

Supporting Information

The Control Effect of Different Scaffolds in Chiral Phosphoric Acid: A Case Study of Enantioselective Asymmetric Arylation

Lihan Zhu, Hend Mohamed, Haiyan Yuan*, Jingping Zhang*

Faculty of Chemistry, Northeast Normal University, Changchun 130024, China

*yuanhy034@nenu.edu.cn; jpzhang@nenu.edu.cn

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Computational Methods

The ee value has been calculated by the Boltzmann distribution of diastereomeric transition states using the basic following equations:

$$ee = \frac{1 - e^{-\Delta G^\ddagger_{R/S}/RT}}{1 + e^{-\Delta G^\ddagger_{R/S}/RT}} \times 100 \quad (1)$$

$\Delta G^\ddagger$ is the difference in the Gibbs free energies between the competing diastereomeric transition states.

Results and Discussion

To identify the stable conformation of the substrate **1a**, the conformational analysis on pointed out that there are ten stable conformers for it. The ten conformers were calculated using M062X/6-311+G(d,p)-SMD (DCM) at 253.15 K, M062X/6-311+G(d,p)-SMD (Toluene), and M062X/6-311+G(d,p)-SMD (DCM) at 298.15 K. The optimized structures were shown in Figure S1.

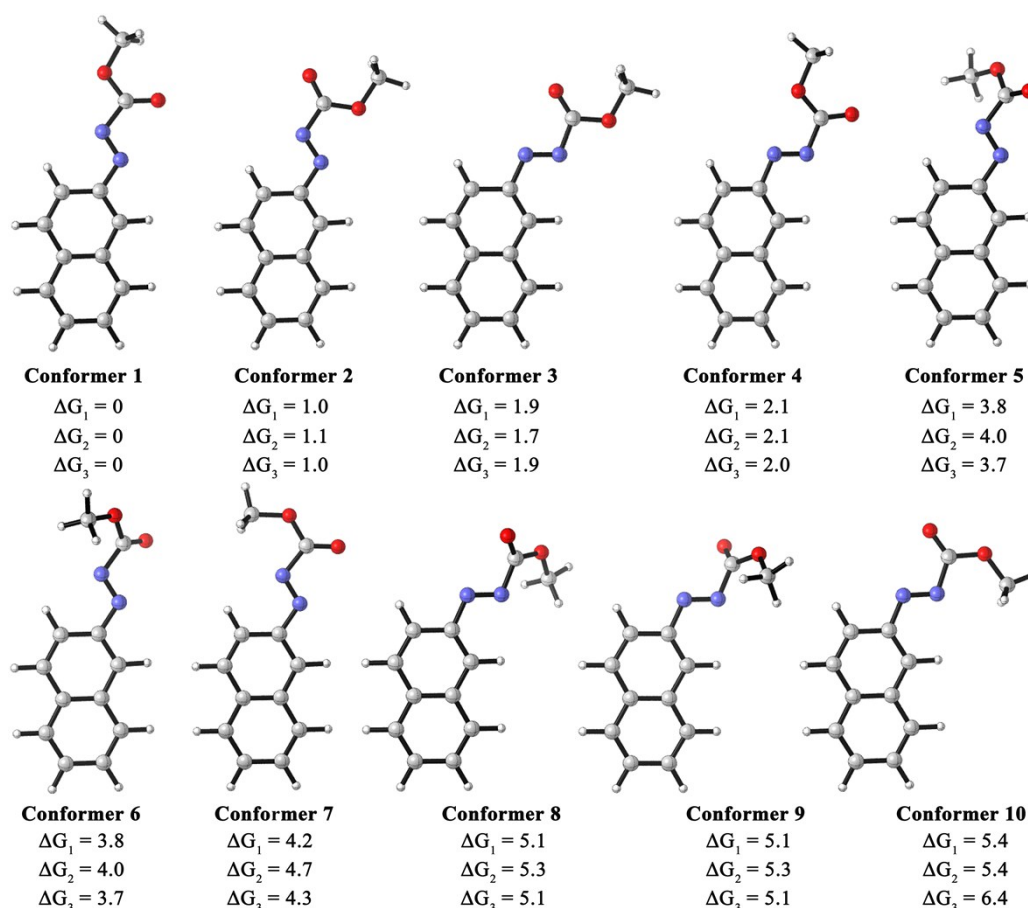


Figure S1. Different conformations of substrate **1a**. ΔG_1 values are computed with M062X/6-311+G(d,p)-SMD (DCM) at 253.15 K, ΔG_2 values are computed with

M062X/6-311+G(d,p)-SMD (Toluene), and ΔG_3 values are computed with M062X/6-311+G(d,p)-SMD (DCM) at 298.15 K. All energies are in kcal/mol.

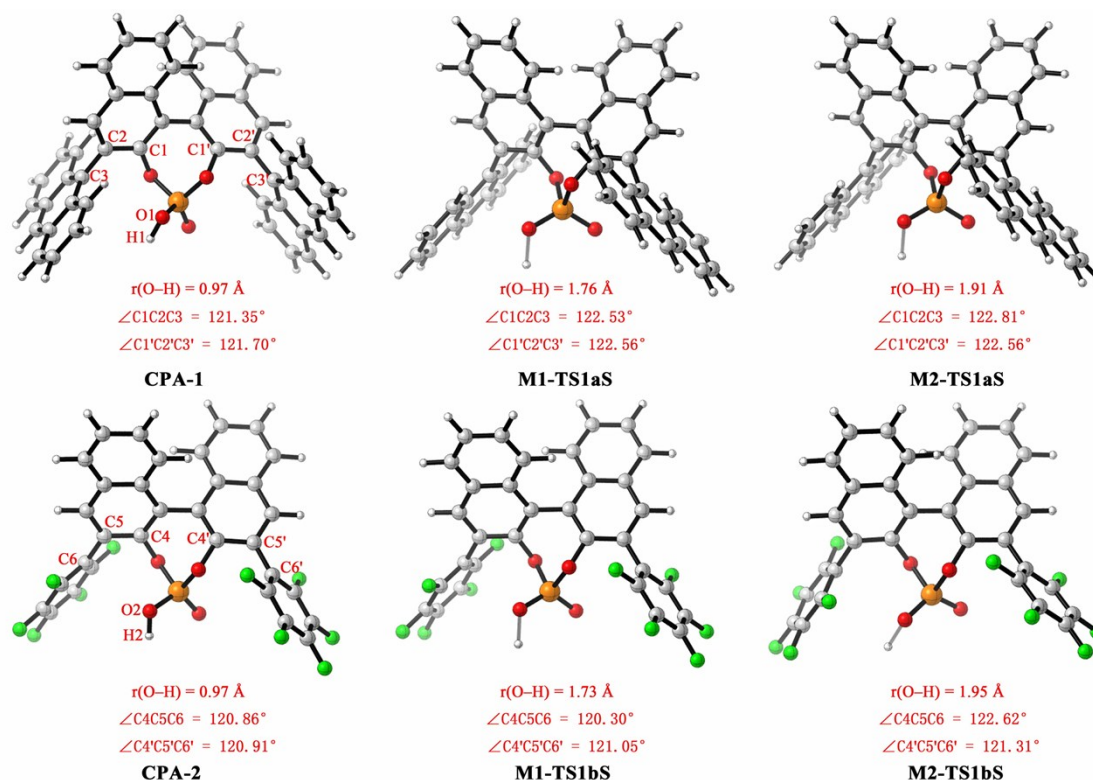


Figure S2. Key angles and lengths for the optimized catalyst structures of **CPA-1**, **CPA-2**, mode M1 and M2 of **TS1aS**, and **TS1bS**. Distances are provided in Å.

The breaking O1–H1 bond (0.97 Å) of the two catalysts have stretched to 1.76 Å (**Ts1aS**) and 1.73 Å (**Ts1bS**) in M1 mode, in comparison with 1.91 Å (**Ts1aS**) and 1.95 Å (**Ts1bS**) in M2 mode. In **TS1aS**, the angle $\angle \text{C1C2C3}$ changes from 121.35° in the native geometry of **CPA-1** to 122.53° and 122.81° in the M1 and M2 mode, $\angle \text{C1'C2'C3'}$ changes from 121.70° in the native geometry of **CPA-1** to 122.56° and 122.56° in the M1 and M2 mode. In the case of **TS1bS**, much larger deviations in $\angle \text{C4C5C6}$ and $\angle \text{C4'C5'C6'}$ from 120.86° and 120.91° in the native catalyst geometry to 122.62° and 121.31° in M2 mode. Thus, the M2 mode exhibits much larger deviations than M1 with respect to the optimized catalyst structures, explaining the much higher distortion energy in M2 mode.

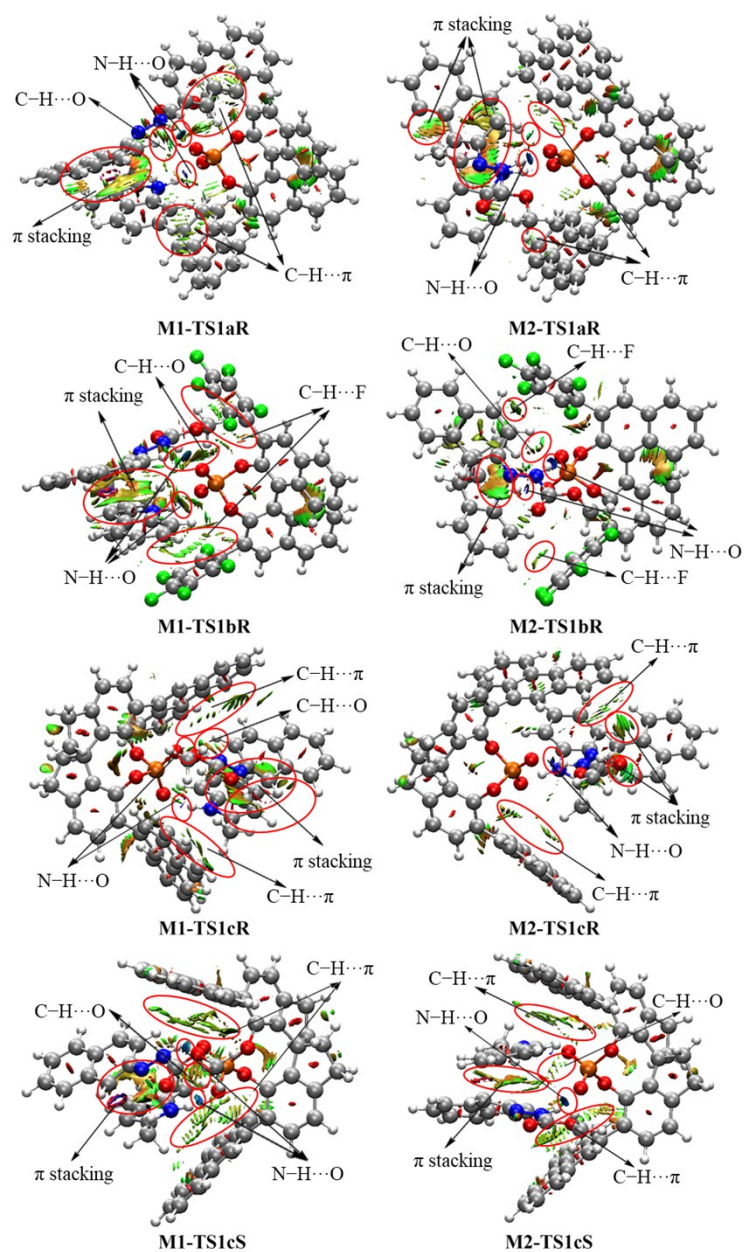


Figure S3. NCI plots for different activation modes of stereocontrolling transition states **M1-TS1aR**, **M2-TS1aR**, **M1-TS1bR**, **M2-TS1bR**, **M1-TS1cR**, **M2-TS1cR**, **M1-TS1cS**, and **M2-TS1cS** (blue: strong attractive; green: weak attractive; and red: strong repulsive).

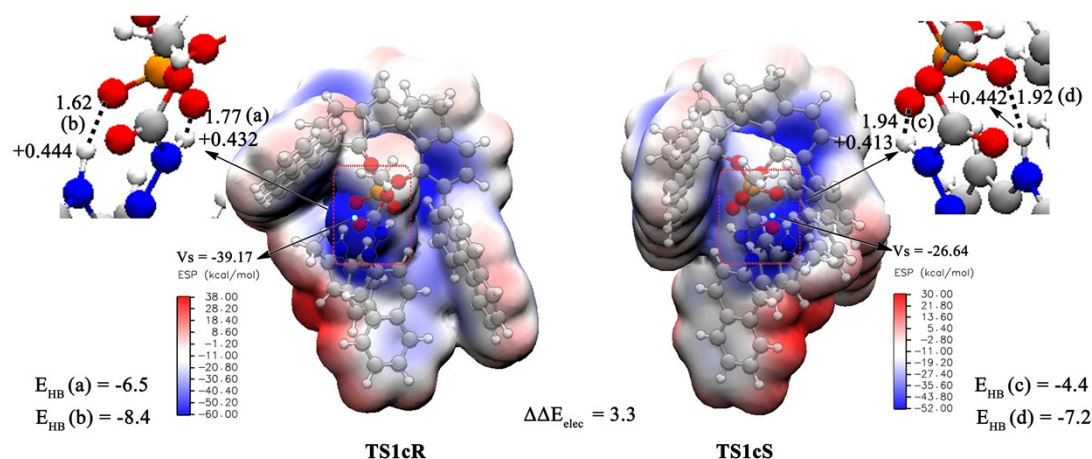


Figure S4. Electrostatic potentials on the monomers' van der Waals surface of **M1-TS1cR** (red = +38 kcal/mol; blue = -60 kcal/mol) catalyzed by **CPA-3**, and **M1-TS1cS** (red = +30 kcal/mol; blue = -52 kcal/mol) catalyzed by **CPA-3**. Red and blue regions represent positive and negative molecular electrostatic potential (MEP) values, respectively. The difference in electrostatic stabilization for **M1-TS1cR** and **M1-TS1cS** of the key N-H and P=O group ($\Delta E_{elec}(c)$ and $\Delta E_{elec}(d)$) is also shown in kilocalories per mole. The cyan spheres represent the position of MEP on the surface.

S1. Cartesian coordinates of optimized structures.**Conformer 1**

C	4.98496700	0.22884800	-0.00049700
C	4.66369200	-1.14956500	-0.00039200
C	3.34695100	-1.55321200	-0.00015800
C	2.29658300	-0.59667500	-0.00002000
C	2.62238100	0.80003400	-0.00012600
C	3.98695500	1.18115400	-0.00036600
C	0.93240400	-0.97553100	0.00021900
C	-0.07182500	-0.02231000	0.00035000
C	0.24999600	1.36778700	0.00024700
C	1.56298700	1.75693500	0.00001500
N	-1.38260200	-0.54203600	0.00059100
N	-2.29324900	0.32777700	0.00071600
C	-3.60267900	-0.29864500	0.00045400
O	-3.86639400	-1.47664200	-0.00011900
H	6.02722300	0.53604000	-0.00068100
H	5.46079400	-1.88755000	-0.00049700
H	3.09218200	-2.61004200	-0.00007700
H	4.23673200	2.23931700	-0.00044700
H	0.64938000	-2.02425800	0.00030400
H	-0.56042200	2.08740900	0.00035700
H	1.81983700	2.81363900	-0.00006500
O	-4.50323500	0.69848400	0.00010000
C	-5.87242800	0.26898600	-0.00063400
H	-6.08643700	-0.33005900	0.88883300
H	-6.46566300	1.18364900	-0.00084800
H	-6.08554400	-0.32989500	-0.89042600

Conformer 2

C	4.93109300	-0.07487800	0.00003600
C	4.47121200	-1.41341600	-0.00003800
C	3.12026200	-1.68131700	-0.00007900
C	2.17231500	-0.62307000	-0.00004700
C	2.63863900	0.73311500	0.00002800
C	4.03491100	0.97370900	0.00006900
C	0.77648300	-0.86104800	-0.00008800
C	-0.12491300	0.18966700	-0.00005600
C	0.33656300	1.53958500	0.00001900
C	1.68235300	1.79296100	0.00006000
N	-1.48446600	-0.18951900	-0.00010300
N	-2.29476500	0.77519800	-0.00007200
C	-3.68097000	0.37202700	-0.00002200
O	-4.55036800	1.21338200	-0.00008700
H	5.99917300	0.12461700	0.00006800
H	5.18916300	-2.22864300	-0.00006300
H	2.75973300	-2.70697000	-0.00013700
H	4.39056300	2.00109900	0.00012600
H	0.38939700	-1.87601400	-0.00014600
H	-0.39670500	2.33770400	0.00004100

H	2.04534200	2.81804800	0.00011600
O	-3.89389400	-0.95301000	0.00012000
C	-5.27847100	-1.33536100	0.00018000
H	-5.78313300	-0.94944000	-0.88966300
H	-5.27857800	-2.42570500	0.00028300
H	-5.78310200	-0.94927200	0.88996700

Conformer 3

C	4.77758900	0.94217200	0.00000000
C	3.95695700	2.09902800	0.00000000
C	2.58778900	1.97608500	0.00000000
C	1.97222800	0.69159600	0.00000000
C	2.80537700	-0.47997800	0.00000000
C	4.21528900	-0.31475000	0.00000000
C	0.56885500	0.53868500	0.00000000
C	0.00000000	-0.72746600	0.00000000
C	0.82350500	-1.88572900	0.00000000
C	2.19094100	-1.76242800	0.00000000
N	-1.39065300	-0.98796500	0.00000000
N	-2.12403900	0.03378400	0.00000000
C	-3.52767300	-0.33945900	0.00000000
O	-4.00464400	-1.44811700	0.00000000
H	5.85847100	1.05328800	0.00000000
H	4.41719800	3.08304100	0.00000000
H	1.95208800	2.85792200	0.00000000
H	4.84598000	-1.20035700	0.00000000
H	-0.07933900	1.40926900	0.00000000
H	0.33485000	-2.85480200	0.00000000
H	2.82342100	-2.64644100	0.00000000
O	-4.22680200	0.80762400	0.00000000
C	-5.65206400	0.64035900	0.00000000
H	-5.97318500	0.09158500	0.88967300
H	-6.06465400	1.64943000	0.00000000
H	-5.97318500	0.09158500	-0.88967300

