

**Transfer Hydrogenation of *ortho*-Hydroxybenzophenone  
Ketimines Catalysed by BINOL-derived Phosphoric Acid  
Occurs by a 14-Membered Bifunctional Transition**

**Structure**

*Jolene P. Reid and Jonathan M. Goodman\**

Centre for Molecular Informatics, Department of Chemistry, University of  
Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom

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## **Full list of authors in the Gaussian09 reference**

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

## Computational Methods

The preferred reaction pathway was first investigated using buta-1,3-diene-1,4-diol-phosphoric acid as a model for the catalyst, before studying the full molecular system. Quantum mechanical calculations were performed using the Gaussian 09 (revision D.01).<sup>1</sup> The B3LYP density functional,<sup>2-3</sup> and split-valence polarized 6-31G\*\* basis set,<sup>4-5</sup> were used for all geometry optimizations. Single-point energies were taken using the M06-2X density functional,<sup>6</sup> and 6-31G\*\* basis set.<sup>4-5</sup> This energy was used to correct the gas-phase energy obtained from the B3LYP calculations.

For the QM/MM hybrid calculations on the full catalyst, transition states were located first, by a conformational search in MacroModel (version 9.9)<sup>7</sup> using the OPLS-2005 force field.<sup>8-10</sup> Selected conformers below 10 kJ mol<sup>-1</sup> of the minimum were optimized using the ONIOM method implemented in Gaussian 09 (revision D.01).<sup>1</sup> The B3LYP density functional,<sup>2-3</sup> and split-valence polarized 6-31G\*\* basis set,<sup>4-5</sup> were used for the high-layer, and the force field UFF,<sup>11</sup> was used for the low-layer. The reactants and the phosphoric acid moiety of the catalyst were included in the high-layer, and the remaining regions of the catalyst were treated as the low-layer. This method has previously been shown to give excellent results when used to describe reactions catalyzed by chiral phosphoric acids.<sup>12-17</sup> The position of the partition within the catalyst was chosen as the phosphoric acid binds directly to the reagents, whereas the remaining catalyst acts as steric bulk and can be adequately described by molecular mechanics. We use the Kekulé bonding structure for all catalysts ensuring that the connectivity in the catalyst backbone is consistent between the structures allowing for accurate energy and geometry comparisons. We have re-optimized the lowest energy TS structures for reaction 1, using the delocalized bonding arrangement and have

concluded that it does not affect the relative energies to an appreciable extent. All calculations were performed with the (*S*)-catalyst for model consistency. Single point energy calculations were performed on the resulting structures using M06-2X density functional,<sup>6</sup> and the 6-31G\*\* basis set,<sup>4-5</sup> using non-default convergence criteria (fine grid density, ultrafine accuracy level) as implemented in the Jaguar program (version 7.9).<sup>18</sup> This energy was used to correct the gas-phase energy derived from the ONIOM calculations. Free energies in solution were derived from structures optimized in the gas phase at the ONIOM (B3LYP/6-31G\*\* :UFF), level of theory by means of a single point calculation using M06-2X/6-31G\*\* with the polarizable continuum model (PCM) as implemented in the Jaguar program (version 7.9), using benzene (probe radius = 2.60 Å) as the solvent.<sup>19</sup> These values were used to correct the Gibbs free energy derived from the ONIOM calculations.

## Buta-1,3-diene-1,4-diol-phosphoric acid Model Results

### TS1

(B3LYP/6-31G\*\*) Energy = -2021.876859

(B3LYP/6-31G\*\*) Free Energy = -2021.445237

M06-2X/6-31G\*\* Derived free energy = -2020.729720

Number of Imaginary Frequencies = 1 (-761.42)

### B3LYP/6-31G\*\* Geometry

C	-5.73420	0.54070	0.71380	H	1.05330	2.08740	2.39160
C	-6.14550	-0.19100	-0.33010	N	0.81180	1.20400	1.97290
C	-5.44680	-0.40900	-1.58980	O	-0.94370	-0.77100	2.49060
C	-4.17150	-0.16890	-1.94150	H	-1.84330	-0.94850	2.06920
H	-7.12040	-0.65940	-0.23090	C	1.81840	-0.51790	-1.37300
H	-6.32800	0.66030	1.61420	C	0.47290	-0.50250	-1.68430
H	-3.84650	-0.36610	-2.95900	N	-0.20120	0.68470	-1.54580
H	-6.04670	-0.83140	-2.39150	H	-1.22000	0.66010	-1.63490
O	-3.12880	0.32530	-1.19850	C	0.35010	1.87950	-1.18480
P	-3.11360	0.50690	0.49380	C	-0.54300	3.07680	-1.30100
O	-4.55710	1.25450	0.75060	H	-1.53240	2.78480	-1.65130
O	-3.11630	-0.87300	1.10520	H	-0.65820	3.55560	-0.32830
O	-2.01530	1.48910	0.73250	H	-0.09750	3.81030	-1.97660
H	-0.17710	1.01700	1.81690	C	-0.36230	-1.64850	-2.18290
C	1.76850	0.21640	1.89810	H	-1.42150	-1.43090	-2.03510
C	0.62910	-3.95580	1.62170	H	-0.17750	-1.82960	-3.24640
C	-0.34020	-3.01710	1.94860	H	-0.11190	-2.56400	-1.64890
C	-0.01200	-1.65620	2.09970	C	1.67900	1.88310	-0.78680
C	1.32310	-1.22910	1.87960	C	2.39090	0.63190	-0.70540
C	2.28200	-2.20870	1.55940	H	2.25150	0.30400	0.70160
C	1.95650	-3.55500	1.43830	H	3.47460	0.66750	-0.67520
H	0.35190	-5.00130	1.51900	C	2.75600	-1.63980	-1.61700
H	-1.37310	-3.31030	2.10800	C	2.34810	3.14900	-0.41140
H	3.30280	-1.90040	1.35790	H	3.99760	-3.43790	-3.10720
H	2.72730	-4.28050	1.19780	H	3.43220	-4.21140	-1.60880
C	3.00830	0.52990	2.74000	C	3.11510	-3.76850	-2.55540
H	3.33450	1.55760	2.55540	H	2.54000	-4.48540	-3.14060
H	2.76570	0.41670	3.80190	C	4.33510	4.10380	0.43110
H	3.84080	-0.13360	2.50440	H	3.81200	4.68250	1.19600

H	5.29400	3.74740	0.80590	O	1.88530	4.26880	-0.52170
H	4.47660	4.73460	-0.44960	O	3.59110	2.92190	0.08990
O	3.91840	-1.62340	-1.25050	O	2.22440	-2.66440	-2.31740

**Additional conformations for Mechanism A (Wang's proposed mode)**

(B3LYP/6-31G\*\*) Energy = -2021.847959

(B3LYP/6-31G\*\*) Free Energy = -2021.415343

M06-2X/6-31G\*\* Derived free energy = -2020.695700

Number of Imaginary Frequencies = 1 (-306.28)

**B3LYP/6-31G\*\* Geometry**

C	-5.86350	1.51710	0.71590	C	-0.27110	0.03390	2.13450
C	-6.62060	0.40670	0.76720	H	0.05280	-0.90260	2.59160
C	-6.44020	-0.88620	0.11980	H	0.21230	0.86830	2.65400
C	-5.51460	-1.25950	-0.77770	H	-1.35320	0.13100	2.23830
H	-7.50800	0.50120	1.38730	H	-0.36000	2.05950	0.68910
H	-6.17390	2.41480	1.24270	N	-0.16930	1.32710	0.01210
H	-5.50730	-2.26030	-1.19930	O	-1.73070	-2.25960	1.15760
H	-7.15730	-1.65670	0.38970	H	-2.33190	-1.44430	1.11980
O	-4.52140	-0.47570	-1.30770	C	3.50650	-0.66050	0.23680
P	-3.61580	0.54720	-0.37120	C	3.90770	-0.65980	-1.08440
O	-4.69770	1.73700	0.03810	N	3.70730	0.49230	-1.80190
O	-3.21480	-0.16710	0.90180	H	3.97640	0.47210	-2.77720
O	-2.61510	1.18970	-1.28070	C	3.18530	1.66660	-1.32930
H	-0.96360	1.27140	-0.65530	C	3.09970	2.77830	-2.33480
C	0.11510	0.09530	0.65250	H	3.42690	2.43940	-3.32190
C	-0.12440	-3.39260	-1.90420	H	2.07030	3.13480	-2.40550
C	-0.86550	-3.37100	-0.73020	H	3.71300	3.62890	-2.03130
C	-0.90770	-2.22990	0.09150	C	4.51920	-1.80190	-1.83930
C	-0.10480	-1.10870	-0.24160	H	4.81060	-1.49310	-2.84780
C	0.58530	-1.13810	-1.46810	H	5.38780	-2.19840	-1.31340
C	0.58380	-2.25320	-2.29950	H	3.79820	-2.62130	-1.91450
H	-0.12840	-4.28100	-2.52980	C	2.79630	1.70190	-0.00260
H	-1.47720	-4.21640	-0.43220	C	2.84970	0.49460	0.77020
H	1.12330	-0.24560	-1.77040	H	1.31990	0.07900	0.74590
H	1.11550	-2.23430	-3.24680	H	2.76300	0.59490	1.84550

C	3.68110	-1.88060	1.07480	H	2.33880	5.41770	1.52940
C	2.28590	2.90240	0.71490	H	1.83820	6.00170	-0.09400
H	2.67500	-3.74240	2.67430	H	0.71140	5.03990	0.91550
H	4.19500	-3.12420	3.36750	O	4.27860	-2.88370	0.73370
C	3.15400	-2.88120	3.14400	O	1.94450	2.87000	1.88210
H	2.62050	-2.58860	4.04670	O	2.27450	4.02470	-0.02880
C	1.75480	5.19600	0.63410	O	3.08330	-1.73630	2.27040

(B3LYP/6-31G\*\*) Energy = -2021.847959

(B3LYP/6-31G\*\*) Free Energy = -2021.415339

M06-2X/6-31G\*\* Derived free energy = -2020.695690

Number of Imaginary Frequencies = 1 (-306.19)

#### B3LYP/6-31G\*\* Geometry

C	5.51490	-1.25960	-0.77760	H	-1.11610	-2.23400	-3.24700
C	6.44050	-0.88630	0.12000	C	0.27110	0.03360	2.13440
C	6.62080	0.40660	0.76720	H	-0.05290	-0.90290	2.59150
C	5.86360	1.51700	0.71600	H	1.35320	0.13060	2.23820
H	7.15750	-1.65680	0.39000	H	-0.21210	0.86800	2.65400
H	5.50750	-2.26040	-1.19920	H	0.36020	2.05920	0.68920
H	6.17400	2.41480	1.24270	N	0.16940	1.32690	0.01210
H	7.50830	0.50130	1.38710	O	1.73040	-2.26000	1.15720
O	4.69750	1.73680	0.03860	H	2.33170	-1.44480	1.11940
P	3.61600	0.54690	-0.37120	C	-2.79610	1.70210	-0.00260
O	4.52200	-0.47560	-1.30770	C	-3.18520	1.66680	-1.32930
O	3.21490	-0.16780	0.90170	N	-3.70750	0.49250	-1.80180
O	2.61530	1.18940	-1.28060	H	-3.97650	0.47230	-2.77710
H	0.96370	1.27110	-0.65520	C	-3.90800	-0.65940	-1.08430
C	-0.11520	0.09510	0.65250	C	-4.51960	-1.80160	-1.83900
C	0.12380	-3.39250	-1.90460	H	-4.81130	-1.49270	-2.84740
C	0.86490	-3.37120	-0.73070	H	-3.79860	-2.62090	-1.91440
C	0.90730	-2.23020	0.09110	H	-5.38800	-2.19810	-1.31290
C	0.10450	-1.10880	-0.24180	C	-3.09950	2.77840	-2.33480
C	-0.58570	-1.13810	-1.46820	H	-3.42700	2.43960	-3.32180
C	-0.58440	-2.25310	-2.29970	H	-3.71250	3.62920	-2.03120
H	0.12760	-4.28090	-2.53030	H	-2.07000	3.13460	-2.40570
H	1.47650	-4.21660	-0.43280	C	-3.50670	-0.66020	0.23690
H	-1.12360	-0.24550	-1.77040	C	-2.84980	0.49490	0.77030

H	-1.32000	0.07900	0.74600	C	-3.15430	-2.88070	3.14430
H	-2.76290	0.59520	1.84550	H	-2.67540	-3.74200	2.67450
C	-2.28550	2.90250	0.71480	H	-2.62070	-2.58820	4.04690
C	-3.68140	-1.88020	1.07500	H	-4.19530	-3.12360	3.36790
H	-0.71040	5.03960	0.91520	O	-1.94420	2.87010	1.88210
H	-1.83710	6.00160	-0.09430	O	-4.27890	-2.88330	0.73400
C	-1.75370	5.19600	0.63390	O	-3.08360	-1.73590	2.27060
H	-2.33760	5.41790	1.52910	O	-2.27380	4.02480	-0.02900

(B3LYP/6-31G\*\*) Energy = -2021.846468

(B3LYP/6-31G\*\*) Free Energy = -2021.413577

M06-2X/6-31G\*\* Derived free energy = -2020.693990

Number of Imaginary Frequencies = 1 (-280.92)

#### B3LYP/6-31G\*\* Geometry

C	6.00550	1.43580	-0.50150	H	-1.01500	-0.21750	1.80600
C	6.68790	0.28780	-0.66320	H	-1.04950	-2.35440	3.06220
C	6.39610	-1.05730	-0.18470	C	0.31750	0.44910	-2.07570
C	5.42230	-1.46220	0.64510	H	-0.02640	-0.41450	-2.64710
H	7.60390	0.39290	-1.23830	H	-0.14590	1.35060	-2.49250
H	6.39860	2.36480	-0.90430	H	1.40190	0.53710	-2.16250
H	5.32500	-2.50270	0.94050	H	0.38750	2.29780	-0.38630
H	7.06030	-1.84210	-0.53640	N	0.21140	1.48170	0.19080
O	4.48210	-0.66730	1.25080	O	1.66620	-2.01390	-1.40760
P	3.66460	0.51000	0.42040	H	2.30520	-1.23440	-1.28800
O	4.83000	1.66050	0.15640	C	-2.83200	1.81500	0.23750
O	3.24320	-0.03520	-0.92850	C	-3.22900	1.58180	1.54300
O	2.69060	1.11630	1.38140	N	-3.67880	0.32900	1.85380
H	1.02500	1.33880	0.82060	H	-3.94900	0.16890	2.81570
C	-0.07860	0.34060	-0.59920	C	-3.80650	-0.73290	0.99000
C	0.08410	-3.41410	1.55310	C	-4.34070	-1.99330	1.60560
C	0.79010	-3.29470	0.36350	H	-3.54440	-2.74250	1.64830
C	0.86580	-2.07080	-0.32710	H	-4.70240	-1.80810	2.62130
C	0.12180	-0.96060	0.15100	H	-5.15260	-2.41120	1.01130
C	-0.53110	-1.09550	1.39090	C	-3.22470	2.57320	2.66760
C	-0.55580	-2.29460	2.09620	H	-3.53790	2.10410	3.60510
H	0.06790	-4.36500	2.07900	H	-2.22400	2.99280	2.79100
H	1.35490	-4.12660	-0.04480	H	-3.88300	3.41520	2.44480



C	-3.41280	-0.53050	-0.31680	H	-0.80310	4.90820	-1.37310
C	-2.82090	0.72210	-0.68670	C	-3.90470	-3.76560	-2.05280
H	-1.28000	0.34920	-0.70300	H	-2.88730	-3.91950	-2.41720
H	-2.74290	0.93200	-1.74680	H	-4.28460	-4.66690	-1.57390
C	-2.42200	3.18110	-0.18280	H	-4.54450	-3.46860	-2.88610
C	-3.46260	-1.54520	-1.41110	O	-2.48620	4.17620	0.51340
H	-1.29260	4.31660	-2.99560	O	-3.11140	-1.29030	-2.54540
H	-2.46590	5.17780	-1.94420	O	-3.91490	-2.75190	-1.02460
C	-1.61640	4.49180	-1.97090	O	-2.00140	3.19790	-1.46450

(B3LYP/6-31G\*\*) Energy = -2021.846468

(B3LYP/6-31G\*\*) Free Energy = -2021.413566

M06-2X/6-31G\*\* Derived free energy = -2020.693977

Number of Imaginary Frequencies = 1 (-280.46)

#### B3LYP/6-31G\*\* Geometry

C	5.51490	-1.25960	-0.77760	H	1.47650	-4.21660	-0.43280
C	6.44050	-0.88630	0.12000	H	-1.12360	-0.24550	-1.77040
C	6.62080	0.40660	0.76720	H	-1.11610	-2.23400	-3.24700
C	5.86360	1.51700	0.71600	C	0.27110	0.03360	2.13440
H	7.15750	-1.65680	0.39000	H	-0.05290	-0.90290	2.59150
H	5.50750	-2.26040	-1.19920	H	1.35320	0.13060	2.23820
H	6.17400	2.41480	1.24270	H	-0.21210	0.86800	2.65400
H	7.50830	0.50130	1.38710	H	0.36020	2.05920	0.68920
O	4.69750	1.73680	0.03860	N	0.16940	1.32690	0.01210
P	3.61600	0.54690	-0.37120	O	1.73040	-2.26000	1.15720
O	4.52200	-0.47560	-1.30770	H	2.33170	-1.44480	1.11940
O	3.21490	-0.16780	0.90170	C	-2.79610	1.70210	-0.00260
O	2.61530	1.18940	-1.28060	C	-3.18520	1.66680	-1.32930
H	0.96370	1.27110	-0.65520	N	-3.70750	0.49250	-1.80180
C	-0.11520	0.09510	0.65250	H	-3.97650	0.47230	-2.77710
C	0.12380	-3.39250	-1.90460	C	-3.90800	-0.65940	-1.08430
C	0.86490	-3.37120	-0.73070	C	-4.51960	-1.80160	-1.83900
C	0.90730	-2.23020	0.09110	H	-4.81130	-1.49270	-2.84740
C	0.10450	-1.10880	-0.24180	H	-3.79860	-2.62090	-1.91440
C	-0.58570	-1.13810	-1.46820	H	-5.38800	-2.19810	-1.31290
C	-0.58440	-2.25310	-2.29970	C	-3.09950	2.77840	-2.33480
H	0.12760	-4.28090	-2.53030	H	-3.42700	2.43960	-3.32180

H	-3.71250	3.62920	-2.03120	C	-1.75370	5.19600	0.63390
H	-2.07000	3.13460	-2.40570	H	-2.33760	5.41790	1.52910
C	-3.50670	-0.66020	0.23690	C	-3.15430	-2.88070	3.14430
C	-2.84980	0.49490	0.77030	H	-2.67540	-3.74200	2.67450
H	-1.32000	0.07900	0.74600	H	-2.62070	-2.58820	4.04690
H	-2.76290	0.59520	1.84550	H	-4.19530	-3.12360	3.36790
C	-2.28550	2.90250	0.71480	O	-1.94420	2.87010	1.88210
C	-3.68140	-1.88020	1.07500	O	-4.27890	-2.88330	0.73400
H	-0.71040	5.03960	0.91520	O	-3.08360	-1.73590	2.27060
H	-1.83710	6.00160	-0.09430	O	-2.27380	4.02480	-0.02900

## TS2

(B3LYP/6-31G\*\*) Energy = -2021.884083

(B3LYP/6-31G\*\*) Free Energy = -2021.451587

M06-2X/6-31G\*\* Derived free energy = -2020.733701

Number of Imaginary Frequencies = 1 (-829.57)

## B3LYP/6-31G\*\* Geometry

C	-4.50410	-1.96290	-0.10240	C	-0.22360	-3.05640	-1.93400
C	-5.66630	-1.52470	0.41060	H	0.58630	-5.03200	-1.60870
C	-6.19830	-0.17200	0.51750	H	2.92540	-4.19590	-1.31420
C	-5.68780	0.97960	0.05580	H	-0.75100	-1.00740	-2.23020
H	-6.30760	-2.31210	0.79660	H	-1.24650	-3.39380	-2.06590
H	-4.28050	-3.02470	-0.13370	C	2.83940	0.72040	-2.80880
H	-6.20740	1.92350	0.18560	H	3.73480	0.14070	-2.60270
H	-7.14930	-0.07700	1.03360	H	3.04970	1.77810	-2.62910
O	-4.52080	1.13890	-0.65350	H	2.55950	0.58350	-3.85940
P	-3.13770	0.33150	-0.26850	H	0.73450	2.01920	-2.42350
O	-3.48680	-1.23820	-0.66710	N	0.59000	1.10250	-2.03190
O	-2.91280	0.41630	1.23200	O	3.70000	-1.73560	-1.43220
O	-2.08010	0.78490	-1.22500	H	3.90900	-1.65220	-0.47700
H	-0.35340	0.89680	-1.68510	C	1.48620	2.02490	0.67400
C	1.67250	0.26400	-1.92930	C	0.15880	1.97370	1.06980
C	0.80020	-3.96890	-1.67440	N	-0.33310	0.79090	1.53900
C	2.10480	-3.51100	-1.50450	H	-1.39440	0.68690	1.56610
C	2.39710	-2.14540	-1.58520	C	0.40660	-0.32850	1.77330
C	1.37160	-1.21190	-1.86550	C	-0.36450	-1.46060	2.39550
C	0.06170	-1.69620	-2.03020	H	-1.43440	-1.29590	2.25300

H	-0.07820	-2.41530	1.95490	H	3.13030	5.70070	0.34630
H	-0.15360	-1.52120	3.46770	H	1.50200	6.38360	0.02390
C	-0.83620	3.10100	1.05550	C	2.18140	5.55550	-0.17490
H	-1.82080	2.73310	1.34380	H	2.37790	5.46680	-1.24580
H	-0.52300	3.89060	1.74270	C	3.20290	-3.30600	3.02980
H	-0.90110	3.54400	0.06080	H	4.13420	-2.89400	3.42360
C	1.75090	-0.31510	1.42920	H	2.69410	-3.90210	3.78620
C	2.26100	0.80300	0.65460	H	3.42460	-3.90970	2.14700
H	2.15490	0.42580	-0.71620	O	3.29120	3.17290	-0.35710
H	3.34070	0.91760	0.61390	O	3.83320	-1.46330	1.27010
C	2.18760	3.22360	0.15950	O	2.28440	-2.24720	2.69770
C	2.70870	-1.38080	1.76190	O	1.51010	4.38170	0.31720

### Additional conformations for *Mechanism B*

(B3LYP/6-31G\*\*) Energy = -2021.885183

(B3LYP/6-31G\*\*) Free Energy = -2021.452716

M06-2X/6-31G\*\* Derived free energy = -2020.733211

Number of Imaginary Frequencies = 1 (-820.51)

### B3LYP/6-31G\*\* Geometry

C	5.49450	1.33260	0.07440	C	0.37440	-3.45690	-1.97200
C	6.13990	0.35360	0.73030	C	0.11510	-2.08320	-2.11860
C	5.73030	-1.01360	1.02750	C	-1.13600	-1.57030	-1.68300
C	4.63540	-1.67630	0.62720	C	-2.04690	-2.46620	-1.08890
H	7.12680	0.63420	1.08680	C	-1.76830	-3.81800	-0.93370
H	5.96640	2.29560	-0.08920	H	-0.30790	-5.37230	-1.28050
H	4.45800	-2.71030	0.90270	H	1.33310	-3.81360	-2.33340
H	6.41020	-1.58630	1.65160	H	-3.00230	-2.08280	-0.74340
O	3.63930	-1.19020	-0.19160	H	-2.49680	-4.47450	-0.46820
P	3.02480	0.32260	-0.00390	C	-2.85530	-0.01710	-2.78460
O	4.24740	1.30780	-0.49790	H	-2.58650	-0.26600	-3.81690
O	2.71440	0.58680	1.45190	H	-3.64660	-0.69660	-2.46600
O	1.94130	0.46490	-1.04430	H	-3.24170	1.00470	-2.74130
H	0.24900	0.80000	-1.72940	H	-0.98150	1.67340	-2.58520
C	-1.61560	-0.15540	-1.89720	N	-0.68710	0.82490	-2.12920
C	-0.54500	-4.31770	-1.38770	O	1.05960	-1.35110	-2.76170

