

Electronic Supplementary Information for

Insights to Ag(I)-catalyzed addition reactions of amino alcohols to electron-deficient olefins: Competing mechanisms, role of catalyst, and origin of chemoselectivity

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1. Test the impact of different computational methods

Table S1. Relative free energies (ΔG) [$\text{kcal}\cdot\text{mol}^{-1}$] between TS1-O and **1+3'** geometries at the different theory levels.

ΔG	Method1	Method2	Method3
TS3	11.8	11.1	10.7
1+3'	0.0	0.0	0.0

Method1: Geometry B3LYP/SDD,6-31g(d), single point energies in solution M06/SDD,6-31+g(d,p).
Method2: Geometry B3LYP/SDD,6-31g(d), single point energies in solution B97D/SDD,6-31+g(d,p).
Method3: Geometry B3LYP/SDD,6-31g(d), single point energies in solution B3LYP-D3/ SDD,6-31+g(d,p).

To test the impact of different computational methods on the calculated results, we additionally computed the rate-determining step by using different computational methods. As summarized in **Table S1**, the free energies calculated by the different methods are very close and have small differences, which indicate that the calculated results should be reliable by using the selected computational method.

2. The possible reaction pathways via TS1'-O and TS1'-N

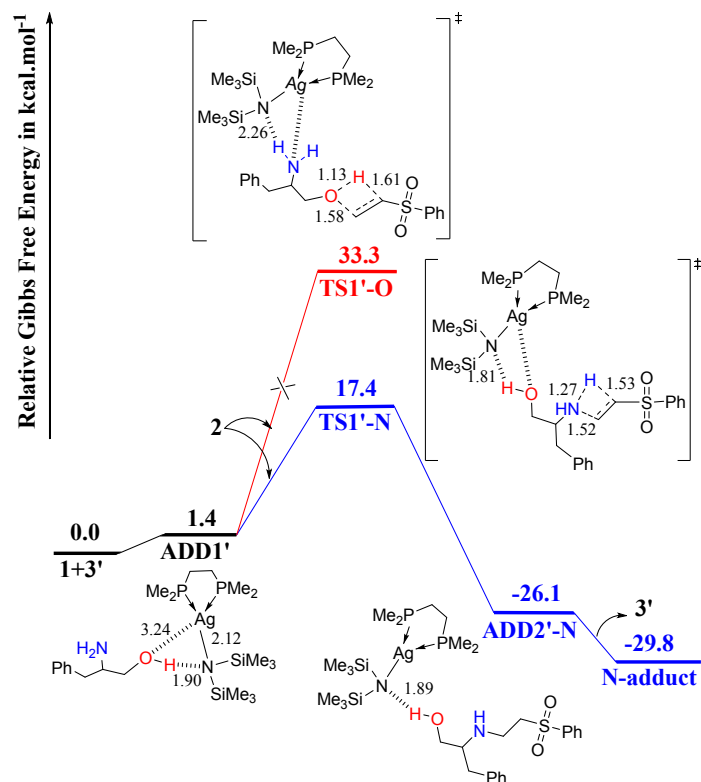


Fig. S1 Computed Gibbs free-energy profiles (253 K) for the possible reaction pathways via TS1'-O and TS1'-N catalyzed by 3' (distances in Å).

3. Chemoselective addition reaction pathways catalyzed by the real system

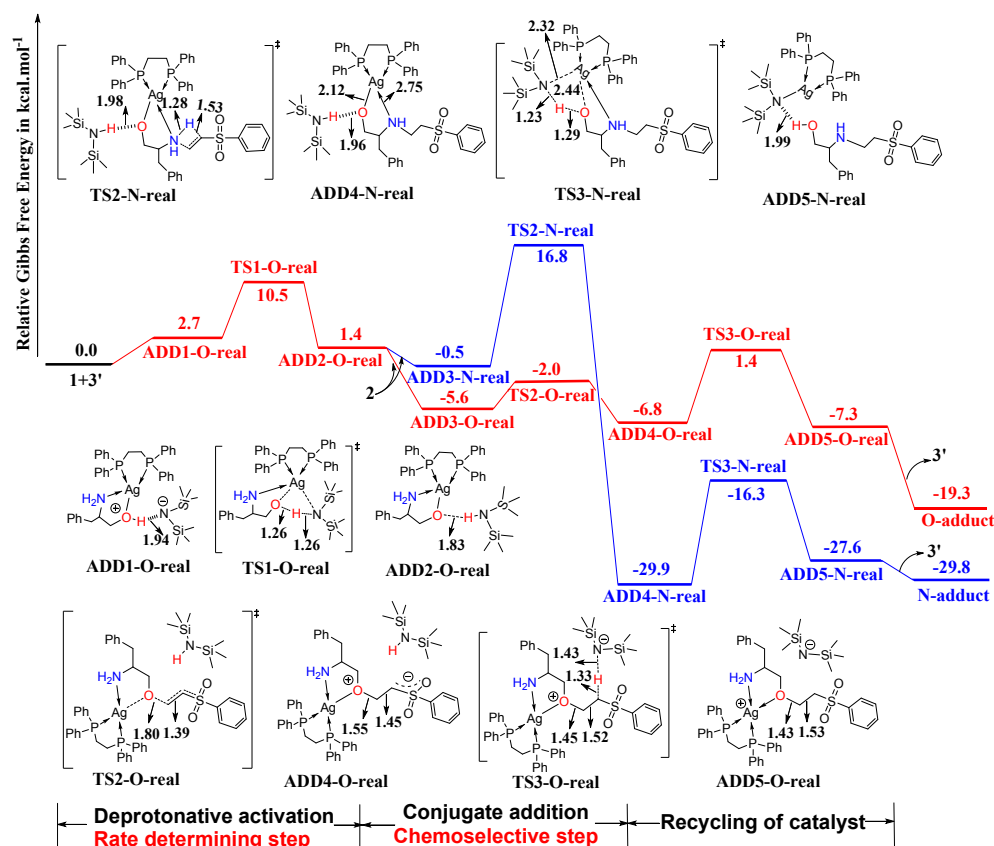


Fig. S2 Computed free-energy profiles (253 K) for chemoselective addition reactions catalyzed by **3** system (distances in Å).

We additionally reoptimized all the structures depicted in **Fig. 2** with the actual dppe ligand by using catalyst **3**. The computed free-energy profiles and energy barriers (**Fig. S2**) showed the same trend and conclusions as the calculated results of the model systems. This indicates that the selected models and the computed results should be suitable and reliable.

4. Compared the hydrogen bond between Int1 and ADD2-O

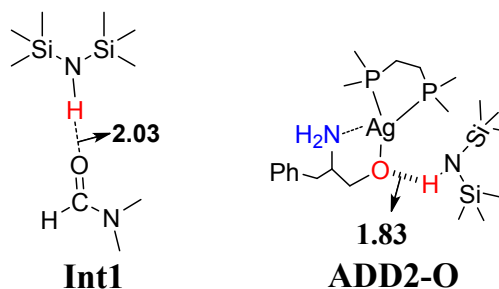


Fig. S3 Computed structures of Int1 and ADD2-O (distances in Å).

In order to study if the HN(SiMe₃)₂ molecule bonded to O atom of adduct or to DMF solution, we compared the hydrogen bond of Int1 (2.03 Å) with that of ADD2-O (1.83 Å), the hydrogen bond of ADD2-O is stronger than that of Int1, so the HN(SiMe₃)₂ molecule hydrogen bonded to O atom of adduct is more favorable than hydrogen bonded to DMF.

5. Parr function analysis

Pioneered by Domingo and coworkers, the nucleophilic (P_k^-) and electrophilic (P_k^+) Parr functions which allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the corresponding radical cations (RC) or anions (RA) of the studied molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

$$P^-(r) = \rho_S^{rc}(r) \text{ for the electrophilic attacks} \quad (1)$$

$$P^+(r) = \rho_S^{ra}(r) \text{ for the nucleophilic attacks} \quad (2)$$

where $\rho_S^{rc}(r)$ is the ASD of the radical cation and $\rho_S^{ra}(r)$ is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic P_k^- and electrophilic P_k^+ Parr functions of the neutral system, respectively.

6. Cartesian coordinates (Å) of the computed structures

1

C	3.11692700	0.62118200	0.04204600
H	3.71491100	0.84865700	0.94416800
H	3.23952800	1.46140000	-0.65104400
C	1.64155200	0.46535200	0.45197700
H	1.33880500	1.36012000	1.02389800
O	3.58865100	-0.54408600	-0.60297800
H	3.18190100	-1.27215700	-0.09249500
N	1.56141600	-0.77329600	1.24587200
H	1.95180600	-0.61912700	2.17452600
H	0.58943100	-1.04703800	1.37752600
C	0.72890800	0.35074100	-0.78839500
H	0.86278300	1.26302400	-1.38309200
H	1.09219100	-0.48387100	-1.39693600
C	-0.73658900	0.16794800	-0.45557700
C	-1.33064500	-1.10286200	-0.47231500
C	-1.53225500	1.26643900	-0.09460400
C	-2.67550500	-1.27319800	-0.13297100
H	-0.73391600	-1.96446100	-0.76382200
C	-2.87567000	1.10169400	0.24250300
H	-1.09320900	2.26209000	-0.08580600
C	-3.45225100	-0.17112200	0.22621800
H	-3.11587100	-2.26670900	-0.15659800
H	-3.47478700	1.96732900	0.51337400
H	-4.49952900	-0.30055300	0.48572800

2

C	5.62405600	-0.98835900	-1.10307800
C	4.25948000	-0.70720800	-1.00746700
C	3.83727700	0.37850900	-0.23731300
C	4.76098500	1.19315500	0.42333200
C	6.12183100	0.90417800	0.32253200
C	6.55379900	-0.18790200	-0.43574000
H	5.96079100	-1.82685100	-1.70697100
H	3.52480200	-1.29885500	-1.54326800
H	4.41278500	2.05269900	0.98731000
H	6.84630500	1.53668000	0.82842200
H	7.61508000	-0.40803100	-0.51421500
S	2.06973000	0.73153600	-0.05949300
O	1.95173300	2.19589600	0.04844000
O	1.41422000	0.00472900	-1.18498400
C	1.48943900	0.01614200	1.41765900
H	1.86831300	0.50340800	2.31104600
C	1.27322015	-1.30626618	1.42693368
H	1.62886615	-1.90059018	0.58418468
H	1.42949815	-1.81375618	2.37754068

3'

Ag	0.05639200	-0.64846800	-0.33163600
P	2.23800800	-1.57340000	-0.54803600
C	3.49644500	-1.03608400	0.72095200
H	4.33479700	-1.74518600	0.67699600
H	3.01911800	-1.17301900	1.69908500
C	4.03506000	0.40009000	0.58569400
H	4.71464300	0.59567300	1.42720200
H	4.63912800	0.48023700	-0.32729800
P	2.73932600	1.76368100	0.48485500
C	3.09056100	-1.30119900	-2.16364100
H	4.10101500	-1.72602900	-2.16369400
H	2.50587300	-1.77149700	-2.96042900
H	3.14633500	-0.22962300	-2.37484400
C	2.29156600	-3.41180000	-0.35714700
H	1.90258100	-3.68791800	0.62800700
H	1.65188500	-3.87665200	-1.11360200
H	3.31170200	-3.79913500	-0.46122000
C	3.89237800	3.22645300	0.59484400
H	3.30044600	4.14342100	0.68480800
H	4.57681400	3.16556600	1.45036900
H	4.48226200	3.30356400	-0.32497100
C	2.09120800	1.74241400	2.23188600
H	2.89231400	1.75059400	2.98210800
H	1.45661300	2.62200000	2.38422800
H	1.45942000	0.86178700	2.38668100
N	-1.88503700	0.05987400	-0.06747200
Si	-2.28681100	1.50243600	-0.93066200
Si	-2.90740200	-0.88879000	0.94976700
C	-4.01509900	0.16604000	2.08790500
H	-4.63981400	-0.47161700	2.72752300
H	-3.41127700	0.80606000	2.74351600
H	-4.68955600	0.81969500	1.52142000
C	-4.05323900	-2.05125500	-0.03269800
H	-4.72313500	-1.48647000	-0.69220800
H	-3.46601200	-2.72831300	-0.66698900
H	-4.67746900	-2.66810300	0.62777200
C	-1.87504200	-2.00428600	2.10290400
H	-1.20231800	-1.40796800	2.73321400
H	-2.52368900	-2.58945800	2.76877300
H	-1.26151200	-2.71773300	1.53570800
C	-4.04790400	1.46717600	-1.65992400
H	-4.26293500	2.39281400	-2.21021700
H	-4.16890100	0.62948700	-2.35818200
H	-4.81751400	1.36263400	-0.88533600
C	-2.15898100	3.06038500	0.15889300
H	-2.38711300	3.97545200	-0.40394000
H	-2.84974200	3.01090800	1.00951900
H	-1.14431900	3.16214600	0.56594500

C	-1.09848700	1.76560900	-2.39635000
H	-0.05927700	1.87383400	-2.05781600
H	-1.13981900	0.92072400	-3.09621700
H	-1.35755700	2.67447100	-2.95635800
4'			
O	-2.76768000	-0.23101400	-1.06526400
C	-3.27692000	-0.11815200	0.09769200
C	-4.79777700	-0.08050900	0.19397500
H	-5.12710100	-0.08440100	1.23522000
H	-5.17196000	0.82317200	-0.30088400
H	-5.22607300	-0.93802600	-0.33541200
O	-2.58655800	-0.02616600	1.15203000
Ag	-0.62884200	-0.16893100	-0.25709500
P	1.36777900	-1.62496700	0.03616400
C	2.66651200	-0.43086600	0.67004200
H	3.65842400	-0.89963300	0.61973500
H	2.44681000	-0.26967900	1.73349800
C	2.67882700	0.91982900	-0.07370100
H	3.46521800	1.56575800	0.33933000
H	2.92397400	0.76291400	-1.13250600
P	1.02879900	1.81350700	-0.03182700
C	2.21581600	-2.38620600	-1.42763900
H	3.19401500	-2.80492600	-1.16201000
H	1.58565500	-3.18288600	-1.83550000
H	2.34919500	-1.63499000	-2.21249600
C	1.47211800	-2.98421800	1.29011200
H	1.07006200	-2.63065200	2.24464000
H	0.85417900	-3.82482800	0.95909000
H	2.50095900	-3.33422400	1.43734400
C	1.39858200	3.27641500	-1.11412100
H	0.55206900	3.96952300	-1.07971600
H	2.30531200	3.80740700	-0.79975700
H	1.51829600	2.94615000	-2.15094800
C	1.04964900	2.58451900	1.65561600
H	1.96104000	3.16787100	1.83487900
H	0.17832200	3.23912400	1.75756500
H	0.96158900	1.80655100	2.42035700
N-adduct			
C	2.60524000	2.00490800	-1.01850700
C	1.93889500	1.06855600	-0.22578600
C	2.54480400	-0.16815000	0.00804900
C	3.80202900	-0.47984900	-0.51667200
C	4.45596900	0.46475900	-1.30764300
C	3.85655700	1.70234500	-1.56037000
H	2.14568600	2.97131700	-1.20416100
H	0.97816700	1.29923300	0.22276800

H	4.26430800	-1.43414200	-0.28512000
H	5.43623300	0.23931700	-1.71774300
H	4.37175600	2.43586600	-2.17450900
S	1.70121000	-1.38388600	1.03451100
O	2.72154900	-2.20964900	1.69903200
O	0.67668300	-0.66709100	1.82142200
C	0.83601100	-2.47465000	-0.14855500
H	1.61871800	-2.89991900	-0.78379500
C	-0.26245900	-1.80998500	-0.97983200
H	0.15611200	-0.94844900	-1.53087200
H	-0.56765200	-2.53924000	-1.74030600
C	-3.44431500	-2.08746800	-1.37883100
H	-2.90551300	-2.70197300	-2.12255500
H	-4.36026700	-1.72626500	-1.86028100
C	-2.55368700	-0.90416300	-0.95246800
H	-2.19684800	-0.38363000	-1.85942400
O	-3.82165200	-2.85780700	-0.25679800
H	-3.00137500	-2.90660500	0.27330300
N	-1.42928600	-1.45705300	-0.17653700
H	0.42381500	-3.26779800	0.48414400
H	-1.13889000	-0.81631300	0.55924500
C	-3.34660700	0.10992800	-0.09751700
H	-4.25789700	0.36850400	-0.65083200
H	-3.67045400	-0.39392900	0.81976400
C	-2.57373800	1.37176400	0.22607500
C	-1.95075600	1.54876300	1.46939700
C	-2.44331100	2.38977000	-0.73226200
C	-1.21034900	2.70181700	1.74555400
H	-2.04245300	0.77864900	2.23126200
C	-1.71022700	3.54474300	-0.46035400
H	-2.93006600	2.27731600	-1.69909600
C	-1.08800300	3.70388600	0.78172800
H	-0.73374500	2.81381900	2.71548900
H	-1.63139800	4.32460100	-1.21370100
H	-0.52155000	4.60572200	0.99874500

O-adduct

C	5.46565700	-1.19565100	-0.75126400
C	4.14200100	-0.77304600	-0.88954600
C	3.72246200	0.37238400	-0.21026000
C	4.60212500	1.11094100	0.58590400
C	5.92102600	0.67716700	0.71905400
C	6.35014100	-0.47569200	0.05486800
H	5.80619100	-2.08229600	-1.27842400
H	3.44472600	-1.30244600	-1.53014800
H	4.26196200	2.02088500	1.07019100
H	6.61593300	1.24380900	1.33223200
H	7.37941100	-0.80770200	0.15913800
S	2.01658900	0.93135400	-0.37816100

O	2.01678000	2.40253200	-0.32319100
O	1.44359400	0.22345200	-1.54541300
C	1.17496100	0.34239200	1.12417500
H	1.69293600	0.82787800	1.95629800
C	1.07672900	-1.19081700	1.29505800
H	1.75337100	-1.71440200	0.60404800
H	1.39754700	-1.44429800	2.31037800
C	-0.75629000	-1.89878000	-0.12696900
H	0.02351200	-1.73756100	-0.88094600
H	-1.07934500	-2.94766900	-0.18827900
C	-1.96360600	-1.00218600	-0.43913800
H	-2.37392300	-1.38983300	-1.39222500
O	-0.23787600	-1.69345600	1.18661600
H	0.16364700	0.75665500	1.02020200
N	-1.54747200	0.39881600	-0.53751900
H	-0.86755600	0.51001900	-1.28924800
H	-2.35068400	0.98433200	-0.75878100
C	-3.06196900	-1.15282200	0.63686100
H	-3.30135700	-2.22003900	0.73128900
H	-2.63854100	-0.82919800	1.59262000
C	-4.32292200	-0.37500300	0.32492300
C	-4.54006200	0.89967100	0.86878300
C	-5.29548700	-0.90075100	-0.53942100
C	-5.69023700	1.62849800	0.55665000
H	-3.79952100	1.32055300	1.54473100
C	-6.44650700	-0.17738200	-0.85298100
H	-5.14997500	-1.89161900	-0.96530800
C	-6.64771700	1.09215600	-0.30556400
H	-5.83898700	2.61352000	0.99174400
H	-7.18909400	-0.60648100	-1.52098400
H	-7.54517700	1.65582600	-0.54620800

TS1-N-non

C	-3.47224800	2.09625600	-0.96739700
C	-2.63430100	0.97963000	-0.92968900
C	-2.96104600	-0.09374700	-0.09772700
C	-4.11902500	-0.06805200	0.68490300
C	-4.94946600	1.05161400	0.64118000
C	-4.62528600	2.13521900	-0.18058700
H	-3.22915900	2.93135500	-1.61917700
H	-1.75014600	0.91880100	-1.55509200
H	-4.37142700	-0.92757600	1.29777200
H	-5.85519200	1.07520000	1.24126500
H	-5.27677600	3.00439000	-0.21448700
S	-1.86102500	-1.52899000	0.00978000
O	-2.73341800	-2.69425200	0.24261600
O	-1.01542600	-1.46180600	-1.22318800
C	-0.76201600	-1.35040400	1.34919100
H	-1.27402900	-1.31224800	2.30860700

C	0.38259900	-0.38600400	1.08999600
H	0.21375400	0.50489200	0.48092900
H	0.87321000	-0.09854000	2.02272700
C	3.24893500	-2.79597300	0.11684400
H	2.85816400	-3.50242100	0.86268700
H	4.34267100	-2.82978100	0.16216800
C	2.77426000	-1.37083400	0.46097200
H	3.01947700	-1.16608800	1.51068900
O	2.88631800	-3.17754800	-1.20171300
H	1.97999200	-3.52263500	-1.18902900
N	1.29474000	-1.37037300	0.36130700
H	0.51516900	-2.16378100	0.89475800
H	0.96332300	-1.39832000	-0.61247400
C	3.45348500	-0.32725300	-0.45389600
H	4.53685900	-0.43469400	-0.30677800
H	3.25376800	-0.61389100	-1.49242500
C	3.05086200	1.11291800	-0.21718600
C	2.23054800	1.78784600	-1.13109700
C	3.48977200	1.80349200	0.92227500
C	1.84913100	3.11333600	-0.90933400
H	1.89166500	1.27189300	-2.02674100
C	3.11002900	3.12674700	1.14860200
H	4.14244200	1.30306000	1.63529100
C	2.28550000	3.78567200	0.23316600
H	1.21502800	3.61997700	-1.63193700
H	3.46276000	3.64579500	2.03591300
H	1.99147700	4.81712500	0.40668700

TS1-O-non

C	5.62405600	-0.98835900	-1.10307800
C	4.25948000	-0.70720800	-1.00746700
C	3.83727700	0.37850900	-0.23731300
C	4.76098500	1.19315500	0.42333200
C	6.12183100	0.90417800	0.32253200
C	6.55379900	-0.18790200	-0.43574000
H	5.96079100	-1.82685100	-1.70697100
H	3.52480200	-1.29885500	-1.54326800
H	4.41278500	2.05269900	0.98731000
H	6.84630500	1.53668000	0.82842200
H	7.61508000	-0.40803100	-0.51421500
S	2.06973000	0.73153600	-0.05949300
O	1.95173300	2.19589600	0.04844000
O	1.41422000	0.00472900	-1.18498400
C	1.48943900	0.01614200	1.41765900
H	1.86831300	0.50340800	2.31104600
C	1.25230100	-1.43420900	1.42783100
H	1.60794700	-2.02853300	0.58508200
H	1.40857900	-1.94169900	2.37843800
C	-0.91633800	-1.90513600	0.04435100

H	-0.15483300	-1.88155000	-0.74091900
H	-1.23177600	-2.93501900	0.23467400
C	-2.09745600	-1.01301000	-0.34788500
H	-2.44681800	-1.41138200	-1.31991200
O	-0.32148400	-1.38917400	1.27059300
H	-0.08993600	-0.24699700	1.23459500
N	-1.61776500	0.36125000	-0.41068400
H	-0.83779500	0.45786300	-1.06076900
H	-2.36168200	0.99571300	-0.68877700
C	-3.27147800	-1.12583800	0.65296100
H	-3.54921800	-2.18471200	0.73596000
H	-2.91630300	-0.80155800	1.63680600
C	-4.48197600	-0.31383100	0.24247700
C	-4.68419900	0.98221300	0.73922600
C	-5.41531600	-0.83085800	-0.66842700
C	-5.78434700	1.74159500	0.33405000
H	-3.97307500	1.39588600	1.45020900
C	-6.51629100	-0.07612400	-1.07430200
H	-5.28103900	-1.83836200	-1.05746300
C	-6.70387300	1.21465700	-0.57419600
H	-5.92363000	2.74320800	0.73233400
H	-7.23049100	-0.49734900	-1.77715200
H	-7.56243300	1.80265700	-0.88720500

ADD1-O

Ag	1.43919500	0.40934400	0.74798200
P	0.03978800	1.94991900	1.91111600
C	-1.35810100	2.74831400	0.96704100
H	-2.13616700	2.99693600	1.70242300
H	-1.77048100	1.96733600	0.31523200
C	-1.01013900	4.01621200	0.16589200
H	-1.93286800	4.40198700	-0.29081000
H	-0.65210900	4.79887900	0.84716600
P	0.30488000	3.81184000	-1.16331000
C	0.82298600	3.34160800	2.84235100
H	0.07393800	3.95361800	3.35795300
H	1.51478900	2.92845500	3.58324900
H	1.39819100	3.97208200	2.15856400
C	-0.88907400	1.05226900	3.23522600
H	-1.49494000	0.26523800	2.77585100
H	-0.18384200	0.57519100	3.92249300
H	-1.54156100	1.72919400	3.79931100
C	0.26503600	5.54757300	-1.84752200
H	0.85663700	5.58489700	-2.76848500
H	-0.75282900	5.89150700	-2.07119900
H	0.72254400	6.24024100	-1.13277300
C	-0.70178700	2.93597000	-2.46355000
H	-1.62654100	3.47526300	-2.70697900
H	-0.10448900	2.82740400	-3.37477800

H	-0.95807400	1.93310800	-2.10840700
N	2.43387500	-1.24415600	-0.15885800
H	0.56880700	-1.70572400	-0.40962600
Si	3.29198600	-0.81289200	-1.60651500
Si	2.91007200	-2.49879300	0.95156100
C	4.75885400	-2.45799400	1.41129700
H	5.00064300	-3.24317700	2.13999900
H	5.40652700	-2.61161600	0.53925700
H	5.03361100	-1.49370200	1.85766900
C	1.93538600	-2.34897100	2.57947300
H	2.19826900	-1.43377200	3.12710300
H	0.85521200	-2.33573800	2.38879000
H	2.14734500	-3.19979500	3.24105600
C	2.52954200	-4.23052100	0.25925600
H	3.08761800	-4.43916900	-0.66060500
H	2.78503400	-5.01217900	0.98688000
H	1.46116100	-4.32795000	0.02909400
C	3.94253400	-2.32570300	-2.56554200
H	4.43244400	-2.00526900	-3.49454600
H	4.68041500	-2.89796400	-1.99026600
H	3.13241500	-3.01294600	-2.83850300
C	2.14315900	0.13009800	-2.79428200
H	2.67782400	0.42377300	-3.70748200
H	1.28455900	-0.48389900	-3.09422400
H	1.75436000	1.04443400	-2.32878200
C	4.78490800	0.32195300	-1.27719000
H	4.46650700	1.25457900	-0.79286100
H	5.51421400	-0.15923700	-0.61421000
H	5.30435600	0.58991100	-2.20713600
C	-1.10167900	-2.07894900	-1.43086600
H	-0.62728400	-1.62466100	-2.31643700
H	-1.10445400	-3.17101500	-1.59179400
C	-2.56279200	-1.61385800	-1.36880200
H	-3.07578200	-2.12084900	-2.20797000
O	-0.40952800	-1.74612400	-0.24828100
N	-2.65285900	-0.14774300	-1.49032500
H	-2.33892900	0.12561500	-2.42084400
H	-3.63364800	0.12693000	-1.43456700
C	-3.24657600	-2.07312600	-0.06377800
H	-3.08343500	-3.15322600	0.04002500
H	-2.73324900	-1.58955000	0.77250000
C	-4.73087200	-1.77494600	-0.02511500
C	-5.23072700	-0.65543800	0.65619900
C	-5.64601000	-2.60234900	-0.69498300
C	-6.59801300	-0.36746400	0.66603100
H	-4.53846000	-0.00851500	1.19070500
C	-7.01205500	-2.32023400	-0.68783000
H	-5.28121100	-3.48210100	-1.22127600
C	-7.49388500	-1.19921900	-0.00695000
H	-6.96256100	0.50363200	1.20484200

H	-7.70222800	-2.97883100	-1.20902900
H	-8.55831000	-0.98034400	0.00291500

TS1-O

Ag	0.87611100	0.20181900	0.63700300
P	-0.29024800	1.84814700	1.90584600
C	-1.43595700	2.98376700	0.96843900
H	-2.18021300	3.35989800	1.68443800
H	-1.96712200	2.34159100	0.25526400
C	-0.78061400	4.17811400	0.25196600
H	-1.56888000	4.76149900	-0.24496600
H	-0.32073600	4.84616800	0.99154600
P	0.55921500	3.74989600	-0.99666700
C	0.67935200	2.98219000	2.99847600
H	0.02838000	3.67483500	3.54487500
H	1.24335300	2.38140100	3.71904300
H	1.39688100	3.55190400	2.40141500
C	-1.46649200	1.06615600	3.10224800
H	-2.18221800	0.44573800	2.55441000
H	-0.91632100	0.41639600	3.78984900
H	-2.01200300	1.82177800	3.67993000
C	0.87584000	5.47190700	-1.64310000
H	1.54173600	5.41479100	-2.51076100
H	-0.04578100	5.98687300	-1.94276000
H	1.38133600	6.07049800	-0.87745000
C	-0.49982300	3.08228900	-2.37593900
H	-1.30496800	3.77463600	-2.65459500
H	0.12557600	2.89523100	-3.25548500
H	-0.93748800	2.12817300	-2.06565000
N	2.33773800	-1.36138100	-0.19100200
H	1.19964800	-1.69365700	-0.58367700
Si	3.39464900	-0.68496300	-1.42114900
Si	2.84075000	-2.52525000	1.03306600
C	4.52349900	-2.08736900	1.79855300
H	4.77698000	-2.80107400	2.59333100
H	5.33864900	-2.11359300	1.06565300
H	4.51141800	-1.08536900	2.24512000
C	1.55923300	-2.57542200	2.43084300
H	1.56796300	-1.64963400	3.02170300
H	0.55264500	-2.70778500	2.01746800
H	1.75944500	-3.40815300	3.11817500
C	2.94228000	-4.27315500	0.29902000
H	3.70012500	-4.34696900	-0.48940900
H	3.18982200	-5.01481900	1.06961600
H	1.97808300	-4.55864900	-0.13943100
C	4.52758100	-1.99018200	-2.21480200
H	5.12895400	-1.54192700	-3.01664200
H	5.22585100	-2.42987500	-1.49244300
H	3.94757900	-2.81017400	-2.65556100

C	2.32619200	0.05480100	-2.80216800
H	2.95473600	0.51312400	-3.57686900
H	1.70683400	-0.71192500	-3.28237300
H	1.65623000	0.83068900	-2.41281100
C	4.49651900	0.69635800	-0.72765800
H	3.88611000	1.51054100	-0.31688600
H	5.15255700	0.33404400	0.07244600
H	5.13423500	1.12119600	-1.51431200
C	-0.83398000	-1.95068900	-1.68368700
H	-0.41537700	-1.46824200	-2.59287400
H	-0.86236900	-3.03694300	-1.90436100
C	-2.30663900	-1.49958400	-1.57688700
H	-2.83476600	-1.97824100	-2.42417700
O	-0.07908400	-1.69282000	-0.54936700
N	-2.42088600	-0.02823000	-1.65150100
H	-2.08750700	0.27009400	-2.56791100
H	-3.40895700	0.22551500	-1.62110500
C	-2.95872500	-2.00985900	-0.27683800
H	-2.77217900	-3.08920400	-0.21219800
H	-2.43424200	-1.54580200	0.56389500
C	-4.44740600	-1.74601900	-0.19845100
C	-4.95831000	-0.63316700	0.48626700
C	-5.36151500	-2.60021900	-0.83594900
C	-6.33132600	-0.37807800	0.53176700
H	-4.26845200	0.03744800	0.99443100
C	-6.73347100	-2.35179900	-0.79368100
H	-4.98904300	-3.47457700	-1.36574000
C	-7.22492700	-1.23726400	-0.10910800
H	-6.70228300	0.48888500	1.07321800
H	-7.42084000	-3.03174500	-1.29087800
H	-8.29385700	-1.04456000	-0.07160400

ADD2-O

Ag	-0.62821700	0.82621100	0.32142700
P	-0.43834700	2.43378900	2.05095800
C	-0.21671500	4.17382800	1.41568200
H	0.17168000	4.78840500	2.23897000
H	-1.21490700	4.56372200	1.17753000
C	0.71067300	4.26283100	0.18609900
H	1.11392200	5.28066200	0.09757800
H	1.57309800	3.59575800	0.31019800
P	-0.14015000	3.78672300	-1.42549700
C	1.03383300	2.22329800	3.15255100
H	1.07394100	2.99933900	3.92619100
H	0.99498300	1.23821100	3.62714900
H	1.94842400	2.26284400	2.55310400
C	-1.81126100	2.63853100	3.27622500
H	-2.74589100	2.85523700	2.74933600
H	-1.94408600	1.70629300	3.83423600

H	-1.60190600	3.44855300	3.98464400
C	1.34932800	3.72741800	-2.54194100
H	1.01697500	3.67466400	-3.58426100
H	1.99880300	4.60403800	-2.42592700
H	1.92809900	2.82180400	-2.33378400
C	-0.82871700	5.45730300	-1.90513300
H	-0.06218900	6.24244800	-1.91804800
H	-1.27896600	5.39130600	-2.90149000
H	-1.62077200	5.75116700	-1.20721900
N	2.77426300	-1.89291100	-0.22671200
H	1.87115300	-1.47677100	-0.53453100
Si	4.13437100	-1.12569600	-0.99012700
Si	2.55477500	-2.98389200	1.10769100
C	4.20751000	-3.75272000	1.63197500
H	4.06141100	-4.41554100	2.49450600
H	4.64949700	-4.35187600	0.82759000
H	4.94271700	-2.99325700	1.92572200
C	1.81776100	-2.07814000	2.61059800
H	2.51491300	-1.31917100	2.98837500
H	0.89205300	-1.56498400	2.31879400
H	1.58179400	-2.76223400	3.43656200
C	1.35290600	-4.37082400	0.63347000
H	1.75522800	-4.97732600	-0.18686100
H	1.14465100	-5.03963800	1.47870300
H	0.39789700	-3.95044600	0.29515500
C	5.44416600	-2.37017700	-1.57135000
H	6.24695700	-1.85916200	-2.11919400
H	5.90919900	-2.90757700	-0.73665500
H	5.00379600	-3.11654700	-2.24348100
C	3.46336200	-0.18244600	-2.49116000
H	4.18357200	0.55343300	-2.87059600
H	3.22014600	-0.86774300	-3.31234000
H	2.53597400	0.33516800	-2.21725900
C	5.01174000	0.11366100	0.15953000
H	4.32320400	0.90942600	0.47300700
H	5.37969600	-0.37776200	1.06943900
H	5.87280100	0.58804700	-0.32974700
C	-0.46846900	-1.01384000	-2.02936000
H	-0.34396300	-0.27344800	-2.85272200
H	-0.14865600	-1.98838300	-2.44737500
C	-1.99332900	-1.11882100	-1.76754500
H	-2.49255400	-1.32603800	-2.72974300
O	0.27060700	-0.68346500	-0.90989900
N	-2.45540000	0.16970300	-1.20417200
H	-2.41232900	0.90115800	-1.91273000
H	-3.42164200	0.10443400	-0.88890200
C	-2.33003000	-2.26373200	-0.79194800
H	-1.94564300	-3.19091300	-1.23549000
H	-1.77030300	-2.09712100	0.13484600
C	-3.80827900	-2.40950800	-0.49931700

