
Prediction on the origin of chemoselectivity in Lewis base-mediated competition cyclizations between allenolate and chalcone: A computational study

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1. Computational details

All theoretical calculations on the possible mechanisms of LBs catalyzed annulation reactions of allenolate with chalcone were performed using Gaussian 09 suite of programs. All structures of the stationary points were optimized by the M06-2X/6-31G(d, p)/def2-TZVP method in solvent using integral equation formalism polarizable continuum model (IEF-PCM) at 298.15 K. The solvent is acetonitrile for NHC/PMe₃ catalysis system and the solvent is toluene for DABCO catalysis system. Moreover, basis sets 6-31G(d, p) and 6-311++G(2d, 2p) were employed for H, C, N, O and P atoms, while basis sets def2-TZVP and def2-QZVP were used for Cs atom. The corresponding vibrational frequencies were calculated at the same level (M06-2X/6-31G(d, p)/def2-TZVP//IEFPCM) to take account of the free energy contributions. The single-point energies of the optimized structures were then refined at the higher basis set 6-311++G(2d, 2p)/def2-QZVP with the M06-2X method and the same solvent effect included and simulated by using IEF-PCM. We confirmed that all the reactants, intermediates, and products have no imaginary frequencies, whereas each transition state has only one imaginary frequency. In addition, we have also made some tests of the different computational methods (such as B3LYP, B3PW91, and ω B97X-D).

2. The optimized structures of stationary points of the most favorable $[\alpha, \beta]$ -[4 + 2] annulation pathway

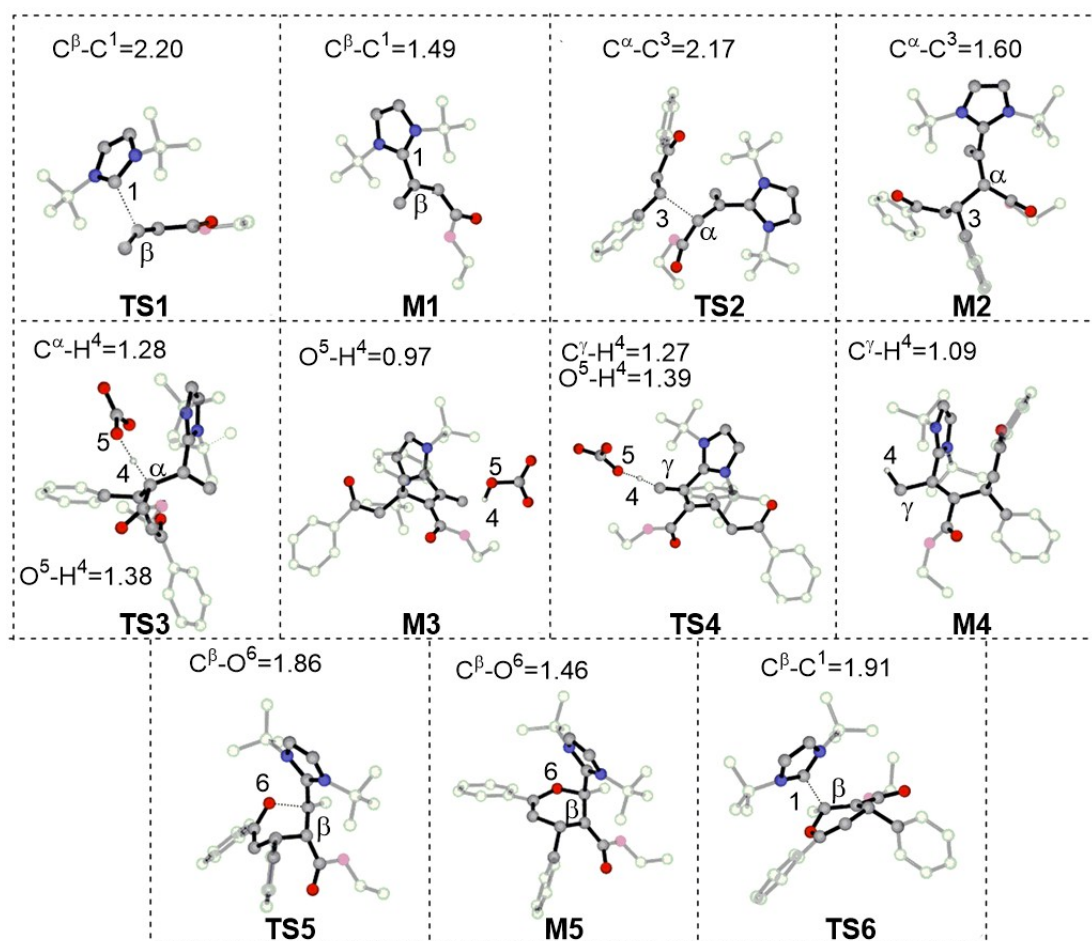


Fig. S1 Optimized structures and geometrical parameters of the stationary points (distance in Å)

3. The discussion for the chirality of α -C and C3 atoms and the choice of TS2

As presented in **Fig. S2**, the chiral centers (α -C and C3 atoms) are formed in this step, we have also considered the chirality of α -C atom, which has had not exist after the next step. Considering with the different isomers associated with the two chiral centers, we must point out that we have actually studied four possible reaction pathways, and the transition states **TS2(RR)** and **TS2(SS)** are with the lower energy barriers. Because the catalyst NHC has no chiral center, thus **TS2(RR)** and **TS2(SS)** are the image of each other (It is the same situation for **TS2(SR)** and **TS2(RS)**), which means they have the same energy in the following steps. **TS2(RR)** leads to the formation of product with *R*-configuration, and **TS2(SS)** leads to the formation of product with *S*-configuration. Therefore, we chose **TS2(RR)** as transition state **TS2** in the main text to discuss.

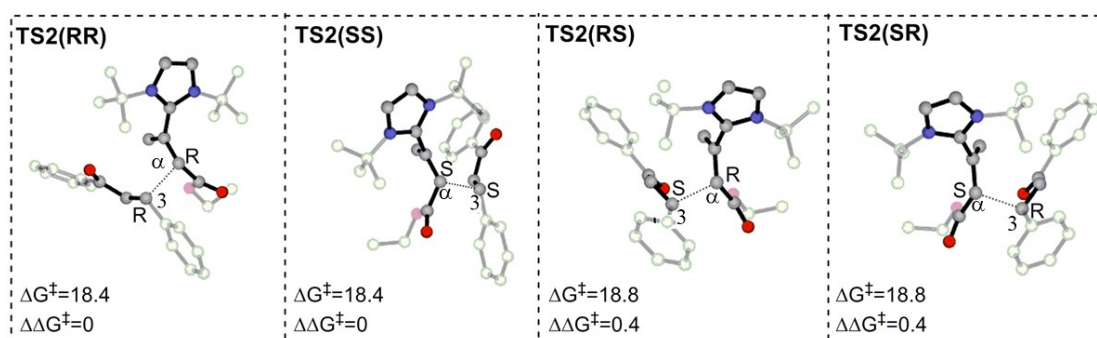


Fig. S2 Possible reaction patterns for the C^α -C3 bond formation step and energy barriers (unit: kcal/mol)

4. The discussion of Cs_2CO_3 -assisted [1, 3]-proton transfer from α -C to γ -C atom

We have also studied the possibility of Cs_2CO_3 -assisted [1, 3]-proton transfer. As shown in **Fig. S3**, the energy barrier is 27.7 kcal/mol and is higher than the energy barrier of CO_3^{2-} -assisted [1, 3]-proton transfer. Therefore, the [1, 3]-proton transfer from α -C to γ -C atom in the most favorable $[\alpha, \beta]$ -[4 + 2] annulation pathway is mainly assisted by HCO_3^- anion.

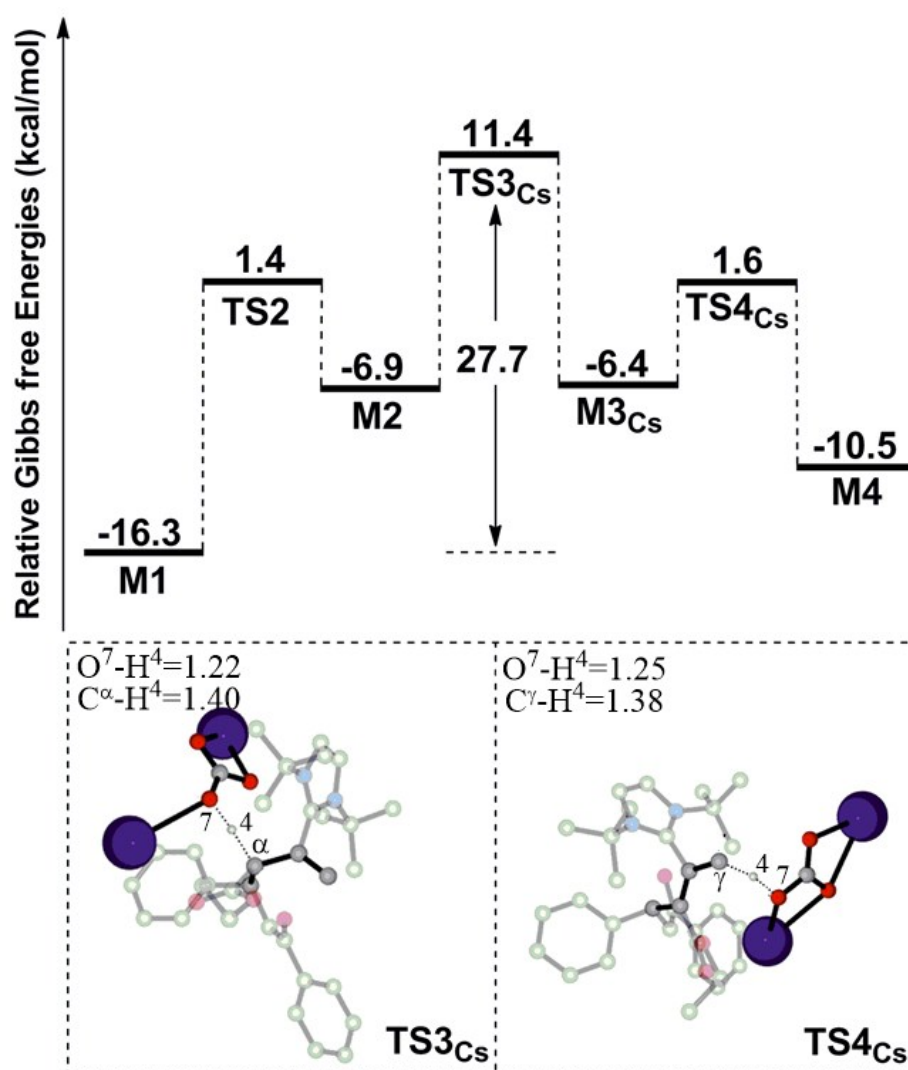


Fig. S3 The relative Gibbs free energy profiles of Cs_2CO_3 -assisted [1, 3]-proton transfer from α -C to γ -C atom and the optimized structures of transition states (distance in Å)

5. Tests of the different computational methods

We have employed at the B3LYP-D3/6-311++G(2d, 2p)//IEF-PCM_{acetonitrile} & B3LYP-D3/6-31G(d, p)//IEF-PCM_{acetonitrile}, B3PW91-D3/6-311++G(2d, 2p)//IEF-PCM_{acetonitrile} & B3PW91-D3/6-31G(d, p)//IEF-PCM_{acetonitrile}, and ω B97X-D/6-311++G(2d, 2p)//IEF-PCM_{acetonitrile} & ω B97X-D/6-31G(d, p)//IEF-PCM_{acetonitrile} methods to re-calculate the first and second steps of the most favorable $[\alpha, \beta]$ -[4 + 2] annulation pathway and the correction of single-point energies of the optimized structures with high basis set. As summarized in **Table S1**, the computed results by using different methods including M06-2X, B3PW91-D3, B3LYP-D3, and ω B97X-D have the same trend and small differences with those discussed above, indicating that the selected method M06-2X functional and basis sets should be suitable and reliable for studying the NHC catalyzed $[\alpha, \beta]$ -[4 + 2] annulation reaction.

Table S1 The energy barriers associated with stereoselectivity-determining step by using different methods (unit: kcal/mol)

	M06-2X	B3LYP-D3	B3PW91-D3	ωB97X-D
$\Delta G^\ddagger_{\text{step 1}}$	16.2	15.4	15.2	17.2
$\Delta G^\ddagger_{\text{step 2}}$	17.7	17.1	17.0	18.9

6. The p -orbital of the center atoms in the $LUMO_{TSs}$ (Only shown the orbital picture of the key atoms)

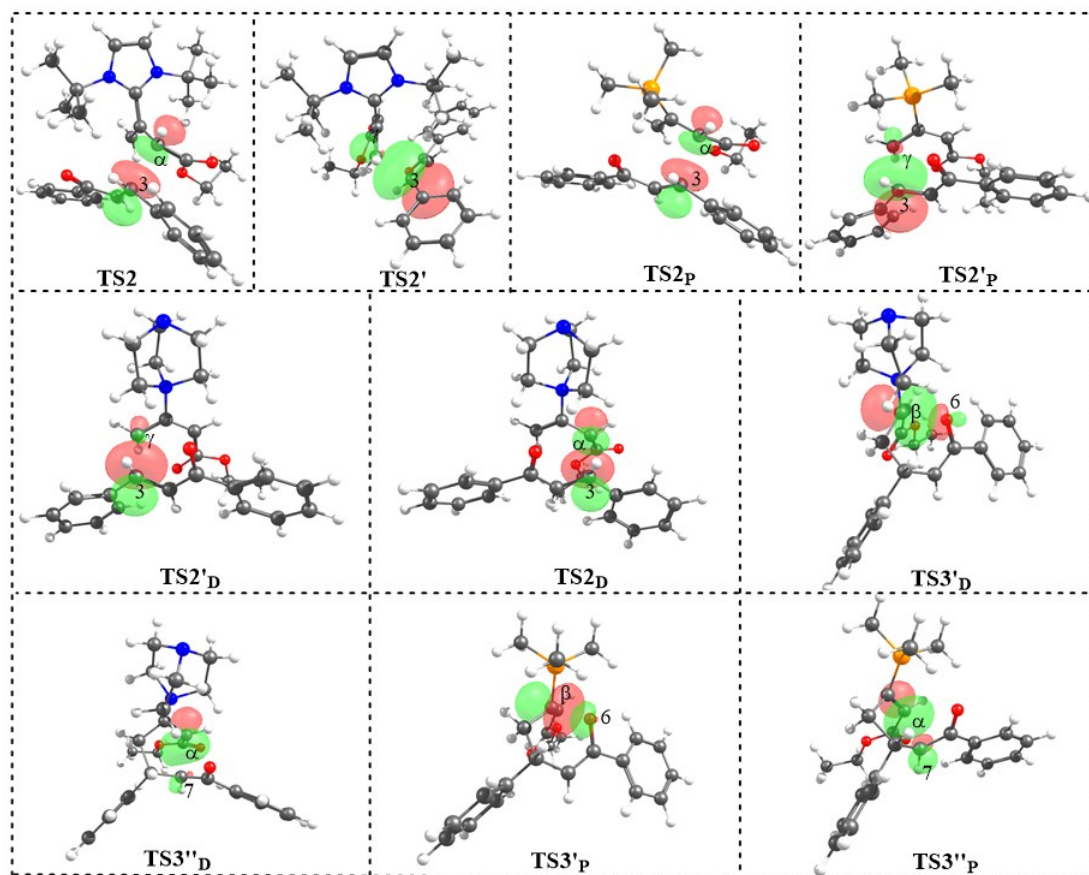


Fig. S4 The p -orbital of the center atoms in the $LUMO_{TSs}$ (Only shown the orbital picture of the key atoms)

7. Cartesian coordinates of stationary points

NHC

C	-0.67718100	1.61520400	0.00386600
C	0.67718100	1.61520400	-0.00386300
C	0.00000000	-0.57012600	0.00000500
N	-1.06374900	0.28333100	0.00771000
H	-1.36587800	2.44333000	0.00785400
H	1.36587800	2.44333000	-0.00785200
N	1.06374900	0.28333100	-0.00770100
C	-2.46012900	-0.22007500	-0.00034700
C	-3.44082100	0.94886700	0.05941600
C	-2.67479200	-1.01489600	-1.29056000
C	-2.65289000	-1.12223300	1.22068900
H	-3.30232100	1.54187000	0.96819400
H	-3.34050500	1.60312600	-0.81145800
H	-4.45883900	0.55218300	0.06643400
H	-1.95366900	-1.83279200	-1.34571100
H	-3.68809400	-1.42580700	-1.31574600
H	-2.53764600	-0.36873600	-2.16277800
H	-3.66614700	-1.53384500	1.22575900
H	-1.93174700	-1.94108100	1.19526800
H	-2.50220400	-0.55238800	2.14243900
C	2.46012900	-0.22007500	0.00034700
C	2.67478900	-1.01493200	1.29053800
C	2.65289400	-1.12219900	-1.22071400
C	3.44082100	0.94886800	-0.05938100
H	2.53764400	-0.36879500	2.16277300
H	1.95366300	-1.83282700	1.34566700
H	3.68809000	-1.42584600	1.31571400
H	2.50220800	-0.55232800	-2.14244800
H	3.66615000	-1.53381000	-1.22579500
H	1.93175000	-1.94104800	-1.19531800
H	4.45884000	0.55218500	-0.06639500
H	3.30233200	1.54189100	-0.96814800
H	3.34049400	1.60310800	0.81150600

R1

C	2.49988700	-0.40477500	-0.00001500
C	3.73798400	-0.00756600	-0.00025400
C	1.24909200	-0.80231200	0.00019700
H	4.26772700	0.16360000	-0.93261400
H	4.26801600	0.16408700	0.93184300
H	0.98918800	-1.85598200	0.00044000
C	0.14496500	0.18924400	0.00013000
O	0.27494700	1.39366200	-0.00005400
O	-1.04236700	-0.42967200	0.00033300
C	-2.19512100	0.43144400	0.00021300

C	-3.41891600	-0.45669900	-0.00043300
H	-2.15289900	1.07346700	-0.88403600
H	-2.15348100	1.07292200	0.88488900
H	-4.32046300	0.15954500	-0.00051100
H	-3.43276400	-1.09251200	-0.88835800
H	-3.43330600	-1.09306600	0.88708700

R2

C	-1.18083400	-0.96599700	0.03818900
O	-1.17640700	-2.18851100	0.09723300
C	-2.48267500	-0.22444400	0.01951200
C	-2.58393600	1.13865200	0.31536200
C	-3.64064200	-0.94961000	-0.28386700
C	-3.82714600	1.76557700	0.30373400
H	-1.70457600	1.71524900	0.58122000
C	-4.87833900	-0.32070600	-0.30856400
H	-3.54587000	-2.00807900	-0.50198000
C	-4.97275600	1.04002400	-0.01417200
H	-3.90006200	2.82102900	0.54390900
H	-5.77020000	-0.88681600	-0.55608200
H	-5.93939900	1.53331400	-0.03043400
C	0.08225500	-0.19176400	-0.03717300
C	1.25788400	-0.82625500	0.09157300
H	0.02852600	0.87474500	-0.22192300
H	1.21795500	-1.90147000	0.26312900
C	2.59714100	-0.23445000	0.02447000
C	3.70844600	-1.07542600	0.17084600
C	2.81273600	1.13684600	-0.18340600
C	5.00170500	-0.56570800	0.11027600
H	3.55008900	-2.13814600	0.33220300
C	4.10298100	1.64556300	-0.24340400
H	1.96972200	1.81098300	-0.29692500
C	5.20146600	0.79647800	-0.09758000
H	5.85092100	-1.23134600	0.22424700
H	4.25611000	2.70764900	-0.40420600
H	6.20831800	1.19830000	-0.14578700

CO₃²⁻

C	0.00000000	0.00000000	-0.00123900
O	0.00000000	0.00000000	1.29619100
O	0.00000000	1.12341700	-0.64763100
O	0.00000000	-1.12341700	-0.64763100

TS1

C	1.07715400	1.82150100	1.34265600
C	2.21598400	1.09341300	1.38073400
C	1.05685800	0.44822500	-0.46460300
N	0.39375100	1.43134000	0.20333000
H	0.72567000	2.58970800	2.01279500

H	3.02388500	1.11840300	2.09235100
N	2.20177400	0.27905300	0.25943600
C	-0.85612800	2.10935100	-0.22616100
C	-0.54056900	3.59681200	-0.42459000
C	-1.35396200	1.52163200	-1.54250900
C	-1.91605500	1.93033100	0.86524300
H	-0.18571700	4.06276400	0.49861500
H	0.22540100	3.72293400	-1.19499500
H	-1.44493900	4.12290200	-0.74185500
H	-1.67109600	0.48518700	-1.42186200
H	-2.21076500	2.11519900	-1.87526500
H	-0.57553200	1.56764800	-2.30837900
H	-2.85615400	2.38636600	0.54049800
H	-2.09119200	0.86899400	1.05453900
H	-1.61545100	2.40897800	1.80167800
C	3.31078400	-0.64318700	-0.10886500
C	3.03290500	-2.04358600	0.44466500
C	3.43493600	-0.68119700	-1.63210900
C	4.61919400	-0.11192900	0.48422800
H	2.85268400	-2.00085600	1.52338600
H	2.16728800	-2.49355500	-0.04611300
H	3.90035000	-2.68565300	0.26587600
H	3.61640900	0.32251900	-2.02663700
H	4.27825300	-1.32182600	-1.90424500
H	2.52947000	-1.08140900	-2.08803200
H	5.44643800	-0.71017600	0.09524500
H	4.78502100	0.93167200	0.20194900
H	4.64060000	-0.19444600	1.57402800
C	-0.03517800	-1.43890900	-0.79863700
C	0.02376200	-1.65189400	-2.09580300
C	-0.44134200	-1.80024900	0.43901800
H	-0.30420500	-2.61552800	-2.47751500
H	0.37308900	-0.89893200	-2.78946300
H	0.27407200	-2.08558000	1.20307100
C	-1.81300300	-1.67678800	0.89252400
O	-2.19535000	-1.92644900	2.02584100
O	-2.67072800	-1.25759600	-0.07045400
C	-4.02894500	-1.06993000	0.34104300
C	-4.75263800	-0.39448700	-0.80329500
H	-4.05032900	-0.45897800	1.24882500
H	-4.46837400	-2.04259100	0.58518900
H	-5.80194600	-0.23908500	-0.54240400
H	-4.29959400	0.57722900	-1.01807700
H	-4.70591900	-1.00693600	-1.70689800
M1			
C	-2.90107300	1.31386800	-0.08671000
C	-3.25774000	0.01234600	-0.14515000

C	-1.05950100	0.09996700	0.13423100
N	-1.53336600	1.36498400	0.09190500
H	-3.51727500	2.19183900	-0.15309900
H	-4.23264300	-0.42199500	-0.27069300
N	-2.10755900	-0.73994000	-0.01467400
C	-0.77543100	2.67337900	0.09490700
C	-1.72055100	3.76430200	0.61153200
C	0.44668800	2.62145400	1.01350300
C	-0.36235800	2.97808000	-1.34597700
H	-2.52653800	3.98769400	-0.09055600
H	-2.14699700	3.49604400	1.58208900
H	-1.13998500	4.68055300	0.73369700
H	1.22571900	1.97107500	0.61927700
H	0.84172500	3.63820400	1.08140800
H	0.17207500	2.28657400	2.01652900
H	0.11223500	3.96271500	-1.37893000
H	0.34876000	2.23033500	-1.70233100
H	-1.23642200	2.99333300	-2.00347300
C	-2.11325300	-2.25040500	0.01067400
C	-0.96573300	-2.80546800	-0.83388100
C	-2.01515400	-2.71520700	1.46428700
C	-3.43632900	-2.73297300	-0.59142200
H	-0.99155100	-2.38804000	-1.84409300
H	0.00648600	-2.59877600	-0.39093300
H	-1.09587800	-3.88843100	-0.90275400
H	-2.81432300	-2.26965200	2.06359500
H	-2.12344700	-3.80274500	1.49669800
H	-1.04844100	-2.44347800	1.89003500
H	-3.39054000	-3.82115400	-0.66358100
H	-4.29432000	-2.48527300	0.03799000
H	-3.59193200	-2.33049900	-1.59615900
C	0.37365200	-0.28698100	0.30003300
C	0.72950500	-0.60153000	1.57441000
C	1.11105500	-0.20530400	-0.92311300
H	1.74626100	-0.86747900	1.82596400
H	0.00274500	-0.52352200	2.37536900
H	0.55421800	-0.07201500	-1.84329200
C	2.50662800	-0.31863100	-1.09106000
O	3.13252200	-0.27237900	-2.15908100
O	3.20041000	-0.47918900	0.09213000
C	4.61494700	-0.56358400	-0.02998200
C	5.17767900	-0.73264900	1.36673400
H	5.00231300	0.34250100	-0.50874700
H	4.88369900	-1.40822400	-0.67359800
H	6.26793300	-0.79810100	1.33195500
H	4.90040800	0.11672200	1.99636400
H	4.79054300	-1.64493200	1.82816200