H	1.48890	-0.69820	-2.15060	H	-2.13930	0.11250	-0.71130
C	-1.98150	-0.25810	1.52890	H	-3.49170	0.78480	0.36560
C	-0.67440	-0.18940	1.97550	C	-2.89530	-1.30780	2.02530
N	0.07740	0.89560	1.61710	C	-2.35570	3.04210	-0.28080
H	1.12240	0.82550	1.73570	H	-5.26760	-2.06140	2.93690
C	-0.39020	1.98890	0.95180	H	-4.71590	-3.22840	1.71710
C	0.58060	3.13380	0.85980	C	-5.07210	-2.20720	1.87200
H	1.56600	2.81800	1.20290	H	-5.97260	-2.02120	1.28730
H	0.65680	3.49950	-0.16470	C	-2.40730	5.32780	-0.85500
H	0.23290	3.96900	1.47400	H	-1.80160	6.21020	-0.65200
C	0.02910	-1.18630	2.85070	H	-2.44260	5.12370	-1.92770
H	1.10910	-1.03380	2.79270	H	-3.42700	5.46720	-0.48940
H	-0.29360	-1.07210	3.89060	O	-2.64900	-2.11780	2.90000
H	-0.22550	-2.20460	2.55860	O	-3.37370	2.87780	-0.93490
C	-1.68060	1.94720	0.44750	O	-1.76290	4.24990	-0.15300
C	-2.42260	0.70440	0.53500	O	-4.10360	-1.25530	1.40200

(B3LYP/6-31G\*\*) Energy = -2021.885009

(B3LYP/6-31G\*\*) Free Energy = -2021.451682

M06-2X/6-31G\*\* Derived free energy = -2020.733064

Number of Imaginary Frequencies = 1 (-884.58)

#### B3LYP/6-31G\*\* Geometry

C	-5.01330	-2.51730	-0.26940	C	5.44690	-2.22430	-1.77250
C	-6.21740	-1.92510	-0.35160	C	5.34710	-0.88010	-1.44050
C	-6.58260	-0.58380	-0.78950	C	4.09760	-0.26090	-1.27350
C	-5.80910	0.36140	-1.34310	C	2.91500	-1.02350	-1.43600
H	-7.04480	-2.55960	-0.04650	C	3.04950	-2.38190	-1.78270
H	-4.93030	-3.55170	0.04900	C	4.28960	-2.98670	-1.95070
H	-6.20950	1.32310	-1.64740	H	6.42710	-2.67440	-1.90050
H	-7.62650	-0.31070	-0.66360	H	6.22920	-0.26390	-1.30200
O	-4.46950	0.24660	-1.63950	H	2.14760	-2.95900	-1.95740
P	-3.39930	-0.39880	-0.56760	H	4.35080	-4.03330	-2.23070
O	-3.77670	-2.00970	-0.56870	C	1.10310	0.61430	-2.29930
O	-3.66910	0.16730	0.81580	H	1.01180	0.13350	-3.27850
O	-2.03540	-0.28480	-1.17980	H	1.83200	1.42070	-2.37880
H	-0.45000	-1.05320	-1.08140	H	0.12430	1.02140	-2.03330
C	1.53160	-0.44630	-1.28740	H	0.75050	-2.15170	-0.44750

N	0.53880	-1.34530	-1.01610	C	1.45170	0.86000	1.06990
O	4.16520	1.05090	-0.94550	H	1.65030	0.30630	-0.16630
H	3.32180	1.52120	-0.81040	H	2.50520	1.06060	1.24470
C	0.60790	2.02800	0.84090	C	1.28870	3.16950	0.21340
C	-0.75250	1.93930	1.06380	C	1.74630	-1.30950	2.34720
N	-1.25030	0.79880	1.62590	H	0.62320	6.30500	-0.20560
H	-2.28820	0.61720	1.48810	H	1.43590	5.25570	-1.41450
C	-0.49750	-0.25810	2.04060	C	1.29270	5.45830	-0.35110
C	-1.27060	-1.35750	2.71200	H	2.26410	5.64960	0.10930
H	-2.33730	-1.23730	2.51560	C	3.96430	-2.12880	2.37090
H	-0.93200	-2.33630	2.37380	H	4.92040	-1.82700	1.94580
H	-1.09460	-1.33230	3.79230	H	4.02230	-2.18930	3.46030
C	-1.78870	2.98640	0.76100	H	3.66030	-3.10060	1.97610
H	-1.60800	3.45090	-0.20800	O	2.37980	3.06280	-0.34190
H	-2.78180	2.53450	0.76740	O	1.39310	-2.27240	3.00540
H	-1.75260	3.78130	1.51270	O	3.03190	-1.11100	1.97150
C	0.87430	-0.22360	1.84420	O	0.64340	4.34380	0.29310

(B3LYP/6-31G\*\*) Energy = -2021.885321

(B3LYP/6-31G\*\*) Free Energy = -2021.452513

M06-2X/6-31G\*\* Derived free energy = -2020.732353

Number of Imaginary Frequencies = 1 (-844.09)

#### B3LYP/6-31G\*\* Geometry

C	-4.82690	-1.45190	0.28360	C	1.62260	0.02890	-1.90240
C	-5.86880	-0.74990	0.76000	C	0.47570	-4.14230	-1.85020
C	-6.10270	0.68860	0.79720	C	-0.42110	-3.20700	-2.34860
C	-5.37700	1.67620	0.25370	C	-0.13750	-1.83020	-2.34120
H	-6.66250	-1.36370	1.17640	C	1.11490	-1.39060	-1.83370
H	-4.83320	-2.53650	0.30430	C	2.00240	-2.36070	-1.32650
H	-5.67100	2.71720	0.33520	C	1.69890	-3.71630	-1.32600
H	-6.99390	1.01070	1.32800	H	0.22090	-5.19830	-1.86510
O	-4.22940	1.52690	-0.49510	H	-1.37900	-3.50530	-2.76130
P	-3.03090	0.50050	-0.03900	H	2.95640	-2.03810	-0.92070
O	-3.67260	-0.99340	-0.29970	H	2.41290	-4.43150	-0.92930
O	-2.72460	0.68270	1.43020	C	2.86690	0.22530	-2.77060
O	-1.93250	0.65020	-1.06270	H	3.64950	-0.48700	-2.50790
H	-0.22360	1.00090	-1.64570	H	3.26510	1.23630	-2.64430

H	2.60030	0.07120	-3.82160	C	1.91410	-0.39000	1.49340
H	1.01600	1.92490	-2.42750	C	2.43570	0.63500	0.60240
N	0.71940	1.04860	-2.02910	H	2.15480	0.16630	-0.68740
O	-1.05820	-1.01810	-2.91790	H	3.51490	0.64080	0.48620
H	-1.48390	-0.41690	-2.25270	C	2.42810	3.12080	0.06700
C	1.76470	1.91870	0.61110	C	2.85290	-1.48300	1.82470
C	0.46260	1.98170	1.08690	H	4.57750	4.66950	-0.14700
N	-0.07980	0.86340	1.64120	H	3.84440	4.45510	-1.74960
H	-1.12920	0.84230	1.73570	C	4.39150	3.95140	-0.94910
C	0.60240	-0.29270	1.91570	H	5.32980	3.54230	-1.32230
C	-0.19690	-1.31800	2.67180	C	3.30060	-3.40550	3.10950
H	-1.26130	-1.08670	2.59420	H	4.23990	-3.00530	3.49750
H	-0.00900	-2.31870	2.28390	H	2.78570	-3.98750	3.87330
H	0.08880	-1.32250	3.72850	H	3.51430	-4.02300	2.23410
C	-0.43010	3.18900	1.07170	O	1.98000	4.25360	0.06630
H	-1.43470	2.91890	1.39860	O	3.95770	-1.59080	1.31650
H	-0.02300	3.96360	1.72730	O	2.39960	-2.33810	2.76750
H	-0.47260	3.62680	0.07350	O	3.64920	2.82420	-0.45470

(B3LYP/6-31G\*\*) Energy = -2021.882880

(B3LYP/6-31G\*\*) Free Energy = -2021.450285

M06-2X/6-31G\*\* Derived free energy = -2020.729828

Number of Imaginary Frequencies = 1 (-720.29)

#### B3LYP/6-31G\*\* Geometry

C	-5.64510	-1.78380	-0.65240	H	-0.11760	-1.34280	-1.20560
C	-6.50940	-0.79590	-0.94130	C	1.62660	-0.20870	-1.27310
C	-6.26940	0.54170	-1.46810	C	5.72470	-0.52440	-2.68610
C	-5.12150	1.09100	-1.89200	C	5.16270	-1.57010	-1.95990
H	-7.55010	-1.04730	-0.75700	C	3.85960	-1.47720	-1.46700
H	-6.00430	-2.74430	-0.29660	C	3.06820	-0.33500	-1.72580
H	-5.08700	2.10080	-2.28880	C	3.67160	0.71610	-2.43750
H	-7.14140	1.18540	-1.54200	C	4.97650	0.63000	-2.91510
O	-3.88750	0.48530	-1.93630	H	6.74040	-0.60720	-3.06100
P	-3.32420	-0.45040	-0.69980	H	5.71750	-2.47860	-1.74960
O	-4.28030	-1.79600	-0.76950	H	3.10620	1.61830	-2.63580
O	-3.58450	0.26180	0.62000	H	5.40130	1.46060	-3.47000
O	-1.93970	-0.88360	-1.06000	C	0.81140	0.92280	-1.89860

H	-0.22560	0.85120	-1.56440	H	-1.22090	3.62280	0.54620
H	0.81750	0.82100	-2.98830	C	0.83880	-0.63340	1.78620
H	1.21120	1.90460	-1.63660	C	1.52120	0.55240	1.32930
H	1.39780	-2.25600	-1.13070	H	1.75600	0.25150	-0.07850
N	0.90220	-1.37810	-1.17720	H	2.58960	0.61350	1.51650
O	3.37290	-2.56250	-0.76380	C	1.60450	3.01890	1.14650
H	3.30740	-2.31880	0.18570	C	1.68770	-1.80100	2.05740
C	0.78550	1.79880	1.34160	H	1.08290	6.18880	1.54060
C	-0.59300	1.75940	1.42360	H	2.06400	5.46110	0.22540
N	-1.19870	0.54910	1.63600	C	1.74300	5.36690	1.26530
H	-2.23860	0.47580	1.38910	H	2.62660	5.35040	1.90710
C	-0.55260	-0.61910	1.86470	C	1.88910	-4.00490	2.87380
C	-1.44540	-1.78310	2.18890	H	1.23170	-4.72600	3.35750
H	-1.22900	-2.62330	1.52790	H	2.27230	-4.40690	1.93310
H	-1.27100	-2.11920	3.21410	H	2.72880	-3.74870	3.52260
H	-2.49010	-1.49700	2.06980	O	2.76030	2.98350	0.76420
C	-1.55200	2.91200	1.30190	O	2.89190	-1.82110	1.80110
H	-2.54550	2.53660	1.04700	O	1.06800	-2.84590	2.63000
H	-1.61370	3.45660	2.25000	O	0.96470	4.17030	1.44950

(B3LYP/6-31G\*\*) Energy = -2021.883476

(B3LYP/6-31G\*\*) Free Energy = -2021.451122

M06-2X/6-31G\*\* Derived free energy = -2020.729368

Number of Imaginary Frequencies = 1 (-645.14)

#### B3LYP/6-31G\*\* Geometry

C	-5.31680	-2.20510	0.23040	O	-1.91500	-0.84570	-0.89080
C	-6.38200	-1.51600	-0.20540	H	-0.30220	-1.38510	-0.76610
C	-6.44960	-0.45760	-1.20530	C	1.56310	-0.59080	-1.19020
C	-5.46870	0.15770	-1.88690	C	5.73690	-1.51280	-1.71440
H	-7.32760	-1.79930	0.24810	C	4.79470	-2.52640	-1.82460
H	-5.41410	-2.99290	0.97050	C	3.43030	-2.25570	-1.64610
H	-5.70170	0.91230	-2.63140	C	3.01000	-0.93630	-1.34160
H	-7.44860	-0.10850	-1.45080	C	3.98510	0.07590	-1.26210
O	-4.11510	-0.04840	-1.81770	C	5.33410	-0.20100	-1.43860
P	-3.33230	-0.59250	-0.47040	H	6.78910	-1.74400	-1.85280
O	-4.01630	-2.06880	-0.19630	H	5.08050	-3.54590	-2.06070
O	-3.64180	0.32760	0.69390	H	3.66910	1.09100	-1.03790

H	6.06590	0.59610	-1.35970	H	-1.76440	3.99180	1.12480
C	0.95180	0.34880	-2.21090	H	-1.47010	3.58780	-0.56010
H	0.93130	-0.15470	-3.18440	C	0.84310	0.05890	1.93800
H	1.55510	1.25240	-2.30960	C	1.45770	0.99560	0.99130
H	-0.07540	0.60030	-1.93710	H	1.62180	0.34120	-0.08040
H	1.04540	-2.14240	0.02520	H	2.51150	1.20670	1.16710
N	0.71950	-1.57760	-0.75120	C	1.40090	3.27070	0.00100
O	2.58500	-3.30710	-1.81190	C	1.67840	-0.94190	2.63050
H	1.66590	-2.98890	-1.74840	H	1.71290	5.24540	-1.74550
C	0.65380	2.18000	0.65120	H	2.36850	5.74310	-0.17070
C	-0.71060	2.14340	0.84790	C	1.45210	5.51450	-0.71930
N	-1.24910	1.07980	1.52070	H	0.77370	6.36690	-0.70600
H	-2.27760	0.89140	1.37200	C	3.83900	-1.90630	2.70910
C	-0.52730	0.08790	2.11680	H	3.44280	-2.92360	2.67010
C	-1.33740	-0.86920	2.94430	H	4.01130	-1.63630	3.75390
H	-2.38680	-0.81890	2.64790	H	4.76060	-1.83020	2.13340
H	-0.96510	-1.88840	2.85030	O	2.54300	3.13740	-0.41800
H	-1.25270	-0.60640	4.00400	O	1.33690	-1.66320	3.55130
C	-1.72620	3.16360	0.40920	O	2.92670	-0.98230	2.09370
H	-2.71290	2.69780	0.35900	O	0.73540	4.44380	-0.07940

(B3LYP/6-31G\*\*) Energy = -2021.880968

(B3LYP/6-31G\*\*) Free Energy = -2021.448221

M06-2X/6-31G\*\* Derived free energy = -2020.727120

Number of Imaginary Frequencies = 1 (-698.69)

#### B3LYP/6-31G\*\* Geometry

C	4.55590	0.95780	-2.15030	O	3.66230	0.14520	0.81750
C	5.83390	0.62520	-1.89760	O	1.93450	-1.29390	-0.52360
C	6.38980	-0.48930	-1.14040	H	0.25610	-1.56070	-0.67360
C	5.75620	-1.54650	-0.61280	C	-1.44940	-0.50860	-1.19840
H	6.56190	1.29970	-2.33960	C	-5.56000	-0.93390	-2.41580
H	4.32600	1.81560	-2.77450	C	-4.68320	-1.99760	-2.57510
H	6.28810	-2.32830	-0.08070	C	-3.34690	-1.89150	-2.16320
H	7.46560	-0.47250	-0.99050	C	-2.88750	-0.68600	-1.57420
O	4.40740	-1.81080	-0.70180	C	-3.79350	0.38090	-1.44640
P	3.28130	-0.64590	-0.41720	C	-5.11610	0.26750	-1.85290
O	3.40250	0.33760	-1.74840	H	-6.59260	-1.03950	-2.73520



H	-4.99950	-2.93300	-3.02410	H	2.41380	-1.19620	2.60240
H	-3.44650	1.30610	-0.99740	H	1.25250	-1.22980	3.95220
H	-5.79800	1.10230	-1.72800	H	1.02970	-2.31150	2.58220
C	-0.62670	0.45800	-2.02930	C	-0.63170	2.03720	1.03890
H	0.39930	0.52010	-1.66110	C	-1.42660	0.80580	1.16500
H	-1.08730	1.44820	-2.03810	H	-1.55440	0.29800	0.00230
H	-0.59740	0.09720	-3.06380	H	-2.49070	0.95280	1.34630
H	-1.26620	-2.21860	-0.12680	C	-1.73410	-1.32650	2.41450
N	-0.77380	-1.62600	-0.78640	C	-1.26830	3.30420	0.63720
O	-2.56130	-2.97340	-2.39920	H	-1.66590	-3.58250	4.73540
H	-1.65190	-2.77430	-2.10920	H	-2.32380	-3.82620	3.08380
C	-0.81920	-0.25300	1.98210	C	-2.17000	-3.10910	3.89360
C	0.54620	-0.25050	2.18480	H	-3.13980	-2.71030	4.19930
N	1.27030	0.82010	1.74510	C	-3.28410	4.32630	-0.05260
H	2.29940	0.65770	1.58630	H	-4.30450	4.01270	-0.27140
C	0.73260	1.97400	1.24580	H	-3.26950	5.03480	0.77860
C	1.73410	3.06590	0.99480	H	-2.83080	4.79990	-0.92640
H	2.72780	2.62940	0.86900	O	-2.80450	-1.54320	1.86580
H	1.46510	3.65670	0.12100	O	-0.74120	4.40190	0.60690
H	1.75670	3.75780	1.84360	O	-2.57690	3.12430	0.29730
C	1.36200	-1.31410	2.86640	O	-1.29780	-2.04430	3.47290

(B3LYP/6-31G\*\*) Energy = -2021.880264

(B3LYP/6-31G\*\*) Free Energy = -2021.446481

M06-2X/6-31G\*\* Derived free energy = -2020.726082

Number of Imaginary Frequencies = 1 (-813.44)

B3LYP/6-31G\*\* Geometry

C	4.20140	-1.37690	-0.30500	O	3.13030	-0.69930	0.20940
C	5.33910	-0.89600	-0.83680	O	2.46490	0.97640	-1.64170
C	5.79040	0.47830	-1.01600	O	1.68970	1.27340	0.84040
C	5.23670	1.61030	-0.55820	H	0.22000	0.95810	1.60840
H	6.02780	-1.66380	-1.17800	C	-1.41810	-0.28290	2.05070
H	4.04620	-2.44740	-0.21560	C	0.38270	-4.17920	1.65740
H	5.67920	2.58320	-0.74560	C	1.08500	-3.17190	2.30040
H	6.70500	0.60850	-1.58760	C	0.54650	-1.88050	2.42720
O	4.10390	1.70090	0.22050	C	-0.73510	-1.60290	1.88050
P	2.73720	0.86550	-0.15370	C	-1.43320	-2.65560	1.25560

C	-0.89070	-3.92700	1.13330	C	0.02400	3.28610	-1.13480
H	0.82480	-5.16750	1.56920	H	1.02210	3.10410	-1.53340
H	2.06560	-3.34600	2.72990	H	-0.50220	3.99390	-1.78190
H	-2.42310	-2.46000	0.85630	H	0.11440	3.74360	-0.15020
H	-1.45320	-4.71360	0.64090	C	-1.99460	-0.50090	-1.39880
C	-2.68660	-0.28210	2.89360	C	-2.45750	0.40240	-0.34450
H	-2.41440	-0.44680	3.94280	H	-2.00530	-0.09020	0.78390
H	-3.35230	-1.09080	2.58870	H	-3.51570	0.31880	-0.10340
H	-3.21700	0.66760	2.79500	C	-2.68830	2.78390	0.35570
H	-1.07390	1.66510	2.51500	C	-2.87050	-1.65280	-1.68320
N	-0.60840	0.81470	2.22470	H	-2.78980	6.01960	0.33010
O	1.29090	-1.00600	3.13570	H	-2.91370	5.00070	1.80140
H	0.89340	-0.11970	3.09200	C	-3.13420	5.06800	0.73350
C	-1.93380	1.76650	-0.40090	H	-4.21070	4.95440	0.58800
C	-0.74040	1.99320	-1.06270	C	-3.37760	-3.47510	-3.08790
N	-0.16970	0.95690	-1.74320	H	-2.96100	-3.92250	-3.98990
H	0.87250	1.02610	-1.91640	H	-3.37340	-4.19320	-2.26470
C	-0.77480	-0.24460	-1.99370	H	-4.40400	-3.14380	-3.26110
C	0.00380	-1.14130	-2.91660	O	-3.50330	2.50590	1.22390
H	1.05960	-0.86060	-2.89000	O	-3.84380	-1.93720	-1.00130
H	-0.10620	-2.18670	-2.63380	O	-2.52890	-2.35380	-2.78800
H	-0.36040	-1.04000	-3.94440	O	-2.41750	4.05850	0.00060

(B3LYP/6-31G\*\*) Energy = -2021.880264

(B3LYP/6-31G\*\*) Free Energy = -2021.446478

M06-2X/6-31G\*\* Derived free energy = -2020.726048

Number of Imaginary Frequencies = 1 (-813.20)

#### B3LYP/6-31G\*\* Geometry

C	-5.23690	1.61030	-0.55770	P	-2.73710	0.86570	-0.15360
C	-5.79040	0.47830	-1.01580	O	-4.10390	1.70090	0.22070
C	-5.33880	-0.89600	-0.83720	O	-2.46500	0.97680	-1.64160
C	-4.20090	-1.37680	-0.30560	O	-1.68960	1.27350	0.84060
H	-6.70510	0.60850	-1.58720	H	-0.22000	0.95790	1.60850
H	-5.67970	2.58310	-0.74470	C	1.41820	-0.28300	2.05070
H	-4.04550	-2.44740	-0.21670	C	-0.38290	-4.17930	1.65750
H	-6.02730	-1.66380	-1.17880	C	-1.08500	-3.17190	2.30080
O	-3.13010	-0.69920	0.20930	C	-0.54640	-1.88060	2.42750

C	0.73510	-1.60310	1.88050	H	0.50220	3.99390	-1.78230
C	1.43300	-2.65570	1.25550	C	-0.00400	-1.14110	-2.91670
C	0.89040	-3.92710	1.13310	H	-1.05960	-0.86010	-2.89050
H	-0.82500	-5.16760	1.56940	H	0.36060	-1.04030	-3.94440
H	-2.06550	-3.34600	2.73040	H	0.10570	-2.18650	-2.63370
H	2.42290	-2.46010	0.85590	C	1.93380	1.76650	-0.40090
H	1.45280	-4.71370	0.64060	C	2.45740	0.40230	-0.34450
C	2.68680	-0.28230	2.89330	H	2.00520	-0.09030	0.78370
H	3.21710	0.66740	2.79480	H	3.51560	0.31870	-0.10340
H	2.41470	-0.44700	3.94260	C	2.87030	-1.65280	-1.68340
H	3.35240	-1.09100	2.58830	C	2.68830	2.78390	0.35570
H	1.07390	1.66490	2.51500	H	2.96050	-3.92260	-3.99000
N	0.60850	0.81460	2.22470	H	3.37290	-4.19330	-2.26470
O	-1.29060	-1.00610	3.13620	C	3.37720	-3.47520	-3.08800
H	-0.89290	-0.11990	3.09250	H	4.40360	-3.14410	-3.26120
C	1.99450	-0.50090	-1.39890	C	3.13440	5.06790	0.73340
C	0.77470	-0.24450	-1.99380	H	4.21090	4.95410	0.58800
N	0.16960	0.95710	-1.74320	H	2.79020	6.01950	0.32990
H	-0.87260	1.02630	-1.91640	H	2.91380	5.00060	1.80140
C	0.74040	1.99320	-1.06260	O	3.84360	-1.93730	-1.00150
C	-0.02390	3.28620	-1.13480	O	3.50330	2.50580	1.22400
H	-1.02210	3.10430	-1.53300	O	2.41770	4.05840	0.00050
H	-0.11390	3.74400	-0.15020	O	2.52860	-2.35390	-2.78810

(B3LYP/6-31G\*\*) Energy = -2021.876616

(B3LYP/6-31G\*\*) Free Energy = -2021.443129

M06-2X/6-31G\*\* Derived free energy = -2020.724939

Number of Imaginary Frequencies = 1 (-887.61)