Conformer 4

C	4.87666200	-0.21702100	0.00004100
C	4.29445800	-1.51028400	0.00009300
C	2.92723200	-1.65369200	0.00007600
C	2.07584400	-0.51193800	0.00000700
C	2.66752900	0.79840600	-0.00004600
C	4.08277700	0.90814500	-0.00002700
C	0.66940600	-0.63288700	-0.00001200
C	-0.13308700	0.49958300	-0.00008200
C	0.45137200	1.79491300	-0.00013600
C	1.81689600	1.93798900	-0.00011700
N	-1.54856400	0.48330100	-0.00010900
N	-2.06521600	-0.66412100	-0.00005400
C	-3.50957700	-0.65260400	0.00000200
O	-4.11698300	-1.69887500	-0.00003500
H	5.95869400	-0.11760600	0.00005500

H	4.93560900	-2.38721700	0.00014600
H	2.47359300	-2.64150600	0.00011600
H	4.53110500	1.89862000	-0.00006700
H	0.20128600	-1.61212900	0.00002500
H	-0.21412200	2.65233800	-0.00019000
H	2.26645500	2.92762800	-0.00015800
O	-4.07357800	0.56450700	0.00012100
C	-5.51013600	0.55813400	0.00018800
H	-5.89147300	0.05007400	0.89006400
H	-5.80491100	1.60784200	0.00026400
H	-5.89155600	0.05017900	-0.88971200

Conformer 5

C	4.82976800	0.32976300	0.07147600
C	4.55281900	-1.01617600	0.41041600
C	3.25207800	-1.46731800	0.44857500
C	2.17376600	-0.59211700	0.14972700
C	2.45471000	0.77140600	-0.19411000
C	3.80387800	1.20310700	-0.22408600
C	0.82453700	-1.02145300	0.17839400
C	-0.20681200	-0.14726700	-0.11673200
C	0.07009900	1.20869100	-0.45995700
C	1.36766500	1.64582300	-0.49557600
N	-1.50036800	-0.71267800	-0.05616000
N	-2.44362200	0.08926300	-0.27918000
C	-3.72994600	-0.56880400	-0.29856700
O	-3.96754200	-1.58458100	-0.89809800
H	5.85987800	0.67425000	0.04438400
H	5.37157700	-1.69215400	0.63985200
H	3.03188400	-2.49998000	0.70719400
H	4.01914700	2.23635800	-0.48500400
H	0.57681000	-2.04839000	0.43125700
H	-0.75892100	1.86784300	-0.69048500
H	1.59014800	2.67714500	-0.75910900
O	-4.69603800	0.12932100	0.32640600
C	-4.36745800	1.31395500	1.07045400
H	-3.64739300	1.09891400	1.86556500
H	-3.96686700	2.09221500	0.41615000
H	-5.31031900	1.64212400	1.51103200

Conformer 6

C	-4.82976800	0.32976300	0.07147500
C	-4.55281900	-1.01617600	0.41041600
C	-3.25207800	-1.46731800	0.44857500
C	-2.17376600	-0.59211700	0.14972700
C	-2.45471000	0.77140600	-0.19411000
C	-3.80387800	1.20310700	-0.22408600
C	-0.82453700	-1.02145300	0.17839400
C	0.20681200	-0.14726700	-0.11673200
C	-0.07009900	1.20869100	-0.45995700

C	-1.36766500	1.64582300	-0.49557600
N	1.50036800	-0.71267800	-0.05616000
N	2.44362200	0.08926300	-0.27918000
C	3.72994600	-0.56880400	-0.29856700
O	3.96754200	-1.58458100	-0.89809700
H	-5.85987800	0.67425000	0.04438400
H	-5.37157700	-1.69215400	0.63985200
H	-3.03188400	-2.49998000	0.70719400
H	-4.01914700	2.23635800	-0.48500400
H	-0.57681000	-2.04839000	0.43125700
H	0.75892100	1.86784300	-0.69048500
H	-1.59014800	2.67714500	-0.75910900
O	4.69603800	0.12932100	0.32640500
C	4.36745800	1.31395500	1.07045400
H	5.31031900	1.64212400	1.51103200
H	3.96686700	2.09221500	0.41615000
H	3.64739300	1.09891400	1.86556500

Conformer 7

C	-2.95733800	-3.85721200	0.00000000
C	-3.83448500	-2.74662200	0.00000000
C	-3.32918200	-1.46537300	0.00000000
C	-1.92634800	-1.24106400	0.00000000
C	-1.03780700	-2.36679800	0.00000000
C	-1.59034600	-3.67111600	0.00000000
C	-1.37196400	0.06156200	0.00000000
C	0.00000000	0.25307900	0.00000000
C	0.88506200	-0.86623000	0.00000000
C	0.37109500	-2.13531100	0.00000000
N	0.40615700	1.60191900	0.00000000
N	1.65159600	1.78566200	0.00000000
C	1.96878300	3.21136100	0.00000000
O	1.18194600	4.12092200	0.00000000
H	-3.36716800	-4.86347200	0.00000000
H	-4.90841100	-2.90954300	0.00000000
H	-3.99642800	-0.60721500	0.00000000
H	-0.91907800	-4.52631900	0.00000000
H	-2.01489100	0.93702400	0.00000000
H	1.95331900	-0.68432700	0.00000000
H	1.03695100	-2.99508500	0.00000000
O	3.29520700	3.43584900	0.00000000
C	4.24049500	2.35372500	0.00000000
H	4.13394400	1.73144400	0.89192400
H	4.13394400	1.73144400	-0.89192400
H	5.21853700	2.83880500	0.00000000

Conformer 8

C	4.67524800	-0.53979700	0.00756100
C	3.95537700	-1.70448100	-0.36223900
C	2.58385800	-1.67178400	-0.45047000

C	1.86502200	-0.47441500	-0.17203200
C	2.59603100	0.70581100	0.20120500
C	4.01172200	0.63503900	0.28166900
C	0.45637500	-0.41484300	-0.25145400
C	-0.21346100	0.76805300	0.02260300
C	0.50866600	1.93701600	0.38263400
C	1.87852500	1.90271300	0.47313400
N	-1.62028600	0.93580800	-0.04469400
N	-2.27823100	-0.11151700	-0.26428400
C	-3.69062000	0.14547400	-0.42577000
O	-4.14788500	0.97068900	-1.17208300
H	5.75910100	-0.57902800	0.07289600
H	4.49454400	-2.62291300	-0.57638500
H	2.02611900	-2.56070000	-0.73435300
H	4.56516900	1.52736000	0.56350600
H	-0.11288900	-1.29552100	-0.53220700
H	-0.05569900	2.84296100	0.57935900
H	2.43349000	2.79519200	0.75040600
O	-4.47263300	-0.71806100	0.24722900
C	-3.88761800	-1.65647000	1.16544100
H	-3.32860500	-1.14569300	1.95512300
H	-4.73317600	-2.18928000	1.60325300
H	-3.22903200	-2.35734700	0.64638400

Conformer 9

C	-4.67524800	-0.53979700	0.00755900
C	-3.95537700	-1.70448100	-0.36223900
C	-2.58385800	-1.67178400	-0.45046800
C	-1.86502200	-0.47441500	-0.17203100
C	-2.59603100	0.70581200	0.20120400
C	-4.01172200	0.63503900	0.28166600
C	-0.45637500	-0.41484400	-0.25145100
C	0.21346200	0.76805300	0.02260500
C	-0.50866600	1.93701700	0.38263500
C	-1.87852500	1.90271400	0.47313200
N	1.62028700	0.93580800	-0.04468900
N	2.27823100	-0.11151600	-0.26428600
C	3.69062000	0.14547500	-0.42576900
O	4.14788600	0.97069400	-1.17207900
H	-5.75910100	-0.57902800	0.07289200
H	-4.49454300	-2.62291400	-0.57638400
H	-2.02611900	-2.56070100	-0.73434900
H	-4.56516900	1.52736100	0.56350100
H	0.11288900	-1.29552200	-0.53220200
H	0.05569800	2.84296100	0.57936000
H	-2.43349100	2.79519300	0.75040300
O	4.47263200	-0.71806300	0.24722600
C	3.88761700	-1.65647400	1.16543600
H	3.32860400	-1.14569800	1.95512000
H	3.22903000	-2.35734900	0.64637800

H	4.73317400	-2.18928500	1.60324700
Conformer 10			
C	4.66684600	0.60177700	-0.00001800
C	3.90557800	1.79855300	-0.00001800
C	2.53205000	1.74481900	-0.00001200
C	1.85256100	0.49289100	-0.00000500
C	2.62578300	-0.71938500	-0.00000500
C	4.04212200	-0.62530700	-0.00001100
C	0.44371200	0.41003600	0.00000100
C	-0.18912700	-0.82587900	0.00000800
C	0.57599600	-2.02401900	0.00000900
C	1.94776900	-1.96927700	0.00000200
N	-1.58888400	-1.02129300	0.00001500
N	-2.28412900	0.02609900	0.00001600
C	-3.71053900	-0.29563000	-0.00001500
O	-4.19580400	-1.39563100	-0.00006800
H	5.75189900	0.65827900	-0.00002200
H	4.41474200	2.75812400	-0.00002400
H	1.94225300	2.65805900	-0.00001300
H	4.62752200	-1.54136100	-0.00001000
H	-0.15738900	1.31360900	0.00000000
H	0.03922400	-2.96720600	0.00001400
H	2.53478600	-2.88401500	0.00000300
O	-4.47970000	0.80772900	0.00000800
C	-3.90592400	2.12515700	0.00007300
H	-3.29801300	2.29505600	0.89208800
H	-3.29798500	2.29513200	-0.89190800
H	-4.76286700	2.80146800	0.00008900
2a			
C	-0.54268400	-0.86911200	0.00005400
C	-0.31199000	0.53409000	-0.00009300
C	-1.41919400	1.39991900	-0.00032700
C	-2.70059800	0.86100600	-0.00041200
C	-2.90378000	-0.53376600	-0.00026400
C	-1.82864900	-1.41687300	-0.00001900
C	1.69489000	-0.51291300	-0.00002200
C	1.11506900	0.73613100	0.00023100
H	-1.27579800	2.47769000	-0.00038200
H	-3.56244700	1.52313000	-0.00055100
H	-3.91688300	-0.92683400	-0.00030400
H	-1.98516900	-2.49286900	0.00012400
N	0.69492500	-1.47733000	0.00031700
H	0.85798800	-2.47214600	0.00051400
C	1.82311700	2.05805700	0.00048100
H	1.56370200	2.65935900	-0.88136700
H	1.56352300	2.65920100	0.88239000
H	2.91097800	1.93203800	0.00057300
C	3.13989600	-0.91418400	-0.00010900

H	3.66732600	-0.53473500	-0.88370500
H	3.66781200	-0.53309700	0.88248000
H	3.24803600	-2.00455600	0.00088400
2b			
C	-1.23473600	-0.64330700	0.00004900
C	-1.27603700	0.77825600	0.00002300
C	-2.52751500	1.41782700	-0.00003900
C	-3.68227400	0.64468000	-0.00007900
C	-3.61604000	-0.76341900	-0.00005400
C	-2.39300800	-1.42631500	0.00001500
C	0.90366100	0.12535400	-0.00002400
C	0.08694100	1.23173200	0.00015700
H	-2.58980600	2.50330900	-0.00002700
H	-4.65447100	1.13036000	-0.00010900
H	-4.53591100	-1.34193800	-0.00007700
H	-2.34246800	-2.51242100	0.00003900
N	0.09665800	-1.00816300	0.00010700
H	0.43473200	-1.95755800	0.00013700
H	0.41718300	2.26071700	0.00024200
C	2.41376900	0.00146600	-0.00004000
C	2.87869400	-0.76266300	1.26286700
C	2.87870600	-0.76269400	-1.26292600
C	3.05429100	1.40126500	-0.00005300
H	2.56681800	-0.23962900	2.17326700
H	2.46522900	-1.77754200	1.30314500
H	3.97155300	-0.85189200	1.27468800
H	2.56669800	-0.23977600	-2.17334700
H	3.97157600	-0.85177300	-1.27481400
H	2.46540300	-1.77764400	-1.30310200
H	4.14663700	1.31402900	-0.00003000
H	2.76076800	1.97288500	-0.88718100
H	2.76074200	1.97291500	0.88704600
2c			
C	0.20932000	-0.65889600	0.00005800
C	0.23350600	0.76416700	0.00002700
C	1.47775300	1.41743900	-0.00013800
C	2.64160000	0.65777000	-0.00026100
C	2.59201800	-0.75071800	-0.00022100
C	1.37653000	-1.42770800	-0.00005400
C	-1.93326200	0.08380700	0.00002800
C	-1.13535700	1.20080400	0.00036000
H	1.52751000	2.50351900	-0.00010700
H	3.60796800	1.15492500	-0.00034900
H	3.51851400	-1.31854400	-0.00029600
H	1.33847300	-2.51431200	-0.00001100
H	-1.49056400	2.22282500	0.00056200
N	-1.11868300	-1.04059400	0.00023200
H	-1.45083500	-1.99272600	0.00031900

C	-3.42237400	-0.04479300	-0.00005400
H	-3.78661600	-0.58407100	-0.88510700
H	-3.78666900	-0.58429800	0.88483600
H	-3.88540000	0.94560600	0.00006400

CPA-1

P	0.00674000	-1.45692300	-0.00066300
O	0.47450600	-2.46856600	-0.96059100
O	-1.06706000	-0.44494900	-0.69032000
O	1.06725900	-0.44629700	0.69438500
C	-1.53403000	0.64903800	0.03563000
C	-0.68121300	1.71562300	0.27311000
C	1.54167800	0.63264000	-0.05378200
C	0.69717200	1.70483900	-0.29972400
C	-1.15711600	2.78959300	1.10388500
C	-2.17623200	4.85777100	2.75270700
C	-0.32346600	3.85213100	1.55047300
C	-2.52140500	2.77473400	1.54307200
C	-3.00545700	3.83458900	2.35664700
C	-0.81926500	4.85573400	2.35314300
H	0.72097400	3.86231800	1.26165800
H	-4.04607300	3.81208500	2.67106100
H	-0.15908200	5.65159500	2.68693900
H	-2.55536800	5.65942100	3.38030700
C	1.17958800	2.76399300	-1.14561900
C	2.21177200	4.80093200	-2.82509500
C	0.35431100	3.82883300	-1.60270500
C	2.54175400	2.73053900	-1.58970300
C	3.03259900	3.77497900	-2.41910700
C	0.85646500	4.81722600	-2.42008200
H	-0.68905900	3.85296000	-1.31088600
H	4.07152000	3.73782000	-2.73752600
H	0.20254100	5.61495700	-2.76173700
H	2.59592000	5.59055900	-3.46479100
C	-3.36338000	1.69440400	1.17466800
H	-4.40253200	1.70730000	1.49324600
C	-2.89572900	0.61990000	0.44798600
C	3.37441700	1.64717800	-1.21069300
H	4.41199400	1.64490000	-1.53423500
C	2.90126300	0.58568500	-0.46827600
O	-0.65935400	-1.99195700	1.36190900
H	-1.11310200	-2.83952000	1.22030100
C	-3.79640900	-0.51943000	0.08233700
C	-4.31612200	-0.60177100	-1.23129300
C	-4.14711000	-1.48750900	1.05278500
C	-4.00921400	0.36016400	-2.24611000
C	-5.20498600	-1.68619700	-1.57996200
C	-5.04071200	-2.56634800	0.69084700
C	-3.64469400	-1.46236600	2.39556600
C	-4.53100200	0.25402800	-3.50870400

H	-3.35150900	1.18738600	-2.00289200
C	-5.72648600	-1.76059500	-2.90926500
C	-5.54192400	-2.63619700	-0.61165100
C	-5.39050100	-3.54316300	1.67567100
H	-2.96143000	-0.67241200	2.68442100
C	-4.00180200	-2.42191700	3.30727600
C	-5.40042900	-0.82107500	-3.84942400
H	-4.27977800	0.99684600	-4.26091700
H	-6.39170800	-2.58480600	-3.15549200
H	-6.21241000	-3.45056200	-0.87879900
C	-4.88937400	-3.47674800	2.94749300
H	-6.06611500	-4.34464800	1.38627400
H	-3.60323200	-2.37978700	4.31733900
H	-5.80265200	-0.88900700	-4.85646200
H	-5.16228000	-4.22587700	3.68569500
C	3.79862300	-0.55346700	-0.09571700
C	4.11295600	-1.54620900	-1.05179200
C	4.35776000	-0.60218100	1.20250300
C	3.55842100	-1.55704200	-2.37218400
C	5.02511200	-2.61028300	-0.69579600
C	5.25908000	-1.67714900	1.54826400
C	4.08129000	0.38334300	2.20354200
C	3.89393400	-2.53036300	-3.27553300
H	2.84950300	-0.78547900	-2.64969200
C	5.35036700	-3.60434200	-1.67088600
C	5.56962800	-2.64687300	0.59053400
C	5.82149200	-1.71884000	2.86224400
H	3.41503100	1.20436600	1.96127300
C	4.64145800	0.30768500	3.45203000
C	4.80601400	-3.56672000	-2.92576700
H	3.45160600	-2.52031500	-4.26783900
H	6.04119600	-4.39516700	-1.38795200
H	6.25373300	-3.45127100	0.85379300
C	5.52314200	-0.75817200	3.79053100
H	6.49626100	-2.53594800	3.10679100
H	4.41229600	1.06798000	4.19397900
H	5.05918900	-4.32945400	-3.65717500
H	5.95721300	-0.80195500	4.78574300
CPA-2			
P	0.04875300	-1.42175700	-0.02751600
O	0.65932900	-2.38662700	-0.95598200
O	-0.99637700	-0.41844200	-0.76116900
O	1.01319500	-0.39729500	0.78248600
C	-1.51810600	0.66605400	-0.05500400
C	-0.69989300	1.74138800	0.24655000
C	1.53826400	0.68175000	0.06720500
C	0.71154800	1.74916600	-0.23622900
C	-1.23503900	2.79276400	1.06884900
C	-2.36563000	4.80968900	2.70724500
C	-0.44296400	3.86382400	1.56619600