C	-4.37222000	-1.88428200	0.67334600
C	-4.66198100	-3.04983000	-1.41187900
C	-5.74319800	-1.98802100	0.92471200
H	-3.72412100	-1.40043700	1.40153900
C	-6.03042300	-3.15796200	-1.16496500
H	-4.24402900	-3.47362500	-2.32274500
C	-6.57763900	-2.62462600	0.00521700
H	-6.15627600	-1.57814800	1.84316000
H	-6.67047500	-3.66355500	-1.88371400
H	-7.64327900	-2.71123900	0.20015400

ADD1-N

Ag	-1.37615100	-1.10246200	-0.18004600
P	-2.89029800	3.26500600	0.32186500
C	-4.13608000	2.61356500	-0.93036000
H	-4.30372500	3.38301700	-1.69773000
H	-5.08791600	2.49765600	-0.39683700
C	-3.78317000	1.30196900	-1.65412200
H	-4.57826400	1.08081500	-2.37832400
H	-2.86039300	1.42485700	-2.23197700
P	-3.56313500	-0.25038600	-0.62040800
C	-1.50286700	3.77819700	-0.80958100
H	-1.86032100	4.21556500	-1.75085800
H	-0.89358100	4.52817500	-0.29194800
H	-0.84941300	2.92174800	-1.00539000
C	-3.69700800	4.92363300	0.61641000
H	-4.64469500	4.78716300	1.14889800
H	-3.04618300	5.53296700	1.25251800
H	-3.89143000	5.47414100	-0.31290100
C	-4.49281000	-1.48834500	-1.63853400
H	-4.49879000	-2.45521100	-1.12607700
H	-5.52622400	-1.16632400	-1.81287200
H	-3.99284800	-1.62196600	-2.60303700
C	-4.67346000	-0.04806900	0.84222900
H	-5.69487400	0.21588800	0.54606600
H	-4.69712700	-0.99494100	1.39099300
H	-4.27215500	0.72273000	1.50553900
H	1.00124100	0.48209100	0.38246900
N	0.44425500	-2.12417700	0.08848800
Si	0.63849300	-2.86970500	1.63935300
Si	1.18374000	-2.62245200	-1.39266200
C	1.28187000	-1.17867000	-2.63273000
H	0.30150700	-0.70820100	-2.78745200
H	1.97112800	-0.39758200	-2.28851400
H	1.64021200	-1.52530200	-3.61129100
C	2.97149700	-3.24953000	-1.16584000
H	3.61619400	-2.48445400	-0.71512500
H	3.02472600	-4.13982300	-0.52744100
H	3.40842300	-3.51825800	-2.13676700

C	0.22541900	-4.01678800	-2.27219300
H	-0.79706100	-3.69564400	-2.51329900
H	0.70869800	-4.32188500	-3.21016300
H	0.14533800	-4.90402200	-1.63219400
C	0.53694800	-4.77457000	1.58620800
H	0.65145200	-5.20552000	2.58986200
H	-0.43409400	-5.10295700	1.19315100
H	1.31362700	-5.21633900	0.94977600
C	2.31495900	-2.43936800	2.44264200
H	2.41026000	-2.88853400	3.44011700
H	3.16010800	-2.78994000	1.83876300
H	2.42159900	-1.35267300	2.55391200
C	-0.70951600	-2.29570400	2.85122200
H	-0.70845700	-1.20438500	2.95726500
H	-1.70803000	-2.61107000	2.51838000
H	-0.54778400	-2.73034000	3.84748000
C	0.79250600	2.25545300	2.34841100
H	-0.20643600	2.58938500	2.05619300
H	1.18446600	2.95156400	3.10733800
C	1.70349800	2.27246200	1.11405900
H	1.71221200	3.31198900	0.75283700
O	0.60221700	0.95597600	2.90179400
N	1.10477100	1.44815600	0.06454800
C	3.17200400	1.90360200	1.48148900
H	3.49205900	2.53681500	2.32155100
H	3.20022500	0.86277300	1.82874800
C	4.13669100	2.07501100	0.32974000
C	4.48200400	0.99500900	-0.49571400
C	4.67913700	3.33518700	0.03526700
C	5.34004300	1.16880900	-1.58470000
H	4.08584100	0.00660100	-0.27510900
C	5.53717600	3.51319400	-1.05007900
H	4.43006300	4.18406400	0.66926200
C	5.86970100	2.42886200	-1.86607900
H	5.59682300	0.31643000	-2.20819800
H	5.95057200	4.49731400	-1.25607700
H	6.54039000	2.56489100	-2.71028700
H	1.43586900	0.65553500	3.29462400
H	1.71392700	1.41870900	-0.75131100

TS1-N

Ag	-1.15761100	-0.08235300	-0.91282400
P	-3.66807300	-2.23141400	0.97005200
C	-5.00783200	-0.93529200	0.70511400
H	-5.67601100	-0.91529300	1.57766900
H	-5.61566200	-1.27718900	-0.14242300
C	-4.51357100	0.49921800	0.44236800
H	-5.37959400	1.16092400	0.30167400
H	-3.96449000	0.88256800	1.31117300

P	-3.39986600	0.73293300	-1.03464700
C	-3.10521200	-1.76907200	2.68497600
H	-3.94323800	-1.63820300	3.38168800
H	-2.44864700	-2.55683500	3.06891400
H	-2.51536200	-0.84755800	2.65757200
C	-4.77689300	-3.67376400	1.38320200
H	-5.31653900	-3.99681000	0.48632000
H	-4.16076500	-4.51471400	1.71860800
H	-5.50569000	-3.43887100	2.16911900
C	-3.48827100	2.55899400	-1.29669200
H	-2.94850400	2.81728000	-2.21271800
H	-4.52621200	2.90201300	-1.37748800
H	-2.99743600	3.07623500	-0.46713200
C	-4.39707200	0.07266800	-2.44367100
H	-5.41239600	0.48598200	-2.44312300
H	-3.90496600	0.34092700	-3.38378300
H	-4.44981300	-1.01832400	-2.38852600
H	1.31814400	0.31310200	-0.12096600
N	1.58828100	1.23937500	0.85532600
Si	1.81948100	2.88711900	0.43208700
Si	1.25449400	0.65910000	2.43992800
C	0.88338200	-1.21448400	2.41368300
H	-0.00052100	-1.46107800	1.81087100
H	1.73108900	-1.79158200	2.02346500
H	0.69048900	-1.57095800	3.43426700
C	2.68401500	0.86043000	3.68675200
H	3.59325400	0.36472700	3.32242100
H	2.93575400	1.91176900	3.86602000
H	2.42949700	0.41164800	4.65658600
C	-0.28229700	1.47471800	3.24055800
H	-1.16286200	1.34101200	2.59585100
H	-0.51638600	1.04525600	4.22420300
H	-0.14691700	2.55512700	3.37748000
C	2.44485400	4.00428200	1.84634100
H	2.55267300	5.03911800	1.49473100
H	1.76058900	4.02210000	2.70349300
H	3.42480400	3.67705400	2.21399700
C	3.13225100	3.12014600	-0.94258700
H	3.28308200	4.18978000	-1.13975700
H	4.09678500	2.70288700	-0.62732000
H	2.89333200	2.66025500	-1.91185500
C	0.22023000	3.71218600	-0.21577800
H	-0.20585000	3.14354800	-1.05237700
H	-0.53405800	3.74371000	0.58245700
H	0.38719400	4.74259400	-0.55783000
C	0.95809500	-0.02913500	-3.28627000
H	0.02323500	-0.51614200	-3.58668100
H	1.62447400	-0.02170800	-4.16294800
C	1.60820600	-0.84917700	-2.15348000
H	1.48138500	-1.90021000	-2.45774300

O	0.57286500	1.29883700	-2.93730000
N	0.91666500	-0.62770500	-0.86791200
C	3.14139400	-0.60537700	-2.05506500
H	3.55589700	-0.65029300	-3.07170000
H	3.32792200	0.40322300	-1.67326200
C	3.85780000	-1.61854600	-1.18724800
C	4.11709300	-1.35989100	0.16641700
C	4.26325800	-2.85056400	-1.72189400
C	4.76256000	-2.30995100	0.96202700
H	3.80039100	-0.41112000	0.59300900
C	4.90614600	-3.80216400	-0.92870200
H	4.08151900	-3.06224700	-2.77430100
C	5.15845700	-3.53375300	0.41859500
H	4.95795700	-2.08987800	2.00863900
H	5.21684900	-4.74864100	-1.36434300
H	5.66365500	-4.27064400	1.03768000
H	1.30720700	1.73589300	-2.47725200
H	1.06879000	-1.45092800	-0.28631500

ADD2-N

Ag	1.31446300	-0.31490700	-0.69540000
P	4.42354700	1.25757900	0.62219100
C	5.18176600	-0.42159900	1.01472400
H	5.72285200	-0.36681600	1.96990900
H	5.93680100	-0.60865800	0.24020000
C	4.20669400	-1.61144900	1.07964800
H	4.77566700	-2.53928300	1.23053300
H	3.53870800	-1.50920800	1.94353900
P	3.10628100	-1.86598200	-0.40447100
C	3.48119100	1.57770300	2.19841800
H	4.07934600	1.38185500	3.09761800
H	3.16080400	2.62507000	2.21136700
H	2.57394200	0.96539000	2.22895800
C	5.93554600	2.30200900	0.94779600
H	6.68495000	2.12152600	0.16951000
H	5.65795800	3.36027200	0.90011800
H	6.38778800	2.10184200	1.92732100
C	2.54834900	-3.61165700	-0.16034900
H	1.94657100	-3.92486700	-1.01887500
H	3.39836700	-4.29449900	-0.04729700
H	1.91714300	-3.67363800	0.73166900
C	4.28785600	-2.00556000	-1.81721100
H	5.09331800	-2.71537800	-1.59663800
H	3.74577400	-2.34666800	-2.70476000
H	4.71708600	-1.02440800	-2.03879400
H	-2.02209700	-0.50345800	0.02193500
N	-2.64433700	-1.14014300	0.53760000
Si	-3.62054600	-2.15806800	-0.50697800
Si	-2.28684800	-1.22049200	2.24621500

C	-1.00691600	0.12058600	2.64034900
H	-0.08931200	-0.02632000	2.05548100
H	-1.38681700	1.12411100	2.41500100
H	-0.73432000	0.09746400	3.70335500
C	-3.82479800	-0.92221900	3.31342600
H	-4.28570600	0.04361200	3.07399900
H	-4.58577700	-1.69687200	3.16584100
H	-3.56549500	-0.91462300	4.38022300
C	-1.55134600	-2.90038900	2.75256600
H	-0.61837900	-3.09819400	2.20854400
H	-1.32682700	-2.93272400	3.82691500
H	-2.23595200	-3.73003400	2.53696800
C	-4.94975100	-3.03819300	0.51820600
H	-5.54112200	-3.69781400	-0.12945100
H	-4.52654100	-3.66244800	1.31454600
H	-5.64093900	-2.32514100	0.98194500
C	-4.44673700	-1.10472100	-1.84276900
H	-5.10555400	-1.71843800	-2.47102500
H	-5.05372800	-0.30372100	-1.40384700
H	-3.69958800	-0.64851200	-2.50345100
C	-2.56043200	-3.47312600	-1.37456500
H	-1.80685800	-3.00076500	-2.01765300
H	-2.03658000	-4.10529300	-0.64671000
H	-3.16916900	-4.12783100	-2.01187800
C	-0.42382700	0.82739500	-3.35620400
H	0.63937200	0.56187800	-3.50057500
H	-0.75767900	1.36598100	-4.25120400
C	-0.54719500	1.70464100	-2.09444800
H	0.24789100	2.47106300	-2.15154400
O	-1.21052600	-0.34964500	-3.22822700
N	-0.42075600	0.81456300	-0.93813800
C	-1.90579800	2.46166200	-2.08574500
H	-1.95836400	3.07444300	-2.99655500
H	-2.71174300	1.72242500	-2.14444700
C	-2.10126600	3.34734700	-0.87548700
C	-2.87114400	2.92301000	0.21824300
C	-1.49573000	4.61189200	-0.80583300
C	-3.02835400	3.73417500	1.34559800
H	-3.35138200	1.94810300	0.18239800
C	-1.64802600	5.42429700	0.31842800
H	-0.90370400	4.96470600	-1.64814400
C	-2.41635800	4.98763000	1.40082500
H	-3.63621800	3.38729300	2.17783500
H	-1.17360500	6.40235100	0.34654700
H	-2.54203800	5.62160300	2.27480500
H	-1.21596100	-0.49335000	-2.25765500
H	-0.60906200	1.35010600	-0.09200700

ADD3-O

C	-0.17817300	-0.04641400	-0.87967200
H	0.61889600	0.53298000	-0.37763100
H	0.29320700	-0.47137400	-1.79559200
C	-1.23585500	0.97468700	-1.35442400
H	-1.69533400	1.41770400	-0.46122600
O	-0.67773800	-1.02917000	-0.04039200
N	-2.31944000	0.24034500	-2.04492200
H	-3.09331800	0.86324000	-2.26936800
H	-1.96962400	-0.12841200	-2.93097500
C	-0.60934500	2.10075900	-2.21010600
H	0.21935000	2.53538300	-1.63620300
H	-0.16478800	1.65487100	-3.11071600
C	-1.59018600	3.18483200	-2.59960300
C	-2.20197400	3.19831100	-3.86160500
C	-1.94311700	4.18968800	-1.68453900
C	-3.13768300	4.17925500	-4.20054300
H	-1.92869800	2.44073000	-4.59356400
C	-2.87621200	5.17149200	-2.01783900
H	-1.47347200	4.20303900	-0.70307700
C	-3.47932700	5.16938500	-3.27858100
H	-3.12836100	5.94338600	-1.29496700
H	-4.20311300	5.93650500	-3.54099700
Ag	-2.68536100	-1.61849600	-0.45598300
P	-4.58727900	-2.98317400	-0.08334000
C	-5.66911200	-2.38079300	1.31473900
H	-6.24806100	-3.23527100	1.69025400
H	-6.39309400	-1.67510200	0.88705600
C	-4.86981700	-1.71149000	2.45135300
H	-5.46342100	-1.71057200	3.37525500
H	-3.95788800	-2.28307000	2.66562700
P	-4.35216400	0.05158800	2.02299400
C	6.51496300	-4.51030700	-1.56875800
C	5.35834700	-3.73306700	-1.63296200
C	5.23865800	-2.62655800	-0.78924700
C	6.25260700	-2.27835000	0.10561100
C	7.40419300	-3.06496400	0.16235000
C	7.53329700	-4.17919200	-0.67049500
H	6.62405300	-5.37037900	-2.22349600
H	4.56346000	-3.96220800	-2.33504900
H	6.14383000	-1.39541200	0.72684100
H	8.20270100	-2.80266500	0.85068000
H	8.43278800	-4.78717400	-0.62466800
S	3.73953000	-1.62975000	-0.85796600
O	4.10737600	-0.27945400	-0.37397300
O	3.13962800	-1.80905300	-2.19088700
C	2.67630400	-2.35738300	0.36518600
H	3.06607000	-2.30191200	1.37715000
C	1.45988600	-2.79049300	0.03546200

H	1.11779600	-2.78698400	-0.99233400
H	0.77287700	-3.15647600	0.78895800
C	-5.81128500	-3.23664000	-1.44956200
C	-4.22352100	-4.72716200	0.42639300
C	-5.77729000	0.97518800	2.80703700
C	-3.04220900	0.31830900	3.31660600
H	-5.59682600	2.05278900	2.73011700
H	-6.70464600	0.75931700	2.26436000
H	-5.92001700	0.71744200	3.86418400
H	-2.78397500	1.38210200	3.35176400
H	-3.36020200	0.00042500	4.31759300
H	-2.13856100	-0.22793700	3.02812400
H	-5.32211600	-3.73876400	-2.29030200
H	-6.66395800	-3.84262100	-1.12160600
H	-6.17499400	-2.26553100	-1.79954700
H	-3.63165900	-4.72276800	1.34695000
H	-5.14295000	-5.30097600	0.59280000
H	-3.62916800	-5.21787900	-0.35058900
H	-3.59302000	4.17253100	-5.18785500
H	2.88412300	1.18299100	0.79746000
N	2.74875300	2.08837300	1.25014900
Si	1.73241500	2.01630800	2.66992300
Si	3.81750800	3.29605700	0.56667100
C	5.62248600	2.96759300	1.05063700
H	6.30931700	3.69497500	0.59829500
H	5.75765100	3.00924000	2.13852900
H	5.92456100	1.96819000	0.71448600
C	3.68887800	3.24116500	-1.31958400
H	4.41387600	3.91435000	-1.79503600
H	3.88257700	2.22559500	-1.68428900
H	2.68748100	3.53298400	-1.65907200
C	3.31770500	5.01713400	1.18542400
H	3.37997700	5.10726600	2.27643400
H	3.98364700	5.77784800	0.75856800
H	2.29398700	5.27001800	0.88503000
C	2.65915700	2.57000200	4.23316300
H	3.53600500	1.93617500	4.41379400
H	3.01239200	3.60566700	4.15819200
H	2.01367800	2.50890800	5.11926800
C	0.20120300	3.12647600	2.49178800
H	-0.42425200	3.08707500	3.39366600
H	0.47328600	4.17582100	2.32567000
H	-0.41305000	2.80089800	1.64312800
C	1.16480600	0.22609700	2.90002500
H	0.51880200	0.14692500	3.78474900
H	0.59999300	-0.15136500	2.03698800
H	2.02077900	-0.44147400	3.06360500

TS2-O

C	-0.11673800	0.10171800	-1.14448300
H	0.90481300	0.33401400	-0.80797000
H	-0.02209100	-0.31904300	-2.16356700
C	-0.90643100	1.41287200	-1.22689300
H	-0.99178100	1.82884800	-0.21560800
O	-0.72992900	-0.80914300	-0.27081700
N	-2.29674400	1.11228100	-1.66412600
H	-2.84971500	1.96866400	-1.67806100
H	-2.27514700	0.77263100	-2.62725800
C	-0.19966500	2.44460400	-2.13789300
H	0.81375300	2.59812900	-1.74727800
H	-0.08402500	2.00947500	-3.13996300
C	-0.92888800	3.76856300	-2.23188900
C	-1.74177000	4.07393000	-3.33356200
C	-0.83552400	4.71273400	-1.19668200
C	-2.44379500	5.28031700	-3.40103500
H	-1.81017400	3.36623300	-4.15761300
C	-1.53432800	5.91857500	-1.25988100
H	-0.19952400	4.50435000	-0.33924200
C	-2.34343900	6.20657300	-2.36224900
H	-1.44033500	6.63825300	-0.45065500
H	-2.88358700	7.14815200	-2.41380900
Ag	-3.02339000	-0.65817400	-0.28949500
P	-4.71921800	-2.45219800	-0.34087200
C	-5.67792700	-2.21994700	1.25049500
H	-6.24957300	-3.13119400	1.47098600
H	-6.41115300	-1.42431600	1.06351300
C	-4.78452500	-1.84564300	2.44984700
H	-5.38918300	-1.79149800	3.36471200
H	-4.03153200	-2.62705000	2.61564000
P	-3.85024100	-0.23620200	2.20346400
C	4.40698700	-5.68923300	-1.74923600
C	3.61020500	-4.54503500	-1.80489100
C	3.82435100	-3.51402900	-0.88743200
C	4.83261300	-3.61147800	0.07456800
C	5.62179700	-4.76151400	0.12675400
C	5.40905600	-5.80167900	-0.78161000
H	4.25033000	-6.49115400	-2.46638400
H	2.83979400	-4.43082200	-2.56042000
H	5.00548500	-2.78408700	0.75505400
H	6.41035300	-4.84065400	0.87081100
H	6.02893600	-6.69371900	-0.74155400
S	2.76309000	-2.04576500	-0.93854700
O	3.65588700	-0.94310800	-0.47350500
O	2.21074400	-1.99112200	-2.31405800
C	1.49577700	-2.30487100	0.18876100
H	1.79556000	-2.21877600	1.22718000
C	0.16607500	-2.36445000	-0.22306500

H	-0.01411200	-2.64145800	-1.25981200
H	-0.54607600	-2.78784800	0.48413100
C	-6.08527800	-2.60732500	-1.58370300
C	-4.12901900	-4.20366700	-0.20361200
C	-5.11638000	1.01076500	2.75170200
C	-2.69898900	-0.26400600	3.65536600
H	-4.66180400	2.00680100	2.76049400
H	-5.95064200	1.03328300	2.04279300
H	-5.50565600	0.79118800	3.75325600
H	-2.19546700	0.70464500	3.73302800
H	-3.22005600	-0.47152900	4.59765900
H	-1.92677400	-1.02178100	3.49198600
H	-5.65992700	-2.87805300	-2.55528100
H	-6.81940600	-3.36878300	-1.29466700
H	-6.59387500	-1.64441800	-1.69472000
H	-3.39883600	-4.28777800	0.60716600
H	-4.95605500	-4.89915300	-0.01714500
H	-3.62451000	-4.48867300	-1.13217200
H	-3.06093900	5.49787400	-4.26911500
H	3.27890400	0.66635100	0.79020500
N	3.45877200	1.59862100	1.17660200
Si	2.52928300	1.97473200	2.59764200
Si	4.72106600	2.39280300	0.25720400
C	6.30166800	1.35244700	0.28190100
H	7.08880700	1.78568000	-0.34883700
H	6.69964600	1.25477400	1.29951900
H	6.08234900	0.34587300	-0.09274900
C	4.17511500	2.60221800	-1.54447600
H	4.97758800	3.01233100	-2.17140100
H	3.88681500	1.62956100	-1.96048000
H	3.31227500	3.27588400	-1.62475800
C	5.07934600	4.10257400	0.99881100
H	5.47905100	4.03453200	2.01728900
H	5.82859700	4.62311700	0.38873800
H	4.18631600	4.73871300	1.02880100
C	3.61203500	2.41459200	4.09348300
H	4.30899100	1.60017300	4.32532100
H	4.20686400	3.31904900	3.91987500
H	2.99747500	2.59372200	4.98576700
C	1.34821100	3.43687400	2.30585500
H	0.78835100	3.69741400	3.21385500
H	1.88949800	4.33489200	1.98338100
H	0.62141700	3.18822200	1.52182000
C	1.48783600	0.45264200	3.03299000
H	0.82168900	0.66623900	3.87959200
H	0.87163200	0.12793600	2.18554300
H	2.12551800	-0.39238200	3.32078000

ADD4-O

C	0.03341700	-0.38819100	-0.56587300
H	-0.96129500	-0.34282200	-0.10841600
H	-0.07677100	-0.04058500	-1.60638300
C	0.54910900	-1.82443000	-0.53824300
H	0.70600100	-2.11206700	0.50830600
O	0.93510000	0.44137500	0.15035200
N	1.89426200	-1.88190100	-1.18200500
H	2.26148900	-2.83147000	-1.12045800
H	1.78994300	-1.68740800	-2.17939400
C	-0.46113900	-2.80182600	-1.18288800
H	-1.41794400	-2.68586900	-0.65989200
H	-0.63694000	-2.49473200	-2.22279100
C	-0.00546800	-4.24544600	-1.13895900
C	0.58919500	-4.85496400	-2.25373900
C	-0.13651300	-5.00074500	0.03719300
C	1.04406400	-6.17516600	-2.19747000
H	0.67684700	-4.29625200	-3.18373300
C	0.31575700	-6.31901700	0.09806400
H	-0.61328500	-4.55449900	0.90708100
C	0.91072700	-6.91086100	-1.01934300
H	0.19483500	-6.88817100	1.01613600
H	1.25795800	-7.93956400	-0.97397100
Ag	3.19968100	-0.21072900	-0.23899000
P	4.84960400	1.50985000	-1.03313200
C	6.08020200	1.56691300	0.37940300
H	6.67536700	2.48692500	0.31055200
H	6.77432600	0.72997100	0.22669300
C	5.42326900	1.46364400	1.77062500
H	6.18736400	1.55062900	2.55415600
H	4.72405300	2.29669100	1.91835400
P	4.44086200	-0.11532400	2.01457000
C	-2.01355300	6.45524600	-1.39629800
C	-1.83886000	5.07008800	-1.38128000
C	-2.41269500	4.31069900	-0.35823300
C	-3.16871300	4.93080900	0.64127000
C	-3.33774700	6.31558100	0.62177600
C	-2.75820600	7.08169200	-0.39376400
H	-1.57638000	7.04555000	-2.19837300
H	-1.28593300	4.56424700	-2.16613300
H	-3.63626200	4.32312800	1.40938800
H	-3.93191600	6.79703700	1.39483600
H	-2.89609500	8.15996100	-0.40949200
S	-2.11735800	2.51457400	-0.29045800
O	-3.39767900	2.00104200	0.28939500
O	-1.76041400	2.15026300	-1.69136100
C	-0.82838400	2.17169400	0.73789300
H	-1.05632100	2.20101300	1.79677400
C	0.49538100	1.92604800	0.22410900

H	0.62922700	2.28997300	-0.80005600
H	1.30299000	2.29875100	0.86839900
C	5.97688800	1.40836100	-2.50106500
C	4.25322300	3.26114600	-1.12522400
C	5.75942600	-1.30725700	2.55235400
C	3.56000600	0.23213300	3.60540400
H	5.29739200	-2.26248300	2.82165100
H	6.45403100	-1.49478900	1.72715400
H	6.32321800	-0.93058100	3.41411100
H	3.06100500	-0.68048300	3.94643800
H	4.24324900	0.57872900	4.38962400
H	2.78792000	0.98879900	3.43594700
H	5.38535000	1.50202500	-3.41728200
H	6.73703200	2.19840100	-2.48975300
H	6.47500300	0.43379100	-2.51871000
H	3.64894800	3.49742800	-0.24426700
H	5.08497800	3.97197400	-1.19604700
H	3.60933700	3.37593800	-2.00286400
H	1.49344900	-6.62916700	-3.07698600
H	-3.69477200	0.05706800	0.46870600
N	-4.06758500	-0.90265500	0.47328100
Si	-4.19516900	-1.52202300	2.09826600
Si	-4.99510200	-1.17563900	-0.98785700
C	-6.45685800	0.02524900	-1.10474000
H	-6.99764900	-0.06912700	-2.05556500
H	-7.17455900	-0.13871600	-0.29133000
C	-3.88078100	-0.90828800	-2.49501500
H	-4.46074100	-0.90627900	-3.42720200
H	-3.35167800	0.04992200	-2.42354000
H	-3.12766500	-1.70253200	-2.57406200
C	-5.64523100	-2.95945300	-1.00068400
H	-6.31703300	-3.16456700	-0.15815200
H	-6.21076200	-3.15248400	-1.92125900
H	-4.82541700	-3.68701200	-0.95931000
C	-5.97135000	-1.51861800	2.77508500
H	-6.38769700	-0.50395100	2.77008200
H	-6.63927800	-2.15055300	2.17627700
H	-6.00750900	-1.89061000	3.80773200
C	-3.55734700	-3.30935800	2.19911400
H	-3.65481800	-3.71134200	3.21607400
H	-4.10772100	-3.97686900	1.52551400
H	-2.49708400	-3.35825100	1.91976400
C	-3.12503500	-0.42037200	3.20580600
H	-3.14805700	-0.75429000	4.25097100
H	-2.08075800	-0.41536500	2.87050200
H	-3.47606600	0.61756100	3.17126100
H	-6.09289700	1.05646000	-1.02217800

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C	0.21523000	0.64532600	-1.40961100
H	0.93883700	1.41495900	-1.13421500
H	0.51330700	0.22134000	-2.38272100
C	-1.17308900	1.26521900	-1.48685700
H	-1.43303700	1.61917800	-0.48367800
O	0.19713600	-0.37757700	-0.41580400
N	-2.17377200	0.21468100	-1.83725200
H	-3.10093400	0.63879000	-1.87880600
H	-1.98019300	-0.12472000	-2.78120600
C	-1.20622700	2.45894800	-2.46629900
H	-0.42548700	3.16451200	-2.16010300
H	-0.93638300	2.10837900	-3.47218000
C	-2.55250600	3.15251000	-2.50003700
C	-3.45703000	2.93920800	-3.54997200
C	-2.93822200	4.00214800	-1.45044400
C	-4.71284800	3.55321300	-3.55449400
H	-3.16745000	2.30184600	-4.38352700
C	-4.19054300	4.61638300	-1.45154900
H	-2.24606500	4.18901700	-0.63228500
C	-5.08354700	4.39258500	-2.50349500
H	-4.46620700	5.27732800	-0.63407100
H	-6.05672700	4.87607900	-2.50665700
Ag	-2.02662600	-1.50525900	-0.31030300
P	-1.82992800	-4.02624000	-0.27063500
C	-3.05527000	-4.49403200	1.06735200
H	-2.86157400	-5.52423200	1.39407700
H	-4.04849100	-4.49439700	0.59965900
C	-3.04250500	-3.54474400	2.28312300
H	-3.76795300	-3.88891900	3.03179300
H	-2.05731900	-3.56487500	2.76638300
P	-3.38085800	-1.75388300	1.84856800
C	5.00083500	-3.52789500	-2.36591100
C	4.40138700	-2.27478600	-2.21337600
C	4.70249300	-1.50235300	-1.08956500
C	5.60872900	-1.96039100	-0.12837300
C	6.20210700	-3.21256400	-0.28749400
C	5.89533700	-3.99910900	-1.40266500
H	4.77911400	-4.12969300	-3.24383500
H	3.72939300	-1.87388300	-2.96524900
H	5.85841800	-1.32736700	0.71766600
H	6.91318500	-3.57087400	0.45232600
H	6.36383100	-4.97222200	-1.52553400
S	3.89781100	0.11166600	-0.85773800
O	4.91890500	0.98096300	-0.24211100
O	3.31797400	0.45403000	-2.17983600
C	2.57933900	-0.12089700	0.30097100
H	3.04448000	-0.51574700	1.20837000
C	1.47527700	-1.03199300	-0.21054900

H	1.73703000	-1.53853000	-1.15167600
H	1.24650000	-1.79990800	0.53292300
C	-2.26766700	-5.22811500	-1.61146800
C	-0.24299300	-4.72945100	0.37661300
C	-5.22847700	-1.72946500	1.68226500
C	-3.12329500	-0.90839000	3.47119400
H	-5.56240300	-0.69691100	1.53748500
H	-5.53951500	-2.30670000	0.80567600
H	-5.72106700	-2.13777400	2.57260200
H	-3.38734600	0.14884700	3.37236000
H	-3.72925400	-1.36034300	4.26527900
H	-2.06552500	-0.95549400	3.74384600
H	-1.52843000	-5.15629000	-2.41547800
H	-2.29077700	-6.26065100	-1.24373100
H	-3.24735800	-4.97583400	-2.02962700
H	0.06864200	-4.18932700	1.27584200
H	-0.34162700	-5.79489300	0.61562500
H	0.54312100	-4.60321000	-0.37415000
H	-5.39505300	3.38103300	-4.38306900
H	2.12199000	1.06236700	0.73499900
N	1.57901700	2.21646600	1.35617800
Si	0.73301800	1.89049400	2.80101300
Si	2.32006500	3.71573300	0.93714900
C	4.06124800	3.92942600	1.67461100
H	4.51528400	4.88899500	1.39139500
H	4.03729300	3.88161700	2.77098500
H	4.71548400	3.12604600	1.31676100
C	2.49595300	3.90696700	-0.95176300
H	3.10270500	4.79107600	-1.18965000
H	2.97715800	3.04401000	-1.42417400
H	1.51836500	4.05294800	-1.43279900
C	1.29511800	5.24110700	1.48065500
H	1.18106400	5.31010100	2.56978300
H	1.77685300	6.16995500	1.14549000
H	0.28625000	5.22079300	1.04619200
C	1.46488600	2.64385600	4.39899000
H	2.49431700	2.29723400	4.55516900
H	1.49462500	3.73971100	4.36546900
H	0.87900800	2.35881700	5.28414300
C	-1.10324900	2.44647400	2.76700000
H	-1.63127500	2.19432800	3.69803600
H	-1.18830500	3.53109800	2.62504100
H	-1.63559700	1.96482300	1.93432500
C	0.65585700	0.00744000	3.15768500
H	0.13418300	-0.17728500	4.10725600
H	0.12229900	-0.52446700	2.35982100
H	1.65690000	-0.43257500	3.24671600

ADD5-O

C	1.19078700	0.31881900	-1.56099600
H	1.88750300	-0.43307900	-1.14958600
H	1.29068700	0.37497300	-2.65803000
C	1.53630700	1.65261000	-0.91852200
H	1.49261100	1.52234400	0.16698500
O	-0.17171900	-0.02480000	-1.24226700
N	0.50704200	2.68138900	-1.25135400
H	0.78368100	3.57081400	-0.83340800
H	0.50002300	2.83748400	-2.26086300
C	2.97246100	2.07261100	-1.30392400
H	3.62949200	1.23509300	-1.03949700
H	3.03000300	2.19914400	-2.39434900
C	3.42076700	3.34080100	-0.60880900
C	3.32096000	4.59086700	-1.23807900
C	3.91346900	3.29450400	0.70542500
C	3.69312400	5.76367900	-0.57473800
H	2.97136900	4.64450600	-2.26778400
C	4.28669500	4.46307800	1.36975900
H	4.01613500	2.33271100	1.20205300
C	4.17455600	5.70256600	0.73346000
H	4.67502700	4.40415700	2.38312600
H	4.47117700	6.61144600	1.25013900
Ag	-1.54437100	1.93525300	-0.52631500
P	-3.97018900	2.14395300	-1.10179600
C	-4.73690800	2.43635700	0.58224000
H	-5.82623800	2.31718100	0.51278500
H	-4.55100600	3.48942700	0.83142000
C	-4.17389300	1.52236700	1.68977600
H	-4.68866100	1.72773400	2.63737500
H	-4.37240800	0.47043600	1.44674300
P	-2.31888500	1.67483200	1.92660400
C	-4.72969400	-3.43179300	-0.76713300
C	-3.36919700	-3.62811400	-1.02121000
C	-2.47762400	-3.68606800	0.05107800
C	-2.92445100	-3.57622400	1.37094400
C	-4.28466000	-3.37759900	1.61562300
C	-5.18517200	-3.29971600	0.54768600
H	-5.43445800	-3.40161500	-1.59388100
H	-2.99590700	-3.76306700	-2.03143600
H	-2.21551000	-3.67855300	2.18713600
H	-4.64511300	-3.30678800	2.63839500
H	-6.24522500	-3.15955100	0.74255900
S	-0.70569100	-3.92149100	-0.26640200
O	-0.16940800	-4.66551100	0.88309800
O	-0.58409200	-4.43157600	-1.64473100
C	-0.04212800	-2.23942800	-0.21847100
H	-0.40320100	-1.79740900	0.71535700
C	-0.48600400	-1.40755100	-1.42506400