TS1-1

C	1. 56403800	-2. 14940600	-0. 51102300
C	0. 30196700	-2. 56819000	-0. 72859800
C	0. 18043400	-0. 50970900	0. 17029700
N	1. 48487400	-0. 90020800	0. 07754700
H	2. 49648300	-2. 64643800	-0. 71470200
H	-0. 04924400	-3. 49214400	-1. 15316800
N	-0. 54391900	-1. 57434800	-0. 27489800
C	2. 73499900	-0. 28693400	0. 64847800
C	3. 52885500	-1. 40954200	1. 33902200
C	3. 56816300	0. 31912200	-0. 47905300
C	2. 41410300	0. 76195600	1. 70659300
H	2. 90128900	-1. 94582600	2. 05620600
H	3. 95402800	-2. 12636500	0. 63398300
H	4. 36295700	-0. 95649700	1. 87940100
H	3. 07054800	1. 19959700	-0. 88333700
H	4. 54429600	0. 61714300	-0. 08635200
H	3. 72969300	-0. 40654800	-1. 28175100
H	3. 34942000	1. 04476900	2. 19601900
H	1. 97908400	1. 65080000	1. 25744400
H	1. 74305300	0. 35169900	2. 46702600
C	-2. 02837300	-1. 81663500	-0. 22781500
C	-2. 25287200	-3. 29366200	0. 13526200
C	-2. 67758400	-0. 97056100	0. 86496500
C	-2. 62554000	-1. 52920300	-1. 60585200
H	-1. 96706700	-3. 97840000	-0. 66600300
H	-1. 71137300	-3. 56334200	1. 04651200
H	-3. 32056300	-3. 43899700	0. 31395600
H	-2. 67269700	0. 08104200	0. 59373100
H	-3. 71143100	-1. 30626700	0. 98482700
H	-2. 16023900	-1. 11053000	1. 81943900
H	-3. 69839500	-1. 74307300	-1. 58514600
H	-2. 46036200	-0. 48444300	-1. 86485900
H	-2. 16557100	-2. 17573800	-2. 36049800
C	-1. 87022700	2. 20728600	1. 75706800
C	-3. 04869000	2. 62987900	2. 12909900
C	-0. 70096500	1. 75460600	1. 38972400
H	-3. 34814200	3. 66531500	1. 99564300
H	-3. 76651200	1. 95114600	2. 58227600
H	0. 12489200	1. 78712100	2. 09044300
C	-0. 47746800	1. 21739900	-0. 02085300
O	-1. 46069800	1. 15729900	-0. 80046200
O	0. 70250500	1. 85174900	-0. 52205600
C	0. 75087600	1. 93215400	-1. 94399800
C	0. 05283100	3. 18031700	-2. 45846000
H	0. 30910600	1. 03172500	-2. 38302800
H	1. 81114400	1. 95908900	-2. 21205100
H	0. 16222100	3. 26073500	-3. 54427300

H	-1.00716500	3.13838600	-2.20645400
H	0.49213700	4.07227900	-2.00280900

M1-1

C	-0.98361400	-2.62746400	-0.13895800
C	0.34258100	-2.78660600	0.01730500
C	-0.07555100	-0.59889200	0.02784600
N	-1.24992600	-1.27305400	-0.15581500
H	-1.73871900	-3.38241200	-0.24320900
H	0.90533100	-3.69880000	0.06487000
N	0.91251000	-1.53456800	0.10205100
C	-2.69452000	-0.81555800	-0.32474600
C	-3.50721800	-1.97652800	-0.92377200
C	-3.27910000	-0.49380500	1.05223200
C	-2.80864100	0.34193400	-1.31790200
H	-3.06441500	-2.35063600	-1.85077600
H	-3.64711500	-2.80315700	-0.22422300
H	-4.49970600	-1.58711100	-1.15702600
H	-2.75641700	0.33891400	1.51445800
H	-4.33682400	-0.24157600	0.93438700
H	-3.20955200	-1.37369000	1.69897300
H	-3.87198100	0.53997900	-1.47561000
H	-2.34128800	1.24831600	-0.94744900
H	-2.37735500	0.05434500	-2.28200800
C	2.42254700	-1.41496600	0.27456700
C	3.06583900	-2.75361900	-0.11972700
C	3.00044700	-0.34932600	-0.65719000
C	2.72314900	-1.14694000	1.75010700
H	2.83319000	-3.56099400	0.57814200
H	2.79486300	-3.05666000	-1.13509800
H	4.14729100	-2.60942500	-0.08860900
H	2.70360400	0.64519000	-0.33775400
H	4.09038700	-0.43421500	-0.62708800
H	2.67472000	-0.52641600	-1.68706400
H	3.80751200	-1.08287400	1.88214700
H	2.25279100	-0.21366500	2.05267800
H	2.35400300	-1.97602200	2.36236000
C	1.26655800	2.36094200	-1.59602100
C	2.24483700	3.16830200	-1.91265100
C	0.30655800	1.54881500	-1.24932800
H	2.15591700	4.24257800	-1.77499000
H	3.17591700	2.78807900	-2.32476900
H	-0.45589700	1.28296800	-1.97694900
C	0.19972000	0.97644600	0.19701600
O	1.19043200	1.22614200	0.97520700
O	-1.09211100	1.45785400	0.70741900
C	-0.99472800	2.50091600	1.65933400
C	-0.60156800	3.83876100	1.04862500
H	-0.28215600	2.22433800	2.44094200

H	-1.99359000	2.56647000	2.10671300
H	-0.65988200	4.63081200	1.80169100
H	0.42088000	3.78596600	0.66865300
H	-1.26994200	4.09661100	0.22153200

TS1-2

C	1.18816600	1.09890400	-1.69149300
C	1.81541600	-0.08857900	-1.82022900
C	1.66107700	0.35952800	0.40156400
N	1.09262500	1.35802100	-0.33119900
H	0.81941600	1.77149900	-2.44840900
H	2.07750600	-0.63556300	-2.70952400
N	2.10756500	-0.52443500	-0.53687600
C	0.59812600	2.67786300	0.15211900
C	1.61531600	3.73914400	-0.28283200
C	-0.77355100	2.95631000	-0.47037900
C	0.46785600	2.69230600	1.67029500
H	2.59248900	3.52956100	0.16167400
H	1.72543300	3.76436200	-1.37038300
H	1.28353300	4.72625800	0.04981200
H	-1.47865100	2.16127900	-0.21213700
H	-1.15624300	3.90302100	-0.08016500
H	-0.72313800	3.04431300	-1.55854500
H	0.19642000	3.70496900	1.97836500
H	-0.32042600	2.01215000	2.00089800
H	1.41194700	2.42654800	2.15165000
C	2.81652400	-1.80198200	-0.25094800
C	3.74599000	-1.60491400	0.94904400
C	1.78408700	-2.91237300	-0.02248600
C	3.68456500	-2.17848600	-1.45750200
H	4.50165700	-0.84995500	0.71446100
H	3.21949000	-1.28467500	1.84694800
H	4.25300000	-2.54903000	1.16363800
H	1.15800200	-3.02374700	-0.91291600
H	2.29679400	-3.86096500	0.15886300
H	1.12859200	-2.70421600	0.82439300
H	4.30375400	-3.03545100	-1.18252600
H	3.08576800	-2.47336400	-2.32274400
H	4.34381400	-1.35348700	-1.74136900
C	-0.62831600	-0.66891700	1.74375900
C	0.67543100	-0.40414000	2.05215000
C	-1.44115800	-0.55459000	0.69880300
H	0.88227400	0.40146200	2.74874800
H	1.32394500	-1.26118500	2.20749700
H	-1.09861500	-0.15126100	-0.26069700
C	-2.86599300	-0.93242100	0.75487800
O	-3.45026600	-1.45416900	1.68433800
O	-3.49300500	-0.61086300	-0.39796600
C	-4.88984000	-0.92509500	-0.45781500

C	-5.39847600	-0.46820000	-1.80752100
H	-5.40471400	-0.41896600	0.36422200
H	-5.01963600	-2.00251900	-0.31622500
H	-6.46522100	-0.68539600	-1.89635700
H	-5.25230600	0.60771400	-1.92886200
H	-4.87135600	-0.98434800	-2.61319700

M1-2

C	1.58594300	1.12787400	-1.67889300
C	2.06348600	-0.13238100	-1.72860300
C	1.43431700	0.27669000	0.36886000
N	1.19704600	1.38023600	-0.37611900
H	1.48923400	1.85620800	-2.46528400
H	2.46191900	-0.67835500	-2.56388300
N	1.96535400	-0.65927600	-0.45449500
C	0.56676500	2.71118900	-0.04292000
C	1.52421200	3.80317300	-0.53623500
C	-0.77255800	2.77697500	-0.78409300
C	0.33208100	2.92267800	1.45061200
H	2.50545400	3.69287200	-0.06724400
H	1.64877100	3.79679700	-1.62081600
H	1.11406000	4.77693900	-0.25874500
H	-1.44479100	1.99495900	-0.42203300
H	-1.23114000	3.75248500	-0.60316200
H	-0.64204300	2.65942600	-1.86308200
H	-0.11896900	3.91198100	1.55871400
H	-0.35657900	2.18797200	1.87252400
H	1.27094100	2.92624300	2.00933800
C	2.43744000	-2.03935900	-0.08172700
C	3.57599100	-1.92534700	0.93797800
C	1.25530500	-2.87630500	0.41915200
C	2.99562900	-2.72040600	-1.33418800
H	4.39142600	-1.32889000	0.52025300
H	3.26943800	-1.47559200	1.88211200
H	3.95634200	-2.92719000	1.15234500
H	0.49882800	-2.95664600	-0.36637900
H	1.61888300	-3.88015100	0.65363300
H	0.77203800	-2.46788700	1.30557100
H	3.32984200	-3.71875800	-1.04581500
H	2.23304200	-2.83496000	-2.10873100
H	3.85645400	-2.18483500	-1.74289200
C	-0.53368700	-0.17855600	1.97322300
C	0.97335900	0.04687900	1.77800900
C	-1.23638300	-0.40175100	0.83500900
H	1.32007900	0.86903100	2.40463100
H	1.48588300	-0.82851300	2.17548700
H	-0.85178300	-0.42531800	-0.19662900
C	-2.69005000	-0.61825900	0.88117300
O	-3.41572600	-0.69352400	1.85728900

O	-3.20538300	-0.72583000	-0.37665200
C	-4.61668700	-0.93234000	-0.45460900
C	-4.98001900	-1.04815900	-1.91956000
H	-5.13208500	-0.09384600	0.02507200
H	-4.88157300	-1.83808800	0.10045400
H	-6.05578100	-1.20474800	-2.02780400
H	-4.70713300	-0.13714500	-2.45762700
H	-4.45955100	-1.89144900	-2.37992200

TS2

C	2.20341800	-3.84646200	-0.92241500
C	3.14683400	-3.35954900	-0.08809900
C	1.46498400	-1.90733600	-0.12846600
N	1.16472500	-2.94422700	-0.94590400
H	2.20454000	-4.75895300	-1.48906000
H	4.09387600	-3.78606800	0.18490400
N	2.68770400	-2.16108200	0.40999000
C	-0.06512700	-3.13636200	-1.80017400
C	0.11419000	-4.39531400	-2.65061800
C	-1.28147900	-3.32486500	-0.89366200
C	-0.18224900	-1.92950200	-2.72430700
H	0.99147400	-4.33303300	-3.30004700
H	0.17008700	-5.30212600	-2.04223700
H	-0.76757700	-4.47966700	-3.28877700
H	-1.52531500	-2.41315500	-0.35326700
H	-2.14324100	-3.58004700	-1.51513500
H	-1.09800300	-4.14577300	-0.19336600
H	-1.05746900	-2.05447500	-3.36522300
H	-0.33360000	-1.01732100	-2.15441000
H	0.71423900	-1.84757300	-3.34683100
C	3.54181500	-1.31425700	1.33141000
C	4.23756800	-0.24137500	0.49190800
C	2.71487900	-0.71090700	2.46696200
C	4.60446400	-2.22068400	1.96608700
H	4.81113900	-0.70610300	-0.31533300
H	3.52996800	0.47073700	0.06693700
H	4.93154500	0.30920900	1.13372800
H	2.15392600	-1.48892900	2.99272100
H	3.41232400	-0.25225200	3.17290800
H	2.02106300	0.05621200	2.13360600
H	5.14289800	-1.62775300	2.70743300
H	4.15215300	-3.07510100	2.47707600
H	5.34169600	-2.57484400	1.24248500
C	0.62839400	-0.71012000	0.21285200
C	-0.27303100	-0.87334200	1.20436700
C	0.95968000	0.55429600	-0.44824900
H	-0.81082800	-0.02805500	1.60683800
H	-0.41920700	-1.84489000	1.66690300
H	1.61460400	0.45698900	-1.31273900

C	1.34265000	1.71998300	0.33563400
O	2.22320200	2.51094100	0.02480400
O	0.58291500	1.90256300	1.44652300
C	0.90007500	3.05054200	2.24552000
C	2.07371800	2.77587700	3.16725300
H	-0.01104800	3.25549200	2.81238000
H	1.10609100	3.89452700	1.58363000
H	2.29108700	3.66062800	3.77138100
H	1.85106000	1.94331200	3.83962400
H	2.96091700	2.52776000	2.57910500
C	-2.74204700	0.01375400	-0.56195500
O	-2.70269500	-0.68955500	-1.59445600
C	-3.77346700	-0.35040400	0.48774400
C	-4.75226700	-1.28581300	0.13706400
C	-3.78808600	0.17580800	1.78489300
C	-5.72867300	-1.67826500	1.04680400
H	-4.72257500	-1.69540900	-0.86707200
C	-4.76214600	-0.21692000	2.69956900
H	-3.02960600	0.88652800	2.09794900
C	-5.73737300	-1.14283600	2.33362700
H	-6.48327200	-2.40223500	0.75399900
H	-4.75612900	0.19741700	3.70305700
H	-6.49557800	-1.44816600	3.04808600
C	-1.91808900	1.15266800	-0.34555700
C	-0.86879400	1.43338100	-1.22658600
H	-2.09437100	1.78723600	0.51412800
H	-0.86032900	0.80617900	-2.11439400
C	-0.39596700	2.81506700	-1.49786100
C	0.36382500	3.06562400	-2.64695600
C	-0.69684100	3.89192900	-0.65513700
C	0.80303900	4.34914300	-2.95349600
H	0.60880400	2.23563200	-3.30594800
C	-0.25189700	5.17674100	-0.95403800
H	-1.28986500	3.72677200	0.23925700
C	0.49765900	5.41226600	-2.10472300
H	1.38294600	4.52169400	-3.85504200
H	-0.49841600	5.99887600	-0.28878800
H	0.83765100	6.41570100	-2.34039600

M2

C	-3.91905100	-2.46190700	0.68647700
C	-4.49333900	-1.63426500	-0.21390500
C	-2.33941100	-1.11809100	-0.09863200
N	-2.58309900	-2.14094800	0.75529300
H	-4.36698100	-3.25015700	1.26208300
H	-5.51642300	-1.59210000	-0.53775800
N	-3.51198500	-0.80351300	-0.70401300
C	-1.63704000	-2.80207700	1.73482200
C	-2.33171200	-4.03188600	2.32550100

C	-0.35386800	-3.26139400	1.03749800
C	-1.36172000	-1.79668500	2.85229700
H	-3.21993900	-3.77439700	2.90672800
H	-2.59487300	-4.75783200	1.55105000
H	-1.62478200	-4.50707000	3.00765200
H	0.35385600	-2.45564000	0.84314400
H	0.15057200	-3.96308900	1.70721200
H	-0.59277300	-3.79020300	0.10998600
H	-0.63980500	-2.22513700	3.55234900
H	-0.94072700	-0.87318000	2.45490500
H	-2.28156800	-1.55841000	3.39325400
C	-3.83650600	0.33660700	-1.64682200
C	-3.95570200	1.60629200	-0.80422500
C	-2.78740700	0.47545100	-2.75117500
C	-5.18312600	0.04155300	-2.31653700
H	-4.74808900	1.49496900	-0.05895600
H	-3.02244500	1.84710200	-0.29343600
H	-4.20889800	2.44556000	-1.45807200
H	-2.62042400	-0.48197700	-3.25225800
H	-3.17653400	1.18581100	-3.48497100
H	-1.83333700	0.85675700	-2.39561300
H	-5.35828400	0.82235800	-3.05840900
H	-5.17418500	-0.92278600	-2.83174600
H	-6.01723500	0.07482800	-1.61271300
C	-1.00556200	-0.52301100	-0.41404500
C	-0.31921500	-1.10777100	-1.39981900
C	-0.52640200	0.70469800	0.34641000
H	0.64329200	-0.72145500	-1.70927600
H	-0.71221100	-1.98769600	-1.90201700
H	-1.24389700	0.93466900	1.14124400
C	-0.47782300	1.97736500	-0.48294200
O	-0.98746100	3.02146600	-0.13713500
O	0.25044500	1.85079400	-1.59769600
C	0.48305000	3.06148800	-2.34814300
C	-0.68999200	3.38682400	-3.25105500
H	1.38726900	2.85492400	-2.92214600
H	0.67933000	3.87032300	-1.64078200
H	-0.47887500	4.30297700	-3.80819600
H	-0.86280200	2.58001500	-3.96730300
H	-1.59597500	3.54042800	-2.65964000
C	2.73046400	-1.02738900	0.40028500
O	2.50129800	-1.85383500	1.34738100
C	3.86457700	-1.38230700	-0.54397200
C	4.24224800	-2.72548100	-0.64276100
C	4.56984900	-0.44152500	-1.30490200
C	5.26631900	-3.12596100	-1.49648100
H	3.70985600	-3.44271200	-0.02662500
C	5.59976200	-0.83536200	-2.15562600

H	4.32635900	0.61273500	-1.21222400
C	5.94964100	-2.18095600	-2.26035000
H	5.53655600	-4.17604700	-1.56427600
H	6.13893400	-0.08792100	-2.73054400
H	6.75423900	-2.48759800	-2.92162600
C	2.02549000	0.13098000	0.13873700
C	0.90659600	0.53746900	1.03720800
H	2.26984500	0.74229500	-0.72086400
H	0.79990400	-0.28828200	1.74923800
C	1.15974700	1.80890000	1.84413200
C	0.56763200	1.98055200	3.09924500
C	1.95491200	2.84226100	1.34081000
C	0.76616800	3.14687200	3.83461300
H	-0.05179900	1.18514500	3.51021600
C	2.14989400	4.01460200	2.06650600
H	2.43708300	2.71428100	0.37535500
C	1.55715200	4.17104000	3.31814600
H	0.30649600	3.25472700	4.81244000
H	2.77171300	4.80518300	1.65722700
H	1.71515500	5.08111800	3.88822000

TS2'

C	0.96631000	-0.52931600	-0.02268400
C	1.17117600	0.36753800	-1.10017600
C	0.01469500	-1.52309700	0.08438600
H	1.09431400	-0.02681600	-2.10427600
H	1.94222600	1.12120200	-0.96069900
H	-0.08872400	-2.05674800	1.02382600
C	-0.73150300	-2.14059600	-1.00143700
O	-1.56536000	-3.02007700	-0.84071000
O	-0.35259700	-1.71726800	-2.22414800
C	-1.02282600	-2.31262300	-3.34170000
C	-0.35854900	-3.62367900	-3.72020900
H	-0.93935100	-1.57428600	-4.14243200
H	-2.07402400	-2.44185700	-3.08767300
H	-0.83178600	-4.04506300	-4.61115100
H	0.70310300	-3.47102600	-3.93245700
H	-0.45488600	-4.34170400	-2.90260600
C	-2.67517100	0.14108200	-0.87047300
O	-2.85334900	-0.42210900	-1.96848800
C	-3.61378400	-0.21554500	0.26197300
C	-4.21351800	-1.47842800	0.23245200
C	-3.92084800	0.65064000	1.31756400
C	-5.07739500	-1.87940300	1.24682500
H	-3.96239500	-2.13707000	-0.59130800
C	-4.79666600	0.25640700	2.32648800
H	-3.49292600	1.64837500	1.34740900
C	-5.37288600	-1.01221300	2.29791800
H	-5.52364000	-2.86910400	1.21833800

H	-5.03282700	0.94318600	3.13367000
H	-6.05120600	-1.32088200	3.08734500
C	-1.65983800	1.10808000	-0.60383800
C	-0.65888700	1.40951100	-1.53262800
H	-1.66156400	1.59107100	0.36631100
H	-0.78139000	0.87753400	-2.47455800
C	-0.05634300	2.76287200	-1.68624000
C	0.86690000	2.99803200	-2.71644400
C	-0.41296900	3.84093300	-0.86695400
C	1.43414500	4.25262800	-2.90416600
H	1.14316200	2.17541600	-3.37193600
C	0.16134000	5.09789400	-1.04538500
H	-1.16368600	3.69812100	-0.09588400
C	1.08936200	5.31000100	-2.06171200
H	2.14662500	4.40769600	-3.70850000
H	-0.12947500	5.91765300	-0.39551400
H	1.53181200	6.29069100	-2.20409800
C	1.90081500	-0.46586100	1.14292600
N	3.07930300	-1.13894500	1.16267300
N	1.74948100	0.12446000	2.35004400
C	3.66575000	-0.95731200	2.39648500
C	3.77718700	-1.88306200	0.04072600
C	2.84220900	-0.17848400	3.13206500
C	0.63977600	1.04332800	2.79152300
H	4.61019300	-1.39050900	2.66930400
C	4.87693200	-2.75161000	0.66176700
C	2.82069600	-2.80282500	-0.72470600
C	4.41546700	-0.85005700	-0.88974200
H	2.95837600	0.17403600	4.14051700
C	0.60932700	2.21997200	1.82064200
C	-0.68422600	0.27914700	2.82092700
C	0.94793000	1.55632800	4.19793200
H	5.68136800	-2.15575800	1.09842300
H	4.47530600	-3.43435300	1.41546500
H	5.31813900	-3.34849200	-0.13810700
H	2.13824300	-2.25541600	-1.37334600
H	3.43212000	-3.45684200	-1.35152600
H	2.23995100	-3.42584100	-0.03973000
H	5.01005400	-1.37358900	-1.64323100
H	3.65355700	-0.25840100	-1.39915700
H	5.07555800	-0.18281600	-0.32853500
H	1.54479400	2.78513600	1.87187000
H	0.46089300	1.87859600	0.79684800
H	-0.21573900	2.88612800	2.08889600
H	-0.60012500	-0.60363900	3.46196000
H	-1.45398600	0.93492600	3.23811400
H	-1.00150200	-0.02700700	1.82411100
H	0.14756900	2.24538200	4.47500400

H	0.96255100	0.74926400	4.93541700
H	1.89064000	2.10812700	4.23701700

M2'

C	1.13627200	-0.52005100	0.04430500
C	0.94462400	0.48235600	-1.06627600
C	0.41332700	-1.63034500	0.24385900
H	1.30842200	0.03514800	-1.99870400
H	1.59166100	1.34106700	-0.86186400
H	0.60062000	-2.25460600	1.11421100
C	-0.60654500	-2.20379800	-0.67601200
O	-1.46317100	-2.97810400	-0.30602900
O	-0.35731200	-1.89981000	-1.95207500
C	-1.21709000	-2.51034800	-2.93708300
C	-0.74141200	-3.91676700	-3.24692700
H	-1.13661600	-1.85696900	-3.80747900
H	-2.23878000	-2.46853500	-2.56464100
H	-1.35283700	-4.34790000	-4.04377300
H	0.30058400	-3.90970700	-3.57737100
H	-0.82787000	-4.55235500	-2.36302200
C	-2.73690500	-0.02721400	-0.68130400
O	-3.05968300	-0.41977500	-1.84948000
C	-3.70707600	-0.35642800	0.44140600
C	-4.61965400	-1.39604700	0.23557100
C	-3.75574500	0.32810100	1.66339100
C	-5.52895100	-1.76608700	1.22297500
H	-4.59623700	-1.90049100	-0.72427600
C	-4.66607900	-0.03430500	2.65326200
H	-3.08896800	1.16789700	1.83883600
C	-5.55449900	-1.08800600	2.44041900
H	-6.22221000	-2.58288000	1.04286700
H	-4.68928900	0.51429900	3.59044800
H	-6.26511200	-1.36938400	3.21143800
C	-1.56622200	0.61872200	-0.32891500
C	-0.54056300	0.98615600	-1.34754300
H	-1.40751200	0.88909300	0.70629000
H	-0.86391400	0.48290300	-2.26501700
C	-0.44266500	2.47873500	-1.67553900
C	0.32915600	2.89947400	-2.76735000
C	-1.09403500	3.45437400	-0.91843400
C	0.45088500	4.24765300	-3.08903200
H	0.83715300	2.15501300	-3.37737400
C	-0.97000300	4.80853600	-1.23113500
H	-1.71586500	3.13743400	-0.08604000
C	-0.19758400	5.21155800	-2.31670200
H	1.04855400	4.54761900	-3.94458800
H	-1.48444200	5.54943500	-0.62626400
H	-0.10506400	6.26433700	-2.56399400
C	2.26877000	-0.32078900	0.99178700