C	-2.61548700	2.74215100	1.45092200
C	-3.15614300	3.77674400	2.26144100
C	-0.99376400	4.84275400	2.36355100
H	0.61260400	3.89929200	1.32392700
H	-4.20740500	3.72648300	2.53373700
H	-0.36531800	5.64600100	2.73800800
H	-2.78647100	5.59193600	3.33243400
C	1.23754300	2.80319500	-1.06061600
C	2.35458700	4.82501800	-2.70144100
C	0.43896300	3.87000600	-1.55637400
C	2.61747400	2.75856000	-1.44572900
C	3.15103300	3.79574900	-2.25770600
C	0.98333300	4.85166200	-2.35478300
H	-0.61629700	3.90031100	-1.31197500
H	4.20165800	3.75011400	-2.53313400
H	0.35026500	5.65185500	-2.72800000
H	2.77025400	5.60910500	-3.32778400
C	-3.41704600	1.65191200	1.03308000
H	-4.46506400	1.63382700	1.31708500
C	-2.89348300	0.60832800	0.30010800
C	3.42523900	1.67070900	-1.03309400
H	4.47051600	1.65489300	-1.32677700
C	2.91092200	0.62449700	-0.29684500
O	-0.74968600	-2.05323500	1.21898700
H	-0.76838700	-3.02144700	1.13881400
C	-3.73604400	-0.54662100	-0.10114200
C	3.75357700	-0.53640700	0.08548000
C	5.36052600	-2.74237400	0.80134500
C	-4.43674200	-1.30245200	0.84563300
C	-5.24183000	-2.37878400	0.48197000
C	-5.36281500	-2.72441000	-0.86140000
C	-4.68171900	-1.99009000	-1.82963200
C	-3.88715100	-0.91439800	-1.44360200
F	-4.34319300	-1.00457400	2.14992300
F	-5.89324900	-3.08395300	1.41464700
F	-6.13270300	-3.75451300	-1.22061900
F	-4.80913900	-2.31124600	-3.12127400
F	-3.27027100	-0.21277900	-2.40120700
C	4.44284800	-1.28279000	-0.87721400
C	5.23867400	-2.37271900	-0.53521400
C	4.69074700	-2.01789700	1.78456800
C	3.90621000	-0.92804800	1.42047700
F	4.34764600	-0.96038500	-2.17443700
F	5.88193300	-3.06618700	-1.48100300
F	6.12235500	-3.78524000	1.14120600
F	4.81931900	-2.36272500	3.07127700
F	3.29895500	-0.23671000	2.39374000

CPA-3

C	-1.12058800	4.68208400	-2.36147700
C	0.24016300	4.38612900	-1.69525400
C	-0.11774600	3.58834000	-0.39521000
C	-1.33029600	2.80270700	-0.88773200
C	-1.95151600	3.48820700	-1.94474600
C	-0.49713000	4.58880700	0.74779100
C	0.85839500	5.04224800	1.33409600
C	1.73274500	3.82680700	1.11272800
C	1.12200600	2.93938900	0.21456900
C	-1.88195500	1.60224400	-0.44896600
C	-3.09522700	1.11715200	-0.97438800
C	-3.71716200	1.85875500	-1.98979400
C	-3.14474000	3.02828800	-2.49166900
C	2.96147000	3.51780900	1.68812000
C	3.57757100	2.30752100	1.37047200
C	2.96604000	1.36463700	0.52669500
C	1.71606700	1.70168900	-0.02316700
O	-1.21345000	0.83881300	0.50901700
O	1.01642500	0.75882200	-0.79222300
P	-0.01555700	-0.17422100	0.04573000
O	0.49877200	-0.90927800	1.21157200
O	-0.58028200	-0.99259300	-1.21445000
H	-1.04689100	4.78299100	-3.45011500
H	-1.55475400	5.61946400	-1.98595800
H	0.82714600	5.28551100	-1.48478200
H	0.83878100	3.74206000	-2.34928700
H	-1.06893400	4.05062000	1.51240300
H	-1.11577800	5.41720000	0.38830200
H	1.25080600	5.91966400	0.80092900
H	0.78825500	5.32228600	2.39125400
H	-4.65294200	1.49115200	-2.40080100
H	-3.62343100	3.56303000	-3.30803900
H	3.43984500	4.20701100	2.37952400
H	4.54591000	2.06609100	1.79853600
H	-1.40099300	-1.47174600	-0.99446900
C	3.66247300	0.08727100	0.19149600
C	3.98554000	-0.16395500	-1.11245100
C	4.06143000	-0.85508000	1.22077600
C	4.74305600	-1.30956800	-1.51173400
H	3.68184500	0.53807600	-1.88453800
C	4.84559000	-1.99751500	0.86751700
C	3.66866300	-0.68563300	2.57021500
C	5.06179300	-1.52141100	-2.87405800
C	5.20155700	-2.22949000	-0.52609700
C	5.23708700	-2.88330800	1.89898000
H	3.02332000	0.14585300	2.82708300
C	4.06167300	-1.57443200	3.55095900
C	5.81437300	-2.60956300	-3.26751300
H	4.70005000	-0.80659900	-3.60959200
C	5.97387600	-3.33239900	-0.96093500

C	4.86389200	-2.67765800	3.21337300
H	5.83832900	-3.75376000	1.66053500
H	3.73951700	-1.42633500	4.57802000
C	6.27420400	-3.52079400	-2.29804500
H	6.05162800	-2.76288700	-4.31680200
H	6.34238500	-4.05453700	-0.24065400
H	5.17923600	-3.37945100	3.98097800
H	6.86858400	-4.37912500	-2.59989700
C	-3.68554900	-0.18593400	-0.54022800
C	-4.20344100	-0.38554400	0.80083700
C	-3.78082900	-1.20156300	-1.45552700
C	-4.17901400	0.65554200	1.75861600
C	-4.77691300	-1.64552800	1.15887000
C	-4.34893900	-2.47886500	-1.13779800
H	-3.41077800	-1.04264200	-2.46629700
C	-4.68192300	0.47307700	3.03113400
H	-3.75965400	1.61527300	1.47848300
C	-5.27913400	-1.79907800	2.47242800
C	-4.84224000	-2.72020700	0.17615200
C	-4.41143400	-3.50091600	-2.11409200
C	-5.23305100	-0.76842900	3.39168300
H	-4.65100900	1.28682300	3.75019700
H	-5.71784400	-2.74359400	2.77389200
C	-5.37850500	-3.99950700	0.45418800
H	-4.02882500	-3.29413400	-3.11088900
C	-4.94390900	-4.73815900	-1.81218500
H	-5.62780600	-0.91982000	4.39261200
C	-5.42905300	-4.98582500	-0.51438100
H	-5.75864100	-4.22577700	1.44409400
H	-4.98640300	-5.51669800	-2.56866100
H	-5.84554500	-5.95885900	-0.26880100

M1-TS1aR

P	-0.61167400	-0.07954700	-0.29276500
O	-0.98661700	1.30541600	0.57355900
O	-2.13854900	-0.64640900	-0.62142400
C	-1.96639500	2.14288600	0.07555800
C	-3.29647000	1.75182500	0.17147500
C	-3.04473200	-0.70583300	0.42197600
C	-3.63022800	0.47414900	0.86282200
C	-4.30873900	2.57323100	-0.43140100
C	-6.23685200	4.25197000	-1.65850800
C	-5.67458700	2.18306300	-0.52054700
C	-3.93051700	3.82771700	-1.00938900
C	-4.92220500	4.65259200	-1.60582500
C	-6.61003100	2.99857700	-1.11782200
H	-5.97614000	1.22237000	-0.11959800
H	-4.61619100	5.60596800	-2.03034200
H	-7.64528200	2.67350300	-1.17892200
H	-6.98643100	4.88761000	-2.12194700

C	-4.50787700	0.43479500	1.99924800
C	-6.22023000	0.25915400	4.25276800
C	-5.03661400	1.60389200	2.61513900
C	-4.84039100	-0.83440400	2.57308000
C	-5.71151900	-0.89021300	3.69444000
C	-5.86748300	1.51759300	3.71025200
H	-4.77006300	2.57648900	2.21792600
H	-5.95990000	-1.86436400	4.10926500
H	-6.25254400	2.42633300	4.16536500
H	-6.88141800	0.20555600	5.11339500
C	-2.56930400	4.21934500	-0.97932100
H	-2.29615700	5.19026800	-1.38514300
C	-1.58106800	3.40542900	-0.46425900
C	-4.28493000	-2.01233000	2.01495700
H	-4.56652800	-2.97368200	2.43742000
C	-3.38837800	-1.97876200	0.96653600
O	0.02219300	0.30693800	-1.60624900
C	-0.16932700	3.90637000	-0.43483700
C	0.33835100	4.47023000	0.76017300
C	0.61051800	3.91730600	-1.61467100
C	-0.40678200	4.48504900	1.98350700
C	1.65334400	5.06950700	0.76656400
C	1.92092000	4.52984300	-1.59816500
C	0.15849400	3.33674000	-2.84426400
C	0.11041200	5.03787600	3.12615100
H	-1.39756200	4.04478300	1.99753100
C	2.15333500	5.63962500	1.97889200
C	2.40458600	5.08850200	-0.41195500
C	2.69159800	4.55682700	-2.80315300
H	-0.80130100	2.83539500	-2.86178100
C	0.92988900	3.38223100	-3.97647100
C	1.40839900	5.62478500	3.12737300
H	-0.47513200	5.03255300	4.04163700
H	3.14479900	6.08643500	1.96612800
H	3.38977700	5.55089100	-0.40576500
C	2.21101400	4.00702500	-3.96128800
H	3.66973800	5.03209700	-2.77783100
H	0.56429400	2.93317000	-4.89598000
H	1.80027900	6.06214800	4.04186700
H	2.80322500	4.04187500	-4.87220900
C	-2.85983700	-3.26763000	0.41570700
C	-1.82369000	-3.95898800	1.08392000
C	-3.47498900	-3.83436500	-0.72468700
C	-1.17212000	-3.43713200	2.24805100
C	-1.39279500	-5.24828500	0.59066600
C	-3.02750200	-5.11775500	-1.21541600
C	-4.54959900	-3.19230000	-1.42150600
C	-0.18807100	-4.14495100	2.88744800
H	-1.45581500	-2.45628200	2.60867300
C	-0.35811700	-5.95016100	1.28570000

C	-2.00007400	-5.78826900	-0.54588800
C	-3.65701500	-5.67954100	-2.37013200
H	-4.90549000	-2.23255700	-1.06303000
C	-5.12897000	-3.76622000	-2.52413300
C	0.22474400	-5.42055400	2.40491300
H	0.28906300	-3.72705100	3.77008200
H	-0.04757300	-6.91969100	0.90304900
H	-1.67165500	-6.75855400	-0.91344300
C	-4.67688100	-5.02688500	-3.00947300
H	-3.30629600	-6.64475800	-2.72836900
H	-5.94233700	-3.25695100	-3.03427600
H	1.00694700	-5.96615700	2.92632600
H	-5.14725700	-5.46666600	-3.88487200
C	3.16366200	1.08304800	0.23997600
C	4.55901300	0.89818500	0.27982800
C	5.26267800	1.21432900	1.44044500
C	4.54327700	1.68514100	2.54413300
C	3.15054900	1.82678500	2.49301700
C	2.42993000	1.52752500	1.33292400
C	3.75710400	0.39805800	-1.82528400
C	4.95810500	0.32333900	-1.01422700
H	6.34094500	1.09679200	1.49310200
H	5.07391000	1.94421600	3.45634700
H	2.61471300	2.19231300	3.36359900
H	1.35353600	1.64122800	1.29498900
N	2.73059500	0.75632400	-1.05899500
H	1.72342600	0.70565600	-1.34635800
C	6.32750600	0.55049200	-1.60334700
H	6.46805800	1.61007900	-1.85147500
H	7.11044300	0.27735000	-0.89035400
H	6.48483300	-0.03099200	-2.51796500
C	7.80831000	-2.34443400	2.48378800
C	8.22565000	-2.27810600	1.14770400
C	7.28609600	-2.09554700	0.13892400
C	5.91621800	-1.97492800	0.43875300
C	5.48972200	-2.08442200	1.79244200
C	6.45686800	-2.25613700	2.79803000
C	4.91267600	-1.77573700	-0.60076300
C	3.52879300	-2.12504600	-0.26562100
C	3.12443800	-2.12646900	1.13068900
C	4.07085800	-2.09134000	2.09847000
N	2.79911700	-2.39459800	-1.32256200
N	1.49776600	-2.63371600	-1.24738500
C	0.83673800	-2.68706200	-2.48958700
O	1.38329000	-2.63285500	-3.56937600
H	8.54005600	-2.48303400	3.27497300
H	9.27826300	-2.37661400	0.89856200
H	7.60599100	-2.06618100	-0.89911800
H	6.13145800	-2.33696000	3.83221400
H	5.20291300	-2.04063200	-1.61320900

H	2.07084500	-2.16031300	1.38526000
H	3.77893700	-2.11309100	3.14517600
O	-0.47572200	-2.80955200	-2.27073100
C	-1.29894800	-2.61683900	-3.43622300
H	-1.05352300	-3.35824700	-4.20003500
H	-2.32228700	-2.73562500	-3.08854400
H	-1.14063100	-1.60931700	-3.82736100
C	3.57177300	0.03139400	-3.25421400
H	4.52329500	0.04260000	-3.79135200
H	3.13329000	-0.97522900	-3.33395300
H	2.88203100	0.72974800	-3.73842900
O	0.11839500	-0.98922500	0.65537700
H	0.93751900	-2.32655800	-0.43077200

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P	-0.57414100	-0.13051800	-0.11813700
O	0.02747700	0.58868400	-1.30097300
O	-1.28873400	-1.48305600	-0.76019100
O	-1.90661100	0.68530700	0.44495600
C	-2.24545500	-2.14579200	-0.01959500
C	-3.51053600	-1.58592100	0.11000200
C	-3.01439800	0.80572700	-0.36632300
C	-3.82130400	-0.30406600	-0.58646600
C	-4.47299900	-2.24250100	0.95226000
C	-6.30371900	-3.60514200	2.63780900
C	-5.73676200	-1.67517500	1.27936800
C	-4.13898200	-3.51029300	1.52982500
C	-5.08307300	-4.17415100	2.35913400
C	-6.62453600	-2.33697700	2.09861900
H	-5.99680400	-0.70063100	0.88316200
H	-4.81346900	-5.14035200	2.77934000
H	-7.57987900	-1.87713400	2.33743200
H	-7.01591800	-4.11873800	3.27787800
C	-4.91889200	-0.18664800	-1.50674500
C	-7.06072700	0.13569800	-3.33827200
C	-5.70099700	-1.29814500	-1.92888200
C	-5.22459700	1.09767700	-2.06314200
C	-6.31302500	1.22886700	-2.96746500
C	-6.73982400	-1.14109100	-2.81965200
H	-5.46361700	-2.28498900	-1.54876500
H	-6.53547000	2.21431400	-3.37018600
H	-7.31605900	-2.00839900	-3.13094600
H	-7.88725600	0.24629000	-4.03491600
C	-2.86468000	-4.07483000	1.27432900
H	-2.63088800	-5.04962500	1.69494900
C	-1.90836000	-3.41757600	0.52828300
C	-4.42684100	2.21405400	-1.70937900
H	-4.68602400	3.19033500	-2.11129900
C	-3.32302200	2.09490500	-0.89008900

O	0.23920500	-0.47493600	1.09572800
H	1.56655600	0.29789700	1.99182200
C	2.89007700	2.81203600	-0.57945100
C	4.29080700	2.86540900	-0.68782900
C	4.98032900	3.92248900	-0.09068700
C	4.24698100	4.89508300	0.59028700
C	2.84892400	4.81551000	0.68584500
C	2.14093900	3.76747900	0.09813800
C	3.46904500	1.04960100	-1.84609500
C	4.71934700	1.65654400	-1.40653600
H	6.06315800	3.99495000	-0.15378600
H	4.76617900	5.72658800	1.05785700
H	2.30553000	5.58210200	1.22980600
H	1.06015500	3.70412300	0.15936300
N	2.44593900	1.68528400	-1.29243800
H	1.44668500	1.32823600	-1.31719100
C	3.26833900	-0.07207000	-2.80566200
C	7.42556400	-2.90238100	-1.27012700
C	8.07327000	-1.68722000	-1.00879600
C	7.34661000	-0.60667300	-0.52103300
C	5.96498000	-0.71384100	-0.27909900
C	5.31933900	-1.96294600	-0.49660000
C	6.06655000	-3.03777200	-1.01121900
C	5.18007600	0.41351700	0.22305300
C	3.91741100	0.09686700	0.89917000
C	3.25657900	-1.15356800	0.56089900
C	3.92981000	-2.11739100	-0.11483500
N	3.51761100	1.00567300	1.76257300
N	2.33610200	0.89160200	2.36235900
C	2.00241700	1.86531300	3.31104500
O	2.73456100	2.72043600	3.75121500
H	7.98966000	-3.74562400	-1.65912800
H	9.14069300	-1.58901300	-1.18418800
H	7.85048400	0.33255900	-0.30875300
H	5.56905800	-3.98898700	-1.18292100
H	5.74357000	1.21180500	0.69626000
H	2.23391700	-1.32699800	0.87783300
H	3.44213400	-3.06476700	-0.32885300
O	0.71728600	1.66254400	3.66653700
C	0.19499400	2.59956200	4.61649400
H	0.80147400	2.60636400	5.52628300
H	0.17169000	3.60607400	4.18966400
H	-0.81888400	2.25967500	4.82730700
H	2.26488800	-0.49272200	-2.70309900
H	4.01473300	-0.85753100	-2.66529600
H	3.37966200	0.30568200	-3.83210600
C	5.93838800	1.65280500	-2.29572500
H	5.77859000	2.31142300	-3.15897500
H	6.81909300	2.02581000	-1.76313200
H	6.17357200	0.65314800	-2.66983800