H	-0.01728800	-1.78667300	-2.33970800
H	-1.57274400	-1.44354400	-1.55540800
C	-4.72767600	3.50782000	-2.10010000
C	-4.88371600	0.65654700	-1.72106700
C	-2.17238000	3.13236000	3.06301500
C	-1.96737900	0.25419300	3.05755000
H	-1.12488200	3.25019000	3.35850000
H	-2.47874500	4.04760100	2.54632300
H	-2.78299600	3.00883200	3.96513700
H	-0.90163000	0.24252400	3.30550100
H	-2.55454500	0.31581300	3.98127700
H	-2.20398200	-0.68508900	2.54733100
H	-4.45795300	3.37842400	-3.15297000
H	-5.82048300	3.51735800	-2.01327100
H	-4.33433800	4.47319900	-1.76637000
H	-4.62671100	-0.22709500	-1.12871000
H	-5.96893400	0.80857500	-1.68520400
H	-4.58770800	0.45965300	-2.75650000
H	3.61663200	6.72064200	-1.08478000
H	1.06601400	-2.31505000	-0.14975500
N	3.14084700	-1.66598900	0.04031800
Si	3.35133500	-1.49395900	1.70543500
Si	4.07310100	-2.48338800	-1.11585900
C	4.79204200	-4.17064700	-0.56816800
H	5.33156000	-4.67075000	-1.38445800
H	5.49524400	-4.05393500	0.26741300
H	3.99581100	-4.84617300	-0.23082400
C	3.03716900	-2.86111300	-2.68454500
H	3.63482900	-3.39331000	-3.43698200
H	2.16789100	-3.49171300	-2.45500500
H	2.66628300	-1.94260700	-3.16191200
C	5.57816900	-1.47767400	-1.75360200
H	6.26397600	-1.23224400	-0.93207500
H	6.15326600	-2.02559500	-2.51317200
H	5.26151600	-0.52689000	-2.20518000
C	3.10209200	-3.09205100	2.72755800
H	2.13788900	-3.56276800	2.49622600
H	3.87908000	-3.82937400	2.48909000
H	3.14155000	-2.90934900	3.81092100
C	5.04196500	-0.78459600	2.27395700
H	5.08283100	-0.62825000	3.36128400
H	5.86230100	-1.46546900	2.01100400
H	5.26138800	0.17763200	1.79054700
C	2.06502300	-0.25814000	2.44590800
H	2.08935600	-0.27340500	3.54447300
H	2.25738500	0.77621800	2.12866400
H	1.04695700	-0.52015500	2.12755000

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C	1.81434300	1.90941100	-1.11513000
H	1.65124300	2.18427300	-2.17614600
H	2.06262400	2.86114800	-0.59187900
C	3.08717000	1.03396500	-1.07624400
H	2.87033700	0.10329100	-1.61663700
O	0.69276600	1.29799900	-0.58013600
N	3.33998600	0.64100300	0.32480000
H	4.11884700	-0.01235800	0.38397700
H	3.59828000	1.46302900	0.87305300
C	4.29006400	1.73855500	-1.74882700
H	3.99242500	2.01600700	-2.76891200
H	4.49172800	2.67759400	-1.21464600
C	5.54446300	0.89334600	-1.79392100
C	6.55977300	1.04581900	-0.83840000
C	5.70451600	-0.09809200	-2.77479400
C	7.69694600	0.23416700	-0.85711200
H	6.46541900	1.82049500	-0.08006300
C	6.83813600	-0.91073600	-2.79871200
H	4.93298600	-0.22774900	-3.53103500
C	7.83932200	-0.74872600	-1.83735200
H	6.94329800	-1.66735300	-3.57216100
H	8.72474500	-1.37845000	-1.85748200
Ag	1.08493400	-0.11074500	1.03587000
P	0.49472800	-1.51967300	2.86841900
C	1.03779600	-3.29520200	2.69716200
H	0.62120800	-3.84775200	3.55086600
H	2.12867700	-3.30718400	2.82067800
C	0.63448200	-3.98386300	1.37893000
H	0.79657900	-5.06602500	1.48223500
H	-0.43629900	-3.84528600	1.18423400
P	1.56504200	-3.36943800	-0.13591100
C	-6.58437800	-1.78913900	-2.69115000
C	-5.25280100	-2.12108800	-2.44299800
C	-4.80375200	-2.16798000	-1.12092000
C	-5.65632800	-1.89877200	-0.04850500
C	-6.98648400	-1.56735800	-0.31037200
C	-7.44749200	-1.50961900	-1.62776500
H	-6.94914900	-1.75271900	-3.71365200
H	-4.57130400	-2.35638900	-3.25376000
H	-5.28338700	-1.96895900	0.96782700
H	-7.66240100	-1.35906000	0.51405300
H	-8.48376800	-1.25079300	-1.82691100
S	-3.08193400	-2.57124400	-0.79507800
O	-3.00283200	-3.06215500	0.60059800
O	-2.59806700	-3.41678200	-1.90327700
C	-2.21939100	-1.01455500	-0.83856000
H	-2.47971900	-0.33947900	-0.02809700
C	-1.25661400	-0.78480300	-1.73011100

H	-1.03756100	-1.51728700	-2.50302800
H	-0.63677800	0.11216300	-1.64635900
C	1.24788800	-1.06376500	4.49785800
C	-1.29346700	-1.68583500	3.30316900
C	3.21350600	-4.20319500	0.14830500
C	0.84623800	-4.53066800	-1.40314900
H	3.83567700	-4.08065300	-0.74499700
H	3.74358300	-3.72824200	0.98120600
H	3.11277100	-5.27547100	0.35984800
H	1.39744800	-4.42012000	-2.34369200
H	0.90176500	-5.58038200	-1.08754600
H	-0.20074400	-4.27287200	-1.59357000
H	0.89111300	-0.07367400	4.79836200
H	0.98436700	-1.78805900	5.27765300
H	2.33754100	-1.01789100	4.40501900
H	-1.84818800	-2.11001800	2.46056800
H	-1.42424000	-2.33051700	4.18098800
H	-1.70447200	-0.69564400	3.52342900
H	8.47344200	0.37590400	-0.10958700
H	-0.52422200	2.68414800	-0.19297400
N	-1.13224100	3.48484200	0.07225200
Si	-1.97155200	4.20467700	-1.27615900
Si	-1.08435900	3.82831200	1.77595900
C	-2.01628100	2.50177400	2.77122300
H	-1.93618000	2.66229100	3.85481400
H	-3.08172500	2.48649500	2.51013100
H	-1.60513200	1.50964600	2.54337500
C	0.71084600	3.83853200	2.39284900
H	0.76638900	3.99714600	3.47795700
H	1.19810900	2.88188700	2.16454500
H	1.28956000	4.63186700	1.90429000
C	-1.86737300	5.51127600	2.16202500
H	-2.91405000	5.56786100	1.84084800
H	-1.84922200	5.69591700	3.24386500
H	-1.32448300	6.33203800	1.67920400
C	-3.85223100	4.25083900	-1.00755600
H	-4.25216500	3.24040600	-0.85781900
H	-4.13213200	4.84952900	-0.13208700
H	-4.36314300	4.68680000	-1.87620000
C	-1.40048400	5.98344600	-1.61864200
H	-1.91367300	6.40568900	-2.49268800
H	-1.60151700	6.64647100	-0.76849600
H	-0.32179100	6.01712800	-1.81485900
C	-1.61834600	3.15535800	-2.81274300
H	-2.09512900	3.59004900	-3.70051400
H	-0.54254500	3.08452500	-3.01079400
H	-1.99933800	2.13435000	-2.69412800

TS2'-O

C	1.08064700	-0.78446600	-1.90892300
H	1.15857600	-0.25081900	-2.87198500
H	1.86547800	-1.56253000	-1.92033400
C	-0.30051800	-1.46703700	-1.84273400
H	-1.06157500	-0.67969900	-1.82908300
O	1.30982300	0.09794500	-0.83796900
N	-0.41068500	-2.15565400	-0.54245500
H	-1.37529400	-2.40124500	-0.31745700
H	0.13981200	-3.01502300	-0.53392300
C	-0.54049900	-2.39063300	-3.05827100
H	-0.41563500	-1.79083200	-3.97070400
H	0.24297500	-3.16165500	-3.08365700
C	-1.90500000	-3.04831500	-3.06106000
C	-2.05459900	-4.41204500	-2.77610600
C	-3.05984300	-2.29395600	-3.32128300
C	-3.31759400	-5.00904700	-2.74974500
H	-1.17070500	-5.01648200	-2.58201400
C	-4.32317300	-2.88531600	-3.29641600
H	-2.96783800	-1.23281500	-3.54176300
C	-4.45695600	-4.24682500	-3.00958700
H	-5.20354200	-2.28338600	-3.50688400
H	-5.44053900	-4.70884500	-2.99402500
Ag	0.22026700	-0.56098700	1.08595400
P	-0.38222700	-0.25529300	3.38512900
C	-2.07839100	-0.86867800	3.86245300
H	-2.28794400	-0.47389100	4.86607300
H	-2.00288100	-1.95913200	3.97069100
C	-3.21348200	-0.48268900	2.88642500
H	-4.15466200	-0.38786300	3.44521400
H	-3.01850800	0.49186800	2.42475400
P	-3.46241500	-1.71534300	1.48987100
C	-3.01651300	5.32915300	-2.59698100
C	-2.56459100	4.10135200	-2.11164900
C	-2.27595200	3.96698100	-0.75167200
C	-2.44093500	5.04113500	0.12599500
C	-2.89112200	6.26583900	-0.36870400
C	-3.17587800	6.41227600	-1.72876000
H	-3.24989300	5.43829100	-3.65281100
H	-2.45417500	3.24506700	-2.76865900
H	-2.23727500	4.90634900	1.18316600
H	-3.02612900	7.10416100	0.30963900
H	-3.52826900	7.36692900	-2.11017100
S	-1.64261000	2.38849200	-0.12568400
O	-2.11524700	2.33555100	1.28642800
O	-2.13095800	1.36081800	-1.08454500
C	0.07564600	2.44208500	-0.15825300
H	0.52565900	2.97069800	0.67400600
C	0.80025700	1.85523500	-1.18674400

H	0.28342800	1.61811100	-2.11228600
H	1.82890800	2.17745200	-1.30990700
C	0.68405600	-1.10446100	4.63855700
C	-0.38480200	1.49212300	3.98013300
C	-4.58863400	-2.93867400	2.34095700
C	-4.70025600	-0.77880700	0.46533800
H	-4.91977200	-3.69276800	1.61877400
H	-4.04382000	-3.46117200	3.13546500
H	-5.47314900	-2.45889700	2.77854600
H	-5.09313800	-1.44053800	-0.31436700
H	-5.53778800	-0.39570200	1.06200200
H	-4.19217300	0.05739800	-0.02527400
H	1.70884100	-0.72907100	4.55867400
H	0.31890300	-0.92935000	5.65741200
H	0.70055700	-2.18167500	4.44540400
H	-1.03593400	2.08361700	3.33065700
H	-0.72240100	1.55785800	5.02127300
H	0.63090600	1.89452100	3.90660400
H	-3.40859100	-6.06983400	-2.53021200
H	3.35395200	0.06670200	-0.66278800
N	4.35880500	-0.07521400	-0.49032000
Si	5.40100200	0.51025300	-1.76655300
Si	4.66387100	-0.79161400	1.07119500
C	4.11396300	0.36958900	2.46971000
H	4.25496400	-0.08801900	3.45837300
H	4.67831900	1.30985500	2.45086600
H	3.05073400	0.62101100	2.36033600
C	3.68532700	-2.40812400	1.25289200
H	3.83256700	-2.86231900	2.24164200
H	2.60926200	-2.22616600	1.12680600
H	3.99015200	-3.14101600	0.49575800
C	6.50619200	-1.17297500	1.28903000
H	7.13112000	-0.27633600	1.20516800
H	6.68131200	-1.59908700	2.28509400
H	6.86453900	-1.90243000	0.55375200
C	6.56208100	1.88609300	-1.16657300
H	5.99276100	2.73277600	-0.76399600
H	7.23816900	1.53807800	-0.37614700
H	7.18672100	2.26245200	-1.98725600
C	6.47026100	-0.87212200	-2.50530000
H	7.08022200	-0.49424600	-3.33625100
H	7.15655700	-1.30031700	-1.76539800
H	5.84857000	-1.68921400	-2.89126600
C	4.30524000	1.21085900	-3.14447200
H	4.92051200	1.55284700	-3.98622000
H	3.60821900	0.45722100	-3.52981200
H	3.71418600	2.06847300	-2.80182600

ADD4'-O

C	-1.12104800	-0.27242900	2.13471700
H	-1.32352800	0.46838900	2.92538700
H	-1.69869400	-1.17465500	2.37638400
C	0.38156100	-0.59413000	2.15281500
H	0.93567300	0.32145800	1.92610800
O	-1.64586300	0.18021500	0.89782300
N	0.71997100	-1.55006000	1.08465600
H	1.72443900	-1.73431900	1.08579200
H	0.24257700	-2.44089200	1.22739100
C	0.78123100	-1.07386700	3.57066300
H	0.46488100	-0.30753700	4.29284900
H	0.21813800	-1.98501900	3.81899300
C	2.26491000	-1.33492900	3.73599800
C	2.74824400	-2.62549100	3.98797800
C	3.19110300	-0.28402300	3.63554200
C	4.11606900	-2.86613600	4.14354400
H	2.04424700	-3.45072300	4.07462500
C	4.55704400	-0.51976700	3.79334900
H	2.84192200	0.72347000	3.42286400
C	5.02567000	-1.81239600	4.04864200
H	5.25657700	0.30930700	3.72262600
H	6.08953100	-1.99332300	4.17840700
Ag	0.51422400	-0.56511500	-1.14942000
P	1.35483100	-1.76281500	-3.09991400
C	3.18563200	-2.12796400	-3.08429700
H	3.49926400	-2.30217300	-4.12262000
H	3.32346200	-3.07993000	-2.55457700
C	4.03586700	-1.01367100	-2.43722400
H	5.05827400	-1.04897200	-2.83748800
H	3.63394000	-0.02287200	-2.68184000
P	4.09389500	-1.12464900	-0.56135400
C	0.12217500	6.24449700	0.76449000
C	0.51026600	4.90321400	0.79492700
C	0.75915800	4.23430000	-0.40548100
C	0.63633000	4.89447600	-1.63169900
C	0.24727500	6.23366800	-1.65269100
C	-0.01424800	6.90839000	-0.45643100
H	-0.06636400	6.77222200	1.69574100
H	0.64689500	4.37921500	1.73501000
H	0.86683200	4.36565300	-2.55108500
H	0.15598500	6.75388600	-2.60256900
H	-0.31549700	7.95236400	-0.47660800
S	1.20466900	2.47466200	-0.38039500
O	2.12538300	2.29842800	-1.53411100
O	1.71865200	2.22069800	0.99232800
C	-0.23637300	1.51262800	-0.65835800
H	-0.65955800	1.87420100	-1.59935400
C	-1.25472600	1.51215300	0.47232700

H	-0.89918300	2.06096200	1.35341300
H	-2.19281900	1.97292900	0.14416100
C	0.65014300	-3.38667800	-3.65083000
C	1.19182000	-0.73666500	-4.63387000
C	5.50717500	-2.32935700	-0.35618800
C	4.95829200	0.47608700	-0.18739800
H	5.73438200	-2.43233300	0.71037600
H	5.21778700	-3.31907600	-0.72791400
H	6.41532100	-2.00836700	-0.88218400
H	5.20977500	0.50590800	0.87757900
H	5.87694600	0.60240600	-0.77438200
H	4.27265800	1.30200300	-0.39857400
H	-0.42516200	-3.27896700	-3.82410800
H	1.12598400	-3.74288200	-4.57220300
H	0.79129000	-4.13434700	-2.86373800
H	1.69163400	0.22380800	-4.47522400
H	1.62762800	-1.23518200	-5.50825700
H	0.13329400	-0.53380400	-4.82570500
H	4.46734000	-3.87508900	4.34442400
H	-3.55678700	-0.51419200	0.49102200
N	-4.53277000	-0.81124700	0.39230000
Si	-4.74988800	-2.01970100	-0.85029900
Si	-5.61510200	0.09430600	1.42520500
C	-7.41464500	-0.36339900	1.05568600
H	-8.08717900	0.25030500	1.66814000
H	-7.67640500	-0.18507000	0.00608400
H	-7.63261600	-1.41279300	1.28427100
C	-5.25317300	-0.26880600	3.25158200
H	-5.89557400	0.32148500	3.91776300
H	-5.41509800	-1.32877700	3.48174400
H	-4.21188200	-0.03192300	3.50426300
C	-5.38631100	1.95567600	1.14329500
H	-5.62898900	2.23127500	0.10992200
H	-6.02796300	2.54810400	1.80836100
H	-4.34927300	2.26103900	1.33053900
C	-5.61499000	-1.33087900	-2.39208800
H	-6.61959800	-0.95696200	-2.15951200
H	-5.04601300	-0.49696500	-2.82154500
H	-5.72326200	-2.09917400	-3.16887500
C	-3.02447900	-2.62599000	-1.35010800
H	-3.08491200	-3.31009600	-2.20655300
H	-2.37068100	-1.78951500	-1.62776600
H	-2.53770700	-3.16382700	-0.52705300
C	-5.75119900	-3.50499900	-0.22785500
H	-5.80097100	-4.29044800	-0.99328400
H	-5.29130800	-3.93925600	0.66806900
H	-6.78236800	-3.23426400	0.02685400

TS3'-O

C	-0.77822100	-0.54233800	-3.36301300
H	-1.03672800	0.13493300	-4.19203100
H	-0.76927300	-1.56194600	-3.77444400
C	-1.87797200	-0.44028200	-2.28923300
H	-1.92203100	0.59440000	-1.93706300
O	0.52523700	-0.29557500	-2.89784700
N	-1.55318200	-1.26228600	-1.10180400
H	-2.25301400	-1.07807000	-0.37763900
H	-1.62582300	-2.25373000	-1.33695200
C	-3.22095400	-0.82141900	-2.97027800
H	-3.28937000	-0.25440300	-3.90977500
H	-3.17504600	-1.88168600	-3.25817900
C	-4.48058300	-0.57434100	-2.16883100
C	-5.22579600	-1.63672600	-1.64141600
C	-4.95262500	0.73213100	-1.96743800
C	-6.41020500	-1.40730400	-0.93668600
H	-4.88364900	-2.65757200	-1.79855600
C	-6.13554300	0.96737300	-1.26674400
H	-4.39082100	1.57119500	-2.37159100
C	-6.87140700	-0.10350700	-0.74953600
H	-6.49065200	1.98643600	-1.13503100
H	-7.80073300	0.07791100	-0.21569000
Ag	0.52099300	-1.18824800	0.42458500
P	-0.05050400	-1.88333100	2.73873400
C	-1.69045200	-1.41172200	3.49108800
H	-1.62309500	-1.58587800	4.57315600
H	-2.43912800	-2.11865200	3.10967700
C	-2.09934900	0.05148200	3.18948400
H	-2.51569100	0.52170500	4.09013400
H	-1.23461200	0.65326500	2.88477600
P	-3.33819200	0.15457700	1.78657400
C	1.67046000	6.06776300	-0.63599100
C	1.16602000	4.81295800	-0.97375800
C	1.14192100	3.80249600	-0.00793100
C	1.59738800	4.03528900	1.28875800
C	2.09937600	5.29708700	1.61916000
C	2.13933000	6.30942000	0.65937300
H	1.69224400	6.85904800	-1.38035100
H	0.78112800	4.62051100	-1.97052600
H	1.55175300	3.23680000	2.02006400
H	2.45773700	5.48676600	2.62732700
H	2.53153800	7.28899700	0.91923000
S	0.44907400	2.18672800	-0.45768200
O	0.33573100	1.42782000	0.82861200
O	-0.84253600	2.47137200	-1.14556400
C	1.61624400	1.40537900	-1.56103800
H	2.45520400	2.09972400	-1.65875500
C	0.99114600	1.06778500	-2.89769700

H	0.16030900	1.72727400	-3.17841100
H	1.76957600	1.14872300	-3.66879500
C	0.04684900	-3.69089700	3.13884100
C	1.11050300	-1.15917700	3.98953400
C	-4.91241300	-0.17384600	2.73359200
C	-3.45193600	1.99686200	1.57134300
H	-5.76354100	-0.08317600	2.05139500
H	-4.90863000	-1.19872300	3.12215800
H	-5.05142000	0.51858800	3.57370400
H	-4.32997700	2.22542500	0.95849200
H	-3.53917500	2.52958200	2.52679500
H	-2.56698500	2.34934000	1.03304800
H	1.04074900	-4.06766200	2.87683500
H	-0.13758300	-3.88472000	4.20225200
H	-0.68971300	-4.24063400	2.54365800
H	1.03123200	-0.06806600	3.96788500
H	0.87697700	-1.51520800	5.00025700
H	2.14171100	-1.42479900	3.74336900
H	-6.97622400	-2.24820500	-0.54395000
H	2.18103500	0.13817000	-1.03788600
N	2.65925100	-0.97359400	-0.57808600
Si	3.96483300	-0.58292400	0.54063800
Si	2.91836300	-2.26450100	-1.76267800
C	4.23791500	-3.54397400	-1.24017000
H	4.30309700	-4.29811700	-2.03639300
H	5.24366100	-3.13251300	-1.10413800
H	3.96358700	-4.07067200	-0.31859200
C	1.38130600	-3.35085900	-2.02632700
H	1.59243800	-4.12251800	-2.77936300
H	1.10017700	-3.86545100	-1.09736200
H	0.52744900	-2.76431200	-2.36829100
C	3.49132600	-1.59503800	-3.44532700
H	4.37638100	-0.95500600	-3.34396000
H	3.75675100	-2.42168600	-4.11757300
H	2.69783000	-1.01423400	-3.92409000
C	5.58394400	-0.14099500	-0.36364200
H	5.99092200	-0.96839800	-0.95545900
H	5.42496000	0.70335000	-1.04649700
H	6.35762500	0.16041000	0.35530500
C	3.55673100	0.95057500	1.57812100
H	4.34761900	1.10079500	2.32542200
H	3.51469100	1.85451300	0.96139800
H	2.59868100	0.86754900	2.09923800
C	4.36177300	-1.97880900	1.77969900
H	4.87851500	-1.56530000	2.65640200
H	3.45226700	-2.47950000	2.13384200
H	5.01033500	-2.74926600	1.35188300

ADD5'-O

C	-1.89643300	0.61832700	-2.70014200
H	-2.08942100	1.59911500	-3.16261800
H	-1.74950700	-0.10875600	-3.52038400
C	-3.10879700	0.21193000	-1.86625300
H	-3.14629500	0.87696300	-0.99368700
O	-0.73030100	0.69509300	-1.89968500
N	-2.96123100	-1.16479900	-1.36769500
H	-3.87429100	-1.50981500	-1.07182400
H	-2.65263800	-1.77664200	-2.12349100
C	-4.39898200	0.44500800	-2.70216200
H	-4.43300500	1.50129700	-3.00102700
H	-4.33991700	-0.14562000	-3.62709500
C	-5.66671300	0.09058800	-1.95366900
C	-6.38719800	-1.07298400	-2.25728400
C	-6.13259000	0.90927400	-0.91203700
C	-7.54413200	-1.40977900	-1.54882900
H	-6.04624900	-1.71522500	-3.06679200
C	-7.28641700	0.57625200	-0.20309300
H	-5.58433800	1.81190000	-0.65223100
C	-7.99768100	-0.58473800	-0.51960300
H	-7.63285400	1.22635200	0.59609800
H	-8.89919200	-0.84115600	0.03047600
Ag	0.93821400	-1.86350300	0.85994200
P	-1.04045900	-1.88649600	2.18837600
C	-2.26125700	-0.49973700	2.04088600
H	-3.12241600	-0.75864300	2.67350100
H	-2.59133300	-0.53027400	0.99613600
C	-1.71036100	0.88957100	2.38751300
H	-1.31670800	0.92041200	3.41390400
H	-0.89070700	1.15095500	1.70909000
P	-3.01101300	2.23122500	2.17580300
C	4.57849900	5.15690200	-1.05632400
C	3.32142700	4.61627500	-1.32858100
C	2.76002700	3.71882900	-0.41745100
C	3.41926400	3.36443500	0.76102300
C	4.67773100	3.91013400	1.02066700
C	5.25607400	4.80089300	0.11312900
H	5.02559200	5.86012200	-1.75323700
H	2.76950700	4.89580700	-2.22012900
H	2.94683700	2.68640000	1.46355100
H	5.20228300	3.64144400	1.93295300
H	6.23526400	5.22377700	0.32030600
S	1.13880300	3.01337800	-0.77186700
O	0.52594300	2.65542000	0.52306400
O	0.45026000	3.93152700	-1.69867300
C	1.53068300	1.48301100	-1.70362200
H	2.43180500	1.70301200	-2.28450800
C	0.39955600	1.10540700	-2.64570600

H	0.14952800	1.96827700	-3.27998900
H	0.75228100	0.28970400	-3.29703000
C	-2.09548200	-3.35768700	1.81437600
C	-0.74161500	-2.04588700	4.00701800
C	-4.00419300	1.97512500	3.73946600
C	-1.99225700	3.70225200	2.69310100
H	-4.71219200	2.80312300	3.85715700
H	-4.59040600	1.05212800	3.67076800
H	-3.37348200	1.92748100	4.63667600
H	-2.62205700	4.59848700	2.70992500
H	-1.54121600	3.57155600	3.68518400
H	-1.19439200	3.85145500	1.95963100
H	-1.51516100	-4.27790100	1.93237700
H	-2.97170200	-3.39741200	2.47194700
H	-2.42900600	-3.28552800	0.77493400
H	-0.18418700	-1.17780300	4.37091700
H	-1.68621600	-2.12040000	4.55837600
H	-0.14123300	-2.93993400	4.20297600
H	-8.09079200	-2.31335900	-1.80628600
H	1.75623700	0.69189800	-0.98175900
N	2.70451700	-2.02342500	-0.26936600
Si	4.13363900	-1.95573400	0.70151400
Si	2.54102400	-2.75013500	-1.82791400
C	3.23249200	-4.52484800	-1.92557200
H	3.08266700	-4.95892900	-2.92326700
H	4.30823200	-4.55825500	-1.71180000
H	2.73470900	-5.17956900	-1.19868700
C	0.70522400	-2.86714500	-2.32989300
H	0.60641200	-3.18676700	-3.37659700
H	0.17507800	-3.60345800	-1.71086300
H	0.18723800	-1.90699000	-2.21445400
C	3.41974000	-1.76034300	-3.20322600
H	4.50254300	-1.71423400	-3.03922900
H	3.25456800	-2.21880900	-4.18750400
H	3.05577200	-0.72622500	-3.25448300
C	5.72966400	-1.75615800	-0.32192800
H	5.89336000	-2.59750100	-1.00661800
H	5.71095000	-0.83902700	-0.92340000
H	6.60442100	-1.70074200	0.33951600
C	4.06952800	-0.46686100	1.88814200
H	4.94193800	-0.44852400	2.55504900
H	4.05725800	0.47622600	1.32815800
H	3.17029200	-0.48923400	2.51865400
C	4.36924100	-3.50534500	1.78706800
H	5.27490000	-3.44076900	2.40516600
H	3.51356200	-3.64244200	2.46208000
H	4.44710600	-4.41108400	1.17271100

ADD3-N

Ag	-0.92381100	-0.99082300	0.28128700
P	0.10309100	-3.15563700	0.54975000
C	-1.21852600	-4.31520400	1.18147900
H	-0.74550500	-5.26426200	1.46772400
H	-1.88143700	-4.53618100	0.33495100
C	-2.02983100	-3.74927100	2.36348800
H	-2.72993800	-4.51137000	2.73120600
H	-1.35640300	-3.51433900	3.19841100
P	-2.96702700	-2.17255200	1.95510600
C	1.43729000	-3.28501400	1.81744800
H	1.68884100	-4.33525300	2.00695200
H	2.32633600	-2.76923600	1.44314200
H	1.12226600	-2.81353200	2.75348900
C	0.81287500	-4.04800800	-0.89492900
H	0.12113700	-4.00751400	-1.74165700
H	1.75212300	-3.55298500	-1.16398400
H	1.02030100	-5.09431500	-0.64199000
C	-3.65785300	-1.75771700	3.63099200
H	-4.36901400	-0.93126900	3.53073600
H	-4.17021300	-2.60931300	4.09553500
H	-2.84995300	-1.42475800	4.29138100
C	-4.47736800	-2.86236800	1.11761800
H	-4.97845000	-3.62362200	1.72795700
H	-5.17777700	-2.04560800	0.91755600
H	-4.20282700	-3.30350600	0.15392500
C	-0.66346500	1.94823700	-0.89621100
H	-0.52210200	1.62858000	-1.95017200
H	-1.21208700	2.90654000	-0.94129800
C	0.74056300	2.29395000	-0.33656400
H	1.20939200	3.05288100	-0.97478600
O	-1.37185900	1.02897400	-0.14322100
N	1.59852200	1.06269300	-0.44447400
H	2.25071300	0.91294900	0.34509400
C	0.69829600	2.79994100	1.11743500
H	-0.02615300	3.62318500	1.14218400
H	0.28335000	2.00789900	1.75069800
C	2.04080200	3.26996400	1.63922700
C	2.84921200	2.43729500	2.42589000
C	2.52095800	4.54824300	1.31176900
C	4.10590800	2.86380000	2.86520200
H	2.49910600	1.44456600	2.69975600
C	3.77104700	4.98009900	1.75330200
H	1.90302400	5.21361800	0.71146000
C	4.56980200	4.13631200	2.53084700
H	4.71659700	2.19874200	3.46956500
H	4.12112000	5.97608000	1.49433600
H	5.54402200	4.47181800	2.87596700
C	7.55657000	0.74088400	-0.67851600

C	6.23532900	0.40477600	-0.37680300
C	5.68830400	-0.77372800	-0.89495400
C	6.45653600	-1.61673400	-1.70472100
C	7.77651800	-1.27477300	-1.99794900
C	8.32771700	-0.09452100	-1.48974900
H	7.98691300	1.65193500	-0.27010200
H	5.63640700	1.02910300	0.27818000
H	6.02302800	-2.53964500	-2.07613500
H	8.37875900	-1.93424900	-2.61778700
H	9.35737600	0.16754400	-1.71873400
S	3.93512300	-1.16233200	-0.61252100
O	3.88448000	-2.64931200	-0.61753500
O	3.62670400	-0.43639300	0.67346500
C	2.90744700	-0.53714200	-1.78874900
H	2.88714000	-1.05593000	-2.73871900
C	2.49628400	0.87850300	-1.68886500
H	3.27659300	1.64322100	-1.54298000
H	1.89634200	1.16590000	-2.55617900
H	0.98890300	0.22868000	-0.41581900
H	-3.21033400	1.14695600	-0.73252900
N	-4.18292100	1.26700500	-1.06165900
Si	-4.49655300	0.49906800	-2.59405500
Si	-5.12342000	2.26888300	0.01457500
C	-6.23088800	1.23106300	1.16130400
H	-6.82703700	1.86082600	1.83458000
H	-6.92834200	0.60971600	0.58579800
H	-5.62472800	0.55957800	1.78348900
C	-3.90918200	3.25974100	1.07758100
H	-3.10127600	2.61278500	1.44046400
H	-3.44748200	4.06491500	0.49210000
H	-4.40449400	3.71881500	1.94285100
C	-6.24732600	3.46859100	-0.93219800
H	-7.00323100	2.95028100	-1.53352300
H	-6.78339700	4.12558100	-0.23469000
H	-5.66445100	4.10652200	-1.60773900
C	-3.50354700	-1.11738000	-2.68265800
H	-3.55571400	-1.57317900	-3.68020300
H	-2.44577100	-0.94182700	-2.44986200
H	-3.88622300	-1.84572900	-1.95808200
C	-6.33879900	0.09133900	-2.78643400
H	-6.51030800	-0.46180400	-3.71890300
H	-6.70529600	-0.52980600	-1.96073100
H	-6.96095300	0.99193500	-2.82618200
C	-3.97249400	1.58475500	-4.06132500
H	-4.50820400	2.54291800	-4.05455500
H	-2.89847100	1.80956300	-4.01796900
H	-4.17115400	1.09793900	-5.02490700

TS2-N

Ag	-0.53028000	-0.91538200	0.21520700
P	0.17025800	-3.03634400	1.01961300
C	-1.17229900	-4.05693300	1.81426800
H	-0.77673600	-5.07511500	1.93460000
H	-1.99266900	-4.12288100	1.08883900
C	-1.69209800	-3.55065000	3.17243900
H	-2.45465200	-4.25287400	3.53833400
H	-0.87646300	-3.56642300	3.90669300
P	-2.39487100	-1.80371000	3.18754500
C	1.52541300	-3.01914200	2.26807000
H	1.69601900	-4.02349500	2.67363700
H	2.43741600	-2.67156500	1.77348600
H	1.27933600	-2.33464800	3.08483000
C	0.81572700	-4.16826100	-0.28501800
H	0.07192700	-4.28695400	-1.07909000
H	1.72242900	-3.71905600	-0.70080300
H	1.05999000	-5.15203500	0.13240800
C	-3.04574900	-1.80092400	4.93672000
H	-3.63207700	-0.89049800	5.10062500
H	-3.67890800	-2.66990500	5.15651600
H	-2.20875100	-1.78681700	5.64323400
C	-3.98904600	-2.08273400	2.26353800
H	-4.53800600	-2.96209300	2.62445900
H	-4.62584200	-1.19920800	2.37948200
H	-3.79233500	-2.19592600	1.19282200
C	-0.58155500	1.84743800	-1.21084600
H	-0.18238700	1.47861500	-2.17843300
H	-1.26357000	2.67901300	-1.46757200
C	0.59533800	2.50265300	-0.44285100
H	0.94661700	3.36524500	-1.02878100
O	-1.28003100	0.87891100	-0.51102100
N	1.73257900	1.54924100	-0.32587500
H	2.30908000	1.72258200	0.50227400
C	0.16584900	2.98580300	0.95556100
H	-0.71116600	3.62914900	0.81574000
H	-0.17831700	2.11750000	1.52703300
C	1.24944900	3.72969300	1.70739100
C	2.00194800	3.09579900	2.70691600
C	1.54795700	5.06671400	1.39967700
C	3.02788200	3.77188100	3.37355800
H	1.77515600	2.06570600	2.97495600
C	2.56690900	5.74670100	2.06575200
H	0.96807900	5.58008600	0.63511800
C	3.31334700	5.09923000	3.05458300
H	3.59884600	3.25942400	4.14317500
H	2.77692900	6.78376800	1.81660100
H	4.10748700	5.62854600	3.57429600
C	7.61421300	0.38534900	-1.70947800