N	3.52644100	-0.77363600	0.78085700
N	2.23618100	0.26705700	2.20831400
C	4.28984100	-0.46027700	1.88434100
C	4.12528700	-1.37650900	-0.47409200
C	3.49094200	0.17859700	2.76871000
C	1.07573200	0.98329700	2.86128900
H	5.33002300	-0.71451900	1.97114800
C	5.43233700	-2.07592000	-0.08601900
C	3.20005000	-2.41834400	-1.11113000
C	4.42552900	-0.22871600	-1.43979000
H	3.72709500	0.56300100	3.74389700
C	0.69302700	2.16525200	1.97049800
C	-0.08435100	0.00959000	3.08692300
C	1.53288100	1.51538000	4.22050300
H	6.20372300	-1.37115600	0.23079100
H	5.27101700	-2.82101800	0.69752200
H	5.81052600	-2.58816000	-0.97197800
H	2.33021200	-1.98347200	-1.60173800
H	3.78106900	-2.94380400	-1.87247700
H	2.86405300	-3.14981600	-0.37141700
H	4.91184100	-0.63302800	-2.33114400
H	3.51265000	0.28260000	-1.74983400
H	5.09767000	0.49781500	-0.97574700
H	1.52876200	2.86570000	1.88734200
H	0.39881800	1.85054300	0.97036400
H	-0.15825500	2.68709400	2.41687100
H	0.26055200	-0.86914100	3.63924500
H	-0.84328700	0.51672100	3.68882600
H	-0.55193100	-0.30901700	2.15660200
H	0.68778000	2.04557700	4.66319500
H	1.81428500	0.70786200	4.90140500
H	2.35837500	2.22538700	4.12819600

TS3

C	2.57692100	3.07978800	0.76967200
C	3.59978700	2.33693600	0.30839700
C	1.71960200	1.44315600	-0.45624100
N	1.41194100	2.55318800	0.25902000
H	2.59132200	3.93599700	1.41923100
H	4.65775800	2.45387900	0.46091700
N	3.07064300	1.33586500	-0.47498100
C	0.10253600	3.19601800	0.64891500
C	0.28691800	4.71947700	0.54382500
C	-1.03519600	2.83269600	-0.29788900
C	-0.19245100	2.80017900	2.09929700
H	0.97438100	5.12689700	1.28713100
H	0.63084600	5.00425200	-0.45462300
H	-0.68581700	5.18538000	0.71801200
H	-1.27590100	1.77528600	-0.32412300

H	-1.92426200	3.35078100	0.06620700
H	-0.80792100	3.18178000	-1.30988800
H	-1.22222100	3.06698000	2.34453900
H	-0.04534200	1.73000500	2.24351600
H	0.48977700	3.32586900	2.77630400
C	4.03257600	0.53282600	-1.32295300
C	3.39675200	-0.67166300	-2.00027100
C	4.55817600	1.49464500	-2.39586200
C	5.16820700	0.04787800	-0.41187700
H	2.96852800	-1.33868400	-1.25387800
H	2.63488900	-0.39045200	-2.72257500
H	4.19848900	-1.19364000	-2.53247600
H	5.05274700	2.36457100	-1.95482000
H	5.28447300	0.96920600	-3.02206000
H	3.73826000	1.84153100	-3.03234600
H	5.78006500	-0.65662400	-0.98164600
H	5.82937300	0.86295000	-0.10422600
H	4.75625900	-0.44826700	0.47223400
C	0.76223300	0.52188700	-1.16099900
C	0.36067100	0.92439900	-2.36993700
C	0.36195900	-0.76781500	-0.47030000
H	-0.32218900	0.32172300	-2.95861500
H	0.71375800	1.85470600	-2.80779800
H	1.40314100	-1.09643100	0.20294200
C	0.09839800	-1.91638500	-1.36546000
O	-0.58571600	-2.88691900	-1.07232600
O	0.76021200	-1.89458200	-2.55672500
C	0.74380700	-3.10627700	-3.31294100
C	1.75400300	-4.09959400	-2.76560200
H	0.99918100	-2.80690600	-4.33204600
H	-0.26363900	-3.52799700	-3.30695100
H	1.76414000	-5.00819500	-3.37351600
H	2.75680900	-3.66456300	-2.77183000
H	1.49351300	-4.36867000	-1.73953700
C	-3.13500600	0.39106800	0.33444700
O	-3.05999100	1.20124000	1.33212800
C	-4.43401900	0.43290400	-0.45424500
C	-5.23100100	1.57917900	-0.34511600
C	-4.90444500	-0.61040800	-1.26543100
C	-6.42901400	1.70167000	-1.04449900
H	-4.88063900	2.36606600	0.31467500
C	-6.10503700	-0.49720600	-1.96185900
H	-4.33473900	-1.53213400	-1.33394200
C	-6.87295700	0.66317800	-1.86150600
H	-7.02226300	2.60717900	-0.94898100
H	-6.44939700	-1.32317500	-2.57804400
H	-7.80972800	0.75022700	-2.40345100
C	-2.15214800	-0.45894100	-0.11252500

C	-0.79358600	-0.57375700	0.55166800
H	-2.33383100	-1.08957900	-0.97559000
H	-0.59463300	0.38434900	1.03928900
C	-0.81894500	-1.56981200	1.71678200
C	-0.00115800	-2.69633300	1.83748100
C	-1.74725500	-1.32636100	2.74243700
C	-0.10950100	-3.55010000	2.93646100
H	0.74927100	-2.89144300	1.08384000
C	-1.85280500	-2.17329500	3.84256500
H	-2.38160300	-0.44664700	2.64923500
C	-1.03496800	-3.29869800	3.94585100
H	0.53961300	-4.41979100	3.00258500
H	-2.57745700	-1.95598800	4.62348000
H	-1.11550000	-3.96484400	4.80009800
C	2.72254600	-0.55554600	1.90040300
O	1.80438400	0.29825500	2.13442400
O	3.79577900	-0.64006200	2.58552300
O	2.57143300	-1.39207100	0.87876600

M3

C	0.88451600	-3.60788500	0.81039700
C	-0.16968100	-3.49902900	1.64535000
C	-0.41331500	-1.98416200	0.03862800
N	0.72768500	-2.66769200	-0.18733400
H	1.72355800	-4.28010000	0.84729000
H	-0.39343500	-4.05906700	2.53422500
N	-0.97950500	-2.49089200	1.16234500
C	1.70695200	-2.65616700	-1.34098000
C	1.42137100	-3.91952900	-2.15763600
C	1.59024600	-1.42944100	-2.24122300
C	3.11237400	-2.67941700	-0.72404500
H	1.50883200	-4.82448500	-1.54960800
H	0.41369300	-3.87379200	-2.58154100
H	2.14251500	-3.98617000	-2.97672900
H	1.76180300	-0.51375400	-1.67100100
H	2.37216300	-1.53214100	-2.99933400
H	0.62297900	-1.38092400	-2.74048500
H	3.84186800	-2.45820200	-1.50721500
H	3.18798600	-1.92152600	0.06453600
H	3.36763300	-3.66076700	-0.31367100
C	-2.28872800	-2.10697400	1.81256400
C	-2.28227000	-0.61268800	2.10866700
C	-3.44895900	-2.48566200	0.88947900
C	-2.42428000	-2.87805800	3.12720700
H	-1.42419100	-0.34261200	2.73142700
H	-2.26554000	-0.02827000	1.18987200
H	-3.19960700	-0.36169600	2.65010600
H	-3.38858700	-3.54197200	0.60873200
H	-4.38639200	-2.32251000	1.42913800

H	-3.45257500	-1.86244700	-0.00428400
H	-3.35071500	-2.54914700	3.60194200
H	-2.49899800	-3.95777200	2.97064800
H	-1.60107900	-2.66311300	3.81424500
C	-0.98016900	-0.91952400	-0.85249100
C	-1.78205800	-1.47941900	-1.80750000
C	-0.53398800	0.42763900	-0.59605100
H	-2.28963900	-0.90312000	-2.56484700
H	-1.94251400	-2.55324600	-1.79752900
H	-3.25407300	0.66565300	-1.21537900
C	-0.82652200	1.50689400	-1.45856300
O	-0.38725900	2.66488200	-1.38737600
O	-1.72578800	1.19753700	-2.47789700
C	-2.11033000	2.27401800	-3.32927200
C	-3.21589200	3.10498800	-2.70083500
H	-2.46008400	1.79907800	-4.25058100
H	-1.23558800	2.88815900	-3.55505800
H	-3.51869300	3.91068600	-3.37657100
H	-4.07829400	2.46684400	-2.49127500
H	-2.85515900	3.54573200	-1.76817100
C	2.93447500	0.53703500	0.66236300
O	2.93789500	-0.29376800	1.65319800
C	4.29230700	0.86169200	0.06624000
C	5.37711100	0.05358200	0.42989000
C	4.54255800	1.92496600	-0.81455900
C	6.65285900	0.27181300	-0.08519200
H	5.17947800	-0.74700400	1.13512400
C	5.81612800	2.15203300	-1.32749100
H	3.73563900	2.59629200	-1.09103500
C	6.88046000	1.32275100	-0.97096100
H	7.47428000	-0.37633300	0.20869900
H	5.98198900	2.98483700	-2.00537200
H	7.87354000	1.50054300	-1.37245900
C	1.82415100	1.09999000	0.08948300
C	0.42577900	0.73925900	0.54978300
H	1.89542600	1.78114200	-0.74981500
H	0.57415100	-0.17640100	1.14104500
C	-0.08690600	1.76222600	1.57554900
C	-1.31870600	2.41731800	1.49877400
C	0.72802600	2.02496900	2.68691400
C	-1.71959700	3.31013600	2.49398600
H	-1.98301300	2.20346300	0.66659800
C	0.32753500	2.90776100	3.68576800
H	1.67610200	1.49396900	2.75270400
C	-0.90085600	3.56352700	3.59128500
H	-2.68234000	3.80778500	2.41043600
H	0.97278800	3.08539800	4.54235500
H	-1.21702100	4.25612000	4.36586900

C	-5.13554900	0.35683200	-1.04760600
O	-5.15154600	0.20506100	-2.29142600
O	-6.06330000	0.25653100	-0.22373900
O	-3.90255400	0.69877000	-0.49221600

TS4

C	0.06727700	-3.35033500	1.57541400
C	-0.94629900	-2.84538100	2.30724300
C	-0.75135100	-1.60886800	0.47793300
N	0.17941000	-2.58685100	0.43077700
H	0.71180800	-4.18786400	1.77776900
H	-1.33108000	-3.16920400	3.25681900
N	-1.45761200	-1.76105100	1.62040200
C	1.13687000	-3.03434200	-0.65404800
C	0.59207500	-4.36551700	-1.18304900
C	1.26013000	-2.04701700	-1.81010000
C	2.51240700	-3.20520700	0.00099800
H	0.51499500	-5.11816800	-0.39419200
H	-0.39538800	-4.22282100	-1.63154800
H	1.27136500	-4.74561100	-1.95022200
H	1.65708600	-1.08705200	-1.47151800
H	1.96994400	-2.48980800	-2.51441500
H	0.31366800	-1.90318700	-2.33261800
H	3.24676400	-3.40416500	-0.78401100
H	2.79663200	-2.29235100	0.53747100
H	2.53730700	-4.05440500	0.68951500
C	-2.73004400	-1.07530800	2.06981400
C	-2.73043800	0.39906300	1.68314100
C	-3.91090600	-1.81051000	1.43395600
C	-2.79738800	-1.17894700	3.59836000
H	-1.80304900	0.88289200	1.99574600
H	-2.90663000	0.54284400	0.61636600
H	-3.55938900	0.87476700	2.21539800
H	-3.87041100	-2.87794500	1.67582000
H	-4.83445700	-1.40422200	1.85943800
H	-3.96225200	-1.67090300	0.34931900
H	-3.63776800	-0.57030500	3.93661800
H	-2.98216600	-2.19819900	3.94490800
H	-1.88570800	-0.79552600	4.06550200
C	-1.01354200	-0.62014200	-0.61216100
C	-2.05149900	-1.11753600	-1.52651900
C	-0.30284300	0.54777000	-0.58830400
H	-1.83424900	-0.92539600	-2.57648400
H	-2.24234600	-2.18142400	-1.36236100
H	-3.13618300	-0.46972300	-1.35596900
C	-0.46150200	1.57126400	-1.64475000
O	0.16272600	2.61907300	-1.68345000
O	-1.39370500	1.26795800	-2.56449100
C	-1.85407900	2.33522300	-3.40251800

C	-2.85561300	3.18197800	-2.63629100
H	-2.32517000	1.83612900	-4.25115900
H	-1.00122500	2.91829200	-3.75659500
H	-3.33448000	3.90499000	-3.30199300
H	-3.60850000	2.52019400	-2.19612500
H	-2.34893000	3.73178700	-1.83787700
C	3.19042800	0.26942700	0.47735200
O	3.13011500	-0.35593300	1.60214600
C	4.53018700	0.24201300	-0.23376800
C	5.45655000	-0.73514800	0.14948500
C	4.90588900	1.13987400	-1.24300800
C	6.69799200	-0.84024600	-0.47325200
H	5.16994400	-1.40462600	0.95372800
C	6.14845700	1.04433600	-1.86329300
H	4.22791800	1.93611600	-1.53418400
C	7.05058500	0.04898400	-1.48656300
H	7.39511600	-1.61422600	-0.16419900
H	6.41855200	1.75530000	-2.63887900
H	8.01945100	-0.02458800	-1.97082000
C	2.14363300	0.90492300	-0.14301600
C	0.75543900	0.86872200	0.46159700
H	2.26341900	1.41037800	-1.09269900
H	0.79179300	0.03369400	1.17528500
C	0.47537500	2.10599400	1.32467100
C	-0.62099100	2.95888000	1.17847900
C	1.38828900	2.37818100	2.35445500
C	-0.79432200	4.05867800	2.02071000
H	-1.36127800	2.76179900	0.40921900
C	1.21491300	3.46859100	3.20031400
H	2.22810600	1.69735800	2.47805700
C	0.12311800	4.32219100	3.03284900
H	-1.65319700	4.70893400	1.88162100
H	1.93219600	3.65493100	3.99471800
H	-0.01214200	5.17722200	3.68802100
C	-5.38442200	-0.33168800	-1.42650600
O	-5.30701300	-1.59907600	-1.56612400
O	-6.48067600	0.31338200	-1.44990800
O	-4.25631100	0.35709600	-1.24560700

Cs₂CO₃

C	0.00207400	1.25503800	0.03541700
O	1.12308500	1.88626800	0.05122200
O	-1.11589300	1.87961200	-0.08912300
O	-0.00060900	-0.05204300	0.14436500
Cs	-2.82557700	-0.33789100	-0.00563200
Cs	2.82439300	-0.33921600	-0.01371700

TS3_{Cs}

C	1.39633800	-3.33140200	2.04894100
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C	2.13434100	-2.41916400	2.70717400
C	0.21131900	-1.45871000	2.15450900
N	0.18972000	-2.74574400	1.73063400
H	1.64128700	-4.34263100	1.77906700
H	3.11344600	-2.51484400	3.14197000
N	1.39300300	-1.26073700	2.78938300
C	-0.79054900	-3.54333800	0.90193000
C	-0.86146500	-4.95561600	1.50436500
C	-2.20495700	-2.97704900	0.92558400
C	-0.23509100	-3.59629100	-0.52410100
H	0.06169200	-5.52562200	1.38620800
H	-1.12054300	-4.91227600	2.56585700
H	-1.64693100	-5.50558500	0.98135000
H	-2.29521000	-1.98180200	0.49819700
H	-2.82130100	-3.65136700	0.32504500
H	-2.60014400	-2.96930800	1.94464200
H	-0.96128900	-4.08930300	-1.17510900
H	-0.02928000	-2.58983300	-0.89048100
H	0.69912600	-4.16725600	-0.54823200
C	1.90508700	-0.16664100	3.69765100
C	1.13016500	1.14019700	3.60209700
C	1.79363800	-0.71023300	5.12739900
C	3.36647500	0.11245900	3.32232300
H	1.19928000	1.55924400	2.59847100
H	0.08551100	1.03316400	3.88491200
H	1.60536800	1.83424700	4.30174000
H	2.36801900	-1.63109700	5.25806000
H	2.17884600	0.03550900	5.82757000
H	0.74699800	-0.91158300	5.37457300
H	3.71226200	0.96156200	3.91752000
H	4.02930200	-0.72596400	3.54786900
H	3.44455000	0.36678000	2.26202200
C	-0.88452300	-0.43877600	2.02679500
C	-1.87751100	-0.56747900	2.91368800
C	-0.73007000	0.62844000	0.96929200
H	-2.71414800	0.12058700	2.91713800
H	-1.86780700	-1.35357200	3.66517600
H	0.64255700	0.75039300	0.70700000
C	-1.12333500	1.99122200	1.32858900
O	-1.02733800	2.95564800	0.56657900
O	-1.55979600	2.19844600	2.60133500
C	-1.77821700	3.55676000	2.99239700
C	-0.47947700	4.24150000	3.38035200
H	-2.45670000	3.49642000	3.84616300
H	-2.27438700	4.09173600	2.18036100
H	-0.67440400	5.27465000	3.68063100
H	-0.00429900	3.72183700	4.21571400
H	0.21053500	4.24970800	2.53322200

C	-3.51495600	-0.73346000	-1.19178900
O	-2.96677000	-1.56298900	-2.00000300
C	-5.02577300	-0.79158400	-1.07902300
C	-5.67138600	-1.98224300	-1.43288500
C	-5.81863800	0.28502100	-0.65910700
C	-7.05485600	-2.10992700	-1.33935300
H	-5.05151800	-2.79999200	-1.78671500
C	-7.20336600	0.16590600	-0.56989200
H	-5.34315900	1.23216900	-0.42093400
C	-7.82948000	-1.03504200	-0.90452000
H	-7.53299200	-3.04740800	-1.60978100
H	-7.79834400	1.01607100	-0.24835800
H	-8.90912000	-1.12735700	-0.83731700
C	-2.84199300	0.14520700	-0.37329800
C	-1.33660700	0.19456800	-0.40664000
H	-3.37062100	0.76928200	0.34189700
H	-0.97389600	-0.82879100	-0.56453700
C	-0.81847300	0.95599300	-1.63333000
C	0.31886400	0.51409400	-2.31901200
C	-1.50536600	2.05730600	-2.16112100
C	0.76722800	1.15594200	-3.47676900
H	0.85393300	-0.34129200	-1.91549300
C	-1.06075100	2.70979800	-3.30875100
H	-2.40576700	2.39061900	-1.65643800
C	0.08286500	2.26262900	-3.97673700
H	1.65131100	0.78758200	-3.99107800
H	-1.61128600	3.56467900	-3.69169500
H	0.42471500	2.76261300	-4.87796800
C	2.46024600	-0.11794300	-0.01471500
O	3.68605200	0.01613500	-0.31839300
O	1.80333000	-1.19474600	-0.17293400
O	1.83070300	0.94872000	0.48387800
Cs	1.52268200	3.53066100	-0.93289300
Cs	3.58763700	-2.27500900	-2.26318500

M3_{Cs}

C	1.92277000	-2.42497400	-2.92633000
C	3.15840100	-2.66039000	-2.43276400
C	1.86163200	-2.04517400	-0.74687800
N	1.11574400	-2.05002200	-1.87185200
H	1.56892700	-2.49464100	-3.93850900
H	4.04863200	-2.97252900	-2.94752900
N	3.11787600	-2.42811800	-1.07172100
C	-0.38116700	-1.88440200	-2.02386600
C	-1.01468000	-3.22981500	-1.66470700
C	-0.92390400	-0.76340200	-1.14178500
C	-0.67327500	-1.50738600	-3.47814800
H	-0.57035400	-4.03867300	-2.25263200
H	-0.89037100	-3.43590600	-0.59945300

H	-2.08524700	-3.18883500	-1.88514100
H	-0.45468400	0.18094600	-1.43039000
H	-2.00221800	-0.70237800	-1.32619100
H	-0.77262600	-0.96389600	-0.08468100
H	-1.74408600	-1.30416000	-3.55476700
H	-0.12915000	-0.59399400	-3.73570900
H	-0.44873300	-2.31224400	-4.18210000
C	4.25300700	-2.86742800	-0.16727600
C	4.42741500	-1.98198400	1.06666000
C	3.95444900	-4.31196300	0.24435600
C	5.55344100	-2.81199700	-0.97591000
H	4.67747800	-0.95843000	0.78583500
H	3.54846200	-1.98081600	1.70823000
H	5.26463300	-2.40043100	1.63245400
H	3.78801500	-4.93992900	-0.63563200
H	4.80973200	-4.70981700	0.79702600
H	3.07338300	-4.35244300	0.88806700
H	6.38155000	-2.99497700	-0.28839300
H	5.60188800	-3.58085200	-1.75024500
H	5.69346600	-1.82440900	-1.42390800
C	1.43028500	-1.60214500	0.61471800
C	0.98001700	-2.64927900	1.37356700
C	1.58671000	-0.18498400	0.84111900
H	0.72979600	-2.56108300	2.41976300
H	0.92145000	-3.63599600	0.92706800
H	-0.98496600	-1.38176700	2.20727000
C	1.27201200	0.39921700	2.08871000
O	1.21891700	1.61521000	2.37171800
O	0.99024800	-0.51537000	3.08498100
C	0.56070100	0.01167700	4.33712100
C	1.73986400	0.42867200	5.19880100
H	0.00077400	-0.80072000	4.80945100
H	-0.11658900	0.85274800	4.16907000
H	1.39343800	0.77389200	6.17705300
H	2.41793900	-0.41532000	5.35092400
H	2.28552800	1.23833300	4.71091800
C	0.70603100	2.24767700	-1.76292300
O	0.71752100	1.48985200	-2.80205100
C	-0.19940800	3.46147200	-1.81502900
C	-1.36541600	3.37114500	-2.58652100
C	0.01194500	4.63276400	-1.07292200
C	-2.30972600	4.39601800	-2.58900600
H	-1.50895400	2.46995400	-3.17528500
C	-0.92536200	5.66422600	-1.08025400
H	0.92299900	4.73787400	-0.49055400
C	-2.09622700	5.54740900	-1.83121100
H	-3.21266200	4.29926000	-3.18539400
H	-0.73820000	6.56611000	-0.50447300

H	-2.82517100	6.35168000	-1.83709400
C	1.30018900	1.99342300	-0.54715400
C	2.07898000	0.72276500	-0.30435900
H	1.24756300	2.71279500	0.25942400
H	1.94483800	0.18137900	-1.24535300
C	3.56825100	1.03519200	-0.22377500
C	4.40940700	0.75095700	-1.30414500
C	4.13442600	1.61556300	0.92063300
C	5.77878300	1.01688700	-1.24383600
H	3.98406000	0.30029900	-2.19998200
C	5.49914600	1.87986600	0.98520700
H	3.48505000	1.84500800	1.76129600
C	6.33141700	1.57587300	-0.09475700
H	6.41354100	0.77779900	-2.09278600
H	5.92107300	2.32119000	1.88391300
H	7.39660300	1.77714000	-0.04001400
C	-2.76545300	-1.10321500	1.50426300
O	-3.56633900	-0.18197300	1.20696100
O	-2.85540700	-2.32160100	1.25490900
O	-1.64450000	-0.66778700	2.18331100
Cs	-1.53806300	2.09244300	1.03036600
Cs	-5.38454800	-2.00472300	-0.23845300

TS4_{Cs}

C	1.59406200	-2.66260900	-2.96083600
C	2.81890000	-2.95892900	-2.47739100
C	1.66142200	-1.99728500	-0.85169600
N	0.87445700	-2.06633300	-1.94360100
H	1.18833200	-2.82742100	-3.94251800
H	3.65127000	-3.42723500	-2.97076400
N	2.86096500	-2.54657900	-1.15884000
C	-0.60213400	-1.77600000	-2.09462100
C	-1.34448500	-3.07045000	-1.75511100
C	-1.04821100	-0.64310600	-1.18034300
C	-0.85150400	-1.34041300	-3.54105500
H	-0.93146400	-3.91841500	-2.30983500
H	-1.30861600	-3.25697400	-0.67802700
H	-2.39475400	-2.95540600	-2.03979500
H	-0.50424700	0.26931400	-1.43746700
H	-2.11621600	-0.48645900	-1.37104400
H	-0.93368400	-0.89211000	-0.12814600
H	-1.89940600	-1.04010300	-3.61744700
H	-0.22743100	-0.47349700	-3.77514100
H	-0.69671500	-2.14325000	-4.26527500
C	3.98820500	-2.99404300	-0.24837600
C	4.20819300	-2.08659700	0.96328700
C	3.63300400	-4.41046000	0.21295700
C	5.28131100	-3.00475600	-1.07161900
H	4.42463100	-1.06016000	0.66242500