C	-2.51807400	3.31037500	-0.55165800
C	-1.71912300	3.92342700	-1.54594300
C	-2.62929300	3.89427600	0.73324500
C	-1.05739300	5.17711000	-1.25864200
C	-1.52017200	3.34585800	-2.84240800
C	-1.93889700	5.13187800	1.01777700
C	-3.42345600	3.32000700	1.77715600
C	-0.28133300	5.80610100	-2.28280500
C	-1.18461600	5.74539600	0.01245100
C	-0.76153800	3.97766900	-3.79246200
H	-1.96322100	2.38066900	-3.05635200
C	-2.05959800	5.71427700	2.31887300
C	-3.51463800	3.90964800	3.01086800
H	-3.95921300	2.39838600	1.58047300
C	-0.14207800	5.23061600	-3.51659900
H	0.20026700	6.75404500	-2.05440600
H	-0.68721300	6.69023500	0.22397400
H	-0.62217500	3.51519000	-4.76598400
H	-1.53437400	6.64604900	2.51655000
C	-2.82207100	5.12276600	3.29017800
H	-4.12407100	3.45091500	3.78491300
H	0.45021500	5.71940300	-4.28572200
H	-2.90935400	5.57882800	4.27288300
C	-0.57998600	-4.06783200	0.29360200
C	-0.30544700	-4.67188800	-0.95650700
C	0.35537600	-4.15950400	1.35090400
C	0.92825700	-5.40160300	-1.14195100
C	-1.21614800	-4.61208500	-2.05965800
C	1.57662000	-4.91117100	1.16113900
C	0.15283000	-3.52402600	2.61916000
C	1.19039000	-6.01605400	-2.40648400
C	1.82841500	-5.51087900	-0.07689900
C	-0.92702700	-5.21336200	-3.25660500
H	-2.15037500	-4.07576000	-1.93771200
C	2.50044700	-5.02456000	2.24768000
C	1.06895900	-3.64877300	3.63027400
H	-0.73179200	-2.91550000	2.76141600
C	0.29328600	-5.92521400	-3.43635900
H	2.12218900	-6.56390700	-2.52923900
H	2.74236500	-6.08732700	-0.21160900
H	-1.63451700	-5.14840000	-4.07882100
H	3.40781400	-5.60440800	2.09375100
C	2.25464600	-4.41729000	3.44915900
H	0.89619600	-3.14828700	4.57906400
H	0.50468200	-6.39793300	-4.39189700
H	2.96615300	-4.50883800	4.26551900

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P	0.62501500	0.00144900	0.02184400
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O	0.22269300	-0.84496100	-1.15889000
O	0.95775600	1.49614700	-0.62754800
O	2.13210600	-0.44901500	0.55440300
C	1.73799100	2.37908500	0.08822500
C	3.10423800	2.14688700	0.18942500
C	3.20490500	-0.29159300	-0.29946500
C	3.70393100	0.98495500	-0.52847000
C	3.89463900	3.02296900	1.00925500
C	5.37537700	4.80274000	2.64770300
C	5.26523400	2.78234300	1.30712100
C	3.27464200	4.17612400	1.59092100
C	4.04714800	5.05600100	2.39636400
C	5.98323500	3.64632000	2.10408900
H	5.74464800	1.89648900	0.90679300
H	3.56045900	5.93132700	2.82026800
H	7.02677600	3.43457900	2.32170400
H	5.95529500	5.47905600	3.26977000
C	4.75973400	1.15312700	-1.48913400
C	6.83621000	1.38973000	-3.40720700
C	5.22845000	2.42798700	-1.91448800
C	5.34640200	-0.00937500	-2.08600300
C	6.39464100	0.14195100	-3.03354400
C	6.23571800	2.54195000	-2.84707900
H	4.77397200	3.32169700	-1.50295200
H	6.83369700	-0.75353200	-3.46727600
H	6.56916500	3.52804700	-3.15951100
H	7.63421100	1.49411400	-4.13727600
C	1.89711600	4.41375100	1.35864700
H	1.44362400	5.30910100	1.77641600
C	1.11377600	3.53751200	0.63552500
C	4.86022100	-1.29170500	-1.72878400
H	5.33251100	-2.16933600	-2.16324700
C	3.79684300	-1.45832700	-0.86597000
O	-0.24385300	0.13620100	1.23952800
H	-1.14993300	-1.11746400	2.07259000
C	-3.00603300	-0.64669000	-2.05054400
C	-4.34837700	-1.06338200	-2.02093400
C	-5.34203000	-0.18332600	-2.44656800
C	-4.95860400	1.09614900	-2.86527000
C	-3.61552300	1.49808500	-2.85201600
C	-2.60442100	0.62383700	-2.44134500
C	-2.95347800	-2.79269500	-1.37729500
C	-4.36562600	-2.43156300	-1.46837900
H	-6.38848400	-0.47347300	-2.44960600
H	-5.71954700	1.79433600	-3.20336100
H	-3.35077500	2.50362900	-3.16463400
H	-1.55986900	0.91542300	-2.41745000
N	-2.20929200	-1.72965100	-1.64234300
H	-1.17724400	-1.58990500	-1.46331500
C	-2.36961300	-4.07995600	-0.92237900

C	-8.35997100	0.10433100	0.69374500
C	-8.42955800	-1.28577300	0.53832100
C	-7.25856100	-2.03763400	0.50476900
C	-6.00127400	-1.42041900	0.62536000
C	-5.93313200	-0.01376600	0.82171400
C	-7.12569100	0.72872400	0.84025800
C	-4.75317400	-2.18428500	0.58068500
C	-3.58585200	-1.56410600	1.22525900
C	-3.52124000	-0.11096400	1.27941500
C	-4.64627000	0.61317900	1.07064300
N	-2.73990400	-2.42810800	1.73745400
N	-1.60404900	-2.02595700	2.30421600
C	-0.79264100	-3.03064500	2.84424100
O	-1.05764600	-4.21181800	2.88256700
H	-9.27192100	0.69463500	0.71744000
H	-9.39372500	-1.77875000	0.45320800
H	-7.31309200	-3.11876500	0.41001300
H	-7.07284900	1.80425600	0.98934700
H	-4.83685700	-3.25032300	0.77541000
H	-2.58328700	0.38017200	1.51668000
H	-4.61162900	1.69607000	1.14908900
O	0.32010700	-2.45002500	3.32452300
C	1.28646400	-3.35295400	3.88204700
H	0.89365300	-3.81481000	4.79288000
H	1.54477200	-4.13156200	3.16259900
H	2.15902000	-2.74007200	4.10425800
H	-1.34322500	-4.19835200	-1.28025700
H	-2.96853200	-4.92716900	-1.26947400
H	-2.35385400	-4.10593700	0.17958300
C	-5.40205000	-3.44005000	-1.90548400
H	-5.31854500	-4.38302800	-1.35497900
H	-6.41206200	-3.04804700	-1.75634000
H	-5.29419400	-3.66286900	-2.97437200
C	3.33953500	-2.84299500	-0.52092900
C	2.53492000	-3.57355600	-1.42503200
C	3.80654700	-3.45083800	0.66835400
C	2.19792700	-4.94870700	-1.13053500
C	2.03178800	-3.00701300	-2.64083900
C	3.46671100	-4.82732500	0.94949200
C	4.63650300	-2.76347900	1.61179300
C	1.39685200	-5.68399700	-2.06069700
C	2.67070700	-5.53700200	0.04544900
C	1.27118600	-3.74691900	-3.50774000
H	2.24324100	-1.96718100	-2.85641300
C	3.97056400	-5.44009000	2.14032100
C	5.09767700	-3.38582800	2.74294800
H	4.90231100	-1.73029400	1.41753000
C	0.95085900	-5.10558400	-3.21927900
H	1.15811400	-6.71932900	-1.82806400
H	2.42041400	-6.57431100	0.25885500

H	0.90076700	-3.29274300	-4.42288500
H	3.71078600	-6.47838900	2.33383800
C	4.76403900	-4.74425500	3.01294700
H	5.72795700	-2.84086800	3.44069800
H	0.35202200	-5.67846800	-3.92289700
H	5.14419100	-5.22386400	3.91104400
C	-0.33263500	3.85385600	0.41310200
C	-0.75779200	4.34833500	-0.84316100
C	-1.24956400	3.75533100	1.48560900
C	-2.12655700	4.77844700	-1.01608200
C	0.12276300	4.46315700	-1.96681600
C	-2.60947300	4.21420300	1.30781400
C	-0.89189300	3.20332400	2.75864300
C	-2.54321500	5.28210700	-2.28874200
C	-3.00970200	4.71356900	0.06545400
C	-0.31641100	4.94563100	-3.17205600
H	1.15626700	4.15556900	-1.85508300
C	-3.51577500	4.14941700	2.41365900
C	-1.79552700	3.14478400	3.78728100
H	0.10646200	2.80411600	2.89057600
C	-1.66855100	5.36102600	-3.33977100
H	-3.57495900	5.60876200	-2.39970200
H	-4.03294700	5.06192200	-0.06321800
H	0.37241300	5.01573800	-4.00949800
H	-4.52803100	4.52257700	2.27202600
C	-3.12240200	3.63559400	3.62026800
H	-1.50172300	2.71192400	4.73952300
H	-1.99769300	5.74767900	-4.30069500
H	-3.82084400	3.59130200	4.45177300

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P	-0.63147200	-0.01823400	-0.18991000
O	-1.07193300	1.32377000	0.70008500
O	-2.12029800	-0.58523600	-0.64758900
C	-1.99364400	2.19325700	0.15321500
C	-3.32998100	1.81602200	0.10037200
C	-3.12144500	-0.65457100	0.30351100
C	-3.74250600	0.51975700	0.71072100
C	-4.26769400	2.67945400	-0.56183400
C	-6.04570700	4.44197100	-1.89360200
C	-5.61997700	2.31215900	-0.81011700
C	-3.82144800	3.95595400	-1.03448200
C	-4.74032900	4.82218300	-1.68629300
C	-6.48232500	3.16809900	-1.45879700
H	-5.96842100	1.33633600	-0.49178400
H	-4.38481600	5.79114100	-2.02899000
H	-7.50797700	2.85948800	-1.64298400
H	-6.73846200	5.10955800	-2.39863600
C	-4.73055100	0.45774700	1.75244600

C	-6.66598700	0.23741100	3.81441300
C	-5.31098900	1.61439600	2.34497600
C	-5.12740100	-0.82311500	2.25553200
C	-6.10990100	-0.90097800	3.27947400
C	-6.25015500	1.50647800	3.34672200
H	-4.99812100	2.59506800	2.00610000
H	-6.40516600	-1.88362700	3.63997900
H	-6.67257900	2.40638400	3.78593100
H	-7.41246800	0.16678700	4.60085100
C	-2.46661600	4.32789700	-0.84924600
H	-2.14525000	5.31300800	-1.17824100
C	-1.54351200	3.47397700	-0.28140900
C	-4.51988100	-1.99083300	1.73154900
H	-4.84459500	-2.95978500	2.10254500
C	-3.51855900	-1.93722600	0.78364600
O	0.08030600	0.40854100	-1.45124100
C	-0.13215800	3.93910900	-0.09270800
C	0.28336700	4.40085500	1.17934100
C	0.74547400	4.01268700	-1.19941700
C	-0.56116000	4.34603600	2.33452500
C	1.60290900	4.97018100	1.33740500
C	2.06015800	4.59286400	-1.03204200
C	0.38939300	3.52604500	-2.49942100
C	-0.13421200	4.80715300	3.55230900
H	-1.55566100	3.92579000	2.23535300
C	2.00709000	5.44471400	2.62510500
C	2.45107100	5.05687700	0.22775500
C	2.93017000	4.68397900	-2.16418100
H	-0.57361300	3.04826500	-2.63100000
C	1.25561000	3.62839300	-3.55618600
C	1.16709900	5.36578900	3.70303800
H	-0.79408900	4.74862900	4.41360900
H	3.00132800	5.87416900	2.72663300
H	3.43647000	5.50410100	0.34680000
C	2.54061900	4.22161900	-3.39203200
H	3.91163600	5.13180200	-2.02501500
H	0.96384300	3.24720100	-4.53099400
H	1.48661200	5.73064300	4.67557400
H	3.21113200	4.29625600	-4.24390500
C	-2.92528100	-3.21444900	0.27320500
C	-1.98318300	-3.92235900	1.05400500
C	-3.39104100	-3.75699100	-0.94688100
C	-1.47501700	-3.42050900	2.29592800
C	-1.50251700	-5.20840200	0.59983000
C	-2.89829100	-5.04000600	-1.39366600
C	-4.35685900	-3.09114400	-1.76875900
C	-0.58150500	-4.14430900	3.04177500
H	-1.79583600	-2.44260200	2.63356500
C	-0.56590400	-5.92734300	1.40726700
C	-1.96991000	-5.72994100	-0.60906300

C	-3.38378400	-5.58179400	-2.62502700
H	-4.74187100	-2.12938400	-1.44787000
C	-4.79653900	-3.64422900	-2.94399500
C	-0.12110200	-5.41727000	2.59658800
H	-0.21438900	-3.74190800	3.98247200
H	-0.21671200	-6.89420000	1.05234200
H	-1.60781900	-6.69986300	-0.94444200
C	-4.30468500	-4.90759800	-3.38153900
H	-3.00284300	-6.54841000	-2.94681700
H	-5.52876800	-3.11631100	-3.54914500
H	0.58758500	-5.97582400	3.20241000
H	-4.66537000	-5.33187100	-4.31476300
C	3.64130700	0.33319200	-2.15789600
C	4.94800600	0.29730200	-1.64646900
C	6.01443100	0.07458400	-2.51820500
C	5.73660400	-0.10321800	-3.87614200
C	4.41907900	-0.07899300	-4.35748900
C	3.34038200	0.13939100	-3.49953200
C	3.44118900	0.78948400	0.03667100
C	4.84836100	0.44933900	-0.18062300
H	7.03984200	0.04725900	-2.15817100
H	6.55487900	-0.26661200	-4.57181900
H	4.23315600	-0.23914200	-5.41520400
H	2.31563100	0.14750000	-3.85303800
N	2.76955400	0.63049800	-1.09146900
H	1.71825600	0.65516000	-1.19675400
C	5.92340700	1.16361400	0.60403900
H	5.74889200	1.11318900	1.68212500
H	6.90988100	0.73376600	0.40998000
H	5.96101800	2.22072400	0.31217100
C	7.06329900	-1.81886400	4.03332200
C	7.75068100	-1.74768700	2.81458500
C	7.03787000	-1.66480000	1.62304100
C	5.63227000	-1.65608500	1.62027600
C	4.93680900	-1.77918400	2.85351200
C	5.67308800	-1.84107200	4.04979700
C	4.86809500	-1.55150400	0.37465500
C	3.47624000	-2.03029700	0.40549300
C	2.79076600	-2.06080900	1.68847900
C	3.49378400	-1.92169100	2.83930100
N	2.98549400	-2.34411500	-0.77113200
N	1.68644100	-2.62728300	-0.89782900
C	1.21170800	-2.79753800	-2.20611000
O	1.89036500	-2.87814800	-3.20382800
H	7.61674100	-1.87533100	4.96662100
H	8.83668500	-1.75806900	2.79883600
H	7.56926000	-1.61901500	0.67547300
H	5.13982900	-1.93083800	4.99306700
H	5.40089800	-1.84507000	-0.52316600
H	1.71876500	-2.20907800	1.72603900

H	2.98029300	-1.97912900	3.79614600
O	-0.13037900	-2.85516300	-2.15464400
C	-0.78225300	-2.84241200	-3.43431500
H	-0.50380900	-3.72615900	-4.01397400
H	-1.84777000	-2.84060200	-3.21538500
H	-0.50298000	-1.94076200	-3.98517500
C	2.79421500	1.26087100	1.29285000
H	3.39530200	0.99874500	2.16471700
H	2.69862600	2.35437800	1.26009200
H	1.79325300	0.83588000	1.40936000
O	0.04903400	-0.94365500	0.78050600
H	1.00120100	-2.28041300	-0.20534300

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P	-0.83351000	0.13559300	0.24528000
O	-0.11756200	1.12941800	-0.62932800
O	-1.39824000	-1.09935200	-0.74522100
O	-2.28991500	0.76176900	0.75215900
C	-2.37200600	-1.92666300	-0.21677500
C	-3.67832800	-1.46588300	-0.12729300
C	-3.25938000	0.96761100	-0.21333100
C	-3.99026800	-0.11701300	-0.67441900
C	-4.66347400	-2.27991600	0.52560900
C	-6.54145100	-3.94399800	1.84454300
C	-5.98689900	-1.82907000	0.78949300
C	-4.29705800	-3.58875200	0.97751500
C	-5.26468400	-4.40441700	1.62380900
C	-6.89808300	-2.63830100	1.43100300
H	-6.27206800	-0.82731000	0.48956100
H	-4.97008300	-5.39847200	1.95177100
H	-7.90053000	-2.26765800	1.62737600
H	-7.27257800	-4.57259100	2.34519800
C	-4.95321900	0.08077300	-1.72140300
C	-6.82544400	0.56557500	-3.79609200
C	-5.65617000	-0.98882500	-2.34330200
C	-5.19117200	1.40856600	-2.20373900
C	-6.14564400	1.62084900	-3.23486100
C	-6.56569900	-0.75190200	-3.35006600
H	-5.46174200	-2.00580000	-2.02374900
H	-6.31847900	2.63740700	-3.58019200
H	-7.08496800	-1.58759600	-3.81147000
H	-7.54932900	0.73748400	-4.58780600
C	-2.96971300	-4.04015900	0.78157600
H	-2.70547300	-5.04355600	1.10470000