C	6.40407500	0.28707200	-1.01925100
C	5.54613700	-0.78035500	-1.29409000
C	5.88558800	-1.75180000	-2.24031100
C	7.09631800	-1.64475500	-2.92398700
C	7.95849400	-0.57554000	-2.66249600
H	8.29092300	1.20837900	-1.49607500
H	6.13105800	1.00778100	-0.25571900
H	5.21783400	-2.58908900	-2.41650600
H	7.37118500	-2.39970700	-3.65564000
H	8.90175800	-0.49702700	-3.19628100
S	3.95061600	-0.88417000	-0.44656900
O	3.68329100	-2.33412000	-0.26991900
O	4.07268800	-0.01082000	0.75025500
C	2.68653500	-0.21583100	-1.43776700
H	2.54595800	-0.78456000	-2.35578500
C	2.64187800	1.30516300	-1.51117800
H	3.57883500	1.85972900	-1.40187300
H	2.13129100	1.63483100	-2.41831800
H	1.63528600	0.27106700	-0.45514200
H	-3.07060900	0.85935400	-1.17936900
N	-4.00366300	0.82889200	-1.62651100
Si	-4.08902100	-0.38260300	-2.87361300
Si	-5.12960300	1.95901700	-0.92190100
C	-6.45458600	1.10151400	0.13769200
H	-7.15346400	1.82840300	0.57226200
H	-7.04571600	0.38975400	-0.45236900
H	-5.99713700	0.54215700	0.96349400
C	-4.12902100	3.12704100	0.18516200
H	-3.45732900	2.56300200	0.84274000
H	-3.50919800	3.80103100	-0.41933500
H	-4.78230600	3.74759100	0.81121700
C	-6.03493300	2.98910500	-2.23302900
H	-6.67867600	2.37384700	-2.87195000
H	-6.67398600	3.74547900	-1.75863000
H	-5.32354900	3.51311200	-2.88281800
C	-3.66558100	-2.09319200	-2.15978600
H	-3.63990100	-2.86986600	-2.93560600
H	-2.67826900	-2.06526600	-1.67880500
H	-4.39951100	-2.39478600	-1.40177600
C	-5.82777900	-0.45891300	-3.62323600
H	-5.89521100	-1.29072200	-4.33587200
H	-6.59787800	-0.61986000	-2.85918700
H	-6.08113800	0.45863800	-4.16621300
C	-2.83611600	-0.02238300	-4.25178100
H	-3.05653700	0.93123400	-4.74658100
H	-1.82090500	0.04655700	-3.84027300
H	-2.83274600	-0.80767400	-5.01902400

ADD4-N

Ag	0.57803200	0.56228600	-0.38167200
P	0.21111900	2.18820100	-2.07872900
C	1.68214700	3.27279900	-2.45875500
H	1.49498900	3.76248300	-3.42460400
H	2.53345000	2.59754300	-2.60654800
C	2.02622900	4.34337100	-1.40663800
H	2.95179300	4.84889500	-1.71707700
H	1.24077200	5.10998400	-1.39748900
P	2.20086100	3.74962100	0.37245600
C	-1.15704900	3.38467400	-1.75865700
H	-1.24357100	4.11757400	-2.56941800
H	-2.09321800	2.82654900	-1.66430900
H	-0.97260900	3.90634000	-0.81500600
C	-0.20991000	1.53421800	-3.75749300
H	0.57037700	0.84335300	-4.09255400
H	-1.16194600	0.99506000	-3.71935000
H	-0.29968000	2.34963300	-4.48484000
C	2.85238000	5.34014100	1.10226300
H	3.14761300	5.16355700	2.14205700
H	3.71769700	5.73583100	0.55530800
H	2.06173400	6.09856400	1.10689000
C	3.78898400	2.78428400	0.26209100
H	4.57033800	3.31887500	-0.29372100
H	4.14914600	2.58760400	1.27737000
H	3.61165300	1.81005800	-0.20373300
C	0.70570900	-1.64858300	1.66264200
H	0.63968500	-2.57489200	1.05022300
H	1.13872100	-1.96591800	2.63192600
C	-0.74779000	-1.19686800	1.96638500
H	-1.27596400	-2.05265700	2.42712000
O	1.49557100	-0.68251200	1.06565400
N	-1.41787200	-0.79952000	0.71186000
H	-2.12743400	-0.09211100	0.88471800
C	-0.78267400	-0.02620400	2.97235800
H	-0.19634600	-0.33176100	3.84760900
H	-0.26271900	0.83134900	2.53034200
C	-2.18327600	0.36169800	3.39920400
C	-2.84657800	1.45337300	2.81889900
C	-2.87201600	-0.39200700	4.36343300
C	-4.15954400	1.77433200	3.17761800
H	-2.32671200	2.06479700	2.08445900
C	-4.17926000	-0.07278100	4.72987800
H	-2.37161400	-1.23531100	4.83507100
C	-4.83113700	1.01100700	4.13384800
H	-4.65068700	2.62650600	2.71481400
H	-4.68862000	-0.66630800	5.48510500
H	-5.84812700	1.26435300	4.42202200
C	-6.78296800	-1.52121800	0.49086800

C	-5.60298400	-0.89865000	0.07990500
C	-5.15522400	-1.10347400	-1.22790300
C	-5.86480000	-1.89922300	-2.13126500
C	-7.04275900	-2.51378200	-1.70667600
C	-7.49730000	-2.32824600	-0.39782900
H	-7.14358800	-1.36930500	1.50393900
H	-5.05109100	-0.25029500	0.75293200
H	-5.50845900	-2.01219800	-3.15015900
H	-7.60871500	-3.13068400	-2.39869400
H	-8.41576600	-2.80888200	-0.07248700
S	-3.62560000	-0.32533900	-1.76781000
O	-3.68881500	-0.13215800	-3.22906000
O	-3.38073000	0.83393800	-0.88206000
C	-2.33002300	-1.57489400	-1.47561700
H	-2.65214400	-2.46006300	-2.03354300
C	-2.01997700	-1.91190300	-0.01737000
H	-2.92285900	-2.30690600	0.48073400
H	-1.29647000	-2.73371200	-0.04420000
H	-1.44847100	-1.14925400	-1.96628700
H	3.12851600	-1.34857400	0.46834900
N	4.04052700	-1.73267500	0.14923100
Si	4.01255600	-2.25775200	-1.50545700
Si	5.19915000	-1.80492800	1.45140700
C	6.95478300	-1.39386400	0.85662400
H	7.64942600	-1.35878700	1.70620000
H	7.34466300	-2.13708700	0.15116100
H	6.98560700	-0.41537900	0.36185200
C	4.66536000	-0.53206700	2.74878400
H	4.96692000	0.47933900	2.44924600
H	3.57340200	-0.52797900	2.84528300
H	5.10633100	-0.73566000	3.73257700
C	5.25913100	-3.52004000	2.26851900
H	5.54261200	-4.29759800	1.54804200
H	5.98477200	-3.55176000	3.09216300
H	4.27820200	-3.79349500	2.67693900
C	4.30074500	-0.81165400	-2.70907100
H	4.25823300	-1.12983600	-3.75935400
H	3.53612300	-0.03692100	-2.56094700
H	5.27884100	-0.34515500	-2.53797000
C	5.33414700	-3.57372500	-1.84806200
H	5.25597200	-3.93312100	-2.88225800
H	6.35117300	-3.18699100	-1.71515900
H	5.21742100	-4.44060500	-1.18663300
C	2.30309000	-2.98429100	-1.89958100
H	2.12009000	-3.89657000	-1.31894300
H	1.51816400	-2.26229800	-1.63877700
H	2.19988000	-3.23145400	-2.96431400

TS3-N

Ag	1.60824000	-0.02154300	-0.13604200
P	1.03311200	1.50859900	-1.89999500
C	2.39796500	2.50715200	-2.70571700
H	2.04810800	2.75894200	-3.71635500
H	3.25609800	1.83579100	-2.83000600
C	2.82166800	3.80390900	-1.99316400
H	3.56427900	4.31874300	-2.61955100
H	1.96033200	4.47943200	-1.91756200
P	3.50388800	3.60043300	-0.25393000
C	-0.27968700	2.76827200	-1.57642100
H	-0.40134900	3.44162900	-2.43339000
H	-1.22568400	2.24698400	-1.40251500
H	-0.02550800	3.35495800	-0.68876200
C	0.35239400	0.62023900	-3.37448100
H	1.07617500	-0.11884800	-3.73188900
H	-0.56865400	0.10136200	-3.09640400
H	0.12306100	1.31954800	-4.18672400
C	3.92723900	5.38771400	0.07567800
H	4.49738300	5.45607700	1.00830000
H	4.51817400	5.84142100	-0.73010500
H	3.00746600	5.96778000	0.20778900
C	5.20693800	2.95377500	-0.65470300
H	5.71750500	3.55808900	-1.41550900
H	5.81343100	2.94901600	0.25696900
H	5.14441400	1.91839800	-1.00461700
C	-0.00773900	-1.67888200	2.40868600
H	-0.11816200	-2.66029000	1.90979200
H	0.05877200	-1.88817500	3.49384600
C	-1.31262400	-0.88685400	2.18515400
H	-2.11217400	-1.42887300	2.72642100
O	1.12492100	-0.99918700	1.96843500
N	-1.64301600	-0.80992700	0.75205100
H	-2.07352100	0.08196100	0.52396600
C	-1.21591100	0.52399800	2.80285500
H	-0.81759900	0.41234300	3.81899100
H	-0.47187900	1.10006200	2.24240900
C	-2.53857800	1.26175900	2.85345200
C	-2.83009300	2.30528500	1.96339500
C	-3.51951000	0.90374600	3.79290700
C	-4.06125900	2.96724200	2.00293300
H	-2.08167200	2.60781100	1.23478500
C	-4.74850300	1.56136900	3.83984200
H	-3.30996800	0.10407300	4.50029000
C	-5.02554500	2.59724900	2.94203000
H	-4.26176100	3.77442600	1.30312500
H	-5.48750100	1.27274900	4.58329300
H	-5.97869900	3.11821600	2.98326100
C	-6.93627100	-0.13242300	0.37214300

C	-5.63847500	0.00692600	-0.12283500
C	-5.29012800	-0.66894300	-1.29482800
C	-6.20909000	-1.46307200	-1.98605600
C	-7.50260900	-1.59187600	-1.48008700
C	-7.86287000	-0.93140100	-0.30179700
H	-7.21719300	0.38906300	1.28230900
H	-4.91793600	0.64302200	0.38041400
H	-5.91665200	-1.94878600	-2.91145400
H	-8.23011200	-2.20124000	-2.00857800
H	-8.87190300	-1.03517500	0.08775500
S	-3.61780600	-0.51701800	-1.94001800
O	-3.65604100	-0.74835800	-3.39432300
O	-3.04748200	0.74168800	-1.40869000
C	-2.69888300	-1.91427700	-1.21330100
H	-3.23689700	-2.81098600	-1.53634400
C	-2.51275200	-1.88781700	0.30358300
H	-3.50179800	-1.88826700	0.80049100
H	-2.04054900	-2.84222000	0.56551000
H	-1.73162500	-1.88195300	-1.72481700
H	2.01328300	-1.64429200	1.41908000
N	2.98888100	-1.84617200	0.60136100
Si	2.85811900	-3.15382100	-0.54374500
Si	4.46302800	-1.37829900	1.42728700
C	5.94457700	-1.23408100	0.23964000
H	6.83696800	-0.88483100	0.77556400
H	6.19933700	-2.19476600	-0.22478200
H	5.74455900	-0.52095700	-0.57000600
C	4.20665600	0.29223700	2.28241900
H	4.00765200	1.10038300	1.56796800
H	3.34439300	0.23839700	2.95672900
H	5.08959400	0.57337500	2.87213300
C	4.93519100	-2.62212200	2.78634200
H	5.15795600	-3.61635900	2.38271300
H	5.81929700	-2.28276500	3.34213300
H	4.11467900	-2.73298300	3.50633900
C	3.48522800	-2.65702400	-2.27159200
H	3.37484300	-3.47941200	-2.99086900
H	2.92373100	-1.79623000	-2.65849100
H	4.54455400	-2.37408500	-2.25031400
C	3.81206600	-4.72292800	-0.04126100
H	3.64044000	-5.52782700	-0.76825200
H	4.89477300	-4.55419300	0.00859200
H	3.49098800	-5.08897600	0.94151800
C	1.03455500	-3.65767200	-0.73151200
H	0.66055500	-4.13997800	0.17989800
H	0.39828300	-2.78588300	-0.92796600
H	0.90833300	-4.36613100	-1.56064100

ADD5-N

Ag	2.06870700	0.35842500	-0.40396400
P	1.40627200	2.66449400	-0.31392000
C	2.76312900	3.93764400	-0.12797800
H	2.33246200	4.89921800	-0.43983000
H	3.53421200	3.68672500	-0.86684100
C	3.38761100	4.09907600	1.26855900
H	4.12981600	4.90914000	1.22572000
H	2.61793200	4.42056500	1.98160300
P	4.18199700	2.55533300	1.98763900
C	0.18147800	3.13089400	0.98422000
H	-0.00936900	4.21054200	0.97550200
H	-0.75690900	2.60170000	0.79054600
H	0.55409400	2.83645700	1.96984400
C	0.61043800	3.26044100	-1.87280000
H	1.28495300	3.09129500	-2.71852400
H	-0.32459500	2.72519600	-2.05903700
H	0.38459900	4.33102400	-1.80661000
C	4.92207300	3.32377200	3.51822400
H	5.56366500	2.58876200	4.01575700
H	5.51795500	4.21905400	3.30015500
H	4.12422500	3.59321000	4.21881200
C	5.70880100	2.45432500	0.92127800
H	6.24300900	3.41093000	0.85521700
H	6.38585400	1.70042600	1.33625500
H	5.44032200	2.12446600	-0.08774500
C	-0.62474200	-3.53834300	0.33012400
H	-0.57845500	-3.63277800	-0.76574000
H	-0.75681900	-4.55235700	0.73768500
C	-1.86465700	-2.70252800	0.70911000
H	-2.75420700	-3.31338300	0.46539200
O	0.57115400	-3.01475000	0.85862400
N	-1.89597900	-1.44547900	-0.05383000
H	-2.14461000	-0.65698200	0.53631200
C	-1.88798500	-2.43144700	2.22876500
H	-1.72654000	-3.38821400	2.74142900
H	-1.02561400	-1.80297400	2.47386400
C	-3.17128700	-1.79802400	2.72485200
C	-3.22605600	-0.44045400	3.07177000
C	-4.34610400	-2.55816200	2.84590300
C	-4.41419600	0.14267200	3.52286800
H	-2.32593600	0.16532300	2.99624600
C	-5.53432000	-1.98321400	3.29676300
H	-4.32315600	-3.61623100	2.59214100
C	-5.57306400	-0.62742400	3.63799000
H	-4.42919700	1.19622600	3.79029000
H	-6.42814600	-2.59495100	3.39238900
H	-6.49453200	-0.17995800	4.00236200
C	-6.96298200	0.56450100	-0.12000700

C	-5.57333700	0.68931700	-0.16317500
C	-4.97946800	1.18496200	-1.32643700
C	-5.73954600	1.56991900	-2.43402100
C	-7.12739500	1.44185100	-2.37496900
C	-7.73611800	0.93619100	-1.22241500
H	-7.43470800	0.18036900	0.77967200
H	-4.96534100	0.42537300	0.69570500
H	-5.24942100	1.98028200	-3.31089900
H	-7.73311900	1.74259500	-3.22492700
H	-8.81756900	0.83845800	-1.18221200
S	-3.18847000	1.33142500	-1.40757000
O	-2.85422300	2.37467100	-2.39687000
O	-2.68478900	1.45221700	-0.02021900
C	-2.61119100	-0.24892600	-2.10529300
H	-3.15358300	-0.35818800	-3.04982400
C	-2.77499500	-1.47849700	-1.21152200
H	-3.84306200	-1.61822300	-0.95574900
H	-2.49754200	-2.33977600	-1.83244100
H	-1.55368600	-0.07116700	-2.32280800
H	1.07497700	-2.48798200	0.19088400
N	2.64146900	-1.66454200	-0.71640200
Si	2.55772500	-2.06461800	-2.40227700
Si	3.83107800	-2.22848100	0.43388700
C	5.59646800	-1.61933700	0.04042700
H	6.30340500	-1.92616300	0.82325200
H	5.96327500	-2.02702000	-0.91004900
H	5.63539600	-0.52550700	-0.03573400
C	3.37696800	-1.61544900	2.17085400
H	3.38053100	-0.52057100	2.24335300
H	2.37673500	-1.97417600	2.43924700
H	4.08650900	-1.99967800	2.91637600
C	3.91695100	-4.12561800	0.53569900
H	4.32495800	-4.58652200	-0.37072800
H	4.55711000	-4.42888300	1.37497500
H	2.91742000	-4.53925600	0.70895900
C	3.91274700	-1.24495700	-3.46542600
H	3.79190800	-1.49300300	-4.52877200
H	3.87941700	-0.15092600	-3.37243500
H	4.91642000	-1.56761300	-3.16200800
C	2.64712000	-3.93515600	-2.75097100
H	2.39964500	-4.13713000	-3.80179300
H	3.64645200	-4.34697100	-2.56832500
H	1.94255000	-4.49841000	-2.12720900
C	0.89443000	-1.47680600	-3.12608500
H	0.05487000	-1.91908100	-2.57726400
H	0.79380600	-0.38493400	-3.06352100
H	0.79866000	-1.75854300	-4.18287200

ADD1'

Ag	-1.29426600	-0.25126300	-0.32193000
P	-1.50727300	-2.59219200	-0.71636600
C	-3.21581200	-3.25880000	-1.05553500
H	-3.09863500	-4.27792200	-1.44919200
H	-3.62660900	-2.65191600	-1.87184500
C	-4.19087700	-3.28092200	0.13570900
H	-5.16026200	-3.66058100	-0.21673100
H	-3.83378900	-3.99465400	0.88919000
P	-4.43942100	-1.64366300	1.03147300
C	-0.86936000	-3.66383300	0.64492100
H	-1.01279800	-4.72693800	0.41967200
H	0.19858200	-3.46734300	0.78164000
H	-1.37877700	-3.41741300	1.58067700
C	-0.57289900	-3.19798900	-2.19172600
H	-0.95276400	-2.71065000	-3.09523100
H	0.48388900	-2.93515800	-2.08549600
H	-0.66435700	-4.28428600	-2.30539600
C	-5.83210400	-2.17166900	2.15450400
H	-6.21558400	-1.29561100	2.68800200
H	-6.66148900	-2.64318200	1.61239200
H	-5.45529900	-2.87553100	2.90447800
C	-5.40846700	-0.69915100	-0.25030700
H	-4.74524200	-0.37095100	-1.05723500
H	-6.23476900	-1.28263700	-0.67623900
H	-5.81985300	0.20389800	0.21340800
C	2.84318200	1.68342700	0.16774200
H	2.69502300	2.55565400	-0.49078500
H	2.95772900	2.06390900	1.19710300
C	4.12362700	0.95008600	-0.26601800
H	4.95269500	1.66873200	-0.21881900
O	1.75337100	0.78259000	0.06901500
N	4.04256500	0.45066800	-1.64760800
H	3.11621000	0.03521400	-1.75806300
C	4.44592600	-0.22186800	0.69399200
H	4.26561900	0.11362500	1.72292500
H	3.72070500	-1.02200000	0.50031500
C	5.86155500	-0.74950000	0.58896900
C	6.28243600	-1.51377500	-0.51082400
C	6.79332200	-0.47835200	1.60081300
C	7.59203100	-1.98825100	-0.59186800
H	5.57827100	-1.71184100	-1.31202600
C	8.10506800	-0.95192300	1.52370600
H	6.48500600	0.10853700	2.46405600
C	8.50936400	-1.71104300	0.42501600
H	7.89801400	-2.57804000	-1.45285200
H	8.80768800	-0.73001200	2.32338500
H	9.52832700	-2.08467300	0.36163000
H	4.07568400	1.23645600	-2.29674700

H	0.88975500	1.27302200	0.05096000
N	-0.92449600	1.82020200	-0.03984000
Si	-1.11311300	2.71513400	-1.51828400
Si	-1.27721900	2.36631700	1.57672100
C	-1.07921900	0.92390200	2.79929500
H	-0.08858100	0.46137100	2.70273600
H	-1.18354900	1.27342600	3.83535400
H	-1.83598300	0.14524000	2.63666500
C	-0.08366600	3.73096700	2.15622300
H	0.95734400	3.38584000	2.12668300
H	-0.14846700	4.63586300	1.54177600
H	-0.30482700	4.01949900	3.19249600
C	-3.04643900	3.04436200	1.77211200
H	-3.78894500	2.29481300	1.46979800
H	-3.25559700	3.32084500	2.81398600
H	-3.21064200	3.93771400	1.15627400
C	-0.08910000	1.89828500	-2.89938000
H	-0.10828500	2.50037100	-3.81733400
H	0.95684400	1.77062300	-2.59628700
H	-0.47838800	0.90222700	-3.15123800
C	-2.91444400	2.77562400	-2.13767000
H	-2.99926700	3.32842600	-3.08295700
H	-3.30417200	1.76316200	-2.31023700
H	-3.57443300	3.25986800	-1.40774900
C	-0.52001200	4.51721300	-1.36885400
H	-1.13469200	5.09633500	-0.66898700
H	0.51825200	4.57464000	-1.02033700
H	-0.57215400	5.02133300	-2.34274300

TS1'-N

Ag	2.17576900	-0.29640500	0.24298600
P	1.69852600	-2.64243200	0.22960900
C	3.19046000	-3.75472300	0.06815300
H	2.84969800	-4.77560200	0.29040200
H	3.88141200	-3.47532600	0.87325000
C	3.91790800	-3.75206300	-1.28763100
H	4.73020200	-4.49196000	-1.24721200
H	3.23104000	-4.08767900	-2.07548100
P	4.61133900	-2.09523500	-1.84552100
C	0.56171200	-3.22873800	-1.09688100
H	0.46189000	-4.32042500	-1.07163400
H	-0.41865300	-2.76931600	-0.93435200
H	0.93839600	-2.92101100	-2.07697400
C	0.93161100	-3.29394800	1.77536200
H	1.55183800	-3.02574700	2.63690100
H	-0.06706900	-2.86760600	1.91256200
H	0.84022300	-4.38561100	1.72897400
C	5.57138800	-2.69603100	-3.32869100
H	6.16883000	-1.86991300	-3.72877000

H	6.24212400	-3.53206600	-3.09271900
H	4.87710700	-3.01226200	-4.11477200
C	6.01348700	-1.89967100	-0.63143100
H	5.62401800	-1.62123200	0.35312700
H	6.62056000	-2.80907100	-0.53439600
H	6.66019200	-1.08082100	-0.96466200
C	-0.83619000	3.04927300	0.87262700
H	-0.61555200	2.71960100	1.89860300
H	-0.62486800	4.13017300	0.81461100
C	-2.32844200	2.81853500	0.59292800
H	-2.91975900	3.28363500	1.39162400
O	-0.10694500	2.31239900	-0.08009100
N	-2.53974800	1.35513500	0.69643900
H	-1.94505800	0.86725600	0.01804200
C	-2.73409600	3.41555100	-0.77505500
H	-2.41752900	4.46776000	-0.76007100
H	-2.13467800	2.92685000	-1.54984500
C	-4.20700900	3.34497900	-1.12190400
C	-4.65992000	2.54471200	-2.17921800
C	-5.15294800	4.09136100	-0.40225800
C	-6.01736900	2.47965000	-2.50264000
H	-3.93939600	1.97122100	-2.75839400
C	-6.51013000	4.02798700	-0.71938100
H	-4.82274700	4.73635500	0.40984600
C	-6.94783300	3.21860200	-1.77090700
H	-6.34567200	1.85393200	-3.32851200
H	-7.22554900	4.61586500	-0.15016100
H	-8.00418000	3.17068200	-2.02094000
C	-5.77188500	-3.45006900	-1.39198900
C	-4.67810600	-2.73845300	-0.89439100
C	-4.36333100	-2.82951600	0.46361000
C	-5.12097300	-3.62905300	1.32451700
C	-6.21173600	-4.33551200	0.81815900
C	-6.54039000	-4.24362300	-0.53763000
H	-6.01873000	-3.38973300	-2.44864900
H	-4.05523700	-2.13664700	-1.54760700
H	-4.84067900	-3.70869100	2.37012100
H	-6.80145600	-4.96397300	1.48010400
H	-7.39018800	-4.79684000	-0.92841000
S	-2.98930000	-1.86163100	1.14068700
O	-2.41570600	-2.68384200	2.22904500
O	-2.13517500	-1.51680400	-0.03665300
C	-3.57056600	-0.35923300	1.79268700
H	-4.26022100	-0.51958300	2.61982500
C	-3.90887300	0.70235900	0.75462300
H	-4.24290600	0.38394000	-0.23478100
H	-4.62026300	1.42891000	1.15172200
H	-2.40990300	0.63936700	1.73249900
H	0.84402600	2.17596900	0.21608800
N	2.59699000	1.79381400	0.44336400

Si	3.18793200	2.10405100	2.05104600
Si	3.19809000	2.53655800	-1.02095000
C	2.42501100	1.68507100	-2.53136000
H	1.33056100	1.69498700	-2.46000400
H	2.70560200	2.20174400	-3.45923400
H	2.75459300	0.64202200	-2.61965200
C	2.72307400	4.37700700	-1.12645000
H	1.63502500	4.49829300	-1.05989300
H	3.17583500	4.97648300	-0.32867600
H	3.04608300	4.80469000	-2.08496700
C	5.09179100	2.43420300	-1.20571900
H	5.43483700	1.39265000	-1.17022500
H	5.41558400	2.85926600	-2.16513700
H	5.61439000	2.98256400	-0.41179800
C	1.94353500	1.48026300	3.34910100
H	2.34319400	1.61094300	4.36357100
H	0.99224100	2.02407600	3.29877700
H	1.71648600	0.41416100	3.21815000
C	4.83704400	1.22424600	2.42832300
H	5.19059400	1.45082900	3.44323400
H	4.72801200	0.13387500	2.35198800
H	5.62368300	1.52469500	1.72575100
C	3.46704000	3.95480600	2.40354300
H	4.27732600	4.37347400	1.79446000
H	2.56650100	4.54866200	2.20573300
H	3.73987400	4.10531000	3.45639000

ADD2'-N

Ag	2.33933800	-0.26734700	0.26036500
P	1.73629300	-2.57491900	0.38967100
C	3.14095800	-3.80289300	0.36010100
H	2.72479800	-4.77408800	0.66253500
H	3.83894500	-3.50201900	1.15116900
C	3.88582800	-3.96650600	-0.97713700
H	4.67159500	-4.72429900	-0.84634800
H	3.19688800	-4.35980900	-1.73587300
P	4.63980300	-2.39972800	-1.69963800
C	0.59429900	-3.17363500	-0.92913800
H	0.44764600	-4.25804600	-0.85900900
H	-0.37026200	-2.67450100	-0.79875900
H	0.99527400	-2.92297100	-1.91545500
C	0.86276200	-3.05047700	1.94456700
H	1.48138400	-2.79873400	2.81175400
H	-0.07746600	-2.49681700	2.00866500
H	0.63984700	-4.12361300	1.96071400
C	5.60430400	-3.19166400	-3.08782000
H	6.24145100	-2.43610600	-3.55989900
H	6.23658100	-4.02233200	-2.74901800
H	4.91327000	-3.56409600	-3.85192500

C	6.02449800	-2.11026800	-0.48513600
H	5.62477400	-1.71518800	0.45445000
H	6.60358700	-3.01917800	-0.27662900
H	6.69960000	-1.34952700	-0.89192800
C	-0.74310000	2.98592100	0.74883900
H	-0.45741000	2.84616500	1.80088600
H	-0.55900300	4.04023400	0.47934600
C	-2.24140600	2.67662800	0.61242800
H	-2.78017900	3.34746000	1.29837700
O	-0.03315800	2.10499600	-0.10119400
N	-2.43858200	1.31166100	1.09354100
H	-1.88374600	0.66346300	0.54028300
C	-2.69992300	2.98810800	-0.84405800
H	-2.33741100	3.99802000	-1.08507100
H	-2.17028900	2.30719800	-1.51858700
C	-4.18930000	2.93502600	-1.11280100
C	-4.72238300	2.03832900	-2.05016600
C	-5.07679800	3.80121000	-0.45444300
C	-6.09375200	1.99334300	-2.31131000
H	-4.04829000	1.37306500	-2.58615300
C	-6.44799800	3.76017600	-0.70972000
H	-4.68776200	4.52213200	0.26165100
C	-6.96383000	2.85230000	-1.63802600
H	-6.48171100	1.29071800	-3.04493700
H	-7.11456900	4.44248500	-0.18793500
H	-8.03129900	2.82167100	-1.83983900
C	-5.82619500	-2.35567100	-1.75254500
C	-4.73437500	-1.97830600	-0.96963800
C	-4.65864900	-2.43612600	0.34735100
C	-5.63878200	-3.26998200	0.89027200
C	-6.72432800	-3.64063600	0.09668700
C	-6.81907300	-3.18083000	-1.21949200
H	-5.89788300	-2.00863800	-2.77897100
H	-3.94511400	-1.35296600	-1.37207700
H	-5.53441500	-3.63429200	1.90701300
H	-7.49174100	-4.29278700	0.50318500
H	-7.66652800	-3.47223500	-1.83354300
S	-3.26139000	-1.95686100	1.37826000
O	-3.09821100	-2.98227000	2.42394700
O	-2.13203600	-1.64636600	0.47041400
C	-3.78455100	-0.41603500	2.20182000
H	-4.77155400	-0.63731500	2.62103100
C	-3.78942800	0.82832200	1.30531400
H	-4.37076500	0.62288300	0.39166200
H	-4.35083100	1.60252600	1.84374300
H	-3.06323300	-0.29416700	3.01657100
H	0.93365600	2.09150300	0.13512800
N	2.79655500	1.81158900	0.27915700
Si	3.40365100	2.29930700	1.83205800
Si	3.27375800	2.45205600	-1.27180200

C	2.46962700	1.43810200	-2.66236800
H	1.38146400	1.40163300	-2.52689100
H	2.66990900	1.89253000	-3.64227700
H	2.84839200	0.40799000	-2.69114700
C	2.69034300	4.24896000	-1.51231100
H	1.60149600	4.31802800	-1.39685600
H	3.14617600	4.94140300	-0.79576700
H	2.93931600	4.60563800	-2.52069500
C	5.15918700	2.42892500	-1.55159700
H	5.56076300	1.41328800	-1.44038900
H	5.41532700	2.78126500	-2.55970000
H	5.68627800	3.07266800	-0.83584800
C	2.26536900	1.65333500	3.21496600
H	2.63623400	1.95879200	4.20254000
H	1.24294400	2.03575000	3.10872300
H	2.20371900	0.55652400	3.21078300
C	5.14467800	1.61968300	2.21175900
H	5.49798100	1.94278300	3.19999800
H	5.14691100	0.52132800	2.20092200
H	5.87824400	1.95528800	1.46843700
C	3.50038800	4.19089700	2.03506800
H	4.24253800	4.64134800	1.36502200
H	2.53609700	4.67099800	1.82805000
H	3.78776900	4.45158700	3.06246900

TS1'-O

Ag	-0.06250600	1.73682900	0.38817200
P	2.22273100	2.39653900	0.62305200
C	2.50890300	4.23365200	0.81128500
H	3.53019200	4.36209700	1.19577300
H	1.83126100	4.57627200	1.60304900
C	2.33518200	5.09408200	-0.45282000
H	2.54233000	6.14226000	-0.19327300
H	3.08588700	4.80441800	-1.19912900
P	0.66090200	4.97811600	-1.30248800
C	3.34427900	1.90850600	-0.75608900
H	4.36605000	2.26659900	-0.58281500
H	3.34409800	0.81682300	-0.83271000
H	2.97064400	2.31979200	-1.69871900
C	3.06710200	1.73947900	2.12583600
H	2.50863700	2.03817700	3.01911400
H	3.10096100	0.64615000	2.08373800
H	4.09004200	2.12786300	2.19872100
C	0.91992200	6.31500200	-2.57946100
H	-0.02346000	6.49635800	-3.10542000
H	1.26546900	7.26113100	-2.14381300
H	1.65291600	5.98055600	-3.32178300
C	-0.39064700	5.91692000	-0.08246900
H	-0.59023400	5.29732800	0.79755700