B3LYP/6-31G\*\* Geometry

C	-3.38610	-2.57080	-0.21960	O	-4.86050	0.01540	-1.10680
C	-4.67370	-2.76260	0.11960	P	-3.34660	0.12200	-0.47860
C	-5.80740	-1.84720	0.10410	O	-2.75410	-1.43950	-0.66050
C	-5.87700	-0.61950	-0.42900	O	-3.43040	0.40750	1.01000
H	-4.89460	-3.77420	0.44920	O	-2.51020	0.96240	-1.38900
H	-2.68760	-3.40160	-0.17980	H	-0.69850	0.45980	-1.80210
H	-6.78450	-0.02540	-0.39830	C	1.34390	-0.08360	-1.68750
H	-6.72030	-2.20830	0.56930	C	3.61980	-3.76110	-1.78840

C	4.20130	-2.60320	-1.27810	H	-0.46710	-1.98090	2.51670
C	3.48160	-1.40520	-1.23620	H	-0.66490	-0.83170	3.82940
C	2.15240	-1.35740	-1.70150	C	-1.57660	3.25040	0.68720
C	1.58870	-2.53550	-2.22370	H	-2.54120	2.85850	1.00870
C	2.30940	-3.72600	-2.26830	H	-1.33330	4.15190	1.25530
H	4.19150	-4.68400	-1.82130	H	-1.64940	3.52820	-0.36410
H	5.22280	-2.59970	-0.91100	C	1.23050	0.13030	1.65480
H	0.58070	-2.50130	-2.62350	C	1.68000	1.13460	0.70080
H	1.85270	-4.61780	-2.68620	H	1.67780	0.48130	-0.50700
C	1.81660	1.02830	-2.61740	H	2.74260	1.35320	0.68350
H	1.71760	0.68520	-3.65260	C	1.48820	3.48030	-0.07360
H	2.85640	1.28130	-2.41410	C	2.27040	-0.75800	2.20030
H	1.19890	1.92190	-2.49450	H	0.54770	6.48700	-0.81290
H	-0.39390	-1.07820	-1.19140	H	1.70190	5.50460	-1.77350
N	-0.00710	-0.28450	-1.68470	C	1.32320	5.72280	-0.77250
O	4.07880	-0.26840	-0.75340	H	2.15510	6.04970	-0.14440
H	4.11460	-0.34200	0.22360	C	2.84780	-2.49220	3.69100
C	0.82160	2.29540	0.51770	H	3.62400	-1.90640	4.18770
C	-0.50890	2.21070	0.88250	H	2.32230	-3.12180	4.40800
N	-0.93170	1.08010	1.53090	H	3.30600	-3.09860	2.90670
H	-1.97480	0.89360	1.51920	O	2.66200	3.48590	-0.40150
C	-0.12290	0.07100	1.96000	O	3.45520	-0.70560	1.87650
C	-0.83720	-0.98570	2.75910	O	1.84070	-1.62560	3.13510
H	-1.90990	-0.93240	2.56160	O	0.68900	4.56200	-0.20750

(B3LYP/6-31G\*\*) Energy = -2021.878551

(B3LYP/6-31G\*\*) Free Energy = -2021.445295

M06-2X/6-31G\*\* Derived free energy = -2020.723662

Number of Imaginary Frequencies = 1 (-732.56)

B3LYP/6-31G\*\* Geometry

C	6.03370	-0.03470	-0.60340	H	6.31800	-3.36300	0.14450
C	6.44840	-1.22590	-0.14920	O	3.42580	-1.92290	-0.75950
C	5.72750	-2.49230	-0.12700	P	3.40690	-0.28710	-0.49090
C	4.43930	-2.76780	-0.39810	O	4.81040	0.22820	-1.17900
H	7.46230	-1.24740	0.24030	O	3.46510	-0.04470	1.00970
H	6.67200	0.84280	-0.58340	O	2.27060	0.25630	-1.30200
H	4.08130	-3.79220	-0.36720	H	0.64030	-0.57190	-1.41290

C	-1.41590	-0.21420	-1.52460	H	1.91050	3.23040	-0.26860
C	-5.29870	-2.17070	-1.66460	H	1.73070	3.82700	1.37810
C	-4.23090	-2.80940	-1.04090	H	2.79750	2.43380	1.04400
C	-2.96620	-2.21190	-0.99120	C	0.78320	-1.34930	2.64790
C	-2.73990	-0.95010	-1.59190	H	1.79200	-1.52250	2.26390
C	-3.83880	-0.33320	-2.21700	H	0.87410	-1.11340	3.71530
C	-5.09790	-0.92430	-2.25840	H	0.17410	-2.24360	2.54690
H	-6.27350	-2.64810	-1.69700	C	-0.62030	2.21090	0.67930
H	-4.34560	-3.79290	-0.59520	C	-1.56830	1.13190	0.84680
H	-3.70490	0.63670	-2.68110	H	-1.61670	0.48470	-0.45860
H	-5.91590	-0.41400	-2.75710	H	-2.61630	1.41160	0.82280
C	-1.17630	0.91800	-2.52550	C	-2.22850	-0.93800	2.10690
H	-0.17000	1.31560	-2.36780	C	-1.17810	3.44500	0.08260
H	-1.89220	1.73300	-2.40990	H	-5.35280	-0.48440	2.81820
H	-1.22690	0.52830	-3.54710	H	-4.29750	-1.76160	3.51140
H	-0.40770	-1.89980	-0.92480	C	-4.52460	-1.16500	2.62600
N	-0.29640	-0.98770	-1.34380	H	-4.76180	-1.82780	1.79020
O	-1.93910	-2.91840	-0.39210	C	-0.84590	5.69270	-0.53650
H	-2.05550	-2.92000	0.57930	H	-1.71650	6.04760	0.01960
C	-1.18180	0.01190	1.66860	H	-0.03460	6.41810	-0.48540
C	0.16730	-0.18520	1.92440	H	-1.13790	5.51360	-1.57380
N	1.04760	0.78970	1.56600	O	-2.09500	-2.14770	2.27800
H	2.07740	0.51190	1.51590	O	-2.31900	3.51530	-0.34520
C	0.70940	1.98250	0.99090	O	-0.32380	4.49030	0.05610
C	1.86110	2.92370	0.77710	O	-3.40900	-0.31990	2.28600

(B3LYP/6-31G\*\*) Energy = -2021.873473

(B3LYP/6-31G\*\*) Free Energy = -2021.439314

M06-2X/6-31G\*\* Derived free energy = -2020.717391

Number of Imaginary Frequencies = 1 (-866.67)

B3LYP/6-31G\*\* Geometry

C	-4.84200	-2.51530	-0.53930	H	-6.28990	1.40800	-1.30640
C	-6.06880	-1.97370	-0.44390	H	-7.55660	-0.40030	-0.42600
C	-6.51910	-0.60660	-0.67310	O	-4.52020	0.41880	-1.58240
C	-5.83120	0.43490	-1.16320	P	-3.33770	-0.30300	-0.69270
H	-6.84290	-2.67930	-0.15530	O	-3.65520	-1.91850	-0.87270
H	-4.69600	-3.57670	-0.36490	O	-3.50310	0.07150	0.76750

O	-2.04190	-0.05370	-1.40790	C	-1.01660	-1.50670	2.54580
H	-0.47410	-0.75690	-1.37700	H	-2.08220	-1.40600	2.33090
C	1.50540	-0.13370	-1.53700	H	-0.65290	-2.45860	2.16190
C	5.46870	-1.61990	-2.34240	H	-0.87180	-1.52420	3.63090
C	4.62740	-2.33250	-1.49700	C	-1.67660	2.95570	0.99810
C	3.34120	-1.86300	-1.21510	H	-2.65150	2.46920	0.93270
C	2.87370	-0.65970	-1.80380	H	-1.67280	3.62940	1.86100
C	3.75920	0.04740	-2.63920	H	-1.51320	3.56860	0.11250
C	5.03690	-0.42080	-2.91640	C	1.10530	-0.23700	1.76430
H	6.46580	-1.99730	-2.54830	C	1.61190	0.88800	0.98270
H	4.94470	-3.25710	-1.02720	H	1.69100	0.43050	-0.23230
H	3.42850	0.97630	-3.08860	H	2.67450	1.08950	1.10800
H	5.69060	0.14360	-3.57290	C	1.42610	3.33130	0.54830
C	1.04880	1.15170	-2.19940	C	2.14060	-1.15450	2.29650
H	0.04590	1.40620	-1.84950	H	1.57030	5.68940	-0.66210
H	0.97920	0.98530	-3.28090	H	2.25160	5.82030	0.97330
H	1.73150	1.97920	-2.00260	C	1.33000	5.68090	0.40370
H	0.67700	-2.00560	-1.70650	H	0.60950	6.46300	0.64120
N	0.51460	-1.07500	-1.34450	C	2.65120	-3.21840	3.30530
O	2.60060	-2.63400	-0.36620	H	3.27740	-2.75450	4.07030
H	1.76680	-2.18420	-0.14770	H	2.09750	-4.06090	3.71900
C	0.75370	2.07350	0.93110	H	3.28030	-3.53920	2.47220
C	-0.59950	1.91610	1.14840	O	2.55430	3.36880	0.08460
N	-1.05520	0.69220	1.55940	O	3.33190	-0.90850	2.24840
H	-2.08410	0.49450	1.42140	O	1.65120	-2.29400	2.83830
C	-0.26350	-0.35400	1.93700	O	0.69200	4.44570	0.77150

### TS3

(B3LYP/6-31G\*\*) Energy = -2021.900629

(B3LYP/6-31G\*\*) Free Energy = -2021.466982

M06-2X/6-31G\*\* Derived free energy = -2020.746243

Number of Imaginary Frequencies = 1 (-764.21)

### B3LYP/6-31G\*\* Geometry

C	-5.58070	-1.36840	0.50490	H	-6.97010	-1.62850	-0.97890
C	-6.24720	-0.92700	-0.57260	H	-5.77610	-2.34660	0.93150
C	-6.15090	0.35330	-1.26280	H	-5.42200	2.30530	-1.63080
C	-5.34230	1.40140	-1.03560	H	-6.84360	0.49400	-2.08770

O	-4.37450	1.53820	-0.07180	H	-1.09800	0.89160	1.65210
P	-3.50080	0.27410	0.52830	C	0.61960	-0.26010	1.85820
O	-4.63320	-0.68630	1.23220	C	-0.18350	-1.25820	2.64250
O	-2.84790	-0.47550	-0.61050	H	-0.13380	-2.24120	2.16990
O	-2.68650	0.85310	1.65610	H	0.23920	-1.38050	3.64300
H	0.76930	0.89480	-2.37480	H	-1.22210	-0.93300	2.71750
C	2.37480	-0.26900	-1.90540	C	-0.40290	3.15030	0.77280
C	0.08870	-3.88780	-1.37300	H	-0.13440	3.92070	1.50200
C	-0.55210	-2.65840	-1.29190	H	-0.31250	3.60410	-0.21450
C	0.17110	-1.46640	-1.47530	H	-1.43640	2.84550	0.94650
C	1.56490	-1.51600	-1.75400	C	1.94430	-0.39230	1.48390
C	2.17900	-2.78100	-1.81590	C	2.53630	0.61400	0.61880
C	1.46040	-3.95680	-1.63740	H	2.47890	0.08040	-0.62490
H	-0.48550	-4.79870	-1.22920	H	3.62180	0.67700	0.62130
H	-1.61440	-2.58530	-1.08370	C	2.60560	2.97770	-0.12320
H	3.23990	-2.84360	-2.02890	C	2.72560	-1.58330	1.87610
H	1.96190	-4.91650	-1.70750	H	2.27950	6.19500	-0.28020
C	3.85330	-0.39390	-2.24680	H	3.84650	5.33070	-0.14760
H	4.36930	-1.04160	-1.53670	C	2.82710	5.28880	-0.53700
H	3.97680	-0.79650	-3.25770	H	2.86850	5.15860	-1.62110
H	4.31920	0.59330	-2.20110	C	4.76650	-2.73080	1.59760
H	2.30020	1.65170	-2.57450	H	4.28740	-3.65770	1.27370
N	1.76350	0.79500	-2.54940	H	5.70440	-2.57610	1.06460
O	-0.43590	-0.26650	-1.38410	H	4.94040	-2.78140	2.67480
H	-1.41410	-0.34710	-1.10340	O	3.63080	2.78920	-0.76560
C	1.83870	1.88740	0.50850	O	2.36870	-2.45770	2.64360
C	0.51570	1.96630	0.91170	O	3.94350	-1.59990	1.26910
N	-0.04810	0.88030	1.51040	O	2.09670	4.21200	0.07740

### Additional conformations for *Mechanism C*

(B3LYP/6-31G\*\*) Energy = -2021.900671

(B3LYP/6-31G\*\*) Free Energy = -2021.466520

M06-2X/6-31G\*\* Derived free energy = -2020.745739

Number of Imaginary Frequencies = 1 (-761.42)

B3LYP/6-31G\*\* Geometry

C	5.57140	1.40150	-1.01630	H	1.39390	-0.07100	-1.22410
C	6.25470	0.25150	-1.11540	C	-1.83040	-0.47030	1.50730
C	6.16740	-0.94870	-0.29250	C	-0.51680	-0.17070	1.81910
C	5.33340	-1.25030	0.71690	N	-0.00850	1.03390	1.42230
H	6.98360	0.22090	-1.92010	H	1.03770	1.17460	1.50880
H	5.75400	2.23250	-1.68950	C	-0.72590	2.03140	0.83470
H	5.42890	-2.18790	1.25470	C	0.03570	3.31350	0.63330
H	6.89280	-1.72520	-0.51800	H	-0.28890	4.06130	1.36320
O	4.31900	-0.49320	1.24500	H	1.10520	3.13630	0.75970
P	3.46910	0.63390	0.39200	H	-0.15560	3.73240	-0.35500
O	4.61660	1.71440	-0.07510	C	0.43500	-1.04820	2.58150
O	2.86010	-0.02300	-0.82560	H	1.43320	-0.60830	2.59230
O	2.61590	1.34450	1.41040	H	0.08320	-1.18550	3.60740
H	-0.97170	0.88900	-2.40530	H	0.47240	-2.04510	2.13810
C	-2.40670	-0.45440	-1.86570	C	-2.04620	1.78550	0.49580
C	0.31750	-3.77010	-1.43660	C	-2.57680	0.43890	0.65360
C	0.80870	-2.47240	-1.37590	H	-2.50160	-0.10660	-0.58400
C	-0.05990	-1.37630	-1.52190	H	-3.66080	0.36860	0.69980
C	-1.44780	-1.59440	-1.74340	C	-2.44400	-1.73830	1.95260
C	-1.90760	-2.92380	-1.78580	C	-2.96790	2.76430	-0.11150
C	-1.04580	-4.00440	-1.64290	H	-5.31630	-3.09310	1.29550
H	1.00310	-4.60500	-1.32260	H	-3.77480	-3.99890	1.45100
H	1.86290	-2.27250	-1.21460	C	-4.34250	-3.12670	1.78380
H	-2.96120	-3.11330	-1.95530	H	-4.45800	-3.17430	2.86900
H	-1.43040	-5.01770	-1.69630	C	-3.49080	5.02480	-0.53330
C	-3.87170	-0.75840	-2.14880	H	-3.56880	4.87330	-1.61250
H	-4.45060	0.16620	-2.08910	H	-4.48760	4.94890	-0.09360
H	-3.98360	-1.18140	-3.15270	H	-3.04600	5.99450	-0.31300
H	-4.27900	-1.45790	-1.41740	O	-1.95290	-2.54570	2.71930
H	-2.58950	1.45370	-2.55120	O	-3.98930	2.44260	-0.70510
N	-1.95260	0.66840	-2.53910	O	-2.60580	4.05430	0.05460
O	0.39870	-0.11090	-1.44850	O	-3.67380	-1.91500	1.39770

(B3LYP/6-31G\*\*) Energy = -2021.885563

(B3LYP/6-31G\*\*) Free Energy = -2021.449725

M06-2X/6-31G\*\* Derived free energy = -2020.732051

Number of Imaginary Frequencies = 1 (-715.06)

B3LYP/6-31G\*\* Geometry



C	5.59800	-0.81040	-0.73970	H	1.18520	-0.56820	-1.42080
C	5.74050	-1.13820	0.55040	C	-1.37390	-0.33630	1.56820
C	5.25740	-0.37290	1.69130	C	-0.00600	-0.14700	1.61740
C	4.29500	0.56500	1.76140	N	0.50220	1.02180	1.11520
H	6.29450	-2.04780	0.76480	H	1.52440	1.10840	1.10110
H	5.98430	-1.41490	-1.55380	C	-0.22150	2.07210	0.62240
H	4.10370	1.06820	2.70520	C	0.60960	3.25280	0.21760
H	5.75120	-0.56840	2.63980	H	1.43370	2.91420	-0.42640
O	3.43770	1.03050	0.80140	H	0.01850	4.00080	-0.29990
P	3.40990	0.63020	-0.85600	H	1.04980	3.72030	1.10650
O	4.99610	0.35670	-1.16170	C	1.03350	-1.09200	2.14050
O	2.63700	-0.67550	-0.93860	H	1.74620	-1.30010	1.33360
O	2.95670	1.86700	-1.54190	H	1.59190	-0.62420	2.95910
H	-1.15470	0.67410	-2.49730	H	0.58350	-2.01110	2.50050
C	-2.64520	-0.38930	-1.59610	C	-1.59440	1.91880	0.53750
C	-0.41990	-4.08290	-1.41660	C	-2.18680	0.63230	0.85600
C	0.26060	-2.87330	-1.47090	H	-2.42970	0.02900	-0.38940
C	-0.45190	-1.66350	-1.54560	H	-3.24590	0.64970	1.09560
C	-1.87180	-1.67320	-1.56890	C	-2.02660	-1.53650	2.14980
C	-2.52500	-2.91630	-1.50040	C	-2.55320	2.95220	0.07980
C	-1.81840	-4.11200	-1.43410	H	-5.08180	-2.60330	1.96980
H	0.14380	-5.00980	-1.36060	H	-3.63080	-3.65700	1.89760
H	1.34460	-2.83160	-1.45190	C	-4.05220	-2.73370	2.30180
H	-3.60850	-2.94760	-1.52010	H	-3.99930	-2.76610	3.39210
H	-2.35070	-5.05710	-1.40130	C	-3.06930	5.23820	-0.17950
C	-4.16640	-0.47230	-1.59900	H	-2.57990	6.18690	0.03650
H	-4.58620	0.53100	-1.49990	H	-3.26720	5.14110	-1.24940
H	-4.51720	-0.91090	-2.53890	H	-4.01200	5.15590	0.36520
H	-4.52870	-1.07570	-0.76520	O	-1.51430	-2.37350	2.86850
H	-2.66000	1.48030	-2.40060	O	-3.64950	2.67550	-0.38580
N	-2.16550	0.59910	-2.45230	O	-2.14580	4.22340	0.26030
O	0.18260	-0.47770	-1.58950	O	-3.33570	-1.59550	1.79320

## ONIOM Results

### TS4-Z

(B3LYP/6-31G\*\*:UFF) Energy = -1868.147992

(B3LYP/6-31G\*\*:UFF) Free Energy = -1866.987286

M06-2X/6-31G\*\* Derived free energy = -4601.397990

M06-2X/6-31G\*\* Derived free energy in solution = -4601.415476

Number of Imaginary Frequencies = 1 (-865.40)

### ONIOM (B3LYP/6-31G\*\*:UFF) Geometry

C	3.08370	1.86990	0.85080	H	4.04310	7.61770	-1.50410
C	5.18790	0.05200	1.35910	H	5.66240	5.72030	-0.98130
C	4.25530	-0.25190	0.44370	H	4.84790	3.60930	-0.19530
C	3.10780	0.67040	0.23780	O	2.06500	0.30610	-0.57240
H	6.03280	-0.60750	1.51980	P	0.69290	0.04420	0.29650
C	5.08270	1.29040	2.15760	O	0.23250	1.53440	0.87440
C	4.07870	2.16530	1.92230	O	1.03910	-0.76450	1.54680
C	3.96520	3.38320	2.76860	N	-3.12580	-0.72210	-0.44750
C	4.86970	3.62810	3.72370	H	-3.63230	-0.20570	0.25440
C	5.98110	2.68450	3.95260	C	-3.68300	-1.86310	-0.95880
C	6.08150	1.57400	3.21380	C	-2.01800	-4.17410	0.86170
H	3.14720	4.07760	2.62760	C	-0.81260	-3.60010	1.21820
H	4.78430	4.51590	4.33700	C	-1.94230	-1.90650	2.51200
H	6.71060	2.89070	4.72510	C	-3.18490	-2.42250	2.17300
H	6.89570	0.88270	3.39220	C	0.56160	-4.09360	0.88000
C	0.37460	4.96650	-0.45290	H	0.91870	-4.76000	1.67300
C	2.13370	2.90390	0.36230	H	0.57270	-4.65780	-0.04830
C	0.79030	2.67850	0.34050	C	-1.65730	-0.76200	3.43950
C	-0.12740	3.77680	-0.09260	H	-0.97560	-1.09960	4.22700
H	-0.27340	5.76610	-0.78530	H	-2.56770	-0.38490	3.89030
C	2.67680	4.19500	-0.16960	H	-1.12900	0.02630	2.89280
C	1.82700	5.18800	-0.50660	C	-4.45020	-1.90880	2.75770
C	2.34810	6.48510	-0.99890	C	-2.18040	-5.37550	0.03140
C	3.66360	6.67060	-1.14270	H	-0.36980	-7.96290	-0.66260
C	4.60030	5.57670	-0.82990	H	-2.15390	-7.99280	-0.46960
C	4.13910	4.40450	-0.37950	H	-6.85510	-0.86380	2.49850
H	1.66440	7.28750	-1.24730	H	-7.52440	-2.40000	1.86090

O	-1.14880	-6.23550	0.04750	C	-3.68870	7.27320	0.14480
O	-3.19840	-5.59400	-0.62120	C	-3.03390	5.97430	0.40440
O	-4.57170	-1.14010	3.69460	C	-2.81280	5.11400	-0.60400
O	-5.51850	-2.41430	2.09600	C	-3.20110	5.49490	-1.98460
Si	4.48350	-1.78500	-0.59620	C	-3.79110	6.67400	-2.21660
Si	-1.96790	3.48940	-0.27190	H	-4.53020	8.55600	-1.29180
C	8.89880	-1.54950	-2.17070	H	-3.87300	7.95590	0.96410
C	8.45770	-2.68230	-1.61270	H	-2.73780	5.73190	1.41720
C	7.07010	-2.77150	-1.11140	H	-2.99570	4.83440	-2.81610
C	6.23650	-1.72310	-1.23070	H	-4.07030	6.95260	-3.22450
C	6.74280	-0.46180	-1.82770	C	-3.89370	2.10200	3.77090
C	8.00150	-0.38250	-2.27580	C	-2.63440	2.55190	3.75060
H	9.91520	-1.48270	-2.53650	C	-2.00940	2.94730	2.47180
H	9.11650	-3.53670	-1.52590	C	-2.69430	2.84320	1.31880
H	6.75420	-3.69380	-0.64960	C	-4.09400	2.35350	1.35360
H	6.10950	0.41370	-1.87740	C	-4.65730	1.99450	2.51310
H	8.36900	0.54160	-2.70300	H	-4.35320	1.81240	4.70690
C	1.41670	-1.68460	-4.15330	H	-2.07150	2.63190	4.67150
C	2.38290	-0.76310	-4.07600	H	-1.00930	3.35820	2.49420
C	3.37020	-0.81420	-2.97730	H	-4.67750	2.29120	0.44980
C	3.30830	-1.78680	-2.05030	H	-5.67790	1.63470	2.53280
C	2.24380	-2.81500	-2.15760	C	-2.74200	0.75040	-4.00700
C	1.34380	-2.76030	-3.14660	C	-1.49180	0.95130	-3.57830
H	0.68810	-1.64430	-4.95260	C	-1.24080	1.80660	-2.40060
H	2.43620	0.03010	-4.81040	C	-2.26650	2.35970	-1.72870
H	4.10920	-0.02990	-2.91410	C	-3.64810	2.15230	-2.22910
H	2.17710	-3.61260	-1.43760	C	-3.87190	1.38650	-3.30390
H	0.56240	-3.50660	-3.21210	H	-2.92710	0.12700	-4.87210
C	3.79700	-5.56840	2.09550	H	-0.66000	0.49370	-4.09660
C	4.07800	-5.71360	0.79580	H	-0.21630	1.97460	-2.10430
C	4.29440	-4.52350	-0.05240	H	-4.48240	2.65130	-1.75740
C	4.20920	-3.28930	0.47360	H	-4.88090	1.24430	-3.66900
C	3.88440	-3.13640	1.91450	N	-0.82240	-2.46830	1.97650
C	3.69390	-4.21720	2.68120	H	0.05390	-1.82720	1.93160
H	3.63730	-6.43910	2.71820	H	1.23640	-3.23810	0.81930
H	4.14840	-6.70280	0.36240	C	-6.80390	-1.95370	2.54450
H	4.51900	-4.66340	-1.10260	H	-6.98800	-2.27480	3.57260
H	3.78600	-2.15570	2.35810	C	-1.29400	-7.40060	-0.78920
H	3.45230	-4.10310	3.73000	H	-1.43050	-7.10910	-1.83270
C	-4.05160	7.60440	-1.09980	C	-3.25160	-3.46510	1.16480

