

Supporting Information

Theoretical Investigations toward TMEDA-Catalyzed [2 + 4] Annulation of Allenolate with 1-Aza-1,3-Diene: Mechanism, Regioselectivity, and Role of Catalyst

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Table 1. The ZPE, δG , E, E+ZPE, and G of SP (stationary points) at the M06-2X/6-31G (d,p) level in gas phase, and E at B2, i.e. M06-2X/6-311++G (d,p) level in solvent toluene (unit: a.u.)

SP	δE	δG	E+ZPE	G	E/B2
R1	0.183147	0.144974	-575.167648	-575.205821	-575.50577332
R2	0.354741	0.296814	-1563.576222	-1563.634150	-1564.27411681
TMEDA	0.225187	0.189326	-347.355673	-347.391533	-347.66895566
TS1A	0.412824	0.363472	-922.517188	-922.566541	-923.169351315
M1A	0.415789	0.365982	-922.527364	-922.577172	-923.1853396
TS2A	0.773345	0.693328	-2486.135438	-2486.215455	-2487.48478409
M2A	0.775403	0.693918	-2486.156893	-2486.238379	-2487.51080735
TS3A	0.770676	0.689410	-2486.137524	-2486.218790	-2487.49017863
M3A	0.775881	0.695307	-2486.158182	-2486.238757	-2487.51033162
TS4A	0.771256	0.691847	-2486.118653	-2486.198062	-2487.46731249
M4A	0.776095	0.694765	-2486.131603	-2486.212933	-2487.49623699
TS5A	0.774577	0.695709	-2486.134978	-2486.213846	-2487.48438016
M5A	0.773026	0.690747	-2486.213072	-2486.295351	-2487.55495261
TS6A	0.769652	0.690707	-2486.199252	-2486.278197	-2487.53703282
M6A	0.775795	0.697122	-2486.202353	-2486.281026	-2487.55074550
TS7A	0.773589	0.694214	-2486.199220	-2486.278594	-2487.54777102
P	0.771859	0.690140	-2486.288884	-2486.370603	-2487.62864193
TS3B	0.774017	0.694758	-2486.104425	-2486.183684	-2487.48135209
M3B	0.772517	0.686619	-2486.200636	-2486.286534	-2487.54531929
TS4B	0.567128	0.497771	-2215.143698	-2215.213055	-2216.25266503
M4B	0.546463	0.478173	-2138.841051	-2138.909341	-2139.87406709
M3C	0.789366	0.706480	-2486.602485	-2486.685371	-2487.98644090
TS4C	0.782253	0.700576	-2486.582271	-2486.663948	-2487.94837355
M4C	0.786272	0.705112	-2486.587266	-2486.668426	-2487.95770998
TS5C	0.782263	0.698657	-2486.585898	-2486.669504	-2487.94908729
M5C	0.789884	0.705207	-2486.621428	-2486.706104	-2487.99731375
TS2A'	0.772529	0.688867	-2486.120823	-2486.204485	-2487.46994126
M2A'	0.775953	0.692653	-2486.144983	-2486.228284	-2487.504041

Cartesian Coordinate for all stationary points

R1

C	-4.13891200	0.26480500	-0.70213700
C	-5.43211700	0.23118800	-0.57248300
C	-2.83458800	0.29784200	-0.83018700
H	-5.99473100	-0.66088800	-0.82899400
H	-5.97662800	1.09044400	-0.19369300
H	-2.36160800	0.62621000	-1.75005400
C	-1.95615700	-0.11948600	0.29343400
O	-2.32084000	-0.50633400	1.37609000
O	-0.66313700	-0.00664900	-0.06369100
C	0.27420600	-0.38679500	0.95766800
H	0.08297000	0.21511000	1.85109900
H	0.10277000	-1.43526500	1.22001000
C	1.65704200	-0.16480800	0.41571000
C	2.32753500	-1.18998300	-0.25146100
C	2.27328300	1.08022200	0.54599500
C	3.59705600	-0.97616900	-0.77943800
H	1.84979400	-2.16050300	-0.35619000
C	3.54224100	1.29824500	0.01924000
H	1.75261700	1.88090400	1.06460700
C	4.20587600	0.26889200	-0.64422400
H	4.11213400	-1.78085100	-1.29416400
H	4.01451300	2.26921000	0.12890900
H	5.19719600	0.43577200	-1.05340700

R2

C	3.09001700	0.88060900	-0.64074600
C	2.26305200	0.20025400	0.15723400
H	2.78198000	1.81006700	-1.10954600
H	2.58300300	-0.73054400	0.61609800
C	0.88089900	0.65911700	0.45563800
C	4.47663000	0.44022800	-0.94450700
O	5.22582000	1.06137300	-1.65875200
O	4.80520200	-0.71552500	-0.34523500
C	6.13997200	-1.17639800	-0.60385400
C	6.31226500	-2.48686600	0.13092500
H	6.84661300	-0.41401500	-0.26248800
H	6.27093900	-1.28629500	-1.68443500
H	7.31945100	-2.87662900	-0.03304400
H	6.16394900	-2.34848200	1.20413400
H	5.59195500	-3.22590300	-0.22690600
C	0.03948900	-0.30841700	1.22142700
C	-0.42224900	0.00903900	2.50054400

C	-0.24727100	-1.55574600	0.65936300
C	-1.17940800	-0.92215700	3.20659900
H	-0.20548900	0.98377800	2.92408900
C	-1.03076400	-2.46664500	1.35741300
H	0.12119200	-1.79570400	-0.33458300
C	-1.49243000	-2.15182900	2.63458600
H	-1.53218000	-0.67956800	4.20371000
H	-1.27691600	-3.42346900	0.90862900
H	-2.09404600	-2.86848000	3.18445600
N	0.55055400	1.82549900	0.03608200
S	-1.02443300	2.46362500	0.17400000
O	-1.27804600	2.79501200	1.56983000
O	-1.06856800	3.48279300	-0.85562200
C	-2.11511000	1.15107400	-0.30998800
C	-2.99990200	0.60440300	0.61869000
C	-2.05206200	0.67420900	-1.61263600
C	-3.81141500	-0.44810900	0.23803000
H	-3.02829500	1.00344200	1.62686200
C	-2.85931900	-0.39209500	-1.99682900
H	-1.37500900	1.13405800	-2.32642000
C	-3.73628300	-0.95801400	-1.06517700
H	-4.50955600	-0.90481300	0.93050300
H	-2.80412300	-0.76295300	-3.01258400
O	-4.55688400	-1.99990500	-1.33041400
C	-4.53852900	-2.53982300	-2.63610100
H	-3.54839800	-2.93711200	-2.88852000
H	-5.26523500	-3.35117600	-2.63784900
H	-4.82847300	-1.78968600	-3.38079400

TMEDA

N	-1.84940300	0.06315800	-0.32481700
C	-0.60065400	0.35644500	0.36492400
H	-0.41848200	1.43150000	0.26266500
H	-0.66817100	0.14562300	1.44994100
C	0.58395300	-0.41511200	-0.21094600
H	0.55040000	-0.35853500	-1.31603100
H	0.49164700	-1.47214900	0.05991900
C	-2.25278100	-1.32182400	-0.15068200
H	-3.21553000	-1.48358600	-0.64290400
H	-1.52827900	-1.99674500	-0.61213600
H	-2.35996600	-1.60096000	0.91513300
C	-2.90064700	0.94990200	0.14108100
H	-2.61224900	1.99015900	-0.03413800
H	-3.82243900	0.75290900	-0.41345900

H	-3.11518300	0.82831000	1.21950300
N	1.85296200	0.06178200	0.32647900
C	2.27368000	1.30333100	-0.30156400
H	3.19876800	1.65385900	0.16451400
H	2.45555000	1.18389900	-1.38609400
H	1.51979800	2.08182900	-0.16837200
C	2.89264900	-0.94077400	0.17006500
H	3.08654900	-1.19391800	-0.88910000
H	3.82603100	-0.57238800	0.60523700
H	2.60944900	-1.85619700	0.69641700

TS1A

C	2.63964600	-1.05600000	-0.76754100
C	3.88746300	-1.43023200	-0.99587300
C	1.37478900	-1.23276700	-1.28625800
H	4.04458400	-2.24263100	-1.69627600
H	4.76582200	-0.98242300	-0.54976000
C	0.32877500	-1.85383900	-0.54279100
O	0.36999800	-2.21930800	0.63222000
O	-0.81173300	-1.99432500	-1.28485200
C	-1.97171200	-2.42670300	-0.56755200
H	-2.61084300	-2.90169900	-1.31527400
H	-1.68069300	-3.15880200	0.18856200
C	-2.67333900	-1.24498700	0.05827100
C	-3.69624200	-0.58731800	-0.62648100
C	-2.24998200	-0.74290100	1.29337900
C	-4.28697900	0.55579300	-0.09329000
H	-4.02837600	-0.97268900	-1.58722000
C	-2.82867800	0.40797500	1.81964300
H	-1.44947800	-1.25484400	1.81832100
C	-3.84768100	1.05989200	1.12804300
H	-5.08513200	1.05589600	-0.63333300
H	-2.48548700	0.79695900	2.77325100
H	-4.29914900	1.95642200	1.54125000
N	2.71645000	0.12830200	0.74585800
C	1.46765200	0.91869400	0.77742200
H	0.63882500	0.21298200	0.71201000
H	1.39882800	1.42079600	1.75191000
C	1.38537300	1.96659000	-0.33079900
H	1.71420800	1.52989800	-1.29224400
H	2.06764100	2.79216900	-0.09853000
C	3.89135400	1.01461400	0.72044600
H	4.79342100	0.43218000	0.90891700
H	3.97582400	1.50308800	-0.25104000

H	3.80569100	1.77358200	1.50927300
C	2.78601900	-0.75559000	1.92565300
H	1.90638200	-1.39919400	1.92617000
H	3.68094500	-1.37548500	1.84227700
H	2.83977700	-0.15405100	2.84219700
N	0.03864800	2.51031800	-0.40372000
C	-0.85819300	1.63024900	-1.14122800
H	-1.88196400	2.00721500	-1.06818200
H	-0.57996800	1.55887800	-2.20924900
H	-0.84778900	0.62079200	-0.72789000
C	0.03727000	3.83287300	-1.00346200
H	0.41776500	3.83154800	-2.04191400
H	-0.98453800	4.22147600	-1.02056900
H	0.65295800	4.51562400	-0.41079300
H	1.16572800	-0.88701100	-2.29125600

M1A

C	2.60270500	-0.87903300	-0.78981200
C	3.61871300	-0.91812500	-1.68200600
C	1.28673300	-1.36382800	-1.05075700
H	3.43737900	-1.42572700	-2.61990600
H	4.58261700	-0.45201700	-1.56295400
C	0.19337000	-1.68211300	-0.23077700
O	0.02458400	-1.54569900	0.99878200
O	-0.83657400	-2.21529800	-0.97983600
C	-2.04019800	-2.44939500	-0.26308600
H	-2.61814400	-3.12057500	-0.90479600
H	-1.82812300	-2.94923900	0.68530600
C	-2.81133300	-1.17360500	-0.01810900
C	-3.31108900	-0.44771000	-1.10132600
C	-3.02267300	-0.69591000	1.27424600
C	-4.03241000	0.72405600	-0.89559000
H	-3.12735100	-0.80969200	-2.10983200
C	-3.74821700	0.47413200	1.48515100
H	-2.59170300	-1.23812500	2.11072300
C	-4.25887900	1.18316900	0.40116700
H	-4.42123800	1.27801800	-1.74477500
H	-3.90841700	0.83727000	2.49564700
H	-4.82483900	2.09521400	0.56502600
N	2.89566300	-0.24173600	0.56085500
C	1.83724400	0.78480900	0.91703100
H	0.91284700	0.22691100	1.05060500
H	2.13234800	1.20381800	1.88353500
C	1.69880900	1.88686300	-0.12786600

H	1. 77062700	1. 45900400	-1. 14410100
H	2. 50919300	2. 61715200	-0. 01516700
C	4. 22629900	0. 42905600	0. 61836900
H	5. 00861100	-0. 31518600	0. 48281700
H	4. 28728500	1. 18517400	-0. 16155800
H	4. 31735500	0. 88982900	1. 60223300
C	2. 90177900	-1. 33329100	1. 59520200
H	1. 89969000	-1. 76109600	1. 64331500
H	3. 64300700	-2. 06866800	1. 28095500
H	3. 18017900	-0. 88822600	2. 55328600
N	0. 44037600	2. 58504800	0. 08675200
C	-0. 70160300	1. 78891200	-0. 35747200
H	-1. 61988200	2. 35654300	-0. 18838900
H	-0. 63820200	1. 53167000	-1. 42977800
H	-0. 78797900	0. 85853500	0. 20973900
C	0. 45048100	3. 86591600	-0. 59947400
H	0. 56277900	3. 76255200	-1. 69460600
H	-0. 48882700	4. 38940400	-0. 40399400
H	1. 27144600	4. 48570700	-0. 22643200
H	1. 14461000	-1. 62687100	-2. 09106500

TS2A

C	0. 95958800	1. 62474600	0. 46546400
C	0. 15622900	1. 51387400	1. 54702200
C	1. 90976000	0. 59305900	0. 16110200
H	0. 32180300	0. 68455500	2. 22223400
H	-0. 64007900	2. 19959000	1. 79322000
C	3. 01873400	0. 52456500	-0. 75896100
O	3. 23189100	1. 15880700	-1. 79045500
O	3. 88323700	-0. 45212200	-0. 36999500
C	4. 89484900	-0. 77710600	-1. 33212100
H	4. 41387300	-1. 15363000	-2. 23915300
H	5. 44650300	0. 13355800	-1. 58760400
C	5. 79683200	-1. 80697700	-0. 71101900
C	6. 54392100	-1. 48635700	0. 42553200
C	5. 89309000	-3. 08977800	-1. 24710400
C	7. 36703100	-2. 43487800	1. 02054900
H	6. 46210000	-0. 48782900	0. 84799800
C	6. 72046200	-4. 04311300	-0. 65555600
H	5. 30415400	-3. 34305300	-2. 12522000
C	7. 45674200	-3. 71736600	0. 47956900
H	7. 94094100	-2. 17680700	1. 90493100
H	6. 78821100	-5. 03930100	-1. 08121200
H	8. 10195200	-4. 45842500	0. 94081100

N	0. 80670200	2. 82172200	-0. 44002900
C	2. 10157300	3. 61287500	-0. 48747000
H	2. 79669300	3. 00902900	-1. 06523000
H	1. 88073900	4. 51964500	-1. 05558200
C	2. 67768700	3. 97468500	0. 87851200
H	2. 62506800	3. 11455700	1. 56779400
H	2. 09925200	4. 78945700	1. 32742100
C	-0. 28943000	3. 73759900	0. 00604800
H	-1. 23931800	3. 20290900	0. 01711600
H	-0. 05790200	4. 12204900	0. 99826800
H	-0. 33401200	4. 55651400	-0. 71154800
C	0. 46988300	2. 38799700	-1. 84772200
H	1. 27970300	1. 76063900	-2. 21346100
H	-0. 48332900	1. 85987800	-1. 82195100
H	0. 39354700	3. 29366300	-2. 45200200
N	4. 04646000	4. 44078700	0. 69464300
C	4. 96285600	3. 32784200	0. 47152400
H	5. 97191100	3. 72074200	0. 32343600
H	4. 98204200	2. 62786400	1. 32755800
H	4. 69073100	2. 76330500	-0. 42361300
C	4. 48110800	5. 21878100	1. 84351100
H	4. 47707500	4. 63328800	2. 78097100
H	5. 49828300	5. 58080800	1. 67345800
H	3. 82831700	6. 08609100	1. 97496800
C	0. 41505600	-1. 01254500	-0. 71819400
C	-0. 59110800	-1. 11331100	0. 21154700
H	0. 24973700	-0. 46644300	-1. 64104000
H	-0. 48218600	-1. 79753300	1. 04554500
C	-1. 79358500	-0. 34200200	0. 14640000
C	1. 51663700	-2. 00659900	-0. 79443300
O	2. 13864000	-2. 23330100	-1. 80821200
O	1. 74006200	-2. 60160300	0. 38834600
C	2. 84471200	-3. 51554800	0. 47350100
C	3. 67327800	-3. 15798900	1. 68896600
H	3. 42971200	-3. 44635500	-0. 44314900
H	2. 42538100	-4. 52404800	0. 54876800
H	4. 56294600	-3. 79421300	1. 72954500
H	4. 00146600	-2. 11909300	1. 61238500
H	3. 09998700	-3. 28681200	2. 61066500
C	-2. 84070400	-0. 70067500	1. 16152700
C	-3. 17008800	0. 12526300	2. 23677900
C	-3. 49937900	-1. 92377700	1. 00114400
C	-4. 15594700	-0. 27113700	3. 13772700
H	-2. 67703600	1. 08431800	2. 34664700