H	0.07269700	6.85952700	0.23634800
H	-1.35874500	6.13909500	-0.54383000
C	-0.44266400	-3.07541100	-1.22918900
H	0.09981800	-2.13136600	-1.34646700
H	-0.46486700	-3.61614600	-2.18004800
C	-1.85701900	-2.86511800	-0.66427700
H	-2.39101600	-2.30137900	-1.44017500
O	0.32031600	-3.92767300	-0.30800500
N	-1.91731200	-2.07162800	0.55247700
H	-1.23241000	-2.36231100	1.24647500
C	-2.58439400	-4.22456000	-0.47483500
H	-2.34064200	-4.88143700	-1.32029800
H	-2.17391200	-4.70655500	0.42093200
C	-4.08867800	-4.09985700	-0.36383100
C	-4.70057800	-3.68122800	0.82719900
C	-4.90565000	-4.39463400	-1.46383300
C	-6.08813500	-3.55999800	0.91129000
H	-4.08001000	-3.43572600	1.68256900
C	-6.29462300	-4.27453100	-1.38342000
H	-4.44916700	-4.72721700	-2.39445900
C	-6.89071900	-3.85644700	-0.19314700
H	-6.54352100	-3.23321000	1.84265700
H	-6.90850200	-4.51071600	-2.24901400
H	-7.97151600	-3.76350700	-0.12531000
C	6.72353800	-2.98062000	-1.66671200
C	5.41815400	-2.62478300	-1.32228400
C	5.03604900	-2.64909000	0.02089300
C	5.94132100	-3.01269300	1.02156900
C	7.24260100	-3.36894000	0.66655900
C	7.63307100	-3.35669400	-0.67546300
H	7.03136100	-2.95721600	-2.70856600
H	4.70553500	-2.30839600	-2.07676600
H	5.63087600	-2.99469800	2.06139700
H	7.95419500	-3.64871300	1.43853900
H	8.64828700	-3.63267700	-0.94718200
S	3.33359900	-2.23784600	0.47851200
O	3.41713200	-1.61829900	1.81828000
O	2.78468900	-1.45772000	-0.66389200
C	2.40833700	-3.70367500	0.60589200
H	2.78040600	-4.37785100	1.37216100
C	1.83440900	-4.26144100	-0.62982800
H	2.05869300	-3.73761500	-1.55866400
H	1.84053500	-5.34418900	-0.74374400
H	-1.82776000	-1.06303300	0.39134000
H	0.82291200	-3.42731300	0.57716100
N	-2.10357400	1.18298500	0.30116500
Si	-2.85735100	1.37669900	1.85160400
Si	-2.80433400	1.42110200	-1.26562900
C	-1.52389200	0.99216000	-2.61218200
H	-1.13112900	-0.02591000	-2.48828300

H	-1.96831600	1.05633400	-3.61462800
H	-0.66997800	1.68158500	-2.58517100
C	-4.32986300	0.32953700	-1.59617600
H	-4.15110800	-0.72690500	-1.36409800
H	-5.19462600	0.64361300	-1.00153300
H	-4.61917700	0.39533300	-2.65381600
C	-3.35612200	3.21676000	-1.59284000
H	-2.50812200	3.90580000	-1.49391900
H	-3.77092800	3.33718900	-2.60271900
H	-4.12724600	3.53402000	-0.87899000
C	-1.95268100	0.33670800	3.16568200
H	-2.35116500	0.53714200	4.16918100
H	-2.07621000	-0.73471700	2.96715100
H	-0.87564600	0.55155900	3.18838100
C	-2.81747400	3.18196500	2.47502900
H	-3.32535000	3.28840200	3.44327800
H	-1.78451800	3.53435000	2.60346800
H	-3.30896100	3.85807500	1.76386000
C	-4.68126000	0.83489900	1.89115400
H	-5.32225700	1.47881300	1.27654500
H	-4.80198900	-0.19490600	1.53622200
H	-5.06372700	0.88292100	2.91961600

TS1-O-Cu-Bu

P	0.94658700	1.17153400	1.59387500
C	-0.20866700	2.63436600	1.43713900
H	-0.00578500	3.31192100	2.27822100
H	-1.22968800	2.25816000	1.58145700
C	-0.09744100	3.40841300	0.10687600
H	-0.47720600	4.42993800	0.24784500
H	0.95493300	3.51110900	-0.18815600
P	-1.00304400	2.62755400	-1.34666200
C	2.56531900	2.02223000	1.91074800
H	2.49490400	2.74408800	2.73340900
H	3.31877600	1.26799700	2.15713600
H	2.90182400	2.54023500	1.00729200
C	0.52305400	0.57075100	3.29622100
H	-0.49296600	0.16354600	3.30489600
H	1.20837300	-0.23764800	3.56901000
H	0.59393200	1.37080500	4.04284800
C	-0.52895900	3.86855300	-2.65698000
H	-1.11240300	3.67850700	-3.56426400
H	-0.69896400	4.90603500	-2.34258800
H	0.52925400	3.74702000	-2.91236400
C	-2.73917300	3.21486800	-0.98657700
H	-2.78674100	4.28592000	-0.75150400
H	-3.37036600	3.01954600	-1.86047400
H	-3.16243500	2.64680200	-0.15154100
H	2.02340900	-1.93370500	-0.24972800

C	0.50747300	-3.31597300	-0.64716900
H	1.00579400	-3.33312900	-1.63817600
H	0.29095800	-4.36723200	-0.39080300
C	-0.84337000	-2.58578900	-0.82733100
H	-1.40469700	-3.07743900	-1.63890700
O	1.31627300	-2.71988300	0.31618200
N	-0.55582900	-1.17231500	-1.18660100
H	-0.19988600	-1.12375000	-2.14090600
H	-1.40186200	-0.60377400	-1.16665300
C	-1.68920600	-2.64179700	0.45825500
H	-1.83528900	-3.70234700	0.70088500
H	-1.09757100	-2.20839600	1.27116000
C	-3.03535600	-1.95496800	0.35231500
C	-3.28183800	-0.73487100	0.99782200
C	-4.07381100	-2.52032800	-0.40549700
C	-4.52142500	-0.09741500	0.89185900
H	-2.49379700	-0.28934000	1.60090100
C	-5.31162200	-1.88758200	-0.51791700
H	-3.90981700	-3.47240100	-0.90616400
C	-5.54053100	-0.67096900	0.13079600
H	-4.69346200	0.84128200	1.41328900
H	-6.10153800	-2.34743500	-1.10633500
H	-6.50671400	-0.18029300	0.04931300
Cu	0.98058200	-0.36893800	0.02045400
C	2.88692400	-1.00638100	-1.00717200
H	2.90210200	-1.58614900	-1.94660900
H	2.75690700	0.04138800	-1.34672200
C	4.25477000	-1.12290500	-0.31556000
H	4.25680500	-0.51522700	0.60384700
H	4.40341100	-2.15967000	0.02352400
C	5.46336300	-0.71082300	-1.17285500
H	5.33099500	0.33058000	-1.50369700
H	5.47378900	-1.31896900	-2.08929700
C	6.80925400	-0.85126800	-0.45123900
H	6.98283200	-1.88876000	-0.13842000
H	7.64881500	-0.55187500	-1.09079900
H	6.84142300	-0.22785900	0.45205000

TS1-O-Cu-HMDS

P	0.21697000	1.59546000	1.90716800
C	-0.72603400	3.00602900	1.12990100
H	-1.38880400	3.41652900	1.90484000
H	-1.36688200	2.54022100	0.37062500
C	0.11056500	4.15329600	0.53609500
H	-0.57410700	4.90659100	0.12017000
H	0.67381700	4.65413300	1.33444900
P	1.36420000	3.66351600	-0.77590100
C	1.36600500	2.43363100	3.09222400
H	0.84717300	3.18050100	3.70515600

H	1.80948000	1.68072000	3.75164000
H	2.17755100	2.91757800	2.54113500
C	-1.07749100	0.90600900	3.03727800
H	-1.89379400	0.50214900	2.43092400
H	-0.65824800	0.08667700	3.62897400
H	-1.47235300	1.67387700	3.71283800
C	1.93827500	5.37475300	-1.25123600
H	2.58233100	5.30694500	-2.13455400
H	1.10619500	6.05434600	-1.47558900
H	2.53510000	5.80476700	-0.43950400
C	0.21068000	3.31721900	-2.19899500
H	-0.51052600	4.12931300	-2.35823900
H	0.79325600	3.17779400	-3.11570100
H	-0.33243600	2.38759600	-2.00452400
N	2.07850900	-1.53323800	-0.19775400
H	0.91274500	-1.57981900	-0.67695500
Si	3.31822900	-0.99821600	-1.32728000
Si	2.27590700	-2.86948900	0.93621800
C	3.94875600	-2.80534100	1.83354300
H	4.01987100	-3.61763200	2.56865000
H	4.79865500	-2.90993300	1.14855500
H	4.07349500	-1.85844400	2.37352900
C	0.90855400	-2.80381100	2.24937800
H	1.04490600	-1.95239700	2.92901800
H	-0.07471000	-2.70598600	1.77549900
H	0.90603900	-3.71705000	2.85910700
C	2.12071100	-4.53955700	0.04720700
H	2.90463700	-4.68279900	-0.70492200
H	2.18457400	-5.37378900	0.75799800
H	1.15287600	-4.61335700	-0.46427900
C	4.25186000	-2.44365500	-2.13875200
H	4.97773100	-2.06030000	-2.86796600
H	4.80918200	-3.04773300	-1.41264800
H	3.56960000	-3.11484400	-2.67430200
C	2.49073700	-0.01297600	-2.71832500
H	3.24031900	0.35593700	-3.43048800
H	1.77285100	-0.62642600	-3.27541900
H	1.95405200	0.85575500	-2.32034400
C	4.60052000	0.11928600	-0.48740900
H	4.12642600	1.02836500	-0.09760900
H	5.09496700	-0.38677000	0.35002300
H	5.37988400	0.42667300	-1.19723700
C	-1.05951800	-1.13301200	-1.81512300
H	-0.61421500	-0.42818900	-2.54730000
H	-1.11770500	-2.11175400	-2.32964100
C	-2.51611200	-0.68227200	-1.57767500
H	-3.06155700	-0.89781600	-2.51684500
O	-0.30686900	-1.23600600	-0.64913400
N	-2.58059700	0.75667100	-1.25004400
H	-2.31111500	1.28745300	-2.07786200

H	-3.55243400	1.00867900	-1.06648200
C	-3.18130300	-1.50540300	-0.45735600
H	-3.03152900	-2.56707900	-0.69074200
H	-2.63939900	-1.30635400	0.47166100
C	-4.65946600	-1.22290000	-0.29050600
C	-5.12834800	-0.35369200	0.70583400
C	-5.60346800	-1.80707400	-1.15035200
C	-6.49065800	-0.07205300	0.83794700
H	-4.41542100	0.09973100	1.39136100
C	-6.96479300	-1.53139800	-1.02242600
H	-5.26362200	-2.49175200	-1.92476100
C	-7.41454600	-0.66009500	-0.02679400
H	-6.82927600	0.60177200	1.62121300
H	-7.67655100	-2.00093900	-1.69691500
H	-8.47523600	-0.44697700	0.07645700
Cu	0.99988900	0.01997800	0.60357900

ADD1-OAc

Ag	0.69127500	0.18584700	-0.19950400
P	2.04227600	2.17140300	0.76954600
C	3.63348100	2.04487700	-0.21514400
H	4.44495200	2.53881600	0.33629700
H	3.48289000	2.62194400	-1.13778400
C	4.03196700	0.59482100	-0.55138900
H	5.00397200	0.57893700	-1.06289300
H	4.13844900	0.01079600	0.37046900
P	2.75924200	-0.31220800	-1.58231300
C	-1.50506400	-2.43934100	-1.30083300
H	-0.46334500	-2.19807900	-1.57393900
H	-1.97446500	-2.90915200	-2.17411700
C	-2.24117500	-1.11906800	-1.00883600
H	-2.21837300	-0.51492600	-1.92654100
O	-1.57134900	-3.37733500	-0.25249100
N	-1.50790200	-0.35876500	0.03153000
H	-1.32961900	-0.95883900	0.85157500
C	-3.71863800	-1.38311500	-0.62462100
H	-4.18628600	-1.93097500	-1.45367800
H	-3.72690300	-2.05453800	0.24031100
C	-4.50541100	-0.12335700	-0.33663700
C	-4.73212800	0.30498700	0.98001400
C	-5.00017300	0.66994600	-1.38416600
C	-5.42610100	1.48929200	1.24336000
H	-4.37198600	-0.30433300	1.80619300
C	-5.69450200	1.85195200	-1.12661900
H	-4.84430500	0.35076800	-2.41287400
C	-5.90872700	2.26743700	0.19043600
H	-5.59427900	1.79803500	2.27198900
H	-6.07373200	2.44695400	-1.95369500
H	-6.45253900	3.18641900	0.39253200

H	-2.06869200	0.43521900	0.33774000
O	1.74687100	-1.27923700	1.47500300
C	0.96755400	-2.08330400	2.07299700
C	1.58416300	-3.01325600	3.12251900
H	2.65823900	-2.84550200	3.23308100
H	1.08642700	-2.85827600	4.08623500
H	1.40363200	-4.05562900	2.83622300
O	-0.27938400	-2.19073000	1.88761400
H	-1.04139200	-3.04615500	0.50949900
C	3.41476200	-2.03980700	-1.51877800
C	3.19961300	0.22500500	-3.30633800
C	2.60472200	1.78317400	2.49010400
C	1.82767100	4.01642300	0.82950500
H	2.75051700	0.70166400	2.56696000
H	3.52315800	2.31728700	2.76274300
H	1.81120400	2.06082600	3.19236600
H	1.58280700	4.39331500	-0.16897900
H	0.99390400	4.26147000	1.49535800
H	2.72891300	4.52616300	1.19133100
H	2.58265100	-0.32203200	-4.02672000
H	2.98868000	1.29230900	-3.43053500
H	4.25677700	0.04206300	-3.53465400
H	2.85369700	-2.67241200	-2.21408700
H	4.48039700	-2.08778600	-1.77286000
H	3.25607600	-2.41730300	-0.50452500

TS1-N-OAc

Ag	-2.12294700	0.04517300	0.04737700
P	-2.27931100	-2.39528200	-0.31042600
C	-4.12811700	-2.68963200	-0.41991900
H	-4.33583800	-3.75853400	-0.27772800
H	-4.42352800	-2.44746400	-1.44931000
C	-4.96078400	-1.85713500	0.57608100
H	-6.02525200	-2.10958200	0.47745400
H	-4.67212600	-2.10799800	1.60554700
P	-4.73069200	-0.00334400	0.39800300
C	-1.75935700	-3.45154800	1.11256800
H	-2.02766800	-4.50284200	0.95387800
H	-0.67524400	-3.35349100	1.22288100
H	-2.22892000	-3.09355100	2.03464800
C	-1.65750500	-3.33480700	-1.77332300
H	-1.94799200	-2.81846300	-2.69421000
H	-0.56421900	-3.38527600	-1.72575100
H	-2.06442600	-4.35335300	-1.78984400
C	-5.77618400	0.61440200	1.80201900
H	-5.84262200	1.70564500	1.74602100
H	-6.78928900	0.19449100	1.78311800
H	-5.30064200	0.35570900	2.75361500
C	-5.80583400	0.38575100	-1.06448200

H	-6.82881500	0.01043900	-0.93967600
H	-5.83745500	1.47109300	-1.20421700
H	-5.37285200	-0.04891000	-1.97096600
C	-0.57679100	2.07135800	-2.52438800
H	-0.56847100	1.21237800	-3.20433000
H	-0.73051600	2.97615600	-3.13333300
C	0.81289100	2.17532300	-1.85312200
H	1.55578800	2.04774400	-2.65278500
O	-1.67008500	1.86494100	-1.64933600
N	0.98550400	1.01938900	-0.94212800
H	0.42751900	1.13445000	-0.07910700
C	1.04321200	3.55642300	-1.18945000
H	0.90477500	4.30560700	-1.98072700
H	0.25317400	3.73530900	-0.45354500
C	2.40451100	3.74988800	-0.55453300
C	2.58866600	3.56530800	0.82301100
C	3.51548600	4.11075300	-1.33144800
C	3.84733900	3.72602200	1.40625100
H	1.73788200	3.29086400	1.44195700
C	4.77562200	4.27102100	-0.75325100
H	3.38968100	4.27534100	-2.40009800
C	4.94576500	4.07728100	0.61966400
H	3.96756800	3.57992800	2.47659500
H	5.62257000	4.55414500	-1.37305200
H	5.92527800	4.20514200	1.07255100
C	5.41650300	-2.59851300	2.00235500
C	4.13407600	-2.29033100	1.54361200
C	3.72935000	-2.74688700	0.28709500
C	4.58502700	-3.51432200	-0.50822200
C	5.86395300	-3.81746600	-0.04129400
C	6.28191100	-3.35704400	1.21083300
H	5.73615600	-2.25264500	2.98185400
H	3.43833500	-1.72507200	2.15485300
H	4.23767000	-3.88435400	-1.46767800
H	6.53230400	-4.41980500	-0.65096800
H	7.27850000	-3.59679000	1.57206300
S	2.08865800	-2.30286300	-0.34431700
O	1.66674500	-3.44615200	-1.18959200
O	1.28306300	-1.95357000	0.85561700
C	2.19834600	-0.89502500	-1.35619100
H	2.80941600	-1.10397700	-2.23423100
C	2.38395500	0.45876600	-0.67985300
H	2.55985700	0.43196300	0.39635800
H	3.13623300	1.09339300	-1.14950200
H	0.88995400	-0.13655600	-1.45874400
O	-1.83330600	3.35504400	0.54161900
C	-1.34475200	2.66741900	1.47529800
C	-1.27929100	3.27732300	2.87269000
H	-1.58567700	4.32532400	2.86003300
H	-1.93744000	2.71293700	3.54364400

H	-0.26520300	3.18795100	3.27687700
O	-0.88061000	1.47715400	1.35735500
H	-1.72138900	2.55367200	-0.91784200

ADD2-N-OAc

Ag	1.99175000	-0.34855800	0.17757100
P	3.07222100	1.55107600	-0.97148800
C	4.88139700	1.07226800	-1.05816000
H	5.49487300	1.95156200	-1.29685900
H	4.98086500	0.37997400	-1.90475500
C	5.40222400	0.40219100	0.23062300
H	6.46737700	0.15737500	0.11989500
H	5.32701400	1.10385500	1.07212400
P	4.44970200	-1.13720300	0.73498200
C	3.10373500	3.16245300	-0.06518400
H	3.76744200	3.89118000	-0.54610300
H	2.08210900	3.55182100	-0.04443900
H	3.42990100	3.00472800	0.96781200
C	2.71524900	2.08240500	-2.70465800
H	2.76212300	1.21821300	-3.37481100
H	1.69737100	2.48124000	-2.72501300
H	3.41659900	2.84948000	-3.05411100
C	5.31145200	-1.56039600	2.32534800
H	4.94571900	-2.52841500	2.68250500
H	6.40117100	-1.61206600	2.21086100
H	5.06805800	-0.81003600	3.08462700
C	5.15447900	-2.41261600	-0.41501500
H	6.25106000	-2.43229200	-0.39355300
H	4.77203900	-3.39807600	-0.13052000
H	4.81717100	-2.21557500	-1.43735800
C	0.10825500	-2.48789100	-2.04146000
H	0.51639100	-1.90203200	-2.87096400
H	0.06641500	-3.54299900	-2.35552200
C	-1.32820300	-1.99825400	-1.76237400
H	-1.84410400	-2.05099500	-2.73373600
O	1.03272700	-2.33800000	-0.97115000
N	-1.28106200	-0.58431500	-1.39057100
H	-0.76163100	-0.45092100	-0.52545200
C	-2.06515000	-2.98008700	-0.79740900
H	-1.88816100	-3.99469500	-1.18329200
H	-1.59225400	-2.94413500	0.18871800
C	-3.56005900	-2.77763200	-0.66338500
C	-4.12589800	-2.31832600	0.53406100
C	-4.42432400	-3.06037800	-1.73342700
C	-5.50456100	-2.13081500	0.65704500
H	-3.47612200	-2.10898700	1.38081200
C	-5.80218200	-2.87330800	-1.61776800
H	-4.01222000	-3.43929800	-2.66692100
C	-6.34859500	-2.40402800	-0.42048200

H	-5.91842900	-1.77428800	1.59701900
H	-6.45088700	-3.10133000	-2.46000600
H	-7.42192200	-2.26104100	-0.32711500
C	-2.55771900	2.03431500	2.89484500
C	-1.90281700	1.99117400	1.66129000
C	-2.33853100	2.85050600	0.64777400
C	-3.39422100	3.74547400	0.84337000
C	-4.03630700	3.77402100	2.08138200
C	-3.61901000	2.91796500	3.10417000
H	-2.22703900	1.37680700	3.69378200
H	-1.07257300	1.30519300	1.50957700
H	-3.68459300	4.41893400	0.04368500
H	-4.85462800	4.46863100	2.24926600
H	-4.11917300	2.94488500	4.06872300
S	-1.51386300	2.84322700	-0.95314200
O	-1.77565100	4.14129600	-1.60348300
O	-0.11814400	2.40454700	-0.74036900
C	-2.39004700	1.59130800	-1.95265500
H	-3.37614100	2.03528400	-2.12602600
C	-2.52755100	0.16705500	-1.39119800
H	-3.02151400	0.20855500	-0.40961900
H	-3.23882800	-0.33634100	-2.05492500
H	-1.83046600	1.58518400	-2.89376600
O	0.29992600	-2.80299500	1.56840300
C	0.01269500	-1.70655300	2.11012600
C	-0.70544300	-1.72755900	3.45988800
H	-0.85042000	-2.75048800	3.81325400
H	-0.12699700	-1.15982300	4.19725100
H	-1.68031800	-1.23366500	3.36588800
O	0.25076500	-0.54478300	1.62556700
H	0.68956800	-2.67646700	-0.09557300

TS1-O-OAc

Ag	-0.96417300	1.00479300	-0.21865600
P	-2.88449800	2.85923800	-1.15071100
C	-1.76769300	4.37056000	-1.12281200
H	-2.38935200	5.27516500	-1.06789100
H	-1.25107000	4.40259900	-2.09174800
C	-0.74306500	4.37971900	0.02611900
H	-0.18749500	5.32767600	0.02588000
H	-1.26102100	4.31266900	0.99079500
P	0.47391400	2.96068700	-0.00943100
C	0.33093900	-2.35756400	-0.98547100
H	0.71912400	-1.49691000	-1.53714500
H	0.70971400	-3.28134000	-1.43063700
C	-1.19234900	-2.37909400	-0.94375400
H	-1.50287900	-2.38311200	-1.99852000
O	0.87292800	-2.30162600	0.37536700
N	-1.72460000	-1.15289500	-0.32561300

H	-1.73561900	-1.22268500	0.72021800
C	-1.73027500	-3.66820400	-0.26440600
H	-1.28534000	-4.53697700	-0.76865900
H	-1.37696900	-3.67742000	0.77239100
C	-3.24010500	-3.78096100	-0.29797100
C	-4.02502400	-3.22861000	0.72731100
C	-3.88405700	-4.41963500	-1.36743300
C	-5.41838800	-3.31476900	0.67519100
H	-3.54168600	-2.72503000	1.56215600
C	-5.27617600	-4.50732200	-1.41853600
H	-3.28795600	-4.86152200	-2.16406700
C	-6.04827500	-3.95350500	-0.39518900
H	-6.01161300	-2.88505200	1.47835600
H	-5.75614300	-5.01229500	-2.25308600
H	-7.13238600	-4.02364300	-0.42976300
H	-2.70499000	-1.06250400	-0.58772500
O	-1.95887300	1.20648600	1.99747700
C	-2.08626700	0.19645000	2.76221100
C	-2.44931800	0.49881400	4.22130100
H	-3.24663700	1.24773600	4.26948600
H	-2.75495500	-0.40893300	4.74735100
H	-1.57498800	0.92326300	4.73028300
O	-1.92261500	-1.01144900	2.43842500
H	1.22827300	-1.26248300	0.71150700
C	7.20266200	-2.05456500	-1.13611400
C	5.86698500	-1.64731700	-1.15348200
C	5.41027700	-0.76397500	-0.17339600
C	6.27087700	-0.27399200	0.81284300
C	7.60272300	-0.68795900	0.82253600
C	8.06808100	-1.58012200	-0.14799100
H	7.56846200	-2.73554100	-1.89989300
H	5.18558600	-1.98307600	-1.92802100
H	5.90242100	0.43683700	1.54569500
H	8.27977900	-0.30799200	1.58274700
H	9.10715800	-1.89792600	-0.13840700
S	3.67000600	-0.26417800	-0.15899900
O	3.66487600	1.13950000	0.31307900
O	3.14098200	-0.59822200	-1.50464900
C	2.80988900	-1.23817100	1.00177000
H	3.14193200	-1.08582600	2.02458000
C	2.41221400	-2.58954700	0.56841600
H	2.76933200	-2.93897000	-0.40014500
H	2.43284600	-3.37068300	1.32633000
C	1.33807200	3.16681200	1.60615300
C	1.73707000	3.51006700	-1.24225700
C	-4.02365400	3.20730500	0.27307300
C	-3.96225300	3.31478000	-2.60213400
H	-3.52425200	2.91529400	1.20213200
H	-4.33877900	4.25754500	0.31531300
H	-4.91442400	2.57726500	0.16974100

H	-3.37517200	3.27600500	-3.52598700
H	-4.77531200	2.58662400	-2.69130700
H	-4.39804500	4.31665000	-2.50209000
H	2.57503100	2.80835700	-1.20351900
H	1.31277900	3.49661600	-2.25120900
H	2.09998600	4.52046600	-1.01705700
H	2.19873800	2.49303000	1.61893300
H	1.67832200	4.19907900	1.75307400
H	0.64885500	2.88731500	2.40870400

ADD1-O-real

Ag	0.75534100	-1.53016100	-0.19293800
P	0.89264500	-0.42701600	1.92575800
C	0.59961400	1.41935100	2.00478100
H	0.44630600	1.67882300	3.05968800
H	-0.36039900	1.58407700	1.50092100
C	1.71485600	2.29949600	1.40959400
H	1.61006300	3.32397100	1.78817200
H	2.69640800	1.95568300	1.75624700
P	1.81447700	2.29490600	-0.46643900
N	0.38969900	-2.70655300	-1.92933000
H	-1.33070700	-1.82522300	-1.71506900
Si	1.35281000	-2.23846700	-3.29742900
Si	-0.09813900	-4.34177200	-1.56641100
C	1.33580500	-5.59615500	-1.64642500
H	0.99318000	-6.60364600	-1.37521300
H	1.77930200	-5.65969800	-2.64787000
H	2.13784400	-5.31964100	-0.94956500
C	-0.82410700	-4.45218300	0.18745000
H	-0.07091000	-4.25790200	0.96275000
H	-1.64077100	-3.73375300	0.32622000
H	-1.22942100	-5.45669100	0.37088900
C	-1.46385500	-4.94707900	-2.74503200
H	-1.12782700	-4.99089600	-3.78700400
H	-1.80714900	-5.95174600	-2.46462400
H	-2.33052400	-4.27582300	-2.70161500
C	0.95962000	-3.23574900	-4.87245100
H	1.56083400	-2.86536100	-5.71337400
H	1.17972200	-4.30424700	-4.76061700
H	-0.09607000	-3.14309100	-5.15466900
C	1.05815800	-0.41123100	-3.73663200
H	1.72596800	-0.09340300	-4.54870400
H	0.02644800	-0.24293700	-4.07005600
H	1.24684800	0.24031300	-2.87420000
C	3.22325400	-2.42303800	-2.97876200
H	3.54063100	-1.78616800	-2.14194000
H	3.48304800	-3.45759500	-2.72236700
H	3.81616300	-2.13658400	-3.85785400
C	-2.57811900	-0.33912600	-2.12398500

H	-1.72639300	0.23326900	-2.52511200
H	-3.15900500	-0.70504700	-2.98862400
C	-3.47392100	0.62100000	-1.33243400
H	-3.89612900	1.31863200	-2.08126800
O	-2.13928400	-1.41106300	-1.31749300
N	-2.69230300	1.33488200	-0.30944500
H	-1.96243700	1.87618300	-0.77114200
H	-3.29592800	2.01596500	0.14988800
C	-4.65819600	-0.11984300	-0.67401900
H	-5.16098500	-0.70886700	-1.45135400
H	-4.25157600	-0.82962900	0.05262600
C	-5.65927200	0.80828100	-0.01816900
C	-5.56593200	1.14063000	1.34211000
C	-6.69652300	1.38474300	-0.76758200
C	-6.47628700	2.02017300	1.93342800
H	-4.77191200	0.70294000	1.94256000
C	-7.60912400	2.26261700	-0.18170200
H	-6.79240700	1.13343000	-1.82199700
C	-7.50191300	2.58459000	1.17343200
H	-6.38669800	2.25859800	2.99044800
H	-8.40813500	2.69093600	-0.78179300
H	-8.21464000	3.26431500	1.63303400
C	3.28250700	3.40843400	-0.68108800
C	4.50229900	2.80251900	-1.02216200
C	3.24737400	4.80157500	-0.50984400
C	5.66274300	3.56555500	-1.16889200
H	4.54053400	1.72726000	-1.18140700
C	4.40460900	5.56561500	-0.66508400
H	2.31016700	5.29472400	-0.26688700
C	5.61534000	4.94900500	-0.99119500
H	6.59887100	3.08025100	-1.43218700
H	4.36102800	6.64387400	-0.53368400
H	6.51519300	5.54605200	-1.11362900
C	0.40019500	3.38896200	-0.95888100
C	0.01847500	3.34521900	-2.31297700
C	-0.32934900	4.21973900	-0.09225600
C	-1.04017000	4.12091400	-2.78776600
H	0.55200300	2.69068200	-2.99772600
C	-1.39823200	4.98731600	-0.56380600
H	-0.07490500	4.27460800	0.96195700
C	-1.75410400	4.94335000	-1.91269700
H	-1.31340700	4.07432100	-3.83853200
H	-1.95111400	5.62056400	0.12534300
H	-2.58584500	5.53950700	-2.27794600
C	2.46193800	-0.68144800	2.84894000
C	2.76885700	0.02421300	4.02545700
C	3.39077000	-1.61199600	2.35749900
C	3.97315000	-0.19943600	4.69275800
H	2.06520500	0.74701400	4.42901400
C	4.59438400	-1.83861100	3.02858800

H	3.17041500	-2.15639100	1.44249300
C	4.88738500	-1.13215600	4.19554300
H	4.19782200	0.35437500	5.60027400
H	5.30192100	-2.56302400	2.63505400
H	5.82547300	-1.30425900	4.71613400
C	-0.45623900	-1.05853100	3.01021100
C	-0.22548600	-1.64237400	4.26348200
C	-1.77049200	-0.98001200	2.51396300
C	-1.29432800	-2.13168400	5.01843400
H	0.78433000	-1.72419500	4.65264400
C	-2.83145900	-1.46679100	3.27807000
H	-1.96656900	-0.54971500	1.53306300
C	-2.59768000	-2.04352500	4.52918500
H	-1.10340700	-2.58566300	5.98727700
H	-3.84309300	-1.41058700	2.88511500
H	-3.42735700	-2.42977300	5.11519500

TS1-O-real

Ag	0.25885400	-1.12772100	-0.20755100
P	0.60925600	-0.53264000	2.08555600
C	0.93170800	1.28121100	2.40577700
H	0.97326700	1.43243500	3.49138700
H	0.03492700	1.80497600	2.05598700
C	2.20060500	1.84899500	1.74503200
H	2.45885300	2.80934500	2.20838600
H	3.05649000	1.18890700	1.93157200
P	2.09316400	2.02315900	-0.12235300
N	0.21888500	-2.33137300	-2.20636000
H	-0.73135000	-1.49701400	-2.22281700
Si	1.55283500	-1.95842700	-3.28002100
Si	-0.45860000	-3.93766700	-1.96971800
C	0.88876900	-5.26148600	-1.74774200
H	0.43204900	-6.24121600	-1.55562300
H	1.52550000	-5.36687800	-2.63431200
H	1.54225100	-5.03032900	-0.89685600
C	-1.55309500	-3.95865500	-0.42108800
H	-0.96565500	-3.87196500	0.50245400
H	-2.26622900	-3.12663900	-0.44409800
H	-2.12418800	-4.89493300	-0.36078000
C	-1.55695100	-4.44258500	-3.43494800
H	-0.99195400	-4.51084300	-4.37151000
H	-2.02990200	-5.41772400	-3.25934000
H	-2.35801000	-3.70770700	-3.58331500
C	1.49158100	-2.92164600	-4.92087300
H	2.32386800	-2.62134000	-5.57125200
H	1.56552900	-4.00648700	-4.77774700
H	0.56004400	-2.72328200	-5.46479600
C	1.50310800	-0.11447700	-3.71825400
H	2.34263300	0.15173700	-4.37365500

H	0.57495300	0.14469100	-4.24182300
H	1.56841400	0.50901700	-2.81898200
C	3.23208000	-2.32614300	-2.46830900
H	3.34853700	-1.74819300	-1.54212200
H	3.33330000	-3.38721900	-2.21013500
H	4.06458100	-2.06551600	-3.13530300
C	-1.98810800	0.44412300	-2.33397500
H	-1.17184500	1.18534400	-2.45294100
H	-2.35235400	0.22240400	-3.35650200
C	-3.14476800	1.15408100	-1.60226600
H	-3.47261900	1.97025500	-2.27637400
O	-1.56303300	-0.71419000	-1.69182600
N	-2.69531400	1.68572300	-0.30204600
H	-1.93939700	2.35126400	-0.46418500
H	-3.45715100	2.21949000	0.11640800
C	-4.33664700	0.19995900	-1.39942200
H	-4.61808600	-0.19000500	-2.38771000
H	-3.98618800	-0.65138700	-0.80958300
C	-5.54783800	0.83314100	-0.74479000
C	-6.00710600	0.38915100	0.50358400
C	-6.25021800	1.87686600	-1.36948800
C	-7.12436600	0.96705600	1.11229200
H	-5.48619000	-0.42944600	0.99466300
C	-7.36430900	2.46035000	-0.76529600
H	-5.92288000	2.23131700	-2.34473500
C	-7.80622200	2.00800900	0.48076400
H	-7.46418200	0.59963600	2.07770800
H	-7.89298300	3.26500200	-1.27067000
H	-8.67651100	2.45903000	0.95038600
C	3.78531500	2.70899500	-0.44592500
C	4.75817100	1.81610900	-0.92335700
C	4.14775100	4.04774500	-0.22805700
C	6.06653600	2.24408900	-1.15738000
H	4.48690100	0.78143800	-1.12023300
C	5.45279200	4.47789000	-0.47165600
H	3.40611900	4.76004300	0.12291900
C	6.41572300	3.57666800	-0.93274000
H	6.80762600	1.53943900	-1.52542400
H	5.71807200	5.51850400	-0.30254000
H	7.43110500	3.91432800	-1.12298500
C	0.99772800	3.50144000	-0.34243600
C	0.49099900	3.71786900	-1.63756200
C	0.61314700	4.38878200	0.67610300
C	-0.35431600	4.79450600	-1.90867300
H	0.75826100	3.03214500	-2.43785300
C	-0.24399900	5.46003000	0.40864900
H	0.97745500	4.25473700	1.69029200
C	-0.72723100	5.66783600	-0.88387800
H	-0.72935200	4.94436300	-2.91751800
H	-0.53147300	6.13256300	1.21279800