H	3.36906400	-2.09260800	1.65690700
H	5.08220200	-2.48289600	1.48736200
H	3.47910000	-5.07365100	-0.64296600
H	4.45325800	-4.80766600	0.81654900
H	2.72564900	-4.39545300	0.82211800
H	6.11136700	-3.20983400	-0.39287600
H	5.29285900	-3.78519000	-1.83481900
H	5.45298000	-2.03097400	-1.53824200
C	1.34600600	-1.44130000	0.49377900
C	0.71583100	-2.40594900	1.39189900
C	1.63870100	-0.11722100	0.67739200
H	1.18291000	-2.49592900	2.37146700
H	0.57985400	-3.38341000	0.92630200
H	-0.44497400	-1.75774300	1.75257700
C	1.51065200	0.46878500	2.02853700
O	1.19813900	1.62426200	2.28531000
O	1.82148900	-0.39768400	3.00659900
C	1.69046100	0.06958000	4.35654700
C	2.91694600	0.85770500	4.77798100
H	1.57773400	-0.83793800	4.95246200
H	0.78254700	0.67068800	4.44109800
H	2.83934400	1.13411100	5.83247000
H	3.81954000	0.25664200	4.64271700
H	3.00516600	1.76909300	4.18334400
C	0.63055500	2.33076800	-1.80615600
O	0.61560200	1.59676400	-2.85792800
C	-0.29330200	3.53217400	-1.79868700
C	-1.46658100	3.45569700	-2.55922400
C	-0.07973700	4.68171600	-1.02526200
C	-2.41643300	4.47443900	-2.52232300
H	-1.61050500	2.57133200	-3.17265000
C	-1.02234900	5.70731600	-0.99313900
H	0.83828200	4.77716300	-0.45250300
C	-2.20026700	5.60494400	-1.73472700
H	-3.32561200	4.38942600	-3.11080700
H	-0.83435900	6.59322600	-0.39349100
H	-2.93436100	6.40409800	-1.70847400
C	1.28800300	2.06421100	-0.62537800
C	2.09787200	0.80280000	-0.46599400
H	1.24051000	2.75174900	0.20794300
H	1.92524100	0.26482800	-1.40419800
C	3.59470500	1.07382900	-0.39778500
C	4.43382100	0.64081400	-1.42864000
C	4.17135400	1.74149700	0.69086200
C	5.81195500	0.85214700	-1.37296300
H	3.99977300	0.11991600	-2.28056800
C	5.54681800	1.94619000	0.75459800
H	3.53142500	2.10327200	1.49154000

C	6.37505300	1.49856900	-0.27577000
H	6.44470200	0.50436500	-2.18459600
H	5.97605600	2.45836700	1.61069400
H	7.44726900	1.65796600	-0.22453000
C	-2.51981300	-1.28864800	1.68291400
O	-3.43180100	-0.39416100	1.70276900
O	-2.69520900	-2.46589400	1.24865700
O	-1.31078400	-0.93022300	2.12314700
Cs	-1.66671800	1.96099000	1.09732300
Cs	-5.32674200	-1.91495000	0.00458500

M4

C	1.49648500	3.21859400	-0.91400700
C	0.37092100	3.38519400	-1.64098400
C	-0.11111100	2.06788600	0.07354700
N	1.19044400	2.41322800	0.15753900
H	2.48251800	3.61668700	-1.07640200
H	0.21653900	3.94854500	-2.54296500
N	-0.63645200	2.68554900	-1.01097200
C	2.24553700	2.15460100	1.21328800
C	2.38596700	3.44622100	2.02383800
C	1.89110900	0.99173500	2.13646800
C	3.55392700	1.83500800	0.47493800
H	2.64500500	4.29323500	1.38282300
H	1.46323300	3.68227500	2.56067900
H	3.18582500	3.31535200	2.75751100
H	1.66806700	0.08359600	1.57035300
H	2.76780600	0.80859000	2.76307000
H	1.06354400	1.22974300	2.80513400
H	4.26217000	1.41082600	1.19036800
H	3.36472900	1.11616500	-0.32677200
H	4.01590400	2.73486200	0.05983100
C	-2.05632100	2.69367800	-1.52975300
C	-2.24864400	1.50192700	-2.46493600
C	-3.06186200	2.66942300	-0.37831000
C	-2.26494100	3.99756500	-2.31076400
H	-1.46960400	1.48330300	-3.23254100
H	-2.23372800	0.55801600	-1.91999000
H	-3.22024600	1.59324500	-2.95781500
H	-2.86378600	3.48009900	0.32872600
H	-4.05592800	2.82493400	-0.80333800
H	-3.07312800	1.71732500	0.15190300
H	-3.32438000	4.06788400	-2.56398100
H	-1.99522900	4.87107900	-1.71154500
H	-1.70909000	4.01496000	-3.25037600
C	-0.84568100	1.21190500	1.04323500
C	-1.27622700	1.91366400	2.31816800
C	-1.03804700	-0.09195300	0.76968500
H	-1.17520100	1.26452100	3.18984100

H	-0.67339600	2.80965200	2.48362200
C	-1.70891800	-0.95592100	1.79925300
O	-1.27943000	-2.02657400	2.16393200
O	-2.85652800	-0.42246600	2.23858400
C	-3.61512600	-1.21698400	3.17472200
C	-4.42201500	-2.27168200	2.44292100
H	-4.25662900	-0.49870400	3.68628700
H	-2.92608400	-1.66381900	3.89380500
H	-5.01359100	-2.84706900	3.15911400
H	-5.10222600	-1.80524500	1.72582800
H	-3.75973100	-2.95459800	1.90614000
C	1.93803400	-0.97064900	-0.79114400
O	1.94732300	-0.02800100	-1.65779600
C	3.27929000	-1.58911300	-0.45174900
C	4.32016200	-1.44971800	-1.37602400
C	3.54717100	-2.25654100	0.74988400
C	5.58155700	-1.98289400	-1.12739200
H	4.10848400	-0.90201700	-2.28833800
C	4.80970300	-2.78594300	1.00692000
H	2.76741000	-2.34414200	1.50083500
C	5.83192700	-2.65660700	0.06715200
H	6.37272900	-1.86946900	-1.86306500
H	4.99953800	-3.29302700	1.94848000
H	6.81598400	-3.06869600	0.26865200
C	0.82000500	-1.46537400	-0.15247900
C	-0.51584600	-0.84420000	-0.44791800
H	0.86279900	-2.30380800	0.53133900
H	-0.29254800	-0.09905200	-1.22391500
C	-1.55097200	-1.81653400	-1.01719200
C	-2.92810900	-1.65146800	-0.82667100
C	-1.12349800	-2.89007700	-1.80527000
C	-3.84680500	-2.53504400	-1.39300900
H	-3.30074200	-0.82494600	-0.22466900
C	-2.03653600	-3.76752200	-2.38259100
H	-0.05629400	-3.02972700	-1.94926000
C	-3.40476700	-3.59768200	-2.17490400
H	-4.90869100	-2.38805600	-1.21924300
H	-1.67901200	-4.59245500	-2.99167500
H	-4.11712300	-4.28777300	-2.61569700
H	-2.32297300	2.22361700	2.25996900

TS5

C	1.27792200	-3.36777800	-1.04461300
C	2.38632700	-2.73602100	-0.61381500
C	0.62999700	-1.77623600	0.36321300
N	0.18881000	-2.81992900	-0.40101700
H	1.19619600	-4.17614000	-1.74650000
H	3.41301600	-2.91763600	-0.87310600
N	1.99581100	-1.78351700	0.29730700

C	-1.15143300	-3.53938600	-0.57634400
C	-2.02022300	-3.44055500	0.67645800
C	-1.83975500	-3.02411100	-1.83962800
C	-0.84840200	-5.04090800	-0.76064900
H	-1.47424100	-3.81963500	1.54651200
H	-2.37211000	-2.43069600	0.85284500
H	-2.88696400	-4.08823400	0.52212500
H	-2.73237300	-3.62993100	-2.02102000
H	-2.12387300	-1.98021900	-1.73368700
H	-1.17496600	-3.13910600	-2.70167500
H	-1.79765600	-5.57437500	-0.68605800
H	-0.43084600	-5.28097000	-1.73996600
H	-0.18299000	-5.41697000	0.02094200
C	3.07212400	-1.11792100	1.15805900
C	3.64539000	0.10655700	0.45081900
C	2.54463000	-0.76755100	2.54617700
C	4.19475300	-2.15330000	1.35866000
H	4.03549700	-0.15848500	-0.53607100
H	2.89198200	0.88605400	0.33487600
H	4.47455500	0.48951000	1.05325000
H	2.06284900	-1.63479000	3.00770200
H	3.40597300	-0.49796000	3.16284700
H	1.86336800	0.07854900	2.53462400
H	4.88500100	-1.75051500	2.10208400
H	3.80132100	-3.10199400	1.73350000
H	4.77737000	-2.33496100	0.45404500
C	-0.10998600	-0.57499100	0.96719900
C	-0.70548200	-0.77206900	2.34861400
C	0.42588000	0.64559400	0.49791500
H	-1.46261200	-0.00588900	2.51694200
H	-1.17101700	-1.75351700	2.41844400
C	0.41505700	1.87845700	1.23107300
O	0.56497700	3.00394200	0.75923700
O	0.32443200	1.72251400	2.59325200
C	0.55411900	2.89505600	3.37684100
C	2.04098600	3.17140600	3.51493900
H	0.10075300	2.68051500	4.34739700
H	0.03994100	3.74413200	2.92177100
H	2.21005900	4.04873900	4.14511900
H	2.54841800	2.31599200	3.96928100
H	2.47551700	3.35899800	2.53056900
C	-2.04566000	0.40972700	-0.57266400
O	-1.67890600	-0.73431400	-0.02112700
C	-3.46693300	0.81058300	-0.38861000
C	-4.09938400	1.69659800	-1.27033900
C	-4.20837300	0.28280500	0.67503900
C	-5.42614300	2.06713500	-1.07596300
H	-3.55045500	2.08211100	-2.12485100

C	-5.53534300	0.65480500	0.87051900
H	-3.72450800	-0.41806400	1.34861100
C	-6.15067500	1.55043000	-0.00249700
H	-5.89953800	2.75360800	-1.77147800
H	-6.09251300	0.24225500	1.70651100
H	-7.18717100	1.83580000	0.14647800
C	-1.12040300	1.19967300	-1.17941500
C	0.30695400	0.75307500	-1.04862300
H	-1.36674100	2.19819500	-1.52392200
H	0.36168400	-0.27944800	-1.41906200
C	1.33356400	1.51789800	-1.86154800
C	1.30495600	2.90476400	-2.04355400
C	2.32426900	0.79076600	-2.53127700
C	2.24817600	3.53871500	-2.84930800
H	0.55207800	3.48781300	-1.52758900
C	3.27557200	1.41908100	-3.33115300
H	2.34702600	-0.29233500	-2.41957500
C	3.24045200	2.80176100	-3.49318500
H	2.20682000	4.61664200	-2.97553200
H	4.03486600	0.82843300	-3.83487100
H	3.97423100	3.29953800	-4.11950900
H	0.03808300	-0.68237400	3.13903300

M5

C	1.01315600	2.68297700	-2.09720600
C	-0.32856300	2.70612400	-2.18148700
C	0.20712000	1.80938400	-0.21339000
N	1.35349800	2.19417400	-0.85250000
H	1.74371300	2.99991100	-2.81905300
H	-0.95238900	3.04941300	-2.98585000
N	-0.83456000	2.21936200	-0.99690400
C	2.80395600	2.44182600	-0.42150400
C	3.01368000	2.44380900	1.08990000
C	3.70344800	1.42634200	-1.11741400
C	3.16645200	3.86532400	-0.89485600
H	2.38731600	3.20493000	1.56367000
H	2.84195900	1.47439300	1.54462600
H	4.05566800	2.72465800	1.26175200
H	3.52067300	1.41075800	-2.19572200
H	4.74585600	1.71346200	-0.95438200
H	3.55615600	0.42560400	-0.71767800
H	4.12545800	4.13045700	-0.44546300
H	3.28877200	3.94504400	-1.97565200
H	2.41878200	4.59047500	-0.56309900
C	-2.32745200	2.40869000	-0.73276500
C	-3.14018800	1.25796200	-1.32617200
C	-2.59438900	2.61578200	0.75268400
C	-2.74705800	3.71528800	-1.43595600
H	-2.85631000	1.09744600	-2.37157200

H	-3.03321000	0.32803400	-0.76728000
H	-4.19429800	1.55243600	-1.31296600
H	-2.00304600	3.45434600	1.13444600
H	-3.65152300	2.86959700	0.86793500
H	-2.40279300	1.72579900	1.34220500
H	-3.74927100	3.96762800	-1.08427900
H	-2.07701800	4.54129100	-1.18328400
H	-2.80862800	3.61699500	-2.52158300
C	0.08722500	0.71345200	0.93816500
C	0.06475500	1.35964800	2.32686000
C	-0.98512700	-0.25799400	0.55838900
H	0.08901800	0.56639000	3.07147400
H	0.94781500	1.98419100	2.44023500
C	-2.11388700	-0.60370600	1.31056500
O	-3.10014400	-1.26519300	0.93406100
O	-2.13300000	-0.11589400	2.62137700
C	-3.32395200	-0.36236600	3.35952300
C	-4.42479900	0.63001700	3.02246500
H	-3.03204500	-0.27108300	4.41001200
H	-3.66533400	-1.38336500	3.17587700
H	-5.32074800	0.42151200	3.61464100
H	-4.10272300	1.65399300	3.23325900
H	-4.67766000	0.55146500	1.96228100
C	1.61972100	-0.98023800	0.09575200
O	1.39773700	0.06601900	0.94193200
C	2.94182600	-1.61006700	0.33333400
C	3.58906000	-2.34864000	-0.66607500
C	3.56500800	-1.47149100	1.57934700
C	4.81789000	-2.94856600	-0.41700200
H	3.14008900	-2.43420600	-1.65072100
C	4.79572900	-2.07467100	1.82596500
H	3.07228700	-0.89613700	2.35570500
C	5.42665400	-2.81637700	0.83099300
H	5.30832200	-3.51186700	-1.20449200
H	5.26150000	-1.96267900	2.80001300
H	6.38824800	-3.28191300	1.02096400
C	0.72189200	-1.40347800	-0.79810300
C	-0.71764500	-0.92516000	-0.79294300
H	0.98569200	-2.23426400	-1.44369800
H	-0.86261500	-0.21784700	-1.63113700
C	-1.55932800	-2.14519600	-1.14149000
C	-1.48240200	-3.31075300	-0.37030300
C	-2.32479900	-2.16978900	-2.30485900
C	-2.17554300	-4.45579600	-0.73733900
H	-0.87577700	-3.29890800	0.53173700
C	-3.02600600	-3.31832900	-2.68027800
H	-2.37531900	-1.27919400	-2.92653700
C	-2.95592300	-4.46446600	-1.89726200

H	-2.11096800	-5.34850900	-0.12201000
H	-3.62063000	-3.31424800	-3.58900100
H	-3.49733500	-5.36006100	-2.18575400
H	-0.82006400	1.96260000	2.50203400

TS6

C	-1.97940900	-1.81117900	-1.87321800
C	-0.73307500	-2.06899900	-2.31503900
C	-0.59705500	-1.70407200	-0.09663500
N	-1.90662600	-1.63589200	-0.50102200
H	-2.90765600	-1.78249000	-2.41900700
H	-0.38162800	-2.27780300	-3.31150900
N	0.10256000	-2.05667200	-1.21303400
C	-3.14184100	-1.98559200	0.29898500
C	-2.92963900	-1.84836900	1.79803000
C	-4.33340900	-1.13188300	-0.13647300
C	-3.42115100	-3.46749900	-0.00822100
H	-2.13226900	-2.51425700	2.13590500
H	-2.70342800	-0.82251900	2.08434600
H	-3.85545800	-2.15708900	2.29052600
H	-4.50595400	-1.16927700	-1.21463100
H	-5.22787300	-1.53106700	0.34955600
H	-4.21264000	-0.09190700	0.16539300
H	-4.25830600	-3.81290700	0.60400100
H	-3.67951700	-3.62106000	-1.05882100
H	-2.54108900	-4.07365800	0.22797800
C	1.43648200	-2.75245100	-1.28499800
C	2.48526000	-1.88623900	-1.98035400
C	1.86882400	-3.18153400	0.11226900
C	1.22352300	-4.03773600	-2.10567500
H	2.10041000	-1.51525700	-2.93632600
H	2.80358300	-1.04295300	-1.36750900
H	3.36112800	-2.50677900	-2.19348300
H	1.11508000	-3.83638200	0.56052300
H	2.80311800	-3.74269000	0.02347900
H	2.04954500	-2.33626400	0.76984800
H	2.12756500	-4.64633100	-2.02719200
H	0.38044800	-4.61448700	-1.71469200
H	1.05582000	-3.83683600	-3.16591600
C	0.15785500	-0.44388200	1.12635300
C	0.28090900	-1.10111300	2.48498300
C	1.30200100	0.16871800	0.50394900
H	0.79052000	-0.41358300	3.16048700
H	-0.71225700	-1.30481300	2.87392000
C	2.66404700	-0.01878500	0.86793800
O	3.62772300	0.38317100	0.20383100
O	2.89914400	-0.66971300	2.05915400
C	4.26998200	-0.87441600	2.40227200
C	4.85132900	-2.08402000	1.69166400

H	4. 26996000	-1. 02168200	3. 48522400
H	4. 84195300	0. 02506300	2. 16636000
H	5. 89831500	-2. 22301800	1. 97528000
H	4. 29842700	-2. 98910200	1. 95682200
H	4. 79609900	-1. 94125300	0. 60945500
C	-1. 24370300	1. 22152700	0. 14574900
O	-0. 98478100	0. 38822400	1. 20496000
C	-2. 59808400	1. 80681800	0. 21812700
C	-3. 28809800	2. 16717000	-0. 94525400
C	-3. 21839500	1. 98656400	1. 46028500
C	-4. 57286600	2. 69293800	-0. 86724700
H	-2. 83139600	1. 99788800	-1. 91555500
C	-4. 50517800	2. 51267400	1. 53512000
H	-2. 68791800	1. 70550300	2. 36419000
C	-5. 18809500	2. 86394800	0. 37269100
H	-5. 10268700	2. 95454100	-1. 77754600
H	-4. 97571600	2. 64573100	2. 50409700
H	-6. 19461900	3. 26506000	0. 43158200
C	-0. 35336500	1. 46326200	-0. 81688100
C	1. 08450800	1. 02876400	-0. 72689200
H	-0. 62748800	2. 13499100	-1. 62351800
H	1. 35219200	0. 49308000	-1. 65395000
C	1. 88926500	2. 32984900	-0. 73586500
C	1. 94118500	3. 14441600	0. 39843800
C	2. 49633600	2. 77826500	-1. 90795700
C	2. 60544200	4. 36584300	0. 36760600
H	1. 46225100	2. 79729400	1. 31104000
C	3. 16012400	4. 00432500	-1. 94644600
H	2. 45949300	2. 15377000	-2. 79787600
C	3. 21913200	4. 80264900	-0. 80741900
H	2. 64284800	4. 98268300	1. 26081000
H	3. 63324400	4. 33353900	-2. 86698000
H	3. 73743200	5. 75608400	-0. 83294000
H	0. 85318600	-2. 02503100	2. 44215100

P

C	0. 16414100	-1. 52206900	0. 47479100
C	0. 48693900	-2. 75909500	1. 26215200
C	1. 00254100	-0. 69442900	-0. 18604700
H	1. 14891000	-2. 52592400	2. 09700700
H	-0. 44369000	-3. 18346000	1. 63828900
C	2. 45695200	-0. 91806400	-0. 30158900
O	3. 16391500	-0. 23276100	-1. 01684200
O	2. 93610000	-1. 92845100	0. 44025700
C	4. 34490200	-2. 19805300	0. 31909400
C	4. 63891700	-3. 00715600	-0. 92935600
H	4. 59448600	-2. 75388700	1. 22378700
H	4. 88604000	-1. 24972600	0. 31649200
H	5. 70204900	-3. 25713000	-0. 96624700

H	4.06438600	-3.93646000	-0.92534800
H	4.38448600	-2.43439600	-1.82305900
C	-1.73513500	-0.30536500	-0.27031400
O	-1.18145700	-1.31789800	0.48908600
C	-3.21219300	-0.33516300	-0.21557300
C	-3.97835100	0.27277800	-1.21757400
C	-3.86470400	-0.97203500	0.84637100
C	-5.36638600	0.26277500	-1.14603300
H	-3.48923700	0.73792100	-2.06731900
C	-5.25499600	-0.98257600	0.91252100
H	-3.27953600	-1.45406000	1.62143400
C	-6.01057700	-0.36352400	-0.07968000
H	-5.94640000	0.73543000	-1.93199600
H	-5.74808600	-1.47644300	1.74354400
H	-7.09432900	-0.37470100	-0.02793600
C	-0.98194500	0.56826000	-0.93885100
C	0.51981600	0.55286700	-0.89983800
H	-1.46619200	1.36383100	-1.49343700
H	0.91619000	0.54478100	-1.92295000
C	1.04180200	1.82307500	-0.23330700
C	0.75354500	2.07654900	1.10961200
C	1.78705500	2.75573400	-0.95342300
C	1.20692400	3.24055600	1.72378500
H	0.16939500	1.35262600	1.67395400
C	2.23865600	3.92482100	-0.34426300
H	2.02127200	2.55765900	-1.99602300
C	1.95057900	4.16917400	0.99664300
H	0.97868800	3.42553900	2.76886300
H	2.81922100	4.64230900	-0.91581300
H	2.30406400	5.07802600	1.47319100
H	0.99892000	-3.49341700	0.63883300

PMe₃

P	0.00007500	0.00004000	0.60581600
C	-0.65461700	1.49013400	-0.27966000
H	-1.69576900	1.65958600	0.00669600
H	-0.07680000	2.37217400	0.00818800
H	-0.59992000	1.36808300	-1.36609900
C	-0.96340600	-1.31192500	-0.27960900
H	-0.59102000	-2.29857100	0.00776800
H	-2.01637700	-1.25105200	0.00722900
H	-0.88396800	-1.20440200	-1.36605500
C	1.61795400	-0.17827000	-0.27969700
H	2.28567700	0.63825200	0.00694200
H	2.09242500	-1.11996300	0.00805200
H	1.48503500	-0.16433600	-1.36616400

R1

C	-2.50087000	-0.40341000	-0.00000400
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C	-3.74039200	-0.01095300	-0.00009400
C	-1.24999400	-0.79841100	0.00006300
H	-4.26975400	0.16218800	0.93180600
H	-4.26966200	0.16205000	-0.93207100
H	-0.98869100	-1.85172900	0.00009200
C	-0.14433000	0.19328900	0.00001600
O	-0.26880900	1.39530400	-0.00001400
O	1.04327900	-0.43288700	0.00002000
C	2.19237400	0.42894900	-0.00001000
C	3.41808900	-0.45729300	0.00003800
H	2.14940800	1.07307900	0.88305900
H	2.14942200	1.07299900	-0.88313800
H	4.32049700	0.15809100	0.00002100
H	3.43186600	-1.09448600	0.88696600
H	3.43188300	-1.09455700	-0.88684000

R2

C	1.18071900	-0.96233900	-0.03782900
O	1.17337800	-2.18231700	-0.09516400
C	2.48461500	-0.22220200	-0.02002000
C	2.59062300	1.14006800	-0.31456400
C	3.63955600	-0.95151600	0.28127600
C	3.83513400	1.76353200	-0.30187600
H	1.71219900	1.71779100	-0.58197600
C	4.87877000	-0.32628400	0.30704300
H	3.53755200	-2.01044100	0.49384100
C	4.97785500	1.03414600	0.01553400
H	3.91193900	2.81900600	-0.54147200
H	5.76902900	-0.89595400	0.55264500
H	5.94615200	1.52438100	0.03265000
C	-0.08294800	-0.18531000	0.03739500
C	-1.25723500	-0.82046700	-0.09087500
H	-0.02915000	0.88110400	0.22443200
H	-1.21079000	-1.89566400	-0.26103500
C	-2.59826200	-0.23230300	-0.02412100
C	-3.70724600	-1.07520900	-0.17103600
C	-2.81913400	1.13750300	0.18358300
C	-5.00168600	-0.56957900	-0.11132100
H	-3.54510100	-2.13743000	-0.33211200
C	-4.11019000	1.64287900	0.24291800
H	-1.97739300	1.81314600	0.29822700
C	-5.20595400	0.79136800	0.09627000
H	-5.84874900	-1.23797700	-0.22586500
H	-4.26634900	2.70460200	0.40398900