H	-3.56510	-2.78660	-0.00160	C	-5.93970	-3.00590	-1.41640
H	-4.15790	-4.06400	1.15750	C	-5.17710	-1.83910	-1.16270
O	-0.34630	-0.50650	-0.63840	C	-5.85930	-0.60960	-1.12270
H	-2.10160	-0.58120	-0.49030	C	-7.22780	-0.50620	-1.33930
C	-2.82970	-2.46720	-2.07460	H	-9.03150	-1.60870	-1.78870
H	-2.94850	-1.85390	-2.97150	H	-7.86660	-3.81230	-1.83920
H	-1.77380	-2.44970	-1.79310	H	-5.28600	0.29170	-0.95010
H	-3.13360	-3.48360	-2.32050	H	-7.70890	0.46630	-1.31630
C	-7.96200	-1.66410	-1.60690	O	-5.46200	-4.27240	-1.48420
C	-7.32130	-2.89540	-1.64170	H	-4.57130	-4.42790	-1.11900

### TS5-E

(B3LYP/6-31G\*\*):UFF) Energy = -1868.150712

(B3LYP/6-31G\*\*):UFF) Free Energy = -1866.986072

M06-2X/6-31G\*\* Derived free energy = -4601.397735

M06-2X/6-31G\*\* Derived free energy in solution = -4601.414528

Number of Imaginary Frequencies = 1 (-867.84)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	1.28950	-2.63450	1.24750	H	-4.05050	-2.38300	1.89240
C	4.08300	-3.04090	0.99950	C	-0.77180	-2.46010	2.82330
C	3.53550	-1.91510	0.52250	C	-2.11690	-2.42600	2.95530
C	2.06120	-1.69720	0.62570	C	-2.73070	-2.43200	4.30330
H	5.14430	-3.22440	0.90810	C	-1.95700	-2.44480	5.39390
C	3.24560	-4.09200	1.59710	C	-0.48780	-2.45050	5.25880
C	1.90870	-3.92530	1.68850	C	0.07630	-2.45390	4.04550
C	1.08010	-5.05780	2.19480	H	-3.80820	-2.42010	4.41040
C	1.65740	-6.19480	2.59940	H	-2.40640	-2.44470	6.37860
C	3.12190	-6.34660	2.53410	H	0.13280	-2.44420	6.14550
C	3.87570	-5.35370	2.05270	H	1.15540	-2.43890	3.96820
H	0.00160	-4.98790	2.22610	O	1.56980	-0.47110	0.22500
H	1.04920	-7.01260	2.96420	P	0.19760	-0.36150	-0.71120
H	3.58290	-7.26820	2.86510	O	-0.39680	-1.89140	-0.80670
H	4.95010	-5.47740	1.99520	O	0.57910	0.08130	-2.10820
C	-2.97930	-2.37390	1.75700	N	0.14690	2.34940	1.89150
C	-0.16850	-2.43060	1.46020	H	1.13030	2.57000	1.85010
C	-0.96400	-2.24930	0.38720	C	-0.69930	3.37840	2.22550
C	-2.44560	-2.30690	0.52800	C	0.67980	4.50550	-0.45060

C	1.02570	3.40270	-1.21520	H	3.31820	2.66500	3.15760
C	-1.28960	3.00610	-1.78510	H	3.20940	0.43390	1.97810
C	-1.68970	4.09000	-1.01730	H	6.29790	1.80630	-0.73410
C	2.40030	2.87710	-1.50700	H	6.39580	3.92130	0.41640
H	3.11350	3.18520	-0.75100	C	3.06690	-0.33490	-4.79550
H	2.34920	1.78800	-1.56690	C	2.68520	-1.36290	-4.03050
C	-2.13400	2.13260	-2.66620	C	3.17510	-1.47380	-2.64130
H	-1.62520	1.17850	-2.80860	C	3.99300	-0.53540	-2.12970
H	-2.27160	2.60890	-3.64310	C	4.43980	0.58150	-2.99790
H	-3.12090	1.96730	-2.24470	C	3.99220	0.68070	-4.25580
C	-3.03850	4.67640	-1.02940	H	2.70530	-0.24960	-5.81200
C	1.62010	5.51250	0.09780	H	2.01260	-2.11350	-4.42470
H	3.49450	7.40490	-0.23530	H	2.85750	-2.32400	-2.05350
H	3.82210	6.42140	1.20610	H	5.12040	1.33030	-2.62460
H	-5.04000	5.93090	-2.35800	H	4.31150	1.50340	-4.88240
H	-5.65980	4.33300	-2.88660	C	-6.75440	-5.73260	-0.53670
O	2.88610	5.41220	-0.36930	C	-5.76590	-5.85700	-1.42910
O	1.27840	6.38680	0.87510	C	-4.76070	-4.78370	-1.57780
O	-3.42410	5.52350	-0.22560	C	-4.82100	-3.68460	-0.80530
O	-3.82330	4.26580	-2.04080	C	-5.93710	-3.54410	0.16380
Si	4.61830	-0.68040	-0.37630	C	-6.84830	-4.51600	0.29300
Si	-3.57930	-2.30060	-0.96550	H	-7.49150	-6.51770	-0.42800
C	9.07600	-2.11370	-0.38840	H	-5.69960	-6.74460	-2.04500
C	8.38430	-2.09940	-1.53410	H	-3.98760	-4.91130	-2.31870
C	6.97590	-1.65130	-1.54460	H	-6.03950	-2.64340	0.75450
C	6.38430	-1.25940	-0.40340	H	-7.66360	-4.40630	0.99640
C	7.15620	-1.27550	0.86240	C	-1.01520	-2.61950	-4.88220
C	8.43180	-1.68130	0.86830	C	-0.94410	-3.58290	-3.95690
H	10.10740	-2.44160	-0.37990	C	-1.77420	-3.50060	-2.73740
H	8.85450	-2.41610	-2.45610	C	-2.60570	-2.46010	-2.55000
H	6.43830	-1.65300	-2.48310	C	-2.68970	-1.40420	-3.58880
H	6.68990	-0.96060	1.78770	C	-1.93130	-1.47820	-4.68940
H	8.99380	-1.69360	1.79320	H	-0.40170	-2.67360	-5.77220
C	4.80500	3.42660	1.88590	H	-0.26980	-4.41830	-4.09330
C	3.95280	2.48330	2.29980	H	-1.67090	-4.26960	-1.98170
C	3.87870	1.18790	1.59220	H	-3.35420	-0.56100	-3.46480
C	4.64560	0.95930	0.51110	H	-1.98790	-0.70120	-5.44080
C	5.61550	1.99810	0.08260	C	-6.14010	1.61360	-1.05960
C	5.68420	3.16830	0.72920	C	-5.08500	1.53550	-0.24060
H	4.86300	4.37310	2.40700	C	-4.26300	0.30780	-0.20630

C	-4.56570	-0.72830	-1.00480	O	-0.75040	0.52830	0.06340
C	-5.72640	-0.62980	-1.92140	H	-0.16870	1.61200	1.23140
C	-6.47370	0.48000	-1.94430	C	-0.07500	4.39100	3.18670
H	-6.74850	2.50770	-1.08040	H	0.90560	4.71340	2.82860
H	-4.82780	2.37390	0.39160	H	-0.71220	5.26640	3.29300
H	-3.41720	0.26520	0.46360	H	0.04610	3.91030	4.16360
H	-5.97610	-1.45730	-2.57370	C	-4.70650	2.19250	3.32310
H	-7.32260	0.55000	-2.61200	C	-4.42580	3.52920	3.04840
N	0.03200	2.67600	-1.80000	C	-3.14070	3.91740	2.65880
H	0.27940	1.69670	-2.12320	C	-2.11000	2.95950	2.55320
H	2.75460	3.25410	-2.47310	C	-2.41620	1.61510	2.82360
C	-5.12800	4.87200	-2.10350	C	-3.69940	1.23320	3.20620
H	-5.64260	4.77940	-1.14590	H	-5.70840	1.90110	3.62530
C	3.79690	6.41510	0.11460	H	-5.18850	4.29680	3.13330
H	4.77020	6.14520	-0.29400	H	-1.63610	0.86920	2.73180
C	-0.71960	4.72190	-0.13460	H	-3.91250	0.18930	3.41240
H	-0.86620	4.11330	1.13970	O	-2.87780	5.24630	2.42660
H	-0.97230	5.71290	0.23110	H	-3.12620	5.47020	1.50330

#### TS4-E

(B3LYP/6-31G\*\*):UFF) Energy = -1868.150242

(B3LYP/6-31G\*\*):UFF) Free Energy = -1866.989436

M06-2X/6-31G\*\* Derived free energy = -4601.403198

M06-2X/6-31G\*\* Derived free energy in solution = -4601.419580

Number of Imaginary Frequencies = 1 (-825.60)

#### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	-2.82620	2.26660	-0.38870	C	-5.98050	2.83920	-2.47990
C	-5.06020	0.78170	-1.26840	H	-2.88490	4.93160	-1.36120
C	-4.09250	0.16900	-0.56910	H	-4.60100	5.94390	-2.70890
C	-2.86660	0.93160	-0.19090	H	-6.63300	4.58910	-3.44210
H	-5.95820	0.25320	-1.55290	H	-6.84130	2.26740	-2.80360
C	-4.93250	2.20140	-1.64940	C	0.18990	4.78530	1.36860
C	-3.86960	2.92120	-1.22940	C	-1.78110	3.07420	0.28830
C	-3.74580	4.34320	-1.65030	C	-0.47310	2.84220	0.03200
C	-4.69480	4.90930	-2.40490	C	0.55510	3.79440	0.54120
C	-5.86760	4.12390	-2.83440	H	0.92730	5.46760	1.77280

C	-2.16840	4.13960	1.26090	C	-8.92580	-2.58600	0.28960
C	-1.21910	4.95820	1.76360	C	-8.22950	-2.36250	1.41020
C	-1.58670	6.02430	2.72450	C	-6.78820	-2.04320	1.33700
C	-2.85670	6.16610	3.11750	C	-6.17250	-1.96500	0.14480
C	-3.89530	5.25380	2.60350	C	-6.94850	-2.22520	-1.09270
C	-3.57360	4.29150	1.73130	C	-8.25300	-2.51660	-1.02290
H	-0.82770	6.69170	3.11350	H	-9.98100	-2.82060	0.34240
H	-3.12440	6.94420	3.82070	H	-8.71990	-2.41580	2.37360
H	-4.91760	5.35870	2.94310	H	-6.25050	-1.87430	2.25890
H	-4.34850	3.61900	1.38910	H	-6.46250	-2.18290	-2.05960
O	-1.85080	0.31050	0.49560	H	-8.81690	-2.70490	-1.92730
P	-0.39930	0.28980	-0.29930	C	-2.30080	-1.91460	4.21770
O	-0.10370	1.83340	-0.82400	C	-2.13050	-2.89470	3.32300
O	-0.54210	-0.50050	-1.59280	C	-2.79360	-2.81790	2.00490
N	3.35060	-0.84180	0.38740	C	-3.56210	-1.76180	1.69340
H	3.86470	-0.22790	-0.22190	C	-3.76180	-0.68750	2.69760
C	3.99830	-1.94890	0.87240	C	-3.15950	-0.75870	3.89080
C	2.19000	-4.24880	-0.63670	H	-1.81230	-1.96770	5.18200
C	1.03920	-3.50250	-0.86620	H	-1.50170	-3.74340	3.55960
C	2.19370	-2.14980	-2.49590	H	-2.64460	-3.62590	1.30710
C	3.39820	-2.77400	-2.21580	H	-4.38740	0.16530	2.46470
C	-0.30080	-3.70470	-0.22690	H	-3.29990	0.03040	4.61810
H	-0.79220	-4.59330	-0.63040	C	-2.61540	-4.57610	-3.14400
H	-0.18870	-3.85570	0.84690	C	-3.28010	-5.04000	-2.07910
C	1.91110	-1.14640	-3.57440	C	-3.83190	-4.09830	-1.08270
H	1.32580	-0.32070	-3.15840	C	-3.65840	-2.77470	-1.23440
H	1.28160	-1.61920	-4.33800	C	-2.95790	-2.26580	-2.43820
H	2.82230	-0.80450	-4.05150	C	-2.45160	-3.12100	-3.33500
C	4.63340	-2.48700	-2.98660	H	-2.20460	-5.26440	-3.87110
C	2.24400	-5.51740	0.10000	H	-3.40750	-6.10560	-1.94020
H	0.02380	-7.51230	1.34630	H	-4.37090	-4.49270	-0.23020
H	1.57130	-8.04090	0.60640	H	-2.85330	-1.20250	-2.60400
H	7.18630	-1.76580	-3.16890	H	-1.93140	-2.74790	-4.20770
H	7.72050	-3.32230	-2.45210	C	4.17170	7.96310	0.20710
O	1.04320	-6.02630	0.43080	C	3.29370	7.62780	-0.74480
O	3.28910	-6.11440	0.36330	C	2.72470	6.26470	-0.78070
O	4.72220	-1.85960	-4.02620	C	3.09620	5.34910	0.13050
O	5.72100	-3.02820	-2.37880	C	4.05420	5.73550	1.19680
Si	-4.35400	-1.58740	0.01490	C	4.56520	6.97260	1.22860
Si	2.35910	3.63750	0.08710	H	4.58870	8.96140	0.23540

H	2.99750	8.35410	-1.49060	H	0.30230	-1.73230	-1.73750
H	2.00520	6.02450	-1.55090	H	-0.92340	-2.82950	-0.40830
H	4.33170	5.03440	1.97080	C	6.96710	-2.83120	-3.06690
H	5.25920	7.25370	2.01010	H	6.93010	-3.27870	-4.06290
C	2.87300	2.19390	-4.34510	C	1.06900	-7.25640	1.17610
C	3.73560	1.78010	-3.41020	H	1.58910	-7.11300	2.12580
C	3.56310	2.19900	-2.00470	C	3.45280	-3.70460	-1.10080
C	2.54760	3.00680	-1.65680	H	3.88340	-2.90790	-0.03180
C	1.59750	3.46540	-2.70110	H	4.29860	-4.38340	-1.07150
C	1.74880	3.07420	-3.97210	O	0.61920	-0.15740	0.71320
H	2.99600	1.88280	-5.37440	H	2.33720	-0.67240	0.45900
H	4.56180	1.13520	-3.68050	C	5.51840	-1.78020	0.90080
H	4.28540	1.86090	-1.28080	H	5.86340	-1.34660	-0.04270
H	0.76920	4.11170	-2.43990	H	6.01370	-2.73510	1.05620
H	1.05020	3.40530	-4.72940	H	5.79070	-1.10290	1.71570
C	4.53210	1.01540	3.31320	C	2.14160	-3.91770	4.24810
C	3.20220	1.14960	3.34940	C	3.22450	-4.50790	3.60080
C	2.50920	1.95250	2.32080	C	3.82030	-3.88160	2.50100
C	3.21020	2.55480	1.34430	C	3.35050	-2.62850	2.04860
C	4.68720	2.41160	1.31920	C	2.24030	-2.06300	2.70210
C	5.31120	1.68180	2.25120	C	1.64530	-2.69620	3.79050
H	5.03940	0.42180	4.06250	H	1.68760	-4.41040	5.10330
H	2.62930	0.66700	4.13070	H	3.63260	-5.45810	3.93170
H	1.43370	2.04750	2.38090	H	1.81640	-1.13100	2.34880
H	5.27200	2.91870	0.56250	H	0.79720	-2.22800	4.27920
H	6.38890	1.58430	2.23330	O	4.86910	-4.49720	1.86010
N	1.09550	-2.47240	-1.74760	H	4.50570	-5.26330	1.36620

### TS5-Z

(B3LYP/6-31G\*\*):UFF) Energy = -1868.149203

(B3LYP/6-31G\*\*):UFF) Free Energy = -1866.987612

M06-2X/6-31G\*\* Derived free energy = -4601.400364

M06-2X/6-31G\*\* Derived free energy in solution = -4601.417016

Number of Imaginary Frequencies = 1 (-894.32)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	0.19980	-3.07410	1.13130	C	2.64850	-4.38750	0.59320
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C	2.48600	-3.11150	0.21680	H	3.76450	1.87680	-2.10210
C	1.17700	-2.42560	0.44110	H	2.48630	0.60660	-2.08070
H	3.58490	-4.90170	0.42310	C	-1.90920	2.33630	-2.76780
C	1.54420	-5.13550	1.21410	H	-2.18140	2.78630	-3.72770
C	0.36430	-4.52560	1.45670	H	-2.74390	2.49110	-2.08590
C	-0.76110	-5.33420	2.00720	H	-1.74720	1.26740	-2.90710
C	-0.58720	-6.62760	2.30150	C	-1.61250	5.13680	-1.37650
C	0.71880	-7.27130	2.07010	C	3.26990	4.28770	-1.06150
C	1.72840	-6.56720	1.54910	H	4.16160	6.59050	1.03520
H	-1.73760	-4.89530	2.16050	H	5.05830	5.07230	0.70280
H	-1.40890	-7.20900	2.69950	H	-3.43220	6.94200	-2.33220
H	0.85370	-8.31740	2.31310	H	-4.58720	5.58830	-2.54620
H	2.68170	-7.04950	1.37140	O	3.17860	5.30510	-0.17270
C	-3.62350	-1.44960	2.23790	O	4.33860	3.87980	-1.47930
C	-1.04410	-2.37800	1.55200	O	-1.54550	6.01080	-0.51430
C	-1.85600	-1.86610	0.60830	O	-2.68500	5.00200	-2.17400
C	-3.25290	-1.47930	0.94860	Si	3.91010	-2.21300	-0.59500
H	-4.62320	-1.15300	2.51780	Si	-4.51860	-1.11170	-0.38370
C	-1.44960	-2.30610	2.98440	C	2.83620	-1.55840	-5.12160
C	-2.68070	-1.84760	3.30400	C	4.02320	-1.15850	-4.65320
C	-3.09290	-1.75760	4.72390	C	4.36990	-1.37180	-3.23280
C	-2.24170	-2.10870	5.69420	C	3.48790	-1.94560	-2.39530
C	-0.88590	-2.58200	5.35410	C	2.18990	-2.42450	-2.93510
C	-0.50620	-2.67240	4.07430	C	1.87910	-2.23120	-4.22270
H	-4.08410	-1.40570	4.98140	H	2.57990	-1.40070	-6.16120
H	-2.54280	-2.04080	6.73160	H	4.73240	-0.67560	-5.31290
H	-0.19640	-2.84850	6.14470	H	5.35190	-1.07750	-2.89480
H	0.49830	-3.00390	3.84610	H	1.48090	-2.93500	-2.29900
O	1.08130	-1.08840	0.11680	H	0.92750	-2.57380	-4.60890
P	-0.23340	-0.52590	-0.73740	C	7.79090	-4.79900	-0.16110
O	-1.38200	-1.70030	-0.66480	C	7.20900	-4.68120	-1.36050
O	0.11280	-0.39050	-2.20680	C	5.98560	-3.86650	-1.51440
N	1.08300	2.43140	1.33700	C	5.45810	-3.23340	-0.45260
H	2.08390	2.39180	1.21700	C	6.10260	-3.37470	0.87510
C	0.50730	3.65880	1.52030	C	7.20900	-4.11570	1.01170
C	1.91810	3.78300	-1.41190	H	8.68600	-5.39670	-0.04720
C	1.73100	2.57870	-2.06810	H	7.63130	-5.18470	-2.22050
C	-0.64910	2.95730	-2.23860	H	5.52280	-3.80790	-2.48960
C	-0.52010	4.18920	-1.62410	H	5.67940	-2.88140	1.74120
C	2.78340	1.58760	-2.46090	H	7.67820	-4.21790	1.98160

C	4.82630	1.69210	1.85120	C	-4.89560	0.70600	-0.41490
C	5.37230	1.52080	0.64310	C	-4.14660	1.64750	0.45150
C	5.08470	0.29730	-0.13480	C	-4.47730	2.94510	0.47580
C	4.23910	-0.63110	0.34350	H	-5.86020	4.48860	-0.32970
C	3.65780	-0.44350	1.69830	H	-7.06730	2.96280	-1.77310
C	3.94080	0.65310	2.41120	H	-6.47200	0.49430	-1.80700
H	5.03550	2.58790	2.42170	H	-3.33520	1.29410	1.07320
H	6.03020	2.27620	0.23340	H	-3.93780	3.63340	1.11250
H	5.57500	0.17200	-1.08590	N	0.46710	2.19590	-2.41110
H	3.02560	-1.20260	2.13750	H	0.32110	1.14820	-2.55400
H	3.52280	0.77910	3.40140	H	2.81920	1.50660	-3.55300
C	-8.59600	-3.18010	0.68620	C	-3.74170	5.95920	-1.96820
C	-7.84000	-3.68280	-0.29600	H	-3.99140	6.03710	-0.90940
C	-6.55480	-3.04180	-0.64580	C	4.42800	5.85600	0.27680
C	-6.12800	-1.96160	0.03190	H	4.95970	6.32580	-0.55420
C	-6.98570	-1.39670	1.10410	C	0.75110	4.55300	-1.01120
C	-8.15090	-1.97690	1.41570	H	0.58820	4.27560	0.31760
H	-9.53760	-3.64830	0.94230	H	0.91640	5.61600	-0.85740
H	-8.16780	-4.56060	-0.83770	O	-0.66430	0.71970	0.00670
H	-5.97910	-3.46530	-1.45360	H	0.52320	1.69310	0.87220
H	-6.68580	-0.49830	1.62810	C	-1.00310	3.56150	1.70700
H	-8.77480	-1.55900	2.19520	H	-1.47950	4.54070	1.73220
C	-2.79250	-2.51280	-4.51620	H	-1.19600	3.05830	2.65980
C	-2.90990	-3.38430	-3.50830	H	-1.43570	2.94930	0.91300
C	-3.48240	-2.95020	-2.21750	C	2.68390	6.31470	4.14580
C	-3.89080	-1.67980	-2.04740	C	1.74850	6.84290	3.26490
C	-3.77220	-0.72430	-3.17560	C	1.02210	6.01630	2.39280
C	-3.24680	-1.11890	-4.34200	C	1.25080	4.61860	2.40750
H	-2.36570	-2.82660	-5.45990	C	2.19800	4.11310	3.31660
H	-2.57540	-4.40620	-3.63180	C	2.91330	4.93680	4.17780
H	-3.53200	-3.66150	-1.40220	H	3.22740	6.97850	4.81220
H	-4.09670	0.30010	-3.06660	H	1.54830	7.90850	3.22370
H	-3.15240	-0.41650	-5.16000	H	2.33770	3.03900	3.36200
C	-5.58630	3.44260	-0.36270	H	3.62760	4.50770	4.87320
C	-6.25450	2.59990	-1.15750	O	0.15100	6.67440	1.59030
C	-5.89940	1.16670	-1.17990	H	-0.33380	6.14360	0.93130

**TS6-E**

(B3LYP/6-31G\*\*):UFF) Energy = -1868.170151

(B3LYP/6-31G\*\*):UFF) Free Energy = -1867.008482

M06-2X/6-31G\*\* Derived free energy = -4601.418309

M06-2X/6-31G\*\* Derived free energy in solution = -4601.435352

Number of Imaginary Frequencies = 1 (-771.73)

