.93769400	1.89898500
C	4.54273800	0.72133200	1.26756600
H	4.45973800	1.64288700	1.84489800
C	-4.01757200	-2.23437600	-0.53377500
C	-2.64740600	-1.01815000	1.06919000
C	4.71518700	-1.62701300	-0.18828900
C	5.86490600	-1.09765700	0.39740400
H	6.82159300	-1.60760900	0.28024000
C	5.77857700	0.08779200	1.13256500
H	6.66634100	0.51769200	1.59760300
C	3.38150600	0.20458800	0.67459200
H	-3.67250900	-0.42984200	2.85812700
O	-1.85808600	1.70548000	-0.73231500
N	-1.55317500	2.96311900	-0.33321500
C	-2.70714700	3.84822600	-0.67655000
C	-0.32090900	3.47876700	-1.02484300
C	-1.32256900	3.01306900	1.14838500
Mo	0.26700900	0.03546200	-0.86165500
S	-0.82692500	-0.80450900	1.76042400
S	2.01048600	-1.70150400	-0.64522500
S	-1.40547600	-1.82924300	-1.27334600

H	-2.52705800	4.88520100	-0.36070000
H	-2.84050600	3.78430700	-1.75694700
H	-3.58097500	3.42816600	-0.17732500
H	-0.17421400	4.53877400	-0.77864200
H	0.52237900	2.86798700	-0.69288100
H	-0.46827700	3.31595900	-2.09192600
H	-1.11968700	4.04472100	1.46535300
H	-2.21304600	2.60045500	1.62400200
H	-0.48308200	2.34888200	1.36181900
H	-4.09946200	-2.74329300	-1.49416100
H	4.76769900	-2.55406600	-0.76016000

ES

Mo	0.26570300	-0.04139000	-0.73580700
S	-0.92849600	-0.57574600	1.67181400
S	2.04442100	-1.68372500	-0.76120700
S	-1.42699400	-1.80779000	-1.27794800
S	1.83775500	1.17982700	0.71693100
O	0.48862200	0.77689200	-2.23444400
C	-4.94166300	-1.21223000	1.60913600
H	-5.77286000	-1.07651100	2.30283900
C	-5.15806200	-1.73335400	0.33093600
H	-6.16214800	-2.00539300	0.00285200
C	-2.76466800	-1.53690100	-0.16785900
C	3.46529800	-0.93149400	-0.02496600
C	-3.64559500	-0.86622900	1.99762700
C	4.54096000	0.87455400	1.19577000
H	4.45886700	1.84205900	1.69252700
C	-4.07205400	-1.89183100	-0.53368600
C	-2.53480400	-1.01515900	1.14514200
C	4.70701600	-1.58709000	-0.05769900
C	5.85122300	-1.02951300	0.51223000
H	6.80072700	-1.56362800	0.46262100
C	5.76910000	0.21418400	1.14475600
H	6.65266700	0.66750000	1.59542400
C	3.38600300	0.32839200	0.61793300
H	-3.46591000	-0.46709100	2.99675600
O	-1.67407900	1.27585800	-0.69497400
N	-1.65510700	2.58114900	-0.26636600
C	-3.00080400	3.13153600	-0.58179100
C	-0.59702900	3.35826300	-0.98669600
C	-1.41817000	2.67065000	1.20999400
H	-3.08846500	4.17039400	-0.23916600
H	-3.13097900	3.05804600	-1.66167200
H	-3.72473100	2.48320800	-0.08551900
H	-0.66401200	4.41734700	-0.70773700
H	0.36747700	2.92417800	-0.70728000
H	-0.75510700	3.19895300	-2.05311200
H	-1.45102300	3.72366000	1.51768100
H	-2.18376300	2.06753300	1.69893000
H	-0.44734300	2.21515000	1.41493200
H	-4.22954500	-2.29176800	-1.53530100
H	4.75856800	-2.55903200	-0.54937800

TS2

S	1.85124300	1.33960700	0.50950400
O	0.59655400	0.67753100	-2.41947300
C	-4.88699500	-0.99966500	1.60058800
H	-5.71128600	-0.80538800	2.28923100

C	-5.13617000	-1.42931800	0.29581600
H	-6.15673000	-1.57180100	-0.06174400
C	-2.72348300	-1.47983600	-0.15551300
C	3.41952700	-0.90297900	0.04279800
C	-3.56837800	-0.81900500	2.02597800
C	4.51964600	1.00166800	1.08748100
H	4.45276500	2.02193500	1.46635300
C	-4.05274800	-1.66212800	-0.55919100
C	-2.45376900	-1.05209700	1.19057400
C	4.64394500	-1.59007100	0.13100900
C	5.78632400	-1.00371300	0.67295200
H	6.71766900	-1.56898000	0.71778000
C	5.72750100	0.30672100	1.15513800
H	6.61049900	0.78373500	1.58109800
C	3.36526800	0.42464000	0.54086200
H	-3.36819600	-0.49388000	3.04779900
O	-1.52613800	1.03327300	-0.70289700
N	-1.71966900	2.45381300	-0.12050300
C	-3.14262300	2.69833200	-0.37576300
C	-0.83004300	3.35410800	-0.86216500
C	-1.41922400	2.43611700	1.32012800
H	-3.44084000	3.68398500	0.00684900
H	-3.30492500	2.63247000	-1.45226800
H	-3.70165000	1.89956700	0.11643700
H	-0.90642900	4.37607700	-0.46770800
H	0.18944600	2.96578800	-0.74933800
H	-1.10661700	3.31177700	-1.91654800
H	-1.54088500	3.44931300	1.72923100
H	-2.08682600	2.71649200	1.79728200
H	-0.39565200	2.07389000	1.45076100
H	-4.23246700	-1.98062500	-1.58597000
H	4.68019000	-2.61312700	-0.24315600

Dioxo_P

Mo	-0.31734300	-0.90196700	0.78554900
S	1.34024500	0.64881300	1.79814300
S	-2.15608500	-1.69524400	-0.70088700
S	0.17188600	0.79306800	-1.24259100
S	-2.31169000	0.81899200	1.36121200
O	-0.46730700	-1.48095500	2.42160100
C	3.53030400	3.58678600	0.10691900
H	4.34833300	4.23276300	0.42323000
C	2.99347900	3.68869000	-1.17989400
H	3.38696600	4.42057400	-1.88522300
C	1.41618400	1.87257900	-0.69952500
C	-3.51783100	-0.58905900	-0.68048000
C	3.00163700	2.64566400	0.98925700
C	-4.69315800	1.37298600	0.12426700
H	-4.72604500	2.23460200	0.78884800
C	1.95389700	2.84843400	-1.56532600
C	1.95236900	1.79211200	0.61637100
C	-4.58129800	-0.81569700	-1.56695000
C	-5.68945000	0.02908200	-1.61604500
H	-6.49707400	-0.16906300	-2.31986600
C	-5.73872500	1.13479500	-0.76178200
H	-6.59043900	1.81483400	-0.78846900
C	-3.56682000	0.52641200	0.20384100
H	3.40529200	2.55470200	1.99692100
O	0.58075000	-2.16918300	-0.01525200
H	1.53775700	2.91956100	-2.56884000
H	-4.52102800	-1.67576000	-2.23265100
N	4.30079700	-2.03012100	-1.24671300
C	5.69620300	-1.96258600	-0.88923000
H	6.20390500	-2.89781200	-1.16118800
H	6.18211500	-1.13720800	-1.42291900
H	5.85520200	-1.79639600	0.20031800
C	3.65478600	-3.13179900	-0.55661600

H	2.58719500	-3.14410700	-0.78903500
H	4.11419100	-4.08139300	-0.86210600
H	3.73961600	-3.04416800	0.54655700
C	3.62852400	-0.77584600	-0.92243300
H	4.08153800	0.04838100	-1.48474200
H	2.56658000	-0.83617100	-1.18143900
H	3.69089600	-0.53412200	0.15547300

Dioxo

Mo	0.00004800	-1.38473600	-0.00004000
S	2.13472700	-0.95157200	1.20912800
S	-2.13435700	-0.95109300	-1.20957600
S	1.08653600	0.62264700	-1.45150800
S	-1.08673600	0.62239500	1.45175600
O	-0.28700200	-2.46536200	1.33596800
C	5.16093800	1.59072800	0.38879600
H	6.13654900	1.80813200	0.82215500
C	4.70229200	2.28796000	-0.73287700
H	5.31707700	3.06312600	-1.19130600
C	2.61585100	0.99221000	-0.72667100
C	-3.08611000	0.29634500	-0.42375400
C	4.34759000	0.60848800	0.95259000
C	-3.45334100	1.99172300	1.26921200
H	-3.09377800	2.53227400	2.14340600
C	3.45306000	1.99216300	-1.26890200
C	3.08624400	0.29618400	0.42355700
C	-4.34750500	0.60858400	-0.95274800
C	-5.16108800	1.59047400	-0.38867300
H	-6.13673800	1.80782600	-0.82200700
C	-4.70260600	2.28746100	0.73321300
H	-5.31755800	3.06237900	1.19183800
C	-2.61593400	0.99206100	0.72675200
H	4.68588100	0.05783600	1.82950700
O	0.28697800	-2.46564200	-1.33584000
H	3.09335000	2.53292800	-2.14290900
H	-4.68566900	0.05811700	-1.82983000

Table S2

Cis-E_{carb}

Mo	0.01763500	-1.86266300	0.79488300
S	-1.63445000	-3.28460700	-0.24316600
S	1.65696900	-0.14175100	0.29205500
S	-1.63469600	-0.16444400	0.26041000
S	1.70096400	-3.26641300	-0.21807200
O	5.80210200	1.75573400	-0.18414500
O	0.00761500	-2.13861200	2.48152300
O	-5.82039700	1.68364800	-0.39288700
N	3.56068500	2.09889000	-0.30152300
H	2.65142000	1.63762600	-0.23352200
N	-3.59981200	2.05133500	-0.12097900
H	-2.68676400	1.60841900	0.00079700
C	-4.66470700	1.22786800	-0.30450200
C	-5.49141500	-2.35482800	-0.97973500
H	-6.38758100	-2.90352100	-1.26693000
C	-5.54074300	-0.98268800	-0.79369800
H	-6.46287000	-0.42480800	-0.92545800
C	-3.16418700	-0.93579200	-0.22221300
C	-2.24063300	3.97064200	0.30202100
H	-1.60462900	3.72376600	-0.55490000
H	-1.80438900	3.49118100	1.18504600
H	-2.21445700	5.05612900	0.44934300
C	3.19551200	-0.89786300	-0.18626900
C	-4.28485800	-3.02630200	-0.79865900
C	4.35628700	-2.97117400	-0.74128100
H	4.30919800	-4.04935800	-0.88995100
C	-4.39780000	-0.24773400	-0.42818100
C	-3.12670100	-2.34261700	-0.41974100
C	4.41997700	-0.19289100	-0.37932400
C	-3.67578100	3.49923200	0.07448700
C	5.58149300	-0.90873700	-0.72114100
H	6.49785800	-0.33758600	-0.83661000
C	-4.52980700	3.83740900	1.29984100
H	-4.55837600	4.92385900	1.45459400
H	-4.10741900	3.37272900	2.19694400
H	-5.54846000	3.46734500	1.16304200
C	-4.25137500	4.17980100	-1.17011900
H	-3.63505800	3.95411100	-2.04656700
H	-4.27010200	5.26884000	-1.03306700
H	-5.26702700	3.82532200	-1.35869800
C	5.55540100	-2.28220300	-0.90568700
H	6.46350500	-2.81800300	-1.17950000
C	3.58283100	3.54503600	-0.07284000
C	4.65183400	1.28749300	-0.26200500
C	2.12663600	4.00353900	-0.12079500
H	1.53008100	3.50401500	0.65025200
H	1.67414400	3.77148900	-1.09092400
H	2.06195700	5.08554300	0.04017000
C	4.17834600	3.87024900	1.30031200
H	5.21439400	3.52922200	1.35623900
H	3.60477100	3.37368300	2.08966900
H	4.14911300	4.95269300	1.48033500
C	4.38327100	4.24636300	-1.17255100
H	3.94520200	4.03714600	-2.15434700
H	5.41682400	3.89249900	-1.17067700
H	4.37185900	5.33274400	-1.01485500
C	3.18206700	-2.30514800	-0.37891700
H	-4.21901800	-4.10346300	-0.94758300

Cis-TS1_{carb} (Cis attack)

Mo	-0.00296900	-0.74320400	-0.35621000
S	1.04299200	-1.93207200	1.77994700

S	-2.15686200	0.15313400	0.11334500
S	1.12799000	1.11306300	0.78655800
S	-1.24813700	-2.83600600	-0.33342300
O	-6.76445300	0.54234900	0.19524400
O	0.22278000	-0.45960400	-2.03807500
O	4.70053900	3.18429700	1.06288600
N	-4.76582500	1.60672700	0.11819200
H	-3.75149400	1.48525500	0.07298700
N	3.93882400	1.73226700	-0.54709300
H	3.40648200	0.86403200	-0.64697300
C	4.14900300	2.12026800	0.74998600
C	4.51060800	-0.54866800	3.37033300
H	5.25688900	-0.89906500	4.08312900
C	4.73180200	0.60905000	2.62907200
H	5.66662300	1.16249000	2.70083700
C	2.51596100	0.39035300	1.61411700
C	3.22280400	1.84081600	-2.82761200
H	2.28591100	1.34615700	-2.54140300
H	3.93251600	1.06018700	-3.12870400
H	3.03380700	2.48338000	-3.69553500
C	-3.41952300	-1.09191800	-0.11405300
C	3.35308100	-1.29892200	3.14481200
C	-3.89723600	-3.46186800	-0.45558000
H	-3.51809800	-4.47452200	-0.59058400
C	3.75738100	1.05578900	1.72457800
C	2.36807300	-0.87803400	2.23989700
C	-4.82388600	-0.83919400	-0.08922200
C	3.78668200	2.66569700	-1.67287400
C	-5.71832600	-1.91364600	-0.25105900
H	-6.77819900	-1.68061500	-0.22527900
C	5.14622400	3.25560200	-2.05017500
H	5.04497300	3.92896900	-2.91202100
H	5.84978700	2.45774700	-2.31723500
H	5.56213700	3.81401700	-1.20720200
C	2.80230500	3.78304300	-1.31866200
H	1.84234400	3.35076200	-1.01880100
H	2.64732100	4.43806100	-2.18579500
H	3.18328500	4.38223200	-0.48736800
C	-5.26672800	-3.21078700	-0.43315300
H	-5.97743700	-4.02726800	-0.55770200
C	-5.27662000	2.95991500	0.33957900
C	-5.52477200	0.48067900	0.09203400
C	-4.05957900	3.88221600	0.32214900
H	-3.53897300	3.82690600	-0.63965300
H	-3.34258100	3.60524800	1.10198500
H	-4.36843400	4.92017000	0.48914700
C	-6.24236900	3.36231100	-0.77844900
H	-7.10379500	2.69132600	-0.79555300
H	-5.74070600	3.31022200	-1.75056700
H	-6.59051800	4.39231600	-0.62530000
C	-5.97551600	3.05927600	1.69872900
H	-5.28175500	2.79048900	2.50192000
H	-6.83177100	2.38247600	1.73698900
H	-6.32256400	4.08622400	1.87252400
C	-2.97017800	-2.42661300	-0.30590000
H	3.21016500	-2.25269000	3.65323200
O	2.60822600	-1.00614900	-0.85707400
N	3.19509900	-2.18619800	-1.21765300
C	4.08837500	-2.64854400	-0.11041200
C	3.98741000	-1.95234600	-2.45772000
C	2.14726400	-3.22501100	-1.47753700
H	4.60544600	-3.57414000	-0.39401800
H	4.79469000	-1.84062000	0.08895400
H	3.44403600	-2.79340100	0.75989700
H	4.47966000	-2.87464700	-2.79167200
H	3.28876200	-1.57960000	-3.20807800
H	4.72241300	-1.17930000	-2.22561100
H	2.62042800	-4.14860600	-1.83330800
H	1.61801700	-3.37729000	-0.53301300
H	1.45274000	-2.80573500	-2.20749100

Cis-ES_{carb} (Cis Attack)

Mo	0.10880500	-0.57344200	-0.40238800
S	0.67511800	-1.32984200	2.28463200
S	-2.11571500	0.24790600	0.04807500
S	1.18488100	1.39615500	0.67980400
S	-1.06048400	-2.70624400	-0.41515100
O	-6.73498000	0.40405800	0.11647800
O	0.30805900	-0.25510300	-2.08367200
O	4.99104100	3.00968900	0.61908500
N	-4.79113700	1.56941300	0.07827100
H	-3.77100200	1.49582600	0.04623800
N	4.05121900	1.38835000	-0.71232000
H	3.35532800	0.64312400	-0.65444700
C	4.30458000	1.98702400	0.49725000
C	4.38087400	-0.22640700	3.52130200
H	5.09940300	-0.55772000	4.27165600
C	4.72950100	0.75807900	2.60184100
H	5.72910700	1.18854600	2.57484900
C	2.47340700	0.66879200	1.65268000
C	3.46705100	1.10689800	-3.01256200
H	2.46600100	0.77275500	-2.70759900
H	4.11154400	0.22146800	-3.10384400
H	3.39376600	1.57184100	-4.00269300
C	-3.30753600	-1.05360700	-0.19859800
C	3.12475100	-0.83453500	3.44470800
C	-3.67492600	-3.44040800	-0.58769500
H	-3.24580900	-4.43043500	-0.73898500
C	3.79109200	1.17163100	1.64176900
C	2.15852700	-0.43946100	2.50148800
C	-4.72489600	-0.87167100	-0.17736200
C	4.05165900	2.09225900	-2.00267200
C	-5.56571100	-1.98472300	-0.36562600
H	-6.63543900	-1.80158000	-0.34191300
C	5.48120900	2.46878500	-2.39156700
H	5.49212600	2.95374700	-3.37699600
H	6.11186800	1.57278800	-2.44163100
H	5.90914400	3.14920300	-1.65107800
C	3.16631800	3.33873200	-1.93570100
H	2.15277400	3.05697100	-1.63322900
H	3.12622400	3.83161900	-2.91596000
H	3.55866600	4.04698900	-1.20084400
C	-5.05529600	-3.25589800	-0.57132700
H	-5.72622800	-4.10182500	-0.71752800
C	-5.36791300	2.89193600	0.31961800
C	-5.49257000	0.40826400	0.02358500
C	-4.19626900	3.87171300	0.32551600
H	-3.66745600	3.85757100	-0.63338600
H	-3.47150800	3.61672100	1.10560200
H	-4.55582200	4.89083700	0.50675100
C	-6.34494300	3.26754400	-0.79781800
H	-7.17488900	2.55867500	-0.83141300
H	-5.83589300	3.25383400	-1.76748200
H	-6.74048200	4.27807700	-0.63086100
C	-6.07804400	2.93493400	1.67569300
H	-5.37696300	2.68516000	2.47855700
H	-6.90127500	2.21768300	1.69684000
H	-6.47445900	3.94115700	1.86429200
C	-2.80246600	-2.36620000	-0.40759400
H	2.87273900	-1.65519200	4.11605900
O	2.29647400	-1.11707200	-0.44134200
N	2.77997800	-2.37480900	-0.78031000
C	4.26115800	-2.24612900	-0.78746600
C	2.26770500	-2.75812800	-2.12808800
C	2.37034900	-3.39130200	0.23629400
H	4.72372400	-3.20565200	-1.04289700
H	4.52058900	-1.47371300	-1.51349800
H	4.55565200	-1.91265400	0.20941900

H	2.67690700	-3.73342000	-2.41454600
H	1.17571700	-2.77838900	-2.06016200
H	2.56569900	-1.97150600	-2.82229200
H	2.79918100	-4.36094400	-0.04238700
H	2.72046200	-3.04364600	1.20910800
H	1.27917000	-3.42296800	0.25896900

Cis-TS2_{carb} (Cis attack)

Mo	-0.18735700	-1.71158900	-0.62180500
S	0.71077000	-1.87499200	1.95319000
S	-1.72537600	0.03579500	0.11560000
S	1.73560500	0.10502800	-0.43413000
S	-2.04807100	-3.14327800	-0.10376900
O	-5.69373800	2.15993300	0.75039700
O	-0.17307400	-1.42065900	-2.31930600
O	5.27149100	2.45499700	0.55699600
N	-3.62288200	2.32103300	-0.17392500
H	-2.76987900	1.78814300	-0.36234200
N	3.11900800	2.78938000	-0.13206700
H	2.24511500	2.26805800	-0.21126400
C	4.07768900	2.11651600	0.57446100
C	3.84003600	0.01798800	3.65176000
H	4.35079900	-0.03894400	4.61254400
C	4.24381800	0.93584800	2.69288500
H	5.07563900	1.61473900	2.86173800
C	2.50210700	0.13410700	1.15133000
C	2.04237800	4.01558000	-1.88242500
H	1.45292800	4.60180600	-1.16810100
H	1.46595800	3.11879900	-2.13710500
H	2.17318600	4.61062900	-2.79346200
C	-3.35246700	-0.66390800	0.15267800
C	2.76074100	-0.81949400	3.38502300
C	-4.71517900	-2.69008900	0.20248800
H	-4.76242900	-3.77807500	0.16026900
C	3.57572900	1.02090200	1.46160900
C	2.06522700	-0.79189800	2.16181500
C	-4.54815900	0.10411700	0.28970200
C	3.40097800	3.63894000	-1.29536400
C	-5.78751000	-0.55219700	0.39697900
H	-6.66989900	0.07096800	0.51173200
C	4.21660400	2.86872100	-2.33872300
H	4.42563400	3.50306300	-3.21035600
H	3.66335400	1.98446000	-2.67134900
H	5.16612500	2.54188100	-1.90623600
C	4.14791700	4.90185600	-0.86615100
H	3.60722500	5.40668700	-0.05832200
H	4.23079700	5.59586800	-1.71308900
H	5.14793400	4.65354900	-0.50432300
C	-5.87784800	-1.93461100	0.35537000
H	-6.84657900	-2.42704500	0.43593100
C	-3.46278200	3.77121400	-0.04313800
C	-4.66335700	1.60300600	0.32806900
C	-2.08329400	4.10087300	-0.61260200
H	-2.00009200	3.77936300	-1.65659500
H	-1.29096000	3.59705100	-0.04833600
H	-1.90128100	5.18080500	-0.56948400
C	-4.54490900	4.49973100	-0.84267400
H	-5.53469300	4.23187300	-0.46555500
H	-4.48844700	4.22309000	-1.90099900
H	-4.40945400	5.58642100	-0.76262100
C	-3.52214000	4.19166100	1.42794300
H	-2.74119400	3.67925600	1.99887600
H	-4.49392300	3.93213800	1.85470500
H	-3.36655200	5.27431300	1.52180500
C	-3.46128200	-2.08289300	0.09768300
H	2.41824800	-1.52764800	4.13722400
O	0.84268700	-3.54513800	-0.82138000
N	2.32312200	-3.67829100	-1.10246500

C	3.12308200	-3.21005400	0.04823600
C	2.62702200	-2.89324700	-2.31365400
C	2.50810600	-5.11676000	-1.32667800
H	4.18579900	-3.40386200	-0.15187700
H	2.94162100	-2.14216000	0.16898500
H	2.76987700	-3.72620800	0.94069700
H	3.68214600	-3.02842400	-2.58466900
H	1.95875300	-3.22915300	-3.10678900
H	2.41499900	-1.84487800	-2.08559700
H	3.55792900	-5.33706200	-1.56219600
H	2.19943600	-5.63435700	-0.41821300
H	1.85532900	-5.41265500	-2.14823500

Dioxo_P carb (Cis/Trans) (Cis attack)

M o	1.48536800	-1.72622200	-0.59733900
S	1.44448700	-1.24451400	2.06030800
S	-1.03697600	-0.85876100	-0.52528400
S	1.78081000	0.76255000	-0.42533900
S	0.21214900	-3.82115200	-0.43162600
O	-5.42117600	-0.72983800	-0.35524600
O	1.69448800	-1.38731100	-2.29209900
O	0.63115900	4.80089400	0.15901400
N	-3.63682300	0.08654000	0.81377900
H	-2.63811300	-0.06738100	0.93930600
N	-0.28658700	3.00651000	-0.92491800
H	-0.30341200	1.99168100	-0.89309800
C	0.38378300	3.58862000	0.11328800
C	0.35620100	2.31416600	3.62965800
H	0.08490000	2.69394400	4.61405000
C	0.33768200	3.15782900	2.52411800
H	0.02669500	4.19702600	2.59958200
C	1.09742800	1.32066800	1.10192600
C	-0.89691000	2.43606900	-3.16826700
H	-1.88046700	2.08372300	-2.83844700
H	-0.21373000	1.57903100	-3.14139900
H	-0.98495000	2.77907300	-4.20510200
C	-2.09104500	-2.23817600	-0.30891000
C	0.67025500	0.96831000	3.46859300
C	-2.34713200	-4.67264700	-0.34198000
H	-1.87978000	-5.65382400	-0.40291400
C	0.66104300	2.65981000	1.25581400
C	1.04520500	0.43652700	2.22006600
C	-3.50108000	-2.13955200	-0.13458500
C	-0.38553200	3.56821400	-2.28115900
C	-4.29672600	-3.29205900	-0.13058900
H	-5.37106400	-3.15491700	-0.03809800
C	0.98954200	4.02366300	-2.77708500
H	0.91395100	4.38919400	-3.80896600
H	1.69426300	3.18627900	-2.75453500
H	1.38235100	4.82511300	-2.14669800
C	-1.36925600	4.73787200	-2.28090700
H	-2.35645300	4.40580600	-1.94146400
H	-1.47218700	5.15053400	-3.29289900
H	-1.01731400	5.52570800	-1.60977600
C	-3.73106300	-4.55552900	-0.23781500
H	-4.35673800	-5.44606100	-0.22632900
C	-4.03701500	1.50176100	0.86879800
C	-4.26108200	-0.86305000	0.06309900
C	-2.96050000	2.20596100	1.68635700
H	-1.96841400	2.04164100	1.25208800
H	-2.93369100	1.83629700	2.71721600
H	-3.13572300	3.28754100	1.70836500
C	-4.07736600	2.09256100	-0.54293100
H	-4.79715900	1.55457000	-1.16600200
H	-3.08607700	2.02308600	-1.00428600
H	-4.36175800	3.15167000	-0.50522700
C	-5.39793700	1.64674400	1.54852200
H	-5.37301600	1.20065900	2.54878000