C	-4.49969100	-2.30361800	1.88822500
H	-3.23998300	-2.55994700	0.15977000
C	-4.82627100	-1.47854600	2.96228300
H	-4.40593300	0.37198700	3.97570400
H	-5.02070200	-3.24460600	1.74090700
H	-5.60093700	-1.77729100	3.66201300
N	-1.96028900	0.52169900	-0.83154800
S	-3.26681700	1.51945800	-0.94922500
O	-3.33481300	2.39649300	0.23055500
O	-3.14330200	2.14373500	-2.26069400
C	-4.71382000	0.49412900	-0.93965000
C	-4.86754700	-0.47419300	-1.93434900
C	-5.63219700	0.61472700	0.09084600
C	-5.93920000	-1.34498900	-1.86931700
H	-4.14254400	-0.54439900	-2.73956200
C	-6.71716700	-0.25505400	0.15615900
H	-5.47708900	1.37080400	0.85283000
C	-6.86046400	-1.24643400	-0.81643900
H	-6.09073600	-2.11688400	-2.61534800
H	-7.42048300	-0.16345100	0.97416400
O	-7.85665100	-2.16506500	-0.82550500
C	-8.78722200	-2.12797300	0.23529400
H	-9.33799500	-1.18020900	0.25048400
H	-9.48284600	-2.94736800	0.05808000
H	-8.29088200	-2.27152700	1.20292300
H	2.04107600	-0.08342000	0.99749000

M2A

C	0.76716800	1.52424000	0.49117800
C	0.10175000	1.38735800	1.63434800
C	1.56186600	0.33583500	-0.01790300
H	0.19928800	0.44875100	2.16599000
H	-0.60675800	2.09802300	2.03164900
C	2.86939000	0.54862500	-0.76619600
O	3.05472700	1.22433700	-1.75401700
O	3.82006200	-0.24297400	-0.25283600
C	5.01409000	-0.36484700	-1.04910800
H	4.72560300	-0.69691700	-2.05163300
H	5.47615300	0.62480300	-1.13555900
C	5.91384800	-1.35226400	-0.36109200
C	6.22292500	-1.19338200	0.99217700
C	6.44264000	-2.43558000	-1.05985800
C	7.03977700	-2.11354000	1.63871000
H	5.80095900	-0.35442900	1.53932100

C	7.26795100	-3.35491700	-0.41499100
H	6.20028100	-2.56527100	-2.11165700
C	7.56312300	-3.19757100	0.93534300
H	7.26801000	-1.98771700	2.69220800
H	7.67274700	-4.19709300	-0.96702000
H	8.19928600	-3.91709600	1.44051800
N	0.67200200	2.80568100	-0.28789000
C	2.00354700	3.54873300	-0.31344100
H	2.55930100	3.16928400	-1.16463300
H	1.76608000	4.59863200	-0.49262100
C	2.81839400	3.43040500	0.97125100
H	3.02906700	2.37359200	1.21737600
H	2.24688500	3.83833900	1.81247400
C	-0.34319300	3.74133500	0.31338900
H	-1.31107000	3.24941700	0.39164500
H	0.01782500	4.06920100	1.28825600
H	-0.41964300	4.59246700	-0.36133200
C	0.24532900	2.54326400	-1.71631800
H	1.00638700	1.92547000	-2.18730100
H	-0.73382500	2.06067500	-1.70233400
H	0.19465200	3.51421000	-2.21181300
N	4.04675800	4.19419400	0.81580700
C	5.03755900	3.44381600	0.05611300
H	5.92243100	4.06471300	-0.10370400
H	5.34932000	2.52256000	0.58639600
H	4.64653000	3.15186200	-0.92170100
C	4.59405300	4.57662200	2.10838500
H	4.85415100	3.70411800	2.73437700
H	5.50039200	5.16807400	1.95614600
H	3.87259500	5.19173400	2.65214400
C	0.67819700	-0.69118500	-0.86500400
C	-0.44981500	-1.27686700	-0.07223600
H	0.29967600	-0.17873000	-1.75145200
H	-0.25620900	-2.18699500	0.48394700
C	-1.70339900	-0.76793900	-0.10442300
C	1.64738300	-1.76072900	-1.34609000
O	2.13321200	-1.79845000	-2.45199500
O	1.98477700	-2.60157700	-0.35785400
C	3.03230000	-3.53792600	-0.65038300
C	3.65711500	-3.95119500	0.66271100
H	3.76090500	-3.05583000	-1.30717800
H	2.59799300	-4.38451800	-1.19177000
H	4.46517700	-4.66457500	0.48105200
H	4.08090200	-3.07683600	1.16402400

H	2.91790800	-4.41525300	1.31982900
C	-2.78627400	-1.49989100	0.62967400
C	-2.84564900	-1.51628800	2.02172700
C	-3.77497100	-2.16353800	-0.10483900
C	-3.87897500	-2.18778000	2.67450100
H	-2.09239100	-0.97585200	2.58700500
C	-4.80177500	-2.83739400	0.54408300
H	-3.73662000	-2.12600500	-1.18964200
C	-4.85581800	-2.85004100	1.93798500
H	-3.92188400	-2.18853400	3.75953700
H	-5.56751700	-3.34372700	-0.03635500
H	-5.66164100	-3.37073300	2.44705700
N	-2.01469100	0.32581200	-0.89173900
S	-3.02710700	1.41834500	-0.32306000
O	-2.80269900	1.71988900	1.11215600
O	-2.94825300	2.57368300	-1.23339500
C	-4.70678700	0.81964100	-0.41009800
C	-5.25249200	0.50449100	-1.65581000
C	-5.41890600	0.58483000	0.75462600
C	-6.50764300	-0.07181800	-1.72440400
H	-4.68047100	0.70285900	-2.55730600
C	-6.68622000	0.00814400	0.69325500
H	-4.96237500	0.82677400	1.70846000
C	-7.22228000	-0.33501100	-0.54752700
H	-6.96197400	-0.33982000	-2.67206500
H	-7.22307400	-0.19171800	1.61238700
O	-8.43092500	-0.93466400	-0.71901100
C	-9.13250200	-1.31702200	0.44221100
H	-9.41618900	-0.44668800	1.04603700
H	-10.03338000	-1.82681600	0.10109200
H	-8.53582700	-2.00072200	1.05921000
H	1.83814900	-0.22263600	0.87858500

TS3A

C	2.60930200	-1.63784700	-0.81570300
C	2.17230900	-2.82521500	-0.40118500
C	1.81334400	-0.39953800	-0.60484000
H	1.20431800	-2.90426700	0.08665000
H	2.72044800	-3.75343800	-0.51547600
C	1.73075900	0.56412400	-1.70915800
O	1.88695500	0.31753400	-2.89383800
O	1.35119000	1.77424400	-1.26363600
C	0.94853800	2.75170000	-2.22481000
H	1.83531500	3.22093100	-2.66528100

H	0.40031400	2.24703200	-3.02641200
C	0.09192900	3.75350200	-1.49666800
C	0.24882300	5.12250700	-1.69973800
C	-0.89288000	3.29611700	-0.61656300
C	-0.58257700	6.02960900	-1.04355900
H	1.02194300	5.48331000	-2.37377600
C	-1.72066400	4.19907200	0.03949800
H	-0.99086100	2.22979400	-0.43581200
C	-1.56902700	5.56949200	-0.17618600
H	-0.45425000	7.09500100	-1.20723900
H	-2.48182500	3.82549700	0.71842700
H	-2.21432100	6.27624000	0.33607300
N	3.96959000	-1.62213500	-1.53556500
C	5.00068100	-2.36100800	-0.71384000
H	4.63068900	-3.36675900	-0.53141500
H	5.89555500	-2.44518800	-1.33624800
C	5.31994000	-1.64887200	0.60177200
H	4.42438600	-1.13504800	0.99435100
H	6.06435600	-0.86785800	0.42195000
C	4.53411000	-0.25008700	-1.79312500
H	4.00441900	0.19559900	-2.62868600
H	4.42275000	0.35844500	-0.89509600
H	5.58770400	-0.38603900	-2.04386600
C	3.78937800	-2.30094600	-2.86168000
H	3.50587300	-3.33842400	-2.69160900
H	2.99464500	-1.76964300	-3.38606900
H	4.73329300	-2.24393300	-3.40769900
N	5.86944100	-2.61307100	1.54222900
C	4.80791900	-3.33950600	2.22571100
H	5.24390100	-4.10876500	2.86767500
H	4.18169200	-2.67472100	2.84667000
H	4.14964500	-3.83628900	1.50777700
C	6.73804900	-1.96528200	2.51444900
H	6.20781600	-1.21150800	3.12220000
H	7.15105900	-2.71928400	3.18919400
H	7.56889500	-1.47443500	2.00133500
C	1.70781100	0.14860100	0.84699400
C	0.28558300	0.37062900	1.30778100
H	2.17915700	-0.60508000	1.49581800
H	0.15781300	1.06215000	2.13284000
C	-0.82653300	-0.15103600	0.75657100
C	2.57858300	1.39367300	1.00228100
O	3.76636700	1.40889200	0.73753100
O	1.92476200	2.46331800	1.43801700

C	2. 62837300	3. 71055600	1. 35192700
C	1. 68058200	4. 78890500	1. 82502100
H	2. 92180000	3. 85581900	0. 30594300
H	3. 53972900	3. 65234100	1. 95423000
H	2. 16140000	5. 76721000	1. 74652000
H	0. 77597900	4. 79170200	1. 21238900
H	1. 39848500	4. 62206600	2. 86734700
C	-2. 15995400	0. 23107600	1. 30723400
C	-3. 16830000	0. 66429700	0. 43663500
C	-2. 42785900	0. 16552200	2. 67532800
C	-4. 41442700	1. 03107000	0. 92849200
H	-2. 96370900	0. 68106000	-0. 63005800
C	-3. 67950700	0. 52940100	3. 16795800
H	-1. 65535800	-0. 20063600	3. 34524700
C	-4. 67443300	0. 96384000	2. 29772100
H	-5. 19093400	1. 35600000	0. 24194700
H	-3. 88025400	0. 46185000	4. 23288800
H	-5. 65294300	1. 23698400	2. 68027300
N	-0. 78828700	-0. 90201600	-0. 43525100
S	-1. 34777000	-2. 42454400	-0. 40992000
O	-0. 98527200	-3. 02062600	-1. 69606900
O	-0. 93121500	-3. 12360200	0. 81933900
C	-3. 12562200	-2. 34829300	-0. 34239000
C	-3. 78217500	-2. 52853600	0. 87470800
C	-3. 83027700	-2. 00420900	-1. 48649400
C	-5. 15024200	-2. 33623600	0. 94579600
H	-3. 20346600	-2. 79789600	1. 75159800
C	-5. 20826300	-1. 80999500	-1. 42279100
H	-3. 29607500	-1. 88387500	-2. 42408500
C	-5. 86509000	-1. 96495200	-0. 19906600
H	-5. 69227200	-2. 44816200	1. 87826100
H	-5. 75126700	-1. 54160700	-2. 32058900
O	-7. 19965100	-1. 77889500	-0. 02139400
C	-7. 95430000	-1. 36386100	-1. 13731700
H	-7. 92678300	-2. 10980700	-1. 94084100
H	-8. 97967100	-1. 25012100	-0. 78636900
H	-7. 59436600	-0. 40414500	-1. 52822100
H	0. 62569400	-0. 80540700	-0. 72810100

M3A

C	1. 36292600	2. 25016300	1. 22447700
C	0. 42075200	3. 00142300	1. 80907800
C	1. 38379500	0. 82033000	1. 13325600
H	-0. 29525700	2. 49733100	2. 44891600

H	0.31387700	4.07549400	1.70413500
C	2.47143800	0.11905200	1.67536800
O	3.48495200	0.59695200	2.20296200
O	2.33925600	-1.25346600	1.55772200
C	3.45944300	-1.99846000	2.00222300
H	3.78693800	-1.63149200	2.97924300
H	3.09135700	-3.02389000	2.11133500
C	4.62294500	-1.96361800	1.03550000
C	4.47138000	-1.51122500	-0.27489000
C	5.87126200	-2.42475800	1.45599200
C	5.55842000	-1.51788000	-1.14738600
H	3.50351300	-1.15170800	-0.61371000
C	6.95377700	-2.43658700	0.58318000
H	5.99769900	-2.77043800	2.47946300
C	6.80080700	-1.98040300	-0.72433400
H	5.42870800	-1.16134300	-2.16501100
H	7.91959400	-2.79514800	0.92577400
H	7.64557500	-1.98497200	-1.40586300
N	2.50168900	3.03594900	0.48083900
C	1.92465600	4.13080000	-0.37659500
H	1.45755400	4.85358500	0.28998100
H	2.76518500	4.63279900	-0.86293400
C	0.93603000	3.63613000	-1.43148000
H	0.22546100	2.91140400	-0.99267700
H	1.48434700	3.11525200	-2.22275100
C	3.31827200	2.12962300	-0.39637700
H	3.92702900	1.49258900	0.24278000
H	2.65442300	1.50749500	-0.99688000
H	3.94754100	2.76866200	-1.01889600
C	3.40296000	3.63540500	1.51433400
H	2.82452100	4.34465900	2.10591600
H	3.75904200	2.81309600	2.13688600
H	4.22634400	4.14305000	1.00653800
N	0.24843500	4.77340200	-2.02235200
C	-0.79954100	5.28433500	-1.14044800
H	-1.27658800	6.14347800	-1.61864600
H	-1.57170700	4.52612500	-0.93017200
H	-0.37923700	5.63575300	-0.19390300
C	-0.34774600	4.39174500	-3.29752300
H	-1.11606500	3.60769400	-3.18203000
H	-0.82124500	5.26647500	-3.75053900
H	0.42940300	4.03342500	-3.97813100
C	0.20169200	0.13772800	0.47242700
C	-0.85819200	-0.38480600	1.40013900