**ONIOM (B3LYP/6-31G\*\*):UFF) Geometry**

O	2.16600	0.23570	-0.76140	H	-1.34310	0.14180	2.55750
P	0.66800	0.08530	-0.11360	H	-2.38260	-0.28270	3.95410
O	0.30260	1.55600	0.56500	C	-0.50600	-3.95320	-0.00470
O	-0.23290	-0.21470	-1.28780	H	-0.27260	-4.97690	0.29460
O	0.67880	-0.87240	1.06120	H	-0.71550	-3.97120	-1.07630
H	-4.30460	-0.07340	-0.16540	H	0.35110	-3.30760	0.18440
C	-5.26440	-1.82090	-0.52890	C	-3.62690	-2.18700	2.38310
C	-2.74930	-2.92790	-3.85380	C	-3.44190	-5.13720	0.00600
C	-2.27360	-2.03410	-2.90420	C	-4.72440	-1.65610	3.22280
C	-3.09300	-1.63860	-1.82950	H	-3.45260	-7.67690	-0.75400
C	-4.40630	-2.16630	-1.70320	H	-3.53920	-6.62430	-2.18590
C	-4.84410	-3.08370	-2.67550	C	-2.89770	-6.96620	-1.37050
C	-4.04100	-3.45610	-3.74740	H	-1.98950	-7.42350	-1.76240
H	-2.10860	-3.21310	-4.68370	C	-5.41010	-0.63800	5.23700
H	-1.27580	-1.61320	-2.96900	H	-5.97180	0.13750	4.71220
H	-5.83960	-3.50410	-2.59520	H	-6.09420	-1.44360	5.51270
H	-4.41830	-4.14790	-4.49380	H	-4.92250	-0.22880	6.12110
C	-6.65470	-2.43270	-0.43870	O	-4.61790	-5.45720	-0.06630
H	-7.29700	-2.02450	-1.22630	O	-5.89800	-1.70580	2.88260
H	-6.61350	-3.51910	-0.52930	O	-4.34440	-1.14570	4.41330
H	-7.09290	-2.18900	0.53200	O	-2.45560	-5.84750	-0.58320
H	-5.71810	-0.32290	0.76520	O	-2.65160	-0.76680	-0.90600
N	-5.22290	-0.49990	-0.09980	H	-1.67200	-0.49860	-1.07380
C	-2.97990	-3.94620	0.74850	C	-4.03060	-3.19890	1.41570
C	-1.69440	-3.43520	0.75300	H	-4.64760	-2.52960	0.40430
N	-1.43220	-2.34110	1.52250	H	-4.92450	-3.76830	1.66180
H	-0.50770	-1.83000	1.37380	C	3.10410	0.58060	0.17390
C	-2.31420	-1.75120	2.38010	C	3.11350	1.83300	0.67290
C	-1.69380	-0.66390	3.21010	C	4.97730	-0.09100	1.59040
H	-0.80360	-1.05320	3.71300	C	4.12250	-0.41150	0.60830

H	5.71450	-0.80820	1.93100	C	-3.84530	7.00110	-1.92200
C	2.22890	2.86100	0.05840	C	-3.25960	5.64970	-1.79880
C	0.88330	2.67470	0.00970	C	-2.62680	5.28790	-0.66940
C	0.00380	3.78490	-0.46340	C	-2.50400	6.26320	0.44090
C	0.55170	4.92000	-0.92080	C	-3.03300	7.48730	0.32490
H	-0.06950	5.72590	-1.28870	H	-4.16630	8.86390	-1.00310
C	4.92320	1.24040	2.22910	H	-4.35810	7.28370	-2.83230
C	4.03120	2.16450	1.80250	H	-3.33940	4.97500	-2.63930
C	3.95440	3.47380	2.50530	H	-1.98180	5.99230	1.34950
C	4.78650	3.74770	3.51670	H	-2.94180	8.19780	1.13630
C	5.77980	2.74750	3.95230	C	-3.34030	2.30820	3.78200
C	5.84280	1.55690	3.34630	C	-4.10280	2.05810	2.71270
H	3.21970	4.21350	2.21650	C	-3.62960	2.42570	1.36300
H	4.72710	4.70150	4.02500	C	-2.41720	2.97900	1.19220
H	6.45130	2.97730	4.76940	C	-1.57240	3.24280	2.38530
H	6.56880	0.82470	3.67750	C	-2.01120	2.92610	3.60970
C	2.82530	4.09250	-0.54430	H	-3.68990	2.04800	4.77260
C	2.01470	5.07890	-0.98560	H	-5.07620	1.60150	2.83330
C	2.59080	6.31330	-1.56860	H	-4.29720	2.26840	0.53520
C	3.91570	6.44740	-1.68490	H	-0.60470	3.71500	2.27870
C	4.80900	5.36000	-1.24460	H	-1.39490	3.12630	4.47650
C	4.29840	4.24390	-0.71220	C	1.92600	-5.22520	2.44550
H	1.94040	7.11120	-1.90510	C	2.01220	-3.95220	2.84730
H	4.33550	7.34870	-2.11250	C	2.75380	-2.96680	2.03360
H	5.87970	5.46350	-1.36480	C	3.33300	-3.33840	0.87840
H	4.97420	3.45060	-0.42310	C	3.24080	-4.75490	0.44520
Si	-1.85770	3.60460	-0.47540	C	2.57400	-5.64690	1.18770
Si	4.23310	-2.09810	-0.18740	H	1.37960	-5.94700	3.03860
C	-3.04500	0.97350	-4.18320	H	1.53470	-3.63930	3.76680
C	-3.99590	1.43710	-3.36550	H	2.80650	-1.94590	2.38530
C	-3.62950	2.26160	-2.19550	H	3.70830	-5.07210	-0.47870
C	-2.33830	2.51690	-1.91820	H	2.50380	-6.67770	0.86570
C	-1.29210	2.01830	-2.84670	C	2.21540	-1.76680	-4.41680
C	-1.62780	1.28440	-3.91470	C	3.27920	-1.01300	-4.11900
H	-3.31150	0.36860	-5.04020	C	3.93660	-1.14520	-2.80200
H	-5.03660	1.21430	-3.56170	C	3.48060	-2.03020	-1.89790
H	-4.42430	2.68960	-1.60350	C	2.30970	-2.87430	-2.24620
H	-0.24850	2.24210	-2.67300	C	1.70760	-2.74300	-3.43430
H	-0.86060	0.91530	-4.58310	H	1.72590	-1.66340	-5.37650
C	-3.73910	7.87360	-0.91310	H	3.65180	-0.29280	-4.83590

H	4.75410	-0.48010	-2.56800	C	6.97820	-1.56010	-0.94370
H	1.92120	-3.59440	-1.54660	C	8.28200	-1.84610	-1.04450
H	0.84680	-3.35290	-3.67760	H	9.85340	-3.36010	-0.62070
C	8.79900	-3.13110	-0.53510	H	8.34380	-4.94250	0.42590
C	7.96590	-4.00350	0.04260	H	5.88690	-4.40560	0.65110
C	6.52680	-3.68840	0.16070	H	6.62310	-0.59840	-1.28590
C	6.04170	-2.53350	-0.32860	H	8.96280	-1.12990	-1.48610

### TS7-E

(B3LYP/6-31G\*\*):UFF) Energy = -1868.159365

(B3LYP/6-31G\*\*):UFF) Free Energy = -1866.997377

M06-2X/6-31G\*\* Derived free energy = -4601.415225

M06-2X/6-31G\*\* Derived free energy in solution = -4601.433118

Number of Imaginary Frequencies = 1 (-783.16)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

O	1.92460	0.34490	-0.60220	H	-4.34650	-3.83940	-2.91660
P	0.36850	0.23530	-0.06420	N	-4.35900	-2.98250	-2.37950
O	-0.05020	1.70750	0.57920	C	-1.95280	-4.62530	-0.73430
O	-0.45640	-0.05250	-1.29530	C	-0.95720	-3.70740	-0.44700
O	0.28650	-0.73430	1.09780	N	-1.01820	-3.02280	0.73140
H	-3.54510	-2.38490	-2.48000	H	-0.38580	-2.18100	0.85580
C	-4.84760	-3.10160	-1.08780	C	-1.92630	-3.25310	1.72810
C	-4.35300	0.16200	1.67980	C	-1.69090	-2.46510	2.98730
C	-3.41110	-0.02290	0.67500	H	-2.62270	-2.02310	3.34060
C	-3.57570	-1.04450	-0.27530	H	-1.32740	-3.12470	3.78090
C	-4.71000	-1.90420	-0.20080	H	-0.95830	-1.67820	2.80270
C	-5.63970	-1.68170	0.82980	C	0.20820	-3.35350	-1.32190
C	-5.48040	-0.65810	1.75830	H	0.78040	-4.24970	-1.56180
H	-4.19820	0.94510	2.41310	H	-0.13590	-2.91820	-2.26260
H	-2.54240	0.62270	0.60950	H	0.84610	-2.62260	-0.82960
H	-6.50770	-2.32620	0.90560	C	-2.94050	-4.16440	1.49390
H	-6.22200	-0.50700	2.53590	C	-2.05540	-5.43480	-1.96270
C	-6.12570	-3.92900	-1.01580	C	-3.99460	-4.54970	2.45680
H	-6.97830	-3.33700	-1.36540	H	-1.26820	-7.32060	-3.67450
H	-6.02390	-4.80270	-1.66540	H	-1.75530	-5.86260	-4.56550
H	-6.31530	-4.28820	-0.00400	C	-1.00290	-6.28410	-3.89480

H	-0.01300	-6.22820	-4.34680	H	1.82390	7.22140	-1.82810
C	-4.74520	-4.58570	4.68770	H	4.23130	7.38660	-1.94840
H	-5.68580	-4.08670	4.44350	H	5.69060	5.46990	-1.11410
H	-4.90870	-5.66580	4.68870	H	4.69100	3.49860	-0.17870
H	-4.37340	-4.25240	5.65620	Si	-2.13860	3.91300	-0.37930
O	-3.08690	-5.99650	-2.30630	Si	4.27610	-1.75180	-0.14330
O	-5.01670	-5.12910	2.12550	C	-3.62170	0.80710	-3.56880
O	-3.72320	-4.23050	3.74100	C	-2.35550	1.23690	-3.58870
O	-0.91470	-5.51610	-2.68310	C	-1.88380	2.20100	-2.57260
O	-2.66840	-1.25310	-1.24480	C	-2.71350	2.63120	-1.60620
H	-1.81940	-0.67330	-1.20180	C	-4.12290	2.16620	-1.60560
C	-3.09540	-4.71200	0.15970	C	-4.54990	1.29990	-2.53290
H	-4.03270	-3.91840	-0.43080	H	-3.96770	0.09770	-4.30920
H	-3.69990	-5.61260	0.07950	H	-1.67220	0.87860	-4.34760
C	2.80410	0.72530	0.38030	H	-0.86240	2.55270	-2.63090
C	2.74510	1.97410	0.88190	H	-4.81670	2.51170	-0.85610
C	4.68900	0.15820	1.83420	H	-5.57530	0.95370	-2.52160
C	3.89780	-0.19120	0.80850	C	-3.86780	8.09560	-1.58860
H	5.48640	-0.49650	2.16340	C	-4.03550	7.05150	-2.40890
C	1.91340	2.99190	0.19190	C	-3.49370	5.72600	-2.04270
C	0.57060	2.83090	0.07890	C	-2.82970	5.56470	-0.88540
C	-0.26380	3.98090	-0.39190	C	-2.64790	6.72540	0.01960
C	0.33690	5.09110	-0.84870	C	-3.13990	7.92440	-0.31510
H	-0.24150	5.92380	-1.22310	H	-4.26430	9.06650	-1.85610
C	4.51030	1.45800	2.51130	H	-4.56830	7.17500	-3.34280
C	3.58990	2.33740	2.05620	H	-3.63950	4.90090	-2.72630
C	3.41330	3.63350	2.76470	H	-2.11410	6.60760	0.95440
C	4.18170	3.93780	3.81710	H	-3.00540	8.77070	0.34600
C	5.20430	2.98450	4.28950	C	-3.87510	3.39500	3.95060
C	5.35930	1.80720	3.67370	C	-2.56060	3.25660	3.74640
H	2.65750	4.33850	2.44420	C	-2.00100	3.40750	2.38710
H	4.05040	4.88190	4.32970	C	-2.81190	3.63760	1.33910
H	5.82480	3.23900	5.13900	C	-4.26550	3.81970	1.58070
H	6.10890	1.11090	4.02870	C	-4.76720	3.70410	2.81640
C	2.56800	4.19980	-0.39480	H	-4.28530	3.29040	4.94660
C	1.80450	5.20110	-0.87910	H	-1.90170	3.04260	4.57800
C	2.43770	6.41000	-1.45670	H	-0.93010	3.35700	2.27170
C	3.76950	6.50420	-1.52470	H	-4.92590	4.09040	0.76840
C	4.61350	5.39890	-1.03430	H	-5.82600	3.84790	2.98860
C	4.05040	4.30650	-0.50580	C	1.80110	-5.32860	1.61920

C	1.70450	-4.11450	2.17160	H	3.00920	-0.67280	-5.67870
C	2.48570	-2.98620	1.62400	H	4.20830	0.96800	-4.35570
C	3.29170	-3.16990	0.56400	H	4.75820	0.49840	-1.93160
C	3.42590	-4.52950	-0.01540	H	2.89250	-3.38990	-2.35560
C	2.71170	-5.54840	0.47840	H	2.33940	-2.90530	-4.63840
H	1.22220	-6.15340	2.01410	C	8.87960	-2.57370	0.25640
H	1.04660	-3.95310	3.01520	C	8.00410	-3.46500	0.73420
H	2.38960	-2.01730	2.09350	C	6.55230	-3.21650	0.61400
H	4.11160	-4.70760	-0.83400	C	6.10180	-2.10160	0.01160
H	2.80880	-6.53770	0.05050	C	7.08020	-1.11040	-0.50000
C	3.26020	-0.88360	-4.64730	C	8.39470	-1.33650	-0.38590
C	3.92340	0.01990	-3.91820	H	9.94310	-2.75400	0.34520
C	4.25850	-0.26810	-2.50860	H	8.35690	-4.36990	1.21200
C	3.90190	-1.43770	-1.94680	H	5.87270	-3.94430	1.03240
C	3.17830	-2.43830	-2.76890	H	6.74240	-0.19070	-0.95500
C	2.87100	-2.17290	-4.04450	H	9.10530	-0.60950	-0.75730

### ***OH-binding Type I Z***

(B3LYP/6-31G\*\*):UFF) Energy = -1868.131155

(B3LYP/6-31G\*\*):UFF) Free Energy = -1866.968850

M06-2X/6-31G\*\* Derived free energy = -4601.388414

M06-2X/6-31G\*\* Derived free energy in solution = -4601.406026

Number of Imaginary Frequencies = 1 (-941.59)

### **ONIOM (B3LYP/6-31G\*\*):UFF) Geometry**

O	-1.46280	-1.27730	-0.90590	C	3.47360	5.08620	-3.31920
P	-0.18230	-0.41610	-0.30760	H	3.46400	4.81140	-5.46030
O	0.76200	-1.49360	0.53020	H	1.78910	2.96670	-5.39200
O	0.53780	0.07980	-1.53480	H	3.23370	5.12860	-1.18500
O	-0.63940	0.59530	0.73310	H	4.21380	5.87960	-3.33010
H	-0.41270	2.99760	-1.65740	C	2.29620	2.22090	0.01780
C	1.39710	3.18290	-0.74730	H	3.28380	2.66100	0.16930
C	3.05060	4.48790	-4.50920	H	1.86630	1.93680	0.97870
C	2.11100	3.46410	-4.48310	H	2.37760	1.30840	-0.57470
C	1.56150	3.01160	-3.27320	H	-0.26170	2.06810	-0.21660
C	1.95740	3.64620	-2.06620	N	0.05560	2.88140	-0.76940
C	2.92370	4.65990	-2.11520	C	-0.34180	5.22410	0.82110

C	-1.25240	4.26040	1.21380	C	2.59230	-4.21530	-1.16730
N	-0.84720	3.32530	2.12870	H	3.59280	-4.50730	-1.46120
H	-1.37830	2.46060	2.16880	C	-3.20050	-4.05010	1.72630
C	0.38160	3.30100	2.75410	C	-1.93320	-4.23950	1.29920
C	0.50250	2.19290	3.75710	C	-1.13970	-5.36400	1.86730
H	-0.30660	2.25820	4.49300	C	-1.68980	-6.19800	2.75720
H	0.39460	1.23890	3.22370	C	-3.08580	-6.00280	3.19230
H	1.45260	2.22320	4.27860	C	-3.80190	-4.98250	2.70820
C	-2.68490	4.13320	0.79410	H	-0.10740	-5.51360	1.58000
H	-3.32500	4.78260	1.40030	H	-1.10880	-7.01360	3.16810
H	-2.82090	4.41350	-0.24690	H	-3.52540	-6.68280	3.91050
H	-3.00610	3.10190	0.93560	H	-4.82340	-4.84050	3.03850
C	1.32300	4.21880	2.35130	C	0.21710	-4.80710	-1.09270
C	-0.61740	6.35930	-0.09580	C	1.46830	-5.10850	-1.50390
C	2.68230	4.40320	2.91680	C	1.71770	-6.34080	-2.28750
H	-1.83660	8.60670	-0.80950	C	0.70240	-7.14900	-2.61040
H	-1.75210	7.50150	-2.19880	C	-0.67200	-6.81150	-2.19430
C	-2.21550	7.67020	-1.22440	C	-0.90640	-5.70320	-1.48210
H	-3.30100	7.69890	-1.31270	H	2.72320	-6.59130	-2.60240
C	4.13510	4.18000	4.75830	H	0.88520	-8.04860	-3.18380
H	4.91080	3.73340	4.13320	H	-1.49210	-7.45970	-2.47500
H	4.33310	5.24990	4.85600	H	-1.92500	-5.46530	-1.20610
H	4.10480	3.70450	5.73790	Si	3.85170	-2.03820	0.00360
O	0.26260	7.05190	-0.56850	Si	-4.49940	-0.59230	-0.23410
O	3.57770	4.94850	2.29790	C	7.53160	-4.92380	0.38810
O	2.83030	3.96500	4.18680	C	7.55060	-3.94600	-0.52460
O	-1.93110	6.57440	-0.33370	C	6.39830	-3.02960	-0.65390
O	0.64460	2.01500	-3.36380	C	5.33070	-3.16400	0.15270
H	0.65560	1.34180	-2.62440	C	5.31200	-4.26020	1.15220
C	1.03950	5.03160	1.17070	C	6.35540	-5.09120	1.26400
H	1.46960	4.23260	0.05630	H	8.37410	-5.59670	0.48230
H	1.70990	5.86400	0.98280	H	8.40900	-3.82510	-1.17260
C	-2.02900	-2.18370	-0.04730	H	6.43420	-2.26690	-1.41790
C	-1.34430	-3.29310	0.30760	H	4.45130	-4.40620	1.78900
C	-3.98810	-2.90860	1.22350	H	6.33680	-5.89190	1.99200
C	-3.45160	-2.02360	0.36950	C	3.01870	-0.34050	4.29730
H	-5.00570	-2.79890	1.56670	C	3.60730	0.43730	3.38260
C	-0.01680	-3.56360	-0.30020	C	3.86020	-0.07670	2.02210
C	0.99210	-2.68070	-0.12500	C	3.51660	-1.33350	1.69700
C	2.38160	-3.07010	-0.50140	C	2.85740	-2.18910	2.71620



C	2.61830	-1.71610	3.94500	H	-3.08660	-0.18030	2.31640
H	2.83130	0.03780	5.29380	H	-6.24510	1.83740	0.13920
H	3.90280	1.44510	3.63650	H	-6.47200	3.45280	1.92410
H	4.33150	0.58050	1.31150	C	-2.56390	1.19420	-4.11560
H	2.54260	-3.19380	2.46630	C	-2.85560	2.00040	-3.08860
H	2.12830	-2.33950	4.68160	C	-3.48700	1.45050	-1.87140
C	4.68680	1.23920	-3.25020	C	-3.77420	0.14140	-1.78790
C	3.68570	0.36860	-3.42100	C	-3.46050	-0.74450	-2.93710
C	3.41960	-0.66540	-2.40010	C	-2.88260	-0.24530	-4.03650
C	4.17560	-0.73390	-1.29070	H	-2.09430	1.59450	-5.00470
C	5.30920	0.21080	-1.12850	H	-2.62280	3.05600	-3.14340
C	5.54170	1.15260	-2.05060	H	-3.70780	2.12120	-1.05780
H	4.87930	2.00020	-3.99500	H	-3.67930	-1.80370	-2.88170
H	3.06320	0.42380	-4.30460	H	-2.64450	-0.89580	-4.86810
H	2.60490	-1.35650	-2.56710	C	-8.91150	-1.97670	-1.04910
H	5.96630	0.13290	-0.27190	C	-8.47170	-1.83320	0.20560
H	6.36760	1.84110	-1.92820	C	-7.08180	-1.40070	0.45810
C	-4.87690	2.57120	3.19760	C	-6.24410	-1.16530	-0.56760
C	-3.96690	1.59480	3.29510	C	-6.74700	-1.30850	-1.95730
C	-3.82720	0.60090	2.21030	C	-8.00860	-1.69660	-2.18250
C	-4.60790	0.67820	1.11860	H	-9.93010	-2.29130	-1.23610
C	-5.61090	1.76510	1.01390	H	-9.13350	-2.03020	1.03910
C	-5.73990	2.65960	2.00170	H	-6.76110	-1.26190	1.48260
H	-4.97780	3.30140	3.98990	H	-6.10970	-1.09580	-2.80180
H	-3.32810	1.53240	4.16660	H	-8.37220	-1.79980	-3.19680

### **OH-binding Type II Z**

(B3LYP/6-31G\*\*):UFF) Energy = -1868.124694

(B3LYP/6-31G\*\*):UFF) Free Energy = -1866.963309

M06-2X/6-31G\*\* Derived free energy = -4601.380958

M06-2X/6-31G\*\* Derived free energy in solution = -4601.399433

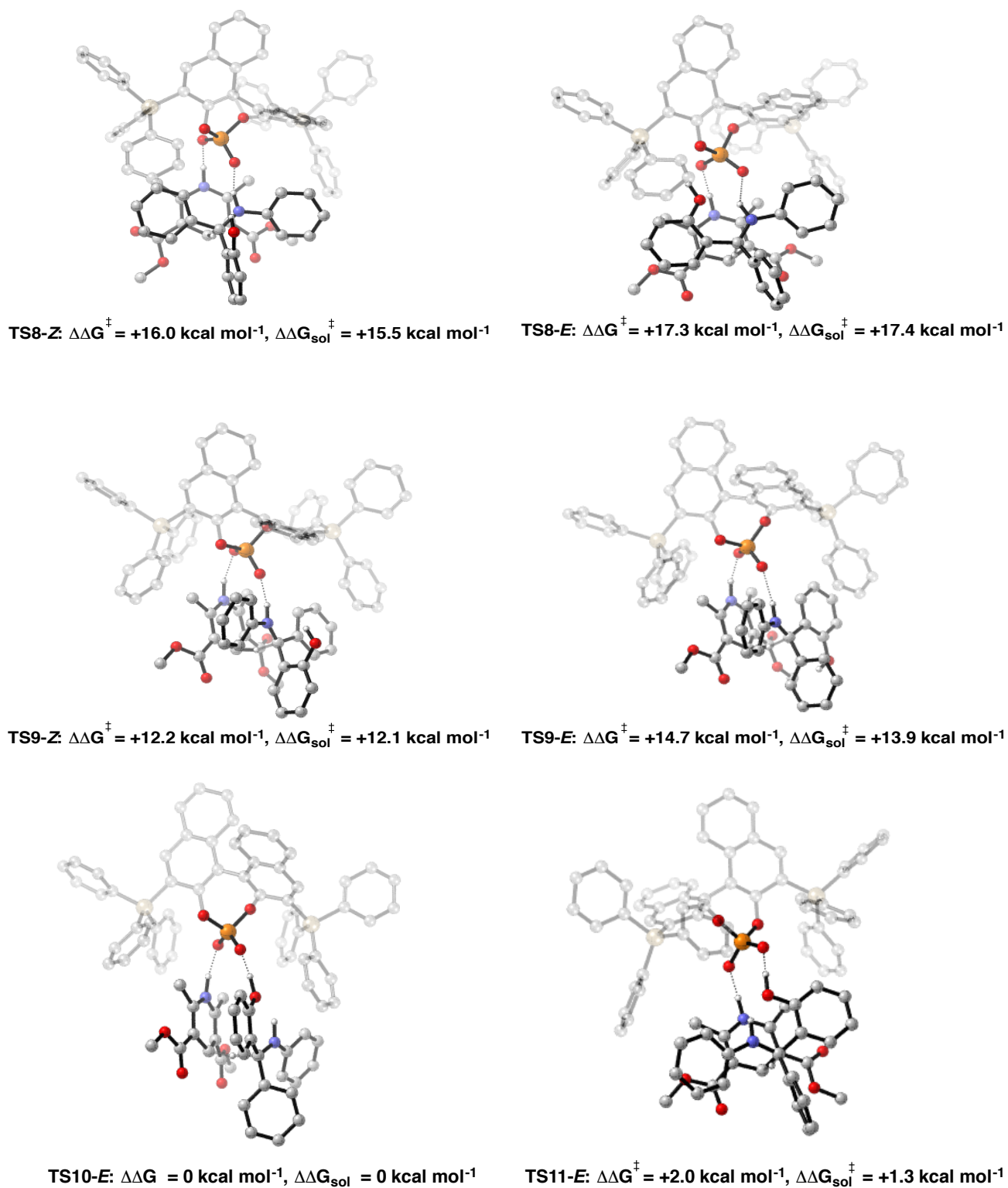
Number of Imaginary Frequencies = 1 (-924.58)