H	-6.21406300	1.19025200	0.14371500
TS1_p			
C	-0.76500400	1.72852100	-0.12210600
C	-1.64572000	2.62631800	0.27424400
C	0.48851500	1.44416000	-0.56072900
H	-1.29349100	3.63333000	0.48602100
H	-2.69930400	2.41379700	0.40394600
H	0.80203100	1.72062500	-1.56091300
C	1.31627900	0.55685900	0.21743700
O	0.98360500	-0.00340100	1.25711500
O	2.53149000	0.35248800	-0.34548300
C	3.39416500	-0.55204600	0.35240300
C	4.68483100	-0.64083200	-0.43236500
H	2.90291100	-1.52696500	0.43535700
H	3.56104700	-0.17911700	1.36769400
H	5.37854400	-1.32075400	0.06735800
H	4.49697300	-1.01730000	-1.44066300
H	5.15683500	0.34138600	-0.50977600
P	-2.00042900	-0.38443600	-0.06423300
C	-2.14235000	-1.34648700	1.49676400
H	-1.15503900	-1.37731600	1.96152100
H	-2.83670500	-0.84441500	2.17457700
H	-2.49929000	-2.36301200	1.30545000
C	-0.94818900	-1.46778100	-1.10386500
H	-0.76729600	-0.98579500	-2.06787200
H	0.01038200	-1.61729500	-0.60194600
H	-1.42490700	-2.43815800	-1.26474200
C	-3.66923200	-0.60602100	-0.81722800
H	-4.40906300	-0.05826600	-0.22857900
H	-3.66574600	-0.20041800	-1.83155700
H	-3.95199100	-1.66262700	-0.85276400
M1_p			
C	0.83408200	0.70132800	-0.00145100
C	1.03208700	2.04858800	-0.00402300
C	-0.35887600	-0.08240400	0.00033200
H	0.17836000	2.71273400	-0.00523000
H	2.02346100	2.48329500	-0.00503800
H	-0.30655600	-1.16458900	0.00147100
C	-1.63732400	0.50543700	0.00120800
O	-1.92909500	1.70912200	0.00098600
O	-2.64647400	-0.44308500	0.00239700
C	-3.97140000	0.07198800	0.00425200
C	-4.91773600	-1.11156500	-0.00542700
H	-4.12616000	0.71116600	-0.87239500
H	-4.12883200	0.69837300	0.88980400
H	-5.95498800	-0.76794400	-0.00374200
H	-4.75708300	-1.72403600	-0.89633000

H	-4.75874900	-1.73771200	0.87622800
P	2.32418700	-0.31512000	0.00004800
C	2.34346900	-1.37557700	-1.46605300
H	1.44345500	-1.99201300	-1.47802600
H	2.35800800	-0.74288900	-2.35562200
H	3.22808600	-2.01505500	-1.45285000
C	2.34350000	-1.37088300	1.46953300
H	2.35916800	-0.73542900	2.35711700
H	1.44286500	-1.98635800	1.48391700
H	3.22751500	-2.01120500	1.45776000
C	3.84239300	0.66434200	-0.00157700
H	3.87924600	1.28912400	-0.89532100
H	3.87882100	1.29259300	0.88975000
H	4.69397200	-0.01907100	-0.00004400

TS2_p

C	0.27450100	1.51437000	0.50748700
C	0.93826100	0.79076100	1.44147900
C	-1.04314900	1.26738800	-0.02422000
H	0.43471000	0.00768200	1.99093300
H	1.96653500	1.00727400	1.71016600
H	-1.40079400	1.94565400	-0.79435500
C	-2.16935300	0.83041700	0.79380900
O	-3.33555800	1.10090000	0.55246300
O	-1.81842100	0.02566300	1.82373500
C	-2.89201500	-0.46316300	2.63976500
C	-3.32190700	0.57582000	3.65848600
H	-2.48674500	-1.35295200	3.12655500
H	-3.72246500	-0.75656600	1.99340500
H	-4.09452200	0.16376500	4.31267400
H	-2.47263100	0.88046600	4.27511300
H	-3.72580800	1.45457300	3.15200200
C	1.68448500	-0.80261200	-0.86707600
O	1.95469800	0.12682900	-1.66989600
C	2.84390200	-1.51077900	-0.20976500
C	4.10834200	-1.37845300	-0.79212200
C	2.71701300	-2.27491900	0.95593300
C	5.21898500	-2.00783800	-0.23764700
H	4.19574500	-0.77302000	-1.68847700
C	3.82698700	-2.90089200	1.51555400
H	1.75217100	-2.36092100	1.44570800
C	5.08078700	-2.77339800	0.91833100
H	6.19282100	-1.90058400	-0.70558500
H	3.71578100	-3.48359000	2.42482600
H	5.94490400	-3.26272600	1.35665300
C	0.35964200	-1.23103900	-0.59197900
C	-0.70765300	-0.54408300	-1.17992100
H	0.18836400	-2.06807900	0.07318900
H	-0.43223400	0.08093100	-2.02635700

C	-2.07246100	-1.11151700	-1.26763000
C	-2.93231500	-0.67516600	-2.28277600
C	-2.54747000	-2.06899000	-0.36129200
C	-4.21959600	-1.18863000	-2.40474000
H	-2.57879200	0.07585200	-2.98525900
C	-3.83545700	-2.58245300	-0.47941900
H	-1.90868900	-2.40534900	0.44975500
C	-4.67662200	-2.14748400	-1.50288300
H	-4.86640900	-0.84089800	-3.20429800
H	-4.18510100	-3.32501900	0.23162600
H	-5.67969400	-2.55143700	-1.59500600
P	1.18901300	2.83781000	-0.30283300
C	0.81430700	2.95185700	-2.06754800
C	2.97168500	2.63407300	-0.10475800
C	0.72034600	4.42039300	0.44567400
H	1.04648700	1.98481800	-2.51522200
H	-0.23524300	3.20931200	-2.21782300
H	1.43680500	3.73780800	-2.50105200
H	3.24709500	2.70235700	0.94879400
H	3.23707200	1.65783500	-0.51756000
H	3.47359000	3.43246500	-0.65576100
H	-0.35806700	4.55822400	0.34291800
H	0.98330700	4.40911800	1.50501500
H	1.24340200	5.23675000	-0.05693300

M2_p

C	0.08660300	1.61757000	0.70137300
C	0.78727700	1.17710700	1.75040100
C	-1.13426400	0.94136600	0.12746900
H	0.46388700	0.30740200	2.30927200
H	1.70046700	1.66375300	2.07829400
H	-1.76596300	1.67523700	-0.38542600
C	-2.05432000	0.36522400	1.18593800
O	-3.17579300	0.77302100	1.39190400
O	-1.51812400	-0.67653900	1.83238800
C	-2.36683600	-1.34316800	2.78724500
C	-2.39920100	-0.59366400	4.10476200
H	-1.92276800	-2.33329400	2.89943100
H	-3.36447800	-1.44255100	2.35317600
H	-2.99512700	-1.15014800	4.83209800
H	-1.38815700	-0.47812600	4.50284800
H	-2.84509000	0.39349800	3.97102800
C	1.68487200	-0.52005600	-0.79532200
O	1.92124200	0.60823900	-1.37513300
C	2.88721500	-1.33166900	-0.37930300
C	4.10214200	-1.11474000	-1.03828000
C	2.85373400	-2.27562500	0.65496100
C	5.24223400	-1.83923800	-0.70080000
H	4.12650000	-0.36185100	-1.81942800

C	3.99260600	-2.99877300	0.99962100
H	1.93260400	-2.42459200	1.21067600
C	5.19180800	-2.78773200	0.31957100
H	6.17352700	-1.66242300	-1.23110400
H	3.94791600	-3.72146400	1.80905300
H	6.08011800	-3.35004000	0.58996700
C	0.42689800	-1.01716600	-0.55459400
C	-0.73767500	-0.17758000	-0.95010300
H	0.27985700	-1.98284200	-0.08941300
H	-0.41957500	0.41425000	-1.81591800
C	-2.00602400	-0.91520800	-1.34189700
C	-2.84472500	-0.36561900	-2.31750700
C	-2.40237600	-2.10796900	-0.72653700
C	-4.04017900	-0.98459100	-2.67450200
H	-2.54967500	0.55954100	-2.80815900
C	-3.59848600	-2.73023400	-1.07872400
H	-1.77311000	-2.55267200	0.03769200
C	-4.42223800	-2.17184300	-2.05371800
H	-4.67056300	-0.54147100	-3.43915100
H	-3.88556200	-3.65655900	-0.59057400
H	-5.35227900	-2.65871300	-2.32889500
P	0.69868600	3.07513500	-0.16635800
C	0.28408900	3.06901500	-1.92215200
C	2.48306000	3.23793100	0.02557300
C	-0.08794500	4.53714100	0.56207100
H	0.79772000	2.21483100	-2.36612300
H	-0.79704100	2.99297300	-2.05599000
H	0.62790200	4.01226600	-2.35277200
H	2.74064700	3.42185400	1.06957600
H	2.91048800	2.30104900	-0.34053800
H	2.81876900	4.08461400	-0.57732900
H	-1.17255700	4.45452600	0.46636900
H	0.17810900	4.59954500	1.61883000
H	0.25493500	5.43373500	0.04132800

TS2'p

C	0.19311900	1.53881500	1.07271000
C	1.56185200	1.43299800	0.82011600
C	-0.65620800	0.48128900	1.39004200
H	2.10744500	0.63675400	1.30660500
H	2.13923200	2.31337500	0.55034800
H	-1.73131200	0.61587900	1.40844800
C	-0.18373800	-0.76806300	1.94350800
O	0.97521700	-1.09660900	2.17346500
O	-1.22321400	-1.59855800	2.24713200
C	-0.87495400	-2.83597600	2.87656400
C	-0.43507900	-3.88493600	1.87078100
H	-1.78099900	-3.15031400	3.39897100
H	-0.08631000	-2.65393100	3.61035500

H	-0.15726000	-4.80471600	2.39255900
H	-1.24051500	-4.12353200	1.17125100
H	0.43323200	-3.53105600	1.30862400
C	-0.85558400	0.09338100	-1.39278000
O	-0.91728800	1.29462800	-1.73965500
C	-2.12476600	-0.71580100	-1.43483200
C	-2.26118700	-1.95813400	-0.80782100
C	-3.21464900	-0.18945900	-2.13506400
C	-3.45991900	-2.66026100	-0.88494500
H	-1.44188200	-2.36208400	-0.22518200
C	-4.41270600	-0.89215300	-2.21841200
H	-3.09799500	0.77747800	-2.61334400
C	-4.53817800	-2.13189600	-1.59372900
H	-3.55591800	-3.62031000	-0.38636900
H	-5.24905900	-0.47394000	-2.77004300
H	-5.47214100	-2.68177000	-1.65422700
C	0.37907600	-0.51550100	-1.00236100
C	1.53544200	0.25365000	-1.04654900
H	0.41818400	-1.56466900	-0.73150300
H	1.46046100	1.17242400	-1.62345400
C	2.89180300	-0.33462100	-0.97893000
C	3.91825600	0.21484500	-1.75656700
C	3.18692800	-1.43513500	-0.16142300
C	5.19849700	-0.33265800	-1.74292900
H	3.70321800	1.07551100	-2.38495400
C	4.46478500	-1.98397900	-0.15072400
H	2.41254300	-1.82637600	0.49358400
C	5.47562700	-1.43888100	-0.94334400
H	5.97890900	0.10504100	-2.35789200
H	4.67912500	-2.83581200	0.48780200
H	6.47281000	-1.86717200	-0.92851300
P	-0.56940200	3.12719400	0.72141300
C	-2.34534500	2.99747700	0.42016800
C	0.20738200	3.95264000	-0.68599200
C	-0.35094700	4.20536500	2.16272000
H	-2.49581000	2.34150800	-0.43944300
H	-2.84724900	2.60079400	1.30429700
H	-2.73282000	3.99717800	0.21078800
H	1.26192600	4.13802900	-0.47619500
H	0.09579600	3.29960100	-1.55226200
H	-0.29412300	4.90877900	-0.85053500
H	-0.83348700	3.74750200	3.02852600
H	0.71590900	4.32058000	2.36414600
H	-0.79562700	5.18360700	1.96762500
M2'p			
C	0.59610700	1.68938500	0.80668200
C	1.79816500	0.81592100	0.66363500

C	-0.54265300	1.32636400	1.41876600
H	1.90186700	0.21773700	1.56772200
H	2.71515800	1.40352600	0.53837100
H	-1.42777400	1.95351400	1.37977700
C	-0.75636400	0.03756700	2.12017400
O	0.08649800	-0.73958700	2.52257600
O	-2.07456600	-0.14132600	2.30700400
C	-2.47932500	-1.39974400	2.87065200
C	-2.56391100	-2.45037200	1.78101200
H	-3.45508800	-1.20407700	3.31775900
H	-1.77399200	-1.68212800	3.65465700
H	-2.90894500	-3.39907700	2.20025000
H	-3.25735500	-2.13188600	0.99830100
H	-1.58105200	-2.60290600	1.32685700
C	-0.68902100	-0.03899100	-1.30199500
O	-0.55763000	1.17667200	-1.70929100
C	-2.05571000	-0.66563200	-1.39451200
C	-2.24153200	-2.01184400	-1.72844900
C	-3.18470100	0.11982800	-1.14189600
C	-3.51943200	-2.56305200	-1.78988400
H	-1.37285100	-2.62482000	-1.95166900
C	-4.46310000	-0.42934200	-1.18730000
H	-3.03967200	1.16845300	-0.89730700
C	-4.63598300	-1.77504100	-1.51379500
H	-3.64513800	-3.60781800	-2.05854100
H	-5.32820700	0.19153400	-0.97313800
H	-5.63263700	-2.20284900	-1.55974900
C	0.31641300	-0.78081200	-0.73155900
C	1.67306700	-0.17483400	-0.57394100
H	0.12709300	-1.77564900	-0.34396300
H	1.87755400	0.43393500	-1.46335100
C	2.76588400	-1.21406600	-0.43410400
C	3.83177000	-1.27343200	-1.33305100
C	2.72506600	-2.13719900	0.61864600
C	4.83231100	-2.23576200	-1.19391100
H	3.87723000	-0.56019400	-2.15223000
C	3.72065300	-3.09869400	0.76047700
H	1.90088700	-2.08822400	1.32847000
C	4.77943800	-3.15165900	-0.14703600
H	5.65276000	-2.26757700	-1.90429200
H	3.67378200	-3.80832600	1.58099300
H	5.55693600	-3.90078000	-0.03612100
P	0.61931200	3.28425200	-0.03578900
C	-1.03798500	3.86976700	-0.43133300
C	1.61480300	3.23419200	-1.53858700
C	1.38849100	4.48359100	1.08668400
H	-1.49399700	3.09781400	-1.05487700
H	-1.61184000	4.03940000	0.48101100

H	-0.94905200	4.81313300	-0.97442700
H	2.63085100	2.90895600	-1.30642500
H	1.12656500	2.53039600	-2.21396500
H	1.64942300	4.24162400	-1.95936400
H	0.78701100	4.56494800	1.99421300
H	2.39435900	4.14749200	1.34796100
H	1.44732200	5.45714400	0.59534100

TS3'p

C	-0.04731100	1.43309500	0.16374800
C	1.40040900	0.98478400	0.30202700
C	-0.99926200	1.06830200	1.12037800
H	1.50916200	0.53322100	1.28645900
H	2.08207000	1.84398100	0.25181100
H	-1.97652100	1.53770000	1.10491200
C	-0.86668600	0.00396800	2.07363200
O	0.08537400	-0.73779000	2.31079900
O	-2.01419100	-0.10966100	2.81420700
C	-2.00671200	-1.12510700	3.81586600
C	-3.36447900	-1.10754100	4.48586500
H	-1.20246900	-0.92873600	4.53274000
H	-1.80014100	-2.09513400	3.35197400
H	-3.41032400	-1.87432000	5.26275900
H	-3.55373000	-0.13525100	4.94729700
H	-4.15455900	-1.30481300	3.75728100
C	-0.40643300	-0.51292300	-1.46951800
O	-0.53593400	0.81078300	-1.51334000
C	-1.61559900	-1.32022800	-1.77726600
C	-1.52410700	-2.62469700	-2.27749300
C	-2.88236000	-0.76816000	-1.55887700
C	-2.67338500	-3.36694000	-2.53074500
H	-0.54590000	-3.05012700	-2.48270700
C	-4.03216000	-1.51026800	-1.81228800
H	-2.94268600	0.24486700	-1.17339300
C	-3.93200400	-2.81298900	-2.29832200
H	-2.58757800	-4.37607600	-2.92189800
H	-5.00919700	-1.07214600	-1.63177100
H	-4.82804100	-3.39022000	-2.50331500
C	0.77124300	-1.03727600	-1.06986900
C	1.86649800	-0.05546500	-0.76660300
H	0.91937600	-2.10017500	-0.91750200
H	2.07690000	0.51684800	-1.68175700
C	3.14479400	-0.71614300	-0.30164200
C	4.35258500	-0.51972500	-0.97115300
C	3.12610800	-1.54016100	0.83079100

C	5.52214700	-1.13576100	-0.52567100
H	4.37718700	0.11894100	-1.85055800
C	4.29075300	-2.15691900	1.27624500
H	2.18462400	-1.67838900	1.35987900
C	5.49366300	-1.95732200	0.59771900
H	6.45454000	-0.97375600	-1.05779300
H	4.26384100	-2.79360100	2.15540200
H	6.40278300	-2.43791800	0.94531300
P	-0.24687300	3.12821000	-0.46855200
C	-1.97008700	3.44934100	-0.89671700
C	0.77308400	3.41178200	-1.93097400
C	0.25903200	4.29494500	0.81748900
H	-2.28315500	2.68896500	-1.61319900
H	-2.59319700	3.40396100	-0.00259300
H	-2.04706400	4.44470900	-1.33885000
H	1.82119500	3.21253800	-1.69815500
H	0.43683700	2.73201800	-2.71316500
H	0.66591500	4.45211600	-2.24505300
H	-0.35768800	4.13521400	1.70368400
H	1.30790000	4.12684900	1.07178500
H	0.13262300	5.31738500	0.45564900

TS3''_p

C	0.05853600	1.82594000	0.57320200
C	1.32869100	1.51101700	-0.13992600
C	-0.54232800	0.73357000	1.19675500
H	2.12841600	1.21887300	0.54309700
H	1.71039400	2.32983200	-0.75915300
H	-1.61739000	0.73082700	1.37253000
C	0.09825600	-0.19161600	2.16786000
O	-0.52481100	-1.01545600	2.81206200
O	1.42449200	-0.03501200	2.30023600
C	2.07684500	-0.92846500	3.21824000
C	3.53419700	-0.52611500	3.27287400
H	1.94623100	-1.95580100	2.86139600
H	1.59208600	-0.84879500	4.19473500
H	4.07272000	-1.18083500	3.96152800
H	3.99782600	-0.60416300	2.28565800
H	3.63383700	0.50381500	3.62311400
C	-1.38277500	-0.49868000	-0.95316300
O	-1.72954200	0.48962300	-1.64069900
C	-2.43214100	-1.51990700	-0.59961100
C	-2.28810800	-2.44408400	0.44152100
C	-3.60784000	-1.53049100	-1.35722200
C	-3.29775200	-3.36620100	0.70560500

H	-1.40560700	-2.42299900	1.07246600
C	-4.61244400	-2.45705100	-1.09902200
H	-3.71226800	-0.79938000	-2.15175400
C	-4.45863800	-3.38045400	-0.06620600
H	-3.17985800	-4.07401000	1.52019800
H	-5.51555800	-2.45987500	-1.70144200
H	-5.24068500	-4.10473300	0.13919400
C	-0.05308500	-0.63653400	-0.45786400
C	1.00524000	0.23447500	-1.06760500
H	0.24565600	-1.59391100	-0.04031200
H	0.59056600	0.65037000	-1.99225700
C	2.28522300	-0.49893300	-1.39535900
C	2.85530100	-0.41080100	-2.66737500
C	2.95342900	-1.24950000	-0.42060500
C	4.05539200	-1.05698200	-2.96217700
H	2.35126000	0.16959200	-3.43609700
C	4.15012500	-1.89795500	-0.70931300
H	2.52385400	-1.31932400	0.57529200
C	4.70727300	-1.80385800	-1.98467800
H	4.47957100	-0.97631800	-3.95842100
H	4.64907100	-2.47688200	0.06248300
H	5.64058900	-2.30868400	-2.21244900
P	-0.95071400	3.12064800	-0.04044000
C	-2.71322100	2.84067900	0.26226500
C	-0.73260900	3.44131900	-1.81241300
C	-0.54741300	4.69336600	0.77994300
H	-3.01436600	1.94786200	-0.28927900
H	-2.89715600	2.71465800	1.33090800
H	-3.26834100	3.71164500	-0.09280400
H	0.31002300	3.68958000	-2.02178400
H	-1.02223000	2.53679100	-2.34882500
H	-1.36137700	4.28641400	-2.10200900
H	-0.73055100	4.59379300	1.85168100
H	0.50934100	4.91825600	0.61789600
H	-1.15739600	5.50400100	0.37386600

M3'p

C	-0.19976800	1.21594100	-0.47732300
C	1.31643300	1.01116300	-0.24770000
C	-1.03453600	1.24492100	0.72759700
H	1.48487500	0.98147800	0.82695900
H	1.91479400	1.83278800	-0.66013100
H	-2.07589700	1.52001800	0.59903900
C	-0.69812600	0.74492100	1.99369500
O	0.36185800	0.26499100	2.43608900

O	-1.77763400	0.85547500	2.86516000
C	-1.55163700	0.38656500	4.18626100
C	-2.83942700	0.58267600	4.96127300
H	-0.72481800	0.93899300	4.64717800
H	-1.25835000	-0.66929800	4.16734900
H	-2.72077200	0.23376200	5.99005300
H	-3.11772800	1.63949100	4.98370200
H	-3.65551900	0.02247900	4.49766800
C	-0.47035100	-1.05244100	-1.14424800
O	-0.70114000	0.25210500	-1.50917300
C	-1.65199900	-1.93549700	-1.18059300
C	-1.51574000	-3.31950100	-1.34559000
C	-2.93326800	-1.38971700	-1.04560500
C	-2.63716800	-4.14175400	-1.35005800
H	-0.52841500	-3.74865600	-1.48824400
C	-4.05436600	-2.21448100	-1.05378800
H	-3.03262100	-0.31657800	-0.92035700
C	-3.91080000	-3.59219800	-1.20405800
H	-2.51824200	-5.21277100	-1.48031300
H	-5.04283500	-1.78024400	-0.94108400
H	-4.78572600	-4.23407600	-1.21413900
C	0.77307200	-1.38220600	-0.77813600
C	1.83033700	-0.31223400	-0.87604400
H	1.02206100	-2.37548700	-0.42211200
H	2.00457200	-0.11921100	-1.94475100
C	3.14236700	-0.72392900	-0.24589700
C	4.31846500	-0.78465900	-0.99299400
C	3.18412500	-1.05097800	1.11499000
C	5.52001800	-1.16814800	-0.39734900
H	4.29431400	-0.53083600	-2.04984400
C	4.38158600	-1.43622100	1.70957200
H	2.26729700	-0.98064500	1.69851000
C	5.55388200	-1.49658800	0.95475400
H	6.42770000	-1.20975200	-0.99149000
H	4.40363700	-1.68851300	2.76549200
H	6.48761900	-1.79639600	1.42014500
P	-0.47785700	2.77257900	-1.44074600
C	-2.24011300	2.98044200	-1.77731600
C	0.39038800	2.71892100	-3.02722300
C	0.10623000	4.17914200	-0.47245900
H	-2.61002200	2.07720300	-2.26611800
H	-2.77609500	3.14333000	-0.84164100
H	-2.38062700	3.84248500	-2.43239300
H	1.46490700	2.62176800	-2.85973400

H	0.02973700	1.85313900	-3.58488900
H	0.19396100	3.63454600	-3.58884900
H	-0.35995200	4.12321000	0.51283600
H	1.19188200	4.13553000	-0.36670300
H	-0.17415800	5.10814600	-0.97212600