H	-0.24923300	0.88114900	-0.19576800
H	-0.58287400	-1.23669300	2.01403700
C	-2.08581900	0.14498200	1.52809100
C	0.69703500	-0.90983800	-0.52063500
O	1.43944300	-0.64256800	-1.44258300
O	0.21023300	-2.12957000	-0.29970600
C	0.73497900	-3.16855000	-1.13675900
C	0.01651600	-4.43939300	-0.74401100
H	1.81704900	-3.22976400	-0.97608100
H	0.55938500	-2.90962800	-2.18417000
H	0.30364000	-5.25988900	-1.40628700
H	0.25238200	-4.71736600	0.28592500
H	-1.06431200	-4.28596800	-0.81670400
C	-3.16892700	-0.46522700	2.33201000
C	-4.18913000	0.32142700	2.87677300
C	-3.19640300	-1.85079900	2.53622500
C	-5.19022000	-0.26155600	3.64534200
H	-4.19288700	1.38768100	2.67943100
C	-4.19498300	-2.42939900	3.31060600
H	-2.44274500	-2.47189400	2.05964800
C	-5.19270000	-1.63545900	3.87202500
H	-5.97456600	0.36018500	4.06492500
H	-4.20411900	-3.50406400	3.46333700
H	-5.97734400	-2.08854900	4.46967700
N	-2.41714400	1.37941500	0.87804100
S	-3.36397800	1.35648800	-0.51405000
O	-4.75227200	1.19671400	-0.12482800
O	-2.91105800	2.52592500	-1.26447100
C	-2.89047100	-0.10433600	-1.40151500
C	-1.82451600	-0.05234200	-2.30100400
C	-3.56511500	-1.29296100	-1.15326300
C	-1.43900100	-1.20462800	-2.96143400
H	-1.31479300	0.88922400	-2.48507200
C	-3.18304100	-2.45365300	-1.81990900
H	-4.39001500	-1.30338800	-0.44718700
C	-2.11849600	-2.40730700	-2.72442400
H	-0.61157500	-1.20253800	-3.66229700
H	-3.71469100	-3.37761200	-1.62779800
O	-1.66108600	-3.48032000	-3.41463500
C	-2.42837300	-4.66836100	-3.37806400
H	-3.45795900	-4.48057200	-3.70304800
H	-1.94693200	-5.35914100	-4.06916000
H	-2.43858900	-5.11149400	-2.37580100
H	-1.61925400	1.98685500	0.70502700

TS4A

C	1.28113400	-2.06500000	-1.00438000
C	0.04960100	-2.72715000	-1.36466300
C	1.38647100	-0.70015600	-0.98847000
H	-0.17484100	-2.52624500	-2.41687600
H	-0.06657300	-3.78085600	-1.13186200
C	2.55833300	0.01530600	-1.51316800
O	3.52464100	-0.49284700	-2.05780600
O	2.41079200	1.35151400	-1.44203100
C	3.51326300	2.11946500	-1.93055800
H	3.77875200	1.77883100	-2.93512500
H	3.12224800	3.13852100	-1.98664400
C	4.71236700	2.04366700	-1.01488600
C	4.55612200	1.82531700	0.35491800
C	5.99016100	2.22496400	-1.54214600
C	5.67593500	1.79087600	1.18295800
H	3.56271400	1.67430500	0.77166000
C	7.10551700	2.19984500	-0.71063000
H	6.11448400	2.37878400	-2.61118300
C	6.95065600	1.98066200	0.65564500
H	5.54815300	1.61950800	2.24738400
H	8.09583300	2.34062000	-1.13209300
H	7.81992600	1.95595700	1.30494900
N	2.47092300	-2.94455100	-0.58996400
C	1.94299800	-4.08534500	0.26870900
H	1.38642000	-4.74910200	-0.38748100
H	2.82155800	-4.63007600	0.62005700
C	1.09702200	-3.62562900	1.45587600
H	0.29767400	-2.93265600	1.13962100
H	1.74055100	-3.09154900	2.16385600
C	3.49282400	-2.20933800	0.24040100
H	4.14249800	-1.63530700	-0.41139900
H	2.96698900	-1.53689000	0.91912900
H	4.06633500	-2.95307700	0.79325800
C	3.12006500	-3.53373900	-1.80559600
H	2.35047500	-4.05642000	-2.37424200
H	3.54359100	-2.71454000	-2.38396300
H	3.89294000	-4.23236000	-1.47850300
N	0.55228700	-4.79446300	2.13257800
C	-0.55229500	-5.38330400	1.36834500
H	-0.95812500	-6.22424000	1.93627800
H	-1.35687100	-4.65695800	1.17539400
H	-0.19526800	-5.78985400	0.41688600

C	0.05275000	-4.39554800	3.44620200
H	-0.75785800	-3.65136300	3.37216200
H	-0.33265800	-5.27584300	3.96669600
H	0.86979700	-3.97784600	4.04175900
C	0.16099800	0.07759200	-0.51628700
C	-0.88774500	0.46685500	-1.51436000
H	-0.32853500	-0.59978700	0.18897200
H	-0.69396200	1.30483200	-2.17533800
C	-2.07357200	-0.18453900	-1.53830800
C	0.63410600	1.18508800	0.41697500
O	1.44714700	0.99514800	1.29846500
O	0.03587800	2.35116800	0.19859000
C	0.42985100	3.42530600	1.06524200
C	-0.40673800	4.62315600	0.67674500
H	1.50341300	3.60297100	0.93632200
H	0.25525400	3.12835100	2.10232500
H	-0.23114100	5.44774000	1.37199500
H	-0.16857800	4.95634900	-0.33619100
H	-1.46582200	4.35345000	0.70789100
C	-3.22482200	0.28742200	-2.35071300
C	-4.21425500	-0.61188600	-2.76092200
C	-3.36100400	1.64202600	-2.68002000
C	-5.29006500	-0.17166300	-3.52440900
H	-4.13171800	-1.64882600	-2.45398200
C	-4.43557000	2.07912600	-3.44554700
H	-2.63498100	2.35544200	-2.30020500
C	-5.40051700	1.17103900	-3.87692500
H	-6.05040900	-0.87956000	-3.83926400
H	-4.53063400	3.13240000	-3.69168200
H	-6.24451100	1.51180000	-4.46867900
N	-2.19354000	-1.38960500	-0.82518600
S	-3.06930300	-1.52105600	0.51730100
O	-4.50761400	-1.60716100	0.27084600
O	-2.43375400	-2.58993300	1.30725500
C	-2.81401300	0.01015400	1.40814000
C	-1.78333500	0.11391000	2.34151600
C	-3.60707900	1.10892000	1.10434500
C	-1.54618500	1.32586700	2.96977400
H	-1.18546100	-0.76212200	2.57672800
C	-3.37436400	2.33137000	1.73137000
H	-4.41003000	1.00190300	0.38053800
C	-2.33884100	2.43788000	2.66203100
H	-0.75630500	1.43839700	3.70479500
H	-3.99808800	3.18338000	1.48806300

O	-2.01216900	3.58975300	3.31164200
C	-2.92609600	4.66416900	3.23632000
H	-3.92648500	4.35387100	3.55920600
H	-2.54682500	5.43224800	3.91007000
H	-2.98733400	5.07616100	2.22203100
H	-1.00688100	-2.14436900	-0.91893800

M4A

C	1.62821600	0.47562900	1.62324200
C	0.74152800	1.53201800	2.22515400
C	1.17116100	-0.48389200	0.80577300
H	1.01118400	1.71156200	3.27092000
H	0.78287400	2.49087600	1.69891400
C	1.84648300	-1.79086700	0.54386200
O	2.47694500	-2.41953100	1.36700900
O	1.62710600	-2.22788300	-0.69930200
C	2.42350400	-3.35434800	-1.09851200
H	2.33916800	-4.14933500	-0.35446900
H	1.97661100	-3.68042200	-2.03929700
C	3.85548200	-2.91214200	-1.27764200
C	4.12119300	-1.71803400	-1.95515100
C	4.90924600	-3.65572700	-0.75206800
C	5.43406100	-1.28228100	-2.10867300
H	3.29297900	-1.11963700	-2.33128000
C	6.22353100	-3.22158700	-0.91260200
H	4.69911900	-4.57020100	-0.20424200
C	6.48747400	-2.03464300	-1.59011900
H	5.63579200	-0.35600800	-2.63787900
H	7.03939400	-3.80604500	-0.49955800
H	7.51091300	-1.69518700	-1.71389300
N	3.09069200	0.55407400	2.04112500
C	3.49393200	2.01531100	2.15829400
H	2.85043100	2.48206400	2.89920500
H	4.51330000	2.01677600	2.55012200
C	3.44188300	2.75958500	0.82280300
H	2.52296300	2.50882100	0.26007000
H	4.28345200	2.43741200	0.20267300
C	4.05539800	-0.05114800	1.04619200
H	4.14275600	-1.11978100	1.20722600
H	3.68165700	0.15104000	0.04139300
H	5.02530800	0.42341700	1.19641600
C	3.26024700	-0.11417000	3.37490500
H	2.60691400	0.37684700	4.09614500
H	2.98240600	-1.16013100	3.25072900

H	4.30335800	-0.01406000	3.68060500
N	3.59436300	4.18330900	1.07540200
C	2.34790500	4.80387600	1.50672100
H	2.52547900	5.86243000	1.70957000
H	1.55326600	4.72351700	0.74383900
H	1.97864000	4.35286700	2.43144600
C	4.10765300	4.86806900	-0.10368200
H	3.42528500	4.79497100	-0.96787900
H	4.25347100	5.92568500	0.12867800
H	5.07510800	4.44562800	-0.38772000
C	-0.13358800	-0.29954300	0.05721500
C	-1.16969300	-1.36597300	0.25192900
H	-0.58953300	0.62934800	0.40777100
H	-1.13177600	-2.26518100	-0.35182500
C	-2.14428700	-1.14987500	1.16859100
C	0.24390200	0.02609900	-1.38327600
O	1.27841100	0.57776400	-1.70740300
O	-0.72526400	-0.29232600	-2.23094700
C	-0.56291100	0.14322500	-3.58907600
C	-1.66624900	-0.51720200	-4.38397000
H	0.43550600	-0.13543700	-3.93844000
H	-0.64828200	1.23395900	-3.61423300
H	-1.68883800	-0.12166600	-5.40250200
H	-1.52238400	-1.59940700	-4.42665800
H	-2.62652500	-0.31672500	-3.90293900
C	-3.28510100	-2.10121500	1.29261600
C	-3.90481100	-2.29365500	2.53126800
C	-3.75508000	-2.81266500	0.18302700
C	-4.94303000	-3.20790600	2.66357900
H	-3.56782400	-1.70011500	3.37401900
C	-4.79602900	-3.72614800	0.31558500
H	-3.31646400	-2.61851400	-0.79211800
C	-5.38781100	-3.93218900	1.55937000
H	-5.41480100	-3.34905700	3.63111000
H	-5.15457900	-4.26776000	-0.55486900
H	-6.20292600	-4.64178800	1.66435000
N	-2.02330200	-0.06151500	2.02752100
S	-3.13340300	1.08404100	1.98380900
O	-4.49806100	0.67373500	2.33237100
O	-2.56638500	2.24737400	2.68169400
C	-3.21502200	1.54113000	0.24177300
C	-2.27658300	2.43164000	-0.28177400
C	-4.12373300	0.91504300	-0.59929700
C	-2.23979100	2.68396700	-1.64426500

H	-1.59687500	2.93497800	0.40159900
C	-4.10730200	1.17437600	-1.97095400
H	-4.85126400	0.23086700	-0.17189100
C	-3.15676000	2.05223100	-2.49181600
H	-1.53172000	3.38295400	-2.07828200
H	-4.82941600	0.68733000	-2.61676600
O	-3.03698300	2.34989100	-3.82099600
C	-4.12714100	2.02393800	-4.65676700
H	-5.06341100	2.43357300	-4.26045100
H	-3.91319100	2.47255300	-5.62719400
H	-4.23717300	0.93998800	-4.78287600
H	-0.29159800	1.16351000	2.24824400

TS5A

C	0.14418600	-1.95335800	0.66312100
C	0.54284900	-2.08648500	2.11744200
C	-1.15632700	-1.59681700	0.29167200
H	0.03111500	-1.29474100	2.66375800
H	0.22299700	-3.02824600	2.56827600
C	-2.19674200	-1.61360300	1.29310100
O	-2.22300000	-2.26144500	2.32856300
O	-3.26964800	-0.85565800	0.91624700
C	-4.43525900	-0.99109600	1.72464200
H	-4.71950400	-2.04572400	1.79279900
H	-4.21177100	-0.64363200	2.73930900
C	-5.51355600	-0.16573400	1.07727500
C	-6.69286600	-0.75016600	0.62102200
C	-5.32069000	1.20756400	0.90098700
C	-7.67089500	0.02330000	-0.00355600
H	-6.84206600	-1.81930300	0.74484000
C	-6.29594700	1.98184200	0.28414800
H	-4.39457500	1.66013300	1.24521400
C	-7.47297300	1.38946600	-0.17477200
H	-8.58396200	-0.44349400	-0.35938000
H	-6.13983600	3.04885600	0.15644700
H	-8.23255300	1.99352000	-0.66106200
N	0.78640900	-3.11723200	-0.19656700
C	2.16965700	-3.50384100	0.29745600
H	2.67745900	-2.60782900	0.63251400
H	2.02177600	-4.14705500	1.16692200
C	3.05238700	-4.23575200	-0.70823300
H	3.25241500	-3.59587100	-1.58267500
H	2.55525200	-5.15063600	-1.05554300
C	0.74058500	-2.86491200	-1.67277000

H	-0.30269500	-2.70852500	-1.94177500
H	1.37206100	-2.01250800	-1.91198200
H	1.09816100	-3.76317300	-2.17521500
C	-0.12024100	-4.29690700	0.04033400
H	-0.26173800	-4.43569900	1.11071900
H	-1.08139900	-4.08883400	-0.42518600
H	0.35585000	-5.17614900	-0.39745500
N	4.28360300	-4.62289000	-0.03275000
C	5.18900200	-3.48558300	0.11994500
H	6.07820800	-3.81496900	0.66406100
H	5.50114300	-3.07189800	-0.85445300
H	4.72458200	-2.67600600	0.68726400
C	4.95084400	-5.69122000	-0.75882900
H	5.23649800	-5.39720500	-1.78520400
H	5.85981300	-5.97793800	-0.22380200
H	4.29988500	-6.56831900	-0.81777600
C	-1.32569400	-0.62294800	-0.88151900
C	-0.94834400	0.67027100	-0.23818600
H	-0.57827900	-0.83272200	-1.64821700
H	-1.70569900	1.39403600	0.04175200
C	0.31309500	0.74522800	0.25095400
C	-2.65747400	-0.75575000	-1.58292000
O	-3.07293500	-1.81504700	-1.99344400
O	-3.27187500	0.41623400	-1.77075500
C	-4.55045400	0.36051100	-2.42130900
C	-4.87378800	1.75952700	-2.89709400
H	-5.28583600	-0.00449900	-1.69618700
H	-4.49774600	-0.35495200	-3.24589300
H	-5.87358600	1.78130800	-3.33844000
H	-4.85229300	2.45946200	-2.05922000
H	-4.15130200	2.09031400	-3.64736100
C	0.71689900	1.86056200	1.14700600
C	1.35026000	1.61858500	2.37160400
C	0.45701600	3.18054100	0.76617400
C	1.71389500	2.67913500	3.19487000
H	1.57746000	0.59805600	2.66366200
C	0.82117400	4.23953200	1.59216200
H	-0.00486500	3.36625700	-0.19926300
C	1.45415500	3.99244100	2.80788200
H	2.20205200	2.47852100	4.14362500
H	0.62041300	5.26000000	1.27907500
H	1.74285300	4.81813300	3.45082900
N	1.11986400	-0.38387600	0.02259300
S	2.76108900	-0.24508500	-0.06841700