### **ONIOM (B3LYP/6-31G\*\*):UFF) Geometry**

O	-1.30620	-1.62520	-0.76060	O	-0.91320	0.62020	0.48920
P	-0.23590	-0.42930	-0.39700	H	2.16160	1.89940	0.54530
O	0.88450	-1.12520	0.62600	C	1.34630	3.34430	-0.65170
O	0.41150	0.03780	-1.66440	C	5.24210	3.92730	-2.39030

C	4.45570	2.84360	-2.76330	O	2.74260	5.11620	2.73880
C	3.19390	2.62900	-2.18530	O	1.74790	3.86040	4.33290
C	2.71960	3.56830	-1.23260	O	-2.53440	6.70380	-0.33610
C	3.53350	4.64260	-0.85790	O	2.51120	1.55310	-2.63730
C	4.79110	4.83040	-1.42550	H	1.79650	1.16920	-2.07230
H	6.21830	4.05980	-2.84830	C	0.41320	5.09150	1.16880
H	4.79820	2.12680	-3.50110	H	1.08680	4.40780	0.10890
H	3.17940	5.32840	-0.09470	H	1.02600	5.98720	1.15690
H	5.40860	5.66730	-1.11610	C	-1.95640	-2.08620	0.35360
C	0.20040	3.43600	-1.65760	C	-1.28240	-2.83630	1.25150
H	0.07030	4.46620	-1.99760	C	-4.01200	-2.24120	1.66580
H	0.44770	2.81330	-2.52000	C	-3.40900	-1.81390	0.54430
H	-0.73390	3.05680	-1.24370	H	-5.06940	-2.05990	1.82050
H	0.44230	1.71850	0.32450	C	0.07030	-3.34570	0.89860
N	1.29650	2.28470	0.20650	C	1.06830	-2.48830	0.55700
C	-0.95400	5.24850	0.68790	C	2.44320	-3.02100	0.31100
C	-1.82940	4.20360	0.86720	C	2.67820	-4.33640	0.42710
N	-1.42150	3.14720	1.65250	H	3.65890	-4.74550	0.22400
H	-1.83990	2.23240	1.47570	C	-3.24770	-2.93280	2.72160
C	-0.28260	3.13110	2.41750	C	-1.93720	-3.20620	2.54010
C	-0.15960	1.92470	3.30090	C	-1.16910	-3.83570	3.64830
H	0.82960	1.84920	3.74060	C	-1.78070	-4.16660	4.79150
H	-0.89500	1.97570	4.11210	C	-3.22070	-3.89740	4.96710
H	-0.36840	1.03620	2.69410	C	-3.91670	-3.30810	3.98880
C	-3.20710	4.05770	0.29190	H	-0.10810	-4.02250	3.54740
H	-3.94040	4.59590	0.90100	H	-1.21850	-4.62490	5.59480
H	-3.26300	4.46100	-0.71700	H	-3.70970	-4.17000	5.89350
H	-3.48240	3.00380	0.27140	H	-4.97110	-3.10460	4.12850
C	0.60510	4.18290	2.27480	C	0.32630	-4.82020	0.89250
C	-1.22430	6.48820	-0.07540	C	1.58450	-5.27700	0.71780
C	1.81420	4.42040	3.10440	C	1.86190	-6.73260	0.74420
H	-3.89820	7.91760	-1.21100	C	0.86310	-7.60470	0.91260
H	-2.47930	8.78290	-0.53360	C	-0.52200	-7.12070	1.05470
C	-2.81620	7.90160	-1.08380	C	-0.78100	-5.80830	1.03710
H	-2.31350	7.87660	-2.05310	H	2.87490	-7.09600	0.62330
C	2.83790	4.17350	5.21970	H	1.06630	-8.66760	0.92950
H	2.93370	5.25520	5.33490	H	-1.33090	-7.83240	1.15830
H	2.58080	3.70570	6.16940	H	-1.80990	-5.48370	1.10810
H	3.78000	3.77440	4.84130	Si	3.81400	-1.92730	-0.34460
O	-0.34520	7.25530	-0.42180	Si	-4.43690	-0.90710	-0.73890

C	2.99170	-1.04650	-4.88640	C	-6.46740	2.86870	1.19520
C	2.06380	-1.66600	-4.14970	C	-5.66090	2.09910	1.93330
C	2.32370	-1.95960	-2.72530	C	-4.99690	0.92610	1.32750
C	3.47360	-1.56830	-2.14670	C	-5.21730	0.60650	0.03810
C	4.51260	-0.91620	-2.98310	C	-6.08950	1.48690	-0.77950
C	4.28270	-0.67000	-4.27890	C	-6.68210	2.55420	-0.23010
H	2.80320	-0.83100	-5.93010	H	-6.94970	3.73150	1.63600
H	1.11860	-1.95130	-4.59340	H	-5.48720	2.33670	2.97480
H	1.55980	-2.47970	-2.16650	H	-4.32750	0.35080	1.94760
H	5.48000	-0.67440	-2.56670	H	-6.23140	1.29530	-1.83200
H	5.04720	-0.20450	-4.88730	H	-7.30970	3.19750	-0.83320
C	7.85960	-4.26060	0.03610	C	-1.78460	0.32310	-4.40080
C	7.30390	-3.69650	1.11470	C	-2.14700	-0.95390	-4.23310
C	6.02920	-2.95940	0.99110	C	-3.00670	-1.33600	-3.09350
C	5.42990	-2.83920	-0.20560	C	-3.41710	-0.40650	-2.21310
C	6.04150	-3.48290	-1.39440	C	-3.02590	1.00930	-2.41510
C	7.19470	-4.15300	-1.27810	C	-2.25250	1.35330	-3.45210
H	8.79250	-4.80200	0.12520	H	-1.14900	0.60370	-5.23070
H	7.78590	-3.77910	2.08010	H	-1.80420	-1.71120	-4.92610
H	5.59120	-2.52030	1.87860	H	-3.27360	-2.37760	-2.96420
H	5.55420	-3.43510	-2.35860	H	-3.35230	1.77170	-1.72470
H	7.63770	-4.62630	-2.14490	H	-1.96620	2.38680	-3.59660
C	4.46890	1.91080	2.27190	C	-7.78100	-3.75080	-2.41500
C	3.71770	0.90760	2.73970	C	-7.61450	-2.52890	-2.93170
C	3.48980	-0.29540	1.91050	C	-6.56030	-1.63850	-2.40360
C	4.00950	-0.37590	0.67210	C	-5.77600	-2.03730	-1.38690
C	4.85670	0.73480	0.17270	C	-5.94870	-3.40840	-0.84040
C	5.07070	1.81710	0.92950	C	-6.90190	-4.21440	-1.32440
H	4.64500	2.79010	2.87450	H	-8.55140	-4.40510	-2.80190
H	3.28200	0.97120	3.72820	H	-8.24960	-2.18990	-3.73990
H	2.92210	-1.11350	2.33270	H	-6.42130	-0.67560	-2.87160
H	5.31790	0.68260	-0.79940	H	-5.30010	-3.78280	-0.06320
H	5.68900	2.62480	0.56040	H	-7.02250	-5.21350	-0.92570



**Figure 1.** Competing TSs for the SiPh<sub>3</sub> catalyzed transfer hydrogenation reaction. ONIOM (B3LYP/6-31G<sup>\*\*</sup>: UFF), single-point energy M06-2X/6-31G<sup>\*\*</sup>. Grayed-out regions were treated with UFF, and the full-colour regions were treated B3LYP/6-31G<sup>\*\*</sup>. Structures generated using CYLview.<sup>20</sup>

## TS8-Z

(B3LYP/6-31G\*\*):UFF) Energy = -2290.932251

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.646833

M06-2X/6-31G\*\* Derived free energy = -5023.892161

M06-2X/6-31G\*\* Derived free energy in solution = -5023.910490

Number of Imaginary Frequencies = 1 (-967.44)

## ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	1.47360	-3.05430	0.88130	O	1.74030	-0.84640	-0.03880
C	4.23960	-3.49640	0.51210	P	0.30890	-0.67910	-0.86920
C	3.71520	-2.29650	0.22380	O	-0.40800	-2.16570	-0.94710
C	2.23670	-2.08840	0.30300	O	0.56020	-0.27860	-2.30420
H	5.30370	-3.67190	0.44030	N	-1.25700	2.61190	1.21840
C	3.38160	-4.60730	0.95030	C	-0.71560	3.87350	1.10350
C	2.05960	-4.40820	1.13200	C	-0.24210	4.39350	-2.23200
C	1.20610	-5.56800	1.52120	C	0.16260	3.15550	-2.69820
C	1.75150	-6.77130	1.73190	C	-1.99020	2.18970	-2.15750
C	3.20390	-6.96540	1.56950	C	-2.44570	3.40770	-1.68880
C	3.97770	-5.94180	1.19450	C	1.45620	2.82210	-3.38080
H	0.13430	-5.46170	1.61970	H	1.38050	3.03640	-4.45290
H	1.12600	-7.60940	2.01100	H	1.65970	1.75710	-3.25100
H	3.63960	-7.94050	1.74530	C	-2.78720	0.92890	-2.30510
H	5.04250	-6.09390	1.06820	H	-3.46770	1.00970	-3.15800
C	-2.69770	-3.05800	1.79310	H	-3.39200	0.75130	-1.41930
C	0.05940	-2.81720	1.25470	H	-2.11420	0.08720	-2.45960
C	-0.83780	-2.59350	0.28050	C	-3.83820	3.73780	-1.33320
C	-2.27900	-2.86100	0.53240	C	0.57520	5.60090	-2.46540
H	-3.73920	-3.27810	1.99740	H	0.85930	8.14960	-3.08470
C	-0.40820	-2.98400	2.65880	H	0.20030	8.67320	-1.49950
C	-1.73300	-3.06850	2.91150	H	-6.73100	2.49540	-2.05020
C	-2.21340	-3.22130	4.30380	H	-6.31830	3.10050	-0.41220
C	-1.33900	-3.25280	5.31590	O	0.04530	6.68540	-1.83740
C	0.10830	-3.13680	5.04850	O	1.58520	5.67120	-3.14270
C	0.55220	-3.00730	3.79270	O	-4.14130	4.75170	-0.72060
H	-3.27370	-3.30420	4.50740	O	-4.75920	2.85700	-1.77910
H	-1.69050	-3.36100	6.33380	Si	4.86190	-0.88470	-0.20980
H	0.80940	-3.15210	5.87290	Si	-3.47820	-3.20620	-0.85740
H	1.61550	-2.91010	3.61500	C	9.31330	-2.34040	-0.11510

C	8.73990	-2.04650	-1.28810	H	-1.30130	-4.79660	-2.00700
C	7.33560	-1.58770	-1.33290	H	-3.82560	-1.57090	-3.42460
C	6.62970	-1.46400	-0.19610	H	-2.68010	-1.57270	-5.53590
C	7.27040	-1.79140	1.10060	C	-7.02800	-0.13970	-0.79670
C	8.54230	-2.20700	1.13750	C	-6.04210	-0.03300	0.10080
H	10.34150	-2.67680	-0.08150	C	-4.91270	-0.98450	0.07690
H	9.30290	-2.14460	-2.20730	C	-4.86780	-1.96160	-0.84380
H	6.89370	-1.36510	-2.29450	C	-5.95500	-2.05970	-1.84930
H	6.71060	-1.69780	2.02280	C	-6.97790	-1.19720	-1.82500
H	9.00830	-2.44680	2.08450	H	-7.86040	0.55150	-0.77490
C	4.61260	2.49880	3.03790	H	-6.07290	0.74720	0.84940
C	5.57670	2.52270	2.11130	H	-4.12980	-0.87380	0.81050
C	5.65700	1.45070	1.09740	H	-5.92680	-2.83330	-2.60660
C	4.75560	0.45270	1.08830	H	-7.77060	-1.27320	-2.55790
C	3.71910	0.40850	2.15240	C	-5.05890	-7.52420	0.09150
C	3.64460	1.38550	3.06450	C	-5.93220	-6.54810	-0.17980
H	4.54710	3.28790	3.77570	C	-5.45050	-5.18330	-0.47950
H	6.29390	3.33300	2.09490	C	-4.13240	-4.91830	-0.50410
H	6.45780	1.48530	0.37130	C	-3.17220	-6.00180	-0.17360
H	3.02150	-0.41190	2.21560	C	-3.61190	-7.23500	0.10370
H	2.88320	1.35390	3.83330	H	-5.41090	-8.52340	0.31300
C	3.90850	0.59860	-4.55660	H	-6.99460	-6.75500	-0.17930
C	4.69930	1.32870	-3.76240	H	-6.18410	-4.41620	-0.67030
C	4.98690	0.87710	-2.38540	H	-2.11140	-5.79740	-0.12060
C	4.43790	-0.25520	-1.91310	H	-2.90860	-8.01920	0.35280
C	3.56370	-1.06090	-2.80180	N	-0.68920	2.09440	-2.56290
C	3.31360	-0.65470	-4.05260	H	-0.26770	1.13090	-2.64290
H	3.69760	0.92780	-5.56570	H	2.27490	3.42340	-2.99340
H	5.13410	2.24990	-4.12790	C	-6.12410	3.19990	-1.48290
H	5.65520	1.46930	-1.77900	H	-6.33680	4.22580	-1.78910
H	3.13100	-1.98930	-2.45410	C	0.77300	7.90760	-2.02280
H	2.67540	-1.24470	-4.69770	H	1.77710	7.82270	-1.59960
C	-1.29240	-3.22760	-5.01590	C	-1.48440	4.48420	-1.46610
C	-0.93470	-4.09820	-4.06610	H	-1.16410	4.37750	-0.19070
C	-1.63420	-4.10380	-2.76490	H	-1.92650	5.47520	-1.41930
C	-2.62980	-3.23260	-2.52170	O	-0.51890	0.25480	-0.00630
C	-3.03020	-2.28180	-3.58880	H	-0.81670	1.81830	0.71730
C	-2.39230	-2.27650	-4.76560	C	-1.88810	6.82470	4.03010
H	-0.77750	-3.21840	-5.96780	C	-1.18560	5.68640	4.41030
H	-0.12660	-4.79560	-4.24510	C	-0.83390	4.72390	3.45780

C	-1.19010	4.90630	2.10300	H	-5.50450	3.14420	2.99540
C	-1.90160	6.05780	1.74540	H	-3.61910	3.98260	1.66060
C	-2.25300	7.01440	2.69550	H	-1.53440	0.27080	2.26640
H	-2.15610	7.56270	4.78040	H	-3.44130	-0.57410	3.61400
H	-0.89590	5.51390	5.44140	C	3.44330	4.22480	-0.01120
H	-2.20710	6.19000	0.71430	C	2.74040	5.32590	0.48140
H	-2.81150	7.89480	2.39510	C	1.40440	5.19720	0.85060
O	-0.13940	3.64470	3.91000	C	0.75000	3.95320	0.76810
H	-0.02960	2.99480	3.20150	C	1.47420	2.84670	0.29720
C	-4.59540	1.23520	3.41300	C	2.80050	2.99190	-0.10220
C	-4.63120	2.51350	2.85620	H	4.47930	4.32690	-0.31970
C	-3.55820	3.00150	2.10950	H	3.22990	6.29110	0.57020
C	-2.42220	2.20120	1.92590	H	0.86130	6.06470	1.20570
C	-2.39700	0.89960	2.45800	H	1.02130	1.86450	0.23000
C	-3.47560	0.42900	3.20080	H	3.31450	2.12610	-0.49710
H	-5.43450	0.86630	3.99480				

### TS8-E

(B3LYP/6-31G\*\*):UFF) Energy = -2290.928236

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.639930

M06-2X/6-31G\*\* Derived free energy = -5023.890010

M06-2X/6-31G\*\* Derived free energy in solution = -5023.907395

Number of Imaginary Frequencies = 1 (-1066.15)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	-0.22220	-3.45880	0.88030	H	-0.29320	-8.79340	1.81200
C	2.10810	-5.01870	0.54960	H	1.75430	-7.70650	1.13260
C	2.14080	-3.71100	0.25300	C	-3.97190	-1.58200	1.76280
C	0.88480	-2.89730	0.31470	C	-1.42130	-2.66280	1.23060
H	2.99820	-5.62840	0.49070	C	-2.13270	-2.09700	0.24140
C	0.86280	-5.66540	0.98220	C	-3.52140	-1.61910	0.49840
C	-0.25620	-4.93190	1.14540	H	-4.96310	-1.21590	1.98480
C	-1.51720	-5.62710	1.53670	C	-1.91480	-2.58720	2.63360
C	-1.52330	-6.94510	1.76610	C	-3.13220	-2.05710	2.88060
C	-0.28290	-7.72800	1.62150	C	-3.63270	-1.96510	4.27160
C	0.84830	-7.12390	1.24510	C	-2.87090	-2.38260	5.28860
H	-2.44820	-5.08370	1.62420	C	-1.52820	-2.93740	5.02830
H	-2.44230	-7.44300	2.04790	C	-1.07170	-3.03370	3.77420

H	-4.61450	-1.55350	4.47040	H	7.18920	-6.09440	-2.11930
H	-3.23510	-2.31060	6.30520	H	5.36630	-4.33960	-2.23590
H	-0.91140	-3.26110	5.85660	H	5.12740	-4.41190	2.09130
H	-0.07870	-3.42910	3.60370	H	6.86110	-6.09340	2.18040
O	0.95440	-1.56630	-0.06260	C	5.06490	0.15530	3.12720
P	-0.32670	-0.80710	-0.88160	C	5.95450	-0.27770	2.22730
O	-1.53900	-1.92150	-0.98010	C	5.54640	-1.24640	1.18860
O	0.12200	-0.51260	-2.29430	C	4.27830	-1.69120	1.13230
N	0.36760	2.75430	1.36040	C	3.31150	-1.24420	2.16830
C	1.39770	3.66430	1.21300	C	3.68150	-0.35770	3.10050
C	1.88400	3.91680	-2.09930	H	5.35920	0.87320	3.88160
C	1.56580	2.65270	-2.56300	H	6.97200	0.09050	2.24910
C	-0.76920	2.98690	-2.00490	H	6.28890	-1.58890	0.48020
C	-0.49740	4.24920	-1.50890	H	2.30320	-1.62700	2.18920
C	2.46860	1.66840	-3.24830	H	2.97080	-0.02510	3.84610
H	3.47160	1.69590	-2.82750	C	3.70000	-1.25740	-4.54560
H	2.55710	1.91050	-4.31290	C	4.74800	-1.00290	-3.75420
C	-2.09610	2.31190	-2.15000	C	4.76790	-1.50810	-2.36590
H	-2.18680	1.91130	-3.16330	C	3.72330	-2.19970	-1.87970
H	-2.92100	2.98590	-1.95250	C	2.56570	-2.48050	-2.76500
H	-2.11240	1.47210	-1.44630	C	2.55700	-2.03470	-4.02720
C	-1.47960	5.27290	-1.08480	H	3.68480	-0.89000	-5.56340
C	3.16150	4.63030	-2.30540	H	5.58690	-0.43210	-4.13060
H	5.80780	4.80410	-2.37160	H	5.64670	-1.32920	-1.76320
H	5.85960	4.03190	-3.99070	H	1.72760	-3.06310	-2.40810
H	-4.57560	5.92460	-1.74250	H	1.71210	-2.24320	-4.67090
H	-3.87250	6.05760	-0.09750	C	-2.73070	-2.08260	-5.04920
O	4.03720	3.98830	-3.11530	C	-2.87690	-3.05680	-4.14440
O	3.40170	5.72120	-1.81600	C	-3.51620	-2.76870	-2.84420
O	-1.16980	6.22350	-0.38230	C	-3.95060	-1.52780	-2.55960
O	-2.72920	5.11810	-1.57060	C	-3.80470	-0.45960	-3.57720
Si	3.79020	-2.93630	-0.16940	C	-3.22070	-0.72180	-4.75290
Si	-4.68860	-1.14510	-0.88850	H	-2.25710	-2.28990	-6.00010
C	7.14730	-6.20410	-0.02130	H	-2.51880	-4.05540	-4.35810
C	6.74240	-5.72730	-1.20440	H	-3.59530	-3.56420	-2.11320
C	5.68310	-4.69850	-1.26630	H	-4.16700	0.53890	-3.38150
C	5.12430	-4.23590	-0.13490	H	-3.11030	0.06200	-5.49110
C	5.57470	-4.77150	1.17290	C	-5.89010	3.36520	-0.54790
C	6.53380	-5.70360	1.22530	C	-4.90280	2.88670	0.21750
H	7.92280	-6.95760	0.02470	C	-4.50120	1.46880	0.10900



C	-5.11790	0.65850	-0.76750	C	1.43870	4.76850	2.25970
C	-6.20770	1.19620	-1.61640	C	1.29980	6.12560	1.95730
C	-6.57230	2.47960	-1.51190	C	1.39900	7.08460	2.96890
H	-6.19100	4.40100	-0.46270	H	1.71460	7.44580	5.07040
H	-4.39730	3.53780	0.91640	H	1.96530	5.03030	5.61710
H	-3.70260	1.10550	0.73980	H	1.07940	6.43770	0.94400
H	-6.71570	0.55100	-2.32240	H	1.28210	8.13510	2.72030
H	-7.36910	2.87050	-2.13130	C	-3.19370	2.96460	3.62790
C	-8.76870	-3.39170	-0.28390	C	-2.65700	4.13620	3.09500
C	-7.93950	-3.78230	-1.25780	C	-1.49440	4.10680	2.32480
C	-6.65410	-3.08230	-1.46360	C	-0.83740	2.88860	2.09730
C	-6.30050	-2.06080	-0.66340	C	-1.39250	1.70350	2.61280
C	-7.24020	-1.61770	0.39770	C	-2.55810	1.74850	3.37040
C	-8.40490	-2.25160	0.57930	H	-4.10100	2.99590	4.22350
H	-9.71040	-3.90350	-0.13280	H	-3.15020	5.08900	3.26570
H	-8.20770	-4.61290	-1.89790	H	-1.12030	5.02370	1.89220
H	-6.01820	-3.41650	-2.26750	H	-0.91710	0.75780	2.38250
H	-7.00400	-0.76240	1.01670	H	-2.97280	0.82560	3.76280
H	-9.08870	-1.92160	1.35080	C	5.40560	2.38730	0.11260
N	0.28230	2.21150	-2.41440	C	5.17800	3.63200	0.70120
H	0.11740	1.17700	-2.52140	C	3.88230	4.00360	1.04040
H	2.03960	0.66960	-3.14950	C	2.77610	3.15140	0.85210
C	-3.67180	6.12780	-1.16940	C	3.03700	1.89050	0.26510
H	-3.28630	7.12380	-1.39520	C	4.33490	1.53320	-0.11510
C	5.28420	4.67080	-3.32080	H	6.40740	2.08190	-0.17420
H	5.11740	5.65090	-3.77370	H	5.99920	4.31660	0.88490
C	0.89250	4.63500	-1.30880	H	3.71710	4.98450	1.46610
H	1.15500	4.32660	-0.00920	H	4.48180	0.57850	-0.60390
H	1.07700	5.70180	-1.22090	O	1.98750	1.06720	0.04660
O	-0.74590	0.33280	0.01130	H	2.20440	0.12950	-0.09540
H	0.44210	1.85770	0.86890	C	1.68370	4.38500	3.58750
C	1.63920	6.69810	4.28640	H	1.79620	3.33170	3.82560
C	1.77970	5.34270	4.59360				