H	-6.17652400	1.14856900	0.96673600
H	-5.64854500	2.71022000	1.65272900
C	-1.52206400	-3.54234800	-0.37007800
H	0.63990300	0.29130600	4.31997100
O	2.88646800	-2.69253700	-0.20859200
N	6.05218100	-0.45484500	0.28811500
C	5.04777900	-0.62452900	1.33376900
C	5.45581300	-0.68802900	-1.01985600
C	6.60795800	0.87851300	0.34693900
H	4.22562400	0.10966100	1.26045000
H	4.59173000	-1.61516200	1.26123200
H	5.52138500	-0.51773600	2.31721100
H	4.67943100	0.05906100	-1.27158200
H	6.23552200	-0.65027700	-1.79154300
H	4.97373800	-1.66884000	-1.03803800
H	5.84390100	1.67033800	0.19665400
H	7.07589800	1.04727300	1.32466000
H	7.37603900	1.00125900	-0.42749000

Dioxo carb (Cis/Trans)

Mo-	1.71708100	-2.20762700	-0.48215500
S	-1.29311200	-2.01213900	2.17520500
S	-0.88662800	0.33641100	-0.53014200
S	0.77443300	-2.46786300	-0.23279700
S	-3.83030600	-0.95161700	-0.38909800
O	-0.88648000	4.78410100	-0.52823100
O	-1.34673100	-2.44975900	-2.16641300
O	4.78773700	-1.12144100	0.39400700
N	0.06774800	3.02132000	0.55630600
H	-0.02228000	2.01436200	0.68767800
N	3.00614700	-0.42940500	-0.86093600
H	1.99217200	-0.48691000	-0.89965000
C	3.56649000	-0.95470500	0.26734500
C	2.17782300	-0.64731000	3.72164400
H	2.52066600	-0.27267100	4.68547500
C	3.05166600	-0.70323500	2.64178100
H	4.07810300	-0.35176900	2.71513300
C	1.28125900	-1.65068500	1.24690800
C	2.58627200	0.07999300	-3.15952100
H	2.14991000	1.04739400	-2.88778100
H	1.77213500	-0.65346800	-3.18333500
H	3.00840800	0.16376100	-4.16714100
C	-2.27837600	1.38179700	-0.37687100
C	0.84869700	-1.02435400	3.55643300
C	-4.71892000	1.59373100	-0.41815400
H	-5.69194400	1.10677800	-0.45262800
C	2.60184700	-1.15982900	1.39545500
C	0.36572200	-1.53017700	2.33505800
C	-2.20387800	2.80234400	-0.27894400
C	3.66910100	-0.33539200	-2.16710100
C	-3.37316000	3.57452900	-0.30807600
H	-3.25485300	4.65400900	-0.26826000
C	4.24856300	-1.69290500	-2.57492000
H	4.70586300	-1.62493300	-3.57027200
H	3.45566700	-2.44706600	-2.60572000
H	5.00721000	-2.01562200	-1.85771300
C	4.77183300	0.72234200	-2.11072800
H	4.35506900	1.69153600	-1.81503100
H	5.24268400	0.83418400	-3.09601400
H	5.53355000	0.43668300	-1.38111500
C	-4.62615200	2.98283400	-0.38144100
H	-5.52742700	3.59311300	-0.39497600
C	1.43698500	3.54665900	0.63356200
C	-0.94883400	3.61002100	-0.12748100
C	2.25468800	2.48531000	1.36085900
H	2.24754800	1.53995900	0.80832600

H	1.85396700	2.28374600	2.36034700
H	3.29861300	2.80422900	1.46248300
C	2.00327500	3.75811100	-0.77324400
H	1.40331900	4.48778700	-1.32307100
H	1.99585700	2.81046600	-1.32343900
H	3.03994400	4.11411400	-0.71805500
C	1.45416400	4.85913600	1.41840400
H	1.06065800	4.70134100	2.42839300
H	0.83966200	5.61226700	0.91912800
H	2.48356300	5.23023100	1.50481000
C	-3.57479400	0.78827100	-0.40854800
H	0.14652000	-0.94038600	4.38365100
O	-2.66581000	-3.60687600	-0.06855600

Trans-E_{carb}

Mo	-0.02129100	-0.02543200	0.81599700
S	-2.31277300	-0.25247300	0.03654900
S	2.29055100	0.23585300	0.11701700
S	-0.35429100	2.23878200	0.03223800
S	0.34216400	-2.24538600	-0.06748200
O	6.68875700	-0.98192800	-0.65996800
O	-0.04482300	-0.06447800	2.52451700
O	-6.59229800	0.89856800	-1.03368200
N	5.24433700	0.65687800	-0.06092500
H	4.26550500	0.89086300	0.11980300
N	-5.30749700	-0.54257300	0.16376400
H	-4.34307800	-0.73975800	0.43863800
C	-5.50418500	0.63371400	-0.49256700
C	-4.79783100	2.94155100	-0.75881500
H	-5.85484600	3.09276500	-0.95726200
C	-3.89880200	3.99616700	-0.77916100
H	-4.24197000	5.00851000	-0.98926300
C	-2.08946900	2.45894400	-0.25244400
C	-5.52525300	-2.82087800	0.86192000
H	-5.35535900	-2.53299100	1.90494400
H	-4.55319000	-3.06710100	0.42166500
H	-6.14813600	-3.72227000	0.84966100
C	2.99510400	-1.36067900	-0.23034900
C	-4.37872300	1.62825600	-0.48067800
C	2.55093100	-3.72732200	-0.63754300
H	1.82422200	-4.53592800	-0.70697600
C	-2.55138600	3.74963800	-0.52584400
H	-1.82590800	4.56226900	-0.53864700
C	-2.99994400	1.36903300	-0.22933800
C	4.38285300	-1.60922300	-0.45768300
C	-6.20907200	-1.69520000	0.08911900
C	4.80398000	-2.91600200	-0.76766700
H	5.86697900	-3.06404300	-0.93023600
C	-6.41769400	-2.12508800	-1.36613400
H	-7.06312400	-3.01164300	-1.41379500
H	-5.45643000	-2.37206800	-1.82868800
H	-6.88106400	-1.31680400	-1.93651600
C	-7.55402300	-1.36589900	0.74035300
H	-7.40772000	-1.06363100	1.78305100
H	-8.20652200	-2.24882800	0.72651400
H	-8.04418500	-0.54808900	0.20796500
C	3.90506700	-3.96559300	-0.86062700
H	4.25373900	-4.96863500	-1.10403900
C	6.22688400	1.73746900	0.01892900
C	5.52205300	-0.62758500	-0.40475500
C	5.44896800	2.99024500	0.41681100
H	4.95422200	2.85571400	1.38439500
H	4.67370400	3.22301400	-0.32064700
H	6.12547000	3.84899600	0.49134400
C	7.28474400	1.43147900	1.08302200
H	7.83426200	0.52421000	0.82355500
H	6.81052900	1.28480000	2.05900600

H	7.99114900	2.26793300	1.16537400
C	6.89833500	1.95980500	-1.33935400
H	6.14758700	2.20248700	-2.09855500
H	7.42979300	1.05798300	-1.65114000
H	7.60973300	2.79380000	-1.27876700
C	2.08537400	-2.44938200	-0.31939400

Trans-TS1_{carb} (Cis Attack)

Mo	0.22372000	-0.23823500	1.28742500
S	-1.36198100	-0.04378800	-0.84837200
S	2.40636600	0.15486200	0.38030900
S	-0.15809100	2.26294400	1.00659200
S	0.57279400	-2.45608000	0.40609900
O	6.68202700	-0.68493100	-0.68136900
O	0.52023100	-0.37081400	2.97763700
O	-5.25661200	1.06221600	-2.78289400
N	4.97258600	0.76698300	-1.08154600
H	3.96955500	0.88208500	-0.93171600
N	-4.26879400	-0.51617000	-1.46051400
H	-3.36343700	-0.69879500	-1.00830600
C	-4.37646400	0.74792800	-1.96370000
C	-3.98433900	3.06797500	-1.34866200
H	-4.93110100	3.22384500	-1.85928600
C	-3.32950700	4.10101700	-0.69199600
H	-3.74812700	5.10698000	-0.68800800
C	-1.59024500	2.54536900	0.02615000
C	-4.37783000	-2.88656500	-1.23398800
H	-4.61852700	-2.77366000	-0.17057900
H	-3.28751800	-2.96019600	-1.31107600
H	-4.81843400	-3.82311700	-1.59475300
C	3.11014100	-1.40533700	-0.12201000
C	-3.45575400	1.76586700	-1.35718900
C	2.80595000	-3.80931000	-0.39321000
H	2.14346800	-4.67299500	-0.34252600
C	-2.15216500	3.82843000	0.00478500
C	-2.19684800	1.49359700	-0.73856600
C	4.45466300	-1.55893300	-0.56397700
C	-4.90999300	-1.70005200	-2.03605300
C	4.95031200	-2.83894200	-0.86511700
H	5.99191400	-2.91267200	-1.16585900
C	-4.53251300	-1.85688400	-3.51240400
H	-4.98152400	-2.76783400	-3.92947100
H	-3.44509500	-1.92654600	-3.61779500
H	-4.88310100	-0.99437900	-4.08545000
C	-6.42907900	-1.60742900	-1.88600000
H	-6.70044300	-1.49969300	-0.82943100
H	-6.90453000	-2.51923900	-2.27150500
H	-6.81177400	-0.74177500	-2.43162300
C	4.13504600	-3.95823700	-0.78505100
H	4.52681000	-4.94412900	-1.03381600
C	5.74952700	2.01033700	-1.01588000
C	5.46131200	-0.46349200	-0.75235100
C	4.75849600	3.14314000	-1.27502100
H	3.95556400	3.14504200	-0.52983700
H	4.29597000	3.03969300	-2.26227700
H	5.27065300	4.11119600	-1.23408000
C	6.37415600	2.18255800	0.37217300
H	7.06924000	1.36571400	0.58166300
H	5.59326200	2.18084200	1.13950200
H	6.91769500	3.13463000	0.43044100
C	6.83675600	2.01890200	-2.09131500
H	6.39070400	1.89670600	-3.08419700
H	7.54325900	1.20280000	-1.92667100
H	7.37808300	2.97419700	-2.07230800
C	2.28191500	-2.55785100	-0.05317100
O	-1.99898500	-0.95156700	2.04677500
N	-2.83683800	-0.21681700	-2.85302800
C	-3.68521200	0.69588200	2.02597700

C	-2.07902200	0.60227900	3.85117500
C	-3.70509500	-1.19043000	3.56910300
H	-4.43952600	1.18533300	2.65344100
S	2.12221500	1.43167100	1.57600500
H	-4.14400700	0.09379300	1.23890600
H	-2.79138800	1.10470300	4.51687100
H	-1.40780700	-0.06939600	4.38403500
H	-1.47622800	1.32224100	3.29040400
H	-4.41665600	-0.67136600	4.22334100
H	-4.22560600	-1.77219300	2.80803100
H	-3.04690800	-1.84439900	4.14079400
H	-1.65322900	4.61365400	0.57103400

Trans-ES_{carb} (Cis Attack)

Mo	0.19075200	1.88556300	-0.01115100
S	-1.50974900	-0.26917300	0.30873000
S	2.12221500	0.47489400	-0.31844900
S	-0.52324800	1.16043000	-2.40970900
S	0.67288400	1.57268300	2.31983200
O	6.23277400	-1.17121300	0.49083900
O	0.77939700	3.43859500	-0.45439600
O	-5.06368200	-3.02551200	-0.44153800
N	4.32968700	-1.53737100	-0.70362200
H	3.36498900	-1.21578500	-0.79938200
N	-3.30869000	-2.56768100	0.92971800
H	-2.50227900	-1.93991500	1.03404100
C	-3.96382600	-2.46765900	-0.25733400
C	-3.80082500	-2.00857300	-2.63143900
H	-4.59964900	-2.74263700	-2.67774100
C	-3.30690200	-1.40194800	-3.77523100
H	-3.70184600	-1.66502900	-4.75606600
C	-1.76927800	-0.08114700	-2.41342700
C	-2.84756100	-2.88096500	3.25514800
H	-2.58582600	-1.82253200	3.35944700
H	-1.92728600	-3.42496200	3.01849300
H	-3.22532100	-3.24257800	4.21849700
C	2.92260800	0.27515400	1.25981000
C	-3.28675500	-1.70093400	-1.35802400
C	2.88394300	0.71143700	3.66108300
H	2.35427400	1.12123900	4.52078900
C	-2.30357600	-0.44271700	-3.65794600
C	-2.23526800	-0.73498400	-1.21783100
C	4.18180400	-0.36884100	1.43340000
C	-3.89753700	-3.08613900	2.16452900
C	4.77311500	-0.41838300	2.70796500
H	5.74856000	-0.89067600	2.78596900
C	-4.21305900	-4.57716700	2.02815500
H	-4.60604200	-4.96840900	2.97610200
H	-3.30489200	-5.13502000	1.77617600
H	-4.94958900	-4.73905100	1.23826800
C	-5.16949300	-2.31033000	2.52328600
H	-4.93973300	-1.24584400	2.64249000
H	-5.59205600	-2.68099600	3.46647300
H	-5.91426300	-2.42130300	1.73120400
C	4.13270500	0.11222900	3.81711700
H	4.59607200	0.05501200	4.80165700
C	4.96381700	-1.98823300	-1.94688100
C	5.00369600	-1.03131000	0.36669600
C	3.82509000	-2.30707500	-2.91327700
H	3.20189600	-1.42516400	-3.09643500
H	3.17790200	-3.09295900	-2.50980900
H	4.22827400	-2.65086800	-3.87257000
C	5.84191500	-0.88021300	-2.53705000
H	6.65015200	-0.62593100	-1.84721800
H	5.24333200	0.01827500	-2.71902600
H	6.27818700	-1.20636400	-3.49015200
C	5.79723600	-3.24597900	-1.69565700

H	5.16985500	-4.04177700	-1.27986700
H	6.60255000	-3.03393300	-0.98901400
H	6.22917300	-3.60599400	-2.63870500
C	2.27356700	0.80770700	2.40756500
O	-1.68394400	2.90362500	0.71531800
N	-2.68193100	3.42704200	-0.11567000
C	-3.50979100	2.33614400	-0.71224700
C	-2.07553300	4.24994100	-1.20216900
C	-3.52436800	4.27616400	0.76057600
H	-4.36620900	2.77688900	-1.23668800
H	-2.87200200	1.78543400	-1.40363400
H	-3.81741500	1.67643600	0.09955200
H	-2.87237200	4.75516900	-1.76107300
H	-1.38891600	4.95283300	-0.73094400
H	-1.50946900	3.56854300	-1.84434200
H	-4.34452700	4.72438300	0.18761500
H	-3.90603800	3.63610200	1.55581100
H	-2.87840200	5.04238500	1.18925900
H	-1.91046700	0.05508900	-4.54299500

Trans-TS2_{carb} (Cis Attack)

Mo	0.18404100	1.93449200	-0.13305900
S	-1.40776000	-0.32296400	0.28974300
S	2.10843800	0.44336700	-0.34957900
S	-0.55765300	1.08058600	-2.49307600
S	0.71577500	1.78829000	2.21043300
O	6.20603900	-1.18556100	0.54038300
O	0.82240200	3.40867900	-0.74187200
O	-5.03597600	-3.03896900	-0.28340200
N	4.28923100	-1.61516600	-0.60911500
H	3.32556500	-1.29480400	-0.71698300
N	-3.27859800	-2.51908800	1.06074000
H	-2.46286400	-1.89726900	1.12820100
C	-3.92939500	-2.48352400	-0.13287400
C	-3.79553100	-2.13546800	-2.52532200
H	-4.60048700	-2.86426400	-2.52548400
C	-3.33008200	-1.57128700	-3.70104000
H	-3.74740400	-1.86988000	-4.66224500
C	-1.76940500	-0.19314700	-2.42410800
C	-2.84085000	-2.69416400	3.40575300
H	-2.55234900	-1.63856000	3.44507000
H	-1.93410100	-3.27592600	3.21016600
H	-3.23354800	-2.98447700	4.38712200
C	2.92174800	0.36032100	1.22430100
C	-3.25245200	-1.78229700	-1.27556000
C	2.92074200	0.98637600	3.58534500
H	2.40976100	1.47554300	4.41399000
C	-2.33236200	-0.60050000	-3.64093700
C	-2.19183600	-0.81810200	-1.19479700
C	4.17372300	-0.28949000	1.43699000
C	-3.88929300	-2.94018700	2.32236800
C	4.77789500	-0.24918500	2.70526900
H	5.74705800	-0.72909600	2.80887700
C	-4.24699300	-4.42754200	2.28158600
H	-4.64945200	-4.74565600	3.25272000
H	-3.35516500	-5.02599000	2.06685600
H	-4.98829400	-4.61984900	1.50301500
C	-5.14059300	-2.10668300	2.61893100
H	-4.88033400	-1.04370400	2.66970100
H	-5.57976500	-2.40204100	3.58096000
H	-5.88249500	-2.24811400	1.82907100
C	4.16003200	0.37735100	3.77648700
H	4.63348900	0.38937500	4.75768200
C	4.90662800	-2.14834500	-1.82810000
C	4.97751500	-1.03999200	0.41616600
C	3.75412700	-2.51356900	-2.76126700
H	3.13605200	-1.63817200	-2.98810700

H	3.10486600	-3.26846500	-2.30536600
H	4.14246200	-2.91644100	-3.70341400
C	5.78870400	-1.08690900	-2.49243300
H	6.60287300	-0.79651600	-1.82385300
H	5.19526100	-0.19713200	-2.72651300
H	6.21602900	-1.47580900	-3.42585900
C	5.72991000	-3.39746000	-1.50963300
H	5.10134700	-4.15459400	-1.02854200
H	6.55301600	-3.15176900	-0.83515400
H	6.13745400	-3.82543500	-2.43508400
C	2.29780400	0.99485500	2.33480500
O	-1.55660700	2.88241900	0.60512000
N	-2.72210000	3.34625400	-0.22343800
C	-3.51273400	2.19013800	-0.69778600
C	-2.20254700	4.13729100	-1.35596700
C	-3.50041600	4.17416600	0.70689500
H	-4.44994700	2.55017400	-1.14296500
H	-2.91677000	1.65855000	-1.43969600
H	-3.69096000	1.53132500	0.15288100
H	-3.04232900	4.56978000	-1.91548000
H	-1.54485600	4.90705100	-0.95175500
H	-1.61916400	3.45920400	-1.98749500
H	-4.38499200	4.58771900	0.20453200
H	-3.79333000	3.54135400	1.54498000
H	-2.84947100	4.97043800	1.06838900
H	-1.97030000	-0.12611500	-4.55168200

Dioxo_P carb (Trans/Trans) (Cis Attack)

Mo	1.50405500	-2.07679900	-0.86592700
S	0.96577200	0.53905700	-0.86478100
S	-0.85932000	-2.20779800	0.38604500
S	0.21765600	-1.77726200	-2.96045700
S	2.08762700	-1.59297200	1.50879900
O	-4.13331800	-0.94603000	3.03295100
O	1.33994100	-3.78028600	-1.16884000
O	-0.92919500	4.42694100	-1.71589000
N	-3.39746000	-0.59532700	0.89957300
H	-2.56721700	-0.72091700	0.32091900
N	-0.62321200	2.95383800	0.00253800
H	-0.35467200	1.98504900	0.17503900
C	-0.79611800	3.26084100	-1.31188700
C	-1.74431300	2.31504900	-3.35092300
H	-2.20581000	3.29546800	-3.43652200
C	-1.97058400	1.32023400	-4.29244800
H	-2.63201700	1.49794600	-5.13875100
C	-0.49150100	-0.17138500	-3.06133100
C	0.10188500	3.05703300	2.27718000
H	0.84266400	2.27047000	2.08751300
H	-0.81719900	2.56563200	2.61433400
H	0.47309700	3.68911100	3.09187400
C	-0.67108900	-1.34035400	1.88809500
C	-0.90781400	2.09423100	-2.24942800
C	0.81786900	-0.64165800	3.70194000
H	1.83246900	-0.53021400	4.08060800
C	-1.35195100	0.08124500	-4.13609700
C	-0.22822600	0.84882700	-2.10021800
C	-1.76681400	-0.87048300	2.66968500
C	-0.14407200	3.89472900	1.02469600
C	-1.55267600	-0.37058700	3.96050300
H	-2.42798700	-0.06539000	4.52822000
C	-1.20252100	4.96249700	1.29844200
H	-0.85776000	5.63950900	2.09091200
H	-2.13822200	4.49771900	1.62624300
H	-1.40046600	5.54165700	0.39343600
C	1.16528600	4.54900400	0.57241600
H	1.92309300	3.78364900	0.37542700
H	1.54449200	5.22016900	1.35378900
H	1.00875100	5.12720900	-0.34225700
C	-0.27149900	-0.26190700	4.48391000

H	-0.11413000	0.13943600	5.48353900
C	-4.67021000	-0.79014000	0.19386800
C	-3.19855100	-0.84220400	2.22294700
C	-4.36491100	-0.57960700	-1.28709100
H	-3.62614000	-1.30617300	-1.64472900
H	-3.95781300	0.42024200	-1.46964800
H	-5.27713800	-0.69421000	-1.88339800
C	-5.19416400	-2.21241200	0.41889100
H	-5.39160600	-2.38398500	1.48042500
H	-4.45646900	-2.94636700	0.07870700
H	-6.12417800	-2.36756500	-0.14334200
C	-5.70070200	0.23299100	0.67198800
H	-5.33322800	1.25102800	0.50640300
H	-5.89708600	0.10282100	1.73894200
H	-6.63896500	0.10949400	0.11554300
C	0.64235300	-1.16970500	2.41762600
O	3.19308700	-1.74482600	-1.16032400
N	5.72275400	0.79665200	0.24100500
C	6.42960600	1.73321700	1.07843200
C	5.66487400	-0.51184000	0.86857400
C	4.37622000	1.26924800	-0.04623500
H	5.94079100	1.88585300	2.06701900
H	7.45183900	1.37888400	1.26416000
H	6.48857200	2.71037000	0.58398700
H	5.17350900	-0.48033800	1.86186200
H	5.08337900	-1.19278300	0.24010400
H	6.68090200	-0.90717900	0.99684600
H	3.77266200	1.40994200	0.87319500
H	4.42122800	2.22606400	-0.57921700
H	3.85011000	0.54003900	-0.66752700
H	-1.52850100	-0.71719100	-4.85463900

Dioxo carb (Trans/Trans)

Mo	3.05353100	0.01475800	-0.06562700
S	0.95372800	-1.08706100	-1.31043300
S	1.10353200	1.24032700	1.32231700
S	2.55154400	-1.97047500	1.33926100
S	2.47657800	1.96974800	-1.49309100
O	-2.82855200	3.13234200	1.98002700
O	4.14342500	0.46792400	1.21182800
O	-2.85958700	-3.19891200	-1.92495300
N	-1.87477000	1.05814800	1.92160400
H	-1.02214000	0.58937500	1.61467100
N	-2.05413200	-1.06749200	-1.76763800
H	-1.22934700	-0.55552600	-1.45413800
C	-2.04763100	-2.38978900	-1.44711900
C	-1.50073900	-3.84304600	0.43489400
H	-2.47557800	-4.27330300	0.21990900
C	-0.72326100	-4.29532800	1.49243900
H	-1.07985800	-5.09472200	2.13989500
C	0.99535700	-2.67091700	0.91312700
C	-2.27784600	0.96503600	-3.00554500
H	-1.18736200	1.06640700	-3.05721900
H	-2.61239000	1.49812800	-2.10915300
H	-2.71041200	1.46034900	-3.88252500
C	0.24529500	2.23979000	0.17820400
C	-1.06098500	-2.80331900	-0.39517200
C	0.33782100	3.57849800	-1.87071500
H	0.88099700	3.86298100	-2.77025800
C	0.51108200	-3.69572800	1.73391800
C	0.22906000	-2.22545600	-0.20421800
C	-1.06246600	2.76253800	0.40364000
C	-2.69440800	-0.50220600	-2.96331100
C	-1.59971000	3.72378500	-0.46334600
H	-2.58526000	4.11482700	-0.22293100
C	-4.21507900	-0.61465600	-2.85552100
H	-4.68792500	-0.15385600	-3.73280600
H	-4.57335900	-0.09597900	-1.96012600
H	-4.51588000	-1.66293600	-2.79557500
C	-2.19680400	-1.22341000	-4.22021800

H	-1.10757900	-1.14277300	-4.29530100
H	-2.64298800	-0.77557600	-5.11776300
H	-2.46573700	-2.28256500	-4.18504400
C	-0.90566600	4.14145800	-1.59075200
H	-1.33834400	4.87701800	-2.26685900
C	-2.45119900	0.51807700	3.15908700
C	-1.97596100	2.35433200	1.52131600
C	-1.91549300	-0.90630300	3.28244100
H	-0.82025300	-0.91269900	3.33232900
H	-2.20748300	-1.51632800	2.42066700
H	-2.30347000	-1.38232800	4.19031200
C	-2.00112200	1.35258400	4.36311700
H	-2.35519800	2.38251800	4.26687700
H	-0.90818100	1.36484800	4.42760800
H	-2.40022600	0.92671100	5.29292200
C	-3.97706400	0.50346500	3.06654600
H	-4.30074800	-0.09758100	2.21038900
H	-4.35903000	1.51993400	2.94289000
H	-4.40445000	0.06525300	3.97794700
C	0.91861400	2.63429500	-1.01676100
O	4.09298500	-0.44932300	-1.38048200
H	1.12315900	-4.01566900	2.57535400

Table S3

Cis-ES_{carb} (Trans Attack)