H	-1.39393200	6.50062700	-1.09053600
C	1.98908700	-1.38743700	2.95467600
C	2.48622400	-0.96388300	4.19960400
C	2.57499100	-2.50472900	2.33957100
C	3.53994300	-1.64322400	4.81138400
H	2.05015700	-0.10494700	4.70189500
C	3.62627500	-3.18771300	2.95473700
H	2.20751800	-2.83225900	1.37019600
C	4.11114200	-2.75692000	4.19015200
H	3.91507200	-1.30269300	5.77274700
H	4.06793400	-4.05080900	2.46444100
H	4.93284500	-3.28393400	4.66743400
C	-0.90127000	-0.80505600	3.10320100
C	-0.90379500	-1.52914700	4.30372000
C	-2.10304200	-0.25142100	2.62448500
C	-2.08822300	-1.68455700	5.02787600
H	0.01251800	-1.97619000	4.67558900
C	-3.27669200	-0.39680700	3.36522900
H	-2.13683600	0.28027100	1.67163700
C	-3.27386700	-1.11291500	4.56495600
H	-2.08014800	-2.25242200	5.95460300
H	-4.19625300	0.04617400	2.99294300
H	-4.19326600	-1.23122900	5.13241500

ADD2-O-real

Ag	0.79178100	0.34444000	-0.01177500
P	0.44311200	-0.72556500	2.07339400
C	0.21780500	-2.58660900	2.00381300
H	0.28986100	-2.97994800	3.02540400
H	1.07969200	-2.97663600	1.45144300
C	-1.09342700	-3.07102000	1.36127800
H	-1.12841200	-4.16741700	1.40032200
H	-1.94454700	-2.71958100	1.95619100
P	-1.44798900	-2.45344300	-0.37984400
N	-1.99208800	3.26585600	-1.03022800
H	-1.11721500	2.74057900	-1.23469700
Si	-3.40902000	2.58410500	-1.77276800
Si	-1.64676600	4.82120400	-0.32376900
C	-3.18043800	5.49344200	0.57421600
H	-2.96323900	6.46824600	1.02955400
H	-4.03279500	5.63472100	-0.10181400
H	-3.50230800	4.81835100	1.37683900
C	-0.22923200	4.61775200	0.91460700
H	-0.54372300	4.02511600	1.78304700
H	0.60034700	4.08615600	0.43327600
H	0.14159200	5.58386400	1.28015600
C	-1.11935600	6.10578900	-1.62050900
H	-1.91065100	6.27227300	-2.36188600
H	-0.87917000	7.07546300	-1.16446800

H	-0.22917800	5.76228100	-2.16208400
C	-4.26299200	3.79082300	-2.96736600
H	-5.15968300	3.34186300	-3.41452700
H	-4.57779100	4.71258100	-2.46216100
H	-3.58941800	4.07765300	-3.78410300
C	-2.88202200	1.04084100	-2.73634500
H	-3.74273300	0.55136300	-3.20976500
H	-2.16409100	1.29793700	-3.52464900
H	-2.39819400	0.31303200	-2.07352400
C	-4.70522600	2.07275300	-0.47742100
H	-4.29138600	1.32793500	0.21450000
H	-5.03463900	2.93135000	0.12133800
H	-5.59817800	1.63812800	-0.94617300
C	1.11073100	1.72709800	-2.64064900
H	0.47672800	1.09402700	-3.30422700
H	1.26849800	2.67595800	-3.19147000
C	2.49341400	1.02671500	-2.56443300
H	2.84787700	0.85346100	-3.59520500
O	0.52976800	1.95156600	-1.40810800
N	2.32715100	-0.25697800	-1.84643200
H	1.82314300	-0.92880500	-2.42450900
H	3.23224300	-0.66968900	-1.62748200
C	3.53321000	1.90201000	-1.83559200
H	3.62161700	2.83753400	-2.40252500
H	3.12948300	2.16351600	-0.85157600
C	4.89576700	1.25704400	-1.69094800
C	5.30340900	0.68928200	-0.47404300
C	5.77909900	1.18731900	-2.78040700
C	6.54912400	0.06759600	-0.34996400
H	4.64153500	0.74757400	0.38767700
C	7.02348200	0.56868900	-2.66108600
H	5.48695800	1.63024100	-3.73046000
C	7.41346900	0.00403300	-1.44347800
H	6.84564600	-0.35858700	0.60541900
H	7.69283000	0.53200400	-3.51701900
H	8.38478400	-0.47422400	-1.34813800
C	-3.05257600	-3.34058300	-0.66506300
C	-4.22721700	-2.57386300	-0.60945700
C	-3.15706800	-4.71893800	-0.91162200
C	-5.47795500	-3.17255800	-0.77692800
H	-4.16117600	-1.50158500	-0.44218700
C	-4.40587100	-5.31572800	-1.08740300
H	-2.25929500	-5.32758900	-0.97873000
C	-5.56902100	-4.54430400	-1.01673300
H	-6.37775800	-2.56491500	-0.73012100
H	-4.47167200	-6.38331900	-1.28183400
H	-6.54087300	-5.01063300	-1.15567600
C	-0.26155300	-3.41198500	-1.43133300
C	-0.10110600	-2.96205700	-2.75551700
C	0.49861700	-4.51421100	-1.00978900

C	0.77603600	-3.60240700	-3.63189600
H	-0.67323800	-2.10274900	-3.09889700
C	1.38904000	-5.14797100	-1.88197200
H	0.40037800	-4.89418600	0.00316200
C	1.52879100	-4.69604200	-3.19468700
H	0.87462300	-3.24594400	-4.65402600
H	1.96868200	-5.99944700	-1.53441000
H	2.21890000	-5.19095300	-3.87254600
C	-1.01536900	-0.15550000	3.03557900
C	-1.37694300	-0.74831100	4.25849300
C	-1.80541200	0.88368500	2.52054800
C	-2.50560300	-0.31005600	4.94984500
H	-0.77094500	-1.54649300	4.67986500
C	-2.93616800	1.32074600	3.21670100
H	-1.54143500	1.35092800	1.57467100
C	-3.28746300	0.72518200	4.42817800
H	-2.77507100	-0.77516200	5.89438600
H	-3.53953400	2.12376200	2.80361300
H	-4.16776900	1.06496800	4.96724700
C	1.87714000	-0.56790800	3.22382600
C	1.85822400	0.30499900	4.32179700
C	3.06170700	-1.26982400	2.93999300
C	2.99103600	0.45958400	5.12418400
H	0.95873900	0.86590300	4.55454700
C	4.18840700	-1.12008900	3.74822000
H	3.11341900	-1.93103500	2.07865500
C	4.15656700	-0.25415000	4.84396500
H	2.95829900	1.14066400	5.97033000
H	5.09286700	-1.67716200	3.51827900
H	5.03593300	-0.13353400	5.47053800

ADD3-O-real

C	1.06756700	-0.29374500	0.62503800
H	1.98862100	-0.69304400	0.15905500
H	1.41363600	0.48059000	1.34692000
C	0.46975400	-1.44431700	1.46805400
H	0.12080100	-2.22101200	0.77539800
O	0.20421900	0.21742900	-0.32798300
N	-0.74065800	-0.94073800	2.15931000
H	-1.24919900	-1.70253800	2.60490000
H	-0.46265000	-0.30061600	2.90493100
C	1.51214100	-2.05686300	2.43295100
H	2.38650700	-2.35331600	1.83925700
H	1.85595500	-1.27245200	3.12137400
C	0.99291800	-3.24238800	3.21682900
C	0.52939700	-3.10184700	4.53318600
C	0.92501800	-4.51441900	2.62622400
C	0.01090900	-4.19173100	5.23724500
H	0.59074900	-2.12953200	5.01827300

C	0.40863400	-5.60594900	3.32459800
H	1.28943400	-4.64824000	1.60970800
C	-0.05278400	-5.44851800	4.63424900
H	0.37173700	-6.58242400	2.84809300
H	-0.45180700	-6.29914300	5.18048800
Ag	-1.84109400	0.37065700	0.44443900
P	-3.87000000	1.67165900	0.52215200
C	-5.19855300	0.70853600	-0.37833600
H	-6.05814500	1.36059700	-0.57613200
H	-5.53326900	-0.08512000	0.30075800
C	-4.67971700	0.11199100	-1.70310500
H	-5.51634200	-0.29286900	-2.28471900
H	-4.22911300	0.90210300	-2.31474400
P	-3.34125800	-1.19139800	-1.45853900
C	5.34761300	6.38598000	0.36191700
C	4.56622100	5.25023200	0.57398400
C	5.02650400	4.01549300	0.11068500
C	6.25170000	3.89429300	-0.54816400
C	7.02428100	5.03821900	-0.75547900
C	6.57186500	6.28055500	-0.30446800
H	5.00447500	7.35178600	0.72216400
H	3.62195100	5.30783600	1.10533600
H	6.59608700	2.91707500	-0.87015700
H	7.98180700	4.95720500	-1.26222700
H	7.17773700	7.16800900	-0.46610300
S	4.01283700	2.54834300	0.36959000
O	4.93129200	1.38793500	0.32067600
O	3.16984600	2.78917700	1.55324300
C	2.98273900	2.46774000	-1.07599200
H	3.53145700	2.29430400	-1.99680800
C	1.65439300	2.49719700	-0.96798500
H	1.16496800	2.63774400	-0.01239200
H	1.02161300	2.37237700	-1.83883800
H	-0.33644900	-4.05831400	6.25883500
H	4.68862000	-0.71773200	-0.31841400
N	4.98167100	-1.68415300	-0.47118200
Si	4.30405400	-2.41241200	-1.90808700
Si	6.27905000	-2.13821300	0.61509200
C	7.93773400	-1.39164300	0.07235200
H	8.74936400	-1.65067500	0.76490700
H	8.22420800	-1.74339600	-0.92649000
H	7.87047800	-0.29741700	0.03206500
C	5.87308800	-1.49922000	2.34774900
H	6.70432400	-1.66575300	3.04486800
H	5.66599200	-0.42303400	2.31936300
H	4.98644600	-1.99837800	2.75682400
C	6.45096800	-4.02597800	0.65207900
H	6.68980200	-4.44572600	-0.33259500
H	7.26024700	-4.31874700	1.33311400
H	5.53118000	-4.50578800	1.00687900

C	5.65434400	-2.98254000	-3.11568600
H	6.28179000	-2.13922000	-3.42912700
H	6.31509700	-3.73614000	-2.66986500
H	5.21637500	-3.42750800	-4.01875400
C	3.22642100	-3.91624900	-1.48820300
H	2.80245000	-4.37190400	-2.39252100
H	3.79811400	-4.69086500	-0.96313900
H	2.39252600	-3.61972300	-0.83983600
C	3.22672000	-1.11767400	-2.77509000
H	2.77316400	-1.54905300	-3.67690300
H	2.41362500	-0.75849800	-2.13258900
H	3.82124100	-0.24950300	-3.08673200
C	-4.28682600	-2.78011400	-1.49436100
C	-5.65218600	-2.87642700	-1.18189500
C	-3.57490600	-3.97016000	-1.73477600
C	-6.28881500	-4.11926500	-1.12471300
H	-6.23657600	-1.98283100	-0.98240500
C	-4.21157800	-5.20852400	-1.68395800
H	-2.51600300	-3.92401700	-1.97667900
C	-5.57295400	-5.28895800	-1.37759400
H	-7.34812000	-4.16879000	-0.88522100
H	-3.64309100	-6.11318000	-1.88337300
H	-6.06867200	-6.25491200	-1.33429700
C	-2.49705500	-1.17736500	-3.09787400
C	-1.15457600	-0.76328900	-3.13919600
C	-3.14787200	-1.53677800	-4.29110500
C	-0.48652500	-0.70016700	-4.36755700
H	-0.62783400	-0.49963100	-2.21881600
C	-2.47391900	-1.47171700	-5.50947100
H	-4.17952100	-1.87869300	-4.26610300
C	-1.14090700	-1.05001300	-5.54869900
H	0.55353300	-0.38593600	-4.39109300
H	-2.98542000	-1.75186100	-6.42703700
H	-0.61498000	-1.00279200	-6.49911700
C	-4.63528800	2.09180900	2.14360300
C	-6.00777400	1.97826700	2.41556500
C	-3.78044100	2.54254400	3.16415700
C	-6.51166500	2.31131300	3.67544200
H	-6.69400700	1.62846200	1.65033100
C	-4.28622000	2.88594700	4.41734400
H	-2.71235800	2.61798700	2.97389400
C	-5.65398100	2.76854800	4.67658700
H	-7.57615200	2.21376300	3.87160400
H	-3.61119100	3.23525000	5.19388600
H	-6.04788800	3.02697300	5.65570000
C	-3.85552100	3.27313100	-0.39899100
C	-2.76061800	3.55955100	-1.22779000
C	-4.91005600	4.19708200	-0.31892100
C	-2.72749500	4.73992400	-1.97481400
H	-1.93186100	2.85714500	-1.27835300

C	-4.87210800	5.37777300	-1.05969600
H	-5.75656300	4.00164500	0.33406900
C	-3.78187400	5.64967600	-1.89141600
H	-1.87431100	4.94910700	-2.61443100
H	-5.69149400	6.08800100	-0.98581100
H	-3.75387900	6.57107600	-2.46691700

TS2-O-real

C	-1.04797700	-0.12101900	-1.17018100
H	-2.10068400	-0.07255500	-0.85324700
H	-0.99790100	0.35686400	-2.16745100
C	-0.65067900	-1.59470600	-1.30917400
H	-0.68525200	-2.05491900	-0.31407400
O	-0.23004400	0.53626800	-0.24093100
N	0.77008800	-1.67033400	-1.74664600
H	1.07945300	-2.64160500	-1.75977900
H	0.83890600	-1.33953200	-2.71059600
C	-1.61463100	-2.35796100	-2.24864900
H	-2.62665500	-2.25782900	-1.83748800
H	-1.62266900	-1.85800500	-3.22712300
C	-1.26077300	-3.82017400	-2.42078200
C	-0.55177400	-4.26821100	-3.54531300
C	-1.60378400	-4.76099000	-1.43677400
C	-0.19093100	-5.61095500	-3.68381800
H	-0.29601400	-3.55982400	-4.33108100
C	-1.24552500	-6.10273400	-1.57064600
H	-2.16822700	-4.43947000	-0.56453500
C	-0.53510700	-6.53287400	-2.69445500
H	-1.52819400	-6.81477900	-0.79954400
H	-0.26021300	-7.57888400	-2.80104000
Ag	1.96446200	-0.16221800	-0.37938200
P	4.14569500	1.00681500	-0.74300900
C	5.15441700	0.42060500	0.72636000
H	6.05523400	1.03704700	0.83286900
H	5.48172600	-0.60425900	0.51211300
C	4.35411200	0.45307800	2.04281500
H	5.01280900	0.17955700	2.87512500
H	3.98787500	1.46890300	2.23524600
P	2.83459800	-0.66013900	2.00488300
C	-3.86479600	6.65675900	-0.82376200
C	-3.41502200	5.36000300	-1.07463000
C	-4.00633700	4.28612600	-0.40497600
C	-5.04842100	4.49616900	0.50104700
C	-5.49002200	5.79689000	0.74935600
C	-4.89794200	6.87773200	0.09121500
H	-3.41410800	7.49533200	-1.34874300
H	-2.62865800	5.16661600	-1.79692600
H	-5.51691100	3.64443800	0.98306800
H	-6.30392400	5.96531000	1.45001100

H	-5.24738200	7.88895700	0.28328400
S	-3.38852200	2.60672500	-0.70130900
O	-4.58364500	1.74497200	-0.46456000
O	-2.77281300	2.63816500	-2.04989600
C	-2.18506800	2.29006800	0.47977500
H	-2.56970400	2.07828000	1.47093300
C	-0.83975400	2.18893600	0.13162200
H	-0.54342400	2.63873100	-0.81329200
H	-0.11549100	2.30667000	0.93561300
H	0.35147400	-5.93581700	-4.56819000
H	-4.90951800	-0.18639300	-0.00738600
N	-5.32138800	-1.12051800	0.09528100
Si	-5.13957000	-1.77753900	1.69907600
Si	-6.43961500	-1.45386200	-1.21123300
C	-8.06880900	-0.50280100	-1.00942900
H	-8.75184300	-0.67764100	-1.85111200
H	-8.59026100	-0.79358600	-0.08905200
H	-7.87466000	0.57517600	-0.95410600
C	-5.63368500	-0.92635900	-2.83841600
H	-6.34155600	-0.97449300	-3.67574800
H	-5.26585800	0.10370700	-2.76363700
H	-4.77905000	-1.56782000	-3.08581100
C	-6.82544900	-3.31148500	-1.25701700
H	-7.30423700	-3.66306600	-0.33471200
H	-7.51092300	-3.53873500	-2.08348200
H	-5.91649700	-3.90584900	-1.40927300
C	-6.80038300	-2.07831300	2.56976900
H	-7.36323700	-1.14336900	2.67840600
H	-7.43373600	-2.78085800	2.01408100
H	-6.65101100	-2.49845500	3.57317800
C	-4.20613300	-3.43144500	1.66981800
H	-4.12036200	-3.86974200	2.67268700
H	-4.70999700	-4.16521600	1.02885500
H	-3.19056600	-3.28960000	1.27889000
C	-4.13135500	-0.53740200	2.71788900
H	-3.90809700	-0.93410600	3.71667400
H	-3.18231400	-0.30536000	2.21924200
H	-4.67603900	0.40621100	2.84142400
C	3.52688000	-2.31214900	2.45562500
C	4.00630500	-3.11635100	1.40652500
C	3.58907700	-2.80999100	3.76647500
C	4.56441800	-4.36944000	1.66376600
H	3.92480600	-2.76613500	0.37978900
C	4.13447600	-4.06964900	4.02070800
H	3.19956900	-2.22133000	4.59082500
C	4.62953000	-4.84903100	2.97318900
H	4.93196400	-4.97594500	0.84026400
H	4.16931400	-4.44320400	5.04074000
H	5.05192600	-5.82959400	3.17499600
C	1.85660100	-0.08280800	3.44631300

C	0.46351000	0.00095200	3.28169800
C	2.42393000	0.30573800	4.67308300
C	-0.34626100	0.43900500	4.33260900
H	0.01716700	-0.24253700	2.32039400
C	1.61217600	0.74791700	5.71796000
H	3.50059500	0.26774700	4.81693400
C	0.22584700	0.80894200	5.55043500
H	-1.42173100	0.49712300	4.19040800
H	2.06151200	1.04657500	6.66144900
H	-0.40432300	1.15377500	6.36584300
C	5.24379800	0.69164200	-2.18791600
C	6.58718100	0.29805400	-2.08514800
C	4.68076400	0.84138800	-3.46747600
C	7.34750400	0.06326200	-3.23389300
H	7.05239000	0.17191400	-1.11249200
C	5.44377900	0.61803400	-4.61244500
H	3.63829300	1.13610300	-3.56446000
C	6.77981200	0.22484600	-4.49792400
H	8.38562200	-0.24347700	-3.13738300
H	4.99348900	0.74326000	-5.59334800
H	7.37311000	0.04222900	-5.38961500
C	4.17892900	2.84045300	-0.54301800
C	2.97750600	3.50743600	-0.26221700
C	5.36571100	3.58514400	-0.64776300
C	2.96352500	4.89220900	-0.07382600
H	2.05080200	2.94319300	-0.19813600
C	5.34908300	4.96683800	-0.46386000
H	6.30229700	3.08801000	-0.88756400
C	4.14805000	5.62187800	-0.17369700
H	2.02559700	5.39591100	0.14262600
H	6.27185500	5.53434300	-0.55092400
H	4.13754100	6.69931800	-0.03305800

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C	-1.11276500	-0.23686600	-1.29992000
H	-2.16424800	-0.18571000	-0.99787900
H	-1.03525900	0.24358400	-2.29066700
C	-0.66464000	-1.69301100	-1.38607800
H	-0.72891900	-2.13243200	-0.38350300
O	-0.31268400	0.44858100	-0.35043700
N	0.77543000	-1.74656500	-1.76590500
H	1.09440500	-2.71534100	-1.75872300
H	0.87503900	-1.42773600	-2.73129100
C	-1.56757100	-2.50238300	-2.34681600
H	-2.60158900	-2.40313600	-1.99586600
H	-1.53014000	-2.03844000	-3.34211900
C	-1.18402500	-3.96433600	-2.44208000
C	-0.39466400	-4.44070700	-3.49934200
C	-1.58272800	-4.87358600	-1.44962600

C	-0.00837600	-5.78212100	-3.56335700
H	-0.09698000	-3.75781200	-4.29296700
C	-1.19953500	-6.21368000	-1.50983900
H	-2.21182100	-4.53023100	-0.63143700
C	-0.40811400	-6.67258100	-2.56612000
H	-1.52633700	-6.90206800	-0.73488500
H	-0.11396800	-7.71755400	-2.61548600
Ag	1.96113300	-0.27722700	-0.38925200
P	4.10976800	0.98714700	-0.71642800
C	5.07382300	0.45209700	0.80126500
H	5.95989300	1.08614400	0.92553200
H	5.42539200	-0.57168200	0.62301500
C	4.22644100	0.50010900	2.08798300
H	4.86218300	0.26371600	2.94891100
H	3.83019700	1.51124000	2.24130700
P	2.74052400	-0.65366100	2.02878800
C	-3.13297500	6.49914100	-1.17305500
C	-3.04490900	5.11096600	-1.29599000
C	-3.64455900	4.29073000	-0.33631700
C	-4.34120800	4.85513800	0.73679500
C	-4.42522300	6.24279400	0.85415300
C	-3.81823000	7.06837800	-0.09687700
H	-2.67577600	7.13729300	-1.92582700
H	-2.54182900	4.65276100	-2.14135100
H	-4.83037900	4.20451900	1.45468300
H	-4.97430900	6.68130500	1.68405700
H	-3.88960200	8.14935300	-0.00547600
S	-3.45332300	2.48112200	-0.44499700
O	-4.73931500	1.98363100	0.13372800
O	-3.15919100	2.23724300	-1.88495100
C	-2.16056000	1.95763000	0.50167900
H	-2.36079500	1.91013500	1.56562800
C	-0.82113700	1.87438100	-0.03479300
H	-0.69789800	2.41117200	-0.98227200
H	-0.04368500	2.17504900	0.67662400
H	0.59628100	-6.13074900	-4.39673500
H	-5.11031500	0.05439700	0.19182000
N	-5.50733600	-0.89197800	0.11354800
Si	-5.38106300	-1.77787500	1.60327800
Si	-6.49486200	-1.00241400	-1.32654000
C	-7.87524300	0.29406800	-1.28694200
H	-8.45350600	0.31398800	-2.21988300
H	-8.57242400	0.10823200	-0.46051800
H	-7.43934600	1.28889300	-1.13560900
C	-5.42590300	-0.68952700	-2.85856700
H	-6.03765800	-0.59277500	-3.76529100
H	-4.84311000	0.23263500	-2.74355000
H	-4.71991400	-1.51401900	-3.02286300
C	-7.25897000	-2.73612000	-1.45185100
H	-7.92331500	-2.96112400	-0.60887900

H	-7.85748900	-2.81843800	-2.36820600
H	-6.49093800	-3.51835300	-1.49250800
C	-7.05395200	-2.08772800	2.44873100
H	-7.57043900	-1.14087500	2.64762000
H	-7.71836900	-2.70103000	1.82774200
H	-6.92790900	-2.60905400	3.40704100
C	-4.56166400	-3.47366200	1.33961900
H	-4.51473000	-4.05032700	2.27264500
H	-5.10866800	-4.07675800	0.60472700
H	-3.53556700	-3.34805200	0.97060200
C	-4.28962400	-0.75812500	2.77034500
H	-4.05606600	-1.31258000	3.68853900
H	-3.34988400	-0.48757700	2.27363300
H	-4.78603900	0.17780000	3.05277700
C	3.46370700	-2.28102300	2.51650300
C	3.93852800	-3.11482800	1.48933400
C	3.56041100	-2.72585600	3.84429300
C	4.52296500	-4.34800400	1.78307900
H	3.83487800	-2.80349200	0.45206200
C	4.13318900	-3.96489100	4.13552400
H	3.17499400	-2.11259500	4.65265600
C	4.62104400	-4.77551300	3.10823100
H	4.88610100	-4.97924300	0.97645500
H	4.19449200	-4.29845200	5.16800000
H	5.06432900	-5.74033500	3.33881600
C	1.70293700	-0.09215100	3.43288700
C	0.30966600	-0.11781600	3.25417300
C	2.22659100	0.37989700	4.64968400
C	-0.54316200	0.29728800	4.27944000
H	-0.10842200	-0.43301000	2.30188900
C	1.37199500	0.79925700	5.66956300
H	3.30119900	0.42471800	4.80586200
C	-0.01293800	0.75306300	5.48719700
H	-1.61793600	0.27141700	4.12408800
H	1.78727300	1.16404300	6.60529800
H	-0.67603900	1.08163100	6.28280800
C	5.25866900	0.65552800	-2.11651900
C	6.60085900	0.27562000	-1.96106400
C	4.73809000	0.77748100	-3.41688600
C	7.40166400	0.02766900	-3.07913000
H	7.03411800	0.17025900	-0.97135300
C	5.54140800	0.54096300	-4.53110800
H	3.69728000	1.06181700	-3.55494000
C	6.87608700	0.16200800	-4.36434200
H	8.43839400	-0.26784300	-2.94189800
H	5.12390400	0.64530100	-5.52877800
H	7.50097900	-0.03050400	-5.23197300
C	4.09672900	2.82408400	-0.56208000
C	2.87143900	3.47742100	-0.36539400
C	5.27591500	3.58604500	-0.62312000

C	2.82501400	4.86637700	-0.21687000
H	1.95032600	2.90194200	-0.33311100
C	5.22717000	4.97150800	-0.47850700
H	6.23214700	3.09936000	-0.79823500
C	4.00164100	5.61313700	-0.27255700
H	1.86873800	5.35884800	-0.06479300
H	6.14420700	5.55231600	-0.53078000
H	3.96636500	6.69351800	-0.16230700

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C	-1.61782700	-0.53888500	-1.48485800
H	-2.63999900	-0.85817900	-1.27067200
H	-1.63111400	0.17326100	-2.32491800
C	-0.76829100	-1.75783800	-1.81221800
H	-0.69707800	-2.36591900	-0.90424200
O	-1.06544300	0.08474900	-0.32086000
N	0.62124400	-1.32429600	-2.13648200
H	1.19654100	-2.14993400	-2.30458000
H	0.60719100	-0.80950100	-3.01877000
C	-1.40149500	-2.61335400	-2.93123500
H	-2.41378100	-2.88328200	-2.60936400
H	-1.51262000	-2.00156200	-3.83719500
C	-0.60034400	-3.86120300	-3.24092100
C	0.17517000	-3.95874400	-4.40478700
C	-0.59433100	-4.94219200	-2.34403800
C	0.93657300	-5.10055900	-4.66971300
H	0.16687400	-3.14008600	-5.12200300
C	0.16580800	-6.08253300	-2.60439900
H	-1.19829900	-4.89168000	-1.44058100
C	0.93545000	-6.16541500	-3.76833200
H	0.15021700	-6.91123900	-1.90146300
H	1.52255500	-7.05662200	-3.97315500
Ag	1.40192000	0.02093000	-0.40031900
P	2.77206800	2.15057400	-0.27122200
C	4.26771200	1.51909900	0.66038800
H	4.92841600	2.34920700	0.93594200
H	4.82645600	0.91111600	-0.06175600
C	3.91532200	0.67752500	1.90118800
H	4.83826400	0.40500000	2.42607000
H	3.29859300	1.25887100	2.59682600
P	2.94782500	-0.87316800	1.46795400
C	-2.94346500	5.84691100	-1.08872900
C	-3.20282500	4.49082700	-1.30937700
C	-3.97444600	3.78039800	-0.38750000
C	-4.50123900	4.41308700	0.74271100
C	-4.23543300	5.76506900	0.95877600
C	-3.45442400	6.48264300	0.04596800
H	-2.35671000	6.40944700	-1.81074000
H	-2.84560100	3.98370300	-2.19984600

H	-5.13071300	3.85281700	1.42734200
H	-4.64926000	6.26413800	1.83109300
H	-3.25998200	7.53940700	0.21101000
S	-4.30388000	2.01035100	-0.65529800
O	-5.70086300	1.80314400	-0.22935600
O	-3.89644100	1.74836500	-2.05756500
C	-3.23681500	1.10060200	0.42619200
H	-3.47571000	1.43106700	1.44051300
C	-1.76225700	1.28762300	0.10084900
H	-1.60092600	2.04250700	-0.68272700
H	-1.20760800	1.59827500	0.98965100
H	1.52269500	-5.15872200	-5.58338600
H	-3.63745000	-0.17127000	0.46445600
N	-3.98758000	-1.54361500	0.66351400
Si	-3.30709200	-2.21505800	2.07894600
Si	-5.39778600	-2.11446900	-0.14802700
C	-7.02039300	-1.44493400	0.58864500
H	-7.90200300	-1.80961300	0.04363700
H	-7.13259700	-1.73915300	1.64028000
H	-7.02273500	-0.34990000	0.54344900
C	-5.39049800	-1.62967500	-1.99250600
H	-6.35764000	-1.87419100	-2.45223700
H	-5.21225200	-0.56098800	-2.15198300
H	-4.62269700	-2.18301100	-2.55150000
C	-5.54675000	-4.02543500	-0.15547500
H	-5.64323900	-4.44590600	0.85331200
H	-6.43245700	-4.33983700	-0.72449500
H	-4.67241100	-4.49671900	-0.62443000
C	-4.54661000	-2.77497000	3.42385800
H	-5.17960200	-1.93615600	3.74011700
H	-5.21443300	-3.56902100	3.06814700
H	-4.02884200	-3.15555400	4.31551400
C	-2.20245400	-3.74896600	1.73904400
H	-1.77924800	-4.17312900	2.66130700
H	-2.77154500	-4.54574100	1.24370300
H	-1.36568300	-3.48404700	1.07651000
C	-2.16015200	-0.96244400	2.95649500
H	-1.69374700	-1.41181800	3.84287100
H	-1.35681800	-0.62657800	2.28994100
H	-2.71276800	-0.07562100	3.29226200
C	4.28733300	-1.99804100	0.87065000
C	4.44004300	-2.19043300	-0.51136700
C	5.17126100	-2.65008900	1.74573600
C	5.46325200	-2.99964400	-1.01092100
H	3.74746100	-1.71056800	-1.19921900
C	6.18824800	-3.46378100	1.24681400
H	5.05544600	-2.53507600	2.81970200
C	6.33887500	-3.63738200	-0.13163600
H	5.56752300	-3.13923000	-2.08351000
H	6.86135500	-3.96724900	1.93552600

H	7.13028900	-4.27440700	-0.51674800
C	2.45663600	-1.55543500	3.10054700
C	1.41151500	-2.49334300	3.12194300
C	3.06736100	-1.19126400	4.31267500
C	1.00020900	-3.06946900	4.32385300
H	0.90279200	-2.76476600	2.20108500
C	2.64607100	-1.76141500	5.51531700
H	3.87191000	-0.46225100	4.32977300
C	1.61627400	-2.70412300	5.52224400
H	0.18640200	-3.78827800	4.32076600
H	3.12355600	-1.46743200	6.44618000
H	1.28792600	-3.14435400	6.45962400
C	2.13480100	3.55221300	0.73556200
C	0.85689100	4.04437300	0.41842200
C	2.84049900	4.14221100	1.79671300
C	0.30260700	5.10583600	1.13297900
H	0.28712800	3.59123300	-0.38828900
C	2.28044500	5.19855000	2.51905400
H	3.82888900	3.78659000	2.07142100
C	1.01405500	5.68242500	2.18792900
H	-0.68639300	5.47049900	0.87093900
H	2.83677900	5.64156300	3.34073500
H	0.57972800	6.50193000	2.75371000
C	3.54655300	2.93825100	-1.74633300
C	3.54943300	2.22831700	-2.95670200
C	4.14516000	4.20717300	-1.69873500
C	4.15502900	2.76602900	-4.09381500
H	3.06777900	1.25436100	-3.00839300
C	4.74311700	4.74646900	-2.83795600
H	4.13255800	4.77978000	-0.77559700
C	4.75196100	4.02645600	-4.03534700
H	4.14966400	2.20685700	-5.02545300
H	5.19983700	5.73135700	-2.79148700
H	5.21548100	4.45077000	-4.92164800

ADD5-O-real

C	1.63359800	1.16675600	-1.15837300
H	2.70973100	1.03462800	-0.93311900
H	1.48053000	1.12128900	-2.25020700
C	1.17304700	2.51132700	-0.62050000
H	1.28860600	2.50764900	0.46918600
O	0.85625000	0.12063000	-0.54058200
N	-0.28676100	2.70494400	-0.87860900
H	-0.57729200	3.59144600	-0.46470600
H	-0.42810900	2.81766200	-1.88436700
C	2.04068200	3.64577400	-1.21430700
H	3.08187700	3.42932600	-0.94794000
H	1.97948200	3.59887400	-2.31071500
C	1.63013200	5.02439600	-0.73828000

C	0.81218800	5.84750400	-1.52736800
C	2.03180700	5.49804200	0.52127600
C	0.39943800	7.10329900	-1.07405700
H	0.51485300	5.51117200	-2.51927400
C	1.62118200	6.75152800	0.97660000
H	2.68477400	4.88566200	1.13790400
C	0.80114700	7.55774000	0.18264600
H	1.95118500	7.10322800	1.95065600
H	0.48768200	8.53622100	0.53676300
Ag	-1.50025400	0.88872600	-0.17016200
P	-3.43768600	-0.31223000	-1.34074600
C	-4.49612200	-0.70620000	0.15719900
H	-5.31652500	-1.38030100	-0.11414700
H	-4.96328900	0.24427500	0.44387700
C	-3.69634500	-1.28707000	1.33901600
H	-4.38666000	-1.55641600	2.14656200
H	-3.17518500	-2.20208700	1.03280200
P	-2.38717200	-0.10062400	1.97986100
C	-0.23637300	-5.69877200	0.07667900
C	0.62732300	-4.83244300	-0.59699400
C	1.83035700	-4.46487500	0.00818500
C	2.19256800	-4.96083200	1.26250300
C	1.32398200	-5.82796800	1.92633400
C	0.11036800	-6.19296200	1.33661100
H	-1.17314100	-5.99332500	-0.38889000
H	0.38761900	-4.46129600	-1.58765700
H	3.14993600	-4.68360400	1.69198900
H	1.59924600	-6.22720600	2.89863800
H	-0.56031100	-6.87311200	1.85527400
S	2.96377700	-3.34280900	-0.85147800
O	4.31452300	-3.64920600	-0.35709800
O	2.63728900	-3.42241300	-2.29062600
C	2.49538100	-1.69151000	-0.26138600
H	2.34753000	-1.77443000	0.81911000
C	1.23160100	-1.19368000	-0.96523700
H	1.38115100	-1.20738200	-2.05139300
H	0.37548100	-1.83263300	-0.72763300
H	-0.22544100	7.72797500	-1.70740400
H	3.37066000	-1.02691400	-0.42891600
N	4.69598300	0.71016100	-0.37407200
Si	5.13304600	1.02359400	1.22253800
Si	5.60729700	0.58947700	-1.79746400
C	6.93353700	-0.78811200	-1.79533600
H	7.41905000	-0.89635100	-2.77538500
H	7.72062700	-0.58502500	-1.05761000
H	6.48344500	-1.75444000	-1.53415700
C	4.48001800	0.17789000	-3.29569800
H	5.07312600	0.09048900	-4.21602200
H	3.95339300	-0.77686500	-3.16203500
H	3.72477000	0.95670500	-3.47226400