## TS9-Z

(B3LYP/6-31G\*\*):UFF) Energy = -2290.939086

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.650511

M06-2X/6-31G\*\* Derived free energy = -5023.898096

M06-2X/6-31G\*\* Derived free energy in solution = -5023.915832

Number of Imaginary Frequencies = 1 (-1002.79)

ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	-3.02620	1.89100	0.96390	C	1.48590	-4.03600	-0.45160
C	-5.59090	0.88840	0.33110	C	0.41980	-3.24560	-0.83390
C	-4.50830	0.13520	0.08620	C	1.68980	-2.36610	-2.69690
C	-3.14520	0.68330	0.35890	C	2.81170	-3.07490	-2.30220
H	-6.58430	0.52250	0.11380	C	-0.91780	-3.20650	-0.16820
C	-5.45800	2.24340	0.89150	H	-1.48790	-2.34110	-0.49740
C	-4.23720	2.73640	1.18930	H	-1.47170	-4.12350	-0.38080
C	-4.13000	4.13210	1.70130	C	1.53340	-1.54630	-3.94400
C	-5.22990	4.86830	1.89760	H	1.46690	-2.20300	-4.81740
C	-6.56040	4.30780	1.59790	H	0.62810	-0.94090	-3.87310
C	-6.67020	3.06550	1.11650	H	2.40530	-0.91270	-4.10440
H	-3.16550	4.57540	1.90850	C	4.01210	-3.13030	-3.16100
H	-5.14570	5.88170	2.26850	C	1.44330	-5.10320	0.56760
H	-7.44630	4.90790	1.76120	H	0.44740	-6.12020	2.89440
H	-7.65020	2.66330	0.89130	H	-0.91910	-6.81150	1.96510
C	0.72110	3.70490	2.00300	H	6.87600	-4.59530	-2.76210
C	-1.69500	2.40420	1.35940	H	6.02150	-4.37820	-4.32560
C	-0.77450	2.62760	0.40070	O	0.19910	-5.48490	0.92580
C	0.44870	3.41090	0.72100	O	2.45010	-5.62430	1.02380
H	1.58970	4.30170	2.25640	O	4.13700	-2.61950	-4.25970
C	-1.36160	2.68050	2.78440	O	5.00310	-3.85590	-2.57850
C	-0.18860	3.27940	3.08520	Si	-4.73150	-1.58110	-0.61810
C	0.17510	3.53080	4.49850	Si	1.48560	4.22550	-0.59780
C	-0.64470	3.14340	5.48200	C	-9.25600	-2.59370	-1.28340
C	-1.91570	2.46480	5.16210	C	-8.77730	-2.43700	-0.04380
C	-2.25760	2.24290	3.88760	C	-7.35060	-2.11340	0.16330
H	1.10790	4.02460	4.74070	C	-6.52980	-1.96650	-0.89070
H	-0.37670	3.32330	6.51500	C	-7.06460	-2.14820	-2.26240
H	-2.56790	2.14130	5.96300	C	-8.35750	-2.44380	-2.44610
H	-3.18580	1.72950	3.67380	H	-10.30060	-2.83180	-1.43690
O	-2.04480	-0.12450	0.16700	H	-9.43300	-2.54820	0.81010
P	-0.79600	0.43880	-0.79740	H	-6.98050	-1.99560	1.17450
O	-0.95900	2.08590	-0.84700	H	-6.41900	-2.04430	-3.12390
O	-0.96400	-0.11940	-2.18580	H	-8.74760	-2.57540	-3.44710
N	2.41630	-1.38000	1.22370	C	-3.26850	-4.84400	2.41480
C	3.64440	-1.81260	0.76410	C	-3.12830	-3.54900	2.71830

C	-3.58730	-2.51230	1.77090	H	1.47670	1.76640	-2.34110
C	-4.12410	-2.86360	0.58820	H	0.78390	1.34230	-4.61770
C	-4.30760	-4.30150	0.27440	C	5.98130	2.95120	-0.29250
C	-3.89360	-5.23860	1.13660	C	5.57330	3.75100	-1.28430
H	-2.93340	-5.60370	3.10880	C	4.14810	4.12410	-1.39540
H	-2.67760	-3.25710	3.65780	C	3.25590	3.66490	-0.50190
H	-3.47860	-1.47580	2.05500	C	3.70730	2.74360	0.57050
H	-4.78230	-4.60080	-0.65150	C	5.00200	2.41750	0.67480
H	-4.02340	-6.28740	0.90300	H	7.02480	2.67700	-0.20890
C	-2.51820	-1.57130	-4.74890	H	6.28700	4.13270	-2.00260
C	-2.45680	-2.65970	-3.97330	H	3.84230	4.79520	-2.18870
C	-3.16520	-2.68680	-2.67660	H	3.00020	2.32160	1.27090
C	-3.85180	-1.61120	-2.25760	H	5.33380	1.74740	1.45600
C	-3.93570	-0.41660	-3.13340	N	0.57590	-2.41120	-1.90560
C	-3.30180	-0.39810	-4.31250	H	-0.14790	-1.67590	-2.08200
H	-1.99480	-1.54810	-5.69590	H	-0.79680	-3.14540	0.91310
H	-1.88250	-3.52060	-4.29000	C	6.21550	-3.94890	-3.33990
H	-3.10960	-3.58260	-2.07920	H	6.66120	-2.95920	-3.46590
H	-4.50540	0.44950	-2.82070	C	0.12820	-6.51380	1.92620
H	-3.35720	0.47780	-4.94570	H	0.76230	-7.35990	1.65520
C	1.15390	8.77620	0.48250	C	2.80390	-3.75950	-1.00840
C	0.05090	8.05350	0.25740	H	3.35380	-2.94900	-0.12660
C	0.16250	6.62210	-0.09030	H	3.51520	-4.57510	-0.91390
C	1.37050	6.04170	-0.19860	O	0.47700	0.09220	-0.04940
C	2.58900	6.84510	0.06960	H	1.83200	-0.77740	0.61720
C	2.48380	8.14130	0.38850	C	6.45040	-3.25210	3.71510
H	1.07420	9.82460	0.73910	C	5.89010	-1.98500	3.82950
H	-0.92550	8.51450	0.33130	C	4.95670	-1.53650	2.88800
H	-0.74340	6.05110	-0.25480	C	4.58190	-2.37270	1.81120
H	3.56990	6.39480	0.02140	C	5.15950	-3.64530	1.71880
H	3.37320	8.72600	0.58510	C	6.08430	-4.09110	2.66000
C	0.05930	3.40540	-4.99190	H	7.16990	-3.58760	4.45620
C	-0.08630	4.62680	-4.46710	H	6.15380	-1.31690	4.64250
C	0.35350	4.89590	-3.08200	H	4.85820	-4.30380	0.91360
C	0.88240	3.91120	-2.33400	H	6.50800	-5.08600	2.57190
C	1.05070	2.56500	-2.92860	O	4.46680	-0.28140	3.06850
C	0.66070	2.32560	-4.18640	H	3.73850	-0.12030	2.45010
H	-0.26050	3.20680	-6.00660	C	0.12160	-2.38330	4.63970
H	-0.52320	5.42230	-5.05670	C	1.12990	-3.25230	4.22270
H	0.24470	5.89910	-2.69830	C	1.90780	-2.96970	3.09870

C	1.68500	-1.78480	2.38130	C	3.58490	-0.13540	-1.16560
C	0.66390	-0.90970	2.79800	C	4.30520	-0.99090	-0.31000
C	-0.11000	-1.21430	3.91310	C	5.68900	-1.14340	-0.52740
H	-0.47940	-2.61710	5.51300	C	6.33410	-0.46070	-1.55310
H	1.31990	-4.16940	4.77320	H	6.10800	0.91000	-3.20580
H	2.65850	-3.67920	2.78240	H	3.68270	1.20450	-2.84680
H	0.46990	-0.01860	2.21360	H	2.52060	0.02940	-1.02530
H	-0.89880	-0.53040	4.21200	H	6.26350	-1.79640	0.11720
C	5.60960	0.37790	-2.40140	H	7.40510	-0.58190	-1.68530
C	4.24120	0.54080	-2.19650				

### TS9-E

(B3LYP/6-31G\*\*):UFF) Energy = -2290.931799

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.643629

M06-2X/6-31G\*\* Derived free energy = -5023.894199

M06-2X/6-31G\*\* Derived free energy in solution = -5023.913005

Number of Imaginary Frequencies = 1 (-978.69)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	-3.90520	0.73920	0.24890	H	-1.70410	5.18690	2.26500
C	-5.49520	-1.42540	-0.61650	C	-3.63720	2.38090	2.22540
C	-4.19140	-1.62180	-0.36470	C	-3.10090	3.52910	2.69290
C	-3.32230	-0.45530	-0.00620	C	-3.57230	4.10150	3.97520
H	-6.13630	-2.24680	-0.90600	C	-4.51500	3.47220	4.68530
C	-6.08870	-0.08140	-0.52250	C	-5.08520	2.20200	4.19630
C	-5.33580	0.96170	-0.11630	C	-4.66980	1.68060	3.03610
C	-5.94410	2.32110	-0.08300	H	-3.15470	5.03070	4.34250
C	-7.22960	2.49550	-0.41020	H	-4.85810	3.88990	5.62300
C	-8.05350	1.34240	-0.81860	H	-5.83570	1.68910	4.78390
C	-7.51320	0.12070	-0.87710	H	-5.08650	0.73870	2.70400
H	-5.35320	3.18560	0.18960	O	-1.99460	-0.66450	0.29430
H	-7.66640	3.48560	-0.38580	P	-0.85370	0.27370	-0.48830
H	-9.09380	1.48970	-1.07870	O	-1.52940	1.75530	-0.77560
H	-8.12190	-0.72010	-1.18580	O	-0.58720	-0.30160	-1.86170
C	-2.06010	4.22610	1.91410	N	3.07240	-0.61650	1.33470
C	-3.15060	1.81600	0.93340	C	4.27550	-0.47120	0.67510
C	-2.07120	2.35560	0.33390	C	2.90460	-3.24250	-0.33460
C	-1.58260	3.69130	0.77960	C	1.62700	-2.80710	-0.63930

C	2.44000	-1.66770	-2.61550	H	-4.38540	-5.14190	-2.66020
C	3.74350	-2.01710	-2.31740	H	-5.73400	-4.22100	1.35420
C	0.38660	-3.13410	0.13100	H	-7.56010	-5.78850	1.12370
H	-0.45160	-2.53890	-0.22140	C	-1.33440	-4.56870	3.51830
H	0.15940	-4.19700	0.03010	C	-1.47490	-5.46040	2.53190
C	1.96190	-0.95230	-3.84560	C	-2.19310	-5.09010	1.29470
H	1.86760	-1.66340	-4.67390	C	-2.67420	-3.84520	1.13180
H	0.98720	-0.49970	-3.65210	C	-2.58650	-2.89050	2.26750
H	2.68090	-0.19880	-4.16060	C	-1.93720	-3.22880	3.38800
C	4.85100	-1.72250	-3.24900	H	-0.80150	-4.83510	4.42190
C	3.26160	-4.20100	0.72720	H	-1.05470	-6.45260	2.63300
H	2.93460	-5.23740	3.18760	H	-2.31720	-5.84120	0.52960
H	1.60140	-6.26840	2.58120	H	-3.07060	-1.92710	2.22150
H	8.06610	-1.91900	-2.86590	H	-1.87720	-2.53060	4.21260
H	7.18150	-2.22970	-4.39750	C	3.97490	3.75190	1.19040
O	2.21610	-4.86040	1.26740	C	2.93960	3.08350	1.71230
O	4.41680	-4.40150	1.07800	C	1.56910	3.35180	1.23650
O	4.74930	-1.32700	-4.39620	C	1.34970	4.27270	0.28220
O	6.05480	-1.95720	-2.66080	C	2.50060	5.02290	-0.27910
Si	-3.50780	-3.36270	-0.47170	C	3.74400	4.76950	0.14670
Si	-0.38610	4.68750	-0.24980	H	4.98130	3.55750	1.53610
C	-0.65020	-3.59990	-4.19720	H	3.09700	2.34510	2.48640
C	-1.42490	-2.52620	-4.01330	H	0.75450	2.80310	1.68810
C	-2.33200	-2.45720	-2.84870	H	2.33970	5.80130	-1.01340
C	-2.37300	-3.46160	-1.95540	H	4.58100	5.32120	-0.26100
C	-1.54530	-4.67040	-2.19670	C	-1.28570	9.21660	0.57350
C	-0.72050	-4.72790	-3.24950	C	-2.17700	8.46120	-0.07800
H	0.02120	-3.64830	-5.04460	C	-1.89050	7.03510	-0.33720
H	-1.38030	-1.69910	-4.70980	C	-0.72940	6.49140	0.06610
H	-2.94770	-1.57620	-2.73170	C	0.24620	7.33120	0.80570
H	-1.59970	-5.51790	-1.53350	C	-0.01790	8.62230	1.04150
H	-0.11250	-5.60770	-3.41580	H	-1.49450	10.26120	0.76530
C	-7.03400	-6.40670	-0.94600	H	-3.11030	8.89250	-0.41620
C	-6.17620	-6.22990	-1.95800	H	-2.63380	6.44250	-0.85280
C	-5.05790	-5.27300	-1.82370	H	1.16730	6.90810	1.18030
C	-4.89790	-4.57830	-0.68450	H	0.69250	9.23160	1.58530
C	-5.85150	-4.77810	0.43300	C	-1.20460	3.88760	-4.80420
C	-6.86380	-5.64470	0.30770	C	-2.21840	3.92020	-3.93280
H	-7.85370	-7.10670	-1.04390	C	-1.95710	4.18470	-2.50320
H	-6.30000	-6.78630	-2.87810	C	-0.69990	4.37640	-2.06370

C	0.41390	4.36880	-3.04290	H	2.10360	2.33400	-2.33610
C	0.17470	4.12880	-4.33800	O	6.75490	0.51900	-0.78270
H	-1.39330	3.69190	-5.85180	H	6.73790	-0.12400	-0.05860
H	-3.23200	3.74880	-4.27150	C	1.86430	-2.09880	5.10850
H	-2.79540	4.19950	-1.81840	C	1.06760	-1.22790	4.36280
H	1.42680	4.56030	-2.72870	C	1.49610	-0.75320	3.12750
H	0.99150	4.11920	-5.04820	C	2.74480	-1.15120	2.60900
N	1.45150	-2.00300	-1.72800	C	3.53860	-2.04320	3.34670
H	0.53870	-1.47070	-1.82360	C	3.09460	-2.49990	4.58910
H	0.52750	-2.93740	1.19460	H	1.52880	-2.46420	6.07420
C	7.19990	-1.65200	-3.47050	H	0.10120	-0.90950	4.74240
H	7.22120	-0.58750	-3.71300	H	0.86580	-0.09460	2.53710
C	2.54010	-5.77850	2.32480	H	4.47610	-2.40930	2.95820
H	3.27860	-6.50900	1.98790	H	3.72580	-3.18430	5.14920
C	4.03230	-2.62410	-1.01810	C	7.83320	-0.73100	3.13630
H	4.36130	-1.64020	-0.20910	C	7.52300	-1.78030	2.27270
H	4.95900	-3.18840	-0.96720	C	6.37470	-1.72690	1.47730
O	0.29610	0.35910	0.48980	C	5.52550	-0.61030	1.53290
H	2.24090	-0.22700	0.88340	C	5.84450	0.43760	2.41180
C	4.25860	2.42230	-2.56420	C	6.98600	0.37660	3.20690
C	5.46270	1.91600	-2.10130	H	8.72590	-0.77580	3.75260
C	5.50460	0.96690	-1.06850	H	8.16600	-2.65340	2.21920
C	4.30370	0.55530	-0.42320	H	6.12010	-2.57270	0.85060
C	3.09710	1.08330	-0.93440	H	5.19710	1.30230	2.46970
C	3.06550	1.98910	-1.98210	H	7.21440	1.19830	3.87880
H	4.24930	3.14270	-3.37650				
H	6.41060	2.21930	-2.53290				
H	2.13540	0.81210	-0.51050				

### TS10-E

(B3LYP/6-31G\*\*):UFF) Energy = -2290.961818

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.674395

M06-2X/6-31G\*\* Derived free energy = -5023.917585

M06-2X/6-31G\*\* Derived free energy in solution = -5023.935180

Number of Imaginary Frequencies = 1 (-1070.60)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	4.36000	1.12580	-0.17150	C	6.03030	-1.02320	0.59260
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C	4.74960	-1.26460	0.27410	H	0.13010	-3.84970	-1.26880
C	3.84730	-0.12860	-0.07270	C	-1.81840	-1.49730	3.20340
H	6.69190	-1.82810	0.88160	H	-0.88790	-0.93800	3.08880
C	6.55620	0.35270	0.61800	H	-2.59750	-0.86830	3.62870
C	5.75990	1.38900	0.27870	H	-1.66090	-2.31250	3.91610
C	6.29250	2.77540	0.39610	C	-4.61400	-2.78860	2.50420
C	7.55440	2.98530	0.78810	C	-2.90920	-3.96420	-1.90010
C	8.42670	1.84390	1.12150	H	-2.75030	-4.32870	-4.53100
C	7.95350	0.59560	1.04700	H	-1.13060	-5.08190	-4.36130
H	5.66520	3.62970	0.17960	H	-6.20720	-2.03730	4.53160
H	7.93610	3.99470	0.87160	H	-5.76770	-3.75810	4.65580
H	9.44720	2.02040	1.43610	O	-1.82920	-4.23670	-2.66350
H	8.59670	-0.23710	1.30340	O	-4.03640	-4.32210	-2.20570
C	2.03160	4.44510	-1.64540	O	-5.70510	-3.20760	2.15430
C	3.54020	2.23290	-0.73180	O	-4.31720	-2.52390	3.79600
C	2.36910	2.54740	-0.13980	Si	4.09970	-3.01610	0.36820
C	1.59150	3.73220	-0.59810	Si	0.01470	4.27040	0.24360
H	1.47450	5.30700	-1.99410	C	1.19650	-3.13030	4.04250
C	3.98540	2.99280	-1.93820	C	0.87150	-3.79800	2.92960
C	3.26510	4.05790	-2.35700	C	1.76540	-3.75930	1.75400
C	3.69690	4.82690	-3.54720	C	2.90650	-3.05200	1.79530
C	4.78650	4.45640	-4.22800	C	3.26040	-2.31470	3.03290
C	5.55610	3.27200	-3.80300	C	2.44730	-2.34910	4.09510
C	5.17720	2.57390	-2.72630	H	0.54430	-3.16020	4.90540
H	3.13050	5.69110	-3.87170	H	-0.04750	-4.36820	2.88700
H	5.10060	5.01790	-5.09830	H	1.48310	-4.31990	0.87760
H	6.42310	2.96290	-4.37260	H	4.18010	-1.74570	3.08490
H	5.74260	1.69430	-2.44990	H	2.70690	-1.80880	4.99610
O	2.56460	-0.40610	-0.48770	C	7.61910	-6.00830	1.12950
P	1.31300	0.32990	0.30990	C	6.66960	-5.85770	2.06070
O	1.89780	1.75670	0.87700	C	5.55350	-4.91510	1.83620
O	0.87450	-0.49000	1.49530	C	5.49180	-4.20180	0.69910
N	-4.65130	0.26010	0.04940	C	6.54310	-4.37740	-0.33140
C	-4.84140	-0.67370	-0.95890	C	7.55190	-5.23260	-0.12550
C	-2.61630	-3.20970	-0.66290	H	8.43650	-6.69870	1.29300
C	-1.38190	-2.71070	-0.28740	H	6.71620	-6.42650	2.98030
C	-2.25470	-2.05370	1.87790	H	4.79640	-4.81720	2.60210
C	-3.50010	-2.56320	1.55790	H	6.49970	-3.81190	-1.25410
C	-0.10400	-2.80310	-1.06970	H	8.31980	-5.35840	-0.87780
H	0.71930	-2.34320	-0.52710	C	2.19560	-4.52000	-3.64530

C	2.67580	-3.27360	-3.56930	H	-0.31960	3.17070	-2.47750
C	3.29560	-2.79260	-2.31680	H	-2.97410	4.51550	0.67400
C	3.34470	-3.58990	-1.23550	H	-4.89560	3.96860	-0.68310
C	2.85270	-4.98550	-1.34270	N	-1.27710	-2.08080	0.92310
C	2.30160	-5.42240	-2.48190	H	-0.38860	-1.56460	1.13880
H	1.73900	-4.87240	-4.56110	H	-0.20620	-2.30880	-2.03700
H	2.60970	-2.61330	-4.42430	C	-5.39080	-2.73570	4.72840
H	3.70840	-1.79490	-2.29890	H	-4.96050	-2.55180	5.71280
H	2.94140	-5.66040	-0.50080	C	-2.10240	-4.93160	-3.89110
H	1.93720	-6.43890	-2.55460	H	-2.58730	-5.89000	-3.69260
C	0.35310	8.91770	0.81030	O	0.31080	0.60130	-0.80210
C	1.36520	8.12000	1.16780	C	-2.07150	-0.57400	-4.28190
C	1.25440	6.65770	0.98880	C	-1.65320	-0.12050	-3.04080
C	0.13260	6.11640	0.48220	C	-2.53710	-0.12080	-1.94210
C	-0.97770	7.01120	0.06830	C	-3.86970	-0.59510	-2.10070
C	-0.87260	8.33640	0.22880	C	-4.25070	-1.05390	-3.37930
H	0.43320	9.98930	0.93900	C	-3.37870	-1.04210	-4.45830
H	2.26920	8.54360	1.58590	H	-1.37810	-0.55510	-5.11820
H	2.10310	6.04010	1.24890	H	-0.64790	0.25300	-2.88160
H	-1.87670	6.61030	-0.37440	H	-5.25830	-1.42020	-3.52440
H	-1.68340	8.98620	-0.07440	H	-3.71780	-1.38560	-5.43030
C	-0.43170	2.31950	4.48800	H	-3.71200	0.65660	0.05250
C	-1.31960	2.03850	3.52890	C	-6.85990	1.34580	3.48000
C	-1.15710	2.60830	2.17720	C	-7.23470	0.21200	2.75850
C	-0.15650	3.46690	1.91820	C	-6.53290	-0.18900	1.62140
C	0.83350	3.76340	2.98370	C	-5.43120	0.56250	1.18100
C	0.70600	3.21310	4.19740	C	-5.05470	1.70510	1.91240
H	-0.54960	1.89990	5.47860	C	-5.75740	2.08740	3.04940
H	-2.16950	1.40790	3.74470	H	-7.41610	1.64710	4.36220
H	-1.85560	2.31410	1.41020	H	-8.08630	-0.38100	3.08000
H	1.67900	4.40460	2.78500	H	-6.82750	-1.09250	1.10810
H	1.43430	3.42480	4.96950	H	-4.21300	2.29900	1.57360
C	-3.71520	3.26100	-2.42710	H	-5.44380	2.97290	3.59430
C	-2.48240	3.06750	-2.90870	C	-8.93050	-1.32850	-2.18650
C	-1.30150	3.36720	-2.07110	C	-8.45010	-0.03810	-1.95330
C	-1.45820	3.86810	-0.83350	C	-7.13440	0.15430	-1.53870
C	-2.83010	4.10680	-0.31840	C	-6.28030	-0.94340	-1.34950
C	-3.89730	3.80650	-1.06850	C	-6.76020	-2.23370	-1.60480
H	-4.57980	3.02290	-3.03310	C	-8.08120	-2.42170	-2.01690
H	-2.34670	2.67270	-3.90710	H	-9.95790	-1.47890	-2.50480



H	-9.09940	0.82080	-2.09500	H	-1.10470	0.50950	-0.71940
H	-6.76090	1.15740	-1.36070	C	-3.77540	-2.94620	0.18050
H	-6.09970	-3.08880	-1.51230	H	-4.40450	-1.90030	-0.39470
H	-8.44170	-3.42810	-2.20750	H	-4.60140	-3.64250	0.06230
O	-2.13790	0.34070	-0.74540				