C	-2.00814800	-3.23584500	0.20814100
C	-4.44786100	2.48476100	-1.66198800
H	-4.63156900	3.48844000	-2.03593500
C	-3.48529700	2.28767300	-0.69591700
O	-0.12836300	-0.47990500	1.42647800
H	0.92879000	2.16233200	0.54526100
C	-0.63088800	-3.76319300	0.01868000
C	-2.69559000	3.44082900	-0.19146300
C	-1.23910200	5.66545200	0.75082300
C	0.18331200	-4.10291600	1.10290300
C	1.44348100	-4.66816800	0.92705500
C	1.92553700	-4.90669500	-0.35612000
C	1.13890800	-4.57927200	-1.45680800
C	-0.11722300	-4.01373300	-1.25728600
F	-0.22776300	-3.88081400	2.35854600
F	2.20915100	-4.95748000	1.99283300
F	3.13928400	-5.43933300	-0.52875600
F	1.59821200	-4.79336800	-2.69523300
F	-0.84107400	-3.69799600	-2.33975100
C	-1.81559500	4.14064000	-1.02245700
C	-1.09166600	5.23975700	-0.56660400
C	-2.11265900	4.99193200	1.59878500
C	-2.82725000	3.90042000	1.11873600
F	-1.64923300	3.76672800	-2.29703500
F	-0.25338900	5.88846800	-1.38672600
F	-0.54388000	6.71621500	1.19851700
F	-2.24809000	5.38391600	2.87380800
F	-3.66055700	3.27177900	1.96587200
C	2.76052600	-1.16481000	-0.76629800
C	4.15419100	-1.09216800	-0.96427200
C	4.68084100	-1.22241800	-2.24871100
C	3.79273200	-1.41096900	-3.31177000
C	2.40770300	-1.43867900	-3.10061400
C	1.86264100	-1.31047700	-1.81986300
C	3.68291600	-1.02177600	1.29826600
C	4.73875500	-0.81198100	0.34369400
H	5.75252400	-1.18799700	-2.41890800
H	4.18228500	-1.53597200	-4.31824500
H	1.73783200	-1.57247100	-3.94454700
H	0.79072700	-1.32197500	-1.67167800
N	2.52806200	-1.10698100	0.62343600
H	1.57301800	-1.03046700	1.03345500
H	5.77811500	-0.98973900	0.59008500
C	3.79874500	-1.22637800	2.79761600

C	4.57641500	-0.07125700	3.46817300
C	2.41829200	-1.36994800	3.46691400
C	4.59008800	-2.55006900	2.99441400
H	5.58243000	0.04049300	3.04498700
H	4.03518800	0.87337800	3.37717200
H	4.69692100	-0.29748700	4.53336900
H	1.85373300	-2.22175500	3.07388400
H	2.56332600	-1.54114900	4.53881900
H	1.81204000	-0.46898800	3.35480500
H	4.69347800	-2.74699800	4.06776700
H	4.06820100	-3.39951400	2.54351000
H	5.59606700	-2.49212500	2.56439500
C	7.52524800	2.05573300	-2.98220300
C	8.03446500	1.66477000	-1.73397800
C	7.16450500	1.43124300	-0.67761600
C	5.77508700	1.58312400	-0.84135600
C	5.25831200	1.98654500	-2.10367100
C	6.15717800	2.21638700	-3.16121600
C	4.85009000	1.34206100	0.25415800
C	3.47680800	1.81948300	0.10629300
C	2.96757800	2.10776500	-1.22412000
C	3.83035400	2.19115900	-2.26422200
N	2.85556500	1.94776400	1.25687600
N	1.58487900	2.31069100	1.33688900
C	1.04291900	2.30122200	2.63721800
O	1.66937500	2.10558400	3.65322000
H	8.20421500	2.23911900	-3.81032900
H	9.10530700	1.54997600	-1.59378000
H	7.55386600	1.13214400	0.29304700
H	5.76622000	2.52878600	-4.12618600
H	5.24676500	1.41140200	1.25970600
H	1.90373000	2.25680000	-1.37187000
H	3.46249300	2.43690700	-3.25675900
O	-0.26769000	2.56120100	2.55549000
C	-0.99290700	2.39314100	3.79113900
H	-2.02773800	2.61758600	3.54747800
H	-0.89420200	1.36127000	4.13415000
H	-0.60868700	3.07822900	4.54995700

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P	-0.74848200	-0.16928000	-0.13928900
O	-0.26154200	0.67395800	-1.29063000
O	-1.41112100	-1.53082700	-0.82604500
O	-2.10824600	0.51328200	0.53351500

C	-2.19148700	-2.33281700	-0.02029800
C	-3.47584600	-1.92700700	0.30802900
C	-3.29769100	0.50804500	-0.16020200
C	-4.01124200	-0.67505000	-0.29892400
C	-4.22931500	-2.71479400	1.24408400
C	-5.64230300	-4.32008000	3.10688100
C	-5.48792100	-2.30368500	1.76406500
C	-3.67927000	-3.95078300	1.71765500
C	-4.41843300	-4.73929500	2.64040900
C	-6.17275900	-3.08347300	2.66974600
H	-5.90430500	-1.35379200	1.44933100
H	-3.98832400	-5.67829400	2.98074200
H	-7.12878400	-2.74179300	3.05726400
H	-6.19614900	-4.92711300	3.81757300
C	-5.21354700	-0.67283600	-1.08683100
C	-7.57672500	-0.57688100	-2.65558600
C	-5.93078400	-1.85793600	-1.41253600
C	-5.70115200	0.56778500	-1.61179000
C	-6.89560900	0.58556100	-2.38183300
C	-7.07756900	-1.81004800	-2.17385700
H	-5.55801700	-2.81390200	-1.06477000
H	-7.25306100	1.53966700	-2.76187100
H	-7.60111000	-2.73183300	-2.41282400
H	-8.48549300	-0.55420000	-3.25049100
C	-2.40026800	-4.36023600	1.26770400
H	-2.00247200	-5.30985200	1.61459400
C	-1.64891800	-3.57292900	0.42230300
C	-4.97065600	1.75545600	-1.37212100
H	-5.35388200	2.69229200	-1.76665400
C	-3.78140000	1.74575800	-0.67447300
O	0.15767000	-0.54764300	0.99829100
H	1.13798800	0.47686300	2.05089500
C	-0.30006500	-4.00051100	-0.02473100
C	-3.03066600	3.01215000	-0.47703400
C	-1.71843300	5.48835100	-0.12779400
C	0.71583000	-4.29462400	0.89043800
C	1.98249900	-4.69751000	0.47732200
C	2.27296700	-4.79119100	-0.87918900
C	1.28203700	-4.51151000	-1.81491400
C	0.01686200	-4.12434500	-1.38275500
F	0.49357500	-4.19214000	2.20743600
F	2.95000600	-4.93852700	1.38015600
F	3.50086800	-5.14299900	-1.27864900
F	1.56137100	-4.59014600	-3.12398900

F	-0.91263400	-3.88324200	-2.31286500
C	-2.63969700	3.79762600	-1.56814800
C	-1.98862700	5.01916900	-1.40941400
C	-2.09199000	4.73160800	0.97887600
C	-2.74068100	3.51359500	0.79712200
F	-2.88939800	3.38816900	-2.81881000
F	-1.62684500	5.74123900	-2.47658300
F	-1.08074800	6.65392900	0.04499400
F	-1.84098300	5.19807800	2.21180500
F	-3.11529900	2.83454400	1.88887200
C	2.46136500	2.81030800	-0.75184600
C	3.84236200	3.05225500	-0.66022200
C	4.28380200	4.26493800	-0.12527200
C	3.33014800	5.20360300	0.27154500
C	1.95540300	4.93721000	0.16583700
C	1.49561000	3.72411500	-0.34619400
C	3.45363200	1.00343300	-1.66893900
C	4.50533800	1.81520600	-1.07886900
H	5.34431200	4.48523300	-0.03194300
H	3.65571700	6.15943000	0.67113600
H	1.23837900	5.68856200	0.48045400
H	0.44007500	3.49255200	-0.43402900
N	2.28067400	1.55391000	-1.35193900
H	1.32315600	1.13391400	-1.46433600
H	5.51604500	1.78296400	-1.46618500
C	3.54011200	-0.14173500	-2.66348700
C	2.52656800	-1.25985700	-2.33736800
C	3.17740300	0.47234100	-4.04739900
C	4.96131000	-0.72556800	-2.74987400
H	2.73742900	-1.70276900	-1.36065800
H	1.49600400	-0.89264600	-2.32919000
H	2.59389400	-2.04745800	-3.09569400
H	3.86112300	1.28468500	-4.31871900
H	3.25286800	-0.30627400	-4.81478500
H	2.15547700	0.86301300	-4.05573200
H	4.98262600	-1.49614900	-3.52785700
H	5.70041400	0.03615000	-3.02308400
H	5.27522800	-1.18959100	-1.81305800
C	8.00175800	-1.91010600	0.38039800
C	8.31285300	-0.54526500	0.28824900
C	7.30671600	0.40353800	0.42050100
C	5.97524000	0.01403900	0.64712800
C	5.66194700	-1.36687700	0.75540600
C	6.69314600	-2.31389100	0.61446600

C	4. 90937800	1. 00257000	0. 80150200
C	3. 64380700	0. 55034300	1. 37514500
C	3. 32038200	-0. 86494800	1. 30820400
C	4. 29704800	-1. 76680500	1. 03373700
N	2. 94713500	1. 49943600	1. 97042000
N	1. 73425000	1. 23779200	2. 43764900
C	1. 10854700	2. 22518700	3. 21398100
O	1. 61824300	3. 24084000	3. 62280000
H	8. 78691200	-2. 65354300	0. 27517600
H	9. 33822600	-0. 23062500	0. 11711700
H	7. 54602400	1. 46269800	0. 35514400
H	6. 45274200	-3. 37089400	0. 69637800
H	5. 22166500	1. 97989700	1. 15375200
H	2. 31493200	-1. 19806500	1. 53761500
H	4. 07984000	-2. 83041300	1. 07295100
O	-0. 15003400	1. 81012600	3. 45166000
C	-0. 92549600	2. 66776600	4. 30336100
H	-0. 44826900	2. 76172000	5. 28269400
H	-1. 03438300	3. 65584000	3. 85468200
H	-1. 89607700	2. 18072500	4. 38963800

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P	-0. 78659100	-0. 09643400	-0. 09764400
O	-0. 30250900	0. 79616600	-1. 20877700
O	-1. 40719200	-1. 46107700	-0. 82543700
O	-2. 17845700	0. 52867500	0. 57217500
C	-2. 14834000	-2. 30202700	-0. 01958700
C	-3. 44550300	-1. 95245700	0. 32297500
C	-3. 36148300	0. 48535000	-0. 13172100
C	-4. 03388100	-0. 72072200	-0. 27437900
C	-4. 15569400	-2. 77160800	1. 26558400
C	-5. 47756500	-4. 43005600	3. 14779100
C	-5. 42740700	-2. 41560800	1. 79430000
C	-3. 54603900	-3. 97925300	1. 73888800
C	-4. 24007200	-4. 79575100	2. 67214700
C	-6. 06817800	-3. 22141600	2. 70942000
H	-5. 88867700	-1. 48718800	1. 47808000
H	-3. 76501800	-5. 71286800	3. 01246600
H	-7. 03574900	-2. 92231800	3. 10345100
H	-5. 99694500	-5. 05812400	3. 86622700
C	-5. 23541600	-0. 75947200	-1. 06164900
C	-7. 60059900	-0. 74380300	-2. 62976000
C	-5. 91477600	-1. 96789800	-1. 38288600
C	-5. 76199700	0. 46350500	-1. 59062300

C	-6.95627400	0.44057400	-2.36070800
C	-7.06300600	-1.95893000	-2.14347900
H	-5.51190700	-2.91033400	-1.03160700
H	-7.34363100	1.38147700	-2.74437100
H	-7.55764500	-2.89753600	-2.37858000
H	-8.50976300	-0.75196800	-3.22447200
C	-2.25563700	-4.33387200	1.27470700
H	-1.81349200	-5.26586400	1.61617500
C	-1.55042900	-3.51735300	0.41791100
C	-5.06749700	1.67404400	-1.35723300
H	-5.47581100	2.59666700	-1.76021800
C	-3.88094200	1.70403900	-0.65619500
O	0.10424800	-0.50011500	1.04526900
H	1.04066100	0.44455800	2.15078500
C	-0.20117000	-3.90417700	-0.06400900
C	-3.15559500	2.98648700	-0.47501600
C	-1.82258800	5.45394400	-0.15483800
C	0.86298100	-4.12553300	0.81463400
C	2.12056200	-4.51613800	0.36210500
C	2.35008700	-4.67043100	-1.00026000
C	1.30711200	-4.46782500	-1.89826700
C	0.05640800	-4.08167900	-1.42797100
F	0.69820300	-3.96460500	2.13406500
F	3.13114000	-4.69616400	1.23195000
F	3.56397000	-5.01238600	-1.44564700
F	1.52503100	-4.61637300	-3.21496500
F	-0.92113300	-3.90139600	-2.32289100
C	-2.74966600	3.74887700	-1.57602600
C	-2.08912500	4.96576000	-1.42975500
C	-2.22196200	4.72494800	0.96098600
C	-2.87999500	3.51069000	0.79158300
F	-2.98515900	3.31594000	-2.82169900
F	-1.69387900	5.65990600	-2.50528500
F	-1.15497200	6.60428000	-0.00306200
F	-1.97594400	5.20274800	2.19082400
F	-3.26837100	2.84975900	1.89126900
C	2.97131800	0.35090900	-1.93879900
C	4.35542900	0.57163300	-1.79508700
C	5.25115900	-0.39609600	-2.25331500
C	4.73174600	-1.55608000	-2.83669400
C	3.34859900	-1.76067000	-2.95202100
C	2.43615100	-0.80405400	-2.49687900
C	3.17780400	2.42681000	-1.07610000
C	4.49539000	1.85095100	-1.10703000

H	6.32402600	-0.25167300	-2.17006200
H	5.41302700	-2.31488800	-3.21130600
H	2.97927300	-2.67408800	-3.40605300
H	1.36261100	-0.93792300	-2.57867800
N	2.30480800	1.49257400	-1.47260700
H	1.26585300	1.47882300	-1.37584100
H	5.38809800	2.46185100	-1.14807800
C	2.77492600	3.86066500	-0.79000600
C	2.93691600	4.61810000	-2.13927100
C	1.31001200	3.96894500	-0.32585300
C	3.68419700	4.51522000	0.26970200
H	3.97039200	4.58034300	-2.50121200
H	2.28732200	4.19544300	-2.91295700
H	2.66307000	5.67005700	-1.99929900
H	1.17238300	3.51388100	0.65803100
H	1.03808100	5.02620100	-0.24134200
H	0.61236600	3.50287000	-1.02824000
H	3.42577900	5.57614900	0.35534900
H	3.53693800	4.05627100	1.25114800
H	4.74446000	4.46023700	-0.00470500
C	8.13303500	-1.36552400	0.67773100
C	8.33923600	0.02233300	0.62605000
C	7.25546500	0.88431000	0.72304100
C	5.94894700	0.38310800	0.87627900
C	5.73964900	-1.02225500	0.93369000
C	6.85116100	-1.87822200	0.83104100
C	4.80370400	1.26714800	0.98380500
C	3.55184100	0.70895900	1.47952000
C	3.34524100	-0.72746000	1.39122300
C	4.40049800	-1.53970000	1.14056400
N	2.76510100	1.60307000	2.04527000
N	1.57857200	1.25927700	2.52067500
C	0.86131200	2.24723900	3.21627400
O	1.24633700	3.37152900	3.44375700
H	8.98023800	-2.04149600	0.60202900
H	9.34386400	0.42021600	0.51641100
H	7.40991600	1.96051000	0.68930100
H	6.69438000	-2.95270500	0.87863900
H	4.99284000	2.29207400	1.27923200
H	2.35762100	-1.13901800	1.56559700
H	4.26638200	-2.61698300	1.13215400
O	-0.30674600	1.70988100	3.59929500
C	-1.16792000	2.58389500	4.34922900
H	-1.39474200	3.48287400	3.77596700

H	-2.07332200	2.00515100	4.52785700
H	-0.69157700	2.86127600	5.29355500

M2-TS1bS

P	0.75886800	0.00881300	0.14361600
O	-0.16792400	-0.68484800	-0.81735200
O	1.73754900	1.06091500	-0.72173600
O	1.91532900	-1.07526600	0.66044600
C	2.86052500	1.54456400	-0.07692600
C	3.95593300	0.71285200	0.11357000
C	2.87788000	-1.48328200	-0.24411100
C	3.93883100	-0.63303300	-0.51904800
C	5.05268000	1.17094900	0.91796200
C	7.16221900	2.14262500	2.54277500
C	6.13492700	0.32928500	1.29775700
C	5.04576000	2.51748200	1.40463700
C	6.12369100	2.97932300	2.20726900
C	7.15843400	0.80213500	2.08882500
H	6.14039200	-0.70336800	0.96805000
H	6.10446700	4.00762000	2.56051600
H	7.96924200	0.13655200	2.37250200
H	7.97864900	2.50263200	3.16262100
C	4.93389300	-1.02928700	-1.47634200
C	6.85162100	-1.90373800	-3.37609800
C	5.98298800	-0.17175200	-1.91264600
C	4.85312700	-2.33446000	-2.05920700
C	5.83608600	-2.74970600	-2.99743800
C	6.91361200	-0.59819100	-2.83391500
H	6.04176800	0.83601500	-1.51960400
H	5.76054400	-3.74892500	-3.41983200
H	7.70128000	0.07911800	-3.15295000
H	7.59617100	-2.22746700	-4.09806200
C	3.96200900	3.36351500	1.07030800
H	3.98614400	4.39867400	1.39901000
C	2.87995300	2.90508400	0.34817800
C	3.77000400	-3.17675700	-1.71252900
H	3.70829400	-4.16216700	-2.16710600
C	2.78046400	-2.77164100	-0.84341100
O	0.18875800	0.73327800	1.33718300
H	-1.27549300	-1.83380300	0.29877600
C	1.79316300	3.84389100	-0.02209500
C	1.64417400	-3.69773900	-0.57702000
C	-0.42370000	-5.57027200	-0.15715500
C	1.09930300	4.58701000	0.93890200