Mo	-0.59015600	-1.79852300	-1.45878700
S	0.40300500	-3.34837500	0.11948300
S	-1.67205400	0.37956800	-1.60369700
S	1.45146800	-0.55592900	-0.96646600
S	-2.81058100	-2.51453100	-0.71454000
O	-3.68941700	3.76482500	-0.48824900
O	-0.44057100	-2.41862800	-3.04153400
O	5.69335900	0.39871000	0.56573900
N	-2.00319100	2.62234900	0.57532900
H	-1.66118500	1.66753600	0.74293400
N	3.79060300	1.20376600	-0.36814400
H	2.83970200	0.97005400	-0.66487000
C	4.50448300	0.22090100	0.23837500
C	4.08879500	-3.16272200	1.76822600
H	4.69261400	-3.80241600	2.41068100
C	4.56447800	-1.92684700	1.36275500
H	5.54176900	-1.56746200	1.67032700
C	2.51854200	-1.50526300	0.08400100
C	3.19327300	3.22764800	-1.49429800
H	2.35087700	3.38051900	-0.81210600
H	2.82030000	2.65830900	-2.35264600
H	3.53094700	4.20777100	-1.84926300
C	-3.20175400	0.23017700	-0.73399800
C	2.82455700	-3.57607000	1.34973300
C	-5.06120700	-1.12702400	0.04311800
H	-5.49682700	-2.11536400	0.19163700
C	3.80579800	-1.07825100	0.53544600
C	2.03656400	-2.77151600	0.52375300
C	-3.86876500	1.37117800	-0.23136500
C	4.33649200	2.49200300	-0.79997200
C	-5.15901000	1.26512200	0.30628100
H	-5.64958800	2.17088800	0.65904900
C	5.49115300	2.28632500	-1.78512900
H	5.87373500	3.25638600	-2.12807300
H	5.14689500	1.72399400	-2.65938800
H	6.30143000	1.72931400	-1.30938500
C	4.81412200	3.30235700	0.40813300
H	3.98768100	3.46303600	1.10880700
H	5.18558900	4.28330200	0.08414700
H	5.61352400	2.77003100	0.92841300
C	-5.76792000	0.01839200	0.41856300
H	-6.77041500	-0.07117400	0.83638200
C	-0.94913100	3.64535900	0.51186100
C	-3.18382200	2.69912600	-0.10757300
C	0.28252100	3.04097800	1.18376700
H	0.57740200	2.10056600	0.69921400
H	0.08477100	2.81963100	2.24024900
H	1.11986900	3.74829500	1.14032500
C	-0.61552200	3.97922700	-0.94468900
H	-1.49307000	4.38709700	-1.45369300
H	-0.30350000	3.07092700	-1.47135400
H	0.19583100	4.71795400	-0.98956400
C	-1.39350500	4.90337500	1.25993600
H	-1.62540800	4.66388900	2.30484600
H	-2.28921600	5.32390300	0.79553700
H	-0.59391300	5.65603700	1.24857600
C	-3.77066700	-1.04615500	-0.49657800
N	-1.12514400	-0.54580900	2.56458600
C	0.24784700	-0.88900500	3.05023100
C	-1.98202800	-1.77293900	2.58275900
C	-1.74416500	0.49141700	3.44219600
H	0.21730800	-1.24933300	4.08612900
H	0.63455600	-1.65528100	2.37509500
H	0.85455400	0.01370100	2.95837800
H	-2.08098900	-2.14765200	3.60972200

H	-2.94792900	-1.49114700	2.15857100
H	-1.50669200	-2.50457300	1.92551600
H	-1.11047000	1.37874900	3.39713000
H	-2.72099800	0.72493100	3.01401300
H	-1.83955600	0.12878400	4.47335500
O	-1.03400400	-0.06699200	1.29173400
H	2.41995800	-4.53715400	1.66675400

Cis-TS1'_{carb} (Trans Attack)

Mo	-0.43105300	-1.72952900	-1.17012200
S	0.88817300	-3.32317800	0.10115800
S	-1.80507500	0.28299400	-1.38212100
S	1.60718200	-0.35924800	-0.84957600
S	-2.62320700	-2.78991100	-0.64732700
O	-4.44266000	3.32916400	-0.34677900
O	-0.26882000	-2.21161200	-2.80127800
O	5.72985100	0.92949900	0.71426000
N	-2.52350000	2.46924800	0.57586500
H	-2.00911400	1.58467900	0.63825400
N	3.98062600	1.42782400	-0.64536800
H	3.07902100	1.08275600	-0.98503900
C	4.68524900	0.56845700	0.13996900
C	4.76786300	-3.01893900	1.18680900
H	5.50285300	-3.67956300	1.64488900
C	5.09046200	-1.70395600	0.89449100
H	6.06559800	-1.29215600	1.13738100
C	2.86137200	-1.31789500	-0.05126100
C	3.04938800	3.43756700	-1.54863900
H	2.05801700	3.15416800	-1.17787400
H	3.14373600	3.05227700	-2.56966300
H	3.10195200	4.53163100	-1.58547300
C	-3.37022200	-0.09867100	-0.62070000
C	3.48134100	-3.48013600	0.91059300
C	-5.04163100	-1.70770100	0.06307400
H	-5.34024200	-2.74740600	0.19499000
C	4.16480200	-0.83390900	0.28880700
C	2.52570100	-2.65417800	0.31699600
C	-4.21328200	0.93765800	-0.16583100
C	4.15508900	2.88256800	-0.65161600
C	-5.49854100	0.64701800	0.31210400
H	-6.12990700	1.47159100	0.63609300
C	5.52316100	3.26204400	-1.22106900
H	5.62623400	4.35440700	-1.26223300
H	5.63446200	2.86805100	-2.23710400
H	6.31942800	2.84705200	-0.59944800
C	3.99572800	3.44345300	0.76495400
H	3.01694000	3.16577100	1.17130100
H	4.06744900	4.53873000	0.75508400
H	4.77118900	3.04168900	1.42154800
C	-5.91816900	-0.67684300	0.40138600
H	-6.91460700	-0.91286600	0.77435700
C	-1.64671200	3.64466100	0.42894900
C	-3.74452900	2.35600900	-0.03155000
C	-0.28207000	3.23104900	0.97761600
H	0.07397200	2.31100200	0.49294700
H	-0.32845400	3.04659100	2.05807400
H	0.45220100	4.02705700	0.80672100
C	-1.49766000	4.02518700	-1.04729700
H	-2.46702900	4.29529900	-1.47515900
H	-1.09412700	3.17864100	-1.61235100
H	-0.81467700	4.87844700	-1.15012600
C	-2.20780200	4.82061200	1.22745300
H	-2.30893900	4.55063200	2.28509400
H	-3.19301000	5.10165200	0.84654800
H	-1.53402300	5.68441500	1.15510900
C	-3.75027400	-1.45077700	-0.42586200
N	-0.82424900	-0.73995700	2.41775000
C	0.60117800	-0.63465000	2.66860100

C	-1.37645300	-2.06966200	2.61204600
C	-1.61531800	0.27632800	3.07793200
H	0.82259100	-0.72286200	3.74783400
H	1.11718800	-1.42791100	2.12391500
H	0.95528300	0.32827200	2.28987000
H	-1.37706600	-2.33435400	3.68612000
H	-2.39611700	-2.08222900	2.21896100
H	-0.78003700	-2.78869400	2.04598300
H	-1.19298300	1.26087500	2.86612400
H	-2.63301900	0.24219200	2.67671000
H	-1.63837100	0.11458400	4.17093200
O	-1.10313500	-0.29291700	0.65274900
H	3.19059600	-4.49932200	1.16352800

Cis-INT1_{carb} (Trans Attack)

Mo	-0.24889900	-1.84352400	-1.39865900
S	0.63400200	-3.22681600	0.37759300
S	-2.76289200	0.20451500	-1.98676100
S	1.62222200	-0.44104700	-0.75167800
S	-2.48268600	-2.83397500	-0.76185500
O	-4.62758400	3.08090600	0.15585700
O	0.13344900	-2.52308500	-2.91458800
O	5.64578300	0.80831600	1.07994000
N	-2.46639700	2.32264300	0.32459600
H	-1.90278400	1.47601100	0.31646000
N	4.13349100	1.17548000	-0.57163500
H	3.25120600	0.84773800	-0.96901300
C	4.65376900	0.42394500	0.43523800
C	4.32405100	-2.95709100	1.99744000
H	4.94100400	-3.57654900	2.64681500
C	4.77845300	-1.71843000	1.57373800
H	5.74134500	-1.32969200	1.89098100
C	2.73131500	-1.36397000	0.28591000
C	3.56434800	3.03394800	-1.96478800
H	2.50956700	2.93503800	-1.68661700
H	3.72821100	2.43369100	-2.86627600
H	3.75910100	4.08418900	-2.20854200
C	-3.56114700	-0.26512300	-0.51239600
C	3.06378700	-3.39536100	1.59859100
C	-4.51976300	-2.00786800	0.86361300
H	-4.58845100	-3.06045300	1.13406900
C	4.00634800	-0.90207700	0.72804000
C	2.26028900	-2.61932900	0.75909800
C	-4.20766600	0.70372300	0.29413500
C	4.47942300	2.57588900	-0.83074500
C	-5.12625400	0.30462300	1.26403800
H	-5.65151400	1.06278500	1.84140600
C	5.94092400	2.69993800	-1.26576900
H	6.17165200	3.74370800	-1.51548800
H	6.12690200	2.08522700	-2.15305900
H	6.60600000	2.36539600	-0.46693600
C	4.22233100	3.42821900	0.41526700
H	3.17140700	3.35399200	0.71484100
H	4.44857800	4.48253100	0.21123500
H	4.84614700	3.08453600	1.24383100
C	-5.30977400	-1.06205900	1.50990900
H	-6.02915100	-1.38694000	2.26097500
C	-1.73421700	3.54785600	-0.02183100
C	-3.81454600	2.14829200	0.21294000
C	-0.25193900	3.18554400	0.04154400
H	-0.02247600	2.35380200	-0.63592100
H	0.03314000	2.86968400	1.05165300
H	0.35969200	4.05182500	-0.23685100
C	-2.09708900	3.99264500	-1.44035900
H	-3.16236800	4.22975400	-1.50825100
H	-1.87744500	3.18884300	-2.14999100
H	-1.51708500	4.88208100	-1.71754100
C	-2.05649800	4.65312300	0.98474000

H	-1.78508400	4.33789200	1.99876400
H	-3.12473100	4.88398600	0.96681500
H	-1.48912800	5.56137700	0.74397200
C	-3.59695200	-1.63870900	-0.13543500
N	-0.83272700	0.48181800	2.44065700
C	0.55371000	0.14572700	2.69034500
C	-1.67237900	-0.69761300	2.53285800
C	-1.29184700	1.51208900	3.33960000
H	0.72484100	-0.17105700	3.74239500
H	0.85364000	-0.67263000	2.03203000
H	1.20053200	1.00614900	2.47846400
H	-1.62847600	-1.16156900	3.54245000
H	-2.71311300	-0.43090200	2.32489200
H	-1.34856300	-1.44745500	1.80178300
H	-0.66382500	2.40658000	3.23856800
H	-2.32344300	1.79012600	3.09392100
H	-1.25704400	1.19463900	4.40703300
O	-1.10794600	-0.01161800	-1.60786700
H	2.67291600	-4.35246200	1.94160600

Cis-TS2'_{carb} (Trans Attack)

Mo	-0.27763800	-1.79618700	-1.42267800
S	0.57783200	-3.21243200	0.36401600
S	-2.83007600	0.24212400	-2.01250300
S	1.59209900	-0.40766700	-0.70117300
S	-2.51069300	-2.80605200	-0.84741600
O	-4.59801700	3.09871100	0.24306700
O	0.14843800	-2.45830000	-2.93554000
O	5.61720200	0.77422600	1.12842600
N	-2.43776500	2.32087800	0.32979800
H	-1.88201100	1.46974100	0.29078600
N	4.16843900	1.11433800	-0.58482300
H	3.29342100	0.78814000	-0.99838200
C	4.64213000	0.38567100	0.46110300
C	4.25374200	-2.99148800	2.02090500
H	4.85853400	-3.62282100	2.67002800
C	4.72808700	-1.75761700	1.60398200
H	5.69488800	-1.38444300	1.92718800
C	2.68975000	-1.36705100	0.31137000
C	3.66177000	2.94110400	-2.04147900
H	2.59881500	2.85871500	-1.78967800
H	3.84498200	2.31741400	-2.92322600
H	3.87397000	3.98289900	-2.30594500
C	-3.57543100	-0.24145800	-0.53036600
C	2.99079800	-3.41211800	1.61212400
C	-4.49599100	-2.00358800	0.85430300
H	-4.55734400	-3.06008600	1.11187500
C	3.97101900	-0.92708000	0.75874100
C	2.20132600	-2.62243800	0.77103000
C	-4.18871800	0.71694300	0.32223500
C	4.53992000	2.50333300	-0.87114500
C	-5.08221700	0.30351900	1.30683600
H	-5.58621400	1.05380000	1.91310900
C	6.01457800	2.59114600	-1.26789200
H	6.27221700	3.62417400	-1.53461900
H	6.21450800	1.95172900	-2.13436200
H	6.64957200	2.26450500	-0.44132100
C	4.26428800	3.39595200	0.34196400
H	3.20345400	3.35520100	0.61013500
H	4.52193600	4.43840200	0.11525300
H	4.85429900	3.06287400	1.19877300
C	-5.26822900	-1.06723300	1.53552100
H	-5.96953700	-1.40145700	2.29931700
C	-1.70169200	3.54511400	-0.00821200
C	-3.78963200	2.15973900	0.25684200
C	-0.22236000	3.17299300	0.04241100
H	-0.00507200	2.33458900	-0.63176600
H	0.07642100	2.86277100	1.05142000

H	0.39123800	4.03234700	-0.25203700
C	-2.07162200	4.00255400	-1.42111200
H	-3.13566500	4.24806800	-1.47919600
H	-1.86421700	3.20162700	-2.13787900
H	-1.48738800	4.88969000	-1.69719800
C	-2.00843900	4.64557800	1.00859000
H	-1.73264900	4.32163000	2.01874100
H	-3.07440900	4.88587300	0.99889000
H	-1.43396500	5.54995100	0.76968100
C	-3.60313900	-1.62033200	-0.16544600
N	-0.79077300	0.46908600	2.47626400
C	0.58774000	0.12850700	2.75617300
C	-1.63942200	-0.70334700	2.56879300
C	-1.25735800	1.51521800	3.35086400
H	0.73717600	-0.17650000	3.81557300
H	0.89571900	-0.70056800	2.11513700
H	1.24459500	0.98207900	2.54763000
H	-1.60437500	-1.16290300	3.58090100
H	-2.67758200	-0.43203700	2.35518900
H	-1.31662700	-1.45846400	1.84224000
H	-0.61625200	2.40150800	3.25334600
H	-2.27982100	1.80254700	3.07929300
H	-1.24949600	1.21214900	4.42331800
O	-1.08892700	-0.01890500	-1.65108500
H	2.58682700	-4.36656400	1.94709400

Dioxo_P_{carb} (Cis/Trans) (Trans Attack)

Mo	-0.25730500	-2.21442200	-0.10693100
S	-0.12335500	-0.82955700	2.07668000
S	-2.06702200	-0.32527200	-0.57789500
S	1.99088000	-0.96005100	-0.29670500
S	-2.43940300	-3.43191800	0.07726100
O	-5.78141800	1.93457200	-1.06166900
O	0.28989500	-3.71927000	0.55133900
O	5.84039900	1.24825800	0.72340300
N	-3.91912400	1.96351700	0.26339200
H	-3.16313600	1.34998800	0.55860500
N	4.93527400	-0.39100000	-0.55212900
H	4.10127100	-0.95790400	-0.71071200
C	4.91155900	0.44709400	0.51726500
C	3.05989900	0.99608000	3.71040600
H	3.27664500	1.48247500	4.66036400
C	4.01342700	0.96640200	2.70514700
H	4.98745900	1.42902000	2.83104100
C	2.48663500	-0.26908100	1.24098600
C	5.49980500	-1.39015500	-2.65048600
H	4.48817300	-1.20771000	-3.02862100
H	5.51024200	-2.38648300	-2.19565300
H	6.19065700	-1.39208200	-3.50093000
C	-3.66958000	-0.96945400	-0.35217800
C	1.81760900	0.40791000	3.49571100
C	-5.09927100	-2.93991300	-0.12021200
H	-5.18234900	-4.01688800	0.01270500
C	3.75516000	0.34379100	1.47307600
C	1.50750600	-0.22580000	2.28407400
C	-4.85103400	-0.17168900	-0.40230700
C	5.91053100	-0.32138200	-1.63962500
C	-6.11162900	-0.77923200	-0.38614400
H	-6.97885600	-0.12936300	-0.47185300
C	7.31849500	-0.61652900	-1.11728800
H	8.03743800	-0.61100800	-1.94680300
H	7.34961300	-1.60270900	-0.64175500
H	7.61421000	0.13378100	-0.37999300
C	5.87094800	1.05646000	-2.30704200
H	4.87025900	1.25629800	-2.70559100
H	6.58849200	1.09806200	-3.13661400
H	6.11796900	1.83601300	-1.58264900
C	-6.24425800	-2.15605100	-0.25271600

H	-7.22991300	-2.61854000	-0.23441800
C	-3.47799800	3.35014900	0.03922000
C	-4.88254400	1.32524800	-0.46235900
C	-2.27061000	3.53903000	0.95259600
H	-1.53565100	2.74644600	0.76912900
H	-2.56342000	3.49708600	2.00718900
H	-1.76497700	4.49384200	0.76399400
C	-3.05877900	3.54500200	-1.42054100
H	-3.90065100	3.34196400	-2.08825100
H	-2.23503200	2.86660800	-1.66817000
H	-2.72069000	4.57622400	-1.58596400
C	-4.59035000	4.32647800	0.41554400
H	-4.88758200	4.18449400	1.46051600
H	-5.46653900	4.16778200	-0.21754600
H	-4.23748200	5.35868400	0.29375800
C	-3.81813400	-2.37547900	-0.16142900
N	0.72052500	3.21843900	-0.80781900
C	1.19350500	3.01933000	0.54842800
C	0.46017800	4.61045200	-1.07888100
C	1.64755400	2.63663200	-1.75458700
H	2.20120400	3.45779900	0.71214800
H	0.50391500	3.48129300	1.26205300
H	1.24626000	1.94938300	0.76715500
H	1.31810200	5.27669900	-0.83835400
H	0.21413600	4.74429900	-2.13926900
H	-0.41449700	4.92482000	-0.49639300
H	1.76952000	1.56871400	-1.53691000
H	1.25610200	2.74033300	-2.77304400
H	2.65235100	3.11382500	-1.71557500
O	0.09325400	-2.27671200	-1.80468400
H	1.05048900	0.43799100	4.26689800

Dioxo_{carb} (Cis/Trans)

Mo	-1.71708100	-2.20762700	-0.48215500
S	-1.29311200	-2.01213900	2.17520500
S	-0.88662800	0.33641100	-0.53014200
S	0.77443300	-2.46786300	-0.23279700
S	-3.83030600	-0.95161700	-0.38909800
O	-0.88648000	4.78410100	-0.52823100
O	-1.34673100	-2.44975900	-2.16641300
O	4.78773700	-1.12144100	0.39400700
N	0.06774800	3.02132000	0.55630600
H	-0.02228000	2.01436200	0.68767800
N	3.00614700	-0.42940500	-0.86093600
H	1.99217200	-0.48691000	-0.89965000
C	3.56649000	-0.95470500	0.26734500
C	2.17782300	-0.64731000	3.72164400
H	2.52066600	-0.27267100	4.68547500
C	3.05166600	-0.70323500	2.64178100
H	4.07810300	-0.35176900	2.71513300
C	1.28125900	-1.65068500	1.24690800
C	2.58627200	0.07999300	-3.15952100
H	2.14991000	1.04739400	-2.88778100
H	1.77213500	-0.65346800	-3.18333500
H	3.00840800	0.16376100	-4.16714100
C	-2.27837600	1.38179700	-0.37687100
C	0.84869700	-1.02435400	3.55643300
C	-4.71892000	1.59373100	-0.41815400
H	-5.69194400	1.10677800	-0.45262800
C	2.60184700	-1.15982900	1.39545500
C	0.36572200	-1.53017700	2.33505800
C	-2.20387800	2.80234400	-0.27894400
C	3.66910100	-0.33539200	-2.16710100
C	-3.37316000	3.57452900	-0.30807600
H	-3.25485300	4.65400900	-0.26826000
C	4.24856300	-1.69290500	-2.57492000
H	4.70586300	-1.62493300	-3.57027200
H	3.45566700	-2.44706600	-2.60572000

H	5.00721000	-2.01562200	-1.85771300
C	4.77183300	0.72234200	-2.11072800
H	4.35506900	1.69153600	-1.81503100
H	5.24268400	0.83418400	-3.09601400
H	5.53355000	0.43668300	-1.38111500
C	-4.62615200	2.98283400	-0.38144100
H	-5.52742700	3.59311300	-0.39497600
C	1.43698500	3.54665900	0.63356200
C	-0.94883400	3.61002100	-0.12748100
C	2.25468800	2.48531000	1.36085900
H	2.24754800	1.53995900	0.80832600
H	1.85396700	2.28374600	2.36034700
H	3.29861300	2.80422900	1.46248300
C	2.00327500	3.75811100	-0.77324400
H	1.40331900	4.48778700	-1.32307100
H	1.99585700	2.81046600	-1.32343900
H	3.03994400	4.11411400	-0.71805500
C	1.45416400	4.85913600	1.41840400
H	1.06065800	4.70134100	2.42839300
H	0.83966200	5.61226700	0.91912800
H	2.48356300	5.23023100	1.50481000
C	-3.57479400	0.78827100	-0.40854800
H	0.14652000	-0.94038600	4.38365100
O	-2.66581000	-3.60687600	-0.06855600

Trans-ES_{carb} (Trans Attack)

Mo	0.08085300	-0.27480500	-1.50142100
S	-2.35356800	-0.10039700	-1.28749900
S	2.35130500	-0.31872400	-0.57923600
S	-0.37486300	-2.60833600	-0.89633600
S	0.32491000	2.10807000	-1.02622600
O	6.47841800	1.17895300	0.86890000
O	0.30499400	-0.38310800	-3.18599600
O	-6.35296800	-0.77856400	0.88716300
N	5.20939700	-0.58490800	0.22823200
H	4.28564500	-0.88086500	-0.10081800
N	-4.88208700	0.71771800	0.02739000
H	-3.97143500	0.82638600	-0.43335500
C	-5.23901000	-0.54723000	0.37803800
C	-4.61918300	-2.86012200	0.77373800
H	-5.60109600	-2.89215200	1.23544400
C	-3.78485300	-3.96444700	0.76428600
H	-4.11014700	-4.90308400	1.21276200
C	-2.05562000	-2.66356300	-0.36036800
C	-4.87845800	3.07842900	-0.33140800
H	-4.63223200	2.93442600	-1.38877400
H	-3.93259800	3.17453900	0.21379000
H	-5.43339700	4.01787000	-0.22916900
C	2.93714700	1.33884200	-0.32605200
C	-4.22016600	-1.63797100	0.19265300
C	2.39900300	3.72710200	-0.33999500
H	1.66001800	4.50843000	-0.51499900
C	-2.51216100	-3.85905000	0.20511400
H	-1.82871800	-4.70736600	0.22166600
C	-2.93567800	-1.54106100	-0.42443900
C	4.25642300	1.67671100	0.11504200
C	-5.70668100	1.91062500	0.20231900
C	4.59972900	3.02966400	0.30020600
H	5.61250100	3.23680700	0.63184300
C	-6.01868800	2.13670400	1.68459900
H	-6.60801900	3.05387200	1.81508000
H	-5.08937100	2.24196200	2.25585600
H	-6.57976900	1.28936400	2.08530900
C	-7.00888400	1.79601200	-0.59536300
H	-6.79046200	1.65263300	-1.65881800
H	-7.60447000	2.71184400	-0.48546800
H	-7.59301600	0.94328300	-0.24291700
C	3.69014500	4.04873300	0.07406500

H	3.97848400	5.08897800	0.22137100
C	6.19483600	-1.62354000	0.52849100
C	5.39390100	0.74456600	0.43369900
C	5.53954000	-2.95277900	0.15920300
H	5.27214400	-2.97761400	-0.90222600
H	4.62127900	-3.11378200	0.73374400
H	6.22535400	-3.78292200	0.36263100
C	7.46254300	-1.42492600	-0.30717800
H	7.92444000	-0.46363800	-0.07079300
H	7.21997100	-1.44219200	-1.37485200
H	8.18029200	-2.23037000	-0.10344100
C	6.54605700	-1.62042000	2.01929200
H	5.64803400	-1.79403500	2.62150400
H	6.97628100	-0.65730400	2.30320700
H	7.26833700	-2.41682300	2.24144200
C	2.01003300	2.40105100	-0.54156900
N	-0.59657200	0.30495800	2.19369900
C	0.65321200	1.07981900	2.47988100
C	-0.98351800	-0.49486100	3.39245400
C	-1.70937200	1.25436600	1.86455900
H	0.51960700	1.71861200	3.36200600
H	1.44904700	0.34858300	2.62518800
H	0.87061000	1.67384300	1.59160600
H	-1.20116600	0.15599600	4.24934300
H	-1.85728600	-1.08213000	3.10458800
H	-0.15209500	-1.16660000	3.60678900
H	-1.40477200	1.79709000	0.96631500
H	-2.59390300	0.65124700	1.64954600
H	-1.88626200	1.93486900	2.70799300
O	-0.37784100	-0.57453600	1.17770500

Trans-TS1'_{carb} (Trans Attack)