M3''_P

C	1.69835600	0.02886100	-0.91931600
C	1.33432700	-1.43403100	-0.82800500
C	0.59254000	0.81671100	-0.22707200
H	1.51510700	-1.89009200	0.16107600
H	1.84176700	-2.06457600	-1.56826400
H	0.44744400	1.82106100	-0.64449400
C	1.00041700	1.02258500	1.21469500
O	1.61215600	1.99576100	1.61782300
O	0.73889100	-0.03873600	1.99618600
C	1.29122000	-0.00618400	3.32313100
C	0.92584600	-1.31345700	3.98926100
H	0.88046100	0.85650600	3.85514300
H	2.37472400	0.12705300	3.24761000
H	1.31918700	-1.33481400	5.00794900
H	-0.15973600	-1.43231900	4.03404000
H	1.34837800	-2.15662800	3.43649800
C	-1.74666100	0.63530800	-1.17103200
O	-2.07397300	0.30686700	-2.29690700
C	-2.39689100	1.81954200	-0.51332200
C	-2.19381600	2.14103900	0.83322400
C	-3.23626900	2.62405300	-1.29136000
C	-2.82102900	3.25226200	1.38963600
H	-1.56005400	1.52392500	1.46335000
C	-3.85873500	3.73530600	-0.73683100
H	-3.38517600	2.36092300	-2.33331000
C	-3.65123700	4.05075400	0.60605200
H	-2.66126100	3.49301100	2.43526500
H	-4.50460000	4.35679800	-1.34829600
H	-4.13665000	4.91805400	1.04193600
C	-0.66352800	-0.09739700	-0.39985400
C	-0.18864100	-1.39536700	-1.08844900
H	-1.07058300	-0.33826400	0.58647200
H	-0.34227400	-1.26918200	-2.16405900
C	-0.94018300	-2.62227400	-0.63003800
C	-1.64260100	-3.41756000	-1.53711700
C	-0.94046800	-2.99197500	0.72158500
C	-2.32561300	-4.55665000	-1.11206600
H	-1.65597100	-3.13715100	-2.58740100

C	-1.61948800	-4.12801000	1.15018500
H	-0.40441200	-2.37477500	1.44057300
C	-2.31485800	-4.91613100	0.23286400
H	-2.86759300	-5.16142800	-1.83270900
H	-1.60850800	-4.39909300	2.20172100
H	-2.84641900	-5.80207500	0.56565500
P	3.28128100	0.62775700	-1.02832700
C	3.25407200	2.40802100	-1.38941500
C	4.20239400	-0.21209400	-2.35393500
C	4.43655600	0.51848400	0.40463000
H	2.69095900	2.58939600	-2.30632800
H	2.77151400	2.91879000	-0.55251900
H	4.27515800	2.77914200	-1.49853700
H	4.25313800	-1.28183900	-2.13855600
H	3.68987200	-0.06079300	-3.30484400
H	5.21846900	0.18452800	-2.40982900
H	3.99407900	1.06260500	1.24298500
H	4.55721800	-0.53154500	0.68437800
H	5.41568500	0.94451700	0.16786700

DABCO

N	0.00000000	0.00000000	1.28589000
C	-0.03976300	1.37639600	0.77791800
C	0.03976300	1.37639600	-0.77791800
H	0.79352600	1.93151300	1.22129100
H	-0.96911500	1.83753400	1.12890900
H	-0.79352600	1.93151300	-1.22129100
H	0.96911500	1.83753400	-1.12890900
C	1.21187500	-0.65376300	0.77791800
C	1.17211300	-0.72263400	-0.77791800
H	1.27597600	-1.65297000	1.22129100
H	2.07590900	-0.07948900	1.12890900
H	2.06950200	-0.27854300	-1.22129100
H	1.10679400	-1.75804500	-1.12890900
C	-1.17211300	-0.72263400	0.77791800
C	-1.21187500	-0.65376300	-0.77791800
H	-2.06950200	-0.27854300	1.22129100
H	-1.10679400	-1.75804500	1.12890900
H	-1.27597600	-1.65297000	-1.22129100
H	-2.07590900	-0.07948900	-1.12890900
N	0.00000000	0.00000000	-1.28589000

TS1_D

C	0.06462100	1.78819400	-0.17185700
C	-0.51510400	2.87689400	0.29656300
C	1.25716200	1.30359700	-0.64732200
H	0.11264500	3.73486700	0.51196300

H	-1.57661400	2.97890800	0.48522100
H	1.63878300	1.62813900	-1.60695500
C	2.01364000	0.38367800	0.14534800
O	1.65799000	-0.14475100	1.19850200
O	3.23488000	0.11437000	-0.39376600
C	4.04441600	-0.79548000	0.34973100
C	5.35577500	-0.94186600	-0.39260100
H	3.52379900	-1.75446700	0.44510000
H	4.19301000	-0.40646300	1.36194300
H	6.01734300	-1.62691200	0.14332500
H	5.18741900	-1.33634500	-1.39750200
H	5.85539600	0.02564700	-0.48147500
N	-3.09775000	-1.42864800	0.01714800
C	-1.96620500	-1.84467000	-0.81877000
C	-0.82049800	-0.80165600	-0.74032100
H	-2.33035300	-1.96011200	-1.84439400
H	-1.61314500	-2.82215700	-0.47879000
H	-0.00061100	-1.14404500	-0.10742400
H	-0.40646000	-0.54117100	-1.71809000
C	-3.67997100	-0.22532600	-0.57786100
C	-2.57449600	0.83746400	-0.84011700
H	-4.43666600	0.16363100	0.11019700
H	-4.18319100	-0.49443600	-1.51115400
H	-2.31987500	0.91805900	-1.90089400
H	-2.88619000	1.82365600	-0.49182400
C	-2.59277800	-1.09317300	1.35379200
C	-1.66366600	0.15254200	1.29528700
H	-2.05082900	-1.96275500	1.73726200
H	-3.44345300	-0.91092900	2.01686700
H	-2.14867700	1.04191600	1.70801400
H	-0.71181100	0.00300700	1.81020300
N	-1.34522800	0.43490900	-0.12296300

M1_D

C	0.03399700	0.99130700	-0.03090100
C	0.02151600	2.34329100	0.01536700
C	-1.04635700	0.06845600	-0.04703900
H	-0.95042300	2.81338500	0.03594900
H	0.89939600	2.96725300	0.04639100
H	-0.88509200	-0.99876500	-0.05445300
C	-2.39095300	0.49774000	-0.01545800
O	-2.83697500	1.64679000	0.00985100
O	-3.26375000	-0.57690800	-0.01544200
C	-4.64057200	-0.23221200	0.01905400
C	-5.42869300	-1.52693900	0.01201200
H	-4.89208400	0.39335000	-0.84480200
H	-4.85622900	0.36140200	0.91474000
H	-6.50182500	-1.32090000	0.03566300

H	-5.20558500	-2.10568200	-0.88791700
H	-5.17242100	-2.13588300	0.88269800
N	3.64178200	-0.98755400	0.03421300
C	2.94971700	-1.12048600	1.31583400
C	1.51979200	-0.53711700	1.23214500
H	3.53849400	-0.60239500	2.07757400
H	2.90214800	-2.17682200	1.59149400
H	0.75562000	-1.30938500	1.17351600
H	1.26975900	0.12871200	2.05962100
C	3.87125200	0.43255200	-0.21582000
C	2.56422500	1.24602600	-0.04675500
H	4.26495200	0.54480800	-1.22957800
H	4.62753500	0.80477800	0.47942400
H	2.53113300	1.80069200	0.89206500
H	2.39748500	1.93712400	-0.87198200
C	2.77941700	-1.50934900	-1.02656600
C	1.55080900	-0.59565500	-1.23823300
H	2.46701700	-2.51947000	-0.74786000
H	3.35094400	-1.58029300	-1.95545400
H	1.66514400	0.08365100	-2.08594400
H	0.62372900	-1.14729300	-1.36925000
N	1.39696000	0.29569400	-0.02549900

TS_{2D}

C	-0.59745200	-0.86830900	0.90428100
C	-0.90001700	0.26913400	1.55728100
C	0.71706400	-1.28485100	0.48858600
H	-0.08554700	0.88017100	1.91280300
H	-1.90328500	0.60306000	1.77315900
H	0.82067600	-2.28849500	0.09217300
C	1.92423000	-1.00996600	1.27429300
O	2.84961900	-1.79201500	1.38456600
O	1.97638900	0.23227100	1.80543900
C	3.18174100	0.55139600	2.50977100
C	3.07787000	2.00374800	2.92190800
H	4.03452100	0.37001800	1.84871800
H	3.28061700	-0.11474700	3.37281400
H	3.97571100	2.30739800	3.46526400
H	2.97226300	2.64417300	2.04150800
H	2.21078800	2.16184400	3.56844600
C	-0.85967900	1.46494200	-1.08964100
O	-1.61889900	0.62280200	-1.63591900
C	-1.47515700	2.78471700	-0.69054300
C	-2.67108800	3.15768700	-1.30973300
C	-0.92671700	3.63133300	0.27893000
C	-3.29575100	4.35840500	-0.98928800
H	-3.09086200	2.48134400	-2.04682500
C	-1.55409100	4.82970000	0.60707000

H	-0.01969400	3.33964400	0.80037600
C	-2.73753400	5.19976800	-0.02928300
H	-4.21878300	4.63954600	-1.48748500
H	-1.12201400	5.47470400	1.36619800
H	-3.22404600	6.13603500	0.22636400
C	0.52475500	1.25679400	-0.87158400
C	1.08628200	0.00972800	-1.17179500
H	1.12139900	2.04629700	-0.43313000
H	0.47132300	-0.60921600	-1.82250700
C	2.54297600	-0.20213400	-1.35528600
C	2.98832100	-1.35927100	-2.00474300
C	3.50248300	0.69816100	-0.87750000
C	4.34391700	-1.61369300	-2.17494600
H	2.25284900	-2.06872900	-2.37789600
C	4.86083800	0.44558100	-1.04408000
H	3.18464000	1.60322400	-0.36919800
C	5.28832200	-0.71116700	-1.69134500
H	4.66442400	-2.51737700	-2.68405600
H	5.58876600	1.15777400	-0.66673000
H	6.34806000	-0.90660000	-1.81981000
N	-1.72655800	-1.78366700	0.46768900
C	-1.76939100	-2.95921900	1.41767700
C	-3.07277600	-1.09445100	0.51538000
C	-1.57254500	-2.30849400	-0.95115900
C	-3.05043700	-3.78307500	1.14032500
H	-1.73681900	-2.54401100	2.42597400
H	-0.85371300	-3.52809200	1.24544100
C	-4.14069200	-2.04825700	-0.06766700
H	-2.96379800	-0.17264400	-0.06154500
H	-3.27062000	-0.87426100	1.56475800
C	-2.58903800	-3.45264600	-1.16491300
H	-0.55413800	-2.66237500	-1.08077500
H	-1.72816800	-1.43815200	-1.59053700
H	-2.81043000	-4.84918500	1.13944300
H	-3.79674900	-3.60886200	1.92006100
N	-3.63934600	-3.41967200	-0.14797500
H	-5.03511700	-2.02455200	0.55977600
H	-4.42758400	-1.73009700	-1.07332200
H	-3.04153900	-3.35375100	-2.15474400
H	-2.09728400	-4.42855300	-1.11739300

M2_D

C	0.40844200	1.04557900	0.92459700
C	1.04916600	0.39091600	1.88814100
C	-0.91680400	0.60717100	0.37942000
H	0.55479000	-0.46026300	2.33344000
H	2.03964400	0.64003900	2.24141000
H	-1.46076200	1.43194200	-0.08529100

C	-1.85835100	0.06457700	1.43170900
O	-1.60296600	-0.76638700	2.27321700
O	-3.08789500	0.56594900	1.24750800
C	-4.14274500	-0.05573800	1.99930400
C	-5.44683000	0.36199600	1.35813100
H	-4.06678400	0.26273100	3.04383700
H	-4.00227500	-1.13950400	1.96266800
H	-6.28593200	-0.09165700	1.89086300
H	-5.56498500	1.44789100	1.38408800
H	-5.46954800	0.02820700	0.31729800
C	1.58215700	-1.34079000	-0.60230700
O	2.02871700	-0.26909200	-1.15784200
C	2.61319800	-2.36589100	-0.20082600
C	3.85600000	-2.33667400	-0.84021300
C	2.40245000	-3.32113800	0.80027500
C	4.85070200	-3.25324900	-0.51600400
H	4.01276600	-1.57383200	-1.59533200
C	3.39677600	-4.23749600	1.13055300
H	1.46037700	-3.32788400	1.34070600
C	4.62416400	-4.21123900	0.47055200
H	5.80658400	-3.22103400	-1.03141700
H	3.21805500	-4.96922100	1.91321900
H	5.39988900	-4.92557200	0.72962400
C	0.25004700	-1.59797100	-0.36491700
C	-0.73660200	-0.55841300	-0.74773500
H	-0.07856400	-2.54229500	0.04815800
H	-0.31911400	-0.01535500	-1.60268700
C	-2.11735500	-1.05009700	-1.13446900
C	-2.82220600	-0.39809100	-2.14955500
C	-2.74471000	-2.10891400	-0.46904300
C	-4.11174100	-0.78839700	-2.50009300
H	-2.34574600	0.42414500	-2.67951700
C	-4.03659400	-2.50071300	-0.81172500
H	-2.22319500	-2.61989500	0.33487500
C	-4.72548800	-1.84376900	-1.83009000
H	-4.63458400	-0.27234100	-3.29955700
H	-4.50526800	-3.32661900	-0.28475500
H	-5.72940600	-2.15495800	-2.10128900
N	1.03003400	2.26288900	0.29437700
C	0.50264200	3.49915900	0.98642700
C	2.54060300	2.24545100	0.44069300
C	0.74578400	2.38655000	-1.19578400
C	1.32800200	4.72170200	0.51083900
H	0.58703400	3.32087000	2.05907200
H	-0.55580500	3.57581800	0.72513400
C	3.12735900	3.42739600	-0.36232800
H	2.85115300	1.26172900	0.07391900
H	2.75015700	2.35974400	1.50437000

C	1.19006600	3.78905700	-1.66573100
H	-0.32220800	2.25357900	-1.35069400
H	1.28300900	1.54729600	-1.64499300
H	0.65878700	5.56080600	0.30515600
H	2.02883400	5.03430900	1.28957700
N	2.09118600	4.40616000	-0.69445800
H	3.91328700	3.91374900	0.22101500
H	3.57192900	3.07224700	-1.29552900
H	1.69936400	3.70296400	-2.62868000
H	0.32832600	4.44941500	-1.80010300

TS2'_b

C	1.03697400	0.50063900	0.94345900
C	1.68809500	-0.72909800	0.88762400
C	-0.30314300	0.66875900	1.23098200
H	1.21907600	-1.51591500	1.46065500
H	2.76616300	-0.80161800	0.79849400
H	-0.81339400	1.60945900	1.10168200
C	-1.13989300	-0.37329200	1.79038400
O	-0.85458800	-1.52748200	2.08138000
O	-2.39173600	0.11439500	2.00796300
C	-3.34334800	-0.81982600	2.51387800
C	-4.62983700	-0.05969800	2.75614100
H	-2.95616300	-1.27523400	3.43045500
H	-3.48229600	-1.62669200	1.78425900
H	-5.40363200	-0.73660300	3.12638100
H	-4.47480700	0.72906700	3.49610800
H	-4.97850000	0.40122700	1.82865500
C	-0.74382400	0.06750800	-1.55356500
O	0.10903800	0.89263500	-1.96374200
C	-2.19629100	0.47029200	-1.61010000
C	-2.52525600	1.63293400	-2.31303700
C	-3.22220900	-0.25216200	-0.99123600
C	-3.84531800	2.06222800	-2.40461500
H	-1.71939000	2.18194200	-2.78865100
C	-4.54360200	0.17209500	-1.08506400
H	-2.99283200	-1.14639300	-0.42160600
C	-4.86029000	1.33186000	-1.79073300
H	-4.08506600	2.96424200	-2.95950200
H	-5.32880100	-0.40378600	-0.60365800
H	-5.89196100	1.66215600	-1.86197400
C	-0.39207300	-1.22283800	-1.06691500
C	0.95043100	-1.57586600	-0.95570500
H	-1.15517500	-1.91160900	-0.72823800
H	1.63746000	-0.99049100	-1.56383500

C	1.36339100	-2.97821200	-0.70649400
C	2.48056900	-3.50655800	-1.36052900
C	0.65349900	-3.79796600	0.18161800
C	2.86712000	-4.82894800	-1.15730700
H	3.04256100	-2.87640800	-2.04554400
C	1.03852600	-5.11812200	0.38229800
H	-0.18083500	-3.37399700	0.73585000
C	2.14447500	-5.64102400	-0.28799100
H	3.73269200	-5.22493700	-1.67980800
H	0.47924900	-5.74117800	1.07366400
H	2.44421300	-6.67166500	-0.12636000
N	1.83108600	1.73231800	0.56103200
C	0.96366000	2.91664000	0.19219100
C	2.66546300	2.13121800	1.75897400
C	2.75855700	1.49072700	-0.61577500
C	1.87480500	4.05200400	-0.32594700
H	0.43967300	3.21045200	1.10242300
H	0.25851200	2.56015600	-0.56131900
C	3.32486000	3.50226400	1.47597300
H	3.39336100	1.33101400	1.90358400
H	1.99091700	2.14734500	2.61636300
C	3.75389800	2.66934600	-0.70632100
H	2.09743200	1.38736600	-1.47718400
H	3.27532100	0.54888100	-0.45421400
H	1.82175300	4.11763500	-1.41578000
H	1.53768800	5.00708800	0.08472800
N	3.26989700	3.82360400	0.05051600
H	2.81527200	4.29722400	2.02699600
H	4.36770900	3.48399800	1.80248400
H	4.73369600	2.38675700	-0.31039100
H	3.88607200	2.95325000	-1.75349100

M2'_D

C	-1.27883200	-0.12792200	0.93000500
C	-1.20902900	1.32824600	0.64614100
C	-0.27051900	-0.78959900	1.51353000
H	-0.72091100	1.80107400	1.49571300
H	-2.18947400	1.79754200	0.53227300
H	-0.21259500	-1.86737900	1.55442600
C	0.93160600	-0.12620300	2.07717500
O	1.03104800	1.00645800	2.50498400
O	1.93140500	-1.01876000	2.15485500
C	3.15830200	-0.52680300	2.71098000
C	4.13653300	-1.67974500	2.72387700
H	2.96158500	-0.13614300	3.71409000

H	3.51229200	0.30850100	2.09729600
H	5.10020700	-1.34540800	3.11535700
H	3.76679300	-2.49040600	3.35605400
H	4.27916300	-2.06486300	1.71157900
C	0.81313900	-0.45015500	-1.27537100
O	-0.30335300	-0.98598100	-1.62268500
C	2.05276200	-1.28754200	-1.46091700
C	1.97411500	-2.40138100	-2.30191600
C	3.27534800	-1.01347100	-0.83748800
C	3.08600600	-3.20479100	-2.53625300
H	1.01615600	-2.61038700	-2.76569600
C	4.39080800	-1.81210100	-1.07164400
H	3.35039900	-0.17386500	-0.15295600
C	4.30232000	-2.91175800	-1.92427400
H	3.00611200	-4.06069500	-3.20051400
H	5.33280700	-1.57829700	-0.58278000
H	5.17291700	-3.53441400	-2.10652600
C	0.91672900	0.82541300	-0.76540400
C	-0.31966700	1.65531500	-0.64258900
H	1.87389800	1.27985600	-0.54083800
H	-0.95826000	1.43914400	-1.50848700
C	-0.02840800	3.14103000	-0.61674100
C	-0.55923200	3.99709000	-1.58197600
C	0.78073900	3.68328100	0.38866700
C	-0.28738400	5.36406100	-1.55284800
H	-1.18563100	3.58616200	-2.36989700
C	1.05419000	5.04673000	0.42024100
H	1.19401600	3.02050900	1.14746900
C	0.52045200	5.89307000	-0.55114000
H	-0.70562400	6.01465400	-2.31504500
H	1.68670600	5.45197400	1.20442000
H	0.73465900	6.95694700	-0.52659000
N	-2.50247100	-0.86811800	0.47016300
C	-2.26371900	-2.35141800	0.29255100
C	-3.58840600	-0.68695800	1.50588600
C	-3.01130200	-0.32176100	-0.85829900
C	-3.61899000	-3.04343400	0.00267900
H	-1.85056800	-2.72738400	1.22584200
H	-1.51773900	-2.41702600	-0.50558800
C	-4.90907600	-1.27951900	0.94727100
H	-3.66260200	0.38163600	1.71485000
H	-3.23823300	-1.19525000	2.40677300
C	-4.20713600	-1.18100700	-1.32465000
H	-2.14465300	-0.35750300	-1.52423300
H	-3.31647800	0.70677500	-0.67097100
H	-3.51936400	-3.69980800	-0.86499900
H	-3.92330000	-3.65788400	0.85424200
N	-4.67248200	-2.06745900	-0.25966100

H	-5.37448300	-1.91438300	1.70524000
H	-5.61189800	-0.47918400	0.70153500
H	-5.03004300	-0.53329500	-1.63745100
H	-3.92208200	-1.79790800	-2.18031200

TS3'd

C	-0.88564900	-0.54303700	0.50243600
C	-1.27555000	0.91311200	0.50452900
C	0.10312200	-1.01126100	1.33180600
H	-0.84674800	1.34811900	1.40508000
H	-2.36094800	1.04040900	0.57236000
H	0.37809700	-2.05686800	1.31569600
C	1.08462300	-0.17402900	2.00283900
O	1.04488900	1.01403100	2.28833900
O	2.15279200	-0.93562200	2.35677700
C	3.23827700	-0.23459400	2.96510000
C	4.38212600	-1.21720900	3.09829200
H	2.92032400	0.15811000	3.93686800
H	3.50858300	0.61973600	2.33766600
H	5.24505400	-0.73056400	3.55915300
H	4.09076700	-2.06801400	3.71902100
H	4.67505600	-1.58983200	2.11382000
C	0.83484200	0.04569800	-1.39901200
O	-0.19050500	-0.78070400	-1.35597600
C	2.17871000	-0.52119000	-1.70225900
C	3.18011000	0.24429400	-2.30978000
C	2.46223500	-1.84654200	-1.36005300
C	4.43988200	-0.29586500	-2.54734600
H	2.95808400	1.26443400	-2.60940500
C	3.72235200	-2.38772000	-1.59385500
H	1.68055000	-2.43649600	-0.89215000
C	4.71722200	-1.61370000	-2.18809100
H	5.20544100	0.30987500	-3.02294600
H	3.93085100	-3.41586100	-1.31254000
H	5.69935800	-2.03641000	-2.37586500
C	0.65363300	1.34464700	-1.06211000
C	-0.75041200	1.74226100	-0.71628600
H	1.46920800	2.05148700	-0.96722700
H	-1.39514300	1.48214100	-1.56837900
C	-0.90314000	3.21620800	-0.41725500
C	-1.77198700	4.01740700	-1.15772700
C	-0.16829500	3.79857300	0.62234600
C	-1.90736100	5.37558800	-0.87420400
H	-2.34296100	3.57350800	-1.96974500
C	-0.30209400	5.15350500	0.90723900
H	0.50331800	3.17219800	1.20734200
C	-1.17223300	5.94687800	0.15960400
H	-2.58460100	5.98615000	-1.46376000

H	0.27370100	5.59416800	1.71556200
H	-1.27466800	7.00436700	0.38242000
N	-2.02847400	-1.51632800	0.19344800
C	-2.84741600	-1.10582800	-1.01419500
C	-1.52473100	-2.91937000	-0.06689400
C	-2.94875100	-1.58654200	1.39357400
C	-4.14053500	-1.94988900	-1.03603400
H	-2.20189200	-1.26603400	-1.87387100
H	-3.05607200	-0.04038200	-0.94001000
C	-2.70860100	-3.77814100	-0.56630400
H	-1.14407400	-3.29299300	0.88358500
H	-0.71340600	-2.81690300	-0.78598700
C	-3.94346900	-2.75321100	1.18545000
H	-3.45229400	-0.62057600	1.46264300
H	-2.31128700	-1.71274500	2.26872100
H	-4.99274000	-1.38203900	-0.65127500
H	-4.36837000	-2.23428300	-2.06649800
N	-3.98799800	-3.15588300	-0.22030900
H	-2.66994400	-3.90173600	-1.65175300
H	-2.65337100	-4.77204300	-0.11471200
H	-3.65175700	-3.62114000	1.78285800
H	-4.94168300	-2.44619700	1.50739200

TS3''_D

C	1.05452200	-1.02438900	0.72336900
C	0.12001500	-1.85196800	-0.07977400
C	0.42900600	0.13791600	1.20240600
H	-0.63001000	-2.31928700	0.56107500
H	0.57951700	-2.66124000	-0.65661600
H	0.99577000	1.04698400	1.38040500
C	-0.67264600	0.10669700	2.20661500
O	-0.99520700	1.07406700	2.86771900
O	-1.29901900	-1.07621300	2.32520300
C	-2.40465000	-1.10685500	3.23977300
C	-2.90818100	-2.53328000	3.28262700
H	-3.17206300	-0.40934000	2.88681300
H	-2.06645900	-0.75849900	4.21919200
H	-3.75662100	-2.60771200	3.96682400
H	-3.23087600	-2.86399000	2.29161500
H	-2.12099300	-3.20614700	3.63021100
C	-0.10401100	1.60976300	-0.90780200
O	0.92869900	1.46279300	-1.59233800
C	-0.53051600	3.01318900	-0.57030000
C	-0.04240800	4.04980300	-1.37186500
C	-1.36734200	3.32123800	0.50713100
C	-0.40231300	5.36862900	-1.12052100
H	0.61896900	3.79357600	-2.19261100
C	-1.71492600	4.64411800	0.76693200