O	3.41468300	-0.49490000	1.22588200
O	3.19545500	-1.11711000	-1.17160800
C	3.09049900	1.42784900	-0.54981500
C	2.62384300	1.89013100	-1.78118600
C	3.76429800	2.26210700	0.32783100
C	2.81894700	3.21547100	-2.11911200
H	2.10098600	1.21508800	-2.45188400
C	3.96669500	3.59650400	-0.01081100
H	4.09903500	1.87072600	1.28236000
C	3.48002000	4.07585500	-1.22938800
H	2.46499600	3.62095600	-3.06015400
H	4.47734100	4.24811900	0.68666300
O	3.59485700	5.35979400	-1.64143600
C	4.20498700	6.27962000	-0.75979900
H	5.24755800	6.00803800	-0.55784900
H	4.17396400	7.24579700	-1.26199600
H	3.65702900	6.34134800	0.18800200
H	1.61768800	-1.95557000	2.24202800

M5A

C	0.06535900	-0.55543300	1.64206000
C	0.01500200	-1.46160800	2.84405800
C	-0.98213100	-0.15046700	0.89353100
H	0.94940600	-1.39610900	3.40344300
H	-0.81831800	-1.18513800	3.48997100
C	-2.34829600	-0.57420300	1.27634000
O	-2.62750400	-1.49538100	2.01476500
O	-3.29593000	0.21116000	0.73258900
C	-4.64759900	-0.09946300	1.10268000
H	-4.88973400	-1.11102600	0.76560300
H	-4.72772300	-0.07823100	2.19346500
C	-5.52266500	0.93226400	0.45217000
C	-6.00865100	0.73239800	-0.84053800
C	-5.79669500	2.13292100	1.10790900
C	-6.75421100	1.72333700	-1.47254600
H	-5.78820300	-0.19877400	-1.35521000
C	-6.54207400	3.12613700	0.47898800
H	-5.41366500	2.29029300	2.11301600
C	-7.01813000	2.92312000	-0.81430000
H	-7.12537400	1.56239300	-2.47942500
H	-6.74749100	4.05867600	0.99533200
H	-7.59779400	3.69699900	-1.30750900
N	-1.76041500	-2.21358900	-1.22392800
C	-1.06691600	-3.20745200	-0.41092700

H	-0.02617700	-2.87217500	-0.30478300
H	-1.51387600	-3.19534000	0.59117200
C	-1.11552500	-4.64565700	-0.94093200
H	-0.48415100	-4.74083600	-1.84880700
H	-2.14491400	-4.87750600	-1.24349700
C	-1.22912400	-2.08505000	-2.56904700
H	-1.63563500	-1.17702300	-3.02391500
H	-0.13675800	-1.99783100	-2.52439900
H	-1.46941700	-2.94618800	-3.21720800
C	-3.20336400	-2.36035800	-1.24728600
H	-3.55878100	-2.54468600	-0.22839800
H	-3.64081200	-1.42591600	-1.61894300
H	-3.55589800	-3.18782200	-1.88861200
N	-0.72677300	-5.61820100	0.07012400
C	0.65811900	-5.44424800	0.47949700
H	0.91314600	-6.20740000	1.22035900
H	1.36203000	-5.54016900	-0.37001500
H	0.81479300	-4.46508700	0.93517500
C	-0.93890900	-6.96691900	-0.41912700
H	-0.32462500	-7.20077500	-1.30992400
H	-0.68724600	-7.68769000	0.36442400
H	-1.99103700	-7.10504700	-0.68549100
C	-0.68553400	0.64509000	-0.37706000
C	0.42465500	1.62253400	-0.08344700
H	-0.35389600	-0.09120100	-1.12220200
H	0.36905300	2.64091300	-0.44930800
C	1.44378800	1.24181100	0.69134600
C	-1.86956900	1.33467900	-1.04324900
O	-2.45401100	0.90416900	-2.00792800
O	-2.13565700	2.51982200	-0.48353000
C	-3.23085900	3.24390900	-1.06529700
C	-3.43123800	4.49321000	-0.23831200
H	-4.11661200	2.60423700	-1.06421000
H	-2.98459500	3.47279500	-2.10729100
H	-4.27026900	5.06897000	-0.63754500
H	-3.65885600	4.22751600	0.79676400
H	-2.53568300	5.11934800	-0.25045600
C	2.61111300	2.09479900	1.00675200
C	3.17855700	2.09628400	2.28508500
C	3.16927800	2.89718600	0.00637600
C	4.28637400	2.89282500	2.55446100
H	2.75935900	1.45678200	3.05507900
C	4.27150800	3.69822500	0.28220400
H	2.75600000	2.85475400	-0.99722800

C	4. 83584200	3. 69440700	1. 55600500
H	4. 72114100	2. 88739500	3. 54886400
H	4. 70045700	4. 31364400	-0. 50282600
H	5. 70265300	4. 31147200	1. 77072200
N	1. 34975500	-0. 02675500	1. 33221400
S	2. 66147200	-1. 14045400	1. 31423700
O	3. 41865200	-1. 02201400	2. 55003000
O	2. 07283700	-2. 42217200	0. 95080200
C	3. 65627800	-0. 54077900	-0. 01332400
C	3. 14787200	-0. 56543800	-1. 31368300
C	4. 90641800	-0. 01167700	0. 27079700
C	3. 90392500	-0. 02972500	-2. 33721800
H	2. 16744300	-0. 99303300	-1. 50654700
C	5. 67368000	0. 51989200	-0. 75967700
H	5. 25631900	0. 00826800	1. 29745300
C	5. 16515100	0. 52351800	-2. 06186300
H	3. 54968300	-0. 01828400	-3. 36154400
H	6. 64365100	0. 94407300	-0. 53431600
O	5. 81411700	1. 04068300	-3. 12690200
C	7. 06848300	1. 65344800	-2. 90072800
H	7. 79892400	0. 93277200	-2. 51639800
H	7. 40145700	2. 02588300	-3. 86823200
H	6. 97756600	2. 48893200	-2. 19687800
H	-0. 14655800	-2. 49696600	2. 53481900

TS6A

C	0. 31500200	-1. 54590300	-1. 11711000
C	0. 21301700	-2. 70104000	-2. 07258400
C	-0. 69433700	-0. 80697800	-0. 60812600
H	0. 84934400	-3. 50958100	-1. 70065500
H	-0. 80802400	-3. 06473000	-2. 15514700
C	-2. 08413200	-0. 93501200	-1. 13902100
O	-2. 68535600	0. 01799300	-1. 59290200
O	-2. 59314600	-2. 17191200	-1. 10123000
C	-3. 86455700	-2. 36056000	-1. 75126400
H	-3. 94217200	-1. 65739900	-2. 58291900
H	-3. 82841000	-3. 38221400	-2. 13492000
C	-5. 01851000	-2. 19768000	-0. 79673500
C	-5. 62910700	-3. 32412000	-0. 24326800
C	-5. 49519600	-0. 92705400	-0. 46023200
C	-6. 69917800	-3. 19140800	0. 63750800
H	-5. 26120300	-4. 31278900	-0. 50515100
C	-6. 56794700	-0. 79504000	0. 41693100
H	-5. 01207700	-0. 05128400	-0. 88696000

C	-7.16986500	-1.92431000	0.96884000
H	-7.16411500	-4.07515500	1.06242600
H	-6.94037600	0.19359700	0.66976200
H	-8.00539900	-1.81598700	1.65316100
C	-0.47103600	0.29927200	0.35508100
C	0.84691200	0.21902100	0.99248000
H	-0.66154400	1.56786100	-0.35816800
H	0.94581000	0.65915000	1.98165800
C	1.83835100	-0.56033500	0.52258500
C	-1.49684900	0.54421300	1.39557100
O	-1.41231100	1.44069900	2.21846600
O	-2.54953800	-0.29957000	1.34138500
C	-3.59357000	-0.13687500	2.31170000
C	-4.03959300	-1.51709600	2.74568000
H	-4.41268100	0.41141000	1.83097000
H	-3.21340600	0.45917400	3.14368000
H	-4.90164700	-1.43955400	3.41365300
H	-4.32509800	-2.11581400	1.87802200
H	-3.23084300	-2.02879800	3.27290400
C	3.02812100	-0.95025000	1.31049200
C	3.49295600	-2.27302200	1.27015600
C	3.70732800	-0.02811700	2.11274600
C	4.59644900	-2.66031100	2.01903000
H	2.97778200	-2.98786200	0.63538100
C	4.81790400	-0.41554900	2.85812000
H	3.37819400	1.00729000	2.12414100
C	5.26752200	-1.73278700	2.81598200
H	4.93454000	-3.69170800	1.98344200
H	5.34036300	0.32007600	3.46275900
H	6.12976600	-2.03548100	3.40281300
N	1.68572600	-1.20622700	-0.76448100
S	2.41188300	-0.29483500	-2.04516200
O	2.59227500	-1.20200500	-3.16944700
O	1.66907300	0.95220400	-2.25542500
C	3.97796900	0.13025900	-1.35510200
C	4.20879000	1.43610400	-0.92585800
C	4.92081200	-0.87046600	-1.16050700
C	5.38835200	1.73232800	-0.26970300
H	3.45795400	2.19738900	-1.10388300
C	6.09974100	-0.58229000	-0.48575800
H	4.71741300	-1.87847700	-1.50835500
C	6.32038000	0.71647600	-0.01603700
H	5.60514900	2.73129500	0.09143600
H	6.81654800	-1.37308900	-0.30719500

O	7.40616600	1.08846100	0.69584100
C	8.33029200	0.08009300	1.05593600
H	8.80555800	-0.35802600	0.17071700
H	9.08773200	0.56932700	1.66710800
H	7.83841000	-0.70934800	1.63575400
H	0.59237100	-2.43114000	-3.06112200
N	-0.77022800	2.73132500	-0.84643100
C	-1.85925100	3.46145900	-0.15595600
H	-1.58227200	3.48147000	0.89982700
H	-1.89287700	4.49139000	-0.53973600
C	-3.23568800	2.82862600	-0.32070700
H	-3.23948400	1.80182700	0.08786400
H	-3.48115200	2.73933200	-1.38397700
C	-0.96351700	2.64722300	-2.30716100
H	-0.07160400	2.20088100	-2.74522700
H	-1.81526000	2.00166700	-2.51593500
H	-1.12830500	3.65172300	-2.71620300
C	0.52333100	3.34784800	-0.50839700
H	0.66442400	3.27876300	0.57353500
H	1.30783900	2.79026500	-1.01931500
H	0.53682900	4.39911000	-0.81803700
N	-4.25729400	3.66442500	0.29863000
C	-4.07691300	3.77295300	1.74120400
H	-4.93120100	4.30584100	2.16683700
H	-3.99164200	2.78776900	2.23193500
H	-3.17924700	4.34608000	1.98189600
C	-5.56972200	3.11753700	0.00647700
H	-5.71026900	2.10867500	0.44157400
H	-6.34427800	3.77417600	0.41214200
H	-5.71188800	3.04336900	-1.07540700

M6A

C	-0.55653600	-1.25371600	1.53983000
C	-0.46232200	-1.90326000	2.88916900
C	0.47465400	-0.91415700	0.72357000
H	-1.17645400	-2.73220700	2.92886200
H	0.53613700	-2.30112300	3.07230100
C	1.85234200	-0.88786400	1.29539500
O	2.42010600	0.15755200	1.55636300
O	2.37934300	-2.08933100	1.54694200
C	3.68839500	-2.08912000	2.13344700
H	3.75923900	-1.28614800	2.87051500
H	3.75736500	-3.05537600	2.63819400
C	4.77124900	-1.95945300	1.09217900

C	4. 90937400	-2. 93658600	0. 10274300
C	5. 67450400	-0. 89902400	1. 13252500
C	5. 94683000	-2. 86306000	-0. 82086200
H	4. 19656000	-3. 75619900	0. 06192400
C	6. 72110300	-0. 82825000	0. 21388400
H	5. 55533700	-0. 12760200	1. 88951100
C	6. 85961500	-1. 81049200	-0. 76297700
H	6. 04593600	-3. 62740200	-1. 58529700
H	7. 43224700	-0. 00924300	0. 26252800
H	7. 67563400	-1. 75706800	-1. 47658200
C	0. 26027600	-0. 41149400	-0. 62049200
C	-1. 07512500	-0. 55217400	-1. 11335800
H	1. 24093200	1. 44135100	0. 19485100
H	-1. 20858700	-0. 55237500	-2. 19217600
C	-2. 10556200	-0. 91178400	-0. 30593800
C	1. 29178200	-0. 25105100	-1. 60041500
O	1. 14487000	0. 20730400	-2. 73516500
O	2. 54348800	-0. 60758300	-1. 15701100
C	3. 57815600	-0. 62870900	-2. 13882700
C	3. 46556700	-1. 85122800	-3. 03098500
H	4. 50711000	-0. 63995800	-1. 56249000
H	3. 53259600	0. 28435500	-2. 74188600
H	4. 32941300	-1. 91062100	-3. 69981800
H	3. 43546500	-2. 75748900	-2. 42105700
H	2. 55583000	-1. 79251400	-3. 63134700
C	-3. 40526800	-1. 42448200	-0. 77228700
C	-4. 07155900	-2. 43664400	-0. 06219300
C	-4. 02061200	-0. 90881500	-1. 92070800
C	-5. 29917600	-2. 92105600	-0. 49491700
H	-3. 61018900	-2. 82771700	0. 83979300
C	-5. 25351600	-1. 39039300	-2. 34976000
H	-3. 53932900	-0. 09762300	-2. 45982000
C	-5. 90074400	-2. 39999600	-1. 64082200
H	-5. 79038000	-3. 71299800	0. 06323200
H	-5. 71623500	-0. 96275300	-3. 23469600
H	-6. 85911700	-2. 78141300	-1. 98084600
N	-1. 90122600	-0. 89314700	1. 13138300
S	-2. 31410200	0. 63508600	1. 84067900
O	-2. 48788800	0. 40989600	3. 27036600
O	-1. 37377100	1. 68931000	1. 42258400
C	-3. 86551900	0. 97920600	1. 07543900
C	-3. 94023300	1. 91519100	0. 04494900
C	-4. 96279500	0. 20330100	1. 42372300
C	-5. 12285000	2. 05616000	-0. 65541000

H	-3.06748100	2.50910600	-0.20161100
C	-6.15090600	0.33228800	0.71570900
H	-4.87504500	-0.52348100	2.22527700
C	-6.21960100	1.23963900	-0.34554400
H	-5.22138400	2.76066300	-1.47345700
H	-6.99330900	-0.29750800	0.97059000
O	-7.30468600	1.39893800	-1.13482600
C	-8.39273800	0.51779600	-0.93444300
H	-8.84955500	0.66676400	0.05085600
H	-9.12110700	0.75647900	-1.70870500
H	-8.07096300	-0.52513900	-1.03600700
H	-0.73428900	-1.21031700	3.69069000
N	1.35359500	2.44561300	-0.03668000
C	2.65379000	2.63919200	-0.75857600
H	2.56690100	2.05369400	-1.67837600
H	2.70325300	3.70232200	-1.01666300
C	3.90429300	2.27811200	0.04158000
H	4.04829000	1.18558400	0.05623000
H	3.78297500	2.59514300	1.08104200
C	1.26985400	3.19252100	1.24889200
H	0.23984000	3.14252700	1.59703300
H	1.91548200	2.70297500	1.97523100
H	1.58529300	4.22304400	1.07108000
C	0.22849100	2.80030500	-0.95281100
H	0.33165600	2.20806900	-1.86436400
H	-0.69928700	2.55112500	-0.44193400
H	0.29709300	3.86985700	-1.16380700
N	5.04682000	3.00433700	-0.50541000
C	5.50001300	2.42676100	-1.76219000
H	6.31658800	3.03162400	-2.16609500
H	5.85661100	1.38775800	-1.64312700
H	4.69093700	2.42843000	-2.49823700
C	6.13863800	3.04490500	0.45226900
H	6.50545900	2.03973100	0.72546500
H	6.97414800	3.60816800	0.02735400
H	5.81480100	3.55241000	1.36520500