C	0.12387900	5.51736300	0.58856100
C	-0.17616400	5.72628700	-0.75360300
C	0.49430800	5.00215200	-1.73372200
C	1.46724700	4.07950300	-1.36297200
F	1.36108900	4.42012800	2.24232000
F	-0.55148400	6.18501900	1.53457000
F	-1.14452500	6.58567800	-1.10037600
F	0.17195100	5.17307200	-3.02350200
F	2.10632200	3.41907200	-2.33437300
C	0.57927600	-3.81932800	-1.47399700
C	-0.45081600	-4.73498700	-1.27089900
C	0.63081200	-5.47800500	0.74618100
C	1.64301400	-4.54949100	0.52665100
F	0.52527300	-3.05287600	-2.56825800
F	-1.46388900	-4.81894600	-2.14442300
F	-1.40633500	-6.45339200	0.04437300
F	0.64978100	-6.25873700	1.83763000
F	2.63437000	-4.47388300	1.43038700
C	-3.10631500	0.75912500	2.41495000
C	-4.50271900	0.77651300	2.26034600
C	-5.30671100	0.33358900	3.31296800
C	-4.68616600	-0.08378700	4.49168400
C	-3.28783300	-0.08626300	4.61824900
C	-2.46553900	0.33409600	3.57297100
C	-3.48446500	1.68041000	0.38727200
C	-4.76313000	1.19943900	0.88231800
H	-6.39058900	0.32802500	3.22909300
H	-5.29580300	-0.41383700	5.32770600
H	-2.83780100	-0.42913700	5.54487700
H	-1.38248800	0.33366500	3.64081700
N	-2.53625300	1.29195200	1.24419800
H	-1.49954700	1.29342300	1.11809700
H	-5.68935800	1.66647800	0.57083400
C	-3.20007800	2.66004200	-0.73353900
C	-3.23202800	4.06044700	-0.04903200
C	-1.81496300	2.41654800	-1.36271800
C	-4.27599300	2.64462300	-1.83260800
H	-4.22548400	4.28067100	0.35754000
H	-2.50779800	4.13042000	0.76819500
H	-2.98942400	4.83279700	-0.78630600
H	-1.73011100	1.40813300	-1.77581100
H	-1.65142600	3.13640600	-2.17136800
H	-1.00553500	2.54440800	-0.63865300
H	-4.09539300	3.48305200	-2.51376000

H	-4.24216100	1.72547600	-2.41808100
H	-5.28778800	2.76126300	-1.42968900
C	-7.47733600	-0.18383800	-3.50754900
C	-8.05529200	-0.04930800	-2.23643200
C	-7.26864100	-0.19730700	-1.10107900
C	-5.89541600	-0.47910200	-1.20807800
C	-5.31208600	-0.62744800	-2.49454800
C	-6.12403100	-0.47208800	-3.63281500
C	-5.06310500	-0.66188300	-0.02122100
C	-3.74109100	-1.26235200	-0.20058800
C	-3.13424900	-1.23224800	-1.52089300
C	-3.90271400	-0.95080300	-2.60334600
N	-3.25025800	-1.78709200	0.90059000
N	-1.99064400	-2.21195400	0.94678800
C	-1.57173900	-2.74020100	2.18172300
O	-2.29807000	-3.12919700	3.06327600
H	-8.09053200	-0.06828400	-4.39685300
H	-9.11552700	0.16552500	-2.13986400
H	-7.71529500	-0.10132800	-0.11381000
H	-5.67874100	-0.58610200	-4.61798400
H	-5.57976700	-1.00226400	0.86947800
H	-2.08799800	-1.48458900	-1.64525600
H	-3.46861000	-0.99951900	-3.59901800
O	-0.22799000	-2.74734500	2.19748100
C	0.37226600	-3.23116800	3.41142200
H	0.00927000	-2.65681000	4.26664300
H	0.13866100	-4.28888800	3.55543500
H	1.44210400	-3.08921200	3.27160500

M1-TS1cR

C	-4.17821000	4.93493300	-1.95475200
C	-2.92731100	5.28903000	-1.12187500
C	-2.90139100	4.23025100	0.03222900
C	-3.47828200	3.02151600	-0.69051000
C	-4.29111700	3.43947100	-1.75358100
C	-3.83247900	4.69890100	1.19950200
C	-2.96950900	5.68616700	2.01492300
C	-1.56800400	5.16124100	1.78849300
C	-1.55153400	4.23018600	0.73919300
C	-3.35467100	1.66245900	-0.39973400
C	-4.14590000	0.71728300	-1.08355700
C	-4.98818500	1.17483800	-2.11186800
C	-5.04636500	2.51946200	-2.47300100
C	-0.40058200	5.48140900	2.47176700

C	0.79043700	4.86916200	2.08632600
C	0.83266700	3.88751300	1.08048400
C	-0.37684200	3.53470500	0.44505000
O	-2.43166600	1.25956000	0.55414800
O	-0.40830900	2.50344200	-0.47957300
P	-0.87598200	0.98776200	0.02839700
O	-0.91756200	0.16477400	-1.23706300
H	-4.07610100	5.21208200	-3.01051200
H	-5.07027800	5.45583700	-1.57825800
H	-2.93037300	6.31724800	-0.74593200
H	-2.02787800	5.16058500	-1.73498900
H	-4.08416000	3.82919200	1.81695200
H	-4.76954300	5.13448500	0.83745300
H	-3.07539200	6.71446500	1.64053500
H	-3.24201700	5.70998400	3.07655300
H	-5.60097900	0.44920900	-2.63919100
H	-5.68009300	2.83836400	-3.29692700
H	-0.40756400	6.20534100	3.28289700
H	1.72073800	5.14183200	2.57597900
C	1.68921000	-1.69272100	-2.21187200
C	2.54767500	-2.80573800	-2.12262900
C	3.83104500	-2.71838700	-2.66084400
C	4.21889500	-1.51263100	-3.25620100
C	3.35551700	-0.40902300	-3.30175400
C	2.06229900	-0.47983700	-2.77466300
C	0.47183900	-3.30905700	-1.23313200
C	1.81604900	-3.83251900	-1.37239800
H	4.51689100	-3.55885800	-2.61587300
H	5.21400200	-1.42811700	-3.68432200
H	3.69400700	0.52171400	-3.74622500
H	1.38095300	0.36417300	-2.78776800
H	1.98024700	-4.89548700	-1.51398100
N	0.45168000	-2.05077100	-1.64896100
H	-0.28101400	-1.30967500	-1.47132200
C	6.69781500	-3.83863800	0.20591300
C	5.98445100	-5.04270600	0.12197500
C	4.59955500	-5.03555700	0.25258100
C	3.90806000	-3.83421700	0.47552200
C	4.62818800	-2.61481600	0.56467300
C	6.02655900	-2.64051100	0.42440100
C	2.45190000	-3.79452600	0.60945100
C	1.87230300	-2.61449600	1.26683600
C	2.60051200	-1.35778800	1.16584800
C	3.91331800	-1.37771600	0.83309600

N	0.77085700	-2.86558100	1.93355200
N	0.10325500	-1.87461900	2.53192900
C	-0.95268000	-2.24663800	3.36598800
O	-1.25525500	-3.37705900	3.67317800
H	7.77968200	-3.84207800	0.10388600
H	6.51076400	-5.97917800	-0.03930900
H	4.04200300	-5.96795100	0.19301500
H	6.57755200	-1.70654900	0.49822100
H	1.96545000	-4.72487400	0.89072800
H	2.09956400	-0.42229300	1.39213500
H	4.47804600	-0.45203700	0.80171600
O	-1.55662000	-1.12202600	3.80348500
C	-2.64784900	-1.34399200	4.70463900
H	-2.29747500	-1.82648400	5.62200900
H	-3.04687000	-0.35295000	4.92335700
H	-3.40916100	-1.97474700	4.23893000
O	-0.08297000	0.57438800	1.23415400
H	0.13802700	-0.89250500	2.19032600
C	-0.71107600	-3.98815600	-0.64304900
H	-0.41764500	-4.89973900	-0.11924900
H	-1.23481400	-3.33925300	0.06460900
H	-1.42341600	-4.25050700	-1.43557100
C	2.16120900	3.28739900	0.75923200
C	2.76753100	3.40983400	-0.55641200
C	2.88567800	2.72725700	1.77517100
C	2.07908900	4.01885200	-1.63330500
C	4.10219400	2.94251900	-0.77209000
C	4.22960300	2.26567000	1.60825600
H	2.43095600	2.62996900	2.75719700
C	2.65547900	4.14534800	-2.88173600
H	1.07731200	4.39486300	-1.46781300
C	4.66259200	3.08528800	-2.06390300
C	4.85671700	2.36595600	0.33298500
C	4.94722300	1.72606500	2.70328900
C	3.95975000	3.66923900	-3.10100600
H	2.10198700	4.61598700	-3.68969400
H	5.67267000	2.73852600	-2.25334300
C	6.19280300	1.91322600	0.21623800
H	4.44884700	1.65785500	3.66728700
C	6.25184900	1.29754500	2.55971100
H	4.42198200	3.77025700	-4.07965200
C	6.87789600	1.39355500	1.30161500
H	6.70677100	1.97722600	-0.73671900
H	6.79264100	0.89023000	3.40949700

H	7.90785200	1.06726600	1.18149900
C	-4.21545200	-0.72252400	-0.69693500
C	-3.96110500	-1.77963000	-1.65872500
C	-4.66578900	-1.05257600	0.55072900
C	-3.37973500	-1.49681500	-2.91981700
C	-4.27918000	-3.13484800	-1.33105000
C	-4.96062300	-2.39908300	0.93382000
H	-4.85465700	-0.26399000	1.27394800
C	-3.15902700	-2.49431100	-3.84974200
H	-3.08252100	-0.47727500	-3.13561300
C	-4.05954900	-4.12908200	-2.31582000
C	-4.79839800	-3.45523600	-0.00818500
C	-5.46373100	-2.68571100	2.22570000
C	-3.51897200	-3.82110100	-3.55117900
H	-2.70741500	-2.25318300	-4.80825200
H	-4.31587800	-5.16168300	-2.10381500
C	-5.14459000	-4.76547300	0.39870900
H	-5.59971500	-1.86222400	2.92290100
C	-5.78944400	-3.97551300	2.59463400
H	-3.36617900	-4.60757300	-4.28590500
C	-5.62564400	-5.02356400	1.66949700
H	-5.03511000	-5.59517800	-0.29139000
H	-6.17256500	-4.18211800	3.59013100
H	-5.87995600	-6.04129200	1.95272000

M2-TS1cR

C	5.64033000	-3.36734700	2.39225500
C	5.94459500	-2.13510400	1.51117800
C	4.92180800	-2.22947100	0.33057600
C	3.72201000	-2.82787700	1.05940800
C	4.15810100	-3.57695900	2.16328800
C	5.46729900	-3.21125800	-0.76224000
C	6.41740100	-2.35258200	-1.62523300
C	5.79174400	-0.97812200	-1.52559000
C	4.86319600	-0.93678000	-0.47585400
C	2.36015000	-2.78032800	0.75939600
C	1.44660600	-3.59830000	1.45194800
C	1.92338700	-4.38308200	2.51161200
C	3.26561900	-4.35298000	2.89540300
C	6.01337700	0.14092800	-2.32243500
C	5.28689200	1.30455300	-2.07051100
C	4.30563600	1.36090300	-1.06641400
C	4.09050700	0.20811700	-0.28334200
O	1.89759500	-1.91004300	-0.21222100

O	3.10056700	0.19378400	0.68142900
P	1.59079900	-0.33830500	0.25044300
O	1.16269100	0.33769600	-1.03326800
O	0.78227500	-0.29138100	1.51031800
H	5.88277400	-3.20177900	3.44846400
H	6.22199700	-4.24280300	2.06970700
H	6.98220500	-2.09338500	1.16384900
H	5.74294700	-1.21797600	2.07612400
H	4.62544300	-3.55599800	-1.37381100
H	5.94980200	-4.09394700	-0.32997700
H	7.43884500	-2.35608900	-1.21820000
H	6.48999700	-2.70982600	-2.65913200
H	1.21735100	-5.00693600	3.05297700
H	3.60262100	-4.93093100	3.75257300
H	6.73970100	0.11433300	-3.13116100
H	5.46565700	2.19161600	-2.67175300
H	-0.45242500	0.69425900	2.19145600
C	-2.15295200	-0.44857500	-2.55232700
C	-3.43774800	0.13643000	-2.61769200
C	-4.45981400	-0.54680300	-3.28083500
C	-4.17996800	-1.80088700	-3.82834100
C	-2.90860800	-2.37839100	-3.71155800
C	-1.86511700	-1.70491800	-3.06868200
C	-1.94010000	1.58290200	-1.62346700
C	-3.35478100	1.40045000	-1.87483900
H	-5.44748800	-0.10775600	-3.38265600
H	-4.96295400	-2.34107100	-4.35698900
H	-2.71956100	-3.36332800	-4.12811200
H	-0.87599100	-2.14190400	-2.97706500
H	-3.99993500	2.25129900	-2.05709700
N	-1.28927900	0.47311400	-1.94033400
H	-0.27107400	0.31662100	-1.65790100
C	-8.21158000	1.91839200	-0.33490200
C	-7.78693700	0.66134700	-0.78164400
C	-6.45028100	0.29252000	-0.65151000
C	-5.52208600	1.17188400	-0.07085400
C	-5.95776900	2.42809600	0.42551200
C	-7.30430700	2.79000400	0.26784800
C	-4.10011700	0.83634600	0.03189400
C	-3.32069100	1.52297600	1.07690700
C	-3.78435400	2.84168000	1.49407700
C	-5.01260400	3.27507600	1.13136300
N	-2.23716300	0.86117800	1.39276900
N	-1.33638400	1.23308100	2.32336400

C	-1.59555400	1.78110800	3.57156400
O	-2.67117100	2.15872700	3.99434800
H	-9.25305600	2.20912300	-0.43775100
H	-8.49986800	-0.02856600	-1.22056300
H	-6.11356800	-0.68432300	-0.98381700
H	-7.64225600	3.75301500	0.64258700
H	-3.83316700	-0.20524200	-0.09285500
H	-3.13342300	3.46329100	2.09610100
H	-5.34617500	4.26586900	1.43042600
O	-0.44112000	1.79427100	4.26902300
C	-0.55017400	2.28682700	5.61145600
H	-1.22659700	1.66094600	6.20029100
H	0.45825200	2.24584700	6.01463800
H	-0.92539600	3.31378800	5.61657000
C	-1.23901100	2.77421700	-1.07054400
H	-0.23326200	2.86646000	-1.52244200
H	-1.83396100	3.69442300	-1.25778800
H	-1.09542400	2.66132800	0.03036100
C	3.57259200	2.63592900	-0.81239000
C	2.81310900	3.29877400	-1.85790800
C	3.67293500	3.22985300	0.41449600
C	2.58118500	2.67401100	-3.10827600
C	2.25588800	4.59531600	-1.62275200
C	3.09855400	4.50738900	0.70475400
H	4.22622600	2.73022200	1.20446700
C	1.87455500	3.30803900	-4.11166600
H	2.95012900	1.66700200	-3.26121600
C	1.54890000	5.22176900	-2.67782100
C	2.40739700	5.22103800	-0.31573000
C	3.23861500	5.08354500	1.99005800
C	1.36588300	4.60152700	-3.89930800
H	1.70823900	2.80402500	-5.06007400
H	1.13233900	6.21266700	-2.53142000
C	1.89025700	6.49891800	0.00310400
H	3.76842700	4.52101900	2.75512200
C	2.71831900	6.33056900	2.27252700
H	0.81916300	5.11108700	-4.68867200
C	2.04003300	7.04375200	1.26587100
H	1.36323400	7.07488000	-0.75010400
H	2.83329700	6.76178700	3.26344000
H	1.63227900	8.02838500	1.47935900
C	-0.00328500	-3.65135600	1.08768800
C	-0.44608200	-4.41427000	-0.06444700
C	-0.92732700	-3.03445900	1.87939000

C	0.48138400	-5.07753200	-0.90434200
C	-1.84136000	-4.52004500	-0.35772000
C	-2.33329300	-3.10209500	1.61380900
H	-0.58963000	-2.44131500	2.72308100
C	0.06691600	-5.81928900	-1.99331300
H	1.53844400	-4.99801700	-0.67545900
C	-2.23239600	-5.29482100	-1.47565400
C	-2.80968900	-3.84363400	0.49487100
C	-3.25566500	-2.43752000	2.45666500
C	-1.30513300	-5.93189200	-2.27950500
H	0.79924600	-6.31939300	-2.62154500
H	-3.28532000	-5.40193000	-1.71297700
C	-4.20663400	-3.88115500	0.26987300
H	-2.87183900	-1.87325000	3.30270100
C	-4.61404600	-2.49522900	2.21484700
H	-1.63961100	-6.52446600	-3.12730000
C	-5.09076100	-3.22544500	1.10885900
H	-4.60564100	-4.43332200	-0.57414200
H	-5.31057100	-1.98125500	2.87168900
H	-6.15905600	-3.28003000	0.91481700

M1-TS1cS

C	-2.78117900	-0.76693000	0.40880300
C	-3.69060200	-1.84407900	0.46776600
C	-4.40346400	-2.08423500	1.64184900
C	-4.17175000	-1.24927900	2.73891300
C	-3.23601800	-0.20856200	2.67028200
C	-2.51943200	0.05425600	1.49947400
C	-2.79728000	-1.68909600	-1.65346300
C	-3.59098000	-2.53599800	-0.81278600
H	-5.11870700	-2.89900600	1.70393300
H	-4.72417900	-1.41184700	3.66051100
H	-3.06953400	0.42133800	3.53880400
H	-1.79557100	0.85735400	1.45135400
H	-4.35617200	-3.18572900	-1.22008700
N	-2.25914000	-0.72476200	-0.89937200
H	-1.50365800	-0.07840300	-1.20400400
C	-4.04985300	-6.34962400	2.66339600
C	-4.44117600	-6.53189700	1.32758100
C	-3.82532700	-5.79760300	0.32324400
C	-2.80935700	-4.87278900	0.62666800
C	-2.40561500	-4.69254600	1.97855500
C	-3.04541800	-5.44479900	2.98135400
C	-2.15502300	-4.09124500	-0.40942700