C	6.52286400	2.19757000	-2.30552900
H	7.24280200	2.50236300	-1.53431700
H	7.07863600	2.08069000	-3.24656000
H	5.81984700	3.03164400	-2.43785100
C	6.99372000	0.91500400	1.66043000
H	7.38794100	-0.08984800	1.46353100
H	7.58704900	1.61914600	1.06241600
H	7.17978600	1.14349500	2.71920000
C	4.58118700	2.76127200	1.83921700
H	4.88781300	2.95790900	2.87607900
H	5.00125600	3.55720300	1.21004100
H	3.48530400	2.84997000	1.80155800
C	4.26209300	-0.15753100	2.46682200
H	4.53275600	0.07647300	3.50603100
H	3.16989700	-0.06678800	2.37784900
H	4.52777600	-1.20503300	2.27486400
C	-3.34329500	0.99574400	3.11422700
C	-3.63156600	2.30343700	2.69399500
C	-3.80335500	0.57098400	4.37128200
C	-4.38145700	3.16226600	3.50103800
H	-3.25506300	2.65462500	1.73586200
C	-4.54512300	1.43158400	5.17986000
H	-3.56621700	-0.42652600	4.72977800
C	-4.83952200	2.72669600	4.74473800
H	-4.59507300	4.17247800	3.16274700
H	-4.88896600	1.09292100	6.15340000
H	-5.41488800	3.39579800	5.37847700
C	-1.32782100	-1.14934800	3.04815800
C	0.01894400	-0.77726000	3.19285300
C	-1.79120900	-2.30025900	3.70895600
C	0.88144000	-1.52733900	3.99433900
H	0.40013000	0.09153200	2.66290100
C	-0.92643800	-3.05071500	4.50661700
H	-2.82347900	-2.62165700	3.60116900
C	0.40776500	-2.66379800	4.65245400
H	1.92243100	-1.23028200	4.08199300
H	-1.29513500	-3.93982900	5.01103800
H	1.07947200	-3.25235100	5.27114100
C	-3.08105700	-1.93869600	-2.12351000
C	-1.91856700	-2.03272000	-2.90761900
C	-3.89218800	-3.07694000	-1.98020600
C	-1.57932000	-3.22793900	-3.54353600
H	-1.27095300	-1.16661400	-3.01577600
C	-3.54987900	-4.27470200	-2.61137300
H	-4.79664000	-3.03797700	-1.37993800
C	-2.39547000	-4.35181200	-3.39455800
H	-0.67288300	-3.28294800	-4.13947100
H	-4.18752500	-5.14664300	-2.49280600
H	-2.13093400	-5.28475800	-3.88431300
C	-4.64581400	0.52579800	-2.45168700

C	-4.78799900	1.91803900	-2.32901900
C	-5.42280000	-0.15571300	-3.40024300
C	-5.70405100	2.61131200	-3.12042800
H	-4.17301500	2.46219500	-1.61507800
C	-6.33026500	0.54182900	-4.19953300
H	-5.31469800	-1.22907000	-3.52283600
C	-6.47616300	1.92328200	-4.05896300
H	-5.80519800	3.68783300	-3.01305600
H	-6.92302600	0.00370300	-4.93422400
H	-7.18247000	2.46270600	-4.68381500

ADD3-N-real

Ag	-0.59627300	-0.40679800	-0.24823400
P	-0.08274900	-2.72130200	0.19055500
C	-1.67948800	-3.51703400	0.72979700
H	-1.50137800	-4.56060800	1.01314500
H	-2.33467800	-3.53672200	-0.14850400
C	-2.36003100	-2.74578800	1.88175200
H	-3.17216500	-3.35149700	2.29884900
H	-1.64447900	-2.56999600	2.69217300
P	-3.01563000	-1.06454700	1.32995200
C	0.03142600	2.56633200	-1.19883500
H	0.24349400	2.24483300	-2.23733500
H	-0.47048300	3.54722700	-1.28515200
C	1.39022900	2.85191700	-0.51390300
H	1.94803400	3.58476300	-1.10964800
O	-0.77994200	1.67591200	-0.51319000
N	2.20239300	1.58722400	-0.53963100
H	2.85198100	1.46668400	0.25851400
C	1.24077500	3.37289900	0.92804600
H	0.52752200	4.20552300	0.88697400
H	0.76985600	2.59371100	1.53733700
C	2.54314100	3.83649300	1.54820400
C	3.29036300	2.99863000	2.38723200
C	3.04830100	5.11466300	1.26129300
C	4.51355800	3.41988400	2.91628200
H	2.91905600	2.00621400	2.63166300
C	4.26428100	5.54163400	1.79300700
H	2.47657700	5.78333800	0.62046500
C	5.00325700	4.69230100	2.62160500
H	5.07883300	2.75045600	3.55849500
H	4.63437900	6.53755500	1.56370600
H	5.95157600	5.02299000	3.03652400
C	8.12014900	1.59376400	-0.83475600
C	6.83812600	1.17648300	-0.46905200
C	6.35928000	-0.05665700	-0.92232200
C	7.15833000	-0.87434400	-1.72858900
C	8.43826000	-0.45183800	-2.08562500
C	8.91979200	0.78466900	-1.64446600

H	8.49750400	2.54871900	-0.47743500
H	6.22047100	1.78033500	0.18723200
H	6.78042300	-1.84020600	-2.04838300
H	9.06440500	-1.09090500	-2.70312300
H	9.91832600	1.11077200	-1.92363300
S	4.64896200	-0.56286300	-0.56659900
O	4.71165800	-2.04397200	-0.48038200
O	4.31465400	0.23176200	0.67461200
C	3.55602100	-0.08659100	-1.75382800
H	3.51245800	-0.69643000	-2.64634100
C	3.11033000	1.31796600	-1.76894000
H	3.87402600	2.10740300	-1.67716100
H	2.50694700	1.52653400	-2.65553300
H	1.56287500	0.77996900	-0.47922700
H	-2.49525100	1.94455300	-1.54470100
N	-3.28835800	2.13172300	-2.17473900
Si	-3.40415000	1.01374200	-3.51075400
Si	-4.32235500	3.43064700	-1.63233100
C	-6.13427900	2.87929200	-1.50894100
H	-6.77406600	3.69453400	-1.14648500
H	-6.53235700	2.56247600	-2.48105400
H	-6.24144900	2.03284700	-0.81980200
C	-3.72140400	3.97311900	0.08076600
H	-2.65659800	4.23546200	0.06248000
H	-4.27670700	4.85169900	0.43257200
H	-3.84700600	3.17693500	0.82381800
C	-4.25279200	4.93289400	-2.79115100
H	-4.59132000	4.68059000	-3.80305400
H	-4.88938600	5.74911000	-2.42486900
H	-3.22919300	5.31877500	-2.87386000
C	-4.27800500	-0.59831800	-3.01935900
H	-4.32608600	-1.31076700	-3.85376500
H	-3.74939700	-1.08439500	-2.18940700
H	-5.30301200	-0.40658500	-2.67992000
C	-4.36176000	1.79440900	-4.94837600
H	-4.43205600	1.08806600	-5.78537300
H	-5.38651700	2.06918300	-4.67066200
H	-3.86232800	2.69799000	-5.31704800
C	-1.65855900	0.57057200	-4.10348400
H	-1.13025300	1.45650500	-4.47604500
H	-1.06066800	0.14394800	-3.28726000
H	-1.68718000	-0.17000300	-4.91302700
C	-4.83487300	-1.36531300	1.19496600
C	-5.34871600	-2.58940400	0.73734600
C	-5.73460500	-0.31248800	1.43614300
C	-6.72095900	-2.76278500	0.54468800
H	-4.68289500	-3.42198000	0.52627500
C	-7.10513300	-0.48733100	1.24457500
H	-5.36334100	0.64607500	1.78716200
C	-7.60449900	-1.71355500	0.79914300

H	-7.09700900	-3.72100200	0.19560400
H	-7.78382300	0.33710200	1.44656400
H	-8.67213700	-1.84822300	0.64936100
C	-2.87921200	-0.04223600	2.85821500
C	-3.37425300	-0.45686200	4.10667500
C	-2.24144400	1.20512500	2.75519300
C	-3.22340200	0.35302000	5.23125700
H	-3.88678500	-1.41098400	4.19909000
C	-2.09856500	2.01753900	3.88503300
H	-1.86058900	1.54102800	1.79223200
C	-2.58406900	1.59211200	5.12136700
H	-3.60717300	0.02123400	6.19253400
H	-1.60832000	2.98319800	3.79447100
H	-2.46999300	2.22367600	5.99847100
C	1.07639500	-3.00089800	1.58850900
C	2.09355100	-2.06262900	1.81190800
C	1.01360200	-4.14434700	2.40374700
C	3.03779300	-2.26179800	2.82057900
H	2.18396000	-1.18591700	1.18067800
C	1.94216500	-4.32941400	3.42711500
H	0.24947400	-4.89924600	2.24275400
C	2.95652200	-3.38986600	3.63567100
H	3.83725900	-1.53752100	2.93831300
H	1.87998100	-5.21407700	4.05535100
H	3.68633500	-3.54656200	4.42544900
C	0.55433300	-3.76902700	-1.17918300
C	1.93095100	-3.73747100	-1.46258600
C	-0.29814400	-4.53386500	-1.99105200
C	2.43738500	-4.47293800	-2.53423600
H	2.61994200	-3.14406000	-0.86743600
C	0.21836900	-5.26527300	-3.06235100
H	-1.36623500	-4.57043400	-1.79948700
C	1.58688600	-5.23772500	-3.33538600
H	3.50413200	-4.43820700	-2.73611600
H	-0.45178500	-5.85760800	-3.67976000
H	1.98701100	-5.80825200	-4.16933700

TS2-N-real

Ag	0.32444000	-0.40454600	0.25294600
P	0.02852700	-2.57231500	-0.71394800
C	1.62625400	-3.14309400	-1.48754400
H	1.44509600	-4.08452900	-2.01921200
H	2.32568900	-3.36198500	-0.67353100
C	2.22790900	-2.08474600	-2.43794300
H	2.94146300	-2.56388800	-3.11785300
H	1.44400300	-1.64720600	-3.06605800
P	3.04924900	-0.67113500	-1.49675500
C	-0.18326700	2.32651800	1.70913000
H	-0.60718500	1.82314400	2.60071100

H	0.37478100	3.19930300	2.09778400
C	-1.36485800	2.92238200	0.90445600
H	-1.83618800	3.70099100	1.52292900
O	0.67567200	1.51529300	0.98677600
N	-2.40006000	1.88500800	0.64049000
H	-2.92142200	2.06163000	-0.22350700
C	-0.89787300	3.55474100	-0.42012000
H	-0.07793500	4.24067600	-0.17421100
H	-0.46520500	2.76558100	-1.04333900
C	-1.98951600	4.29076000	-1.16870900
C	-2.65428100	3.69542000	-2.25060300
C	-2.38333600	5.58005000	-0.77615900
C	-3.68818100	4.36155400	-2.91482300
H	-2.35415400	2.70424600	-2.58456800
C	-3.41036800	6.25053900	-1.43939800
H	-1.87246600	6.06404300	0.05400600
C	-4.06925100	5.64088400	-2.51100700
H	-4.19046500	3.87907800	-3.74897000
H	-3.69489100	7.25086800	-1.12313900
H	-4.86960300	6.16271100	-3.02874900
C	-8.28824900	0.99580300	1.19210600
C	-7.01456700	0.82533100	0.64460100
C	-6.27572700	-0.31307200	0.97505000
C	-6.79746100	-1.28450100	1.83426200
C	-8.07022800	-1.10567400	2.37529500
C	-8.81391300	0.03533100	2.05869700
H	-8.87219100	1.87543100	0.93463400
H	-6.59979500	1.54597000	-0.05223100
H	-6.21794300	-2.17569600	2.05349900
H	-8.48549000	-1.85980100	3.03841500
H	-9.80591600	0.17036400	2.48131200
S	-4.59834500	-0.51839800	0.32263300
O	-4.41958000	-1.97267300	0.11320500
O	-4.51305800	0.41490300	-0.83712500
C	-3.42999400	0.02651200	1.49492700
H	-3.40639500	-0.62503300	2.36710600
C	-3.39891500	1.53165100	1.71935600
H	-4.32571700	2.10223900	1.59932800
H	-2.95518500	1.76480900	2.68962900
H	-2.26598900	0.60950700	0.68845000
H	2.29122800	1.48159700	2.12664000
N	3.04246100	1.44870900	2.83401300
Si	2.93401300	0.04770700	3.86610500
Si	4.25840300	2.68233100	2.62571100
C	5.97743600	1.94639900	2.29336500
H	6.72712000	2.73480700	2.14458400
H	6.32186200	1.32476300	3.12951800
H	5.97024200	1.31334000	1.39765900
C	3.75376300	3.75120400	1.14489900
H	2.77029700	4.20995700	1.30485000

H	4.47585300	4.56118200	0.98084900
H	3.69520400	3.16178300	0.22258100
C	4.40333300	3.80649700	4.14910400
H	4.71418200	3.24928100	5.04080000
H	5.14215300	4.60212300	3.98503500
H	3.44229600	4.28356600	4.37729800
C	3.49709700	-1.53329900	2.97600500
H	3.39063600	-2.42276800	3.61129000
H	2.89763200	-1.69032600	2.06983300
H	4.54595400	-1.46085600	2.66363000
C	4.00880500	0.27473500	5.41164300
H	3.94586900	-0.61662000	6.04880000
H	5.06748500	0.42411800	5.16734000
H	3.67881200	1.13272500	6.00877100
C	1.13283100	-0.20923400	4.40135600
H	0.76813500	0.64365100	4.98651100
H	0.47857400	-0.31812300	3.52671100
H	1.02161600	-1.11319200	5.01417900
C	4.84063400	-1.13134600	-1.57983800
C	5.27899900	-2.46452000	-1.62103800
C	5.80992200	-0.11749700	-1.46996400
C	6.64046900	-2.77463300	-1.57049100
H	4.56273000	-3.27823200	-1.69340200
C	7.16857600	-0.42717200	-1.42386600
H	5.50004100	0.92341500	-1.43213800
C	7.59048400	-1.75822700	-1.47439300
H	6.95553000	-3.81438900	-1.60895200
H	7.89884800	0.37418200	-1.34819300
H	8.64923600	-1.99941000	-1.43592600
C	2.94107000	0.71329800	-2.71496200
C	3.47004700	0.64428500	-4.01518400
C	2.27629900	1.88237500	-2.30996400
C	3.32475300	1.71526900	-4.89607100
H	4.00656900	-0.24497000	-4.33592100
C	2.13470500	2.95600100	-3.19571000
H	1.87394900	1.95133200	-1.30087600
C	2.65435000	2.87266500	-4.48744900
H	3.73618200	1.64991700	-5.90016900
H	1.62047500	3.85707600	-2.87202600
H	2.54385500	3.70762000	-5.17452300
C	-1.17614900	-2.65913700	-2.09758100
C	-2.03328700	-1.57728500	-2.33514500
C	-1.28736700	-3.80865900	-2.89926300
C	-2.98497700	-1.63620700	-3.35590400
H	-1.98489200	-0.69663600	-1.70316900
C	-2.22517500	-3.85993100	-3.92798000
H	-0.65450700	-4.67224700	-2.71254500
C	-3.07488700	-2.77259100	-4.15761400
H	-3.66585400	-0.80235100	-3.49348900
H	-2.30194100	-4.75202100	-4.54388300

H	-3.81503400	-2.82185000	-4.95180500
C	-0.47238100	-3.93179200	0.41974700
C	-1.82863600	-4.03322000	0.77741400
C	0.45499400	-4.81996300	0.98576100
C	-2.24037300	-5.01707300	1.67620100
H	-2.56681100	-3.35023700	0.36430400
C	0.03364100	-5.80048600	1.88656300
H	1.50905000	-4.76003500	0.73381600
C	-1.31413900	-5.90249900	2.23253900
H	-3.29203200	-5.08660600	1.94027500
H	0.76220700	-6.48415200	2.31416400
H	-1.64040700	-6.66689500	2.93274600

ADD4-N-real

Ag	-0.17796100	-0.16040600	-0.11414200
P	-0.23472500	-2.44932800	-0.81337100
C	-1.96231200	-3.14288400	-0.96554100
H	-1.87625000	-4.21510100	-1.18230300
H	-2.43288200	-2.66652400	-1.83350700
C	-2.81260500	-2.91267400	0.30216300
H	-3.63141200	-3.64041900	0.32865100
H	-2.21448900	-3.09188100	1.20179000
P	-3.49211800	-1.15057500	0.41479800
C	0.30076400	2.64554900	0.94844400
H	0.44390000	3.29656200	0.06101300
H	0.02520700	3.33133400	1.77431500
C	1.68850600	2.06616600	1.32577300
H	2.37147700	2.92659300	1.46218300
O	-0.69683100	1.70686200	0.74010300
N	2.19183100	1.18751800	0.25177600
H	2.85092300	0.50502400	0.62135500
C	1.64064900	1.29606500	2.66239000
H	1.10724300	1.92911600	3.38229000
H	1.03043300	0.39568100	2.52727100
C	3.00370700	0.93501900	3.21714300
C	3.53354200	-0.35728400	3.08747100
C	3.78435500	1.90663400	3.86481700
C	4.80398600	-0.66895200	3.58166200
H	2.94792800	-1.13200600	2.59786700
C	5.05009600	1.60031100	4.36432300
H	3.38744900	2.91248400	3.98602500
C	5.56680000	0.30839500	4.22274700
H	5.19298700	-1.67698300	3.46519000
H	5.62967200	2.36652400	4.87354000
H	6.55025900	0.06518600	4.61641300
C	7.25926900	2.08187500	0.75759900
C	6.22695100	1.23642200	0.34722900
C	6.05126300	1.00407700	-1.01890400
C	6.88936500	1.58266100	-1.97626700

C	7.91600500	2.42574900	-1.55143400
C	8.09706900	2.67727500	-0.18807800
H	7.40478100	2.26745700	1.81756300
H	5.58413100	0.75066300	1.07363700
H	6.74990000	1.35543400	-3.02829400
H	8.57849700	2.87955000	-2.28289600
H	8.89916100	3.33415400	0.13720000
S	4.71907200	-0.07519800	-1.56591700
O	5.14014400	-0.71908500	-2.82450400
O	4.30881500	-0.90509600	-0.41130400
C	3.32950900	1.03536300	-1.97339200
H	3.67380100	1.63745400	-2.81961700
C	2.82888000	1.92577000	-0.83732600
H	3.65543400	2.56597300	-0.47934500
H	2.08656800	2.59901800	-1.27832800
H	2.54807600	0.35209400	-2.32285000
H	-2.00781700	2.70324000	-0.31394100
N	-2.60502300	3.30206400	-0.91049900
Si	-2.47693600	2.94136600	-2.60863000
Si	-3.70330600	4.31499800	-0.00806100
C	-5.51911300	3.94396500	-0.42754500
H	-6.20118200	4.57053700	0.16213000
H	-5.74084700	4.12909900	-1.48626200
H	-5.76167600	2.89426500	-0.22128700
C	-3.42450100	3.99245000	1.83661700
H	-2.38465100	4.19435300	2.11959900
H	-4.06974500	4.63588000	2.44840100
H	-3.63983100	2.95091200	2.10012000
C	-3.40441700	6.16085700	-0.34192700
H	-3.56799900	6.41720100	-1.39525300
H	-4.07729000	6.78762200	0.25823300
H	-2.37369300	6.43959900	-0.09060300
C	-3.47602600	1.40559200	-3.10532400
H	-3.33100500	1.14306700	-4.16203700
H	-3.17871000	0.54482500	-2.49348600
H	-4.54933200	1.56159000	-2.94148900
C	-3.08690300	4.40410100	-3.65100500
H	-3.00689000	4.16970100	-4.72030600
H	-4.13762800	4.64694500	-3.45115500
H	-2.49477100	5.30722800	-3.46243100
C	-0.65786900	2.60437400	-3.03886600
H	-0.04309300	3.49899700	-2.87963000
H	-0.25915300	1.80371700	-2.40172800
H	-0.54160200	2.29198800	-4.08482900
C	-5.27337100	-1.40096800	-0.02916700
C	-5.68645700	-2.36234800	-0.96591400
C	-6.23841300	-0.50727300	0.47014100
C	-7.02001400	-2.44279300	-1.37430700
H	-4.96923200	-3.05992900	-1.39051300
C	-7.57010300	-0.58958600	0.06525600

H	-5.94736200	0.25186800	1.19100800
C	-7.96817500	-1.55939600	-0.85834900
H	-7.31544300	-3.19969900	-2.09674000
H	-8.29857100	0.10645600	0.47318300
H	-9.00573000	-1.62221100	-1.17508700
C	-3.57414700	-0.91419500	2.24773300
C	-4.35257900	-1.72236300	3.09481500
C	-2.79224600	0.11110000	2.80665600
C	-4.34433600	-1.51771100	4.47403100
H	-4.97721100	-2.50542800	2.67250400
C	-2.79040400	0.31262400	4.19200200
H	-2.18363500	0.74911500	2.16454900
C	-3.56095600	-0.49848800	5.02509300
H	-4.95067800	-2.14900000	5.11901300
H	-2.18857100	1.11290400	4.61511000
H	-3.55863800	-0.33614300	6.10010000
C	0.54341100	-3.61774900	0.38116600
C	0.70868000	-3.22465500	1.71791400
C	0.93186600	-4.91205700	-0.00056400
C	1.24300200	-4.10958800	2.65756300
H	0.41975100	-2.22236200	2.02380900
C	1.47170100	-5.79190200	0.93712800
H	0.82477200	-5.22858400	-1.03435400
C	1.62659700	-5.39318600	2.26752900
H	1.36379100	-3.79104800	3.68928500
H	1.77460500	-6.78874000	0.62820500
H	2.04943600	-6.08025600	2.99545300
C	0.57125400	-2.84159500	-2.41829500
C	1.95891700	-2.63623100	-2.52315300
C	-0.13846400	-3.27276700	-3.54886300
C	2.62005400	-2.85700900	-3.73085600
H	2.53049100	-2.30729100	-1.65868300
C	0.52709300	-3.49277400	-4.75819100
H	-1.20923800	-3.44145400	-3.50182900
C	1.90310900	-3.28469200	-4.85207400
H	3.68818300	-2.67250400	-3.78931200
H	-0.03620600	-3.82667200	-5.62556300
H	2.41602500	-3.45163600	-5.79540100

TS3-N-real

Ag	0.97090000	0.96271500	-0.21345200
P	0.99474100	-0.68911900	1.53143900
C	2.62957100	-1.20550900	2.29991500
H	2.38228200	-1.70588900	3.24432600
H	3.17316300	-0.28979800	2.55670500
C	3.51215700	-2.13540800	1.44735800
H	4.24956300	-2.62330800	2.09694400
H	2.90990700	-2.94521400	1.02110900
P	4.36641300	-1.31412700	-0.00976900

C	-1.74187900	1.97628000	-2.41554400
H	-2.02937700	2.88234800	-1.84436700
H	-1.81336000	2.26037100	-3.48602400
C	-2.84336900	0.91826800	-2.18432500
H	-3.75257600	1.30009600	-2.69223600
O	-0.45862700	1.54838900	-2.10331500
N	-3.11876800	0.71573000	-0.75308700
H	-3.43243100	-0.23583300	-0.57802700
C	-2.47232500	-0.41852100	-2.86026800
H	-2.08479700	-0.18667600	-3.85953700
H	-1.64392900	-0.86425600	-2.30109500
C	-3.62916200	-1.38984800	-2.97642700
C	-3.80417500	-2.43873700	-2.06126800
C	-4.57587800	-1.24826000	-4.00440200
C	-4.89107900	-3.31273000	-2.16388400
H	-3.08311800	-2.57807400	-1.25985500
C	-5.66017400	-2.11894100	-4.11395900
H	-4.45404300	-0.44742600	-4.73093300
C	-5.82342000	-3.15677900	-3.19104500
H	-5.00397400	-4.11596500	-1.44026900
H	-6.37368300	-1.99357200	-4.92486900
H	-6.66304000	-3.84165400	-3.27875500
C	-8.21777600	-0.60572800	-0.77812100
C	-6.95590400	-0.64335700	-0.18221800
C	-6.77262400	-0.00459100	1.04629900
C	-7.82118700	0.65295400	1.69509700
C	-9.07701700	0.68149800	1.08862600
C	-9.27275800	0.05721100	-0.14689900
H	-8.36986000	-1.10021000	-1.73296100
H	-6.13481900	-1.17397000	-0.65248000
H	-7.65577600	1.11022100	2.66526500
H	-9.90336600	1.18409300	1.58321800
H	-10.25323000	0.08218600	-0.61470700
S	-5.14890400	-0.03471700	1.82421600
O	-5.34642100	0.08183800	3.28299400
O	-4.40250800	-1.18517500	1.27074400
C	-4.32576800	1.49927200	1.27948400
H	-4.94365700	2.31170700	1.67438100
C	-4.10661400	1.64511800	-0.22646000
H	-5.08200500	1.59220700	-0.74927600
H	-3.73767600	2.66613300	-0.38110500
H	-3.37136000	1.48403000	1.81588900
H	0.40972500	2.46193700	-1.82498800
N	1.43896600	2.93615400	-1.33908100
Si	1.22637300	4.28205700	-0.23381100
Si	2.67233600	2.83135300	-2.59405000
C	4.37718300	3.38851700	-1.96785100
H	5.13236900	3.25935200	-2.75469200
H	4.38989700	4.44618500	-1.67706100
H	4.69688500	2.80126600	-1.09883600

C	2.79395100	1.04531400	-3.20686500
H	3.18411700	0.37336800	-2.43247700
H	1.79977100	0.68657100	-3.49878700
H	3.45534600	0.97255300	-4.08069500
C	2.20466900	3.90967200	-4.08675300
H	2.15730600	4.97474700	-3.83265800
H	2.93169900	3.79426500	-4.90148500
H	1.22163700	3.61759000	-4.47674200
C	2.49776800	4.24326300	1.17755100
H	2.35410000	5.09238500	1.85880700
H	2.39822500	3.32239700	1.76674000
H	3.52726000	4.28566300	0.80357600
C	1.36509400	5.97766700	-1.08513800
H	1.16619300	6.78562700	-0.36869900
H	2.36265600	6.15341000	-1.50576700
H	0.64029400	6.07381200	-1.90263900
C	-0.50098800	4.18651500	0.54697800
H	-1.28613600	4.33563700	-0.20367400
H	-0.68083300	3.21444100	1.02332500
H	-0.61843600	4.96300300	1.31436900
C	0.24910300	-2.31095000	1.09026500
C	-0.03967800	-3.28580300	2.06039900
C	0.02859900	-2.60901500	-0.26211400
C	-0.53877600	-4.53122000	1.68178300
H	0.11112400	-3.06811000	3.11418400
C	-0.46558400	-3.86044600	-0.64039200
H	0.23917300	-1.85737400	-1.01845000
C	-0.74993800	-4.82112200	0.33071100
H	-0.76585000	-5.27462700	2.44098200
H	-0.63503700	-4.07739000	-1.69125800
H	-1.13904500	-5.79249700	0.03793700
C	0.06171300	-0.10916100	3.01134300
C	0.70990200	0.65734400	3.99454700
C	-1.31661400	-0.35072900	3.13789700
C	0.00021800	1.15440800	5.08866600
H	1.77069600	0.87650000	3.91425200
C	-2.02322300	0.14614000	4.23646500
H	-1.84846300	-0.92632700	2.38584100
C	-1.36593600	0.89764100	5.21321600
H	0.51892100	1.74155500	5.84193900
H	-3.08875300	-0.04912100	4.31677400
H	-1.91812500	1.28322800	6.06597400
C	5.24001000	-2.79905100	-0.69846800
C	4.69466800	-3.39028800	-1.84906300
C	6.39280700	-3.36561400	-0.13189500
C	5.27377000	-4.53097500	-2.40912200
H	3.81558800	-2.94881900	-2.31295400
C	6.97712000	-4.50033500	-0.69598000
H	6.84292100	-2.91136600	0.74662100
C	6.41695400	-5.08747600	-1.83349200

H	4.83818700	-4.97672000	-3.29956100
H	7.87189500	-4.92576700	-0.24847900
H	6.87467500	-5.97003000	-2.27264900
C	5.74577900	-0.37377000	0.79478400
C	6.44789900	0.52835800	-0.02507800
C	6.11968400	-0.46910800	2.14494900
C	7.49901300	1.29284500	0.48018900
H	6.16461200	0.63322100	-1.06944500
C	7.16400000	0.30658000	2.65644100
H	5.60295100	-1.15097200	2.81382400
C	7.85853200	1.18637800	1.82587500
H	8.02880200	1.97976300	-0.17423900
H	7.43497600	0.21861400	3.70557600
H	8.66992100	1.78907100	2.22487100

ADD5-N-real

Ag	-1.61776900	0.41667600	-0.73473000
P	-1.21190000	-1.67235600	0.37040000
C	-2.71909600	-2.67119300	0.85346200
H	-2.36810600	-3.59879600	1.32146500
H	-3.21963400	-2.96205100	-0.07661800
C	-3.71122400	-1.96174800	1.78875000
H	-4.45666300	-2.69070000	2.12856600
H	-3.19022900	-1.60474100	2.68419500
P	-4.57690800	-0.47715700	1.00597100
C	2.00614300	2.88751100	-0.89778700
H	2.03936100	2.53592200	-1.94036700
H	2.08465300	3.98927800	-0.92494700
C	3.23512700	2.34172900	-0.15263200
H	4.11174900	2.88468600	-0.55753800
O	0.81580700	2.48177200	-0.25832200
N	3.38606400	0.89689500	-0.36347300
H	3.75922900	0.43960700	0.46418000
C	3.15016900	2.66797700	1.35526500
H	2.85061100	3.71835400	1.45531300
H	2.34067500	2.07017400	1.78449300
C	4.44280200	2.43581300	2.11063400
C	4.63917000	1.28558700	2.88893700
C	5.48602800	3.37289600	2.03987900
C	5.84092600	1.07518200	3.57213700
H	3.84506300	0.54664200	2.96332800
C	6.68584800	3.16975200	2.72163700
H	5.34906000	4.27663300	1.44956400
C	6.86825600	2.01706300	3.49190300
H	5.96964500	0.17567900	4.16846200
H	7.47519900	3.91489100	2.66026300
H	7.79849600	1.86053600	4.03204800
C	8.60437600	0.05800800	0.17938400
C	7.28293300	-0.38568600	0.25580500

C	6.85254700	-1.37478400	-0.63105100
C	7.71395400	-1.93751500	-1.57669000
C	9.03185500	-1.48511700	-1.64155300
C	9.47396600	-0.48695600	-0.76802200
H	8.94825400	0.82623700	0.86568500
H	6.60389400	0.01378600	1.00146900
H	7.35922600	-2.72904700	-2.22894200
H	9.71499300	-1.91668900	-2.36758700
H	10.50197300	-0.13910000	-0.82236900
S	5.14887500	-1.95265000	-0.54847300
O	5.12504900	-3.34763700	-1.03072900
O	4.62290900	-1.62406700	0.79320100
C	4.24577000	-0.95339300	-1.77962000
H	4.72146600	-1.17935100	-2.73891300
C	4.20436000	0.55252300	-1.51486000
H	5.23776300	0.94756900	-1.45816600
H	3.75750400	1.00551000	-2.40891300
H	3.23772300	-1.38118600	-1.77144200
H	0.06087700	2.47804100	-0.90293500
N	-1.63218200	2.27672000	-1.78222100
Si	-1.49755300	2.02468600	-3.49370000
Si	-2.48409000	3.57284000	-0.98690900
C	-4.29990500	3.73756100	-1.54054800
H	-4.80693600	4.54671700	-0.99824700
H	-4.38109500	3.96011900	-2.61216200
H	-4.85828600	2.81201900	-1.35079700
C	-2.47297700	3.30407600	0.89281700
H	-3.02202700	2.39867200	1.17973100
H	-1.44268300	3.21417000	1.25864400
H	-2.94027600	4.15270600	1.41038300
C	-1.65053000	5.25911300	-1.28336800
H	-1.65998700	5.55694800	-2.33749900
H	-2.16008000	6.04665400	-0.71226500
H	-0.60467500	5.23562700	-0.95245300
C	-3.03370700	1.18629600	-4.25510200
H	-2.92405000	1.05495000	-5.34016600
H	-3.19803400	0.19284600	-3.81677600
H	-3.94052100	1.77909100	-4.08116800
C	-1.22348800	3.63292900	-4.47722000
H	-1.05789400	3.40614400	-5.53876700
H	-2.08809600	4.30524000	-4.41871200
H	-0.34937900	4.18747400	-4.11529700
C	-0.02360700	0.88484800	-3.88524200
H	0.92845100	1.34375600	-3.59109600
H	-0.10038500	-0.07410100	-3.35625500
H	0.02900700	0.66813700	-4.96069000
C	-5.80944100	-0.09253600	2.33316800
C	-7.17501100	0.09043300	2.06134500
C	-5.35227500	0.15931100	3.63948600
C	-8.05761400	0.48703600	3.06824100