TS7A

C	-0.52039700	-1.47386100	1.48256800
C	-0.35095200	-1.97050100	2.88975100
C	0.49954500	-1.05972300	0.66979600
H	-0.97161500	-2.85902800	3.03285800
H	0.68457200	-2.22247800	3.11957300
C	1.87670000	-0.98941800	1.23477500

O	2. 41713500	0. 06536900	1. 52316600
O	2. 44726800	-2. 17620700	1. 44315200
C	3. 77137300	-2. 14719700	1. 99643400
H	3. 83614100	-1. 36353200	2. 75429100
H	3. 88554500	-3. 12437000	2. 47050800
C	4. 81672600	-1. 95219100	0. 92695600
C	4. 91825800	-2. 87133900	-0. 12080800
C	5. 72136000	-0. 89447800	0. 99564200
C	5. 92429800	-2. 74598700	-1. 07298600
H	4. 20181500	-3. 68620300	-0. 18392300
C	6. 73564800	-0. 77113100	0. 04603600
H	5. 63189700	-0. 16713400	1. 79909900
C	6. 83996500	-1. 69749400	-0. 98777000
H	5. 99670400	-3. 46678800	-1. 88146400
H	7. 44874900	0. 04457500	0. 11627800
H	7. 63102300	-1. 60391400	-1. 72487100
C	0. 23731600	-0. 55007900	-0. 64629500
C	-1. 10196800	-0. 65626500	-1. 09122700
H	1. 32548400	1. 34343300	0. 44089100
H	-1. 29113900	-0. 50549800	-2. 15028600
C	-2. 09362500	-1. 12859800	-0. 27064400
C	1. 24910700	-0. 23111800	-1. 62406100
O	1. 05452600	0. 32579800	-2. 70122400
O	2. 51424200	-0. 57131000	-1. 23042500
C	3. 54119500	-0. 44293300	-2. 21607600
C	3. 47228100	-1. 57093300	-3. 22838500
H	4. 47453600	-0. 47247100	-1. 64805200
H	3. 44671900	0. 52606600	-2. 71744700
H	4. 33064800	-1. 52174900	-3. 90474000
H	3. 49039400	-2. 53476100	-2. 71381100
H	2. 55500100	-1. 49408600	-3. 81505400
C	-3. 43527800	-1. 52173600	-0. 74862400
C	-4. 16366500	-2. 50192700	-0. 05466100
C	-4. 01916500	-0. 94443000	-1. 88367900
C	-5. 42174100	-2. 89624700	-0. 48978000
H	-3. 72291900	-2. 93792900	0. 83575100
C	-5. 28150200	-1. 33858900	-2. 31677800
H	-3. 49498700	-0. 15378600	-2. 41268300
C	-5. 99053700	-2. 31727300	-1. 62417700
H	-5. 96182500	-3. 66367900	0. 05706100
H	-5. 71903500	-0. 86363800	-3. 19067600
H	-6. 97321100	-2. 62892300	-1. 96615100
N	-1. 86393300	-1. 31288500	1. 10795200
S	-2. 42602400	0. 40043800	2. 07467400

O	-2.84648500	0.10005600	3.45184900
O	-1.34866300	1.40772000	1.86678700
C	-3.84072000	0.95141400	1.15561700
C	-3.70504100	1.88813000	0.13252400
C	-5.04370800	0.28228000	1.35071300
C	-4.77684200	2.14755800	-0.70303900
H	-2.76610000	2.41449600	0.01037600
C	-6.12287800	0.53317400	0.51362900
H	-5.12478400	-0.45095700	2.14736400
C	-5.97794500	1.44823200	-0.53409600
H	-4.70835700	2.86365800	-1.51453700
H	-7.04773400	-0.00925000	0.66154200
O	-6.94364500	1.71699100	-1.44426600
C	-8.14202400	0.97181300	-1.36120100
H	-8.67875800	1.18374600	-0.42887000
H	-8.75222400	1.28466900	-2.20780100
H	-7.93770500	-0.10299500	-1.42869700
H	-0.70405700	-1.22110900	3.60734200
N	1.31814700	2.35779800	0.23692600
C	2.55812000	2.68811100	-0.53602200
H	2.44620600	2.17985200	-1.49853500
H	2.54298800	3.77055000	-0.70039500
C	3.86524700	2.31382400	0.16163400
H	4.05105100	1.23080700	0.06846600
H	3.78836900	2.52933400	1.23106500
C	1.23817300	3.02950500	1.56552200
H	0.24170300	2.84730400	1.96777200
H	1.97750500	2.58461400	2.22773600
H	1.42766500	4.09552300	1.42418100
C	0.11148800	2.66590100	-0.58523700
H	0.20732600	2.16797500	-1.55138000
H	-0.74760800	2.28107000	-0.03934200
H	0.05979000	3.75076900	-0.70366500
N	4.95027000	3.12900900	-0.37358500
C	5.34617900	2.68944000	-1.70337500
H	6.12309500	3.35488800	-2.08917100
H	5.73618800	1.65518500	-1.70405100
H	4.49818600	2.73675200	-2.39253400
C	6.09595300	3.11143200	0.52022700
H	6.51050100	2.09761000	0.66162700
H	6.88532000	3.74824700	0.11176500
H	5.81124900	3.50715700	1.49902300

P

C	-1.20699400	-1.06995000	1.89607200
C	-0.80000700	-0.73197500	3.30323500
C	-0.27452600	-1.22622300	0.85097400
H	-1.70162000	-0.52010800	3.87747700
H	-0.25333400	-1.55430500	3.76918300
C	1.20018400	-1.06772200	1.03034800
O	1.92935900	-0.54189800	0.21834900
O	1.65806300	-1.59124700	2.17480400
C	3.07352700	-1.44899400	2.36231000
H	3.34292000	-0.39212200	2.27523100
H	3.24009400	-1.78327700	3.38868400
C	3.86280000	-2.27956800	1.37938000
C	3.49136100	-3.59780300	1.11212400
C	4.97552300	-1.73847500	0.73792100
C	4.23380500	-4.36707200	0.22083600
H	2.61281100	-4.01465100	1.59657200
C	5.71781100	-2.50623300	-0.15596300
H	5.25243600	-0.70459300	0.93151500
C	5.34778200	-3.82340000	-0.41615900
H	3.94426100	-5.39475000	0.02347100
H	6.58062100	-2.07355800	-0.65231700
H	5.92439000	-4.42463500	-1.11196500
C	-0.76739500	-1.40369600	-0.44387500
C	-2.13492700	-1.43992800	-0.66832300
H	1.54095900	3.03216900	-0.90960100
H	-2.50791000	-1.57960100	-1.67582200
C	-2.99006200	-1.33667300	0.43170100
C	0.16339200	-1.54672200	-1.61208000
O	0.08056900	-0.87209300	-2.60979700
O	1.04162200	-2.53030900	-1.40024400
C	2.21649500	-2.57776100	-2.22866300
C	2.38893200	-3.98949200	-2.74676100
H	3.04809600	-2.27552400	-1.58106300
H	2.10690800	-1.85689400	-3.04107400
H	3.33898500	-4.07605700	-3.28059100
H	2.39556800	-4.69821900	-1.91591900
H	1.57698100	-4.25403600	-3.42819500
C	-4.46630800	-1.45515700	0.29265700
C	-5.23566800	-1.79460200	1.41229700
C	-5.10868500	-1.26113600	-0.93479000
C	-6.61057700	-1.96578300	1.29743200
H	-4.73232700	-1.92693300	2.36352400
C	-6.48484700	-1.42842800	-1.04739800
H	-4.54032400	-0.93787000	-1.80147500

C	-7.23941000	-1.79066700	0.06560400
H	-7.19312400	-2.24140700	2.17088400
H	-6.96770200	-1.26049300	-2.00465100
H	-8.31277800	-1.92603700	-0.02392700
N	-2.51926000	-1.15214000	1.67225400
S	0.11081300	1.78451100	-0.01015800
O	0.26858900	1.74330300	1.48353300
O	0.59572000	3.22651900	-0.56245400
C	-1.64389700	1.96576500	-0.28005300
C	-2.13840600	1.89282500	-1.58424100
C	-2.50027600	1.98467000	0.80697000
C	-3.50557700	1.86556800	-1.79018700
H	-1.45188200	1.83369700	-2.42480600
C	-3.87951500	1.95235100	0.60746600
H	-2.07402800	1.99286000	1.80611200
C	-4.38115100	1.88989400	-0.69355400
H	-3.93212700	1.80621600	-2.78590400
H	-4.54151400	1.94409400	1.46416800
O	-5.69916700	1.81613600	-0.99951400
C	-6.60662000	1.71580400	0.07993000
H	-6.60200600	2.63019100	0.68532400
H	-7.59215800	1.57835900	-0.36453400
H	-6.37149200	0.85158300	0.71269600
H	-0.15148400	0.14870600	3.29054100
N	2.91299500	2.44603800	-1.61064600
C	3.87228300	1.84645600	-0.66420700
H	3.76654600	0.75761000	-0.70092500
H	4.90165400	2.08820200	-0.97425700
C	3.59821800	2.27611000	0.77331900
H	4.35327100	1.80313700	1.43754800
H	2.62362300	1.87383800	1.06915900
C	3.44597000	3.65818200	-2.23276600
H	2.68381300	4.09196400	-2.88653500
H	3.68756800	4.37854300	-1.45046400
H	4.34409900	3.44277900	-2.83389000
C	2.48290900	1.48198200	-2.62463900
H	2.03665900	0.61644100	-2.13119600
H	1.72123500	1.94176200	-3.26146600
H	3.32089700	1.15423200	-3.26079500
N	3.56773800	3.72013700	0.94443800
C	4.90368600	4.27865700	1.02656700
H	4.84592000	5.36960700	1.08443500
H	5.45893400	3.91477100	1.91177900
H	5.48334600	4.01974400	0.13445400

C	2.76961800	4.09902900	2.10135000
H	3.20614800	3.73222300	3.04922900
H	2.70703100	5.18974700	2.15690900
H	1.76199600	3.68987300	1.99625800

TS3B

C	-0.56066900	1.06755100	-0.77374200
C	-1.18278100	0.89095500	-1.98483500
C	-1.10880200	0.15135700	0.34099500
C	-2.62556200	0.23888800	0.43338700
O	-3.23520100	1.04952600	1.09657300
O	-3.21802800	-0.72519600	-0.27463000
C	-4.64410400	-0.75843000	-0.23170400
H	-4.98173300	-0.53916200	0.78581200
H	-5.02820000	0.03404400	-0.88622000
C	-5.10557900	-2.11989900	-0.68137000
C	-6.34495500	-2.59536500	-0.25159000
C	-4.32333100	-2.91004900	-1.52478400
C	-6.80405400	-3.84248200	-0.66340200
H	-6.95118600	-1.98772800	0.41626200
C	-4.78075400	-4.16125600	-1.92982300
H	-3.35155400	-2.54970700	-1.84632700
C	-6.02073700	-4.62950600	-1.50366400
H	-7.76818400	-4.20346700	-0.31967700
H	-4.16329600	-4.77224300	-2.58052800
H	-6.37344700	-5.60542300	-1.82125700
N	-0.37634700	2.73036300	-0.46749400
C	-1.75742600	3.25616500	-0.19893100
H	-2.40514200	2.67742600	-0.85892400
H	-2.00066300	3.00970100	0.83699400
C	-1.95411500	4.75486700	-0.42135200
H	-2.05927300	4.96497700	-1.50436800
H	-1.09480000	5.33691500	-0.06614100
C	0.17322700	3.30962600	-1.73032400
H	1.03624000	2.71146600	-2.02864900
H	-0.59364600	3.27128300	-2.49943100
H	0.46026300	4.34590000	-1.54307400
C	0.51486400	3.17586300	0.63914700
H	0.19160900	2.74200500	1.58048600
H	1.54098900	2.89794900	0.42102300
H	0.44777200	4.26329700	0.71074200
N	-3.11813100	5.21086600	0.32291700
C	-4.32406100	4.48259400	-0.05045300
H	-5.17466500	4.90671600	0.48888200

H	-4.53561600	4.54753200	-1.13437900
H	-4.24312600	3.42935200	0.23126600
C	-3.30386400	6.63776400	0.12631900
H	-3.50750200	6.90004700	-0.92849200
H	-4.14443800	6.98394100	0.73300800
H	-2.40706300	7.17662400	0.44604000
C	-0.50590800	0.27223800	1.74200300
C	0.99243400	0.33236700	1.75175600
H	-0.91399900	1.17534800	2.22700400
H	1.45428300	0.33601500	2.73389900
C	1.75847700	0.49611900	0.66140700
C	-0.93973400	-0.85222900	2.68606100
O	-0.44085100	-1.03901000	3.76795300
O	-1.93726300	-1.58791300	2.18857000
C	-2.42099400	-2.65703300	3.01878300
C	-3.64163300	-3.22892300	2.33344600
H	-2.64329000	-2.25520300	4.01110400
H	-1.62077500	-3.39506400	3.12891600
H	-3.40401300	-3.54510900	1.31477900
H	-4.01523000	-4.09062000	2.89173400
H	-4.43873600	-2.48273100	2.27944000
C	3.22387600	0.74518300	0.83849200
C	3.97547100	0.01412000	1.76253900
C	3.86129600	1.74745900	0.09634500
C	5.32657600	0.28950000	1.95326700
H	3.50037600	-0.79520200	2.30939000
C	5.20614500	2.03517600	0.30033500
H	3.29692100	2.27461200	-0.66873300
C	5.94461700	1.30745700	1.23122100
H	5.89885600	-0.30137800	2.66219700
H	5.68187600	2.82253700	-0.27644500
H	6.99663200	1.52658900	1.38693900
N	1.20764400	0.71474700	-0.62834700
S	1.52877600	-0.44240900	-1.81912800
O	0.54093400	-1.52284700	-1.76059000
O	1.73168500	0.29950200	-3.06175700
C	3.06048800	-1.20812200	-1.35719400
C	4.26430800	-0.65522900	-1.76553500
C	3.02466800	-2.32781700	-0.52492500
C	5.46126000	-1.18409400	-1.29559600
H	4.25891000	0.20300200	-2.42980300
C	4.21181600	-2.86241600	-0.05961700
H	2.06618600	-2.75601100	-0.25165900
C	5.43079000	-2.27091100	-0.41681300

H	6.39754100	-0.73237400	-1.59751500
H	4.23061400	-3.72367400	0.59869800
O	6.53325000	-2.82395700	0.14145400
C	7.78048700	-2.22487000	-0.14240000
H	7.79120000	-1.17298600	0.16726300
H	8.52153800	-2.78213800	0.42956400
H	8.02163400	-2.29070200	-1.20978600
H	-0.86405000	-0.84188300	-0.04931700
H	-0.78370300	1.29716200	-2.90291900
H	-1.74533500	-0.02547300	-2.09655400