C	-0.91221600	-3.40583600	-0.07220500
C	-0.60658600	-3.15208400	1.32360700
C	-1.32465100	-3.77613100	2.28830800
N	-0.21602600	-3.06846600	-1.13616000
N	0.87367200	-2.32720800	-1.07196900
C	1.36002600	-1.88350300	-2.32150700
O	0.89347100	-2.19521700	-3.39488900
H	-4.53129400	-6.92230100	3.45135500
H	-5.22028700	-7.24717400	1.08046400
H	-4.12248500	-5.93614400	-0.71401000
H	-2.73820400	-5.31210300	4.01570100
H	-2.20167400	-4.47000700	-1.42538900
H	0.20098700	-2.47707700	1.58091900
H	-1.08476000	-3.61316700	3.33571600
O	2.40001400	-1.07849000	-2.11118600
C	2.79689300	-0.29407100	-3.25005300
H	3.57875900	0.36423600	-2.87846900
H	1.94254500	0.28808200	-3.59980000
H	3.17449000	-0.94250900	-4.04394900
H	1.07845700	-1.72706700	-0.25077600
C	-2.46936900	-1.86484700	-3.09265200
H	-3.08288500	-2.65795800	-3.52821700
H	-1.40901900	-2.12404200	-3.22621100
H	-2.66307700	-0.93656100	-3.64058200
C	3.09748000	4.37359900	3.50763700
C	1.95606000	4.86682200	2.59185000
C	2.28940500	4.26385300	1.18730500
C	2.91399500	2.93794500	1.59411200
C	3.48716800	3.05810800	2.86804900
C	3.34152200	5.16651500	0.45716900
C	2.50938900	6.28006800	-0.21075800
C	1.19539100	5.58292000	-0.48534700
C	1.11174200	4.38024700	0.23216800
C	3.05506100	1.75208500	0.86908400
C	3.92324000	0.74569200	1.34220900
C	4.52708700	0.91982000	2.59951600
C	4.28768000	2.04545400	3.38446000
C	0.16175000	5.98554800	-1.32173300
C	-0.96775900	5.17619200	-1.42123100
C	-1.06641200	3.94707200	-0.74761800
C	0.01667700	3.53115200	0.05513700
O	2.31826400	1.58289900	-0.30156100
O	0.01881400	2.28903700	0.67785800
P	0.76117500	1.00821900	-0.12048200

O	0.13925200	0.86779300	-1.48716200
O	0.74739000	-0.15616800	0.83446800
H	2.78167100	4.25638900	4.55099500
H	3.94057600	5.07919500	3.51266100
H	1.85635200	5.95699200	2.56682900
H	1.00155000	4.45019600	2.93339400
H	3.84128400	4.56724700	-0.31233000
H	4.11153200	5.54460100	1.13732700
H	2.37009500	7.13592100	0.46537100
H	2.97739600	6.67238900	-1.12114700
H	5.19067200	0.13979000	2.96243800
H	4.73607900	2.13321000	4.37109100
H	0.22426400	6.91419800	-1.88361000
H	-1.80280200	5.48653800	-2.04281200
C	4.32720000	-0.44513800	0.53494300
C	4.01974300	-1.79610900	0.96187900
C	5.12641200	-0.25442300	-0.55615900
C	3.19707500	-2.03702700	2.08981900
C	4.55560900	-2.91026600	0.24343000
C	5.66788500	-1.33901100	-1.31659200
H	5.38520700	0.75832900	-0.85596400
C	2.93005700	-3.32258200	2.52054500
H	2.75938200	-1.18933700	2.60346100
C	4.25759700	-4.21235400	0.71116000
C	5.38974100	-2.68078300	-0.92842000
C	6.48994600	-1.09136500	-2.44176100
C	3.46966400	-4.42037100	1.82718000
H	2.30164400	-3.48389700	3.39256800
H	4.65654600	-5.07555800	0.18974600
C	5.94804400	-3.72370000	-1.70438500
H	6.69724400	-0.05961200	-2.71719100
C	7.02139000	-2.13081500	-3.17895200
H	3.26412600	-5.43347600	2.16273700
C	6.74322700	-3.45899800	-2.80498000
H	5.75267900	-4.75830600	-1.44403200
H	7.64950200	-1.92690500	-4.04197400
H	7.15522800	-4.28256500	-3.38201700
C	-2.34195400	3.18786700	-0.92452000
C	-3.34779800	3.17237100	0.12106300
C	-2.63182500	2.64377000	-2.14307200
C	-3.09944300	3.76139900	1.38435000
C	-4.62422800	2.57721500	-0.12619700
C	-3.89929900	2.04542700	-2.43654500
H	-1.87432900	2.65723600	-2.92131700

C	-4.05683200	3.75986600	2.37985000
H	-2.13518300	4.22459200	1.56220200
C	-5.58151500	2.59367900	0.91522500
C	-4.90893400	1.99728200	-1.43228700
C	-4.16426400	1.51592700	-3.72268800
C	-5.30971700	3.16808300	2.14249300
H	-3.84298200	4.22008100	3.34090400
H	-6.55818000	2.15013700	0.75548300
C	-6.14525600	1.39509100	-1.76570000
H	-3.38655100	1.58104700	-4.48059600
C	-5.38447100	0.94016000	-4.01961900
H	-6.06866900	3.16538700	2.92039000
C	-6.38045700	0.87690700	-3.02686200
H	-6.93559400	1.33443500	-1.02544000
H	-5.57675500	0.54244500	-5.01253200
H	-7.34270400	0.42453800	-3.25185300

M2-TS1cS

C	-2.81679300	5.64705700	-2.34588800
C	-1.49128700	5.73177900	-1.55646600
C	-1.71831000	4.81967000	-0.30534700
C	-2.60032400	3.73809600	-0.91256200
C	-3.31628300	4.26056600	-1.99868300
C	-2.49750800	5.61684400	0.79513100
C	-1.41050400	6.41252400	1.54602400
C	-0.20319700	5.50993100	1.41804700
C	-0.41573500	4.53247900	0.43337500
C	-2.81453500	2.42193500	-0.50512600
C	-3.84448400	1.65666500	-1.09046500
C	-4.59170500	2.23436600	-2.13131900
C	-4.31679800	3.51395100	-2.61218200
C	0.98238100	5.54703300	2.14200000
C	1.96355500	4.59590500	1.86934100
C	1.76601700	3.57477900	0.92481300
C	0.53784700	3.53124900	0.23246400
O	-1.98392600	1.87015400	0.45960500
O	0.26750200	2.49726700	-0.65158100
P	-0.57290100	1.17398300	-0.09002200
O	-0.86025500	0.33871200	-1.31256100
H	-2.67645300	5.78507100	-3.42435300
H	-3.52637500	6.42105300	-2.02004800
H	-1.21049400	6.75458400	-1.28464200
H	-0.67707000	5.30827800	-2.15555900
H	-2.96712300	4.89966700	1.47789600

H	-3.28931000	6.24526200	0.37477500
H	-1.22954800	7.38814900	1.07238100
H	-1.67679400	6.61499600	2.58997000
H	-5.39276600	1.65260800	-2.57849800
H	-4.88262800	3.91742300	-3.44840100
H	1.14770000	6.30304100	2.90573100
H	2.90900000	4.62456900	2.40338900
C	-1.05736200	-2.99756400	0.32802500
C	-0.46393700	-4.27158000	0.20088400
C	-0.56332400	-5.17870200	1.25954400
C	-1.26646400	-4.79504400	2.40125200
C	-1.84558600	-3.52002000	2.50280300
C	-1.74374100	-2.59043000	1.46657500
C	-0.14208600	-3.04645300	-1.72622400
C	0.26089800	-4.26572900	-1.06512900
H	-0.10572100	-6.16272600	1.19859200
H	-1.36047900	-5.49002700	3.23027700
H	-2.38602600	-3.24891600	3.40467200
H	-2.17371000	-1.59842800	1.54463400
H	0.51915600	-5.15396700	-1.62576300
N	-0.83546200	-2.29749500	-0.86874100
H	-1.02021500	-1.26859800	-1.02883000
C	4.63275200	-3.84004100	-3.98884900
C	4.23887500	-5.04584100	-3.38864400
C	3.45444900	-5.02332700	-2.24265800
C	3.04151700	-3.80372400	-1.67923300
C	3.44968700	-2.58097500	-2.27193100
C	4.24795000	-2.62549400	-3.43537800
C	2.21839000	-3.75944700	-0.46866300
C	2.11886000	-2.49378400	0.24596900
C	2.41705400	-1.26853200	-0.47390100
C	3.07300100	-1.32388500	-1.65942300
N	1.78588100	-2.61766200	1.51621800
N	1.51555500	-1.53822300	2.23932800
C	1.31121200	-1.72510300	3.61058100
O	1.43545600	-2.75987900	4.22150700
H	5.24516000	-3.85633000	-4.88621500
H	4.54935100	-5.99452800	-3.81698600
H	3.15171000	-5.95604800	-1.77150200
H	4.56184900	-1.69068600	-3.89304600
H	2.24439200	-4.63482100	0.17298800
H	2.17564200	-0.31105400	-0.02960900
H	3.35868200	-0.40300900	-2.16002500
O	0.99144200	-0.52589400	4.14660100

C	0.71869300	-0.55373700	5.55325000
H	-0.13269100	-1.20596700	5.76688700
H	1.58909800	-0.91266900	6.10941300
H	0.48660800	0.47674300	5.82301800
O	0.09827900	0.58763000	1.11659900
H	1.17488600	-0.65178300	1.81527000
C	0.12811900	-2.59938600	-3.11910600
H	-0.89685800	-2.31774000	-3.60825200
H	0.80772300	-1.63484200	-3.10174800
H	0.64883000	-3.44986700	-3.71833000
C	2.88178400	2.60067500	0.72805300
C	3.65750200	2.56978000	-0.49906600
C	3.26424400	1.81658300	1.78035600
C	3.29867500	3.36230000	-1.61602500
C	4.82222200	1.74292800	-0.58413200
C	4.41711600	0.96889000	1.73408900
H	2.66913300	1.82280800	2.68932100
C	4.03612400	3.34076100	-2.78326000
H	2.42270400	3.99640800	-1.54515200
C	5.55692300	1.74708300	-1.79463900
C	5.22036900	0.93176600	0.55902500
C	4.76918400	0.17481100	2.85141200
C	5.17607900	2.52286500	-2.87380400
H	3.73603000	3.95601000	-3.62714700
H	6.44556100	1.13167800	-1.88582100
C	6.36337000	0.09798600	0.56533200
H	4.13380000	0.21149900	3.73288500
C	5.88843900	-0.63268000	2.82561900
H	5.76397800	2.50416100	-3.78791400
C	6.69263700	-0.66578200	1.67073000
H	7.00424000	0.04659100	-0.30831100
H	6.14718200	-1.24006300	3.68853700
H	7.57699200	-1.29691600	1.64415800
C	-4.21645600	0.30188500	-0.58889300
C	-4.27253800	-0.84975400	-1.47213500
C	-4.60683300	0.16057100	0.71414700
C	-3.78219800	-0.78113100	-2.80010300
C	-4.80730000	-2.08841100	-0.99656900
C	-5.12041400	-1.06730300	1.23886800
H	-4.55877600	1.01802400	1.37950300
C	-3.85264100	-1.86831900	-3.65014100
H	-3.32656000	0.14214100	-3.13743000
C	-4.86710600	-3.18016000	-1.89592200
C	-5.25489400	-2.20004300	0.38533400

C	-5.52502100	-1.15703500	2.59264900
C	-4.41056400	-3.07687600	-3.19595900
H	-3.48436100	-1.78753100	-4.66709300
H	-5.27452300	-4.12853000	-1.56317800
C	-5.80490600	-3.38174700	0.93526500
H	-5.41486300	-0.28015900	3.22636600
C	-6.05197000	-2.32715500	3.10171000
H	-4.47531200	-3.93383400	-3.86149000
C	-6.19434100	-3.44759900	2.26089000
H	-5.92699400	-4.26339800	0.31562400
H	-6.36014800	-2.38332000	4.14231200
H	-6.61259300	-4.37054600	2.65362200

TS1bR'

H	0.25244900	-0.75768800	2.12802600
C	1.72020400	-1.75103000	-2.07136300
C	2.59032500	-2.85919800	-2.03061300
C	3.88620800	-2.72711300	-2.53154500
C	4.27405800	-1.48467200	-3.04416500
C	3.40007600	-0.38774200	-3.04143800
C	2.09693900	-0.50126500	-2.54845800
C	0.50190100	-3.46317400	-1.24634100
C	1.85543700	-3.92914900	-1.36697000
H	4.57748700	-3.56461700	-2.52704200
H	5.27592600	-1.36585000	-3.44812900
H	3.73809300	0.56914800	-3.42610000
H	1.40672200	0.33489000	-2.52786400
N	0.47671600	-2.16457500	-1.57375300
H	-0.26887000	-1.45196300	-1.41668300
H	2.09915400	-4.97958100	-1.45914700
C	-0.74975400	-4.25846600	-0.93563500
C	-0.44981800	-5.48347000	-0.04898600
C	-1.82659100	-3.40088800	-0.24475500
C	-1.28382100	-4.74886800	-2.31166800
H	0.32843800	-6.12727700	-0.47561800
H	-0.15806100	-5.17741300	0.95953700
H	-1.35872400	-6.08807700	0.04080100
H	-2.07135400	-2.49425800	-0.80484500
H	-2.74657200	-3.98560200	-0.15496900
H	-1.51518500	-3.11964800	0.76283100
H	-2.20255100	-5.32550200	-2.15897000
H	-1.51801500	-3.90469200	-2.96822500

H	-0.55337200	-5.38801500	-2.82095600
C	6.76152500	-3.95234500	0.26204400
C	6.01647400	-5.14245300	0.22914000
C	4.63670100	-5.09652100	0.37439100
C	3.97562500	-3.86768900	0.56097300
C	4.72846200	-2.66271300	0.59242000
C	6.12545300	-2.73037900	0.44070100
C	2.53865400	-3.79154700	0.72857500
C	1.97667600	-2.56666400	1.28347700
C	2.73589300	-1.33515900	1.14361100
C	4.04940900	-1.40066400	0.81695400
N	0.84615200	-2.75463300	1.93322700
N	0.19108400	-1.74014300	2.47913500
C	-0.92040600	-2.07083700	3.27166400
O	-1.30974900	-3.19145200	3.51068500
H	7.84181200	-3.98845800	0.14997300
H	6.51888500	-6.09631700	0.09642200
H	4.05422100	-6.01505500	0.35638200
H	6.70102800	-1.80907800	0.47328800
H	2.02009200	-4.70006600	1.01055100
H	2.25755300	-0.37913600	1.33136900
H	4.63730300	-0.49288100	0.74658400
O	-1.44992500	-0.93003700	3.74001700
C	-2.62005900	-1.09741200	4.55422200
H	-2.92606000	-0.08726600	4.82499200
H	-3.41171700	-1.59498900	3.99013600
H	-2.38258000	-1.68353500	5.44660800
C	-2.29889000	6.10743000	1.60812700
C	-3.24635800	5.21339100	0.78112500
C	-2.32856200	4.55902100	-0.30567700
C	-1.03288000	4.41101700	0.47602900
C	-0.97482900	5.38639600	1.48215600
C	-2.14315800	5.54585500	-1.50726600
C	-3.39868400	5.33970900	-2.38006800
C	-3.75539300	3.89542000	-2.10469100
C	-3.04482500	3.40974100	-0.99740000
C	0.05331200	3.56101400	0.25516500
C	1.27801000	3.80991900	0.91244700
C	1.31461300	4.82865800	1.88287600
C	0.19417800	5.59011900	2.20445700
C	-4.65158100	3.07950800	-2.78371000
C	-4.85263600	1.78259900	-2.31835100
C	-4.12192400	1.24785800	-1.24097100
C	-3.15135700	2.06804500	-0.62387900

O	-0.08802800	2.49640900	-0.62217700
O	-2.31552900	1.57444600	0.36682400
P	-0.77440100	1.08010300	-0.05155200
O	-0.85393100	0.16464600	-1.24519000
O	-0.09121500	0.68774600	1.22820900
H	-2.62116200	6.21647500	2.65036600
H	-2.23869600	7.12254800	1.19034500
H	-4.09025200	5.75727000	0.34470600
H	-3.65342500	4.41921800	1.41747600
H	-1.25031900	5.24811900	-2.06918000
H	-2.00197900	6.58131000	-1.18096300
H	-4.21259200	6.01372900	-2.07687100
H	-3.21246900	5.53237600	-3.44318900
H	2.25658900	5.01781500	2.38884100
H	0.24765500	6.34412100	2.98586000
H	-5.20762200	3.44797000	-3.64224600
H	-5.59882300	1.15129600	-2.79140300
C	2.57182700	3.11780600	0.63606300
C	3.22899000	3.21162000	-0.65808700
C	3.24805000	2.55656200	1.68463400
C	2.58750400	3.80598300	-1.77157700
C	4.57108100	2.73989100	-0.81101000
C	4.59289000	2.07997600	1.57739200
H	2.75864000	2.49029100	2.65267500
C	3.21929500	3.92195100	-2.99415900
H	1.57841300	4.18041700	-1.65622100
C	5.19027500	2.87632100	-2.07626800
C	5.27461100	2.16804600	0.32960100
C	5.25932500	1.54333100	2.70571200
C	4.53473700	3.45123200	-3.14882500
H	2.70098700	4.38174000	-3.83112400
H	6.20844100	2.53016300	-2.21699500
C	6.61051200	1.70303500	0.27206000
H	4.72034600	1.48648700	3.64839200
C	6.56458300	1.10184600	2.61958600
H	5.04126000	3.54616300	-4.10582000
C	7.24375400	1.18310200	1.38833400
H	7.16508200	1.75672400	-0.65849300
H	7.06555500	0.69550300	3.49387800
H	8.27434200	0.84560700	1.31380000
C	-4.47933900	-0.13808100	-0.81830700
C	-5.02145800	-0.42062900	0.50131300
C	-4.47681300	-1.13014800	-1.76033600
C	-5.12595200	0.58861300	1.48863500

C	-5.51650700	-1.72885800	0.80231100
C	-4.97755900	-2.44582400	-1.50658000
H	-4.08402100	-0.91618900	-2.75087700
C	-5.67847600	0.33382900	2.72814600
H	-4.77219200	1.58544400	1.25771800
C	-6.06450700	-1.95978800	2.08685600
C	-5.48839800	-2.76918000	-0.21755900
C	-4.97084000	-3.42811600	-2.52529700
C	-6.14808700	-0.95561600	3.03286400
H	-5.75358400	1.13140800	3.46254400
H	-6.44626100	-2.94276900	2.33948300
C	-5.95554300	-4.08757800	-0.00242800
H	-4.58561600	-3.15710200	-3.50566100
C	-5.44182900	-4.70455700	-2.28779000
H	-6.58697200	-1.16355500	4.00534500
C	-5.93280700	-5.03558500	-1.01030000
H	-6.34282500	-4.37523400	0.96883600
H	-5.43594800	-5.44843700	-3.08007900
H	-6.30083900	-6.03897900	-0.81352300