Mo	0.07451300	0.07447700	-1.67448000
S	-2.19392800	0.26186400	-0.82435000
S	2.49121400	-0.10509800	-1.36201600
S	-0.33070700	-2.31905600	-1.20784100
S	0.50760100	2.48566900	-1.24080100
O	6.27236600	0.25778000	0.38438800
O	-0.06968500	0.11021700	-3.37503000
O	-6.38584800	-0.77352400	0.48061400
N	4.26826900	-0.66100800	1.02254300
H	3.25924300	-0.52886200	0.89395400
N	-4.66585100	0.67415400	0.84185000
H	-3.69515400	0.83898000	0.56820200
C	-5.16878200	-0.52909300	0.43967900
C	-4.64506300	-2.89072700	0.20437600
H	-5.66479900	-3.01215800	0.55853000
C	-3.82937600	-3.98088600	-0.06228600
H	-4.20245100	-4.99441500	0.08175800
C	-2.01666100	-2.48152200	-0.71045600
C	-4.46869400	3.01469000	1.28631000
H	-3.76797600	3.12961300	0.45157700
H	-3.88074700	2.80720700	2.18739100
H	-4.99376600	3.96580900	1.42869300
C	3.02222100	1.44129300	-0.64391700
C	-4.17248200	-1.57778200	0.03470900
C	2.69775600	3.80934700	-0.25712500
H	2.05982400	4.68941900	-0.33349900
C	-2.52486000	-3.77209300	-0.50087200
H	-1.86377700	-4.61603500	-0.69424400
C	-2.85689100	-1.35895700	-0.46283600
C	4.25601500	1.52624400	0.03718600
C	-5.46759400	1.89031400	1.01791500
C	4.74089600	2.76587100	0.47728600
H	5.70657900	2.79439000	0.97755800
C	-6.41053600	1.74124500	2.21210500
H	-6.97076100	2.67250100	2.36796700

H	-5.84088700	1.52651200	3.12272300
H	-7.11389200	0.92346900	2.04286400
C	-6.26372000	2.20071000	-0.25299700
H	-5.58529700	2.31482400	-1.10485900
H	-6.82972000	3.13331400	-0.13183700
H	-6.96151800	1.38856700	-0.47067400
C	3.96985700	3.91062600	0.30542100
H	4.33758900	4.87782800	0.64688100
C	4.67949600	-2.07421000	1.08866900
C	5.03678400	0.31777300	0.45444200
C	3.42246600	-2.87050700	1.43163800
H	2.61008900	-2.64871700	0.72771900
H	3.06897700	-2.63128800	2.44212700
H	3.63423900	-3.94510600	1.39786400
C	5.21763500	-2.54127400	-0.26721900
H	6.11071800	-1.97403500	-0.54166900
H	4.45835500	-2.39029700	-1.04101300
H	5.47409100	-3.60745800	-0.22451800
C	5.74227900	-2.25787500	2.17191900
H	5.35976900	-1.92306300	3.14316500
H	6.63238300	-1.67151200	1.92976800
H	6.02161900	-3.31642600	2.25684700
C	2.18660600	2.58414200	-0.71599400
N	0.39938100	0.09763700	2.09477700
C	1.51685500	0.09631900	3.01441600
C	-0.49291800	-1.03644500	2.24590000
C	-0.27120000	1.38588500	2.05806200
H	1.18039200	0.27305500	4.05226800
H	2.03139900	-0.86511800	2.95683200
H	2.21716700	0.88190100	2.71529700
H	-0.96480300	-1.04250600	3.24532400
H	-1.26369400	-0.98090500	1.47530700
H	0.07586900	-1.95604400	2.08865100
H	0.45417000	2.14929400	1.76565700
H	-1.05912200	1.35422700	1.30279400
H	-0.70137300	1.62756500	3.04825300
O	1.25037800	-0.11955600	0.48533600

Trans-INT1_{carb} (Trans Attack)

Mo	0.23704600	-0.89598800	1.73559100
S	2.36426100	-0.10113400	0.86175800
S	-2.99463200	-0.21215700	1.77621600
S	0.74225700	-2.81383400	0.32693400
S	-0.27683900	1.52496300	2.09194700
O	-5.75475700	1.69431600	-1.40124400
O	0.52525500	-1.46778600	3.31442400
O	6.45874900	-0.06171200	-0.84934000
N	-4.99179900	-0.24535000	-0.50138800
H	-4.32803700	-0.63506600	0.17486100
N	4.50941400	1.12546900	-0.87729500
H	3.53783700	1.04410500	-0.57764700
C	5.22083600	-0.03426600	-0.77027600
C	5.00157300	-2.40406800	-1.28805000
H	5.99929100	-2.27440900	-1.69921100
C	4.32738900	-3.61376000	-1.37487200
H	4.79311800	-4.47091700	-1.85930600
C	2.42115800	-2.63751400	-0.21266700
C	3.88260700	3.42602900	-0.73290800
H	3.17626500	3.19710600	0.07352500
H	3.34082600	3.34972400	-1.68250600
H	4.22191400	4.46081900	-0.61160600
C	-2.85165500	1.31700000	0.93760300
C	4.40622300	-1.29068900	-0.67513000
C	-1.67252100	3.45279000	0.83505000
H	-0.80420900	4.05044200	1.10774800
C	3.03737600	-3.71645400	-0.85742000
H	2.47767900	-4.64661200	-0.94797600

C	3.12208100	-1.41023300	-0.07544200
C	-3.83475200	1.84402000	0.03235900
C	5.07366000	2.46990900	-0.71081000
C	-3.75573400	3.19104900	-0.33996200
H	-4.53243100	3.57036200	-0.99671900
C	6.02358500	2.79323800	-1.86399200
H	6.40664800	3.81677100	-1.76065600
H	5.49928900	2.71759400	-2.82274000
H	6.86313600	2.09474000	-1.87303500
C	5.80525200	2.58223100	0.63003200
H	5.12182100	2.35068400	-1.45323200
H	6.19114400	3.59992400	0.77183300
H	6.64220300	1.87994400	0.66557100
C	-2.70650600	4.00094800	0.08777000
H	-2.67329000	5.04985200	-0.20310400
C	-5.80338600	-1.17079400	-1.29068900
C	-4.94906300	1.10122800	-0.66201600
C	-5.39225800	-2.57129400	-0.84016900
H	-5.59391800	-2.71583200	0.22700000
H	-4.32000900	-2.73321300	-0.99913500
H	-5.94565500	-3.33154000	-1.40225100
C	-7.29306800	-0.94613100	-1.01909200
H	-7.57744200	0.07018300	-1.30192800
H	-7.51263300	-1.08570300	0.04506000
H	-7.89753200	-1.66135000	-1.59219100
C	-5.50994100	-1.00684800	-2.78435700
H	-4.44712100	-1.17638100	-2.98460400
H	-5.76766300	0.00135300	-3.11616300
H	-6.09128500	-1.73359800	-3.36596200
C	-1.69831900	2.11098400	1.25037200
N	-0.34948900	0.14144100	-1.59598600
C	-0.58695800	1.53744000	-1.88838200
C	-1.50989900	-0.67129700	-1.89151300
C	0.80396900	-0.33012700	-2.33050100
H	-0.68718200	1.72304300	-2.98198100
H	-1.50365800	1.87925600	-1.40166000
H	0.24694100	2.14127100	-1.50923300
H	-1.75928700	-0.66566200	-2.97786800
H	-1.32042000	-1.70149300	-1.57004300
H	-2.37550500	-0.29644600	-1.33566900
H	1.68970800	0.25183900	-2.05370200
H	0.99680300	-1.37826300	-2.08865500
H	0.65400100	-0.23736900	-3.43048900
O	-1.67734500	-1.23111000	1.26813000

Trans-TS2'_{carb} (Trans Attack)

Mo	0.14969000	-0.71089000	-1.87426500
S	-2.05051400	-0.13893500	-0.95278400
S	3.30502200	0.35511500	-1.93711000
S	-0.09788800	-2.58966500	-0.35657700
S	0.37138900	1.78143200	-2.04243400
O	5.75965600	1.21035100	1.34766700
O	-0.09055100	-1.29864100	-3.45798700
O	-6.17224800	-0.67524700	0.43094200
N	4.08551900	-0.31977300	0.99066400
H	3.23775900	-0.46141000	0.44382900
N	-4.43248000	0.77707000	0.71761700
H	-3.42588200	0.83065100	0.57706000
C	-4.95299800	-0.47077000	0.51769500
C	-4.40387300	-2.76261000	1.15681600
H	-5.42491700	-2.77818700	1.52957500
C	-3.55578900	-3.85123900	1.31302600
H	-3.90133600	-4.75040900	1.42110000
C	-1.78796000	-2.64145500	0.15618300
C	-4.12000900	3.14698000	0.55476000
H	-3.26037000	2.99671500	-0.10923900
H	-3.74816900	3.19148100	1.58429600

H	-4.57671500	4.11290800	0.31208700
C	2.89123400	1.61346800	-0.82821300
C	-3.96165700	-1.59396400	0.51980100
C	1.51871100	3.54572300	-0.30256600
H	0.61505100	4.12944600	-0.47493500
C	-2.25138100	-3.77719300	0.83016500
H	-1.56158600	-4.60843200	0.96954700
C	-2.65707300	-1.53639100	-0.03770300
C	3.71088000	1.92735500	0.29188800
C	-5.14178700	2.02446200	0.39273100
C	3.53523200	3.13316000	0.96624600
H	4.20556000	3.37334700	1.78868800
C	-6.30694600	2.23498400	1.35936600
H	-6.80344700	3.19096800	1.14791400
H	-5.94610000	2.25676400	2.39351700
H	-7.03264400	1.42417900	1.26406600
C	-5.64311100	1.99100600	-1.05360300
H	-4.80416200	1.83349700	-1.73898000
H	-6.13171600	2.93987500	-1.30942300
H	-6.36086400	1.17831400	-1.19047000
C	2.46210300	3.96676800	0.62969500
H	2.31978800	4.91137100	1.15326700
C	4.82467900	-1.55632300	1.27505300
C	4.64689000	0.92185700	0.88609900
C	3.82945300	-2.69402500	1.06293500
H	3.43319800	-2.68146900	0.04142700
H	2.97273700	-2.60282800	1.73946700
H	4.31304200	-3.66050600	1.24492900
C	5.99984700	-1.70501400	0.30460300
H	6.70794400	-0.88141600	0.43099000
H	5.63494600	-1.69156800	-0.72769400
H	6.52264600	-2.65371500	0.48238000
C	5.32168700	-1.54471300	2.72042000
H	4.47831700	-1.43570900	3.41109200
H	6.01073500	-0.71166200	2.88076100
H	5.83693300	-2.48636700	2.95048600
C	1.68378000	2.35148000	-1.02601700
N	-0.14326100	0.94593300	2.83697800
C	-1.08780600	-0.15852100	2.89293500
C	1.07618700	0.52022200	2.16941200
C	-0.72507200	2.06468000	2.11338100
H	-1.35774200	-0.53804200	1.89300300
H	-0.65209600	-0.99164700	3.45657100
H	-2.00750500	0.16044000	3.39915500
H	0.89599600	0.17276200	1.12964800
H	1.78973500	1.34999500	2.13053800
H	1.53594700	-0.30986200	2.71828600
H	-1.65674400	2.37391400	2.60416300
H	-0.02692800	2.90930600	2.11789300
H	-0.94937600	1.81938700	1.05532800
O	2.05102600	-0.89946700	-1.41889700

Dioxo_P carb(Trans/Trans) (Trans Attack)

Mo	0.02387300	-3.11899400	0.30598900
S	-2.07851800	-1.35277900	0.01954400
S	1.48847700	-0.91716500	0.46399000
S	-0.50411800	-2.34580100	2.61105300
S	0.76125100	-2.77059100	-2.01627700
O	4.54718200	2.31256800	-0.64159700
O	-1.13843900	-4.22921000	-0.36415200
O	-4.27247400	2.62135500	0.79333200
N	2.92097300	1.67539300	0.80407600
S	2.15974400	1.01586600	0.96357200
N	-3.55095200	1.13015600	-0.75720600
H	-2.99808800	0.27974300	-0.90245900
C	-3.59672400	1.61389500	0.50897700
C	-2.69117700	1.64131700	2.75605700

H	-3.22823100	2.58415500	2.79291600
C	-1.94848200	1.19055400	3.83432700
H	-1.87736300	1.78364900	4.74446800
C	-1.34800800	-0.79857100	2.57197800
C	-3.97947200	0.77081700	-3.08369800
H	-4.28581900	-0.26211800	-2.88625400
H	-2.90487300	0.76396300	-3.29704000
H	-4.50574600	1.12489100	-3.97735900
C	2.26393400	-0.60447900	-1.06882600
C	-2.77400800	0.91463700	1.55659300
C	2.56444800	-1.31881300	-3.39665100
H	2.30829600	-2.01338100	-4.19468900
C	-1.28065100	-0.02798200	3.73551200
H	-0.68449800	-0.40046900	4.56653400
C	-2.08431800	-0.33542500	1.43312600
C	3.16838100	0.47428200	-1.31999700
C	-4.29642500	1.67359800	-1.89315300
C	3.74836100	0.60449900	-2.59070300
H	4.43816800	1.43188200	-2.72985300
C	-3.84615500	3.10496700	-2.19631100
H	-4.39877900	3.50259600	-3.05773600
H	-2.77644100	3.12494200	-2.43395600
H	-4.02145900	3.74795000	-1.33056600
C	-5.80256900	1.64210200	-1.61510400
H	-6.13014800	0.61605800	-1.41583400
H	-6.35513500	2.01712500	-2.48655800
H	-6.04221100	2.25912900	-0.74648600
C	3.45853600	-0.27582500	-3.62297000
H	3.91936100	-0.15086900	-4.60137100
C	3.26083100	2.58068000	1.90145500
C	3.60105000	1.55171100	-0.35997300
C	2.24434700	2.30282100	3.00814200
H	2.28103600	1.25503500	3.32658300
H	1.22141700	2.50325600	2.66958700
H	2.44714000	2.93760300	3.87802900
C	4.67690500	2.29054700	2.40806600
H	5.40234800	2.44061800	1.60444800
H	4.74939500	1.25498900	2.75633700
H	4.92554400	2.95571200	3.24512200
C	3.15601500	4.04192500	1.45639800
H	2.13599600	4.26802400	1.12564400
H	3.84230500	4.23576800	0.62842800
H	3.39903100	4.71062100	2.29247100
C	1.96047000	-1.48664000	-2.14709200
N	0.58709400	2.18321100	-1.32171800
C	1.06484700	3.36076700	-1.99370000
C	-0.22337300	2.48771500	-0.16711400
C	-0.07509500	1.26886800	-2.22244400
H	0.24737800	3.98226600	-2.42824000
H	1.63112900	3.98710300	-1.29340600
H	1.74218000	3.07084300	-2.80630800
H	-1.16191900	3.02905400	-0.41415000
H	-0.49099200	1.55558400	0.34243500
H	0.35195900	3.10755700	0.53270100
H	0.61255300	0.97622900	-3.02525600
H	-0.37473900	0.36326700	-1.67909000
H	-0.98496100	1.71356900	-2.68412500
O	1.20129200	-4.14498700	1.06035700

Dioxo carb (Trans/Trans)

Mo	3.05353100	0.01475800	-0.06562700
S	0.95372800	-1.08706100	-1.31043300
S	1.10353200	1.24032700	1.32231700
S	2.55154400	-1.97047500	1.33926100
S	2.47657800	1.96974800	-1.49309100
O	-2.82855200	3.13234200	1.98002700
O	4.14342500	0.46792400	1.21182800

O	-2.85958700	-3.19891200	-1.92495300
N	-1.87477000	1.05814800	1.92160400
H	-1.02214000	0.58937500	1.61467100
N	-2.05413200	-1.06749200	-1.76763800
H	-1.22934700	-0.55552600	-1.45413800
C	-2.04763100	-2.38978900	-1.44711900
C	-1.50073900	-3.84304600	0.43489400
H	-2.47557800	-4.27330300	0.21990900
C	-0.72326100	-4.29532800	1.49243900
H	-1.07985800	-5.09472200	2.13989500
C	0.99535700	-2.67091700	0.91312700
C	-2.27784600	0.96503600	-3.00554500
H	-1.18736200	1.06640700	-3.05721900
H	-2.61239000	1.49812800	-2.10915300
H	-2.71041200	1.46034900	-3.88252500
C	0.24529500	2.23979000	0.17820400
C	-1.06098500	-2.80331900	-0.39517200
C	0.33782100	3.57849800	-1.87071500
H	0.88099700	3.86298100	-2.77025800
C	0.51108200	-3.69572800	1.73391800
C	0.22906000	-2.22545600	-0.20421800
C	-1.06246600	2.76253800	0.40364000
C	-2.69440800	-0.50220600	-2.96331100
C	-1.59971000	3.72378500	-0.46334600
H	-2.58526000	4.11482700	-0.22293100
C	-4.21507900	-0.61465600	-2.85552100
H	-4.68792500	-0.15385600	-3.73280600
H	-4.57335900	-0.09597900	-1.96012600
H	-4.51588000	-1.66293600	-2.79557500
C	-2.19680400	-1.22341000	-4.22021800
H	-1.10757900	-1.14277300	-4.29530100
H	-2.64298800	-0.77557600	-5.11776300
H	-2.46573700	-2.28256500	-4.18504400
C	-0.90566600	4.14145800	-1.59075200
H	-1.33834400	4.87701800	-2.26685900
C	-2.45119900	0.51807700	3.15908700
C	-1.97596100	2.35433200	1.52131600
C	-1.91549300	-0.90630300	3.28244100
H	-0.82025300	-0.91269900	3.33232900
H	-2.20748300	-1.51632800	2.42066700
H	-2.30347000	-1.38232800	4.19031200
C	-2.00112200	1.35258400	4.36311700
H	-2.35519800	2.38251800	4.26687700
H	-0.90818100	1.36484800	4.42760800
H	-2.40022600	0.92671100	5.29292200
C	-3.97706400	0.50346500	3.06654600
H	-4.30074800	-0.09758100	2.21038900
H	-4.35903000	1.51993400	2.94289000
H	-4.40445000	0.06525300	3.97794700
C	0.91861400	2.63429500	-1.01676100
O	4.09298500	-0.44932300	-1.38048200
H	1.12315900	-4.01566900	2.57535400

Table S4

Cis-E_{acylam}

Mo	-0.00001600	-1.77299400	0.75832000
S	-1.67729200	-0.09605900	0.17617000
S	1.67726200	-0.09607200	0.17614100
S	-1.65170000	-3.28616300	-0.18281400
S	1.65164600	-3.28617800	-0.18282700
O	-0.00000500	-1.96260900	2.45474900
C	-5.57976400	-0.95069400	-0.69618900
H	-6.49676800	-0.38621400	-0.81161700
C	-5.53807400	-2.33620000	-0.85747100
H	-6.45260500	-2.87208500	-1.10923600
C	-3.15556900	-2.37149500	-0.36543500
C	5.85187800	4.50300200	-0.03741800
H	6.34296200	4.48568100	-1.01452800
H	6.61692500	4.27302600	0.70982400
H	5.47167500	5.51515100	0.14885700
C	3.17425300	-0.97404100	-0.20483500
C	-4.39546800	-0.27973200	-0.37525900
C	4.34622300	-3.03654900	-0.69788500
C	-4.34628600	-3.03651500	-0.69781900
C	-3.17429400	-0.97401900	-0.20478000
C	4.39542700	-0.27976200	-0.37535400
C	4.70526300	3.49984900	0.02027600
C	5.57971000	-0.95073400	-0.69630900
H	6.49671400	-0.38625900	-0.81176700
C	4.05667200	3.54694900	1.40934400
H	3.71322200	4.56595700	1.62962300
H	4.77048400	3.25640100	2.18805800
C	3.18910900	2.88392000	1.49138000
C	3.65941100	3.85847500	-1.04247800
H	4.08705700	3.80371200	-2.04967300
H	3.29596600	4.88209300	-0.88457200
H	2.79174800	3.19145700	-1.01265000
C	5.53801100	-2.33624100	-0.85757000
H	6.45253300	-2.87213400	-1.10935100
C	-4.70516800	3.49990500	0.02018800
C	-5.85180600	4.50305500	-0.03708000
H	-6.61658800	4.27306300	0.71042900
H	-6.34323500	4.48575100	-1.01401600
H	-5.47154100	5.51520100	0.14908300
C	-4.05610300	3.54695700	1.40902900
H	-3.18853100	2.88389800	1.49073900
H	-4.76965100	3.25640400	2.18798400
H	-3.71255100	4.56595000	1.62921100
C	-3.65967400	3.85857000	-1.04291400
H	-4.08765900	3.80381800	-2.04996500
H	-2.79198700	3.19157100	-1.01339200
H	-3.29619300	4.88219200	-0.88511500
C	3.15551600	-2.37151900	-0.36548200
C	-5.27080500	2.08428000	-0.25887000
O	-6.46588300	1.90416800	-0.51324200
N	-4.32570200	1.11696400	-0.19718700
H	-3.37426600	1.40264000	0.02973500
N	4.32567700	1.11693900	-0.19732500
C	5.27081700	2.08422400	-0.25895000
O	6.46591300	1.90405800	-0.51319800
H	3.37424900	1.40263300	0.02960200
H	-4.31714000	-4.11766800	-0.82502900
H	4.31706900	-4.11770200	-0.82508200

Cis-TS1_{acylam} (Cis Attack)

Mo	0.18659700	-1.23190200	0.28367100
S	-1.25809600	0.64521800	-0.46734700
S	2.11556400	0.12056200	-0.12612900

S	-0.90409700	-2.22414300	-1.84475300
S	1.74323900	-3.06325300	-0.10962300
O	-0.00001900	-1.18593800	2.00495200
C	-4.96989900	-0.08398200	-2.01883500
H	-5.93307400	0.41247100	-2.01309400
C	-4.75764800	-1.29198800	-2.68566300
H	-5.58132300	-1.75076600	-3.23252500
C	-2.43259300	-1.37638100	-1.93987500
C	6.80621600	4.19044800	-0.09102000
H	7.39375400	3.99229200	-0.99205400
H	7.45359700	3.98295600	0.76559500
H	6.53079900	5.25229400	-0.07696700
C	3.53388900	-0.95616300	-0.09189500
C	-3.89106400	0.48821100	-1.33292600
C	4.50286500	-3.17397400	-0.08812000
C	-3.51830800	-1.92572700	-2.64536400
C	-2.61972700	-0.12971800	-1.29169300
C	4.84193900	-0.41906000	-0.08199900
C	5.54976800	3.32787700	-0.05221300
C	5.97120100	-1.24386100	-0.07014700
H	6.95800400	-0.79684900	-0.05809200
C	4.76482600	3.62681700	1.23132600
H	4.51272200	4.69400100	1.27949900
H	5.35491800	3.37844800	2.12046400
H	3.82809500	3.06285400	1.28520400
C	4.67375500	3.64543600	-1.27046700
H	5.19341900	3.40220900	-2.20377800
H	4.42789400	4.71488600	-1.28934200
H	3.72919400	3.09156600	-1.26439800
C	5.78278300	-2.62668500	-0.07624700
H	6.65243800	-3.28306700	-0.07051700
C	-4.65504600	3.65873900	0.63907400
C	-5.87626500	4.54781300	0.84369800
H	-6.71417700	3.97961600	1.25733000
H	-6.21669600	4.97416600	-0.10452400
H	-5.63222800	5.36821300	1.53038800
C	-4.21990800	3.06590200	1.98604000
H	-3.31085100	2.46092900	1.89465800
H	-5.00486600	2.42692700	2.40743000
H	-4.01408600	3.86834200	2.70630600
C	-3.50669300	4.49381800	0.05998800
H	-3.77219400	4.90372400	-0.92082700
H	-2.58659300	3.91239800	-0.06078100
H	-3.27924300	5.33522800	0.72730900
C	3.36353000	-2.35257400	-0.08692200
C	-5.03346000	2.50818000	-0.32913700
O	-6.18309900	2.37991400	-0.76399800
N	-3.98974700	1.69418300	-0.60455400
H	-3.09267800	1.91015100	-0.16666100
N	4.91703500	0.98907700	-0.07893400
C	5.97187600	1.83691100	-0.07198600
O	7.16075100	1.50179800	-0.07569500
H	3.98418500	1.39899000	-0.07292300
H	-3.37255800	-2.88141900	-3.14583000
H	4.36276500	-4.25427300	-0.09578200
N	-2.86958900	-2.35708800	1.86461700
C	-2.21495600	-2.97354200	3.06233700
H	-2.10295400	-4.03592400	2.84187700
H	-1.23314000	-2.50169100	3.13986300
H	-2.82502600	-2.81714100	3.96220500
C	-3.06380900	-0.88800000	2.10422200
H	-2.07271600	-0.45494700	2.24264200
H	-3.52112200	-0.47966400	1.20089300
H	-3.70869900	-0.73727400	2.97930900
C	-4.20469800	-2.97854200	1.63063100
H	-4.61626800	-2.50897400	0.73562400
H	-4.03284100	-4.03776500	1.43733200
H	-4.86484500	-2.83332800	2.49627600
O	-2.11160600	-2.59162100	0.75281300

Cis-ES_{acylam} (Cis Attack)