M3B

C	-0.25892600	0.49514200	-1.21225600
C	-0.77445700	1.08482100	-2.28577400
C	-1.01592200	-0.17384500	-0.08514000
C	-2.51280700	-0.00375600	-0.23145400
O	-3.09837300	1.04545300	-0.10072500
O	-3.11875800	-1.15641600	-0.53408500
C	-4.54559700	-1.09289900	-0.61590900
H	-4.92872600	-0.54431000	0.25039300
H	-4.82032400	-0.52282400	-1.51142800
C	-5.08671100	-2.49608500	-0.66048600
C	-6.33258000	-2.76873700	-0.09564800
C	-4.37038600	-3.52701600	-1.27037800
C	-6.86515700	-4.05340600	-0.14686100
H	-6.88533800	-1.97073900	0.39432200
C	-4.90042100	-4.81328700	-1.31436200
H	-3.39347900	-3.31908900	-1.69533900
C	-6.14826800	-5.07939300	-0.75622100
H	-7.83469100	-4.25370600	0.29798600
H	-4.33596700	-5.61072000	-1.78717900
H	-6.55818800	-6.08359400	-0.79236800
N	-0.12518900	3.47725000	0.44589200
C	-1.51506200	3.79308700	0.14541300
H	-1.80094200	3.18871800	-0.72221600
H	-2.13659600	3.44790000	0.98167900
C	-1.83666800	5.27176400	-0.10375700
H	-1.48627600	5.57064400	-1.11337800
H	-1.29263200	5.89399200	0.61853300
C	0.79586600	3.86272800	-0.60511900
H	1.78563900	3.44944800	-0.38400400
H	0.45468500	3.44756600	-1.55856400
H	0.90328900	4.95639800	-0.71755900
C	0.32402100	3.93863700	1.74436800

H	-0.36747600	3.59097100	2.51928900
H	1.31229000	3.51152300	1.94821300
H	0.40967000	5.03625900	1.83009000
N	-3.25771500	5.54696600	0.06117900
C	-4.06989100	4.75834800	-0.85190400
H	-5.12329500	5.01548800	-0.70895000
H	-3.81243900	4.94477400	-1.91283500
H	-3.95388800	3.69100500	-0.64880000
C	-3.52277700	6.96109300	-0.12216700
H	-3.27792800	7.31208200	-1.14286700
H	-4.58086700	7.16716400	0.06379300
H	-2.93016000	7.54406600	0.58895600
C	-0.53246700	0.40895600	1.25554500
C	0.94902400	0.61865300	1.27817200
H	-1.00853400	1.39756400	1.35885500
H	1.38307000	0.90810300	2.22901100
C	1.72863000	0.56956600	0.18999600
C	-0.97322000	-0.42404700	2.44862800
O	-0.34571200	-0.56748700	3.46817100
O	-2.17728700	-0.97095300	2.23330800
C	-2.70172900	-1.80886300	3.27507900
C	-3.96720500	-2.43477900	2.73185000
H	-2.88215700	-1.19546500	4.16309700
H	-1.94606100	-2.55630000	3.53352000
H	-3.75615300	-2.99260000	1.81576700
H	-4.39794900	-3.11740200	3.46805100
H	-4.70871800	-1.66511700	2.50035000
C	3.17477900	0.90237400	0.23745000
C	3.95496300	0.51252900	1.32978600
C	3.77438800	1.60848500	-0.81322500
C	5.30647900	0.83843200	1.38124000
H	3.50213000	-0.07495400	2.12316100
C	5.12569300	1.93314600	-0.75742700
H	3.17368100	1.88067400	-1.67657000
C	5.89630800	1.55012500	0.33898100
H	5.90093900	0.52534400	2.23463400
H	5.57943800	2.48494200	-1.57476500
H	6.95136800	1.80319200	0.37874800
N	1.16848400	0.35518000	-1.10741100
S	1.70841200	-1.00450300	-2.06225200
O	0.61669100	-1.97119300	-2.07226800
O	2.21128200	-0.45883700	-3.31165200
C	3.04713600	-1.69885700	-1.15064200
C	4.34816100	-1.40553900	-1.53459000

C	2.77522200	-2.47059700	-0.01929800
C	5.40940700	-1.85538200	-0.75992900
H	4.51980300	-0.80644000	-2.42246300
C	3.82869300	-2.91606200	0.75575500
H	1.74858700	-2.70406000	0.24433500
C	5.14615900	-2.58691700	0.40261800
H	6.42182300	-1.60668800	-1.05074700
H	3.66699400	-3.50439400	1.65180600
O	6.10070300	-3.01865200	1.25474000
C	7.43679600	-2.63426200	0.99526700
H	7.53020300	-1.54255800	0.95577200
H	8.02860800	-3.02325000	1.82275300
H	7.80004500	-3.06427500	0.05498400
H	-0.78200800	-1.24329200	-0.14123100
H	-0.11591200	1.47474000	-3.05406300
H	-1.84641000	1.17524500	-2.41989300

TS4B

C	-0.53649600	-1.32346300	0.13521800
C	-1.01521100	-2.44582500	0.77227500
C	-1.27182800	-0.39383400	-0.68926400
C	-2.45939900	-0.72019400	-1.43927700
O	-2.93422800	-0.00909100	-2.31290700
O	-3.12274100	-1.84385300	-1.00979700
C	-4.47450800	-1.95451700	-1.46800000
H	-4.53551300	-1.67423000	-2.52017600
H	-4.73177400	-3.00873600	-1.34662200
C	-5.35717200	-1.07867100	-0.61104900
C	-5.76277700	-1.52658600	0.65201300
C	-5.71158800	0.20877600	-1.02421300
C	-6.51903200	-0.70461800	1.48795500
H	-5.49784100	-2.53300500	0.97093800
C	-6.48586100	1.01978000	-0.19798200
H	-5.36079000	0.56508600	-1.98769000
C	-6.88814000	0.56761100	1.05769500
H	-6.83318700	-1.06374300	2.46267000
H	-6.76807200	2.01439700	-0.53039200
H	-7.48525600	1.20642000	1.70048900
C	-0.63123800	0.89073900	-1.17477100
C	0.50786900	1.30217600	-0.28380300
H	-0.29645900	0.82810700	-2.22041400
H	0.74973400	2.35735600	-0.20575500
C	1.18158300	0.42676500	0.46885900
C	-1.62754500	2.04862300	-1.16884200

O	-1.59533700	2.98679500	-1.92062300
O	-2.48503300	1.95887700	-0.12881400
C	-3.43358900	3.02308400	0.00203600
C	-4.01975800	2.92755300	1.39390300
H	-4.19530200	2.90156500	-0.77626700
H	-2.92616700	3.97570600	-0.16968000
H	-4.78857700	3.69241500	1.53223200
H	-4.47802900	1.94808400	1.55277700
H	-3.24172600	3.07278800	2.14673400
C	2.28224000	0.83309900	1.37570900
C	2.45127300	0.21655600	2.61965600
C	3.17675000	1.83160200	0.97763400
C	3.49687700	0.60383200	3.45221300
H	1.77597700	-0.57989300	2.91573600
C	4.21747800	2.21742600	1.81337000
H	3.07687500	2.26998500	-0.01113500
C	4.38195600	1.60238700	3.05289700
H	3.62205900	0.12021900	4.41581100
H	4.91471900	2.98286100	1.48735700
H	5.20197700	1.89496100	3.70086400
N	0.79589200	-0.94183600	0.48590700
S	1.97900000	-2.18948500	0.23609300
O	2.28602500	-2.78602200	1.52715200
O	1.49017300	-3.01722100	-0.85221000
C	3.40003600	-1.29894800	-0.32175400
C	3.36937400	-0.67805700	-1.56263200
C	4.52639800	-1.23893600	0.49953100
C	4.47625600	0.04653700	-1.99234900
H	2.48405900	-0.75358500	-2.18751000
C	5.62977000	-0.52751600	0.07108400
H	4.50896500	-1.73106800	1.46601200
C	5.60586200	0.12563300	-1.16927300
H	4.44868900	0.53629300	-2.95740300
H	6.52357500	-0.44632500	0.67894900
O	6.72760200	0.80896400	-1.48704700
C	6.77163000	1.46398100	-2.73881800
H	5.99456100	2.23344600	-2.81342400
H	7.75249400	1.93344100	-2.79959600
H	6.65740700	0.75132400	-3.56345300
H	-2.25680800	-0.05680000	0.63219200
H	-2.17677200	-1.29775700	1.55040600
H	-1.86613000	-2.97795600	0.37147700
H	-0.34655900	-2.98408900	1.43408500
O	-2.76369400	-0.43195700	1.52205600

H	-3.67077000	-0.67454800	1.24937000
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M4B

C	-0.48465300	-1.37041900	0.10412800
C	-0.93898600	-2.74706800	0.52221500
C	-1.22227700	-0.45842400	-0.55662000
C	-2.58734700	-0.69611800	-1.08130900
O	-3.03326500	-0.03431100	-1.99592800
O	-3.27623400	-1.68045500	-0.48672000
C	-4.59943500	-1.91221200	-1.00801300
H	-4.56494800	-1.85071700	-2.09756300
H	-4.83090400	-2.93453000	-0.70365100
C	-5.61395200	-0.94667200	-0.44671400
C	-6.25842300	-1.23089600	0.75914600
C	-5.93549600	0.22880200	-1.13079800
C	-7.21580600	-0.36047800	1.27339600
H	-6.01304000	-2.14527800	1.29349100
C	-6.89414000	1.09897400	-0.61822800
H	-5.42177900	0.45547000	-2.05956800
C	-7.53719300	0.80506100	0.58181400
H	-7.71401200	-0.59417200	2.20878000
H	-7.14155200	2.00663300	-1.16015800
H	-8.28646100	1.48320900	0.97813300
C	-0.68574200	0.90854900	-0.92263200
C	0.48693600	1.26232100	-0.05054000
H	-0.41636500	0.95848100	-1.98640900
H	0.70991800	2.31269400	0.10648600
C	1.20383200	0.34008500	0.59818700
C	-1.73843100	2.00239400	-0.74562700
O	-1.76600500	3.01844500	-1.39137900
O	-2.56704800	1.72705200	0.26820300
C	-3.65641200	2.64265100	0.45102500
C	-4.44153500	2.15430100	1.64662400
H	-4.26036900	2.64061000	-0.46251000
H	-3.25301500	3.64977800	0.59069400
H	-5.32169700	2.78338200	1.80148600
H	-4.77870000	1.12770000	1.48014900
H	-3.82569000	2.18179200	2.54879500
C	2.34242500	0.68298300	1.48237300
C	2.60001100	-0.05013100	2.64532300
C	3.18981300	1.74059100	1.13596200
C	3.68737300	0.28031100	3.44898100
H	1.95919600	-0.88834700	2.90032600
C	4.27072500	2.07000900	1.94371900

H	3.02002400	2.27404700	0.20529900
C	4.52461800	1.33784300	3.10177300
H	3.88212600	-0.29358700	4.34935300
H	4.92875600	2.88454400	1.65789600
H	5.37596500	1.58693100	3.72708800
N	0.83510700	-1.03327200	0.52278900
S	2.03534600	-2.20716600	0.03832400
O	2.43068100	-2.95282600	1.22157400
O	1.46084100	-2.89779300	-1.10645100
C	3.40652100	-1.23557600	-0.49704200
C	3.29164000	-0.47343700	-1.65182400
C	4.57027700	-1.22951000	0.27378800
C	4.34887600	0.34324300	-2.03831500
H	2.38002200	-0.51060600	-2.24118300
C	5.62543000	-0.42915300	-0.11536700
H	4.61640200	-1.83179700	1.17448500
C	5.51360600	0.37170700	-1.26127700
H	4.25823400	0.94336500	-2.93488300
H	6.54439200	-0.38364500	0.45753500
O	6.58776300	1.14122600	-1.53716400
C	6.52298800	1.99227300	-2.66475200
H	5.70105600	2.71139200	-2.57133300
H	7.47141200	2.52662200	-2.69383900
H	6.40018200	1.41796500	-3.58990900
H	-1.20919400	-3.35002500	-0.34529000
H	-0.15081800	-3.25749300	1.07515800
H	-1.81574800	-2.65957700	1.16496200

M3C

C	-0.51177100	-0.25881500	-0.56159600
C	-1.20117700	-1.35606100	-0.90290500
C	-1.18258500	1.05932100	-0.21867100
C	-2.52116200	1.20727900	-0.91523200
O	-2.65547000	1.59862500	-2.04418200
O	-3.53216800	0.82513000	-0.10926900
C	-4.86841900	0.94803300	-0.64839100
H	-5.47724300	1.35258700	0.16267200
H	-4.84504100	1.65566900	-1.47895100
C	-5.35344000	-0.41086300	-1.07618000
C	-6.38623300	-1.05429800	-0.39492300
C	-4.70835700	-1.07145800	-2.12780600
C	-6.76083400	-2.35222800	-0.74265400
H	-6.90160700	-0.53824700	0.41156900
C	-5.07016000	-2.37278500	-2.46496000

H	-3.92675100	-0.55574800	-2.68164100
C	-6.09449500	-3.01716600	-1.76898900
H	-7.57370800	-2.84116100	-0.21533600
H	-4.56796800	-2.87697900	-3.28441300
H	-6.38499500	-4.02651100	-2.04155000
N	-1.89682900	-0.02328400	2.91090700
C	-2.53302800	-1.06078900	3.70885000
H	-2.22800400	-1.03568300	4.76899200
H	-3.61559800	-0.90314700	3.68954300
C	-2.21205900	-2.44357500	3.15809000
H	-2.83791400	-3.21386200	3.61705400
H	-1.16418300	-2.71099500	3.31508000
C	-0.46380900	0.06256300	3.19475800
H	-0.01649900	0.85643300	2.59107700
H	-0.26308900	0.27676400	4.25687300
H	0.04755300	-0.86788800	2.92560100
N	-2.44742100	-2.49298700	1.67876500
C	-3.85984300	-2.17763300	1.30636500
H	-4.00020500	-2.39024100	0.24515900
H	-4.52902700	-2.79841800	1.90529200
H	-4.02830700	-1.11591000	1.48189500
C	-2.01512900	-3.79739200	1.10968900
H	-2.60309100	-4.58986500	1.57540100
H	-2.18774600	-3.78768000	0.03438100
H	-0.95457400	-3.94235900	1.31638600
C	-0.26164400	2.23200400	-0.56778200
C	1.02879800	2.00818500	0.17141800
H	1.45095800	2.81698700	0.75885100
C	1.56259800	0.78102300	0.21418600
C	-0.92135600	3.52797700	-0.13517500
O	-1.99550300	3.58375800	0.42173100
O	-0.16520600	4.58114200	-0.41911900
C	-0.71152000	5.86859900	-0.05697400
C	0.27297100	6.91789300	-0.51823500
H	-0.86489100	5.88604500	1.02587200
H	-1.68833400	5.97306300	-0.53619400
H	0.41413700	6.86358000	-1.59942100
H	-0.10342100	7.91172600	-0.26673000
H	1.24146500	6.78139900	-0.03248900
C	2.74513100	0.42416400	1.03528500
C	2.92901800	-0.88454500	1.49190400
C	3.69261600	1.39744700	1.37496500
C	4.03399600	-1.21176100	2.27193700
H	2.21285400	-1.64791100	1.20253000