H	-1. 71678300	2. 53822000	1. 17176900
C	-1. 24134100	5. 66901500	-0. 04858600
H	-0. 02774200	6. 16384100	-1. 75780100
H	-2. 35303900	4. 87500600	1. 61416500
H	-1. 51970000	6. 69874300	0. 15387900
C	-0. 84837700	0. 49526300	-0. 38342600
C	-0. 68793400	-0. 84510500	-1. 04965800
H	-1. 83973100	0. 72548500	0. 00099100
H	-0. 07042200	-0. 70101200	-1. 94265700
C	-1. 99497800	-1. 47434800	-1. 46869300
C	-2. 20404700	-1. 90000100	-2. 78173600
C	-3. 01489100	-1. 68870400	-0. 53359700
C	-3. 39698100	-2. 51648400	-3. 15517100
H	-1. 42339300	-1. 74144600	-3. 52143100
C	-4. 20823400	-2. 30056300	-0. 90116200
H	-2. 85957500	-1. 36788200	0. 49377900
C	-4. 40438200	-2. 71899200	-2. 21660400
H	-3. 53919200	-2. 83659800	-4. 18298600
H	-4. 98755400	-2. 45159400	-0. 15967400
H	-5. 33450700	-3. 19757000	-2. 50618600
N	2. 48334600	-0. 96606100	0. 24221800
C	3. 19703400	0. 27971200	0. 69415500
C	3. 20384200	-2. 15113700	0. 84237700
C	2. 65665000	-1. 04310100	-1. 26584700
C	4. 71832200	0. 10140400	0. 47891800
H	2. 95227900	0. 42852800	1. 74637500
H	2. 77523600	1. 09481800	0. 09992700
C	4. 62239700	-2. 25743300	0. 23734500
H	2. 58786600	-3. 02717900	0. 63703200
H	3. 20454000	-1. 98055600	1. 92052800
C	4. 15102600	-0. 84533900	-1. 61344600
H	2. 01701100	-0. 26577800	-1. 68561400
H	2. 30424300	-2. 02966200	-1. 56831300
H	5. 13801800	1. 02087500	0. 06345700
H	5. 22335800	-0. 09743600	1. 42837400
N	4. 99543200	-1. 00964100	-0. 42977000
H	5. 34801500	-2. 47674300	1. 02526600
H	4. 67385100	-3. 06559700	-0. 49758400
H	4. 45519500	-1. 56733000	-2. 37606000
H	4. 31963200	0. 15697700	-2. 01669500

P'

C	0. 62532300	-1. 01826100	0. 26427000
C	-0. 77379100	-1. 53623700	0. 41274100
C	1. 72100000	-1. 79437700	0. 22854500
H	-1. 12750200	-1. 27047900	1. 41778100
H	-0. 78585200	-2. 62407800	0. 32706800
H	1. 59851000	-2. 86707400	0. 30195200

C	3.09469100	-1.28372400	0.09883100
O	3.44829300	-0.12892200	-0.00714000
O	3.96991800	-2.31155500	0.10579300
C	5.34928000	-1.94475000	-0.02399500
C	6.15967000	-3.22156800	0.02221700
H	5.61350300	-1.26082700	0.78820500
H	5.48646900	-1.40591700	-0.96657400
H	7.22305800	-2.99195000	-0.07708000
H	6.00350800	-3.74142300	0.97010000
H	5.87098900	-3.88956200	-0.79238400
C	-0.30438800	1.11763700	-0.16486000
O	0.75757000	0.32737800	0.22915000
C	0.06349000	2.54636000	-0.10026400
C	-0.91968300	3.54097100	-0.06261400
C	1.41480500	2.91159500	-0.07871700
C	-0.55884200	4.88213500	-0.02828400
H	-1.96927800	3.26408500	-0.03910900
C	1.76850500	4.25699800	-0.04077100
H	2.17423400	2.13524900	-0.09464500
C	0.78722400	5.24434200	-0.01941600
H	-1.32925500	5.64586700	0.00515100
H	2.81790900	4.53375400	-0.02851000
H	1.06807900	6.29223900	0.01207200
C	-1.45788300	0.60407700	-0.60296900
C	-1.71828200	-0.87896800	-0.61081700
H	-2.22185400	1.27389300	-0.98024200
H	-1.48944000	-1.28214400	-1.60730800
C	-3.15868800	-1.22654900	-0.28881900
C	-3.81101200	-2.25212000	-0.97390500
C	-3.83829800	-0.55905900	0.73406000
C	-5.11769300	-2.60617400	-0.64585700
H	-3.29128000	-2.77489900	-1.77303900
C	-5.14336200	-0.91038900	1.06419000
H	-3.33692600	0.24400200	1.26957600
C	-5.78731300	-1.93556500	0.37408800
H	-5.61348300	-3.40402900	-1.18970000
H	-5.65968000	-0.38229100	1.85962900
H	-6.80648100	-2.20786100	0.62871800

M3''_D

C	-0.48815300	0.73037200	-0.68571600
C	0.78291000	0.48958500	-1.48661700
C	-0.44502700	-0.23275700	0.47814200
H	1.69452400	1.00390200	-1.12466000
H	0.68026400	0.74949400	-2.54923700
H	-1.40265400	-0.36353500	0.99040200
C	0.57555300	-0.18583800	1.61951900
O	0.42223100	-0.74627300	2.68538800

O	1. 69819500	0. 47925700	1. 30919500
C	2. 77282100	0. 41047900	2. 25617500
C	3. 98855100	1. 00303100	1. 57895900
H	2. 93179300	-0. 63590300	2. 53193400
H	2. 48547300	0. 95798100	3. 16008400
H	4. 85170500	0. 95622000	2. 24748100
H	4. 21788400	0. 44191600	0. 66842400
H	3. 81282000	2. 04957100	1. 31454700
C	-1. 35930600	-1. 94227700	-1. 11430900
O	-1. 37027500	-2. 09672700	-2. 31934500
C	-2. 59250600	-2. 28593100	-0. 31978000
C	-3. 80309500	-2. 38849400	-1. 01093700
C	-2. 55806000	-2. 57305900	1. 04924800
C	-4. 96628300	-2. 75459900	-0. 34510000
H	-3. 80550000	-2. 17985400	-2. 07561800
C	-3. 72154200	-2. 95389000	1. 71265000
H	-1. 62889400	-2. 49614500	1. 60702000
C	-4. 92587100	-3. 04023200	1. 01928600
H	-5. 90377300	-2. 82346100	-0. 88771300
H	-3. 68595700	-3. 18175100	2. 77297900
H	-5. 83215500	-3. 33202600	1. 54081200
C	-0. 10693200	-1. 50381200	-0. 35267400
C	0. 99716800	-1. 05296500	-1. 33036000
H	0. 19005500	-2. 35031000	0. 27844000
H	0. 78921700	-1. 53048200	-2. 29209300
C	2. 42561200	-1. 41983300	-0. 96213100
C	3. 44340300	-1. 02237500	-1. 84023000
C	2. 79872600	-2. 13945200	0. 17551000
C	4. 77771800	-1. 32619200	-1. 59482600
H	3. 17436300	-0. 46363000	-2. 73384700
C	4. 13638200	-2. 44633200	0. 42935000
H	2. 05415200	-2. 45637800	0. 90051800
C	5. 13275800	-2. 04343600	-0. 45248300
H	5. 54172000	-1. 00462100	-2. 29630900
H	4. 39460900	-3. 00243400	1. 32584200
H	6. 17257900	-2. 28313100	-0. 25451900
N	-0. 75474700	2. 17940200	-0. 36238300
C	-2. 13633400	2. 29712300	0. 21460700
C	0. 19095200	2. 88665800	0. 58535000
C	-0. 74092700	2. 94491600	-1. 65772100
C	-2. 41577900	3. 76852700	0. 60042600
H	-2. 18211300	1. 63230700	1. 07794700
H	-2. 80448300	1. 90348800	-0. 55262300
C	-0. 12473300	4. 40179600	0. 59133100
H	1. 20566100	2. 65620500	0. 26000300
H	0. 03640400	2. 43214400	1. 56611800
C	-1. 35397000	4. 34570000	-1. 44099500
H	-1. 29089800	2. 32551800	-2. 36804100

H	0.30289100	2.99543300	-1.97351200
H	-3.41750300	4.05819700	0.27176400
H	-2.37001600	3.90563700	1.68465300
N	-1.43253700	4.66362900	-0.01385500
H	-0.12265100	4.78348300	1.61603200
H	0.62847400	4.95932100	0.02680800
H	-0.74821300	5.10376500	-1.94479000
H	-2.36420400	4.39752800	-1.85713300

NHC/B3LYP-D3

C	-0.67862600	-1.62307500	-0.00006900
C	0.67862600	-1.62307500	0.00006900
C	0.00000000	0.56845800	0.00000000
N	-1.06815100	-0.28627100	-0.00003900
H	-1.36596000	-2.45138600	-0.00023700
H	1.36596000	-2.45138600	0.00023700
N	1.06815100	-0.28627100	0.00003900
C	-2.46884600	0.22085300	-0.00000500
C	-3.45686700	-0.94883600	-0.00023700
C	-2.66862400	1.07236300	1.26213800
C	-2.66845700	1.07281600	-1.26188400
H	-3.34206600	-1.57447300	-0.89011100
H	-3.34222900	-1.57467700	0.88951700
H	-4.47461500	-0.55084000	-0.00031100
H	-1.93548900	1.88072000	1.28633200
H	-3.67567700	1.49988000	1.27586700
H	-2.53881400	0.46113900	2.16077700
H	-3.67524600	1.50095900	-1.27525200
H	-1.93478200	1.88068600	-1.28588700
H	-2.53922800	0.46179200	-2.16074100
C	2.46884600	0.22085300	0.00000500
C	2.66862400	1.07236500	-1.26213700
C	2.66845700	1.07281400	1.26188500
C	3.45686700	-0.94883600	0.00023500
H	2.53881400	0.46114200	-2.16077600
H	1.93548900	1.88072200	-1.28633000
H	3.67567700	1.49988200	-1.27586500
H	2.53922800	0.46178800	2.16074100
H	3.67524600	1.50095700	1.27525400
H	1.93478200	1.88068400	1.28588900
H	4.47461500	-0.55084000	0.00030900
H	3.34206700	-1.57447400	0.89010900
H	3.34222900	-1.57467600	-0.88951900

R1/B3LYP-D3

C	-2.51071000	-0.40575500	0.00008700
C	-3.75723900	-0.03305300	0.00033600
C	-1.25184700	-0.78376600	-0.00021200

H	-4.29694600	0.12967800	0.93008100
H	-4.29736500	0.12951800	-0.92919300
H	-0.98269000	-1.83636500	-0.00033000
C	-0.14866500	0.20618400	-0.00048500
O	-0.27381300	1.41819900	-0.00000200
O	1.04169000	-0.42565300	-0.00032500
C	2.21412300	0.42606100	-0.00001800
C	3.42975400	-0.47690900	0.00040400
H	2.17899100	1.06897100	0.88412600
H	2.17952400	1.06885100	-0.88427300
H	4.33826900	0.13193400	0.00061800
H	3.44209300	-1.11469500	0.88855000
H	3.44260700	-1.11483400	-0.88763500

R2/B3LYP-D3

C	1.18232300	-0.96986900	-0.03449800
O	1.18184000	-2.20427600	-0.08021400
C	2.48109000	-0.22568100	-0.01749800
C	2.57931500	1.15238200	-0.26524500
C	3.65288400	-0.95650700	0.23706800
C	3.82290400	1.78304800	-0.25496300
H	1.69589100	1.73823900	-0.49002300
C	4.89170100	-0.32518900	0.25872200
H	3.56495400	-2.02162100	0.41861600
C	4.97923000	1.04844500	0.01209300
H	3.88824300	2.84739500	-0.45641000
H	5.78948200	-0.89892800	0.46586200
H	5.94547500	1.54293700	0.02603600
C	-0.07741600	-0.20094100	0.02299200
C	-1.26566800	-0.83219200	-0.06992900
H	-0.02480500	0.87146200	0.16217700
H	-1.23163200	-1.91224900	-0.20049900
C	-2.59627100	-0.23746500	-0.01569500
C	-3.71465500	-1.08172900	-0.14407800
C	-2.81488900	1.14321000	0.16155800
C	-5.00873800	-0.56860900	-0.09794500
H	-3.55791400	-2.14775700	-0.28047400
C	-4.10660700	1.65428200	0.20772300
H	-1.97143100	1.81769000	0.26351000
C	-5.20848200	0.80136100	0.07834400
H	-5.85894600	-1.23550900	-0.19880300
H	-4.25911900	2.72005400	0.34496000
H	-6.21523600	1.20520900	0.11485700

TS1/B3LYP-D3

C	-1.11008300	1.80967000	-1.35762600
C	-2.24052400	1.06322500	-1.39317200
C	-1.07516600	0.44740200	0.46671600

N	-0.42005500	1.43626900	-0.21012000
H	-0.77058700	2.57943400	-2.03044800
H	-3.04471100	1.06955600	-2.10803300
N	-2.21904600	0.25362100	-0.26209300
C	0.81136600	2.14903100	0.23495600
C	0.44074200	3.62409500	0.46895100
C	1.33361500	1.54855300	1.54069300
C	1.87708600	2.03262200	-0.86574300
H	0.06522100	4.09836700	-0.44164700
H	-0.32785800	3.70568600	1.24296400
H	1.32426600	4.17855700	0.79739600
H	1.67295500	0.52393900	1.40326200
H	2.17886800	2.15427900	1.88030400
H	0.56153800	1.56193800	2.31289400
H	2.79963500	2.51807700	-0.53561800
H	2.09528700	0.98618000	-1.07961800
H	1.55717600	2.51795300	-1.79186200
C	-3.32164600	-0.68151900	0.11317100
C	-3.03381700	-2.07950300	-0.45478000
C	-3.43165300	-0.73023800	1.64178400
C	-4.64432900	-0.15467300	-0.46428600
H	-2.87061800	-2.03062000	-1.53550100
H	-2.15438400	-2.51927100	0.01701900
H	-3.88745700	-2.73752600	-0.26750300
H	-3.62003600	0.26806000	2.04653500
H	-4.26640900	-1.38038900	1.91886400
H	-2.52100600	-1.12334600	2.09049100
H	-5.46348400	-0.76755600	-0.08079000
H	-4.82177800	0.88195800	-0.16455000
H	-4.67471200	-0.21731800	-1.55510600
C	0.06776400	-1.45805200	0.78849800
C	-0.00527100	-1.69079400	2.08180300
C	0.49139400	-1.79581900	-0.45022700
H	0.32768000	-2.65483000	2.46172200
H	-0.37088000	-0.95691400	2.78630400
H	-0.22010300	-2.07289900	-1.22074600
C	1.85617000	-1.64792200	-0.91059800
O	2.23567500	-1.87982000	-2.05642900
O	2.71840100	-1.23176600	0.06208800
C	4.08940500	-1.04914200	-0.34049300
C	4.82611200	-0.43175800	0.83121100
H	4.12423500	-0.40540800	-1.22442300
H	4.51277300	-2.01919300	-0.62121800
H	5.88084900	-0.29420300	0.57579800
H	4.40160200	0.54344100	1.08517500
H	4.76604700	-1.07554900	1.71340300

M1/B3LYP-D3

C	2. 91271300	1. 33162900	0. 08100300
C	3. 27846200	0. 02944200	0. 13357200
C	1. 06659000	0. 10185600	-0. 14839200
N	1. 53927500	1. 37575800	-0. 09850700
H	3. 52108600	2. 21309200	0. 15303200
H	4. 25497400	-0. 39945400	0. 25392000
N	2. 12951700	-0. 73355700	-0. 00308700
C	0. 76532700	2. 68250400	-0. 09171200
C	1. 71784600	3. 80406100	-0. 53498300
C	-0. 41907200	2. 64157700	-1. 06431800
C	0. 28736300	2. 93565500	1. 34419700
H	2. 50327000	4. 00328300	0. 19734300
H	2. 17477900	3. 58480900	-1. 50386500
H	1. 13394400	4. 72101600	-0. 63462700
H	-1. 19492800	1. 95625300	-0. 73328400
H	-0. 83996800	3. 64934900	-1. 11105500
H	-0. 09718400	2. 35490000	-2. 06780200
H	-0. 20130200	3. 91279800	1. 39227700
H	-0. 42712200	2. 16836500	1. 64631200
H	1. 13159900	2. 93865700	2. 03957800
C	2. 13602600	-2. 25076700	-0. 00805200
C	1. 07831900	-2. 77819500	0. 96854900
C	1. 88549500	-2. 74293500	-1. 43919600
C	3. 51525300	-2. 73620000	0. 45904200
H	1. 27094200	-2. 40802800	1. 97939000
H	0. 07009300	-2. 48814400	0. 68119000
H	1. 14065800	-3. 86944200	0. 98409000
H	2. 61431000	-2. 30646800	-2. 12831500
H	1. 99553200	-3. 83056200	-1. 46566900
H	0. 88087000	-2. 47969700	-1. 76989400
H	3. 47884800	-3. 82562300	0. 52031400
H	4. 30935000	-2. 47648300	-0. 24534700
H	3. 76870900	-2. 35229000	1. 45073800
C	-0. 36255600	-0. 29029000	-0. 31723100
C	-0. 73188100	-0. 59609800	-1. 59585300
C	-1. 10922000	-0. 22187200	0. 90282200
H	-1. 75460300	-0. 85021500	-1. 83349000
H	-0. 01970100	-0. 50987100	-2. 40769800
H	-0. 55058000	-0. 09684600	1. 82255800
C	-2. 50467200	-0. 33288200	1. 08543500
O	-3. 11468700	-0. 28715000	2. 16930000
O	-3. 21980000	-0. 49011100	-0. 09813000
C	-4. 64151200	-0. 56272200	0. 04020400
C	-5. 22621100	-0. 75461100	-1. 34726900
H	-5. 01881500	0. 35489300	0. 50666000
H	-4. 90971100	-1. 39227000	0. 70406600
H	-6. 31789600	-0. 80944500	-1. 29344500
H	-4. 95502100	0. 07922700	-2. 00192400

H	-4.85740700	-1.68003600	-1.80016900
TS2/B3LYP-D3			
C	3.41022500	-2.94111700	-0.85828400
C	4.11706300	-2.17469500	0.00290200
C	2.02973300	-1.37805000	-0.05776400
N	2.11928100	-2.45000900	-0.89496400
H	3.73223400	-3.78762200	-1.43278100
H	5.14821200	-2.25269400	0.28813900
N	3.26400400	-1.21211200	0.50842500
C	1.04613100	-3.06250400	-1.77730100
C	1.66537300	-4.21144200	-2.58508700
C	-0.07804500	-3.62530900	-0.89810200
C	0.55352300	-1.98485300	-2.74326600
H	2.47846700	-3.87416900	-3.23334300
H	2.02027200	-5.02543300	-1.94747500
H	0.87946500	-4.61530900	-3.22571900
H	-0.68577600	-2.83408400	-0.46791200
H	-0.73416400	-4.23613700	-1.52306800
H	0.33879600	-4.26267800	-0.11274700
H	-0.12198200	-2.44041000	-3.47097300
H	-0.01438400	-1.22582700	-2.21731000
H	1.39509300	-1.53623600	-3.27886900
C	3.76352400	-0.15515400	1.48158700
C	4.08236800	1.11542100	0.68329300
C	2.74877500	0.09171400	2.60303500
C	5.05644300	-0.67143300	2.13655600
H	4.80940100	0.89509700	-0.10342700
H	3.19614800	1.55830600	0.23387300
H	4.52322700	1.85544800	1.35709500
H	2.49368500	-0.84547100	3.10455400
H	3.21484300	0.75621500	3.33439700
H	1.83255800	0.55968600	2.26297500
H	5.34522200	0.04617800	2.90658900
H	4.90892600	-1.64214700	2.61707100
H	5.88927000	-0.73657800	1.43331200
C	0.82630500	-0.55121000	0.26174100
C	-0.01111200	-1.03004500	1.20459900
C	0.71096700	0.78076300	-0.37757400
H	-0.83728100	-0.43788900	1.56297200
H	0.15121600	-2.00373700	1.65270800
H	1.41106600	0.92407300	-1.19715900
C	0.71099900	1.98884000	0.46367800
O	1.32486900	3.01743500	0.20017600
O	-0.10427800	1.89032000	1.54557300
C	-0.24375000	3.07739200	2.36020100
C	0.87905900	3.20091000	3.37570500
H	-1.21184800	2.95484800	2.85027900

H	-0.28201100	3.94746900	1.70235800
H	0.71044100	4.07967800	4.00617200
H	0.92176600	2.31878700	4.02051300
H	1.84099900	3.31620400	2.87143800
C	-2.65714500	-0.79127400	-0.59011600
O	-2.38883200	-1.55212300	-1.56698000
C	-3.65061200	-1.30308600	0.43257900
C	-4.41342400	-2.43234200	0.10084900
C	-3.82521700	-0.73825500	1.70631700
C	-5.33264000	-2.97222300	0.99846100
H	-4.25722400	-2.87196600	-0.87804300
C	-4.74073900	-1.27760100	2.61011400
H	-3.23173600	0.11867300	2.00647000
C	-5.50161800	-2.39562800	2.25969500
H	-5.91659500	-3.84441000	0.71759800
H	-4.85544000	-0.82850400	3.59258100
H	-6.21331700	-2.81571200	2.96421000
C	-2.12987800	0.50326300	-0.41379300
C	-1.09234600	1.00305900	-1.25139700
H	-2.49297100	1.11767600	0.39892300
H	-0.89417800	0.34899300	-2.09524700
C	-1.06308600	2.43723100	-1.66313100
C	-0.32831900	2.81437600	-2.79805900
C	-1.74842800	3.43842000	-0.95837700
C	-0.27470000	4.14275500	-3.21535700
H	0.20786700	2.05050300	-3.35542800
C	-1.69374100	4.76978300	-1.36954800
H	-2.33588600	3.17321100	-0.08691300
C	-0.95675800	5.12965300	-2.49944800
H	0.29678900	4.40846700	-4.09993200
H	-2.23361600	5.52739900	-0.80884500
H	-0.91821300	6.16574500	-2.82166000

NHC/B3PW91-D3

C	-0.67848200	-1.61873100	0.00000600
C	0.67848200	-1.61873100	-0.00000600
C	0.00000000	0.56711900	0.00000000
N	-1.06419200	-0.28670400	0.00001900
H	-1.36659500	-2.44753600	0.00002400
H	1.36659500	-2.44753600	-0.00002400
N	1.06419200	-0.28670400	-0.00001900
C	-2.45793600	0.21961300	-0.00000200
C	-3.44471600	-0.94435500	0.00013900
C	-2.65362200	1.06936900	1.25764500
C	-2.65367000	1.06912000	-1.25781000
H	-3.33199100	-1.57012300	-0.89024600
H	-3.33190400	-1.56996700	0.89062100
H	-4.46158100	-0.54380200	0.00014900

H	-1. 91536600	1. 87382400	1. 27919600
H	-3. 65851400	1. 50197700	1. 27132700
H	-2. 52580400	0. 45811600	2. 15660200
H	-3. 65857800	1. 50169000	-1. 27156400
H	-1. 91544700	1. 87360200	-1. 27952700
H	-2. 52584100	0. 45769600	-2. 15664800
C	2. 45793600	0. 21961300	0. 00000200
C	2. 65362200	1. 06936700	-1. 25764600
C	2. 65367000	1. 06912200	1. 25780900
C	3. 44471600	-0. 94435500	-0. 00013800
H	2. 52580400	0. 45811400	-2. 15660200
H	1. 91536600	1. 87382300	-1. 27919700
H	3. 65851400	1. 50197600	-1. 27132800
H	2. 52584100	0. 45769800	2. 15664800
H	3. 65857800	1. 50169100	1. 27156300
H	1. 91544700	1. 87360300	1. 27952500
H	4. 46158100	-0. 54380200	-0. 00014800
H	3. 33199100	-1. 57012200	0. 89024800
H	3. 33190400	-1. 56996800	-0. 89062000

R1/B3PW91-D3

C	-2. 50428200	-0. 40411600	0. 00011500
C	-3. 74956100	-0. 02923500	0. 00040800
C	-1. 24665000	-0. 78466100	-0. 00024800
H	-4. 28747600	0. 13425400	0. 93124100
H	-4. 28805400	0. 13379900	-0. 93017000
H	-0. 98118900	-1. 83861900	-0. 00038800
C	-0. 14576500	0. 20337700	-0. 00060500
O	-0. 27055500	1. 41353400	-0. 00002100
O	1. 03975700	-0. 42748300	-0. 00038200
C	2. 20403300	0. 42367300	-0. 00001300
C	3. 42024800	-0. 47159200	0. 00048600
H	2. 16760400	1. 06753000	0. 88396800
H	2. 16824000	1. 06739700	-0. 88412000
H	4. 32605000	0. 14098200	0. 00074700
H	3. 43622600	-1. 10913600	0. 88864000
H	3. 43684300	-1. 10928800	-0. 88754800