Mo	0.16853700	-1.16006700	0.30985200
S	-1.29806900	0.70986400	-0.47644000
S	2.11221100	0.15910600	-0.16696900
S	-0.83108900	-2.10583400	-1.94115800
S	1.69857400	-3.02165500	-0.00665000
O	0.01067300	-1.02413800	2.03194700
C	-4.98755000	-0.13812100	-2.01888600
H	-5.97082900	0.31641700	-1.99072400
C	-4.72894100	-1.31415800	-2.72505200
H	-5.53658700	-1.79107700	-3.28027600
C	-2.39250200	-1.32241100	-2.00048000
C	6.85887600	4.16394600	-0.18193000
H	7.43135000	3.94537500	-1.08817700
H	7.51470500	3.95747300	0.66836300
H	6.59971400	5.23002000	-0.17912200
C	3.51450900	-0.93450500	-0.07395600
C	-3.92774700	0.45897500	-1.32456700
C	4.45589900	-3.16282000	0.03313800
C	-3.46284800	-1.89445100	-2.71364500
C	-2.62918900	-0.10287600	-1.31142400
C	4.83023200	-0.41533200	-0.07487200
C	5.59022800	3.32089500	-0.11414300
C	5.94880400	-1.25313300	-0.02173700
H	6.94096500	-0.81802900	-0.01992500
C	4.82604700	3.65116100	1.17420700
H	4.58562700	4.72163700	1.20736500
H	5.42574200	3.41157000	2.05934600
H	3.88506000	3.09671300	1.24875500
C	4.70422600	3.63277000	-1.32614900
H	5.20740100	3.36560000	-2.26193200
H	4.47671100	4.70597800	-1.35933100
H	3.74957900	3.09700600	-1.30006300
C	5.74299800	-2.63251900	0.02813800
H	6.60408400	-3.29921200	0.06555600
C	-4.80271300	3.54717600	0.72971700
C	-6.05834000	4.37730900	0.97089600
H	-6.86222300	3.76596000	1.39095000
H	-6.43511200	4.80267900	0.03620600
H	-5.83798200	5.19655100	1.66698500
C	-4.32288700	2.94556600	2.05725200
H	-3.38734700	2.38686600	1.94186500
H	-5.07152400	2.26132500	2.47345000
H	-4.14559800	3.74067600	2.79301200
C	-3.70014900	4.44370800	0.15343000
H	-3.99875100	4.86440000	-0.81315600
H	-2.75876900	3.90421800	0.00491600
H	-3.49826700	5.27827200	0.83730200
C	3.32733600	-2.32802200	-0.00739000
C	-5.14356200	2.40450800	-0.26179600
O	-6.28921300	2.24575300	-0.69746400
N	-4.07179100	1.63625000	-0.55868800
H	-3.17996000	1.87273000	-0.11844100
N	4.92489800	0.99075100	-0.12308900
C	5.99091300	1.82393100	-0.10636500
O	7.17502100	1.47289900	-0.07468400
H	3.99698300	1.41224600	-0.14395300
H	-3.28037900	-2.82585700	-3.24694100
H	4.30160300	-4.24063800	0.07076300
N	-2.69529600	-2.40406400	1.78208000
C	-2.02997600	-2.97344200	2.99712300
H	-1.79508000	-4.01234300	2.76266700
H	-1.10850900	-2.40275600	3.13082500
H	-2.69586300	-2.90272000	3.86736500
C	-3.04395200	-0.96463700	2.02357200
H	-2.10744700	-0.43372100	2.19506600

H	-3.51521300	-0.59372900	1.11080800
H	-3.72469800	-0.89194300	2.88074700
C	-3.94873400	-3.15183600	1.48663900
H	-4.37540500	-2.71121300	0.58418600
H	-3.66433100	-4.18483700	1.28532200
H	-4.64747100	-3.08715500	2.33054500
O	-1.88114200	-2.56076400	0.68807100

Cis-TS2_{acylam} (Cis Attack)

Mo	-0.21626800	-1.67964200	-0.60224100
S	0.45685700	-1.52017200	2.05071100
S	-1.87108100	0.09689000	-0.18905500
S	1.71991800	0.17953200	-0.47520400
S	-2.06364300	-3.14517300	-0.11052700
O	-0.07426700	-1.56724900	-2.31315000
C	3.54157000	0.49428900	3.71434300
H	3.97493900	0.57442600	4.71090700
C	4.09907000	1.22187200	2.66277300
H	4.95835800	1.86743300	2.79710600
C	2.38967900	0.27584200	1.15053400
C	-3.43170000	-0.72446500	-0.09117500
C	2.44002300	-0.32778900	3.50448500
C	-4.77698000	-2.74080700	0.05644700
H	-4.82342500	-3.82859900	0.09072800
C	3.52009400	1.10359800	1.39595600
C	1.83360100	-0.46276000	2.23711800
C	-4.63195700	0.02877900	-0.02065300
C	-5.88312600	-0.58778800	0.07934200
H	-6.77400900	0.02584000	0.12707200
C	-5.94217000	-1.98028300	0.11776800
H	-6.91021900	-2.47329600	0.19988600
C	-3.51834100	-2.13235300	-0.04890000
H	2.00953200	-0.89012100	4.33101600
O	0.84242400	-3.50413300	-0.50920200
N	2.33579000	-3.65986800	-0.65148200
C	3.04872400	-3.02904300	0.47976700
C	2.72932500	-3.04887400	-1.93455100
C	2.53273800	-5.11466500	-0.65570700
H	4.11413400	-3.29078700	0.42144700
H	2.91560100	-1.95033600	0.40020000
H	2.58783500	-3.37142400	1.40675200
H	3.80705300	-3.18704800	-2.09383100
H	2.14201200	-3.51938300	-2.72350700
H	2.47576000	-1.98586100	-1.87873400
H	3.59483500	-5.35767000	-0.79412800
H	2.17018500	-5.49917600	0.29787400
H	1.92901800	-5.53037000	-1.46287400
C	-5.46708200	4.60492200	-1.17805700
H	-6.55556500	4.53235600	-1.09962500
H	-5.16551400	4.17843200	-2.14142400
H	-5.17903600	5.66381600	-1.17264700
C	-4.79926100	3.86574800	-0.01511900
C	-3.28173200	3.95001700	-0.16378500
H	-2.96982900	5.00123500	-0.16819800
H	-2.92905000	3.50022800	-1.09816700
H	-2.75042800	3.45789500	0.65773900
C	-5.21822100	4.52611800	1.30262100
H	-6.30272100	4.46213900	1.43130900
H	-4.92068300	5.58239400	1.31168500
H	-4.74278600	4.03437700	2.15841600
N	-4.46853900	1.43048700	-0.05373200
C	-5.37665600	2.42944000	0.00337500
O	-6.60300300	2.28058600	0.07860700
H	-3.48185900	1.67688600	-0.11595600
C	5.21998200	3.10960000	-1.36378600
C	6.43453100	4.02716900	-1.44695300
H	7.34487100	3.50425900	-1.13959000

H	6.32260100	4.88930800	-0.78317800
H	6.56245000	4.38762300	-2.47550100
C	5.42019400	1.91231200	-2.30230900
H	4.55243000	1.24337800	-2.31311400
H	6.29312200	1.32031800	-2.00422000
H	5.58389600	2.26077100	-3.33074500
C	3.96452000	3.88113400	-1.78686800
H	3.77210100	4.72104300	-1.11033900
H	3.07058400	3.24942200	-1.79363500
H	4.09293800	4.28533100	-2.79947900
C	5.07436200	2.61329000	0.09836800
O	5.87244400	2.95894300	0.97670500
N	4.01431100	1.79185300	0.26970000
H	3.44245800	1.57838700	-0.54920700

Dioxo_P_{acylam} (Cis/Trans) (Cis Attack)

Mo	0.37654700	1.66455600	-1.27158500
S	-1.86796300	0.64332900	-0.84087600
S	1.30564700	-0.84170600	-0.78732300
S	0.17756600	1.78636300	1.39313400
S	2.79744000	2.05165700	-0.99761600
O	0.02682900	1.17014200	-2.90351800
C	-3.61257300	-0.45356300	2.65695500
H	-4.51065100	-0.98598000	2.94252200
C	-2.71716900	0.04952500	3.60139500
H	-2.92638900	-0.09127800	4.66095100
C	-1.26120500	0.92567800	1.85120500
C	2.84100000	-6.62457900	0.83643600
H	3.33784600	-6.61260200	1.81095600
C	3.58350100	-6.94967400	0.10194200
H	2.02696800	-7.35941000	0.86636000
C	3.00202400	-0.66567900	-0.43860100
C	-3.32593200	-0.26635900	1.30221900
C	5.03806500	0.67325000	-0.32326900
C	-1.56369000	0.71685400	3.21187300
C	-2.16459800	0.42862500	0.88038400
C	3.78126800	-1.78527600	-0.02998200
C	2.28581900	-5.24907000	0.48445200
C	5.15312800	-1.68419900	0.20407600
H	5.70488900	-2.56775300	0.50077800
C	1.58797400	-5.31345600	-0.88014100
H	0.78842700	-6.06484800	-0.85817300
H	2.29312400	-5.59327500	-1.67089300
H	1.13566300	-4.35689200	-1.16209200
C	1.27537000	-4.81396300	1.55267900
H	1.75298700	-4.72225700	2.53423000
H	0.47156300	-5.55609900	1.63679900
H	0.81023600	-3.85048900	1.32035500
C	5.77646700	-0.44561200	0.04770700
H	6.84631800	-0.35499700	0.22729600
C	-5.88057300	-1.76933100	-1.09810400
C	-7.23464500	-2.45328100	-0.94559900
H	-7.95165600	-1.80023500	-0.43997700
H	-7.15293300	-3.36411400	-0.34581900
H	-7.63278800	-2.71697400	-1.93323900
C	-6.04190900	-0.50509800	-1.95131800
H	-5.09035400	0.00831700	-2.12458400
H	-6.72140400	0.20898400	-1.47308600
H	-6.45999400	-0.76403000	-2.93245200
C	-4.89895100	-2.72723100	-1.78423300
H	-4.73050600	-3.62241700	-1.17583100
H	-3.92427600	-2.26509900	-1.97026000
H	-5.30110700	-3.04829500	-2.75351600
C	3.65820600	0.58090500	-0.56167100
C	-5.35560900	-1.39381000	0.31065700
O	-5.99740000	-1.65556500	1.33091800
N	-4.15356400	-0.76697700	0.27584000

H	-3.74271100	-0.61094500	-0.64106900
N	3.06314600	-2.98402700	0.12386000
C	3.46147000	-4.24309700	0.42429800
O	4.62762100	-4.59422000	0.62939800
H	2.06765200	-2.82540400	-0.03538900
H	-0.86674300	1.09694000	3.95502300
H	5.52038900	1.64269900	-0.42998500
N	0.91462200	6.12615200	1.33522300
C	1.94111900	5.21388700	0.84697900
H	2.93183200	5.59507900	1.12376900
H	1.80523500	4.22620000	1.29626500
H	1.90436500	5.07313500	-0.24772900
C	-0.41035400	5.58722700	1.05891400
H	-0.49673600	4.58044300	1.48006200
H	-1.16971100	6.23741500	1.51216500
H	-0.61264800	5.49800000	-0.02365400
C	1.06393700	7.42436900	0.72376900
H	0.30622800	8.11507300	1.11573400
H	2.05526300	7.83658400	0.95076800
H	0.95548600	7.39770100	-0.38298500
O	0.26962100	3.39896000	-1.34888700

Dioxo_{acylam} (Cis/Trans)

Mo	-0.06413200	-2.38678500	-0.81560400
S	1.95770500	-0.92170800	-0.59275500
S	-1.56995800	-0.08708900	-0.82995700
S	0.05126900	-1.97372500	1.79980200
S	-2.34776700	-3.22572300	-0.38134300
O	0.40584300	-4.04910600	-0.65170400
C	3.68171800	0.65993500	2.72810000
H	4.55002900	1.27167800	2.93565400
C	2.82377400	0.22254200	3.73768900
H	3.02988300	0.50211800	4.77000800
C	1.41810400	-0.95125300	2.12384100
C	-4.30628200	5.41843000	-0.10108700
H	-4.74627500	5.49487600	0.89733300
H	-5.13290400	5.42314400	-0.81760800
H	-3.68192100	6.30295000	-0.27899900
C	-3.13681600	-0.56041000	-0.24089400
C	3.39677600	0.29585700	1.40915300
C	-4.77898700	-2.26467500	3.35247400
C	1.71465000	-0.56025500	3.44560200
C	2.27400200	-0.50656200	1.08686600
C	-4.12544700	0.41744000	0.06894300
C	-3.46433800	4.15464800	-0.23725400
C	-5.40802300	0.06605200	0.49097200
H	-6.12585300	0.84924700	0.70365700
C	-2.88059100	4.08004100	-1.65375500
H	-2.27432200	4.97177400	-1.85845900
H	-3.67652700	4.03274300	-2.40547900
H	-2.23902800	3.20372200	-1.79461400
C	-2.32026900	4.19117800	0.78317100
H	-2.70531900	4.20500300	1.80867800
H	-1.71572700	5.09534500	0.63734500
H	-1.65151200	3.32939800	0.69270200
C	-5.72876400	-1.28512100	0.62512400
H	-6.72628900	-1.57198000	0.95375900
C	5.85075300	1.62765100	-1.19008500
C	7.13052000	2.45477800	-1.14520600
H	7.90221500	1.95774500	-0.55046700
H	6.95298800	3.43182400	-0.68715700
H	7.51287200	2.60643500	-2.16228800
C	6.14649400	0.26476500	-1.82861200
H	5.24830400	-0.35313900	-1.93106200
H	6.87178400	-0.30066900	-1.23313500
H	6.56768300	0.40266200	-2.83264000
C	4.79598400	2.36350300	-2.02531000
H	4.54160100	3.33008100	-1.57687900
H	3.86829000	1.79062600	-2.12509400

H	5.17919500	2.55039100	-3.03655400
C	-3.48636500	-1.92141500	-0.07256500
C	5.33685200	1.43320300	0.25901500
O	5.93647100	1.91127700	1.22572200
N	4.19642100	0.70305600	0.32059600
H	3.81579200	0.36965600	-0.56114800
N	-3.70391900	1.75056800	-0.07725700
C	-4.36916800	2.92481300	0.02401100
O	-5.56938200	3.04735000	0.29100200
H	-2.71364900	1.77965900	-0.32636100
H	1.05127800	-0.89658100	4.23932300
H	-5.02344200	-3.31847600	0.47101000
O	0.19200000	-2.06072600	-2.50910000

Trans-E_{acylam}

Mo	-0.00001600	0.00000000	0.89625000
S	-2.30018800	-0.33753900	0.15913500
S	2.30021100	0.33753900	0.15930800
S	-0.41967800	2.26186000	0.10667200
S	0.41968900	-2.26187200	0.10673000
O	-0.00008100	0.00001400	2.60344800
C	-4.95307400	2.69259500	-0.53398000
H	-6.02345700	2.77626900	-0.67659200
C	-4.11341500	3.80678400	-0.56117700
H	-4.54182800	4.79351000	-0.73314600
C	-2.16645300	2.41195200	-0.13357500
C	8.34604900	1.63021300	-0.46028000
H	8.69350800	1.22437800	-1.41435000
H	8.86740900	1.08140500	0.32944500
H	8.63054100	2.68809000	-0.39958600
C	2.99491500	-1.27470100	-0.10632900
C	-4.38579800	1.43375500	-0.31254200
C	2.74146800	-3.67039600	-0.36881400
C	-2.74146200	3.67041500	-0.36880200
C	-2.99489600	1.27470500	-0.10646300
C	4.38581600	-1.43374500	-0.31242900
C	6.83430200	1.48961900	-0.32166300
C	4.95308000	-2.69257400	-0.53396200
H	6.02345800	-2.77624500	-0.67660900
C	6.39211600	2.04681900	1.03676800
H	6.71089400	3.09241300	1.13573000
H	6.83783400	1.47916500	1.86098400
H	5.30526200	2.02255900	1.16754800
C	6.14156500	2.27361900	-1.44311400
H	6.41988000	1.88075600	-2.42734500
H	6.43689000	3.32994200	-1.40482000
H	5.05049700	2.23123700	-1.36404000
C	4.11341700	-3.80675800	-0.56121600
H	4.54182400	-4.79347500	-0.73325800
C	-6.83428100	-1.48963700	-0.32158600
C	-8.34602500	-1.63025300	-0.46018300
H	-8.69347600	-1.22474100	-1.41439700
H	-8.86738600	-1.08118000	0.32935400
H	-8.63053000	-2.68810700	-0.39916200
C	-6.14156100	-2.27380600	-1.44291600
H	-5.05048700	-2.23142500	-1.36392600
H	-6.41991300	-1.88113400	-2.42721400
H	-6.43686500	-3.33012800	-1.40442400
C	-6.39211300	-2.04665700	1.03694900
H	-6.83776200	-1.47881100	1.86107100
H	-5.30525400	-2.02244600	1.16766400
H	-6.71097500	-3.09220600	1.13610800
C	2.16646600	-2.41194400	-0.13351300
C	-6.46579100	0.01135600	-0.43661000
O	-7.32196500	0.87057600	-0.66883100
N	-5.14285500	0.24515500	-0.27063400
H	-4.54403100	-0.55726500	-0.08057700

N	5.14288400	-0.24514800	-0.27051500
C	6.46579700	-0.01135900	-0.43666700
O	7.32192600	-0.87055600	-0.66914000
H	4.54409700	0.55726400	-0.08028400
H	-2.08936900	4.54214000	-0.39165000
H	2.08937200	-4.54211600	-0.39171200

Trans-TS1_{acylam} (Cis Attack)

Mo	-0.27371700	-0.63690700	1.22673700
S	1.42510200	0.12179000	-0.78452300
S	-2.42136500	-0.50223500	0.13774400
S	0.24127300	-2.75340700	0.01251400
S	-0.55764300	1.79837700	1.38681900
O	-0.67152100	-1.14834900	2.81465200
C	4.63287200	-2.34655600	-1.29404600
H	5.67016900	-2.22567700	-1.58435900
C	4.09166700	-3.59115500	-0.97256500
H	4.72483100	-4.47725800	-1.00987500
C	1.92006700	-2.58590100	-0.49690000
C	-8.11161600	-0.98093500	-2.25836500
H	-8.17967000	-0.24033600	-3.06036200
H	-8.84586500	-0.69840400	-1.49817900
H	-8.38489300	-1.96389500	-2.66220200
C	-3.03948500	1.15020700	0.36790500
C	3.79998900	-1.22374200	-1.23647600
C	-2.74597300	3.45276200	1.07215500
C	2.75794900	-3.70727800	-0.58225200
C	2.43620400	-1.31276100	-0.85675500
C	-4.35889000	1.47978700	-0.02778200
C	-6.70364000	-1.03367100	-1.67559800
C	-4.87257500	2.77049700	0.13224600
H	-5.88870600	2.98163700	-0.17822600
C	-6.65770900	-2.06690800	-0.54340100
H	-6.96890700	-3.05042600	-0.91822900
H	-7.33250600	-1.78773600	0.27373400
H	-5.65339100	-2.17850300	-0.12202000
C	-5.71158200	-1.43779500	-2.77363700
H	-5.69689800	-0.69874600	-3.58221300
H	-6.00070500	-2.40478600	-3.20476000
H	-4.68838400	-1.53745600	-2.39691000
C	-4.04964900	3.75192500	0.68639900
H	-4.43574900	4.76261900	0.81490800
C	5.42335900	2.11248300	-2.11188000
C	6.84362800	2.58654200	-2.39953100
H	7.26330400	2.06492700	-3.26412400
H	7.50721000	2.38604800	-1.55269500
H	6.84554200	3.66578600	-2.59794300
C	4.52398500	2.43133800	-3.31275700
H	3.48466300	2.13768400	-3.13281500
H	4.86959100	1.90803400	-4.21145100
H	4.53668900	3.50915600	-3.52186000
C	4.88372700	2.83658700	-0.87222700
H	5.46828300	2.58358700	0.02031500
H	3.83482600	2.59232200	-0.66611400
H	4.94278300	3.92341300	-1.01537500
C	-2.22853800	2.15715800	0.92426700
O	1.98646500	-0.99518300	2.10178600
N	2.59829000	-0.03393100	2.86359800
C	3.84061000	-0.65598800	3.39962000
C	2.96396200	1.15933300	2.03741400
C	1.71175000	0.39570400	3.99139600
H	3.48351400	1.89716800	2.66139100
H	3.59197500	0.80220700	1.21981100
H	2.03943300	1.56127500	1.61770700
H	0.82987500	0.86885800	3.55090400
H	1.39822600	-0.50903500	4.51135300
H	2.25693000	1.08557200	4.64684300

H	4.40728300	0.06264400	4.00387100
H	3.53667800	-1.51860000	3.99240300
H	4.41750500	-0.99432700	2.53789300
C	5.44843300	0.57746400	-1.88810900
O	6.48393500	-0.08026800	-2.04991400
N	4.24412700	0.08170500	-1.53212100
H	3.46320300	0.73610000	-1.41707700
N	-5.10097700	0.42022700	-0.58685500
C	-6.33996900	0.37034100	-1.12911800
O	-7.12859200	1.31799700	-1.20428200
H	-4.54910000	-0.43690300	-0.59704800
H	2.34886300	-4.67814600	-0.30713700
H	-2.10216200	4.22267700	1.49574400

Trans-ES_{acylam} (Cis Attack)

Mo	-0.26042200	-1.18277700	0.96299800
S	1.33838500	0.43612100	-0.78388600
S	-2.37310400	-0.54440600	-0.06502000
S	0.29893600	-2.60818700	-1.03145400
S	-0.55365600	0.96281500	2.12648300
O	-0.74815400	-2.29012600	2.17643600
C	4.66951100	-1.56566700	-2.02639500
H	5.69915800	-1.30168400	-2.23809100
C	4.19483300	-2.87001700	-2.15604700
H	4.87219200	-3.65909300	-2.48229700
C	1.96885600	-2.19180100	-1.41264400
C	-8.01096400	0.10803300	-2.54919600
H	-8.06441900	1.11249800	-2.97882200
H	-8.75089200	0.06355800	-1.74474100
H	-8.28679700	-0.62038500	-3.32207400
C	-2.98814000	0.86458100	0.82475000
C	3.77822500	-0.57107000	-1.60777100
C	-2.71576800	2.64482400	2.45284900
C	2.86756300	-3.17527800	-1.85075700
C	2.41576000	-0.84409100	-1.31125600
C	-4.29004100	1.36007000	0.56356000
C	-6.61033700	-0.19486700	-2.02883200
C	-4.80458100	2.47053100	1.23988800
H	-5.80770400	2.81185500	1.01485100
C	-6.58117800	-1.60795000	-1.43338300
H	-6.89252500	-2.34171100	-2.18806200
H	-7.26362800	-1.69113800	-0.58004400
H	-5.58186400	-1.89351000	-1.08887700
C	-5.60582100	-0.10895800	-3.18455200
H	-5.57794800	0.90130600	-3.60752100
H	-5.89227700	-0.80292000	-3.98529600
H	-4.58791400	-0.36595800	-2.87409000
C	-4.00121900	3.10763100	2.18584200
H	-4.38738600	3.97603000	2.71863800
C	5.25897800	2.90904400	-1.14415300
C	6.65134000	3.52134200	-1.24785500
H	7.05470600	3.41721400	-2.25930700
H	7.35276000	3.02397700	-0.57148700
H	6.61137100	4.58791400	-0.99270200
C	4.30981800	3.62526200	-2.11222000
H	3.28497600	3.24651300	-2.03966100
H	4.63972500	3.50220800	-3.15002200
H	4.28374800	4.70033700	-1.89072000
C	4.73397600	3.07126300	0.28820300
H	5.36193100	2.52462400	1.00212800
H	3.70557700	2.70672300	0.39716700
H	4.74012200	4.13042900	0.57661200
C	-2.19931500	1.52347600	1.78718800
O	1.83765400	-1.74138100	1.44969900
N	2.56617500	-1.17913800	2.49259400
C	3.80526900	-1.99491300	2.58179200
C	2.92351600	0.24006900	2.19448800

C	1.79202700	-1.25881100	3.76707300
H	3.51169300	0.64754000	3.02553600
H	3.48620200	0.24227200	1.25935100
H	1.99298800	0.79339000	2.04561200
H	0.89956200	-0.63785600	3.64882600
H	1.48375600	-2.29718300	3.88958100
H	2.41735300	-0.91183400	4.59776800
H	4.46327500	-1.60646300	3.36717100
H	3.50164300	-3.02075600	2.78957200
H	4.28446700	-1.95056800	1.60261800
C	5.34925100	1.40321400	-1.50698200
O	6.42570900	0.87954300	-1.82220600
N	4.15678400	0.77565700	-1.43142100
H	3.33326000	1.31286500	-1.13197100
N	-5.01618600	0.65519700	-0.41650500
C	-6.25043300	0.84482800	-0.93769800
O	-7.03903400	1.73749000	-0.60929500
H	-4.46436500	-0.12235500	-0.77963100
H	2.50952700	-4.20078100	-1.92593100
H	-2.08708600	3.14741100	3.18693800

Trans-TS2_{acylam} (Cis Attack)

Mo	-0.61345100	0.59561600	1.09664100
S	2.75478000	-0.98169400	-1.68359500
S	-2.69871100	-0.31737300	0.17456000
S	0.24032500	-1.64504100	0.52998200
S	-1.45280700	2.64106900	0.04650500
O	-0.86171300	0.73491300	2.78165800
C	4.66773300	-1.79619100	1.82132400
H	5.70606900	-1.81142100	2.13301100
C	3.62342000	-2.04700100	2.70967000
H	3.83873200	-2.27755800	3.75214100
C	1.97924200	-1.68662900	0.93240000
C	-5.65095600	-3.18023300	-0.06912500
H	-5.27313100	-2.78870300	0.88169700
H	-4.84025200	-3.10509700	-0.80165900
H	-5.85672500	-4.24687300	0.07895600
C	-3.69553900	1.06326800	-0.30304400
C	4.36116700	-1.49256900	0.49532300
C	-3.95507400	3.43142800	-0.78147800
C	2.30658000	-1.98673300	2.26344100
C	3.01848300	-1.43216900	-0.00639600
C	-5.05863900	0.88365900	-0.64984800
C	-6.92295200	-2.47133800	-0.53014300
C	-5.85694200	1.95857400	-1.05272500
H	-6.89500700	1.78232400	-1.30472400
C	-7.40554600	-3.09397100	-1.84373000
H	-7.63130600	-4.15799300	-1.69958100
H	-6.64023100	-3.01490200	-2.62361200
H	-8.30666100	-2.58461400	-2.19725900
C	-8.01327500	-2.63881300	0.53308700
H	-7.69404200	-2.22228200	1.49499800
H	-8.23787600	-3.70220700	0.68385900
H	-8.92726300	-2.12291200	0.22500100
C	-5.29066500	3.23175900	-1.11729200
H	-5.90448000	4.07476700	-1.43078100
C	7.27976500	-0.37120800	-1.66404300
C	7.07388000	-1.40524000	-2.77624800
H	6.01377500	-1.56720400	-2.99829600
H	7.50951700	-2.37248500	-2.50063500
H	7.56071800	-1.06731300	-3.70121100
C	6.60709900	0.94780100	-2.06902400
H	6.71203500	1.69908000	-1.27692000
H	5.53571100	0.81306800	-2.26457600
H	7.07100500	1.35041900	-2.97981600
C	8.77184100	-0.14040800	-1.45225000
H	9.27452000	-1.06450400	-1.15036100