C	4. 78941700	1. 07196300	2. 16330900
H	3. 59177000	2. 40679100	0. 98776700
C	4. 96620000	-0. 23534700	2. 61276800
H	4. 17277500	-2. 23490100	2. 60664400
H	5. 51696100	1. 83757100	2. 41316500
H	5. 82825000	-0. 49321200	3. 21927000
N	0. 91890400	-0. 28675200	-0. 51905900
S	1. 63901500	-0. 51947400	-2. 12036800
O	0. 93314400	-1. 64030600	-2. 71212800
O	1. 66805100	0. 78129400	-2. 76836800
C	3. 27111300	-1. 01660700	-1. 71685200
C	4. 26909100	-0. 05845900	-1. 60019700
C	3. 51712300	-2. 36700300	-1. 45272500
C	5. 53404600	-0. 43772800	-1. 16796200
H	4. 04934600	0. 97892900	-1. 83306900
C	4. 77351400	-2. 74682000	-1. 02960500
H	2. 72680300	-3. 09746800	-1. 58966800
C	5. 78073200	-1. 78084400	-0. 85952600
H	6. 30683500	0. 31268600	-1. 06396900
H	5. 01528000	-3. 78155300	-0. 81522400
O	6. 95226600	-2. 24802900	-0. 39723500
C	8. 00313800	-1. 32161500	-0. 17982900
H	7. 70601100	-0. 56044800	0. 55047100
H	8. 83705100	-1. 90110500	0. 21220100
H	8. 30274700	-0. 83812100	-1. 11573200
H	-1. 37528400	1. 07792600	0. 85514100
H	-1. 87553600	-1. 73602900	1. 25726900
H	-2. 27655800	-1. 30052800	-1. 05375100
H	-0. 68568700	-2. 26903400	-1. 17195800
H	-0. 08942100	2. 26903400	-1. 65217600
C	-2. 54574800	1. 26927200	3. 14676100
H	-2. 09966400	2. 03834100	2. 51098600
H	-3. 60313100	1. 20128600	2. 87851500
H	-2. 46145500	1. 58644200	4. 19807900

TS4C

C	-0. 45560200	0. 22975300	-0. 76530300
C	-0. 96278700	-1. 06116800	-1. 06305400
C	-1. 37506700	1. 23551100	-0. 09757000
C	-2. 83808500	1. 00205800	-0. 46130200
O	-3. 31362200	1. 41441100	-1. 49005600
O	-3. 49153100	0. 31848900	0. 47497500
C	-4. 91402700	0. 12697700	0. 25652200
H	-5. 35748400	0. 18897700	1. 25107700

H	-5.27790200	0.94836000	-0.36314000
C	-5.16696000	-1.21553600	-0.37479100
C	-5.75678300	-2.24236500	0.36198700
C	-4.76563200	-1.45912100	-1.69277300
C	-5.92968600	-3.50612100	-0.20038800
H	-6.08031600	-2.05345000	1.38260200
C	-4.92377000	-2.72554600	-2.24939800
H	-4.34063300	-0.64896100	-2.27966300
C	-5.50297600	-3.75157200	-1.50254700
H	-6.39761200	-4.29650500	0.37754400
H	-4.61361900	-2.90740700	-3.27347000
H	-5.63637900	-4.73469400	-1.94202700
N	-0.86935600	-0.64043100	2.56737700
C	-0.96209000	-1.99269500	3.10042700
H	-0.37677400	-2.10434800	4.03189800
H	-2.00594300	-2.18485200	3.36603100
C	-0.48636700	-3.06036400	2.12593800
H	-0.66182200	-4.04635000	2.58370700
H	0.59219400	-2.97863300	1.94565100
C	0.52107500	-0.23930800	2.42342400
H	0.57855800	0.80604600	2.10141900
H	1.09302500	-0.33179000	3.36397500
H	1.01240200	-0.85245600	1.65799300
N	-1.15921500	-3.00335100	0.81748900
C	-2.62364100	-2.94253000	0.93328200
H	-3.06493000	-3.04059700	-0.06219800
H	-3.00564100	-3.75399100	1.56731000
H	-2.90932300	-1.97097200	1.34115800
C	-0.76016200	-4.14445400	-0.01378500
H	-1.15653700	-5.08411800	0.39124300
H	-1.14573700	-4.00872800	-1.02765300
H	0.33010800	-4.21724900	-0.05229200
C	-1.00690800	2.66811100	-0.48456100
C	0.45244600	2.87579600	-0.21656000
H	0.80251700	3.81580600	0.19576000
C	1.31646900	1.87733200	-0.39731000
C	-1.86430800	3.62507300	0.33263500
O	-2.70347600	3.25790100	1.12119300
O	-1.56352000	4.88892100	0.07000200
C	-2.34030900	5.88325100	0.78003200
C	-1.86869900	7.23878800	0.30873300
H	-2.18698600	5.73455500	1.85237300
H	-3.39676200	5.70751500	0.56187300
H	-2.02586700	7.34997300	-0.76589500

H	-2.42932500	8.02176700	0.82352000
H	-0.80697400	7.37633200	0.52385200
C	2.75043500	1.99201200	-0.01703600
C	3.33182400	1.12124600	0.90794500
C	3.50855000	3.04597700	-0.53599900
C	4.64929500	1.30772800	1.31471300
H	2.76425900	0.28398300	1.30080800
C	4.82533400	3.22868200	-0.12984700
H	3.06452200	3.70113700	-1.27887200
C	5.39800000	2.36103400	0.79867100
H	5.08751800	0.62525800	2.03601200
H	5.40684800	4.04567300	-0.54352900
H	6.42487500	2.50733500	1.11714400
N	0.82301500	0.62147700	-0.93785700
S	1.89393600	-0.07617800	-2.22635200
O	1.03253100	-0.88194100	-3.05787900
O	2.58289000	1.07718200	-2.74898600
C	2.99076400	-1.08636500	-1.30666600
C	4.34859600	-0.80125600	-1.33508100
C	2.47544600	-2.14972800	-0.55916300
C	5.22522700	-1.59751900	-0.60677500
H	4.70995400	0.05308100	-1.89956900
C	3.34100400	-2.92644100	0.18074900
H	1.40796700	-2.35486700	-0.55775000
C	4.72407200	-2.65680700	0.15875500
H	6.28425500	-1.37497200	-0.62842600
H	2.99514400	-3.76294700	0.77872900
O	5.47469600	-3.47069000	0.91171600
C	6.87976600	-3.26101000	0.94171200
H	7.11673400	-2.26792800	1.33819000
H	7.28022400	-4.02424500	1.60563600
H	7.31403100	-3.37629600	-0.05629300
H	-1.27468900	1.09822300	0.98352300
H	-0.90803200	-1.79186700	0.00012000
H	-2.03912000	-1.07757900	-1.23840800
H	-0.42151200	-1.65200800	-1.79330700
H	-1.24658000	2.84130400	-1.54369700
C	-1.59024200	0.28779400	3.43529900
H	-1.55536500	1.30039000	3.02100900
H	-2.64095800	-0.00767500	3.48877000
H	-1.17533700	0.31725100	4.45659900

M4C

C	-0.52403200	0.61024800	-0.57857700
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C	-1.14098400	-0.69666300	-0.86001800
C	-1.38658800	1.64972100	0.10618300
C	-2.86465300	1.38038600	-0.17023100
O	-3.41035700	1.77287600	-1.17040000
O	-3.40725000	0.64848200	0.79183700
C	-4.80377400	0.28405800	0.63928000
H	-5.18866000	0.25366600	1.65940300
H	-5.30297500	1.07635100	0.07854200
C	-4.93779700	-1.05384700	-0.03774900
C	-5.25901200	-2.19284400	0.70334300
C	-4.75976500	-1.16577800	-1.42122400
C	-5.39935800	-3.42916500	0.07575300
H	-5.43172700	-2.10708800	1.77346100
C	-4.88885100	-2.40257900	-2.04673000
H	-4.54496600	-0.27310100	-2.00332600
C	-5.21172900	-3.53506100	-1.29969200
H	-5.66663800	-4.30459200	0.65876600
H	-4.76011300	-2.47973800	-3.12163800
H	-5.32905100	-4.49540800	-1.79141400
N	-1.41057400	-1.90706000	2.07549400
C	-1.54757800	-3.35951600	2.17396500
H	-1.37007100	-3.69842100	3.21204900
H	-2.59021800	-3.60244600	1.93720500
C	-0.61377000	-4.16428700	1.27518100
H	-0.91648000	-5.22420500	1.37381100
H	0.41625500	-4.10188300	1.64996500
C	-0.04811800	-1.46815900	2.32827700
H	-0.01422900	-0.37173900	2.30069100
H	0.33040600	-1.78867100	3.31481200
H	0.62062900	-1.85261900	1.55290200
N	-0.60483100	-3.75021500	-0.12530400
C	-1.95363800	-3.72327600	-0.68084700
H	-1.90492500	-3.47549800	-1.74573200
H	-2.46455200	-4.69749600	-0.58213500
H	-2.56340400	-2.96374700	-0.18370100
C	0.22191900	-4.66889800	-0.90069600
H	-0.19436900	-5.69044300	-0.92244600
H	0.30910700	-4.30882400	-1.93041800
H	1.22731700	-4.72541700	-0.47162600
C	-0.99890100	3.05024300	-0.36550100
C	0.47709200	3.21446300	-0.14154200
H	0.87140700	4.15362000	0.23154000
C	1.29063700	2.16877500	-0.28331100
C	-1.81190400	4.07078300	0.42288600

O	-2.68146500	3.76076600	1.19970300
O	-1.43525000	5.30934400	0.14167200
C	-2.16985300	6.35948400	0.81970500
C	-1.61901300	7.67845400	0.33199400
H	-2.04146100	6.22249900	1.89678200
H	-3.23022800	6.23458900	0.58634900
H	-1.75352000	7.77894700	-0.74673100
H	-2.14595000	8.49840200	0.82429900
H	-0.55523800	7.76455200	0.56321900
C	2.70847500	2.13757800	0.15603300
C	3.06799800	1.31198100	1.22580100
C	3.66185300	2.96518100	-0.43851500
C	4.37473800	1.31708500	1.69973100
H	2.32310300	0.66443400	1.68282600
C	4.96986400	2.96645500	0.03847500
H	3.37734100	3.58389500	-1.28360400
C	5.32614000	2.14445400	1.10568400
H	4.64872800	0.67935000	2.53387800
H	5.71026000	3.61105400	-0.42320700
H	6.34522500	2.15408700	1.47855000
N	0.72694200	0.92860800	-0.79216900
S	1.77966400	0.10090600	-2.10337300
O	0.83725900	-0.69596500	-2.84650500
O	2.43853300	1.24834500	-2.67238000
C	2.88735800	-0.88375500	-1.18967600
C	4.22686900	-0.50685300	-1.15713000
C	2.40968600	-2.01419800	-0.51365300
C	5.12692200	-1.27418800	-0.43249700
H	4.55305200	0.38945700	-1.67585800
C	3.30524900	-2.75486900	0.22796000
H	1.36123600	-2.31102000	-0.55572200
C	4.66650200	-2.39410000	0.27323500
H	6.16910400	-0.98318600	-0.40753700
H	2.99330500	-3.63373800	0.78197200
O	5.44133600	-3.18375100	1.02366200
C	6.82914800	-2.88939700	1.11186800
H	6.98941500	-1.89646400	1.54498500
H	7.25216900	-3.64705600	1.76804000
H	7.30340700	-2.94798000	0.12718700
H	-1.21678900	1.56375900	1.18983900
H	-1.50210400	-1.05831300	0.12908400
H	-2.02545400	-0.56719500	-1.49417500
H	-0.48231000	-1.44386900	-1.27991900
H	-1.26667200	3.17424000	-1.42547800

C	-2.33045800	-1.27170500	3.01152200
H	-2.26538700	-0.18488800	2.92049600
H	-3.35437600	-1.56830200	2.76832000
H	-2.12147900	-1.55544900	4.05708700

TS5C

C	0.22624700	0.78521900	-0.60265000
C	0.21668800	2.09212800	0.12263600
C	1.47553600	0.04755100	-0.77503800
C	2.70871000	0.93425000	-0.75014600
O	3.29477700	1.26350800	-1.74867500
O	3.05423500	1.27755000	0.49566000
C	4.05214300	2.33192400	0.60349200
H	4.47678500	2.20125500	1.59937900
H	4.81783400	2.16753500	-0.15550700
C	3.36521100	3.66114100	0.45052000
C	2.75081000	4.25517100	1.55547300
C	3.24429500	4.25666400	-0.80767000
C	2.01073200	5.42366300	1.40560300
H	2.85639600	3.79901400	2.53722500
C	2.50314000	5.42657500	-0.95752000
H	3.72265400	3.79334600	-1.66523200
C	1.88223500	6.00684000	0.14628600
H	1.54273700	5.88481100	2.26915400
H	2.41369100	5.88748800	-1.93566400
H	1.30896500	6.92051500	0.02771000
N	1.75939500	-1.49458100	1.54801700
C	3.13950700	-1.49937500	2.06862900
H	3.80600900	-1.65367500	1.21459100
H	3.33976600	-0.49572200	2.45461200
C	3.43303100	-2.57374000	3.11606900
H	4.48609100	-2.46170400	3.43837100
H	3.36199300	-3.55784700	2.64015700
C	0.79527600	-0.78499600	2.38437700
H	-0.11107900	-0.59282700	1.79150900
H	0.52755500	-1.35490400	3.28047400
H	1.21896800	0.17965500	2.67907200
N	2.51251500	-2.56009400	4.24542400
C	2.76232100	-1.42563700	5.12337300
H	2.03767500	-1.42881900	5.94179300
H	3.77696300	-1.44903300	5.55862600
H	2.64715200	-0.48376000	4.58008500
C	2.61081600	-3.80192800	5.00157200
H	3.61739500	-3.96018600	5.42574200

H	1. 89209900	-3. 78772500	5. 82475600
H	2. 37230100	-4. 65026700	4. 35405400
C	1. 47491100	-0. 82122000	-2. 03288300
C	0. 21458600	-1. 63962200	-2. 03581300
H	0. 22870000	-2. 67179600	-2. 37095400
C	-0. 90818500	-1. 12863400	-1. 53465000
C	2. 69718600	-1. 72803900	-2. 03024800
O	3. 47474900	-1. 80956100	-1. 10739200
O	2. 76794100	-2. 42653400	-3. 15489400
C	3. 90891300	-3. 30699100	-3. 29930800
C	5. 13453300	-2. 52419000	-3. 72343500
H	3. 59766300	-4. 02422600	-4. 05910300
H	4. 06823200	-3. 82332300	-2. 35008000
H	5. 41565500	-1. 80522200	-2. 95143400
H	5. 97095200	-3. 20959300	-3. 87904700
H	4. 94493400	-1. 99205400	-4. 65776100
C	-2. 14430700	-1. 91377600	-1. 29422700
C	-2. 58114800	-2. 11991500	0. 01737100
C	-2. 83858000	-2. 49334800	-2. 35836600
C	-3. 70550100	-2. 90139400	0. 26367900
H	-2. 04425700	-1. 66150900	0. 84463200
C	-3. 96660300	-3. 26944900	-2. 10894600
H	-2. 50560800	-2. 30518700	-3. 37407700
C	-4. 40044000	-3. 47334800	-0. 79944400
H	-4. 03897800	-3. 06108900	1. 28379500
H	-4. 50813000	-3. 71406100	-2. 93711600
H	-5. 27748800	-4. 08306100	-0. 60801700
N	-0. 89618200	0. 23741000	-1. 06145500
S	-2. 30633600	1. 26565900	-1. 65829000
O	-1. 75112400	2. 59692300	-1. 70037500
O	-2. 67611700	0. 53389600	-2. 84336400
C	-3. 57025100	1. 17297200	-0. 45624800
C	-4. 55858500	0. 20121400	-0. 60051300
C	-3. 62637500	2. 13201000	0. 56497800
C	-5. 60390600	0. 15428200	0. 30966400
H	-4. 51393000	-0. 51112600	-1. 41924400
C	-4. 66327300	2. 07958900	1. 47085900
H	-2. 89078700	2. 92796500	0. 61522700
C	-5. 65579200	1. 08755400	1. 35421800
H	-6. 36919300	-0. 60228500	0. 19348600
H	-4. 75544000	2. 80565100	2. 26996300
O	-6. 61576200	1. 12665500	2. 28370000
C	-7. 66835900	0. 17458100	2. 21519300
H	-7. 27936500	-0. 84403600	2. 31555000