TS1bS'

H	-1.37545300	1.58947700	-0.37999400
C	2.50882700	0.93588300	0.41961800
C	3.31118600	2.08474900	0.55380700
C	3.89051300	2.38701700	1.78369900
C	3.63586000	1.53082700	2.86024200
C	2.80423200	0.41355900	2.71534800
C	2.22121300	0.09232400	1.48604000
C	2.67279500	1.82206000	-1.65942200
C	3.26550100	2.77262800	-0.73875900
H	4.52604400	3.25895600	1.90396900
H	4.09044800	1.73740800	3.82548500
H	2.61828900	-0.23382900	3.56646100
H	1.57724300	-0.76990900	1.38363900
N	2.13931300	0.83235800	-0.94070600
H	1.46575000	0.11463900	-1.28284500
H	4.03230000	3.46418400	-1.06753700
C	2.71117100	1.84500100	-3.17591800
C	4.21093800	1.73744200	-3.57001100
C	1.94807000	0.64997000	-3.77743100
C	2.14452800	3.16294900	-3.75174800
H	4.78494700	2.60201000	-3.21909800
H	4.67248400	0.83243000	-3.16308500

H	4. 28953800	1. 70382400	-4. 66288200
H	0. 88294500	0. 68120200	-3. 54014300
H	2. 04807300	0. 67734300	-4. 86778200
H	2. 35427800	-0. 30570700	-3. 42887500
H	2. 25774100	3. 14471300	-4. 84151100
H	1. 08464300	3. 27562900	-3. 51582400
H	2. 69890500	4. 03520600	-3. 38391400
C	3. 20009400	6. 65854500	2. 70173000
C	3. 66751600	6. 83594000	1. 39155500
C	3. 18786400	6. 02089400	0. 37309100
C	2. 23842600	5. 01945200	0. 63768300
C	1. 75640500	4. 84438100	1. 96267300
C	2. 25559900	5. 67780500	2. 97989700
C	1. 73049400	4. 15029700	-0. 42302700
C	0. 51735400	3. 37183800	-0. 13667100
C	0. 14244700	3. 13289600	1. 24636100
C	0. 73586600	3. 84590700	2. 23176900
N	-0. 09571900	2. 97319700	-1. 22239500
N	-1. 16399500	2. 18732800	-1. 19473900
C	-1. 61875800	1. 75555700	-2. 45345600
O	-1. 18262700	2. 14166100	-3. 51609500
H	3. 57264100	7. 29340600	3. 50100300
H	4. 39783700	7. 60944100	1. 17220400
H	3. 54456200	6. 15726400	-0. 64566400
H	1. 88660500	5. 54852800	3. 99435700
H	1. 76724800	4. 55282000	-1. 42880300
H	-0. 62020800	2. 39864300	1. 47966700
H	0. 43339700	3. 69725100	3. 26492000
O	-2. 60772500	0. 88033700	-2. 26204400
C	-3. 04705400	0. 12462800	-3. 40233500
H	-2. 80148800	-0. 91997200	-3. 20486000
H	-4. 12730000	0. 25824300	-3. 48453300
H	-2. 55028700	0. 48270800	-4. 30421400
C	-2. 35560500	-6. 21722700	-1. 47423800
C	-3. 32041400	-5. 25659400	-0. 74469000
C	-2. 43700200	-4. 56308100	0. 34231200
C	-1. 10508700	-4. 47909100	-0. 38894100
C	-1. 01856900	-5. 52302700	-1. 32202500
C	-2. 30598200	-5. 49513600	1. 59627300
C	-3. 55935600	-5. 19708500	2. 44407100
C	-3. 84302900	-3. 75108800	2. 10352800
C	-3. 13227100	-3. 36211700	0. 96019300
C	-0. 01339400	-3. 63190800	-0. 17961800
C	1. 24004000	-3. 96219900	-0. 74046900

C	1.30585700	-5.05127300	-1.62785400
C	0.18240700	-5.80437000	-1.96177800
C	-4.66472300	-2.84827600	2.76836200
C	-4.77843800	-1.55627300	2.26237000
C	-4.05429100	-1.12470000	1.13652000
C	-3.18624900	-2.04206500	0.50666200
O	-0.17554500	-2.47523000	0.57345700
O	-2.37330000	-1.68134400	-0.56299300
P	-0.83355100	-1.13521700	-0.21068500
O	-0.91216500	-0.02791300	0.80269900
O	-0.10041400	-0.92575300	-1.51238500
H	-2.62868100	-6.37459400	-2.52435200
H	-2.34401700	-7.20957800	-1.00146200
H	-4.19402000	-5.75855500	-0.31586900
H	-3.68167400	-4.49189800	-1.44161200
H	-1.40879700	-5.20466300	2.15512700
H	-2.20141900	-6.55046700	1.32462000
H	-4.40050800	-5.84400800	2.15567200
H	-3.39424900	-5.35626000	3.51613400
H	2.27032700	-5.29995000	-2.06082000
H	0.25732200	-6.61205800	-2.68569300
H	-5.21780700	-3.14177800	3.65723100
H	-5.44232300	-0.84506700	2.74609300
C	-4.34972900	0.25182000	0.63244800
C	-5.10856600	0.38884300	-0.49366700
C	-4.00217900	1.43109000	1.40243800
C	-5.56741700	1.65907200	-0.96674100
H	-5.39704200	-0.49834500	-1.05176000
C	-4.46048700	2.71845500	0.98115200
C	-3.22165200	1.33071000	2.58031600
C	-6.35524500	1.75068500	-2.13884500
C	-5.24774200	2.84072300	-0.23882400
C	-4.13837500	3.83806800	1.78532100
H	-2.83367500	0.35985000	2.86294200
C	-2.93004000	2.44439400	3.34412400
C	-6.80592300	2.97088100	-2.60224000
H	-6.60544600	0.83474100	-2.66994600
C	-5.72221100	4.07564800	-0.74001100
C	-3.39938100	3.70919700	2.94595600
H	-4.48310500	4.82489100	1.49621600
H	-2.33638800	2.34078500	4.24886800
C	-6.48041500	4.14336700	-1.89518500
H	-7.40759200	3.02727800	-3.50536600
H	-5.48951100	4.99795900	-0.21881800

H	-3.17773300	4.58856900	3.54517000
H	-6.82728300	5.10809500	-2.25568000
C	2.52498200	-3.27076800	-0.42661900
C	3.08575200	-3.28374900	0.91551100
C	3.27491600	-2.76802600	-1.45416900
C	2.37450700	-3.83722500	2.00753100
C	4.39672100	-2.75899300	1.14517500
C	4.59892300	-2.25561000	-1.27185000
H	2.86110700	-2.77258300	-2.45940200
C	2.90648700	-3.85688100	3.28197000
H	1.39210600	-4.25841500	1.83280500
C	4.91104700	-2.79347000	2.46271300
C	5.17431500	-2.23500300	0.03019000
C	5.35211200	-1.79399200	-2.37812100
C	4.18660100	-3.32462800	3.51274700
H	2.33696600	-4.28766300	4.10101500
H	5.90082300	-2.39891300	2.66401200
C	6.48685600	-1.72429800	0.16570000
H	4.90237500	-1.83896700	-3.36748700
C	6.63630800	-1.31135600	-2.21537900
H	4.61273000	-3.33772300	4.51252000
C	7.20345100	-1.27207700	-0.92771400
H	6.95629800	-1.68641700	1.14253600
H	7.20688700	-0.96867300	-3.07445900
H	8.21184600	-0.89099300	-0.79037000

TS1cR'

C	2.81865700	1.47154900	0.69777300
C	4.22487800	1.48466300	0.81150000
C	4.81623500	1.64730900	2.06382200
C	3.98230700	1.77930400	3.17784300
C	2.58776700	1.73173900	3.04734200
C	1.97612800	1.57457200	1.80032600
C	3.62185600	1.33933800	-1.41065700
C	4.74909000	1.24532300	-0.53056400
H	5.89624700	1.67559400	2.17164300
H	4.42219200	1.92073100	4.16109700
H	1.96292300	1.82647900	3.93032200
H	0.89763100	1.53062600	1.70846600
H	5.74795100	1.51427700	-0.85233800
N	2.50656600	1.36938400	-0.67276000
H	1.54580900	1.20696100	-1.04789400
C	7.90461300	-1.47330300	2.54883900

C	8.33269700	-0.99513200	1.30064100
C	7.40814100	-0.79901000	0.28361600
C	6.04414100	-1.07691700	0.48775100
C	5.60964100	-1.56890800	1.74941600
C	6.56239800	-1.75716900	2.76719500
C	5.05953800	-0.87822800	-0.56381000
C	3.74326200	-1.48863600	-0.39488500
C	3.30826600	-1.86495100	0.93932300
C	4.21108600	-1.90192100	1.94832100
N	3.09111600	-1.60983900	-1.52987600
N	1.84191300	-2.04195200	-1.58477100
C	1.23221700	-1.92738400	-2.85301700
O	1.78687600	-1.54286400	-3.85635100
H	8.62647700	-1.62693700	3.34612700
H	9.38404800	-0.78339500	1.12938900
H	7.73528700	-0.43255400	-0.68693400
H	6.23474400	-2.13622200	3.73183900
H	5.42086900	-0.86346500	-1.58718400
H	2.26817500	-2.11484800	1.11666600
H	3.90084500	-2.20989700	2.94322400
O	-0.03888200	-2.33077000	-2.75164300
C	-0.85988600	-2.03458900	-3.90135900
H	-0.44488700	-2.50910600	-4.79294500
H	-1.84083500	-2.43686900	-3.66202500
H	-0.90974300	-0.95225200	-4.03553300
H	1.21766500	-1.98257100	-0.75843300
C	3.58751800	1.29025600	-2.89687600
H	3.15194100	0.34250900	-3.24639900
H	2.97191500	2.10843900	-3.28792200
H	4.59567200	1.38578100	-3.30810300
P	-0.67176400	-0.09105900	-0.31934400
O	-0.07004800	0.55352400	-1.54359900
O	-2.11668600	-0.80447500	-0.73329300
O	-1.25072300	1.12074000	0.68464800
C	-2.97882700	-1.09975000	0.30935200
C	-3.73911800	-0.08222900	0.86800700
C	-2.33607900	1.84836900	0.22918700
C	-3.60426400	1.28959800	0.30434700
C	-4.56696300	-0.37424400	2.00415400
C	-6.16564000	-1.03786600	4.25017500
C	-5.27508000	0.62751200	2.72496400
C	-4.65398300	-1.72543600	2.47247000
C	-5.47498900	-2.02830000	3.59220100
C	-6.05179400	0.30386300	3.81533000

H	-5.18954900	1.66204600	2.41360700
H	-5.53574100	-3.06135200	3.92624200
H	-6.57797500	1.08906600	4.35152300
H	-6.78633200	-1.27884900	5.10869000
C	-4.72019100	2.01664500	-0.23240200
C	-6.86506700	3.51976200	-1.32098700
C	-6.03225700	1.47231300	-0.31683300
C	-4.50734700	3.33462500	-0.75222900
C	-5.60486000	4.06808900	-1.27837900
C	-7.07306100	2.20360900	-0.84473900
H	-6.20849800	0.46149800	0.03170800
H	-5.42394500	5.07050900	-1.65903700
H	-8.06424000	1.76185400	-0.90194700
H	-7.69687100	4.08632600	-1.73014600
C	-3.89830300	-2.73283000	1.82546400
H	-3.97093400	-3.75492400	2.18699300
C	-3.05785000	-2.44368500	0.77217900
C	-3.19726500	3.87149800	-0.76099100
H	-3.04246600	4.86887200	-1.16412600
C	-2.11700900	3.15055500	-0.30135900
O	0.15853000	-1.02790100	0.51558900
C	-0.74942300	3.72923800	-0.39294000
C	-0.05939300	4.16699800	0.73910400
C	-0.11430100	3.88923400	-1.62861100
C	1.20310700	4.74876400	0.65998500
C	1.15552200	4.45189200	-1.72961600
C	1.81438600	4.88683200	-0.58301100
C	-2.24112600	-3.51725600	0.15099900
C	-1.27894800	-4.21921500	0.88412500
C	-2.41445600	-3.89229900	-1.18204300
C	-0.51822200	-5.23757200	0.31525900
C	-1.66409600	-4.90180300	-1.77386000
C	-0.71022100	-5.57905500	-1.02085000
F	-1.06260900	-3.92366300	2.17258700
F	0.39900600	-5.88789100	1.04488500
F	0.01843800	-6.55262400	-1.57654500
F	-1.84705300	-5.21400700	-3.06437500
F	-3.32659700	-3.26232100	-1.94082600
F	-0.61029400	4.02078000	1.95260400
F	1.83579600	5.15598900	1.76664700
F	3.03727700	5.42097800	-0.67534100
F	1.76426500	4.54606200	-2.92361000
F	-0.71736300	3.49600900	-2.75417000

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C	3.05317000	0.37268500	-2.10117500
C	4.42218100	0.65630400	-1.92760300
C	5.36898700	-0.29730000	-2.30412300
C	4.91387800	-1.51281100	-2.82487300
C	3.54414100	-1.78163100	-2.96369000
C	2.58163600	-0.83374400	-2.60264600
C	3.13983300	2.48063400	-1.31727300
C	4.49165000	1.97688300	-1.30103700
H	6.43199000	-0.10535600	-2.19473800
H	5.63548400	-2.26722700	-3.12513300
H	3.22260900	-2.74142500	-3.35415300
H	1.51730700	-1.01845700	-2.70459700
H	5.33895700	2.64444700	-1.40579400
N	2.32220300	1.50434600	-1.70447600
H	1.27905100	1.45138200	-1.59522300
C	8.25207200	-0.79572600	0.80047100
C	8.38647200	0.59011200	0.62773400
C	7.25607000	1.39818500	0.62109500
C	5.97605700	0.84335900	0.79268100
C	5.83837200	-0.55886800	0.97508800
C	6.99401300	-1.36020300	0.97268100
C	4.77459200	1.67030900	0.77852900
C	3.55195500	1.09700600	1.34076000
C	3.42349400	-0.35151900	1.37812300
C	4.52160600	-1.12549000	1.20332900
N	2.71719800	1.99331600	1.82584900
N	1.54707900	1.62049300	2.33197200
C	0.76060700	2.62475800	2.91482300
O	1.06549000	3.79147400	3.01531500
H	9.13466000	-1.42927100	0.80443600
H	9.37125000	1.03124400	0.50403400
H	7.35652700	2.47364900	0.49159900
H	6.89123300	-2.43283300	1.11520700
H	4.90295200	2.72808800	0.98943200
H	2.45769700	-0.80014200	1.57948700
H	4.43792000	-2.20576900	1.27878600
O	-0.37202500	2.05158900	3.35475700
C	-1.27986900	2.92019500	4.05283900
H	-1.43043700	3.84911100	3.50380600
H	-0.88550800	3.14551700	5.04840700
H	-2.21169800	2.36084400	4.12791400
H	1.06943600	0.74314600	2.03726800

C	2.65878300	3.80390800	-0.84245500
H	3.42706600	4.56800900	-0.99328200
H	2.44376000	3.75603600	0.23747000
H	1.75095200	4.11243400	-1.36689200
P	-0.69197700	-0.01770200	-0.15274100
O	-0.23196500	0.81837400	-1.31814800
O	-1.36135600	-1.38943900	-0.81270700
O	-2.05238600	0.65327100	0.52873400
C	-2.16062200	-2.15683900	0.00969500
C	-3.45527400	-1.74515800	0.29014500
C	-3.21570200	0.66849300	-0.21149200
C	-3.95854800	-0.49528600	-0.34914000
C	-4.23025200	-2.51175500	1.22642300
C	-5.68891400	-4.07261300	3.09238900
C	-5.50833600	-2.09725500	1.69355700
C	-3.68305200	-3.72571100	1.75892700
C	-4.44557000	-4.49231700	2.68088300
C	-6.21603100	-2.85575200	2.59976700
H	-5.92272300	-1.16168200	1.33621400
H	-4.01799000	-5.41521200	3.06555600
H	-7.18762700	-2.51204900	2.94442200
H	-6.26056700	-4.66360400	3.80251100
C	-5.13868600	-0.46443500	-1.16909300
C	-7.45295100	-0.31736300	-2.80413000
C	-5.89162400	-1.62903200	-1.48744500
C	-5.56262300	0.78216800	-1.73713000
C	-6.73447300	0.82491800	-2.53947700
C	-7.01525200	-1.55656300	-2.28067900
H	-5.56473400	-2.58931300	-1.10645700
H	-7.04484700	1.78183100	-2.95247600
H	-7.56767700	-2.46324800	-2.51230400
H	-8.34415900	-0.27426000	-3.42398200
C	-2.38054700	-4.13147000	1.37459500
H	-1.97920700	-5.05814300	1.77599900
C	-1.61393400	-3.36482600	0.52628300
C	-4.78642600	1.94778100	-1.51788400
H	-5.11046400	2.88600300	-1.96062400
C	-3.62134800	1.90407300	-0.78731300
O	0.22883500	-0.37844900	0.97969900
C	-0.23292800	-3.76062900	0.14814700
C	-2.76376500	3.10923800	-0.62010200
C	-1.06607000	5.33543200	-0.27788600
C	0.79637100	-3.83110400	1.09039400
C	2.10025000	-4.15946100	0.72779700

C	2.40693400	-4.41166900	-0.60455000
C	1.39925700	-4.36347800	-1.56279600
C	0.10295500	-4.03277800	-1.18182600
F	0.55353300	-3.57085900	2.38014000
F	3.07797800	-4.18666800	1.65131500
F	3.66384200	-4.69727600	-0.96318800
F	1.69120100	-4.60779400	-2.85111400
F	-0.83800300	-3.98452500	-2.13174100
C	-1.94058000	3.55966300	-1.65531400
C	-1.09765900	4.65544100	-1.49097700
C	-1.89202100	4.92173900	0.76296600
C	-2.71142000	3.81065100	0.58586900
F	-1.93782200	2.93734800	-2.83678600
F	-0.26954500	5.03216400	-2.48159900
F	-0.24884300	6.38079200	-0.11904900
F	-1.88018700	5.58059200	1.93118400
F	-3.46824600	3.41658500	1.62154100