H	8.94830900	0.59123300	-0.65885600
H	9.23203500	0.22331000	-2.38012000
C	-3.15301000	2.35926200	-0.37135100
O	1.36243100	0.93791300	0.83368400
N	2.09846400	2.22443700	0.47318400
C	3.51274000	1.83507800	0.65020500
C	1.82570800	2.53474300	-0.94520900
C	1.68469700	3.28733300	1.39744900
H	2.46819000	3.36737000	-1.25860100
H	2.05170700	1.62015900	-1.50705000
H	0.77138000	2.79700100	-1.04867700
H	0.59456300	3.36824600	1.35348200
H	1.98483500	2.99321000	2.40449600
H	2.15401200	4.23570400	1.11085000
H	4.15408900	2.71482900	0.51871200
H	3.62228900	1.40318300	1.64605700
H	3.73120200	1.07162800	-0.10257600
C	6.65545600	-0.86458500	-0.33234400
O	7.32649900	-0.92280200	0.70698200
N	5.34953900	-1.17750000	-0.45515100
H	4.87158800	-1.02485200	-1.36074900
N	-5.54076300	-0.43823400	-0.54825000
C	-6.77115400	-0.95181100	-0.77937500
O	-7.75338900	-0.30621800	-1.16212900
H	-4.81068600	-1.07051000	-0.22787800
H	1.48478800	-2.15148300	2.95740400
H	-3.51152900	4.42471800	-0.83056400

Dioxo_P_{acylam} (Trans/Trans) (Cis Attack)

Mo	-0.09709900	2.74894200	-0.25310500
S	-0.98389800	0.23105100	0.01116200
S	2.33909300	1.50669700	-0.25660700
S	-0.46971900	2.09173700	-2.60376700
S	0.35480500	2.37464900	2.16930700
O	0.77047300	4.10480000	-0.90780800
C	-2.62294900	-1.92836500	-3.01444500
H	-3.13608600	-2.87822000	-3.10268900
C	-2.39071600	-1.11009500	-4.12017100
H	-2.72725300	-1.42996100	-5.10478200
C	-1.29800100	0.54476100	-2.71327800
C	6.76436600	-2.72229900	-1.21074800
H	6.48184400	-3.69651500	-0.80180700
H	7.60068900	-2.35324000	-0.60950600
H	7.10647900	-2.85828800	-2.24431400
C	2.43749500	0.75031200	1.30898700
C	-2.18417000	-1.50641800	-1.75841100
C	1.76343700	0.57267100	3.64578700
C	-1.74023800	0.11099500	-3.97302900
C	-1.50890400	-0.26705700	-1.57670200
C	3.37812500	-0.28852400	1.55691600
C	5.59054900	-1.74982600	-1.17572500
C	3.52975400	-0.86056100	2.82071800
H	4.26706200	-1.64113900	2.96299200
C	6.03023700	-0.39693200	-1.74857200
H	6.40353000	-0.52647300	-2.77261900
H	6.83516400	0.04286000	-1.14905300
H	5.21065400	0.32877600	-1.78598100
C	4.43661800	-2.30823400	-2.01772700
H	4.07447100	-3.25886200	-1.61162900
H	4.77293700	-2.48697900	-3.04704700
H	3.58537500	-1.62165800	-2.06236300
C	2.72061800	-0.41319500	3.86527000
H	2.82875200	-0.85316200	4.85507600
C	-3.06446100	-3.80307900	1.14363700
C	-3.68354500	-5.18924200	1.28268100
H	-3.08556200	-5.94356400	0.76239100
H	-4.68722000	-5.21911700	0.84938400

H	-3.74672100	-5.46385300	2.34279100
C	-1.65890000	-3.80599700	1.75717300
H	-1.18773700	-2.81760400	1.74827300
H	-0.99404300	-4.49317100	1.22289800
H	-1.70849900	-4.13125000	2.80369800
C	-3.93844000	-2.77458400	1.87266800
H	-4.94262000	-2.72767400	1.43509900
H	-3.51338600	-1.76468100	1.82596000
H	-4.04091100	-3.04267800	2.93196600
C	1.60442800	1.15537800	2.37897600
O	-1.59579400	3.43773000	0.30095500
N	-4.92041800	1.60184100	1.10398300
C	-6.01858100	0.81395900	1.60715000
C	-4.47947700	1.09839400	-0.18602000
C	-3.81487600	1.60407800	2.04814800
H	-4.13925600	0.04358500	-0.13459300
H	-5.30178000	1.15962700	-0.90916400
H	-3.63502000	1.69256800	-0.54703700
H	-2.97856000	2.18124700	1.64389900
H	-4.14124500	2.05187400	2.99493800
H	-3.43956700	0.58108800	2.25694200
H	-5.74650500	-0.25248900	1.77219100
H	-6.36520800	1.21973300	2.56587200
H	-6.85706400	0.83645800	0.89978900
C	-3.00683100	-3.43411200	-0.35829800
O	-3.49982600	-4.15821400	-1.22793200
N	-2.39020600	-2.24808000	-0.58283200
H	-2.02535900	-1.74620100	0.22711700
N	4.11495400	-0.70086300	0.43324900
C	5.12977700	-1.58583600	0.29364500
O	5.65739900	-2.22048900	1.21254000
H	3.77646400	-0.22185000	-0.40338700
H	-1.56390400	0.75054800	-4.83555500
H	1.11354600	0.90050700	4.45453600

Dioxo_{acylam} (Trans/Trans)

Mo	-3.38924400	-0.01373400	0.00908600
S	-1.27911300	-0.84234800	1.50232200
S	-1.31012300	0.84935600	-1.50705200
S	-2.85314300	-2.22847100	-0.98987800
S	-2.87789300	2.21062500	1.00184700
O	-4.46075100	0.21784200	-1.33843900
C	1.45666000	-3.42519800	-0.02571900
H	2.49898600	-3.65480800	0.16053400
C	0.70596500	-4.11999200	-0.97401100
H	1.16561900	-4.93478300	-1.53124700
C	-1.22315900	-2.70446500	-0.53705800
C	4.68751200	0.30859000	-3.05618500
H	5.25215900	0.24849300	-2.12087500
H	4.99363400	1.22997800	-3.56078800
H	4.96200800	-0.54860700	-3.68301700
C	-0.54701800	2.04489200	-0.49243700
C	0.85487100	-2.37829300	0.67532400
C	-0.64340100	3.75042800	1.24620000
C	-0.60852700	-3.74997600	-1.24378100
C	-0.51389100	-2.03820700	0.48947600
C	0.82052600	2.38869000	-0.67922400
C	3.18622400	0.29520700	-2.79049000
C	1.41922100	3.43865900	0.01996400
H	2.46078900	3.67138600	-0.16660500
C	2.42809400	0.36527400	-4.12251700
H	2.69931300	-0.48973300	-4.75481200
H	2.67258800	1.28325500	-4.67022300
H	1.34276900	0.33820000	-3.97867500
C	2.80582500	-0.99376700	-2.05198100
H	3.27786500	-1.04776000	-1.06446200
H	3.13569700	-1.87052600	-2.62309300
H	1.72594700	-1.10157300	-1.90051600
C	0.66777400	4.12857900	0.97128500

H	1.12491300	4.94509500	1.52804800
C	3.22163400	-0.27896400	2.77705100
C	4.70473800	-0.34231600	3.12516800
H	5.32007000	-0.35495400	2.22114700
H	4.94179600	-1.24915800	3.69026800
H	4.98377700	0.53203000	3.72576100
C	2.93388700	0.98869200	1.96256400
H	1.86911400	1.11267400	1.73536600
H	3.47326400	0.98863900	1.00800800
H	3.24785700	1.88064800	2.51898000
C	2.39276700	-0.25608000	4.06735100
H	2.56027200	-1.16158600	4.66234100
H	1.31838700	-0.17820500	3.86995100
H	2.67697500	0.60941700	4.67913100
C	-1.25532000	2.70340200	0.53953800
C	2.85858700	-1.52605300	1.93823500
O	3.69547300	-2.38768000	1.64884400
N	1.55524700	-1.54872400	1.56586300
H	0.95813600	-0.77929800	1.87380400
N	1.52280000	1.55683000	-1.56604200
C	2.82737400	1.53091100	-1.93260000
O	3.66561400	2.38915500	-1.63692500
H	0.92444000	0.78909000	-1.87601600
H	-1.17551700	-4.25614700	-2.02239300
H	-1.20918000	4.25085400	2.02935900
O	-4.44501800	-0.26171700	1.36613200

Table S5

Cis-ES_{acylam} (Trans attack)

Mo	-0.01659800	-1.43357100	-1.24229100
S	1.74780700	0.19611500	-0.64045600
S	-1.83132000	0.18074900	-0.83990000
S	1.71489300	-3.05456800	-0.60687400
S	-1.72827400	-3.08130500	-0.68108000
O	0.03594400	-1.46643200	-2.94288000
C	5.63815900	-0.76777400	0.15245600
H	6.54886600	-0.21514400	0.34916900
C	5.60407200	-2.16260700	0.14800300
H	6.51851200	-2.72174300	0.34308200
C	3.22055400	-2.14741400	-0.35574000
C	-5.93573300	4.66825800	0.19115600
H	-6.35162800	4.56538400	1.19745400
H	-6.75495100	4.49623500	-0.51306400
H	-5.57132800	5.69534200	0.06217700
C	-3.23846100	-0.76989000	-0.33808700
C	4.45391500	-0.06846000	-0.09829900
C	-4.33439600	-2.87793500	0.15781300
C	4.41344900	-2.84098000	-0.09824200
C	3.23011300	-0.73643500	-0.36404800
C	-4.44111700	-0.11339800	0.02755500
C	-4.79705100	3.68040000	-0.03699600
C	-5.57304300	-0.81868600	0.44964300
H	-6.46905600	-0.27245200	0.71918400
C	-4.25359300	3.84618500	-1.46129800
H	-3.91349700	4.87823500	-1.61798700
H	-5.02730100	3.62906000	-2.20612200
H	-3.40488700	3.18417400	-1.66292700
C	-3.67324000	3.95478200	0.97009200
H	-4.02182400	3.80818900	1.99866100
H	-3.32576000	4.99191100	0.87537900
H	-2.80936100	3.30017500	0.81558700
C	-5.50533400	-2.21044800	0.50963800
H	-6.37745100	-2.77694600	0.83491800
C	4.71589100	3.72841500	0.09111600
C	5.82873800	4.72328600	0.40120700
H	6.65789100	4.62001200	-0.30480000
H	6.23841600	4.55919100	1.40188900
H	5.44138100	5.74809000	0.34280200
C	4.16993300	3.99371200	-1.31698400
C	3.33241000	3.33518300	-1.56936300
H	4.94726800	3.85022800	-2.07559900
H	3.81041900	5.02795800	-1.39218500
C	3.58331800	3.89141800	1.11315300
H	3.93522100	3.67465300	2.12808900
H	2.73671200	3.22831700	0.90544000
H	3.20844500	4.92287000	1.09925300
C	-3.19244500	-2.17853500	-0.26422300
C	5.29505200	2.29378200	0.17964900
O	6.47301700	2.08942900	0.49102700
N	4.38039100	1.33832200	-0.10666100
H	3.43283300	1.64154000	-0.33577900
N	-4.40151300	1.29316200	-0.05152000
C	-5.33999300	2.24173100	0.16329600
O	-6.51415000	2.03400600	0.48982400
H	-3.46747800	1.60408300	-0.32248100
H	4.38523000	-3.92989500	-0.09274500
H	-4.28322200	-3.96540500	0.20328400
N	0.06493200	-1.63787900	2.56456400
O	-0.45303000	-0.99366800	1.48342100
C	-0.58998000	-1.07738200	3.78215000
H	-1.66289800	-1.22770200	3.65858300
H	-0.22079600	-1.56712800	4.69305900
H	-0.37357500	-0.00897500	3.79399600
C	-0.21304200	-3.10819800	2.49078400

H	0.28919000	-3.48028200	1.59509200
H	0.15354800	-3.60663300	3.39795300
H	-1.29077000	-3.22082300	2.36771200
C	1.54411600	-1.41307500	2.64539600
H	1.70181700	-0.33467100	2.60430500
H	1.95186200	-1.85267300	3.56448600
H	1.98301200	-1.87265900	1.75973900

Cis-TS1'_{acylam} (Trans Attack)

Mo	0.01623100	-1.41240400	-1.08449000
S	1.87551100	0.18756400	-0.53183200
S	-1.84599700	0.20955500	-0.73440100
S	1.66549700	-3.06466100	-0.39846600
S	-1.78096200	-3.07975500	-0.78509900
O	0.10624500	-1.35892000	-2.79222100
C	5.69985700	-0.96319400	0.32008400
H	6.64377400	-0.45709900	0.48375800
C	5.58081800	-2.35093800	0.40201000
H	6.45773900	-2.95163800	0.63972900
C	3.20714700	-2.22054600	-0.12972400
C	-6.01549100	4.64517500	0.35251000
H	-6.43365300	4.47272500	1.34859100
H	-6.83272600	4.52256700	-0.36362200
H	-5.65114900	5.67873600	0.29941700
C	-3.29764600	-0.76422800	-0.41745100
C	4.56224900	-0.20915600	0.01923900
C	-4.42815000	-2.88544000	-0.12206700
C	4.35259300	-2.96867700	0.18130900
C	3.29731300	-0.81396500	-0.20865900
C	-4.51749300	-0.11596200	-0.10125200
C	-4.87569500	3.67661700	0.05681200
C	-5.68134900	-0.83556500	0.18847800
H	-6.59367200	-0.30164100	0.42348500
C	-4.32339200	3.95115100	-1.34744100
H	-3.98045300	4.99112500	-1.42165800
H	-5.09323500	3.79378600	-2.11092400
C	-3.47475300	3.30411400	-1.59179800
C	-3.75861700	3.87202400	1.08919400
H	-4.11001900	3.63957400	2.10065100
H	-3.41878100	4.91553000	1.08162000
H	-2.88615500	3.24151200	0.88836000
C	-5.61787800	-2.22900900	0.17165500
H	-6.51382800	-2.80703700	0.39646300
C	5.07584200	3.56433500	-0.11364200
C	6.25657700	4.50538600	0.09758300
H	7.06120400	4.29683800	-0.61365600
H	6.67759900	4.39041400	1.10031800
H	5.93354700	5.54581800	-0.03360600
C	4.53347600	3.73555900	-1.53750000
H	3.65112600	3.11495200	-1.72460300
H	5.29091800	3.46890200	-2.28299200
H	4.24514200	4.78092200	-1.70796400
C	3.96949400	3.89730500	0.89529900
H	4.32043000	3.75781900	1.92401600
H	3.08220200	3.27026800	0.75861800
H	3.65784900	4.94391300	0.78346700
C	-3.25049200	-2.17659000	-0.42483200
C	5.55786300	2.10731700	0.10412900
O	6.72253000	1.85324500	0.42940400
N	4.57846000	1.19482000	-0.08991900
H	3.65164500	1.53775800	-0.34897000
N	-4.46901000	1.29283100	-0.07696100
C	-5.42536900	2.22878600	0.12494600
O	-6.62136200	2.00138100	0.33332200
H	-3.51590700	1.61875200	-0.23875600
H	4.25880900	-4.05210100	0.24325500
H	-4.38498800	-3.97365500	-0.12909400
N	-0.16225300	-1.39825400	2.54531300

O	-0.77717100	-0.69183200	0.99692600
C	-0.96497700	-0.61824200	3.46514700
H	-2.01681500	-0.75180200	3.20226600
H	-0.78953200	-0.93087300	4.51069500
H	-0.70966100	0.43618600	3.34380300
C	-0.52112100	-2.80661400	2.54154100
H	0.05433900	-3.31249300	1.76260200
H	-0.31518000	-3.26276600	3.52811500
H	-1.58240800	-2.89461300	2.29757200
C	1.26285700	-1.15009000	2.67740200
H	1.45794400	-0.09578700	2.46861100
H	1.61203100	-1.41352800	3.69268100
H	1.79735400	-1.74884300	1.93778600

Cis-INT1_{acylam} (Trans Attack)

Mo	0.31779800	-1.56408900	-1.28856700
S	2.01586800	0.05499900	-0.59747200
S	-2.53494200	-0.00545300	-1.79101400
S	1.55672500	-3.05200400	0.19061300
S	-1.62867100	-3.07325400	-0.86112500
O	0.76581500	-1.95467900	-2.88323900
C	5.50601600	-0.94476500	1.27585500
H	6.43216500	-0.43817000	1.51897500
C	5.27104400	-2.27261500	1.63290100
H	6.03816000	-2.82287500	2.17645200
C	3.06771400	-2.21800500	0.59565700
C	-6.06310500	4.40848500	0.81990400
H	-5.97031400	4.32801300	1.90676700
H	-7.10072200	4.17314400	0.56778500
H	-5.85399700	5.44495800	0.52754700
C	-3.39543800	-0.90657900	-0.55406400
C	4.50621000	-0.25382500	0.58430200
C	-3.92759500	-2.98626900	0.57143000
C	4.07339200	-2.89894500	1.30035400
C	3.27960500	-0.87134700	0.23841600
C	-4.44178200	-0.28088400	0.18547700
C	-5.09625000	3.46526400	0.11276500
C	-5.26227600	-1.01280300	1.04271300
H	-6.06865700	-0.51501700	1.56625300
C	-5.25414800	3.61637500	-1.40554800
H	-5.05664700	4.65372200	-1.70480200
H	-6.27130700	3.36092800	-1.72361600
H	-4.55851500	2.97516500	-1.95764900
C	-3.65637400	3.81274300	0.51192600
H	-3.48554000	3.63840000	1.57989500
H	-3.45516700	4.87142200	0.30505700
H	-2.91296700	3.22544800	-0.03788200
C	-5.00716100	-2.38113200	1.19608300
H	-5.65330200	-2.97147700	1.84448800
C	5.34932100	3.34816900	-0.34062900
C	6.51923200	4.28672700	-0.06716400
H	7.45448800	3.87498200	-0.45643800
H	6.65996400	4.44055400	1.00674100
H	6.33626000	5.25977400	-0.53983800
C	5.18456200	3.16479200	-1.85460700
H	4.32659600	2.53240500	-2.10426800
H	6.07644300	2.70563800	-2.29540700
H	5.03149800	4.13853500	-2.33738300
C	4.06444200	3.94909600	0.24188900
H	4.13608600	4.05544000	1.32976100
H	3.18045000	3.33994200	0.02627600
H	3.88896300	4.94517500	-0.18408900
C	-3.07162700	-2.26516800	-0.28862300
C	5.65122100	1.97861700	0.31920000
O	6.71983300	1.76228600	0.89898600
N	4.64147600	1.08838400	0.17619700
H	3.81130500	1.39446700	-0.33000000

N	-4.57122200	1.10566400	0.00132000
C	-5.43462100	2.01044500	0.52220600
O	-6.40520500	1.74540400	1.23654600
H	-3.82661900	1.44214400	-0.61622700
H	3.89517000	-3.93665500	1.57909000
H	-3.69506100	-4.03323200	0.75704600
N	-0.53830300	-0.56226600	1.89379500
O	-0.91136300	0.07046400	-1.33672900
C	-0.94107500	0.81232500	1.69866200
H	-1.87034300	0.84427300	1.12094800
H	-1.10466100	1.34684900	2.66313300
H	-0.16970800	1.33588500	1.12377200
C	-1.56887800	-1.33615100	2.54954900
H	-1.31485600	-2.40118800	2.49890900
H	-1.68847900	-1.04754100	3.61877200
H	-2.53051600	-1.18920400	2.05186000
C	0.69470600	-0.63961100	2.64831500
H	1.47757100	-0.06284400	2.14849400
H	0.56410900	-0.24530400	3.68239400
H	1.02787500	-1.68054700	2.70544100

Cis-TS2'_{acylam} (Trans Attack)

Mo	0.30014900	-1.56252300	-1.30792400
S	2.02099700	0.04806600	-0.60399600
S	-2.59490100	-0.02303300	-1.84882600
S	1.47698700	-3.02359500	0.27640000
S	-1.66105600	-3.07757700	-0.96649800
O	0.81204200	-2.00203900	-2.87291500
C	5.44091600	-0.95990200	1.38220300
H	6.37208600	-0.46452200	1.62939100
C	5.16849000	-2.26886900	1.78006300
H	5.91013700	-2.81567500	2.36112300
C	2.99146600	-2.20548400	0.68827700
C	-6.03333200	4.42153000	0.81638800
H	-5.93599900	4.36080900	1.90400600
H	-7.07058300	4.17562800	0.57225300
H	-5.83266500	5.45399700	0.50432000
C	-3.39687000	-0.90419800	-0.58190800
C	4.47395600	-0.27376100	0.64155400
C	-3.88818800	-2.98137200	0.57937300
C	3.96596300	-2.88160400	1.44058500
C	3.24141100	-0.87658700	0.28850600
C	-4.40311200	-0.27127700	0.21401900
C	-5.06295000	3.47277400	0.12175300
C	-5.18894800	-0.99886600	1.10307200
H	-5.97049600	-0.49610300	1.65905800
C	-5.23295600	3.59231300	-1.39796600
H	-5.05037200	4.62639500	-1.71754500
H	-6.24909000	3.31868100	-1.70385000
H	-4.53427800	2.94962100	-1.94451600
C	-3.62371300	3.84053700	0.50448700
H	-3.45176600	3.70617000	1.57793800
H	-3.42682000	4.89180400	0.25911000
H	-2.87992400	3.23487800	-0.02444900
C	-4.93914000	-2.37090600	1.24664200
H	-5.56193000	-2.95634000	1.92149800
C	5.42808000	3.26800100	-0.39990500
C	6.60706800	4.19359000	-0.12089600
H	7.54650300	3.75010800	-0.46255400
H	6.71439200	4.38383200	0.95100300
H	6.46028700	5.15154100	-0.63523900
C	5.31812700	3.02133000	-1.90984500
H	4.45510700	2.39851500	-2.16591100
H	6.21477900	2.52219800	-2.29389400
H	5.20863200	3.97558300	-2.44105100
C	4.13509200	3.92009800	0.10488800
H	4.16599200	4.07026100	1.18958300

H	3.24660900	3.32113900	-0.12095300
H	3.99876500	4.90124200	-0.36770800
C	-3.06803100	-2.26517000	-0.31786100
C	5.67351100	1.92354600	0.33022200
O	6.71199600	1.71270100	0.96394200
N	4.65259900	1.04656500	0.18224500
H	3.84846900	1.34794500	-0.36655100
N	-4.53287900	1.11387000	0.02930800
C	-5.38003600	2.02365700	0.56759900
O	-6.31903300	1.76635000	1.32581300
H	-3.81782500	1.44244900	-0.62577400
H	3.75967800	-3.90494400	1.75047200
H	-3.65185800	-4.02860200	0.75831500
N	-0.58553000	-0.46373800	1.87251200
O	-0.84022200	0.03661800	-1.42873000
C	-1.03093200	0.88542000	1.60788200
H	-1.96269600	0.85829400	1.03375600
H	-1.20945100	1.46484700	2.54332000
H	-0.27906500	1.40328200	1.00239500
C	-1.59291000	-1.23910800	2.56008000
H	-1.29709200	-2.29426200	2.57359600
H	-1.73732600	-0.89710000	3.61050200
H	-2.55210200	-1.15802200	2.04418100
C	0.64767400	-0.46849200	2.62907200
H	1.40826000	0.11980000	2.10887400
H	0.50228800	-0.04409000	3.64928700
H	1.01927600	-1.49428900	2.72251400

Dioxo_P_{acylam} (Cis/Trans) (Trans Attack)

Mo	-0.16633200	-2.58014500	-0.95999800
S	1.83016500	-1.06049700	-0.89256200
S	-1.51551400	-0.31826700	-0.21840800
S	0.59746900	-2.72463700	1.59894000
S	-2.37516300	-3.46169200	-0.31717400
O	0.29000500	-4.24343700	-1.14507700
C	4.42867800	-0.27304400	2.12930900
H	5.31415300	0.33740200	2.25189700
C	3.91663800	-1.05631000	3.16509000
H	4.42408600	-1.06153700	4.12883700
C	2.07252200	-1.82565400	1.76233500
C	-4.47913100	4.81365700	-1.34992200
H	-5.51046800	4.95576300	-1.01675100
H	-4.50525800	4.34572300	-2.34070100
H	-3.99617500	5.79351400	-1.45188000
C	-3.18503900	-0.80522100	-0.11033900
C	3.76583400	-0.28459200	0.89822600
C	-4.90388400	-2.53256000	0.02038900
C	2.76422500	-1.81050200	2.99159500
C	2.60062400	-1.06458100	0.69002000
C	-4.22767200	0.16083900	-0.02458500
C	-3.70873700	3.94771500	-0.35066300
C	-5.56693400	-0.20933600	0.11189100
H	-6.32260600	0.56318600	0.17835200
C	-2.28818300	3.72676800	-0.86998400
H	-1.79958100	4.69538200	-1.03313100
H	-2.28138200	3.18557200	-1.82241100
H	-1.65812100	3.16831300	-0.17003200
C	-3.66154800	4.66646600	1.00306300
H	-4.67546600	4.87176400	1.36117000
H	-3.11978900	5.61704000	0.91460700
H	-3.15108400	4.05757300	1.75657200
C	-5.89535600	-1.56427300	0.14494600
H	-6.93655300	-1.86310400	0.25328200
C	5.20605400	2.07677500	-1.72475500
C	6.42431600	2.98967700	-1.80623100
H	7.35210600	2.42062500	-1.69521200
H	6.41007600	3.73768500	-1.00898200