H	-8.32606800	0.39917800	3.05219500
H	-8.22128800	0.27159400	1.27556100
H	1.62539200	-0.65292400	0.21388200
H	0.93357900	2.02446700	0.94099900
H	0.55937000	2.89637100	-0.54110700
H	-0.76712200	2.34720400	0.50492600
H	1.54612200	-0.20005900	-2.93740000
C	1.27418400	-2.82251900	1.17831600
H	0.34005600	-2.71794100	0.61399700
H	2.01638900	-3.30688900	0.53786100
H	1.08211900	-3.44361100	2.06260500

M5C

C	0.10373600	0.87035700	-0.69929000
C	-0.00517400	2.01851300	0.26126800
C	1.24782600	0.35253400	-1.19399000
C	2.61082500	0.78599200	-0.79117600
O	3.50790400	0.92926600	-1.58771800
O	2.77058800	0.89884600	0.54485800
C	4.00481700	1.53044100	0.98432000
H	4.14925800	1.16010000	2.00182300
H	4.81867000	1.18681200	0.34384100
C	3.85611000	3.02518200	0.96062100
C	3.29949800	3.68671000	2.05765500
C	4.22166600	3.75483300	-0.17279800
C	3.10798800	5.06395200	2.02477500
H	3.02405700	3.11984100	2.94415100
C	4.03103600	5.13327000	-0.20452400
H	4.64966600	3.23698600	-1.02608800
C	3.47436400	5.78722900	0.89173200
H	2.68182600	5.57360600	2.88257200
H	4.31975400	5.69799300	-1.08458700
H	3.33046800	6.86231600	0.86586200
N	1.50893300	-2.10839100	1.13867300
C	2.86904100	-2.21062100	1.77997000
H	3.54756700	-2.52642700	0.98354100
H	3.13834000	-1.19134400	2.06389700
C	2.94284000	-3.18788700	2.94397600
H	3.98134600	-3.15823200	3.32254800
H	2.78502400	-4.20477500	2.57037900
C	0.57900800	-1.17113500	1.83039200
H	-0.32698800	-1.09821900	1.22540700
H	0.36185000	-1.58187500	2.81533200
H	1.06228900	-0.19499800	1.89071800

N	1. 96421500	-2. 92691700	3. 98863300
C	2. 31494300	-1. 74183400	4. 76478200
H	1. 55108100	-1. 56770600	5. 52594800
H	3. 29048400	-1. 84823800	5. 26789900
H	2. 35366300	-0. 85479800	4. 12517900
C	1. 83969900	-4. 08313900	4. 87247200
H	2. 78442200	-4. 32112100	5. 38857100
H	1. 07674100	-3. 88291400	5. 62759600
H	1. 52957800	-4. 95952100	4. 29671600
C	1. 19763800	-0. 66643900	-2. 32627000
C	0. 02187300	-1. 58044100	-2. 06516800
H	0. 09279500	-2. 63772700	-2. 30313300
C	-1. 08692500	-1. 10050500	-1. 49328200
C	2. 46278600	-1. 50426300	-2. 30990700
O	2. 82264900	-2. 09670700	-1. 29953100
O	3. 08044200	-1. 55474700	-3. 46250100
C	4. 34172000	-2. 26744000	-3. 50993900
C	5. 44990700	-1. 40138400	-2. 94715800
H	4. 48462200	-2. 47942300	-4. 56919400
H	4. 23099400	-3. 20425100	-2. 95982200
H	5. 27719000	-1. 19684000	-1. 88890500
H	6. 40755600	-1. 91562900	-3. 05671200
H	5. 49707400	-0. 45016000	-3. 48016900
C	-2. 25979200	-1. 93657900	-1. 14607000
C	-2. 88304500	-1. 78474000	0. 09771700
C	-2. 72746600	-2. 91073300	-2. 03380100
C	-3. 94245900	-2. 61194600	0. 45835700
H	-2. 55465800	-0. 99484700	0. 76854000
C	-3. 78993400	-3. 73152200	-1. 67288700
H	-2. 27777000	-2. 99207200	-3. 01856500
C	-4. 39584500	-3. 58779200	-0. 42511400
H	-4. 42010800	-2. 48371600	1. 42439000
H	-4. 15747500	-4. 47461500	-2. 37252300
H	-5. 22819700	-4. 22673300	-0. 14947800
N	-1. 12471700	0. 26015400	-1. 06717000
S	-2. 34613200	1. 23668700	-1. 85994500
O	-1. 69837700	2. 50681700	-2. 12184600
O	-2. 85304400	0. 39004500	-2. 91988700
C	-3. 62228200	1. 48151700	-0. 67201400
C	-4. 71520500	0. 62213600	-0. 66657900
C	-3. 54164300	2. 56126200	0. 21306200
C	-5. 73465600	0. 81566600	0. 25901000
H	-4. 76968100	-0. 18800100	-1. 38708900
C	-4. 55235800	2. 75351500	1. 13288500

H	-2.71085400	3.25600200	0.15239700
C	-5.65191700	1.87923100	1.16573600
H	-6.58676900	0.14793600	0.25473600
H	-4.53650300	3.58494900	1.82791300
O	-6.57925900	2.15483400	2.09775100
C	-7.73941000	1.34176000	2.15384900
H	-7.48104400	0.30167400	2.38106000
H	-8.35086000	1.74857500	2.95711400
H	-8.29551900	1.38547600	1.21153100
H	1.71691500	-1.73756300	0.19370100
H	0.95803800	2.26548800	0.70293500
H	-0.37157500	2.89873000	-0.27185300
H	-0.72270600	1.77187500	1.05080700
H	1.11629500	-0.16754200	-3.29987900
C	0.86174500	-3.42896400	0.90764200
H	-0.04274800	-3.25957900	0.32027400
H	1.55494500	-4.06349500	0.35393600
H	0.60708700	-3.86417300	1.87432000

TS2A'

C	1.79178800	1.24884300	0.21377800
C	0.76529600	0.83972400	1.03622700
C	3.06419100	0.66706200	0.28415400
H	1.02415500	0.12766600	1.80933500
H	-0.18808000	1.33646200	1.12935200
C	4.20731800	0.65735000	-0.56595200
O	4.50041200	1.35734700	-1.53843300
O	5.07394100	-0.31862300	-0.14969000
C	6.24329400	-0.48196100	-0.93425600
H	5.98117100	-0.48422500	-1.99683800
H	6.91521200	0.37154000	-0.77346700
C	6.91664400	-1.77379400	-0.54624200
C	6.59544800	-2.45440100	0.62782900
C	7.90773200	-2.29135000	-1.38215800
C	7.25606100	-3.63693500	0.95603800
H	5.82627600	-2.05289200	1.27942100
C	8.57052800	-3.46776000	-1.05237400
H	8.15723400	-1.76846000	-2.30241500
C	8.24460400	-4.14652600	0.11993200
H	6.99875500	-4.15904100	1.87304000
H	9.33679400	-3.85928300	-1.71394300
H	8.75814600	-5.06710400	0.37783400
N	1.46232300	2.28052500	-0.84107900
C	2.44547800	3.43082800	-0.77706800

H	3.41531500	3.01195800	-1.03805600
H	2.14776700	4.12893600	-1.56401800
C	2.47233200	4.12946800	0.57919400
H	2.36064500	3.39220300	1.39584900
H	1.63538800	4.83150200	0.65485300
C	0.07294600	2.83428400	-0.70252300
H	-0.67106800	2.04727400	-0.82119600
H	-0.04169600	3.29310400	0.27784900
H	-0.05377600	3.58577600	-1.48148700
C	1.55741000	1.64109200	-2.20245500
H	2.59676100	1.38087800	-2.39155000
H	0.94209900	0.74317200	-2.20719700
H	1.19999800	2.36987600	-2.93177100
N	3.70915500	4.88830800	0.69200500
C	4.84548200	4.01963900	0.97701700
H	5.75382600	4.62581600	1.02437100
H	4.72883700	3.48675900	1.93776500
H	4.98222300	3.27616300	0.18802000
C	3.59371000	5.91162500	1.71808500
H	3.40854700	5.48899800	2.72237700
H	4.51984800	6.49065800	1.75884300
H	2.77483600	6.59379600	1.47388000
C	-0.34564000	-0.87974800	-0.16541900
C	-1.34810800	-1.31123000	0.65723600
H	-0.60784500	-0.15382400	-0.92664700
H	-1.23794000	-2.18201300	1.29360000
C	-2.53392100	-0.49933100	0.75984500
C	0.93939500	-1.56810900	-0.43084400
O	1.52482700	-1.45748100	-1.48634000
O	1.40482900	-2.27283200	0.60584900
C	2.67471100	-2.92053100	0.38123700
C	3.12530900	-3.49677500	1.70403600
H	3.38498900	-2.18430300	-0.00648100
H	2.53833600	-3.69462600	-0.38007400
H	4.08147400	-4.00929600	1.56999000
H	3.25933700	-2.70166300	2.44265700
H	2.39520400	-4.21062100	2.09249900
C	-3.73976100	-1.10053900	1.39732900
C	-4.33799200	-0.50468800	2.51143000
C	-4.26577200	-2.28505400	0.87320600
C	-5.46145100	-1.09061500	3.08665900
H	-3.93298600	0.42054900	2.90600600
C	-5.40460500	-2.85074800	1.43605900
H	-3.79188800	-2.74130900	0.00883700

C	-6.00158000	-2.25476100	2.54509200
H	-5.91973800	-0.63123600	3.95654900
H	-5.82259700	-3.75829800	1.01214400
H	-6.88449100	-2.70160300	2.99162400
N	-2.44041700	0.72075500	0.28980900
S	-3.71479500	1.77004700	0.06691800
O	-4.19767600	2.29608200	1.34122500
O	-3.21542400	2.69869200	-0.94185200
C	-5.00757800	0.79565300	-0.66210600
C	-4.77907400	0.18604200	-1.89767500
C	-6.18698700	0.58337400	0.03374900
C	-5.73494300	-0.66418900	-2.41999200
H	-3.85511600	0.37959600	-2.43407500
C	-7.15650400	-0.26752200	-0.49110800
H	-6.32931400	1.06550100	0.99501000
C	-6.92207100	-0.90360400	-1.71236600
H	-5.59526600	-1.16119600	-3.37332100
H	-8.06988500	-0.43808100	0.06484300
O	-7.78189300	-1.77019400	-2.29765700
C	-8.98353700	-2.06308900	-1.61562500
H	-9.59805200	-1.16442400	-1.48717000
H	-9.51778000	-2.78049500	-2.23728600
H	-8.78352200	-2.50744600	-0.63320000
H	3.14411900	-0.03889100	1.10318300

M2A'

C	1.68311800	1.16069600	0.05436600
C	0.57457500	0.50931800	0.81910300
C	2.93321000	0.69417100	0.22713500
H	0.98660500	0.08642100	1.73644000
H	-0.25310900	1.17400400	1.06770600
C	4.20966800	0.83225500	-0.51078000
O	4.53979400	1.66223600	-1.33358800
O	5.01181300	-0.17180000	-0.13637500
C	6.28428100	-0.24790200	-0.78988600
H	6.14134300	-0.13644200	-1.86860800
H	6.89605600	0.59589700	-0.44963000
C	6.91996500	-1.57051900	-0.45366400
C	6.58847000	-2.27358500	0.70485500
C	7.89136500	-2.08516600	-1.31253000
C	7.22422400	-3.47782400	0.99680300
H	5.82900400	-1.88053500	1.37344500
C	8.53150300	-3.28344500	-1.01582900
H	8.14499200	-1.54644900	-2.22200900

C	8. 19785600	-3. 98407000	0. 14051000
H	6. 95928100	-4. 01931100	1. 89976100
H	9. 28349200	-3. 67502500	-1. 69295400
H	8. 69211800	-4. 92218600	0. 37042200
N	1. 30068400	2. 15580300	-1. 00416800
C	2. 10903400	3. 43104800	-0. 86217200
H	3. 15335800	3. 15970700	-0. 99155700
H	1. 81261000	4. 06664300	-1. 69982700
C	1. 86916700	4. 14758800	0. 46622900
H	1. 73589500	3. 41544600	1. 28745300
H	0. 94904800	4. 73540300	0. 41047800
C	-0. 16650100	2. 53785900	-0. 95368800
H	-0. 81140900	1. 67308700	-1. 09444900
H	-0. 40787500	2. 97579800	0. 01155200
H	-0. 32819700	3. 27111700	-1. 74297000
C	1. 56362900	1. 54351900	-2. 35822800
H	2. 63868400	1. 45801100	-2. 49795000
H	1. 09644100	0. 55842300	-2. 39143000
H	1. 13250600	2. 20836500	-3. 10697100
N	2. 97813100	5. 05255500	0. 71147000
C	4. 14691900	4. 34853900	1. 21900800
H	4. 97162000	5. 05585500	1. 33539500
H	3. 95452200	3. 87349400	2. 19811500
H	4. 47279800	3. 57503300	0. 51815200
C	2. 59680900	6. 12098300	1. 62341000
H	2. 31027600	5. 74621600	2. 62186700
H	3. 43738000	6. 80860100	1. 74522900
H	1. 75501400	6. 68066000	1. 20839500
C	-0. 06540600	-0. 67783800	-0. 00066300
C	-1. 22020800	-1. 27410000	0. 74301000
H	-0. 44573300	-0. 27026600	-0. 94327500
H	-1. 13518000	-2. 24758800	1. 20872500
C	-2. 34875500	-0. 51839700	0. 84551500
C	1. 05434300	-1. 61188300	-0. 38702500
O	1. 51367400	-1. 69464800	-1. 50540300
O	1. 58215700	-2. 25924500	0. 66295700
C	2. 75784800	-3. 03826300	0. 37858700
C	3. 25151600	-3. 60615800	1. 68999800
H	3. 50517300	-2. 38820700	-0. 09086000
H	2. 49835500	-3. 82008000	-0. 34067900
H	4. 15557500	-4. 19570400	1. 51676800
H	3. 49050800	-2. 80258300	2. 39265100
H	2. 49469700	-4. 24718500	2. 14711900
C	-3. 56647600	-1. 09885200	1. 48901000

C	-4.19100900	-0.46781200	2.57016300
C	-4.10845700	-2.28416100	0.98438000
C	-5.33603000	-1.02134000	3.13402700
H	-3.79260700	0.47049600	2.93975500
C	-5.26034000	-2.83001100	1.54326200
H	-3.63269800	-2.75467200	0.12926400
C	-5.87663900	-2.19895900	2.62034200
H	-5.81395700	-0.52570400	3.97355300
H	-5.68026400	-3.74290800	1.13113400
H	-6.77695900	-2.62060800	3.05732100
N	-2.29681200	0.75279300	0.32601600
S	-3.54645400	1.71655400	0.06006600
O	-4.16642900	2.27038100	1.27206300
O	-3.07208600	2.69545300	-0.93423400
C	-4.79500600	0.69801800	-0.71403500
C	-4.48165200	0.00257500	-1.88282800
C	-6.01436800	0.50502700	-0.08510700
C	-5.38982300	-0.89763400	-2.41007800
H	-3.51782800	0.16096700	-2.35773500
C	-6.93660900	-0.39946500	-0.60956500
H	-6.21987200	1.04249800	0.83469600
C	-6.61570200	-1.11115600	-1.76559400
H	-5.17668000	-1.46261100	-3.31089500
H	-7.87830000	-0.55463600	-0.09768200
O	-7.42630200	-2.03822500	-2.34266800
C	-8.63915900	-2.33292400	-1.68701000
H	-9.29695100	-1.45632500	-1.64663500
H	-9.11980800	-3.11728000	-2.27145900
H	-8.46165000	-2.69414000	-0.66635000
H	3.00784600	-0.05863000	1.00603400