R2/B3PW91-D3

C	1. 17947100	-0. 96703000	-0. 03937800
O	1. 17786000	-2. 19866600	-0. 08959300
C	2. 47562200	-0. 22509000	-0. 01932700
C	2. 57610100	1. 14782500	-0. 28172300
C	3. 64193600	-0. 95407600	0. 25219100
C	3. 81870200	1. 77626300	-0. 26894400
H	1. 69430100	1. 73175600	-0. 52155400
C	4. 87970700	-0. 32465000	0. 27748600
H	3. 54987400	-2. 01781600	0. 44451200

C	4.97023600	1.04421500	0.01626200
H	3.88742100	2.83834100	-0.48289800
H	5.77549500	-0.89681300	0.49905700
H	5.93715900	1.53817600	0.03275200
C	-0.07570200	-0.19656900	0.02231600
C	-1.26211100	-0.82836400	-0.07583900
H	-0.02225300	0.87555800	0.17036100
H	-1.22442800	-1.90827300	-0.21417800
C	-2.59051200	-0.23617000	-0.01757800
C	-3.70658500	-1.07978200	-0.14881100
C	-2.80888300	1.14143400	0.16666800
C	-4.99926700	-0.56842300	-0.09820800
H	-3.54914800	-2.14548500	-0.29097000
C	-4.09919300	1.65076100	0.21715400
H	-1.96558700	1.81665800	0.27082700
C	-5.19908900	0.79877500	0.08521600
H	-5.84955200	-1.23548700	-0.20128400
H	-4.25233000	2.71608500	0.35995700
H	-6.20641900	1.20191800	0.12526200

TS1/B3PW91-D3

C	-1.03564600	1.72890300	-1.39968000
C	-2.16993200	0.98788100	-1.43731100
C	-1.08431500	0.47422500	0.49609400
N	-0.39917100	1.41646600	-0.21069400
H	-0.66553100	2.46004300	-2.10042000
H	-2.94671800	0.95656700	-2.18280200
N	-2.19735900	0.25091200	-0.26441600
C	0.80913500	2.14001800	0.25098800
C	0.41569900	3.60400000	0.48191100
C	1.31591300	1.53726800	1.55534900
C	1.89238400	2.04157200	-0.82631400
H	0.03972400	4.06893700	-0.43404300
H	-0.36224000	3.67210400	1.24802400
H	1.28617400	4.17451400	0.81828900
H	1.65705700	0.51242700	1.41174900
H	2.15636300	2.14174200	1.90893100
H	0.53374000	1.54118600	2.31743700
H	2.80487300	2.52930400	-0.47275800
H	2.12137500	0.99809100	-1.04506700
H	1.59113300	2.53380900	-1.75499900
C	-3.30982600	-0.65737900	0.11228300
C	-3.05028400	-2.05479300	-0.45643000
C	-3.41111400	-0.70908800	1.63551800
C	-4.61962000	-0.10249000	-0.45552400
H	-2.89352900	-2.00966800	-1.53845700
H	-2.17315300	-2.50600900	0.01116500
H	-3.91190800	-2.70041000	-0.26257900

H	-3.57736900	0.29085700	2.04582400
H	-4.25593500	-1.34541300	1.91464600
H	-2.50311900	-1.12060900	2.07480900
H	-5.45158700	-0.69645300	-0.06890000
H	-4.77006100	0.93785500	-0.15297400
H	-4.65834500	-0.16231700	-1.54648600
C	0.06445500	-1.47074600	0.79560900
C	-0.01793000	-1.70943900	2.08536300
C	0.46693700	-1.76062900	-0.45584800
H	0.28774900	-2.68530000	2.45873300
H	-0.36687600	-0.96761600	2.79096400
H	-0.25534200	-2.00097300	-1.22916800
C	1.83031100	-1.60539600	-0.91987200
O	2.19375500	-1.78553500	-2.07705200
O	2.69768700	-1.24933700	0.06107400
C	4.06203100	-1.06594500	-0.34273900
C	4.80609400	-0.47710700	0.83324200
H	4.09645400	-0.40602400	-1.21517400
H	4.47897400	-2.03287100	-0.64484300
H	5.85992000	-0.33992900	0.57482700
H	4.38845500	0.49536100	1.10762800
H	4.74815900	-1.13702700	1.70340500

M1/B3PW91-D3

C	2.88887000	1.35784100	0.07586100
C	3.27170900	0.06088500	0.12713800
C	1.06393400	0.10580500	-0.14807000
N	1.51951100	1.38194600	-0.09879500
H	3.48593200	2.24835900	0.14550600
H	4.25461000	-0.35650900	0.24481900
N	2.13573900	-0.71251200	-0.00614600
C	0.73007200	2.66784100	-0.09114300
C	1.66281300	3.80266100	-0.52420900
C	-0.44537900	2.60949100	-1.06520500
C	0.24223400	2.90789400	1.33816500
H	2.43833300	4.01570400	0.21533900
H	2.13061100	3.59428700	-1.49060100
H	1.06307400	4.70932400	-0.62654200
H	-1.20805700	1.90545800	-0.73941400
H	-0.88682400	3.60875800	-1.10782200
H	-0.11420100	2.33451500	-2.06923500
H	-0.25943000	3.87836900	1.38779600
H	-0.46502200	2.12868500	1.62974700
H	1.08200200	2.91762900	2.03905600
C	2.15670700	-2.21967500	-0.00652300
C	1.11518400	-2.74874100	0.97824100
C	1.89659800	-2.71817900	-1.42814300
C	3.53959400	-2.69008700	0.44700800

H	1.31863600	-2.37892900	1.98721800
H	0.10294800	-2.45751400	0.70123400
H	1.17798300	-3.84003800	0.99181300
H	2.61406400	-2.27845600	-2.12713500
H	2.01434000	-3.80508700	-1.45149000
H	0.88503900	-2.46246200	-1.74681500
H	3.51233900	-3.77984300	0.51159800
H	4.32492200	-2.42709500	-0.26662600
H	3.79948700	-2.30226100	1.43590700
C	-0.35591000	-0.30319800	-0.31417800
C	-0.72014100	-0.61447300	-1.59225200
C	-1.10001300	-0.23908500	0.90397000
H	-1.74098800	-0.87948100	-1.82989900
H	-0.00795400	-0.51526400	-2.40355400
H	-0.54160500	-0.11165800	1.82429000
C	-2.49490400	-0.35257100	1.08242900
O	-3.10610500	-0.30497900	2.16282500
O	-3.20056100	-0.51305900	-0.09758000
C	-4.61679100	-0.58156700	0.03787900
C	-5.19863600	-0.77097500	-1.34661300
H	-4.99291700	0.33688700	0.50437600
H	-4.88896700	-1.41047900	0.70160800
H	-6.29032000	-0.82323200	-1.29438900
H	-4.92508900	0.06244300	-2.00064700
H	-4.83202200	-1.69705500	-1.79964200

TS2/B3PW91-D3

C	3.19995100	-3.11644900	-0.87502800
C	3.94947300	-2.40356600	-0.00406400
C	1.92839800	-1.46540900	-0.08463000
N	1.95352500	-2.53482900	-0.92239800
H	3.46541400	-3.98285800	-1.45112500
H	4.96996400	-2.55329100	0.29400500
N	3.16228700	-1.38781700	0.49098100
C	0.85403100	-3.04681100	-1.81631800
C	1.39259700	-4.20809000	-2.65257300
C	-0.30309300	-3.54927500	-0.95456400
C	0.44603100	-1.91150800	-2.74579200
H	2.23566800	-3.91144300	-3.28291200
H	1.67716700	-5.06767900	-2.03925400
H	0.58546600	-4.53073700	-3.31329900
H	-0.83068800	-2.72626200	-0.47848600
H	-1.01884000	-4.06689600	-1.59731300
H	0.06361200	-4.25578600	-0.20388300
H	-0.30612300	-2.27391600	-3.44891900
H	-0.00978200	-1.10323100	-2.18303800
H	1.31164700	-1.54570800	-3.30571400
C	3.71749700	-0.36449000	1.45356000

C	4.09732200	0.88168300	0.65391400
C	2.72481200	-0.06168600	2.57417800
C	4.97996300	-0.94430800	2.10152600
H	4.80375900	0.62120900	-0.13946200
H	3.22999700	1.37061400	0.21295800
H	4.58293800	1.59799900	1.32245900
H	2.41825500	-0.98292700	3.07691000
H	3.22992000	0.57574000	3.30395800
H	1.83462200	0.45803800	2.23498200
H	5.31061300	-0.23987300	2.86723800
H	4.78372400	-1.90359500	2.58840100
H	5.80533800	-1.05590100	1.39432500
C	0.78491600	-0.56608300	0.23611400
C	-0.08181600	-0.99555200	1.17813000
C	0.75614700	0.76653100	-0.38901500
H	-0.85692300	-0.34510200	1.55153100
H	0.01713900	-1.98150200	1.61917400
H	1.45610800	0.87885300	-1.21445300
C	0.80642600	1.96717300	0.45128800
O	1.46759300	2.96572500	0.19367900
O	-0.00933600	1.89989800	1.52968300
C	-0.08576400	3.08341900	2.34348600
C	1.04146500	3.14731100	3.35299100
H	-1.05791200	3.01173700	2.83637400
H	-0.08170500	3.95663300	1.68736200
H	0.92424900	4.03460800	3.98288200
H	1.03863700	2.26550200	3.99958600
H	2.00663300	3.20935100	2.84524400
C	-2.67235900	-0.65898100	-0.60764100
O	-2.46707100	-1.37697700	-1.62411300
C	-3.63407000	-1.18736500	0.43101600
C	-4.38108400	-2.32661600	0.10711100
C	-3.79622400	-0.63084600	1.70762300
C	-5.27211500	-2.88748000	1.01734100
H	-4.23191300	-2.75628300	-0.87829400
C	-4.68514400	-1.18941000	2.62313400
H	-3.21553100	0.23761700	2.00210800
C	-5.42940200	-2.31927900	2.28184500
H	-5.84420600	-3.77009500	0.74343700
H	-4.79259900	-0.74518300	3.60898800
H	-6.12104700	-2.75512200	2.99724100
C	-2.09781900	0.61268900	-0.39964700
C	-1.07070000	1.09550000	-1.24660900
H	-2.41793400	1.21358400	0.44221000
H	-0.91019100	0.45092400	-2.10804400
C	-0.97191400	2.53265600	-1.61075800
C	-0.22363000	2.90794100	-2.73527000
C	-1.60468700	3.54130300	-0.87230300

C	-0.10561900	4.24266000	-3.10939100
H	0.27262000	2.13567600	-3.31838000
C	-1.48297700	4.87930100	-1.23903300
H	-2.20511600	3.27547200	-0.00892500
C	-0.73288500	5.23757100	-2.35851100
H	0.47563100	4.50838600	-3.98805000
H	-1.98242000	5.64483100	-0.65154300
H	-0.64271400	6.28077400	-2.64699600

NHC/ ω B97X-D

C	-0.67610700	-1.61596900	-0.01448300
C	0.67610700	-1.61596900	0.01448200
C	0.00000000	0.56606300	-0.00000200
N	-1.06479000	-0.28408900	-0.02873300
H	-1.36381400	-2.44468600	-0.02878800
H	1.36381400	-2.44468600	0.02878700
N	1.06479000	-0.28409000	0.02872900
C	-2.46053100	0.21972500	0.00168800
C	-3.44725600	-0.93001400	-0.20912700
C	-2.70125800	0.86992300	1.36914700
C	-2.62880400	1.25040900	-1.11957700
H	-3.26789000	-1.44341600	-1.15857000
H	-3.40515700	-1.66117200	0.60339800
H	-4.46062000	-0.52158300	-0.23392800
H	-1.98115000	1.67558400	1.52975700
H	-3.71368000	1.28092600	1.42467200
H	-2.58156900	0.13224500	2.16871200
H	-3.63539100	1.67721700	-1.08695700
H	-1.89567100	2.05081400	-1.00777900
H	-2.48123200	0.78006100	-2.09662800
C	2.46053100	0.21972400	-0.00168800
C	2.70125800	0.86993300	-1.36914300
C	2.62880300	1.25040100	1.11958500
C	3.44725600	-0.93001500	0.20911900
H	2.58157000	0.13226000	-2.16871200
H	1.98114900	1.67559400	-1.52974700
H	3.71368000	1.28093700	-1.42466300
H	2.48123000	0.78004700	2.09663200
H	3.63539100	1.67720900	1.08696800
H	1.89567100	2.05080800	1.00779000
H	4.46062000	-0.52158500	0.23392000
H	3.26789300	-1.44342200	1.15856000
H	3.40515500	-1.66116900	-0.60340900

R1/ ω B97X-D

C	-2.50193100	-0.40447900	0.00000000
C	-3.74543500	-0.02628600	-0.00003600
C	-1.24745700	-0.78978300	0.00002200

H	-4.27841400	0.13743100	0.93192900
H	-4.27826600	0.13775300	-0.93202800
H	-0.98713000	-1.84366900	-0.00000400
C	-0.14540200	0.20133200	0.00006400
O	-0.27669400	1.40810200	0.00007900
O	1.03969100	-0.42045500	-0.00005100
C	2.20364600	0.42651800	-0.00010700
C	3.42001100	-0.47250300	0.00005500
H	2.17290500	1.06898400	0.88435300
H	2.17297600	1.06873800	-0.88475200
H	4.32572500	0.13916200	-0.00005700
H	3.43382100	-1.10902400	0.88835300
H	3.43381900	-1.10935300	-0.88800600

R2/ωB97X-D

C	1.18146400	-0.96971600	-0.07573400
O	1.17922200	-2.19364300	-0.15682000
C	2.48237800	-0.22712600	-0.03127100
C	2.58969900	1.13838500	-0.31619900
C	3.63727000	-0.95014700	0.28895700
C	3.83041500	1.76746500	-0.27569900
H	1.71617600	1.71766300	-0.59495200
C	4.87274200	-0.31937600	0.34274100
H	3.54377000	-2.01032700	0.49730100
C	4.97076400	1.04268600	0.06022200
H	3.90627800	2.82496700	-0.50571600
H	5.76063700	-0.88608100	0.60329200
H	5.93571400	1.53759600	0.10008700
C	-0.08074700	-0.19943900	0.00592400
C	-1.26056500	-0.82734200	-0.11726300
H	-0.02592300	0.86608600	0.19642900
H	-1.22516900	-1.90238300	-0.28750300
C	-2.59758400	-0.23297200	-0.03680100
C	-3.71201400	-1.07961600	-0.11287400
C	-2.81155200	1.14535500	0.11782900
C	-5.00319300	-0.56935300	-0.02947600
H	-3.55995200	-2.14798100	-0.23671200
C	-4.10015300	1.65482900	0.19925800
H	-1.96901200	1.82731100	0.16975100
C	-5.20010700	0.79942400	0.12805200
H	-5.85350900	-1.24087800	-0.08673400
H	-4.25011900	2.72265200	0.31920400
H	-6.20556500	1.20217900	0.19411500

TS1/ωB97X-D

C	-1.07957800	1.81485100	-1.35630200
C	-2.21618900	1.08807100	-1.38955700
C	-1.04853000	0.43813200	0.44411700

N	-0.38793000	1.42335000	-0.22173300
H	-0.73364700	2.58187000	-2.02979500
H	-3.02258700	1.11156000	-2.10215900
N	-2.19861000	0.26999300	-0.27071400
C	0.84980300	2.11770200	0.21740600
C	0.50515800	3.59736200	0.44377600
C	1.36501400	1.52158100	1.52538500
C	1.91389000	1.97701400	-0.87796800
H	0.14102100	4.07670300	-0.46892100
H	-0.26322400	3.69479900	1.21615200
H	1.39817300	4.13612500	0.77213700
H	1.69845400	0.49306600	1.39191300
H	2.21510500	2.12228000	1.86218300
H	0.59374500	1.54479600	2.29875800
H	2.84527900	2.44494700	-0.54691500
H	2.11063300	0.92402400	-1.08503800
H	1.60770100	2.46451500	-1.80774500
C	-3.31453300	-0.63945800	0.10820300
C	-3.05647400	-2.04544200	-0.44602300
C	-3.43341300	-0.67391000	1.63398800
C	-4.62534700	-0.09633600	-0.47591700
H	-2.87822100	-2.00737300	-1.52495000
H	-2.19530800	-2.50685600	0.04091300
H	-3.92985700	-2.67849600	-0.26485600
H	-3.59911000	0.33125100	2.03163800
H	-4.28467200	-1.30198200	1.91172500
H	-2.53568200	-1.08863100	2.09099400
H	-5.45594700	-0.68342700	-0.07708900
H	-4.78160900	0.94993300	-0.19854500
H	-4.66169300	-0.18433700	-1.56515900
C	0.04600400	-1.45141200	0.81178400
C	-0.02178700	-1.65190600	2.10919500
C	0.46021900	-1.83334800	-0.41720100
H	0.30876500	-2.60926000	2.50428100
H	-0.37631200	-0.89636300	2.79639500
H	-0.25759400	-2.13444800	-1.17239700
C	1.82609800	-1.70915200	-0.87963700
O	2.20452800	-1.98251000	-2.01133000
O	2.68236000	-1.26419400	0.07151500
C	4.04209400	-1.07047900	-0.33009400
C	4.74226100	-0.33131900	0.78993600
H	4.06895200	-0.50085500	-1.26377300
H	4.50438100	-2.04429700	-0.52121300
H	5.79494400	-0.18232700	0.53618200
H	4.28213300	0.64752400	0.95010600
H	4.68873300	-0.89622000	1.72428900

M1/ωB97X-D

C	2. 93915800	1. 25085400	0. 06597500
C	3. 25914300	-0. 05725400	0. 12353000
C	1. 06448800	0. 08958800	-0. 14653500
N	1. 57293400	1. 34216700	-0. 10686700
H	3. 58231800	2. 10851700	0. 13196800
H	4. 22391100	-0. 51308500	0. 24378800
N	2. 09023700	-0. 77993500	-0. 00177900
C	0. 85138200	2. 67072800	-0. 08861500
C	1. 82548900	3. 74923600	-0. 58195500
C	-0. 37095100	2. 67037700	-1. 01009700
C	0. 44085700	2. 95552000	1. 35913000
H	2. 63596500	3. 94078300	0. 12495700
H	2. 24808300	3. 49445400	-1. 55763200
H	1. 27072500	4. 68364000	-0. 68608200
H	-1. 16127300	2. 02147300	-0. 63832200
H	-0. 75303000	3. 69366100	-1. 04811900
H	-0. 10387700	2. 36279200	-2. 02361800
H	-0. 01448700	3. 94797100	1. 41505800
H	-0. 28693700	2. 21564900	1. 69797900
H	1. 31088900	2. 93769000	2. 02191400
C	2. 05153300	-2. 29029100	-0. 00609100
C	0. 95243500	-2. 79254900	0. 93359300
C	1. 83492300	-2. 77732000	-1. 44130000
C	3. 39875200	-2. 81418200	0. 50651800
H	1. 09401800	-2. 39084800	1. 94062100
H	-0. 04297800	-2. 51962900	0. 58857400
H	1. 01877600	-3. 88226800	0. 98417200
H	2. 59327300	-2. 35839300	-2. 10903800
H	1. 92152700	-3. 86698900	-1. 46420200
H	0. 84550600	-2. 49447000	-1. 80198900
H	3. 32321500	-3. 90037500	0. 58513000
H	4. 22046400	-2. 59647400	-0. 18042100
H	3. 63695000	-2. 42207400	1. 49896300
C	-0. 37709900	-0. 25814900	-0. 31606300
C	-0. 74657000	-0. 54571100	-1. 59235100
C	-1. 11815700	-0. 17481000	0. 90554000
H	-1. 77423600	-0. 77446000	-1. 83665100
H	-0. 02408700	-0. 48215600	-2. 39842200
H	-0. 55672700	-0. 06271100	1. 82603700
C	-2. 51370900	-0. 27402800	1. 08290400
O	-3. 12345000	-0. 22839300	2. 16174100
O	-3. 22103800	-0. 42026000	-0. 09228700
C	-4. 63469500	-0. 50054900	0. 03369800
C	-5. 20718800	-0. 69217400	-1. 35683100
H	-5. 02378500	0. 41352400	0. 49636900
H	-4. 90613800	-1. 33407300	0. 69058000
H	-6. 29735700	-0. 76283100	-1. 30803800
H	-4. 94339600	0. 14856300	-2. 00461500

H	-4.82234800	-1.61000600	-1.81037400
TS2/ωB97X-D			
C	3.05258500	-3.23717300	-0.94324600
C	3.84615600	-2.56902200	-0.08384500
C	1.87747200	-1.54277100	-0.11987600
N	1.83349400	-2.59990700	-0.96562600
H	3.27203300	-4.10996900	-1.52856800
H	4.86458000	-2.77207900	0.18694100
N	3.11900900	-1.52116200	0.43523100
C	0.69464600	-3.04993300	-1.84744600
C	1.16649400	-4.21906700	-2.71819300
C	-0.46608500	-3.52592500	-0.97116900
C	0.31578700	-1.88308600	-2.75473800
H	2.01100100	-3.94672600	-3.35726400
H	1.42202500	-5.10373200	-2.12839400
H	0.33563700	-4.49178200	-3.37184900
H	-0.93281900	-2.69911500	-0.44183600
H	-1.22663000	-3.97613100	-1.61277100
H	-0.11712100	-4.28089200	-0.26025200
H	-0.48526700	-2.19546400	-3.42686100
H	-0.06061100	-1.04690300	-2.17458000
H	1.17894100	-1.56882700	-3.34913600
C	3.74560000	-0.52932100	1.39343900
C	4.17770600	0.70326500	0.59386700
C	2.79342800	-0.17641800	2.53856400
C	4.99123600	-1.17718700	2.01722200
H	4.85250000	0.41161000	-0.21603400
H	3.33031200	1.24425000	0.17516700
H	4.71807800	1.38288300	1.25868300
H	2.44236700	-1.08135500	3.04193800
H	3.35077500	0.42524200	3.26081000
H	1.93060500	0.40047500	2.22056700
H	5.36956200	-0.49505200	2.78063400
H	4.75721100	-2.12893300	2.50169900
H	5.79767000	-1.32301800	1.29494600
C	0.77982100	-0.58217300	0.22240900
C	-0.07805900	-0.97237600	1.18603800
C	0.81868300	0.73833100	-0.41161900
H	-0.81452500	-0.28825500	1.57801000
H	-0.00365600	-1.95680600	1.63584000
H	1.48854300	0.80561900	-1.26604000
C	0.91980400	1.94385000	0.39370500
O	1.59213100	2.92551800	0.09703100
O	0.15220000	1.92053000	1.51189900
C	0.17693800	3.09471700	2.33252700
C	1.36188100	3.09448100	3.28070200
H	-0.76702500	3.06770300	2.88117700

H	0.18753600	3.97661100	1.68843400
H	1.33200600	3.98666800	3.91296000
H	1.34345700	2.21325300	3.92779000
H	2.29877800	3.09851100	2.71862800
C	-2.72831800	-0.57120400	-0.57994400
O	-2.55715900	-1.26528900	-1.60607000
C	-3.66590400	-1.11627800	0.48085100
C	-4.42291800	-2.24752600	0.16163200
C	-3.79890800	-0.56811800	1.76181100
C	-5.30025100	-2.80797000	1.08355800
H	-4.30013500	-2.67614800	-0.82713500
C	-4.67580700	-1.12569200	2.68818600
H	-3.20868700	0.29432900	2.05387600
C	-5.43270000	-2.24574900	2.35166900
H	-5.88166600	-3.68477900	0.81424900
H	-4.76569600	-0.68520800	3.67643800
H	-6.11780600	-2.67846900	3.07414300
C	-2.14447300	0.70929800	-0.38063300
C	-1.16327200	1.19153900	-1.25033100
H	-2.45050500	1.30762100	0.46819600
H	-0.99467400	0.56140300	-2.11805400
C	-0.98869600	2.63477000	-1.55016100
C	-0.29084600	3.01205900	-2.70346800
C	-1.51912100	3.64517600	-0.73957800
C	-0.12462700	4.35109900	-3.03850900
H	0.12759900	2.23905500	-3.34321900
C	-1.35010600	4.98634100	-1.06797000
H	-2.07182200	3.38453400	0.15682900
C	-0.65200200	5.34642000	-2.21839000
H	0.41631400	4.61860200	-3.94113100
H	-1.76822000	5.75328800	-0.42298100
H	-0.52241700	6.39324700	-2.47434400