H	6.44110800	3.50468300	-2.77469000
C	5.26649100	1.04436300	-2.85726000
H	4.38444700	0.39645400	-2.88603900
H	6.14794000	0.40095300	-2.75986500
H	5.32768000	1.55531000	-3.82653200
C	3.92739900	2.91359300	-1.86285800
H	3.83984800	3.63779800	-1.04547700
H	3.02293700	2.29569100	-1.85342000
H	3.94007500	3.46913900	-2.80909600
C	-3.55568100	-2.17101600	-0.11702100
C	5.21095700	1.37133700	-0.34561000
O	6.06271000	1.62566500	0.50891900
N	4.19245100	0.48660300	-0.20226900
H	3.56266200	0.38099500	-0.99358000
N	-3.81187700	1.50259100	-0.13779300
C	-4.52576500	2.65257500	-0.13034600
O	-5.74348900	2.73367100	0.07001300
H	-2.80805800	1.55381600	-0.30777000
H	2.36025500	-2.39906900	3.81240800
H	-5.16129200	-3.58974500	0.01927700
N	0.70587700	2.44390400	2.33771700
O	-0.23685800	-2.00671300	-2.60144000
C	-0.68435500	2.84394700	2.38855200
H	-0.79930100	3.84791500	1.95920400
H	-1.35418200	2.14950000	1.83917300
H	-1.02396700	2.87789400	3.43112600
C	1.18163000	2.43711000	0.96295100
H	2.24334100	2.16466300	0.94736500
H	0.63955300	1.71458500	0.32123400
H	1.07337900	3.43976000	0.52802200
C	0.86508200	1.11523800	2.91581500
H	0.53559600	1.12921600	3.96153500
H	0.28509100	0.34218000	2.37721500
H	1.92050600	0.82796900	2.89094400

Dioxo_{acylam} (Cis/Trans)

Mo	-0.06413200	-2.38678500	-0.81560400
S	1.95770500	-0.92170800	-0.59275500
S	-1.56995800	-0.08708900	-0.82995700
S	0.05126900	-1.97372500	1.79980200
S	-2.34776700	-3.22572300	-0.38134300
O	0.40584300	-4.04910600	-0.65170400
C	3.68171800	0.65993500	2.92810000
H	4.55002900	1.27167800	2.93565400
C	2.82377400	0.22254200	3.73768900
H	3.02988300	0.50211800	4.77000800
C	1.41810400	-0.95125300	2.12384100
C	-4.30628200	5.41843000	-0.10108700
H	-4.74627500	5.49487600	0.89733300
H	-5.13290400	5.42314400	-0.81760800
H	-3.68192100	6.30295000	-0.27899900
C	-3.13681600	-0.56041000	-0.24089400
C	3.39677600	0.29585700	1.40915300
C	-4.77898700	-2.26467500	0.35247400
C	1.71465000	-0.56025500	3.44560200
C	2.27400200	-0.50656200	1.08686600
C	-4.12544700	0.41744000	0.06894300
C	-3.46433800	4.15464800	-0.23725400
C	-5.40802300	0.06605200	0.49097200
H	-6.12585300	0.84924700	0.70365700
C	-2.88059100	4.08004100	-1.65375500
H	-2.27432200	4.97177400	-1.85845900
H	-3.67652700	4.03274300	-2.40547900
H	-2.23902800	3.20372200	-1.79461400
C	-2.32026900	4.19117800	0.78317100
H	-2.70531900	4.20500300	1.80867800
H	-1.71572700	5.09534500	0.63734500

H	-1.65151200	3.32939800	0.69270200
C	-5.72876400	-1.28512100	0.62512400
H	-6.72628900	-1.57198000	0.95375900
C	5.85075300	1.62765100	-1.19008500
C	7.13052000	2.45477800	-1.14520600
H	7.90221500	1.95774500	-0.55046700
H	6.95298800	3.43182400	-0.68715700
H	7.51287200	2.60643500	-2.16228800
C	6.14649400	0.26476500	-1.82861200
H	5.24830400	-0.35313900	-1.93106200
H	6.87178400	-0.30066900	-1.23313500
H	6.56768300	0.40266200	-2.83264000
C	4.79598400	2.36350300	-2.02531000
H	4.54160100	3.33008100	-1.57687900
H	3.86829000	1.79062600	-2.12509400
H	5.17919500	2.55039100	-3.03655400
C	-3.48636500	-1.92141500	-0.07256500
C	5.33685200	1.43320300	0.25901500
O	5.93647100	1.91127700	1.22572200
N	4.19642100	0.70305600	0.32059600
H	3.81579200	0.36965600	-0.56114800
N	-3.70391900	1.75056800	-0.07725700
C	-4.36916800	2.92481300	0.02401100
O	-5.56938200	3.04735000	0.29100200
H	-2.71364900	1.77965900	-0.32636100
H	1.05127800	-0.89658100	4.23932300
H	-5.02344200	-3.31847600	0.47101000
O	0.19200000	-2.06072600	-2.50910000

Trans-ES_{acylam} (Trans Attack)

Mo	-0.07054400	0.19218400	-1.42758100
S	2.36302700	-0.10054500	-1.15980500
S	-2.38346700	0.40390000	-0.60569300
S	0.44193800	2.54203200	-0.89112600
S	-0.44599900	-2.18622000	-0.91570900
O	-0.23734700	0.25135300	-3.11989000
C	4.77726900	2.65503000	0.64762000
H	5.78322500	2.65664500	1.04997900
C	3.96167900	3.78651200	0.67305300
H	4.34307500	4.71175300	1.10452200
C	2.12754900	2.56296000	-0.37917400
C	-8.27147300	1.54051200	0.91373600
H	-8.44473900	1.10757000	1.90305900
H	-8.91686500	1.00413500	0.21196600
H	-8.57309800	2.59516700	0.93351900
C	-2.99896900	-1.24227800	-0.36510800
C	4.26301900	1.48297500	0.08067500
C	-2.69462200	-3.65035400	-0.28163100
C	2.66414500	3.74043300	0.17062400
C	2.95303200	1.41820000	-0.45337700
C	-4.35500000	-1.44726100	-0.00037100
C	-6.80532900	1.42718000	0.51063200
C	-4.87833500	-2.72673600	0.20931400
H	-5.92137600	-2.83509400	0.48156600
C	-6.60867300	2.04168300	-0.88038900
H	-6.94430600	3.08660400	-0.88058800
H	-7.18781000	1.50061900	-1.63690800
H	-5.56023300	2.03326100	-1.19526500
C	-5.93567200	2.18013600	1.52542400
H	-6.03141300	1.74341300	2.52583200
H	-6.24828600	3.23054600	1.58407000
H	-4.87461300	2.16600400	1.25532000
C	-4.03237300	-3.82635100	0.06380100
H	-4.42554100	-4.82968900	0.22369900
C	6.55007100	-1.56448000	0.21381900
C	7.92513700	-1.86714100	0.79897100
H	7.94605900	-1.68232800	1.87696600

H	8.69335600	-1.23070800	0.35062900
H	8.18634500	-2.91723300	0.61709400
C	5.50117300	-2.46401500	0.88097000
H	4.50455000	-2.34203700	0.44169700
H	5.42086600	-2.24889800	1.95288700
H	5.78224900	-3.51925600	0.76905800
C	6.56620900	-1.83724800	-1.29521100
H	7.28452000	-1.18516200	-1.80477000
H	5.58564200	-1.67625500	-1.75463300
H	6.85738500	-2.87787000	-1.48881100
C	-2.16219900	-2.37029700	-0.50234000
C	6.21769700	-0.07151000	0.47371600
O	7.01947100	0.68033900	1.03924900
N	4.99507700	0.27788300	0.01551400
H	4.42965000	-0.45183700	-0.42091700
N	-5.12411700	-0.27398100	0.12690500
C	-6.41088000	-0.07133600	0.49337100
O	-7.21859300	-0.95601600	0.79626700
H	-4.55781800	0.54641900	-0.09188200
H	2.02469500	4.62093900	0.21524100
H	-2.03342200	-4.50927800	-0.39041000
N	0.47554400	-0.32520900	2.25124400
O	0.31103500	0.53477600	1.20794100
C	0.85696600	0.49625600	3.43691600
H	1.02445600	-0.13586900	4.31887300
H	1.75994000	1.04294800	3.15940100
H	0.04580800	1.20485600	3.60536100
C	-0.80437500	-1.05292200	2.52857900
H	-1.02489100	-1.65757000	1.64821700
H	-0.70672500	-1.67714600	3.42581800
H	-1.57777500	-0.29305700	2.64544000
C	1.56778000	-1.31455800	1.97707000
H	2.46008600	-0.73711200	1.73073100
H	1.72557300	-1.95326500	2.85609500
H	1.26130500	-1.89642400	1.10451700

Trans-TS1'_{acylam} (Trans Attack)

Mo	0.00369400	-0.13628200	-1.20218400
S	2.41011400	-0.37704900	-0.66926700
S	-2.34623000	0.24388700	-0.66676700
S	0.49747100	2.28421100	-0.94341100
S	-0.58102300	-2.49167600	-0.62534900
O	0.05814600	-0.25665600	-2.90747600
C	4.95284800	2.71162200	0.13601400
H	6.00146000	2.80338200	0.39043400
C	4.11533100	3.82105700	0.01855800
H	4.52455000	4.81796600	0.18024200
C	2.20508200	2.40116700	-0.52918600
C	-5.76897400	2.37469800	1.20803800
H	-4.71655200	2.27955200	0.91931500
H	-5.87023100	1.98097100	2.22549400
H	-6.00768600	3.44555400	1.23471100
C	-3.09967900	-1.34498100	-0.35861200
C	4.40451500	1.44283200	-0.07770000
C	-2.96689400	-3.74882500	-0.10362700
C	2.76994000	3.66972400	-0.29794000
C	3.04162200	1.26709100	-0.42160600
C	-4.48425900	-1.42849800	-0.07754400
C	-6.71201700	1.64955400	0.23927200
C	-5.11250400	-2.65362900	0.17054000
H	-6.17476700	-2.67809600	0.37947600
C	-8.15738900	1.89855100	0.65594600
H	-8.37224600	2.97426700	0.63832600
H	-8.34763700	1.51806700	1.66365600
H	-8.85517400	1.38917700	-0.01489900
C	-6.49011900	2.18325700	-1.18122900
H	-5.45278500	2.06648300	-1.51167300

H	-6.73175900	3.25303500	-1.22455800
H	-7.13037700	1.66299300	-1.90227100
C	-4.33211500	-3.81088800	0.15166000
H	-4.80308700	-4.77471700	0.34333100
C	6.84737800	-1.45785400	0.31654700
C	8.32878800	-1.58545500	0.65364200
H	8.55175200	-1.14521600	1.63007200
H	8.94629300	-1.06235500	-0.08177800
H	8.61852100	-2.64345400	0.67098300
C	6.01804400	-2.19383500	1.37563300
H	4.94556800	-2.18042000	1.15552300
H	6.15904200	-1.74930500	2.36713300
H	6.32771400	-3.24529100	1.43017300
C	6.58115500	-2.07979000	-1.06029400
H	7.13755800	-1.55379800	-1.84386400
H	5.52000000	-2.05062200	-1.32889200
H	6.89693200	-3.13087500	-1.06771600
C	-2.32233100	-2.52408300	-0.36403100
C	6.47598900	0.04659000	0.28251600
O	7.32946300	0.92517000	0.44059200
N	5.15962700	0.25913000	0.05048900
H	4.56613800	-0.56040800	-0.07464400
N	-5.17192300	-0.19699500	-0.05820300
C	-6.44319800	0.12354500	0.27876300
O	-7.32814100	-0.67922700	0.59054600
H	-4.54089500	0.57043800	-0.28551600
H	2.12181900	4.54067600	-0.38397100
H	-2.36362600	-4.65539000	-0.10764400
N	-0.08464200	0.11458600	2.44463900
O	0.92385900	-0.16386900	0.96363200
C	-0.63330100	1.45633300	2.34869000
H	-1.11886300	1.74957300	3.29885700
H	0.17880200	2.14596700	2.10696900
H	-1.35750500	1.48167800	1.53100000
C	-1.08158100	-0.93527800	2.55345000
H	-0.59258900	-1.89947800	2.39686800
H	-1.57556200	-0.90673200	3.54209900
H	-1.82604000	-0.80242200	1.76703700
C	0.96410900	0.00917400	3.43800000
H	1.74312000	0.73583000	3.19654900
H	0.57072700	0.19576400	4.45432000
H	1.39620100	-0.99179700	3.38345700

Trans-INT1_{acylam} (Trans Attack)

Mo	-0.25495000	-0.58181300	-1.66604600
S	2.99958300	-0.15172400	-1.79491700
S	-2.34797500	0.14771800	-0.63790400
S	0.36039200	1.85438400	-1.69695000
S	-0.76851900	-2.67406800	-0.52874500
O	-0.60343500	-0.91151200	-3.29862200
C	4.15561200	2.84661700	0.68558100
H	5.00833300	3.05622400	1.31898000
C	3.13402500	3.78208400	0.47993600
H	3.20858300	4.76029900	0.95328900
C	1.88535900	2.22283000	-0.92377900
C	-7.86992300	2.35587700	1.11196100
H	-7.96094800	2.17409900	2.18675700
H	-8.65184400	1.76945000	0.62100600
H	-8.05310700	3.42006300	0.91783100
C	-3.11911600	-1.31149300	0.02481400
C	4.05836400	1.61100400	0.04759200
C	-3.07071400	-3.66091500	0.61857100
C	2.01625100	3.47172700	-0.27949500
C	2.97444200	1.31244000	-0.83015100
C	-4.43259200	-1.24451100	0.55053800
C	-6.48641900	1.96669100	0.60317100
C	-5.06295900	-2.36737300	1.09582200

H	-6.06931000	-2.27531400	1.48571900
C	-6.40449600	2.22538000	-0.90638100
H	-6.62492100	3.27885800	-1.12112000
H	-7.12966800	1.61084700	-1.45143100
H	-5.41125400	2.00673100	-1.31184000
C	-5.42264800	2.80606500	1.32156400
H	-5.42912400	2.61247200	2.39986700
H	-5.62032900	3.87480700	1.16915300
H	-4.41128700	2.60387000	0.95377700
C	-4.36511800	-3.57471700	1.12323700
H	-4.84180200	-4.45819200	1.54657200
C	6.72459900	-0.92334700	1.00531600
C	7.96576100	-0.91116800	1.89042300
H	7.71780400	-0.61356200	2.91308300
H	8.70910100	-0.19935800	1.52018700
H	8.41684300	-1.91084200	1.91479000
C	5.70353500	-1.92228900	1.56529800
H	4.82319300	-2.02652500	0.92205500
H	5.34969000	-1.61596800	2.55566000
H	6.16130500	-2.91503000	1.66059700
C	7.11531500	-1.33884900	-0.41809500
H	7.82560700	-0.62901600	-0.85665600
H	6.24855000	-1.40139900	-1.08515200
H	7.59055500	-2.32806100	-0.40480200
C	-2.43243800	-2.54088700	0.06230800
C	6.11254100	0.49918000	0.99175500
O	6.62027100	1.43175700	1.62018300
N	4.99402000	0.57970200	0.23093800
H	4.69117900	-0.25609400	-0.27718700
N	-5.04413200	0.02327700	0.48556600
C	-6.25926300	0.46132600	0.89131100
O	-7.12560700	-0.23120600	1.43429300
H	-4.41930200	0.70159400	0.05092000
H	1.19534700	4.18032700	-0.37319000
H	-2.52714200	-4.60434800	0.64676100
N	0.53911400	-0.14909300	1.65362300
O	1.68246300	-1.10658300	-1.31846200
C	0.80665500	1.20294900	2.08928600
H	0.92303500	1.26993100	3.19506700
H	1.72579300	1.57601600	1.63099000
H	-0.01978000	1.85553900	1.78395100
C	-0.58898600	-0.69234000	2.38034100
H	-0.78385700	-1.71765500	2.05448100
H	-0.40242300	-0.69353200	3.47883100
H	-1.48321400	-0.09369700	2.17723900
C	1.69933200	-1.00163500	1.78755200
H	2.54027700	-0.56420600	1.23981900
H	2.00241300	-1.14011200	2.85112400
H	1.47864400	-1.97776200	1.34217700

Trans-TS2'_{acylam} (Trans Attack)

Mo	0.23489400	-0.61573800	1.69060100
S	-3.03644100	-0.11921300	1.84584200
S	2.32313100	0.14032300	0.62276100
S	-0.36634700	1.82190600	1.80253100
S	0.76521600	-2.69920400	0.52150800
O	0.62684000	-0.96804900	3.31016700
C	-4.06308700	2.84900900	-0.71175600
H	-4.89117000	3.06239700	-1.37623100
C	-3.03505600	3.77466900	-0.48490700
H	-3.08037700	4.74783300	-0.97202300
C	-1.85650400	2.21232700	0.97420300
C	7.83313900	2.38232500	-1.11547200
H	7.92121100	2.21522400	-2.19289400
H	8.61666000	1.78958100	-0.63479000
H	8.01646000	3.44376900	-0.90722000
C	3.09564800	-1.30971200	-0.04907400

C	-4.00759300	1.62129600	-0.05820400
C	3.06262400	-3.65793100	-0.65173200
C	-1.94467500	3.45403900	0.30984000
C	-2.96123200	1.31769700	0.86908700
C	4.40374200	-1.23006300	-0.58799900
C	6.45126600	1.98546300	-0.60823500
C	5.03655500	-2.34434600	-1.14743100
H	6.03754700	-2.24139000	-1.54812300
C	6.37478700	2.21966900	0.90573000
H	6.59707000	3.26919300	1.13710700
H	7.10115000	1.59548200	1.43802600
H	5.38277900	1.99525200	1.31116300
C	5.38553700	2.83680800	-1.30925100
H	5.38891400	2.66163000	-2.39072800
H	5.58379100	3.90276400	-1.13924000
H	4.37515000	2.62883100	-0.94205000
C	4.34909500	-3.55746600	-1.17298900
H	4.82802700	-4.43428700	-1.60714500
C	-6.69343900	-0.87953300	-1.04810800
C	-7.90994800	-0.85863600	-1.96672800
H	-7.62729500	-0.59637100	-2.99003400
H	-8.64266800	-0.11680800	-1.63584900
H	-8.38764600	-1.84624900	-1.97597700
C	-5.68310200	-1.91617500	-1.55671300
H	-4.81823200	-2.01963000	-0.89264100
H	-5.30365500	-1.64621800	-2.54821100
H	-6.16049900	-2.90142800	-1.63331700
C	-7.13274700	-1.25061000	0.37336600
H	-7.83531200	-0.51238200	0.77619500
H	-6.28616100	-1.31965200	1.06523700
H	-7.63375900	-2.22726100	0.36957700
C	2.42004200	-2.54627200	-0.08267200
C	-6.04586800	0.52710200	-1.05260100
O	-6.50380500	1.45177600	-1.72949300
N	-4.95422400	0.60371900	-0.25357400
H	-4.68940700	-0.22284400	0.28916000
N	5.00777700	0.04086400	-0.52059300
C	6.22360600	0.48464500	-0.91872100
O	7.09096700	-0.20075800	-1.46887000
H	4.38310800	0.71246200	-0.07559600
H	-1.11338100	4.14876900	0.41690200
H	2.52776100	-4.60611900	-0.67708000
N	-0.55014600	-0.16863100	-1.64113200
O	-1.63574500	-1.14843400	1.37879800
C	-0.81175800	1.18300300	-2.07994100
H	-0.95547900	1.24453000	-3.18283100
H	-1.71399000	1.57012300	-1.60127200
H	0.03043300	1.82722500	-1.80070200
C	0.55269100	-0.72983000	-2.39106200
H	0.74680500	-1.75379900	-2.06126200
H	0.33807700	-0.73917600	-3.48442200
H	1.45711300	-0.13712400	-2.21802700
C	-1.72310100	-1.00884300	-1.73509800
H	-2.54181600	-0.55919800	-1.16430300
H	-2.05998800	-1.15039300	-2.78793400
H	-1.49934000	-1.98451100	-1.28988800

Dioxo_P acylam (Trans/Trans) (Trans Attack)

Mo	1.16955300	-3.17442800	0.02180300
S	-1.38265400	-2.13044400	-0.37535100
S	1.75302600	-0.64929000	0.63976800
S	0.22249300	-2.97462400	2.32142200
S	2.02175500	-2.30041100	-2.13049000
O	2.54130200	-3.88415800	0.80924100
C	-3.07724100	0.19424500	2.50226900
H	-3.86548000	0.93565100	2.54283100
C	-2.34399300	-0.16191100	3.63385300
H	-2.55597800	0.32158200	4.58604300

C	-1.03859200	-1.74753100	2.33165200
C	1.67532700	5.28705000	2.02025900
H	1.00290200	5.59365100	1.21337100
H	2.60905600	5.84295700	1.89295700
H	1.22216000	5.56911400	2.97867500
C	2.55429400	0.03864600	-0.74908200
C	-2.78368100	-0.42190300	1.28338100
C	3.40457800	-0.12581800	-3.02638700
C	-1.34116300	-1.12257000	3.55041300
C	-1.74933300	-1.39186600	1.15836100
C	3.04402500	1.37256600	-0.71155200
C	1.91668100	3.78169500	1.98449300
C	3.73851900	1.92612100	-1.78709200
H	4.09421600	2.94728900	-1.71731400
C	2.86726100	3.38881000	3.12254000
H	2.44028100	3.68738300	4.08855900
H	3.84103000	3.88132200	3.01522800
H	3.03812600	2.30805900	3.15558700
C	0.57883500	3.04979800	2.15885200
H	-0.09759800	3.27272100	1.32854500
H	0.09806200	3.36928600	3.09176900
H	0.67832400	1.95862100	2.20196400
C	3.91493000	1.16630100	-2.94399500
H	4.44546400	1.59419700	-3.79309200
C	-5.00195700	0.77010700	-1.61428700
C	-6.47833600	0.35943300	-1.58767900
H	-7.03301400	0.98308200	-0.88035600
H	-6.59171800	-0.68707300	-1.28160800
H	-6.92411600	0.46993700	-2.58452400
C	-4.89607300	2.22796500	-2.07191700
H	-3.84940500	2.55047000	-2.12462400
H	-5.41792000	2.88495300	-1.37005400
H	-5.33767300	2.34838100	-3.06941900
C	-4.24515100	-0.12761800	-2.59114600
H	-4.30486900	-1.18661600	-2.31658400
H	-3.18358800	0.13574800	-2.66278600
H	-4.67531200	-0.02307500	-3.59466800
C	2.72058600	-0.69986100	-1.94210800
C	-4.50099500	0.71535800	-0.15138300
O	-5.05928600	1.42221900	0.69685200
N	-3.47938900	-0.13606400	0.09220200
H	-3.06864400	-0.64771700	-0.68964700
N	2.77350500	2.08692600	0.46985300
C	2.57041000	3.42346900	0.62856000
O	2.90066800	4.28728700	-0.18570700
H	2.33636500	1.48020200	1.16130100
H	-0.76553500	-1.39830200	4.43137000
H	3.52315500	-0.71040200	-3.93651100
N	-0.12596200	2.69057600	-1.27076100
O	0.51788100	-4.47989000	-0.92559300
C	-1.06662100	1.67658300	-0.83682000
H	-1.90247100	1.55553900	-1.55838000
H	-0.56977700	0.70454600	-0.72307700
H	-1.50195200	1.95042200	0.13150800
C	-0.75010600	3.98933100	-1.33410600
H	-0.00774200	4.74863900	-1.60598700
H	-1.57606200	4.03123400	-2.08120700
H	-1.17598000	4.25364700	-0.35828000
C	0.44464600	2.34382200	-2.55633900
H	0.88859900	1.34475100	-2.51488100
H	-0.32485100	2.34889500	-3.36075800
H	1.23412600	3.05610400	-2.81909100

Dioxo acylam (Trans/Trans)

Mo	-3.38924400	-0.01373400	0.00908600
S	-1.27911300	-0.84234800	1.50232200
S	-1.31012300	0.84935600	-1.50705200
S	-2.85314300	-2.22847100	-0.98987800
S	-2.87789300	2.21062500	1.00184700

O	-4.46075100	0.21784200	-1.33843900
C	1.45666000	-3.42519800	-0.02571900
H	2.49898600	-3.65480800	0.16053400
C	0.70596500	-4.11999200	-0.97401100
H	1.16561900	-4.93478300	-1.53124700
C	-1.22315900	-2.70446500	-0.53705800
C	4.68751200	0.30859000	-3.05618500
H	5.25215900	0.24849300	-2.12087500
H	4.99363400	1.22997800	-3.56078800
H	4.96200800	-0.54860700	-3.68301700
C	-0.54701800	2.04489200	-0.49243700
C	0.85487100	-2.37829300	0.67532400
C	-0.64340100	3.75042800	1.24620000
C	-0.60852700	-3.74997600	-1.24378100
C	-0.51389100	-2.03820700	0.48947600
C	0.82052600	2.38869000	-0.67922400
C	3.18622400	0.29520700	-2.79049000
C	1.41922100	3.43865900	0.01996400
H	2.46078900	3.67138600	-0.16660500
C	2.42809400	0.36527400	-4.12251700
H	2.69931300	-0.48973300	-4.75481200
H	2.67258800	1.28325500	-4.67022300
H	1.34276900	0.33820000	-3.97867500
C	2.80582500	-0.99376700	-2.05198100
H	3.27786500	-1.04776000	-1.06446200
H	3.13569700	-1.87052600	-2.62309300
H	1.72594700	-1.10157300	-1.90051600
C	0.66777400	4.12857900	0.97128500
H	1.12491300	4.94509500	1.52804800
C	3.22163400	-0.27896400	2.77705100
C	4.70473800	-0.34231600	3.12516800
H	5.32007000	-0.35495400	2.22114700
H	4.94179600	-1.24915800	3.69026800
H	4.98377700	0.53203000	3.72576100
C	2.93388700	0.98869200	1.96256400
H	1.86911400	1.11267400	1.73536600
H	3.47326400	0.98863900	1.00800800
H	3.24785700	1.88064800	2.51898000
C	2.39276700	-0.25608000	4.06735100
H	2.56027200	-1.16158600	4.66234100
H	1.31838700	-0.17820500	3.86995100
H	2.67697500	0.60941700	4.67913100
C	-1.25532000	2.70340200	0.53953800
C	2.85858700	-1.52605300	1.93823500
O	3.69547300	-2.38768000	1.64884400
N	1.55524700	-1.54872400	1.56586300
H	0.95813600	-0.77929800	1.87380400
N	1.52280000	1.55683000	-1.56604200
C	2.82737400	1.53091100	-1.93260000
O	3.66561400	2.38915500	-1.63692500
H	0.92444000	0.78909000	-1.87601600
H	-1.17551700	-4.25614700	-2.02239300
H	-1.20918000	4.25085400	2.02935900
O	-4.44501800	-0.26171700	1.36613200