H	-7.55566700	-0.07998100	1.05917300
C	-6.23598200	0.54798200	4.64605500
H	-4.29598000	0.06071800	3.87794500
C	-7.59419700	0.71165400	4.36493300
H	-9.11111700	0.61924100	2.83505600
H	-5.86050500	0.72911900	5.64992100
H	-8.28230700	1.01869400	5.14786700
C	-5.58523300	-1.32924000	-0.29255100
C	-5.47241900	-0.86041800	-1.61094700
C	-6.41930500	-2.43321300	-0.04050100
C	-6.16966600	-1.47886800	-2.65321900
H	-4.83274800	-0.00773700	-1.82244500
C	-7.11612400	-3.05046300	-1.07903400
H	-6.53584800	-2.80549000	0.97427700
C	-6.99075700	-2.57480200	-2.38842400
H	-6.06842300	-1.10049700	-3.66682100
H	-7.75862400	-3.90165600	-0.86837200
H	-7.53456800	-3.05728700	-3.19635500
C	-0.26089300	-2.88748700	-0.63425000
C	1.08132000	-3.19565200	-0.36520700
C	-0.88387100	-3.47069900	-1.75135800
C	1.77967200	-4.08613600	-1.18673500
H	1.59239600	-2.74163800	0.47826600
C	-0.18716600	-4.36446400	-2.56398100
H	-1.91358500	-3.22364200	-1.99833100
C	1.14527300	-4.67458300	-2.28218200
H	2.82282700	-4.30128100	-0.97517500
H	-0.68514800	-4.81183800	-3.42014100
H	1.69037700	-5.36638400	-2.91858400
C	-0.30177100	-1.48011100	1.95419800
C	-0.09946800	-2.56300600	2.82798600
C	0.17258400	-0.21045000	2.31835300
C	0.55092500	-2.37679500	4.04658000
H	-0.43903000	-3.55833500	2.55467600
C	0.81741800	-0.02669900	3.54508400
H	0.05311000	0.63086600	1.64034200
C	1.00416700	-1.10537300	4.40996700
H	0.70372200	-3.22227700	4.71169800
H	1.17223300	0.96231100	3.82099500
H	1.50483600	-0.95920300	5.36329300

TS1'-N-real

Ag	-1.45688600	0.55118600	-0.73232100
P	-1.36531800	-1.83682400	-0.51231900
C	-3.00293500	-2.69320800	-0.22886300
H	-2.81632100	-3.77360700	-0.26810700
H	-3.65618100	-2.44806400	-1.07407500
C	-3.69985800	-2.33874800	1.09542700
H	-4.51880500	-3.04801300	1.26301100

H	-3.00179000	-2.46074500	1.93041800
P	-4.36526300	-0.57359400	1.15543900
C	2.30294000	3.19837000	-1.09514500
H	2.29865400	2.90867600	-2.15767500
H	2.09608500	4.27959700	-1.04194500
C	3.69836800	2.93314800	-0.51408200
H	4.44568900	3.44264800	-1.13537400
O	1.38102700	2.44425800	-0.34269100
N	3.94162600	1.47776600	-0.66093600
H	3.18317500	0.94459600	-0.22166100
C	3.79165700	3.44880800	0.94245100
H	3.44762300	4.49220200	0.92052100
H	3.06120100	2.90094300	1.54557600
C	5.16123800	3.39470300	1.58758000
C	5.40665600	2.56294200	2.68795300
C	6.21340700	4.19273700	1.11185800
C	6.66692200	2.51568100	3.28856900
H	4.59895900	1.94876800	3.08028300
C	7.47474900	4.14772400	1.70634300
H	6.04139400	4.86271200	0.27157500
C	7.70677100	3.30574000	2.79706400
H	6.83400300	1.86306800	4.14152400
H	8.27511900	4.77505700	1.32257400
H	8.68807400	3.27145200	3.26240900
C	6.27854900	-3.47807300	2.02683200
C	5.40866400	-2.74236600	1.21850500
C	5.63511300	-2.68969500	-0.15862400
C	6.70986500	-3.37250100	-0.73609100
C	7.57284700	-4.10424500	0.07897700
C	7.36110500	-4.15397600	1.46032500
H	6.10583200	-3.52884100	3.09879500
H	4.54469700	-2.23460400	1.63407500
H	6.84959300	-3.34442900	-1.81228700
H	8.40675300	-4.64241300	-0.36376700
H	8.03528200	-4.72633700	2.09198900
S	4.55074500	-1.69083000	-1.21434900
O	4.41565100	-2.44527300	-2.47936100
O	3.34201400	-1.42301000	-0.38045400
C	5.28456700	-0.14854000	-1.54022700
H	6.19912100	-0.25199600	-2.12207900
C	5.27808900	0.81884000	-0.36577200
H	5.30662500	0.41668400	0.64936200
H	6.06298300	1.56986900	-0.46969800
H	4.13460700	0.85600300	-1.74262700
H	0.44911100	2.55300400	-0.70107600
N	-1.32483300	2.65908500	-1.07592000
Si	-1.58512600	3.00974000	-2.76209000
Si	-1.86234400	3.63683900	0.26673200
C	-1.58458500	2.69858100	1.89509200
H	-0.53493100	2.39139000	1.98614200

H	-1.82331100	3.33177000	2.76015200
H	-2.21526100	1.80294600	1.95700900
C	-0.87003800	5.25550500	0.41273100
H	0.19835300	5.04068300	0.53752300
H	-0.98140200	5.90064200	-0.46571900
H	-1.19668300	5.83020600	1.28949600
C	-3.70420700	4.11305400	0.18080600
H	-4.34484100	3.22323100	0.14083400
H	-3.99968300	4.69354000	1.06486100
H	-3.92967700	4.72436400	-0.70210700
C	-1.25274800	4.83444500	-3.19943100
H	-0.24215300	5.14575800	-2.90817400
H	-1.34695000	4.98789300	-4.28257700
H	-1.96078900	5.51588600	-2.71204600
C	-0.42014300	1.96076800	-3.83742700
H	-0.57836000	2.17169100	-4.90342200
H	0.63483000	2.16189900	-3.61414000
H	-0.58318300	0.88574200	-3.68731000
C	-3.35753000	2.62692800	-3.35090300
H	-3.59195900	1.56070000	-3.23233400
H	-4.10257500	3.19667200	-2.78193100
H	-3.48754200	2.87619900	-4.41268100
C	-5.78245400	-0.72218700	-0.02708200
C	-5.83007200	0.18138300	-1.10020900
C	-6.78091000	-1.70805200	0.06636300
C	-6.84392300	0.10102300	-2.05966900
H	-5.06709000	0.95035900	-1.18637300
C	-7.79423200	-1.78777800	-0.88824400
H	-6.77540600	-2.40901200	0.89716200
C	-7.82594700	-0.88375400	-1.95500000
H	-6.86177300	0.80850800	-2.88418400
H	-8.56046200	-2.55393400	-0.80110300
H	-8.61572500	-0.94807900	-2.69885200
C	-5.17395600	-0.59570500	2.82145300
C	-4.40138600	-0.93023300	3.94866500
C	-6.49436600	-0.16401300	3.02624400
C	-4.94183500	-0.86756100	5.23274700
H	-3.36497400	-1.23715500	3.82959700
C	-7.03229400	-0.09517100	4.31321200
H	-7.11015500	0.11651000	2.17747000
C	-6.26187400	-0.45173400	5.42041700
H	-4.32830700	-1.13954500	6.08784200
H	-8.05831800	0.23792400	4.44748600
H	-6.68260100	-0.39968600	6.42094200
C	-0.35507200	-2.41696400	0.90993200
C	0.01227800	-3.76606800	1.04242000
C	0.02302900	-1.50442000	1.90529500
C	0.73639500	-4.19242300	2.15435700
H	-0.25060000	-4.48006600	0.26669300
C	0.74407300	-1.93529700	3.02167000

H	-0.23691900	-0.45395400	1.80245600
C	1.09993400	-3.27828300	3.14745400
H	1.02264100	-5.23683000	2.24328800
H	1.03224600	-1.21809000	3.78548400
H	1.66472500	-3.61376000	4.01327100
C	-0.66924600	-2.69615200	-1.97885500
C	0.71903700	-2.64405100	-2.19367800
C	-1.48780300	-3.33038500	-2.92719400
C	1.27745700	-3.22751100	-3.33161200
H	1.37894900	-2.16154800	-1.47674600
C	-0.92383800	-3.90857700	-4.06647400
H	-2.56367500	-3.38005800	-2.79040400
C	0.45623000	-3.85876700	-4.26939800
H	2.35408700	-3.17740500	-3.46528800
H	-1.56734200	-4.39895900	-4.79239600
H	0.89105500	-4.31036900	-5.15727300

TS1-N-OAc-real

Ag	0.92067400	-0.10086700	-0.03778600
P	1.51330600	2.28015000	-0.25605500
C	3.37711900	2.23266900	-0.39531300
H	3.79716000	3.23814300	-0.27701600
H	3.61162600	1.90677500	-1.41605700
C	4.03550300	1.27650900	0.62074500
H	5.12404200	1.39601200	0.56626500
H	3.72698200	1.53967800	1.64005600
P	3.54764600	-0.51259100	0.33270600
C	-0.52513500	-2.20633400	-2.74138400
H	-0.60265600	-1.32798800	-3.39088800
H	-0.26215100	-3.06870800	-3.37381500
C	-1.90945900	-2.47808400	-2.11136500
H	-2.63995000	-2.42646700	-2.93119200
O	0.51684400	-1.91996000	-1.82429500
N	-2.23466100	-1.35398900	-1.20355400
H	-1.62204800	-1.34544400	-0.37151400
C	-1.99276800	-3.88936300	-1.47599300
H	-1.69292000	-4.59447400	-2.26369300
H	-1.24163400	-3.97660700	-0.68537500
C	-3.35516000	-4.29207600	-0.95087900
C	-3.63007700	-4.28239800	0.42326600
C	-4.37557500	-4.68532200	-1.83028200
C	-4.89063500	-4.64181900	0.90573700
H	-2.84824700	-3.99135200	1.12061700
C	-5.63720000	-5.04307200	-1.35339700
H	-4.17688600	-4.71708300	-2.90011000
C	-5.89952500	-5.02020800	0.01871400
H	-5.08213600	-4.62833000	1.97556200
H	-6.41301200	-5.34635300	-2.05174200
H	-6.88037500	-5.30138300	0.39248400

C	-6.17303200	1.21219500	2.78518500
C	-5.03460900	1.17692000	1.97697600
C	-5.06584000	1.79246000	0.72309000
C	-6.21511800	2.45008100	0.27554600
C	-7.34677900	2.48182000	1.09049100
C	-7.32852100	1.85979400	2.34244600
H	-6.15390700	0.74084100	3.76438900
H	-4.11905700	0.70290400	2.31523900
H	-6.20605800	2.94724100	-0.68927700
H	-8.24114200	2.99839800	0.75213900
H	-8.21182500	1.88769600	2.97507800
S	-3.61602400	1.69900000	-0.36248300
O	-3.62712900	2.94622600	-1.16049200
O	-2.47080000	1.42295900	0.54645900
C	-3.76705600	0.35196300	-1.45029200
H	-4.54573900	0.54127500	-2.18818100
C	-3.68826800	-1.04473900	-0.84800500
H	-3.82478400	-1.13349800	0.23176700
H	-4.35070700	-1.75391400	-1.34455400
H	-2.37901200	-0.20673700	-1.72720000
O	0.74126900	-3.39744600	0.39618000
C	0.14925800	-2.74679800	1.29957700
C	0.02950800	-3.37521800	2.68428500
H	0.11568000	-4.46325500	2.62958100
H	0.84613800	-2.99571500	3.31120800
H	-0.91110700	-3.08666000	3.16176500
O	-0.35505900	-1.57783700	1.15752300
H	0.59938500	-2.60380600	-1.09400300
C	4.32841200	-1.41496200	1.73638200
C	3.89116600	-2.73325300	1.96116100
C	5.29891300	-0.86784400	2.59067100
C	4.43227200	-3.48846300	3.00199800
H	3.11468200	-3.16125500	1.33050700
C	5.82857400	-1.62368500	3.63931400
H	5.64807700	0.15067500	2.44904600
C	5.40074600	-2.93614300	3.84387100
H	4.08770800	-4.50680400	3.16098400
H	6.57699500	-1.18497100	4.29428200
H	5.81453300	-3.52317000	4.65951700
C	4.58631300	-0.96156000	-1.12893700
C	3.93870500	-1.35322600	-2.31113400
C	5.99025000	-0.91757100	-1.10044600
C	4.68586000	-1.67550900	-3.44857800
H	2.85380600	-1.42485300	-2.33557900
C	6.73156900	-1.24265200	-2.23523000
H	6.50759900	-0.64467100	-0.18396800
C	6.07889700	-1.61817000	-3.41369900
H	4.17491800	-1.97802700	-4.35889700
H	7.81747100	-1.20800700	-2.20065700
H	6.65792900	-1.87239300	-4.29770900

C	0.96886700	3.36630900	-1.63342100
C	1.84077600	3.98945700	-2.53917600
C	-0.41668900	3.54546600	-1.78010400
C	1.33019400	4.77868100	-3.57301300
H	2.91623500	3.86935300	-2.44971000
C	-0.92093700	4.33899900	-2.80862700
H	-1.11181500	3.06935100	-1.09589500
C	-0.04806900	4.95558800	-3.70881000
H	2.01364300	5.25612700	-4.27072000
H	-1.99694800	4.45389400	-2.89662100
H	-0.43931800	5.56955200	-4.51599900
C	1.20638800	3.26784700	1.26966700
C	0.23002200	2.81917400	2.17157500
C	1.89522100	4.46136600	1.54240100
C	-0.03912800	3.54588400	3.33455700
H	-0.34008000	1.92158700	1.95004600
C	1.62804900	5.18028500	2.70630000
H	2.63267000	4.84254100	0.84057000
C	0.66206100	4.72031800	3.60653500
H	-0.80267400	3.19251100	4.02187500
H	2.16784500	6.10178600	2.90844900
H	0.45276700	5.28343900	4.51228700

TS1-O-OAc-real

Ag	-1.30091700	0.13596300	-0.18023300
P	-3.73510200	-0.40298800	0.42394600
C	-3.49583100	-1.91265800	1.52007800
H	-4.46124900	-2.40278400	1.69370200
H	-3.13899900	-1.55170300	2.49112700
C	-2.50148000	-2.92501900	0.91876700
H	-2.43157600	-3.81414300	1.55687600
H	-2.87187000	-3.26502300	-0.05506600
P	-0.78347100	-2.24124300	0.57588400
C	1.63548000	1.55457400	1.29737400
H	1.07213600	0.86611500	1.93106400
H	2.54887000	1.86399600	1.81570600
C	0.74967200	2.73380900	0.89624900
H	0.30930400	3.10409900	1.83282600
O	2.00049400	0.75279500	0.13740300
N	-0.34508600	2.26489900	0.03005900
H	0.00332200	2.16931700	-0.94688900
C	1.55767200	3.89640100	0.25515800
H	2.36420800	4.18031700	0.94445600
H	2.02608400	3.52805200	-0.66430800
C	0.70835200	5.10752900	-0.06828900
C	0.09951400	5.23860200	-1.32659700
C	0.49005500	6.10709700	0.89052100
C	-0.70924500	6.34097400	-1.61223300
H	0.26186000	4.47106700	-2.08047300

C	-0.31690700	7.20972700	0.60552800
H	0.96399500	6.02501800	1.86699900
C	-0.92026000	7.32917100	-0.64835000
H	-1.17057000	6.42869900	-2.59256100
H	-0.46957800	7.97732200	1.36001500
H	-1.54614100	8.18871300	-0.87357500
H	-1.07373500	2.97573600	0.00443800
O	-1.06548900	0.20820300	-2.53515100
C	-0.22734700	0.95421700	-3.14711800
C	-0.08341200	0.69203200	-4.64999600
H	0.49422900	1.48347600	-5.13326700
H	0.42983500	-0.26540100	-4.80454900
H	-1.06970600	0.60949400	-5.11811400
O	0.48752900	1.85075900	-2.63110900
H	2.54621000	-0.22671000	0.30317900
C	8.57555000	1.40521600	-0.48544700
C	7.33554600	1.16618700	0.10985900
C	6.78721600	-0.11657400	0.05314200
C	7.46515800	-1.16298800	-0.57751100
C	8.70249600	-0.91353700	-1.17172800
C	9.25603300	0.36920000	-1.12937800
H	9.01307000	2.39891300	-0.43965000
H	6.80292100	1.95159000	0.63563600
H	7.03449700	-2.15916100	-0.57933900
H	9.23871600	-1.72250000	-1.66052800
H	10.22147600	0.55868600	-1.59087700
S	5.16119600	-0.42585900	0.78342200
O	5.19857000	-1.82415700	1.26450000
O	4.91774800	0.68550100	1.73774000
C	3.94308500	-0.30781200	-0.45780000
H	4.06433800	-1.01186400	-1.27546700
C	3.34741200	1.01178100	-0.70245800
H	3.81033700	1.87477500	-0.22543800
H	2.96524100	1.21728800	-1.70019700
C	-0.15826300	-3.42098800	-0.69235900
C	-0.14043000	-3.00522400	-2.03417000
C	0.25901700	-4.72223600	-0.36707500
C	0.27840400	-3.88987700	-3.03209200
H	-0.44703500	-1.99427700	-2.29842800
C	0.68200900	-5.59636000	-1.36789400
H	0.26694700	-5.04774700	0.66934800
C	0.69008200	-5.18173900	-2.70259000
H	0.28996500	-3.56142200	-4.06811700
H	1.00714200	-6.59984400	-1.10591500
H	1.02203600	-5.86385200	-3.48106900
C	0.20323400	-2.62816400	2.08108600
C	-0.37626300	-2.87365400	3.33558500
C	1.60637900	-2.56812100	1.98900200
C	0.42755300	-3.05666600	4.46458000
H	-1.45563300	-2.92813100	3.44533200

C	2.40838800	-2.75036500	3.11496800
H	2.08812800	-2.39077500	1.03117800
C	1.81758000	-2.99410900	4.35828700
H	-0.03838200	-3.25068900	5.42750200
H	3.48703300	-2.68794400	3.00412100
H	2.43837900	-3.13263500	5.23930100
C	-4.74133300	-1.08070600	-0.96143900
C	-4.22675600	-0.98556800	-2.26529500
C	-5.97776700	-1.71885000	-0.75570500
C	-4.94248800	-1.52378800	-3.33998200
H	-3.26616400	-0.50529300	-2.44442300
C	-6.68709400	-2.25033900	-1.83143100
H	-6.39487100	-1.78856700	0.24588200
C	-6.16829000	-2.15359500	-3.12661100
H	-4.53564700	-1.44726100	-4.34464300
H	-7.64267900	-2.73946100	-1.66110200
H	-6.72144700	-2.56924000	-3.96484400
C	-4.89968400	0.63050400	1.41337000
C	-4.59887300	0.92821600	2.75459400
C	-6.02007300	1.24298300	0.82842800
C	-5.40959800	1.78836400	3.49469400
H	-3.72270700	0.49482500	3.23023800
C	-6.82646600	2.10876600	1.56972900
H	-6.26859000	1.04085500	-0.20864000
C	-6.52864000	2.38109100	2.90546600
H	-5.16331300	1.99807500	4.53231800
H	-7.69083700	2.56944900	1.09864500
H	-7.15854100	3.05340300	3.48140000

AgHMDS/dppe 3

Ag	1.25241900	-0.06265600	-0.34693900
P	0.23969700	1.99577900	0.31477200
C	-1.15801400	1.83668400	1.54710700
H	-1.36310100	2.83345400	1.95783600
H	-0.79043200	1.21255700	2.36998800
C	-2.46079000	1.24520400	0.98287400
H	-3.21981400	1.26221300	1.77389200
H	-2.83590500	1.88255500	0.17490000
P	-2.30058000	-0.49642000	0.26926900
N	2.23143700	-1.84280900	-0.84060200
Si	1.72490100	-2.63829300	-2.28801100
Si	3.57699900	-2.23935800	0.16764900
C	3.83042400	-4.12059500	0.35720600
H	4.68743300	-4.33504200	1.00943400
H	2.94851900	-4.60066500	0.79980700
H	4.02219100	-4.61257800	-0.60423500
C	5.22076000	-1.51733300	-0.46926300
H	5.46174500	-1.89655300	-1.46987300
H	5.16042100	-0.42328800	-0.54070600

H	6.06173600	-1.76304700	0.19321200
C	3.33368600	-1.54930500	1.92793500
H	2.40637400	-1.92287000	2.38061700
H	4.16668500	-1.83914900	2.58278200
H	3.28454500	-0.45172000	1.92967900
C	3.17333700	-3.10759600	-3.43552000
H	2.81066300	-3.59970500	-4.34791600
H	3.73943600	-2.21782400	-3.73887200
H	3.87830300	-3.79542600	-2.95249000
C	0.74738900	-4.23792600	-1.94302000
H	0.41428400	-4.71780500	-2.87314100
H	1.35195100	-4.96810800	-1.39139800
H	-0.14648200	-4.02907400	-1.34076600
C	0.57018300	-1.51637200	-3.30711500
H	-0.32855200	-1.24805800	-2.73596200
H	1.07916800	-0.58948300	-3.60377900
H	0.23845100	-2.02066400	-4.22480200
C	1.41665400	3.14835400	1.13679200
C	2.37895500	3.80342100	0.34851100
C	1.44551600	3.32792900	2.52765000
C	3.33547400	4.62797500	0.93743800
H	2.37844900	3.67052600	-0.73022600
C	2.40923200	4.15169600	3.11541100
H	0.72462500	2.82617500	3.16514200
C	3.35364200	4.80432600	2.32379700
H	4.06984300	5.12967700	0.31335600
H	2.41805000	4.28001500	4.19435600
H	4.10249200	5.44380700	2.78267500
C	-0.50173100	2.99239500	-1.04169300
C	-0.90518400	4.32307800	-0.83943800
C	-0.70695400	2.39800800	-2.29593800
C	-1.50523000	5.04175600	-1.87264700
H	-0.73809900	4.80244100	0.12155600
C	-1.31037300	3.12049100	-3.32879400
H	-0.39431000	1.37123100	-2.46533800
C	-1.70963300	4.44065300	-3.11834100
H	-1.81021600	6.07158900	-1.70751900
H	-1.46132500	2.65015500	-4.29643600
H	-2.17491500	5.00370300	-3.92288500
C	-2.01031800	-1.48570300	1.80564800
C	-0.95077600	-2.40759300	1.79120300
C	-2.76495400	-1.34479600	2.98421800
C	-0.65366900	-3.16947300	2.92550200
H	-0.34494700	-2.52006900	0.89560700
C	-2.46640000	-2.10279300	4.11639600
H	-3.60086800	-0.65043700	3.01590700
C	-1.40853400	-3.01698800	4.08837900
H	0.17000400	-3.87742700	2.89601200
H	-3.05999700	-1.98351700	5.01928900
H	-1.17663000	-3.60724600	4.97102300

C	-4.08106200	-0.80571300	-0.13984100
C	-4.69054600	0.01938500	-1.10314100
C	-4.81818400	-1.88394500	0.37373500
C	-6.00465100	-0.20476300	-1.51142900
H	-4.13285700	0.84072900	-1.54828700
C	-6.13120900	-2.11433000	-0.04451300
H	-4.36913300	-2.54799900	1.10540300
C	-6.73180100	-1.27356400	-0.98170400
H	-6.45797700	0.45068300	-2.25071300
H	-6.68439400	-2.95472400	0.36714500
H	-7.75392200	-1.45322300	-1.30389800

OAc⁻

O	0.69616100	1.16619500	0.00000500
C	0.22056900	0.00178000	-0.00002400
C	-1.35421400	-0.05490400	-0.00000700
H	-1.73338300	-1.08501600	-0.00052200
H	-1.75037100	0.47185900	0.88082500
H	-1.75047200	0.47283600	-0.88020500
O	0.80835100	-1.10881200	0.00000600

AgOAc/dppe 4

O	0.24419900	-1.23602100	3.45360800
C	0.39652300	-2.45997400	3.12849600
C	0.66798200	-3.44990300	4.25523900
H	1.59843700	-3.17821000	4.76636900
H	-0.13469400	-3.39419300	4.99845700
H	0.74613400	-4.47003500	3.87347800
O	0.33725100	-2.87495400	1.93710600
Ag	-0.07623900	-0.53568600	1.31494100
P	-1.75726900	0.35315400	-0.27291000
C	-0.75122500	0.61902000	-1.83351000
H	-1.31634300	1.22206000	-2.55431800
H	-0.59655000	-0.37102800	-2.27985000
C	0.60871900	1.29320000	-1.56568100
H	1.11756900	1.45442100	-2.52364600
H	0.45637700	2.27784100	-1.10608600
P	1.69322200	0.30273000	-0.39642700
C	-2.44583500	2.03235700	0.06155000
C	-1.98365700	2.72688500	1.18991900
C	-3.39810400	2.64387300	-0.77025600
C	-2.44987000	4.01343200	1.47209400
H	-1.26475900	2.25285700	1.85419100
C	-3.86742800	3.92531200	-0.48413300
H	-3.78825300	2.11256200	-1.63418800
C	-3.39117700	4.61371800	0.63555800
H	-2.08353600	4.53855700	2.34994600
H	-4.60861000	4.38584300	-1.13206500

H	-3.76016500	5.61143600	0.85765100
C	-3.18553600	-0.65558500	-0.84225300
C	-3.83472600	-1.44727100	0.11942700
C	-3.64658500	-0.68705400	-2.16862800
C	-4.93160800	-2.23440200	-0.23186900
H	-3.46791900	-1.45515400	1.14269200
C	-4.73872200	-1.48250100	-2.52007100
H	-3.15440000	-0.09880400	-2.93758200
C	-5.38543600	-2.25343500	-1.55218200
H	-5.42189800	-2.84221700	0.52345700
H	-5.08219200	-1.50056200	-3.55103000
H	-6.23404100	-2.87347500	-1.82820800
C	3.15750900	1.39296100	-0.14573400
C	3.48135600	2.49196900	-0.95747700
C	3.98379900	1.09861500	0.95247500
C	4.60890400	3.26920500	-0.68273500
H	2.85761900	2.75264100	-1.80741100
C	5.11575100	1.86838200	1.21850700
H	3.73139200	0.26619800	1.60505300
C	5.43016200	2.95697900	0.40173900
H	4.84473900	4.11854500	-1.31875000
H	5.74486400	1.62484700	2.07031800
H	6.30687700	3.56309700	0.61348000
C	2.30379200	-1.06277700	-1.47828800
C	1.99200100	-2.38405500	-1.11857000
C	3.05396300	-0.82522100	-2.64230400
C	2.41211300	-3.44623100	-1.92581400
H	1.43428000	-2.58659100	-0.20599800
C	3.47298500	-1.88780900	-3.44096900
H	3.32543600	0.19094500	-2.91835800
C	3.14832500	-3.20088700	-3.08466000
H	2.16573700	-4.46484900	-1.63888700
H	4.05564500	-1.69408100	-4.33798300
H	3.47677400	-4.02868800	-3.70784200

HMDS-

N	-0.00004100	0.00106900	0.00174600
Si	-1.64478600	0.00036200	0.00039200
Si	1.64467800	0.00041400	-0.00006300
C	2.44891100	1.70240400	-0.41085300
H	3.54904700	1.66656600	-0.40068300
H	2.13571000	2.05129900	-1.40437000
H	2.13335100	2.46600000	0.31310500
C	2.44963100	-0.49571500	1.67836700
H	2.13332400	0.18741700	2.47846400
H	2.13789800	-1.50637000	1.97541800
H	3.54970000	-0.48199500	1.64230000
C	2.44549600	-1.20750900	-1.26915300
H	2.12927000	-0.96231700	-2.29222500

H	3.54560500	-1.18299100	-1.24386400
H	2.13005400	-2.24143700	-1.07325200
C	-2.44953800	1.75032900	-0.03908900
H	-3.54956800	1.71210000	-0.04877800
H	-2.14391200	2.33847800	0.83700300
H	-2.12692800	2.30684600	-0.92957300
C	-2.44669500	-0.90907800	-1.49675500
H	-3.54681700	-0.88705500	-1.46744600
H	-2.12890900	-0.45273900	-2.44419800
H	-2.13423800	-1.96185600	-1.52531200
C	-2.44770100	-0.84215700	1.53562400
H	-2.13239400	-1.89177400	1.61151800
H	-2.13220800	-0.34317300	2.46205200
H	-3.54780700	-0.82499500	1.50417500

7. Absolute energies and Imaginary frequency for the computed structures

Geometries	$E(\text{gas phase})/\text{a.u.}$	$G(\text{gas phase, 298K})/\text{a.u.}$	$E(\text{DMF})/\text{a.u.}$	$G(\text{DMF, 298K})/\text{a.u.}$	Imaginary Frequency (cm^{-1})
1	-480.73844	-480.56585	-480.55351	-480.38092	0
2	-858.19771	-858.09015	-857.99901	-857.89145	0
TS1-N-non	-1338.88420	-1338.58490	-1338.54017	-1338.24088	-1465.54
TS1-O-non	-1338.87601	-1338.57657	-1338.52163	-1338.22219	-1461.41
N-adduct	-1338.97223	-1338.66671	-1338.62220	-1338.31668	0
O-adduct	-1338.96676	-1338.66089	-1338.60569	-1338.29982	0
Geometries	$E(\text{gas phase})/\text{a.u.}$	$G(\text{gas phase, 253K})/\text{a.u.}$	$E(\text{DMF})/\text{a.u.}$	$G(\text{DMF, 253K})/\text{a.u.}$	Imaginary Frequency (cm^{-1})
1	-480.73844	-480.55882	-480.55351	-480.37389	0
2	-858.19771	-858.08320	-857.99901	-857.88450	0
3'	-1941.36288	-1940.97358	-1941.07754	-1940.68823	0
4'	-1296.53552	-1296.31668	-1296.35377	-1296.13494	0
N-adduct	-1338.97223	-1338.65591	-1338.62220	-1338.30588	0
O-adduct	-1338.96676	-1338.65014	-1338.60569	-1338.28907	0
ADD1-O	-2422.11327	-2421.52733	-2421.64043	-2421.05449	0
TS1-O	-2422.09867	-2421.51642	-2421.62563	-2421.04338	-1049.93
ADD2-O	-2422.12546	-2421.54243	-2421.63936	-2421.05633	0
ADD1-N	-2422.10254	-2421.51779	-2421.63281	-2421.04805	0
TS1-N	-2422.07976	-2421.49805	-2421.61533	-2421.03361	-1237.43
ADD2-N	-2422.10519	-2421.52159	-2421.62979	-2421.04619	0
ADD3-O	-3280.32128	-3279.61098	-3279.66639	-3278.95609	0
TS2-O	-3280.31319	-3279.59700	-3279.66606	-3278.94987	-153.45
ADD4-O	-3280.31544	-3279.59771	-3279.68050	-3278.96277	0
TS3-O	-3280.28836	-3279.56771	-3279.66817	-3278.94753	-1199.59
ADD5-O	-3280.30002	-3279.57563	-3279.68156	-3278.95717	0
ADD3'-O	-3280.33947	-3279.62434	-3279.68089	-3278.96576	0
TS2'-O	-3280.32876	-3279.60960	-3279.67336	-3278.95420	-213.38
ADD4'-O	-3280.34875	-3279.62822	-3279.69826	-3278.97773	0
TS3'-O	-3280.29834	-3279.57668	-3279.66449	-3278.94283	-1345.67
ADD5'-O	-3280.34681	-3279.62422	-3279.69667	-3278.97408	0
ADD3-N	-3280.31436	-3279.59345	-3279.66804	-3278.94713	0
TS2-N	-3280.28688	-3279.57062	-3279.63406	-3278.91779	-1635.82
ADD4-N	-3280.36290	-3279.64292	-3279.71364	-3278.99365	0
TS3-N	-3280.33550	-3279.61531	-3279.69932	-3278.97913	-1090.42
ADD5-N	-3280.35090	-3279.62782	-3279.71270	-3278.98962	0
ADD1'	-2422.11371	-2421.53119	-2421.64240	-2421.05988	0
TS1'-N	-3280.28271	-3279.56414	-3279.63740	-3278.91883	-1568.85
ADD2'-N	-3280.35297	-3279.63259	-3279.70857	-3278.98819	0
TS1'-O	-3280.25078	-3279.53481	-3279.60957	-3278.89360	-1297.41
TS1-O-Cu-HMDS	-2472.45645	-2471.87318	-2472.02545	-2471.44218	-1115.76
TS1-O-Cu-Bu	-1756.93258	-1756.44956	-1756.56119	-1756.07818	-1147.91
ADD1-OAc	-1777.30321	-1776.88345	-1776.92853	-1776.50878	0
TS1-N-OAc	-2635.45893	-2634.90757	-2634.91761	-2634.36624	-1609.63
ADD2-N-OAc	-2635.53057	-2634.97473	-2634.98500	-2634.42916	0

TS1-O-OAc	-2635.43635	-2634.88631	-2634.88952	-2634.33948	-1391.07
ADD1-O-real	-3189.03020	-3188.24571	-3188.17621	-3187.39172	0
TS1-O-real	-3189.01544	-3188.23530	-3188.15937	-3187.37923	-1106.93
ADD2-O-real	-3189.04229	-3188.25953	-3188.17654	-3187.39378	0
ADD3-O-real	-4047.24026	-4046.32842	-4046.20119	-4045.28935	0
TS2-O-real	-4047.23214	-4046.31608	-4046.19973	-4045.28367	-160.54
ADD4-O-real	-4047.23408	-4046.31510	-4046.21034	-4045.29135	0
TS3-O-real	-4047.20390	-4046.28297	-4046.19915	-4045.27822	-1170.77
ADD5-O-real	-4047.21613	-4046.29455	-4046.21369	-4045.29211	0
ADD3-N-real	-4047.22441	-4046.30395	-4046.20174	-4045.28127	0
TS2-N-real	-4047.19650	-4046.28061	-4046.16962	-4045.25374	-1636.96
ADD4-N-real	-4047.27569	-4046.35304	-4046.25083	-4045.32818	0
TS3-N-real	-4047.24918	-4046.32977	-4046.22584	-4045.30644	-964.06
ADD5-N-real	-4047.26717	-4046.34376	-4046.24787	-4045.32446	0
TS1'-N-real	-4047.19442	-4046.27645	-4046.17088	-4045.25291	-1553.69
TS1-N-OAc-real	-3402.37430	-3401.62330	-3401.44633	-3400.69534	-1601.54
TS1-O-OAc-real	-3402.35344	-3401.60283	-3401.42133	-3400.67072	-1333.09
AgHMDS/dppe 3	-2708.27891	-2707.69115	-2707.60986	-2707.02211	0
OAc ⁻	-228.49317	-228.46756	-228.56120	-228.53558	0
AgOAc/dppe 4	-2063.45487	-2063.03791	-2062.88378	-2062.46682	0
HMDS ⁻	-873.34316	-873.15257	-873.26263	-873.07204	0

Note: $E(\text{gas phase})$ is the potential energy in gas phase, $G(\text{gas phase})$ is the free energy in gas phase, $E(\text{DMF})$ is the potential energy in DMF, $G(\text{DMF})$ is the free energy in DMF.