Figure S1

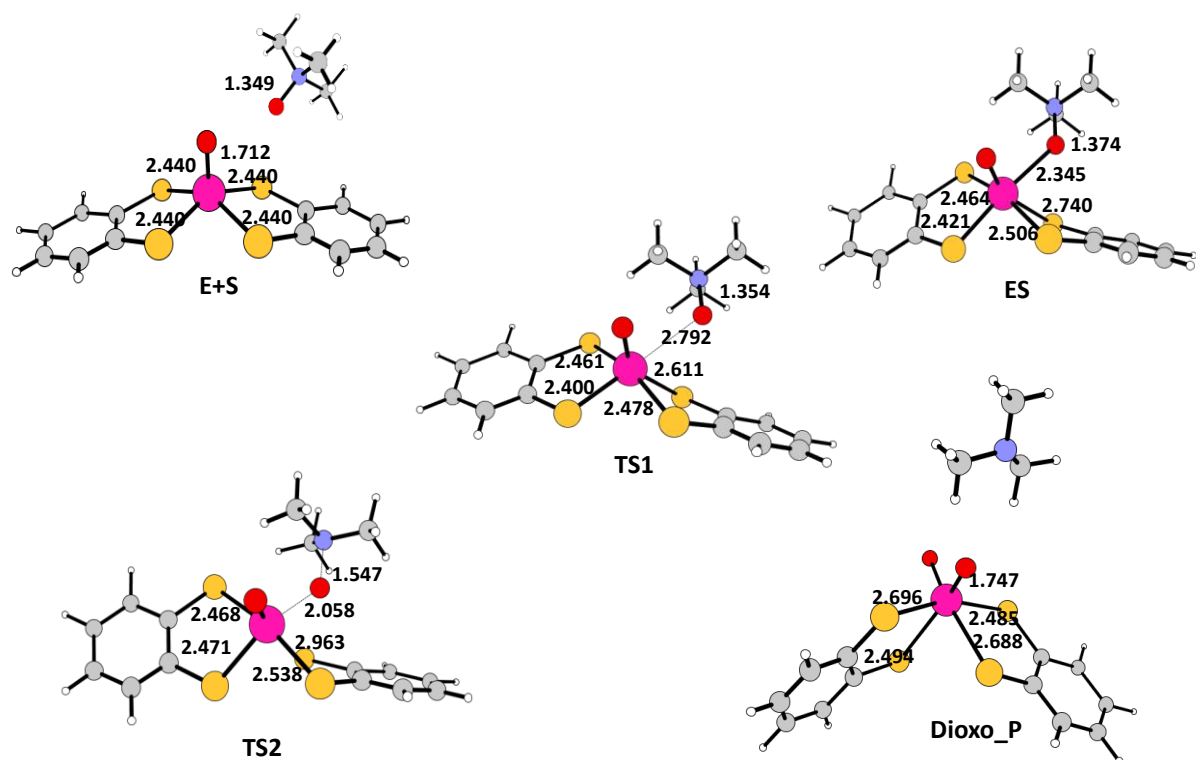


Figure S2

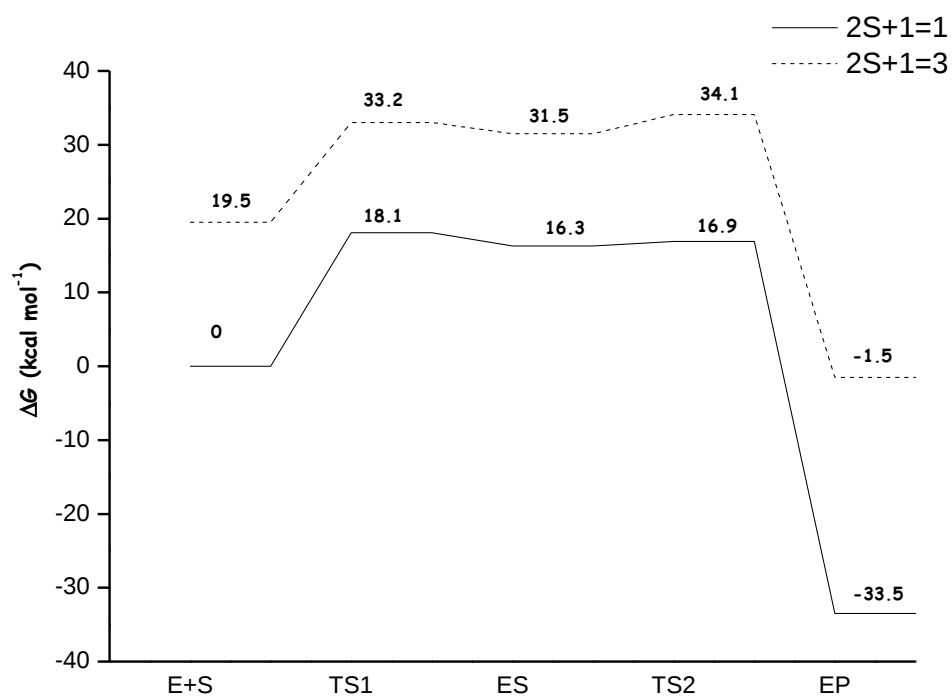


Figure S3

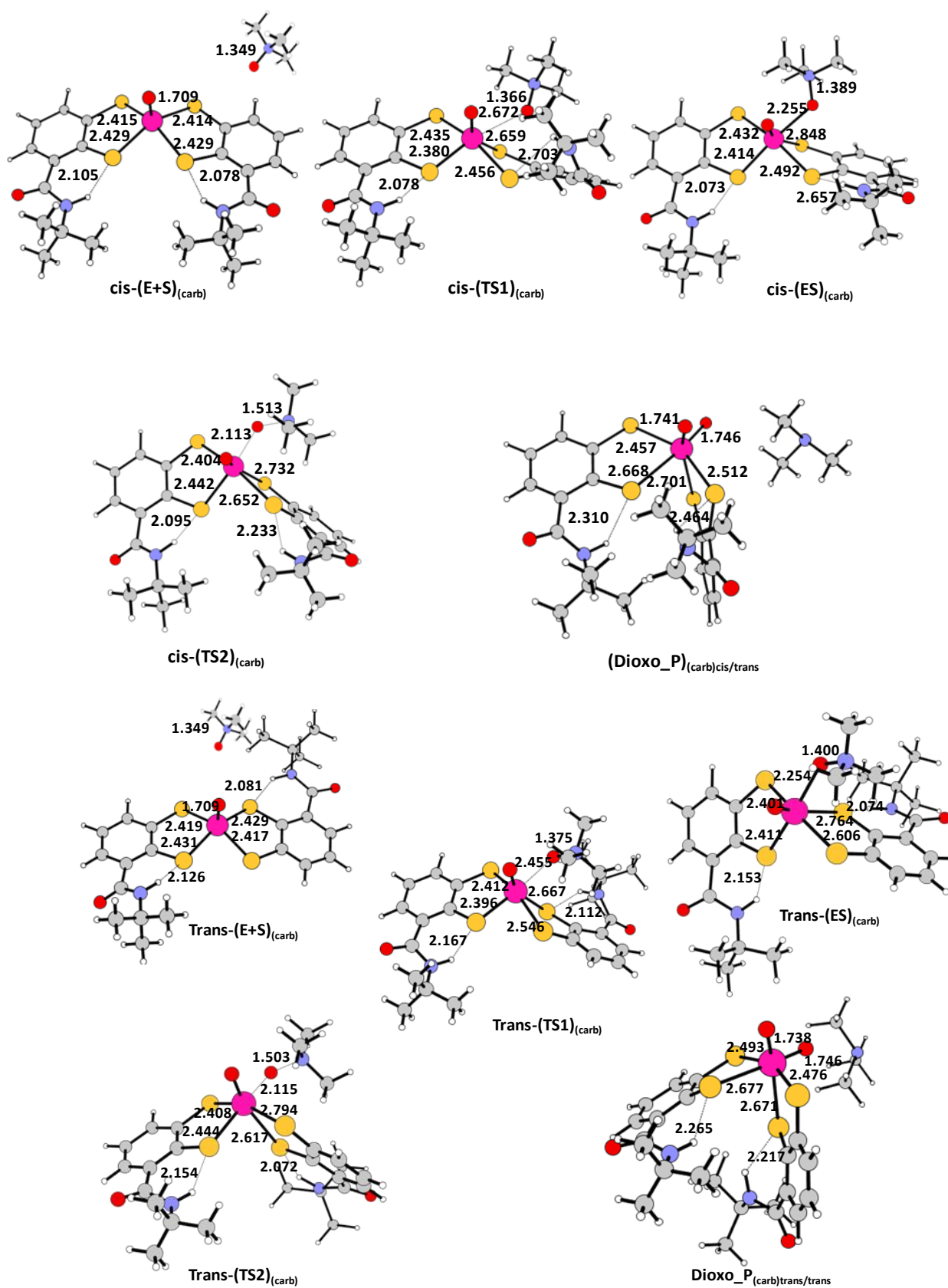


Figure S4

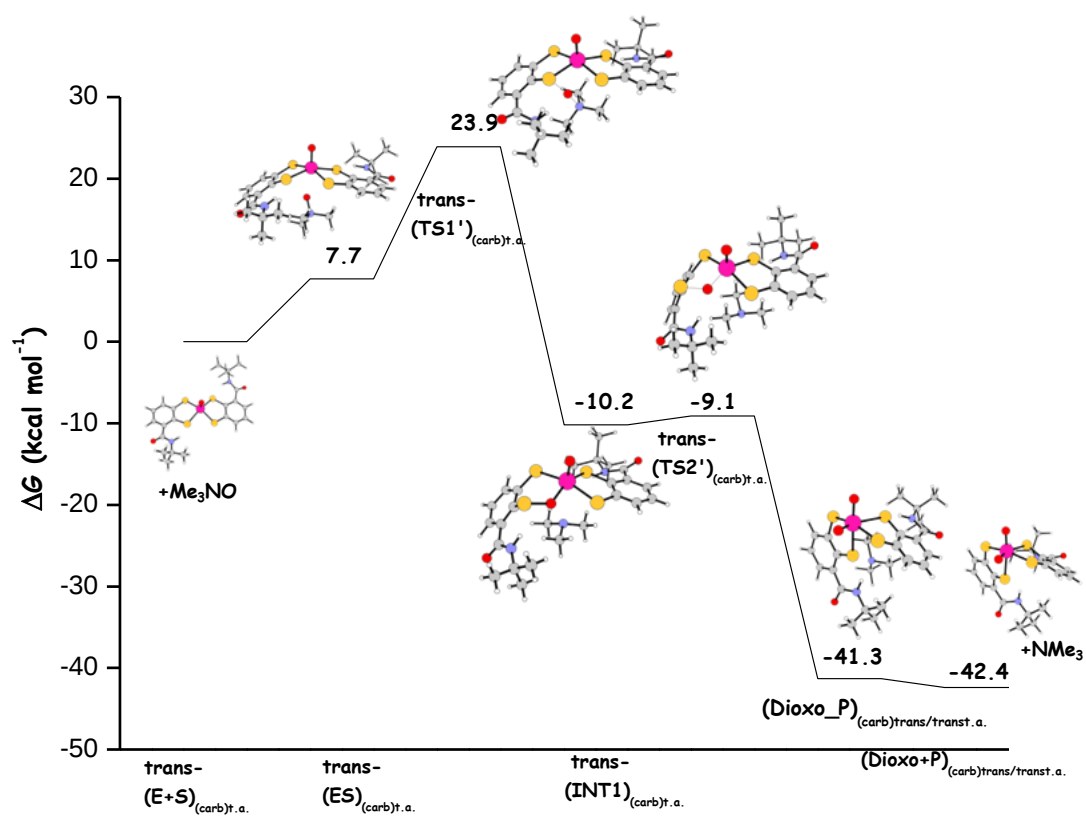


Figure S5

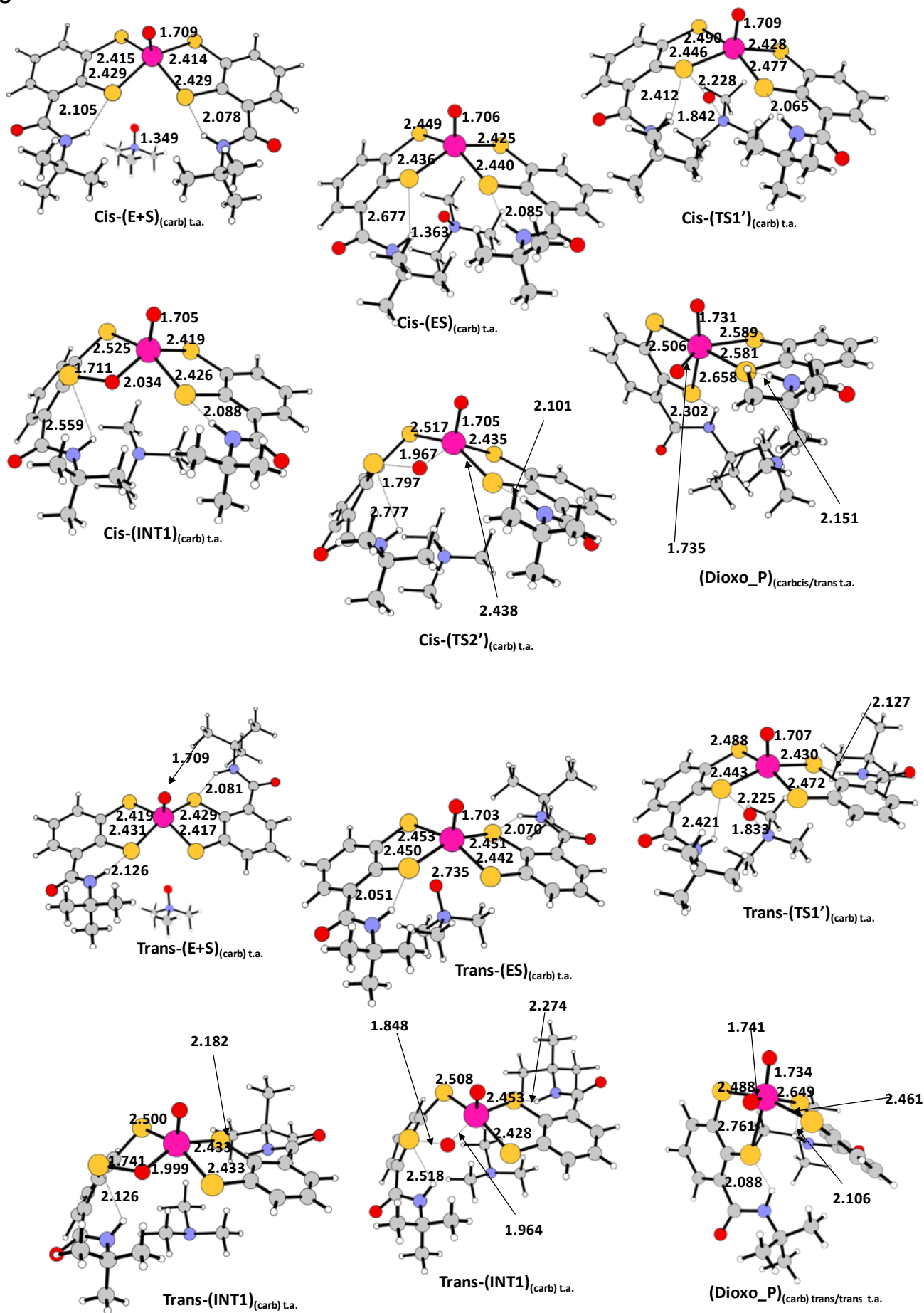


Figure S6

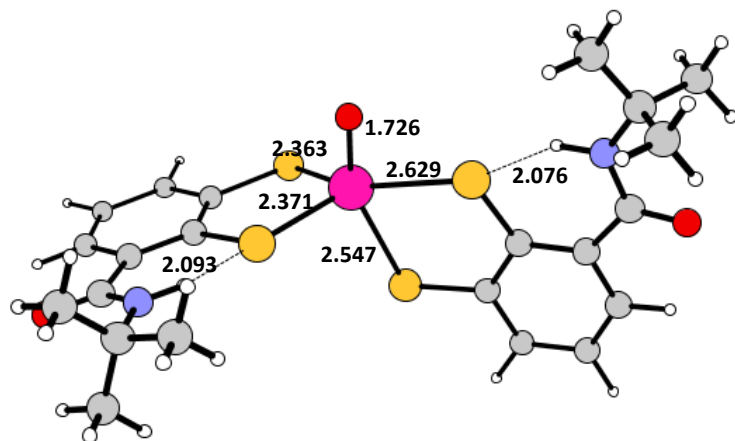


Figure S7

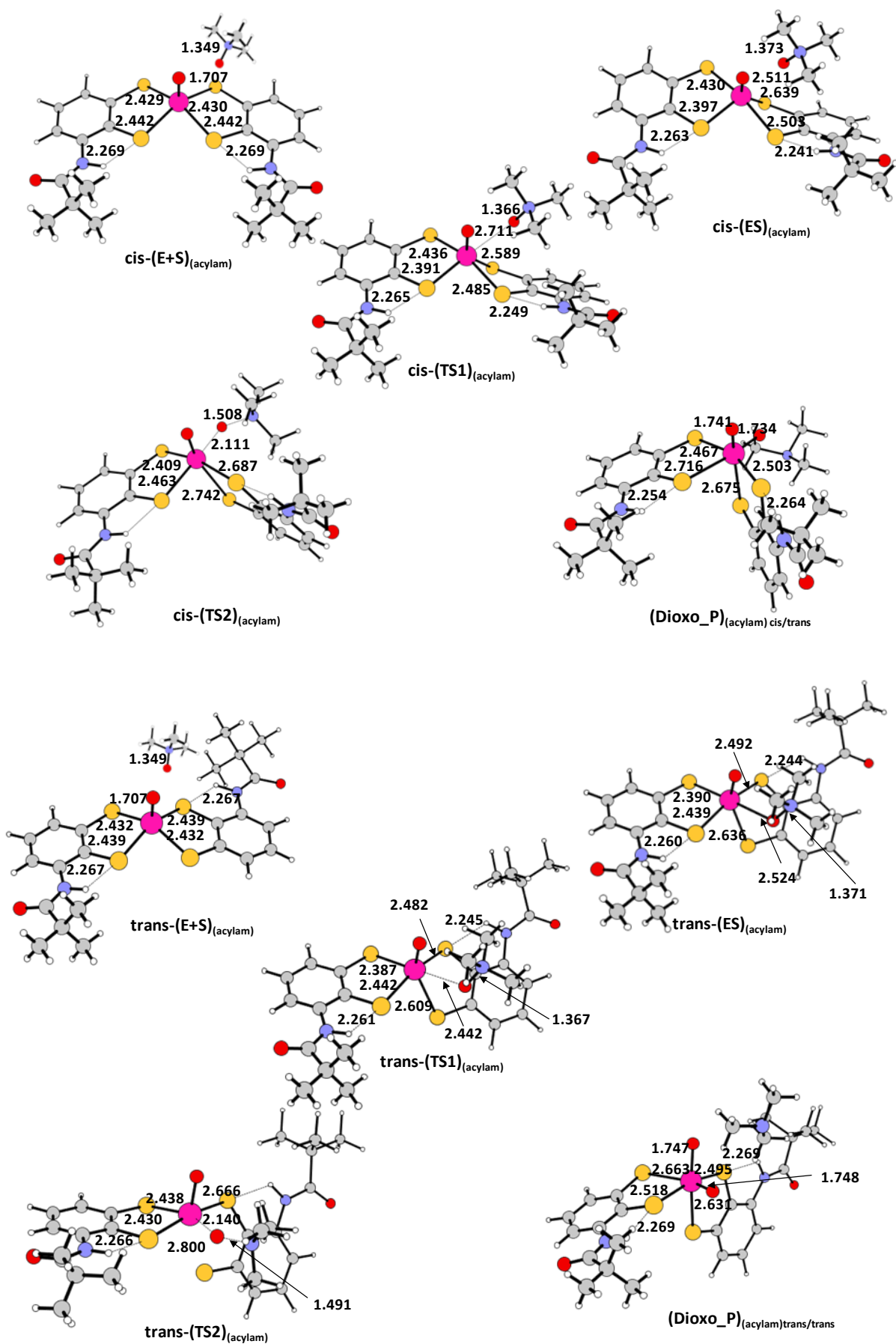


Figure S8

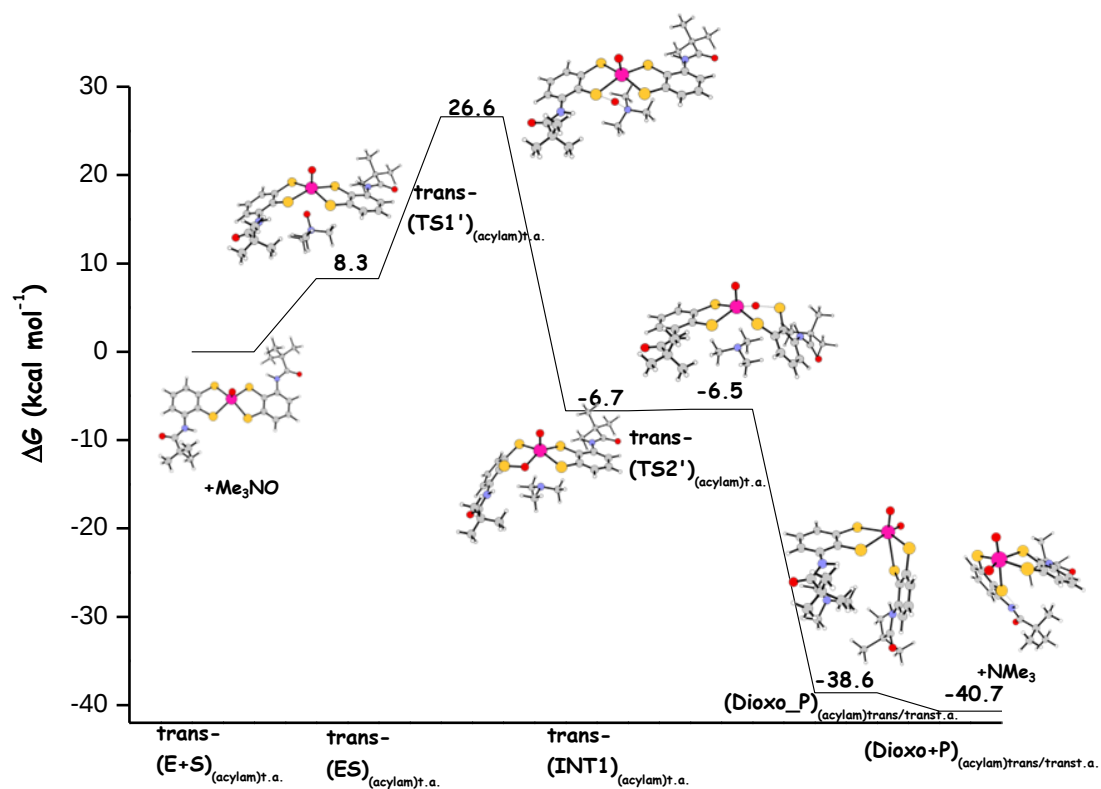
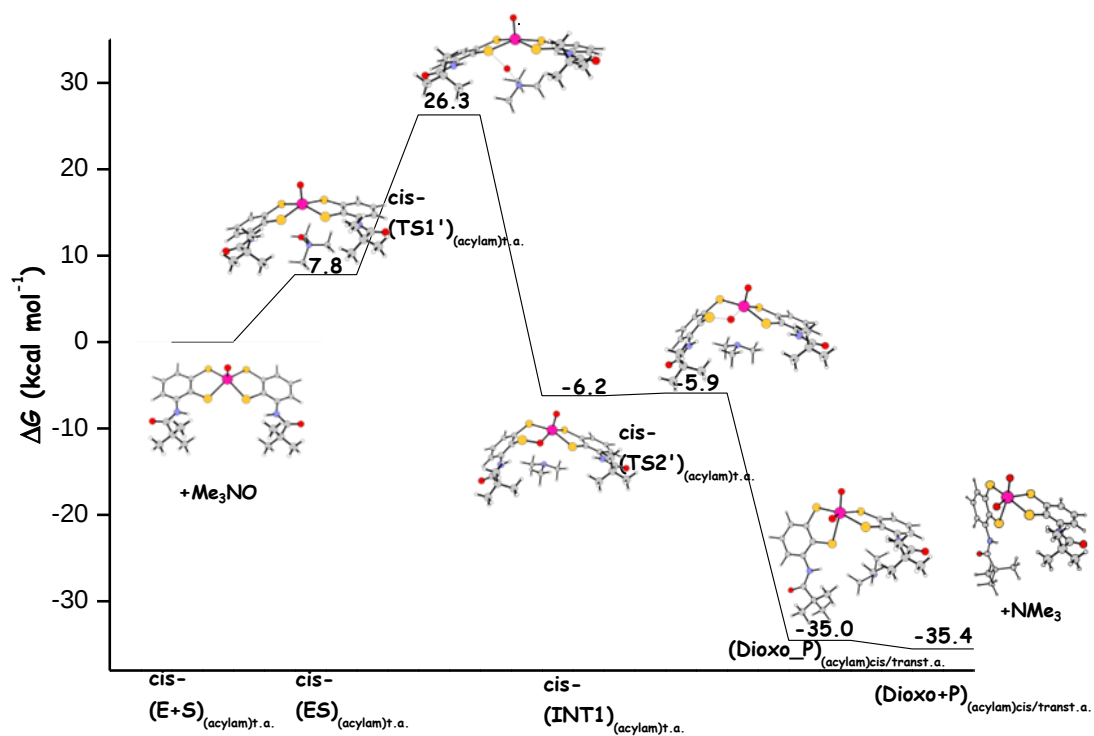


Figure S9