### TS11-E

(B3LYP/6-31G\*\*):UFF) Energy = -2290.952347

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.668906

M06-2X/6-31G\*\* Derived free energy = -5023.914410

M06-2X/6-31G\*\* Derived free energy in solution = -5023.933177

Number of Imaginary Frequencies = 1 (-1039.63)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	-3.71420	1.70230	0.97630	C	-7.73050	2.06120	-0.66730
C	-2.64860	4.24770	1.58440	C	-6.47600	1.96940	-0.21160
C	-2.07760	3.50580	0.62230	H	-8.40010	-1.22990	-1.33370
C	-2.58510	2.12880	0.37420	H	-9.47650	0.92950	-1.44270
H	-2.33220	5.27110	1.74820	H	-8.20830	3.02890	-0.75050
C	-3.76120	3.70770	2.39340	H	-5.95420	2.88010	0.04710
C	-4.28410	2.49500	2.10270	O	-1.93900	1.30390	-0.50640
C	-5.39000	1.96130	2.94130	P	-1.26710	0.00480	0.25170
C	-5.88530	2.69040	3.94810	O	-2.51710	-0.87880	0.86020
C	-5.33000	4.02640	4.24010	O	-0.46950	0.44180	1.46330
C	-4.32150	4.50920	3.50570	N	4.38580	-0.15260	-1.15270
H	-5.79930	0.97760	2.75140	C	4.77450	-1.43350	-0.79680
H	-6.69090	2.29930	4.55610	C	4.26800	0.21280	2.04980
H	-5.73800	4.61180	5.05390	C	2.93980	0.59800	2.01270
H	-3.91590	5.48810	3.72900	C	2.22270	-1.69290	2.30000
C	-5.79720	-1.76590	-0.54420	C	3.53170	-2.13980	2.28710
C	-4.41160	0.50570	0.42870	C	2.40510	1.99720	1.92110
C	-3.77480	-0.69240	0.33390	H	1.33740	1.97180	1.69740
C	-4.51590	-1.88490	-0.17020	H	2.56240	2.52440	2.86620
H	-6.34210	-2.61630	-0.93240	C	1.00410	-2.53160	2.54520
C	-5.80750	0.64120	-0.09620	H	0.09770	-1.93480	2.43520
C	-6.47120	-0.45730	-0.51860	H	0.98600	-3.36750	1.84500
C	-7.86280	-0.34510	-1.01550	H	1.03860	-2.96880	3.54590
C	-8.46080	0.84850	-1.07750	C	3.84690	-3.55380	2.56590

C	5.42660	1.11780	2.18890	H	1.48210	0.60570	-2.97910
H	5.77620	4.26990	2.82440	H	0.98600	2.09250	-0.97330
H	6.89980	2.95350	3.29830	H	-1.87510	4.25020	-3.41450
H	5.33820	-5.45700	3.65690	H	-1.39830	2.82040	-5.28600
H	5.02820	-5.85160	1.95270	C	-0.80970	-3.30950	-4.12380
O	5.10050	2.41510	2.38290	C	-1.47390	-2.21870	-3.72700
O	6.58220	0.72510	2.16390	C	-2.38840	-2.28870	-2.56850
O	3.06300	-4.41320	2.92580	C	-2.53100	-3.43650	-1.88210
O	5.17140	-3.81380	2.37830	C	-1.82680	-4.65290	-2.35950
Si	-0.84990	4.32340	-0.53180	C	-1.00780	-4.58990	-3.41670
Si	-3.65240	-3.52990	-0.39050	H	-0.13640	-3.25900	-4.96950
C	3.11640	5.61870	1.60340	H	-1.33780	-1.27990	-4.24830
C	3.08320	5.48080	0.27350	H	-2.91450	-1.39040	-2.27800
C	1.83820	5.04930	-0.39510	H	-1.99410	-5.60660	-1.87720
C	0.73840	4.77560	0.32890	H	-0.49770	-5.47950	-3.76240
C	0.78820	4.91390	1.80520	C	-6.92950	-6.82880	-0.96860
C	1.91300	5.32290	2.40590	C	-6.15980	-6.47550	-2.00460
H	4.02390	5.94520	2.09360	C	-5.11940	-5.43940	-1.83610
H	3.96430	5.69720	-0.31620	C	-4.93310	-4.85670	-0.63920
H	1.82440	4.97810	-1.47540	C	-5.79750	-5.24470	0.50170
H	-0.07530	4.68270	2.41090	C	-6.74160	-6.18060	0.34480
H	1.94810	5.42240	3.48300	H	-7.69310	-7.58590	-1.09150
C	-2.96500	8.25890	-1.94860	H	-6.29960	-6.94510	-2.96970
C	-3.62570	7.09570	-1.96940	H	-4.53240	-5.15310	-2.69730
C	-2.95490	5.85550	-1.52860	H	-5.67400	-4.76960	1.46620
C	-1.67620	5.88610	-1.11470	H	-7.37190	-6.46170	1.17850
C	-0.95220	7.18100	-1.08540	C	-1.47600	-4.75640	3.58000
C	-1.56420	8.30350	-1.48310	C	-2.50960	-3.90870	3.61330
H	-3.45510	9.16870	-2.27020	C	-3.17680	-3.50530	2.35860
H	-4.65330	7.06040	-2.30740	C	-2.73240	-3.96060	1.17350
H	-3.51130	4.92610	-1.54280	C	-1.57440	-4.88800	1.14550
H	0.07270	7.23270	-0.74540	C	-0.99000	-5.27420	2.28630
H	-1.03460	9.24720	-1.46290	H	-0.98900	-5.05750	4.49830
C	0.10770	1.58350	-4.22130	H	-2.86760	-3.52560	4.56000
C	0.75140	1.39780	-3.06480	H	-4.04060	-2.85570	2.41810
C	0.46420	2.27050	-1.90550	H	-1.18910	-5.26440	0.21280
C	-0.45060	3.25070	-2.00600	H	-0.14540	-5.95070	2.26170
C	-1.14730	3.46100	-3.30000	N	1.98010	-0.36850	2.07650
C	-0.88500	2.66750	-4.34550	H	0.98060	-0.07280	1.90110
H	0.31570	0.94290	-5.06850	H	2.93610	2.55860	1.15170

C	5.55940	-5.17380	2.62510	H	6.86750	4.48170	-1.88750
H	6.63270	-5.21190	2.43950	H	8.12730	2.56430	-0.91760
C	6.21160	3.31510	2.53160	H	7.03320	0.41530	-0.51630
H	6.74660	3.41440	1.58450	H	3.36520	2.00620	-2.11930
O	-0.56030	-0.77330	-0.83890	H	4.45670	4.17980	-2.47040
C	1.83170	-4.59120	-1.12870	C	8.72900	-2.62170	-2.07560
C	1.40070	-3.27580	-1.06400	C	8.36030	-2.79730	-0.74240
C	2.32850	-2.22010	-0.96680	C	7.09110	-2.41170	-0.30450
C	3.72670	-2.49680	-0.94680	C	6.17970	-1.83880	-1.19800
C	4.12010	-3.85140	-1.00980	C	6.55300	-1.67610	-2.54130
C	3.20050	-4.88550	-1.10190	C	7.81820	-2.06400	-2.97560
H	1.10090	-5.39150	-1.20010	H	9.71740	-2.91900	-2.41310
H	0.34740	-3.01910	-1.07700	H	9.06040	-3.23300	-0.03580
H	5.17690	-4.08770	-0.99820	H	6.80990	-2.56520	0.73070
H	3.54490	-5.91290	-1.15970	H	5.84640	-1.24240	-3.24160
H	3.37130	-0.04790	-1.20390	H	8.09270	-1.92970	-4.01770
C	6.37670	3.52730	-1.72460	O	1.90050	-0.95110	-0.88720
C	7.08080	2.45020	-1.18560	H	0.85180	-0.86390	-0.88560
C	6.46810	1.21480	-0.97140	C	4.59500	-1.20400	1.93440
C	5.11680	1.03880	-1.31150	H	4.82800	-1.39780	0.63260
C	4.40770	2.13140	-1.84970	H	5.59070	-1.45690	2.28730
C	5.02920	3.35790	-2.05070				

### **OH-binding Type I Z**

(B3LYP/6-31G\*\*):UFF) Energy = -2290.938419

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.650397

M06-2X/6-31G\*\* Derived free energy = -5023.894756

M06-2X/6-31G\*\* Derived free energy in solution = -5023.912640

Number of Imaginary Frequencies = 1 (-994.35)

### **ONIOM (B3LYP/6-31G\*\*):UFF) Geometry**

C	2.98810	1.95830	-0.98720	C	4.17900	2.83770	-1.18890
C	5.56850	1.02480	-0.31250	C	4.04210	4.23290	-1.69540
C	4.50320	0.24130	-0.08750	C	5.12420	5.00040	-1.86850
C	3.13080	0.75140	-0.38510	C	6.46440	4.47530	-1.54850
H	6.56750	0.68730	-0.07600	C	6.60040	3.23380	-1.07170
C	5.40770	2.37720	-0.87210	H	3.06940	4.65090	-1.91650

H	5.01830	6.01330	-2.23520	H	-6.02790	-2.43210	4.47630
H	7.33590	5.10070	-1.69290	O	-0.09810	-5.52530	-0.97330
H	7.58710	2.85790	-0.83100	O	-2.34630	-5.71300	-1.05380
C	-0.79080	3.69050	-2.05300	O	-4.94690	-3.94640	2.62530
C	1.64810	2.44000	-1.39480	O	-3.97390	-2.73280	4.26060
C	0.71150	2.63180	-0.44500	Si	4.76070	-1.46550	0.62860
C	-0.52860	3.38620	-0.77130	Si	-1.61340	4.14830	0.54220
H	-1.67210	4.26660	-2.31080	C	2.48880	-1.49750	4.72730
C	1.32480	2.72370	-2.82030	C	2.45290	-2.58430	3.94780
C	0.14290	3.30090	-3.12860	C	3.17860	-2.59760	2.66050
C	-0.20790	3.56330	-4.54310	C	3.85730	-1.51200	2.25470
C	0.63270	3.20650	-5.52070	C	3.91200	-0.31850	3.13440
C	1.91340	2.55020	-5.19300	C	3.26140	-0.31210	4.30460
C	2.24350	2.31870	-3.91720	H	1.95210	-1.48420	5.66700
H	-1.14780	4.04050	-4.79100	H	1.88590	-3.45380	4.25410
H	0.37430	3.39470	-6.55470	H	3.14270	-3.49210	2.05950
H	2.58270	2.25150	-5.98930	H	4.47360	0.55630	2.83160
H	3.17990	1.82270	-3.69750	H	3.29550	0.56290	4.94060
O	2.05000	-0.08660	-0.21380	C	9.30080	-2.34680	1.37220
P	0.77950	0.43790	0.74240	C	8.83860	-2.20690	0.12430
O	0.89930	2.08840	0.80090	C	7.40680	-1.92550	-0.10760
O	0.95270	-0.11620	2.13210	C	6.56440	-1.80030	0.93200
N	-2.40760	-1.47620	-1.26710	C	7.08110	-1.96390	2.31300
C	-3.62440	-1.92120	-0.78790	C	8.37880	-2.22120	2.51920
C	-1.40530	-4.09940	0.40930	H	10.34920	-2.55380	1.54390
C	-0.35340	-3.28580	0.78230	H	9.51170	-2.30020	-0.71810
C	-1.63200	-2.42020	2.65150	H	7.05050	-1.82010	-1.12510
C	-2.73700	-3.15850	2.26870	H	6.41850	-1.87770	3.16340
C	0.98080	-3.22130	0.11040	H	8.75560	-2.33950	3.52700
H	1.53370	-2.34200	0.43300	C	3.42140	-4.78630	-2.39830
H	1.55570	-4.12470	0.32570	C	3.25290	-3.49750	-2.71380
C	-1.47100	-1.56950	3.88050	C	3.67480	-2.44240	-1.76940
H	-1.37040	-2.20230	4.76790	C	4.20540	-2.77130	-0.57760
H	-0.58140	-0.94550	3.77790	C	4.42110	-4.20160	-0.25020
H	-2.34740	-0.94090	4.03440	C	4.04150	-5.15540	-1.10990
C	-3.98770	-3.31980	3.04220	H	3.11270	-5.55960	-3.08950
C	-1.34830	-5.16960	-0.60690	H	2.80550	-3.22410	-3.66050
H	1.04220	-6.80560	-2.04570	H	3.54340	-1.41100	-2.06250
H	-0.59740	-7.43150	-1.66720	H	4.89090	-4.48150	0.68420
H	-5.01180	-2.34830	5.95350	H	4.19450	-6.19860	-0.86630

C	-0.23880	3.32930	4.95340	O	-0.47740	0.05810	-0.01570
C	-0.70400	2.32990	4.19680	C	-6.45840	-3.44310	-3.66900
C	-1.13200	2.59110	2.80720	C	-5.88500	-2.18800	-3.83760
C	-1.04450	3.82580	2.28830	C	-4.94210	-1.71100	-2.91990
C	-0.55070	4.93520	3.14280	C	-4.56840	-2.50810	-1.81330
C	-0.16380	4.69640	4.40220	C	-5.16270	-3.76810	-1.66420
H	0.07550	3.14020	5.97160	C	-6.09780	-4.24140	-2.58100
H	-0.76830	1.33000	4.60260	H	-7.18620	-3.80000	-4.39190
H	-1.49760	1.77010	2.20980	H	-6.14690	-1.55000	-4.67500
H	-0.50510	5.94640	2.76610	H	-4.87630	-4.39020	-0.82550
H	0.19650	5.50670	5.02280	H	-6.53600	-5.22450	-2.44620
C	-6.06410	2.75140	0.12630	H	-1.83240	-0.85310	-0.67470
C	-5.70350	3.56530	1.12490	C	-0.10100	-2.53340	-4.66000
C	-4.29260	3.97880	1.26980	C	-1.12590	-3.38440	-4.24600
C	-3.36640	3.54480	0.39840	C	-1.90740	-3.08500	-3.12890
C	-3.76550	2.61010	-0.68320	C	-1.67130	-1.90010	-2.41530
C	-5.04720	2.24540	-0.81650	C	-0.63360	-1.04280	-2.82870
H	-7.09700	2.44660	0.01870	C	0.14340	-1.36470	-3.93700
H	-6.44490	3.92720	1.82520	H	0.50190	-2.78080	-5.52830
H	-4.02480	4.65710	2.07060	H	-1.32700	-4.30090	-4.79340
H	-3.02990	2.20870	-1.36630	H	-2.67010	-3.78230	-2.81470
H	-5.34120	1.56600	-1.60440	H	-0.42860	-0.15250	-2.24670
C	-1.36690	8.72710	-0.43090	H	0.94490	-0.69390	-4.23250
C	-0.25350	8.02870	-0.18100	C	-5.58500	0.29260	2.36670
C	-0.33880	6.58740	0.13140	C	-4.21920	0.46450	2.14960
C	-1.53380	5.97350	0.18320	C	-3.56400	-0.22190	1.12430
C	-2.76310	6.75010	-0.11300	C	-4.28310	-1.09620	0.28710
C	-2.68160	8.05540	-0.40000	C	-5.66280	-1.26020	0.51980
H	-1.30640	9.78290	-0.66140	C	-6.30650	-0.56990	1.54070
H	0.71200	8.51680	-0.20860	H	-6.08370	0.83830	3.16230
H	0.57540	6.03700	0.31830	H	-3.66310	1.14570	2.78360
H	-3.73240	6.27290	-0.11200	H	-2.50230	-0.04890	0.97400
H	-3.57870	8.62070	-0.61720	H	-6.23620	-1.93290	-0.10430
N	-0.52210	-2.44920	1.85010	H	-7.37340	-0.70720	1.68740
H	0.18500	-1.69660	2.01630	O	-4.44410	-0.46770	-3.15420
H	0.85470	-3.16900	-0.97090	H	-3.71680	-0.28340	-2.54110
C	-5.18830	-2.87530	5.01600	C	-2.72170	-3.84650	0.97690
H	-5.40410	-3.92990	5.20230	H	-3.30060	-3.04920	0.10410
C	-0.01600	-6.55810	-1.96890	H	-3.42790	-4.67000	0.90320
H	-0.39150	-6.19020	-2.92670				

### **OH-binding Type II Z**

(B3LYP/6-31G\*\*):UFF) Energy = -2290.899494

(B3LYP/6-31G\*\*):UFF) Free Energy = -2289.612808

M06-2X/6-31G\*\* Derived free energy = -5023.863942

M06-2X/6-31G\*\* Derived free energy in solution = -5023.884257

Number of Imaginary Frequencies = 1 (-1059.74)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

C	-2.80120	2.20280	0.73020	O	-0.95040	1.82170	-0.67720
C	-1.56660	4.50560	1.77810	P	-0.58980	0.25480	-0.24410
C	-1.03390	3.88370	0.71350	O	-1.96620	-0.44630	0.39730
C	-1.58700	2.56890	0.28370	O	0.38740	0.25080	0.92930
H	-1.17900	5.46240	2.10820	N	2.01850	-1.95750	0.05430
C	-2.76670	3.96000	2.44140	C	3.16130	-1.88540	-0.72350
C	-3.38780	2.87970	1.92070	C	5.99690	-1.14730	1.02580
C	-4.61520	2.35880	2.57920	C	5.79700	0.14320	1.46200
C	-5.11230	2.97240	3.65960	C	3.79210	-0.54740	2.69760
C	-4.44160	4.16730	4.20870	C	4.03160	-1.86820	2.36130
C	-3.32880	4.63650	3.63290	C	6.67920	1.33880	1.23580
H	-5.11230	1.47580	2.19860	H	6.22160	2.24120	1.65040
H	-6.00530	2.59080	4.13750	H	7.65470	1.19400	1.70530
H	-4.85200	4.66140	5.07990	C	2.65790	0.02640	3.49590
H	-2.84190	5.51360	4.04090	H	1.80680	0.20120	2.81980
C	-5.31620	-0.70790	-1.14760	H	2.33470	-0.65910	4.27350
C	-3.58770	1.22090	-0.04260	H	2.94430	0.97970	3.95070
C	-3.17820	-0.06270	-0.13210	C	3.47570	-3.06860	3.04460
C	-4.16240	-1.09580	-0.57910	C	7.15880	-1.61900	0.23330
H	-6.03390	-1.43190	-1.50670	H	9.95010	-0.29130	-0.72570
C	-4.85150	1.64980	-0.70900	H	9.74530	-2.00160	-0.22160
C	-5.66240	0.71980	-1.25350	H	1.58390	-4.62950	4.06200
C	-6.91710	1.12790	-1.92760	H	2.94050	-4.49000	5.21250
C	-7.24000	2.42250	-2.01920	O	8.13770	-0.70050	0.07860
C	-6.34460	3.44930	-1.45330	O	7.22790	-2.74240	-0.22970
C	-5.21300	3.08900	-0.83690	O	3.84620	-4.19390	2.77020
H	-7.57700	0.37980	-2.34910	O	2.59370	-2.80480	4.02790
H	-8.15590	2.72060	-2.51300	Si	0.19840	4.83310	-0.31710
H	-6.60240	4.49650	-1.54590	Si	-3.88570	-2.91750	-0.25940
H	-4.56170	3.86050	-0.44760	C	4.33890	4.76030	1.88160

C	4.18310	5.49990	0.77790	H	-4.46430	-4.85300	-2.41880
C	2.87780	5.53220	0.08660	H	-6.68130	-3.05200	0.84170
C	1.84490	4.80820	0.55220	H	-8.65730	-4.29340	0.21200
C	2.02610	3.98860	1.77700	C	-3.62540	-3.86890	4.32880
C	3.20570	3.97530	2.40930	C	-3.60310	-2.59650	3.91710
H	5.29410	4.73560	2.38970	C	-3.67220	-2.28210	2.47480
H	5.01200	6.07700	0.38920	C	-3.72090	-3.27150	1.56450
H	2.76880	6.14970	-0.79620	C	-3.77810	-4.67950	2.03310
H	1.21170	3.39500	2.16980	C	-3.72830	-4.96070	3.34090
H	3.33300	3.38790	3.30850	H	-3.57770	-4.10010	5.38500
C	-1.47810	9.21640	-0.52350	H	-3.53910	-1.79300	4.63950
C	-2.16900	8.20540	-1.06090	H	-3.70220	-1.24430	2.18410
C	-1.63870	6.82810	-0.99490	H	-3.89130	-5.48850	1.32390
C	-0.45140	6.58170	-0.41350	H	-3.77510	-5.98820	3.67790
C	0.29590	7.70710	0.20420	C	-0.50400	-4.56730	-3.02860
C	-0.18970	8.95350	0.14620	C	-0.82470	-5.22860	-1.91270
H	-1.86590	10.22580	-0.56960	C	-1.84770	-4.68330	-0.99820
H	-3.11920	8.39320	-1.54390	C	-2.43550	-3.50490	-1.26210
H	-2.23350	6.02920	-1.41170	C	-2.05950	-2.76630	-2.49160
H	1.22440	7.53520	0.72760	C	-1.15330	-3.27720	-3.33360
H	0.35510	9.77040	0.60170	H	0.22600	-4.98030	-3.71150
C	0.43600	3.06760	-4.66960	H	-0.35400	-6.17720	-1.68970
C	-0.75180	3.27490	-4.09200	H	-2.13710	-5.27350	-0.14350
C	-0.82420	3.85320	-2.73460	H	-2.53420	-1.82400	-2.73200
C	0.30000	4.16140	-2.06150	H	-0.89330	-2.74550	-4.23960
C	1.61100	3.96260	-2.72830	N	4.66890	0.38860	2.20720
C	1.67440	3.43540	-3.95700	H	4.46420	1.35470	2.41670
H	0.49160	2.63850	-5.66160	H	6.84860	1.49270	0.16970
H	-1.66280	3.00920	-4.61240	C	2.10920	-3.95910	4.74310
H	-1.79780	3.97130	-2.27950	H	1.42890	-3.56450	5.49730
H	2.52800	4.25290	-2.24340	C	9.26890	-1.14110	-0.69620
H	2.63390	3.28950	-4.43630	H	8.95660	-1.42120	-1.70450
C	-7.70450	-5.32810	-1.50950	O	-0.17000	-0.42180	-1.51520
C	-6.57440	-5.47440	-2.21130	C	3.63510	-4.47530	-4.14260
C	-5.36210	-4.71900	-1.83130	C	2.63750	-3.51090	-4.11330
C	-5.39060	-3.88130	-0.78060	C	2.43890	-2.69060	-2.98610
C	-6.64590	-3.72450	-0.00650	C	3.29610	-2.86980	-1.86950
C	-7.74180	-4.41010	-0.35330	C	4.31340	-3.83140	-1.92830
H	-8.59260	-5.88090	-1.78720	C	4.48580	-4.64310	-3.04620
H	-6.54520	-6.14650	-3.05920	H	3.75360	-5.09540	-5.02690

H	1.97470	-3.35480	-4.95800	C	3.66660	1.91150	-0.96910
H	4.99480	-3.92940	-1.08880	C	3.10140	0.68870	-0.61750
H	5.27700	-5.38550	-3.06290	C	3.63770	-0.50210	-1.12490
H	1.56070	-1.08560	0.36460	C	4.74120	-0.41850	-1.99590
C	0.06840	-5.28430	1.78950	C	5.28310	0.81220	-2.36340
C	-0.32690	-3.97070	2.05520	H	5.15670	2.95730	-2.12780
C	0.30200	-2.89510	1.44340	H	3.23650	2.81270	-0.55910
C	1.37590	-3.11170	0.55510	H	2.23310	0.69110	0.03500
C	1.77820	-4.43250	0.29130	H	5.16790	-1.32710	-2.40370
C	1.12020	-5.49950	0.90130	H	6.11840	0.84350	-3.05690
H	-0.43920	-6.12030	2.26120	O	1.49990	-1.74190	-3.11630
H	-1.12590	-3.77250	2.75920	H	1.06040	-1.35450	-2.31500
H	-0.02080	-1.88100	1.64880	C	4.98620	-2.15230	1.30490
H	2.59760	-4.64040	-0.37750	H	4.15520	-2.18830	0.12780
H	1.44790	-6.51020	0.67730	H	5.31330	-3.18500	1.23940
C	4.74790	1.99110	-1.84600				



## TSs for Protonation

The reaction is catalysed by phosphoric acids through a proton transfer that activates the imine. This can happen through direct protonation of the imine by the phosphoric acid (**PT2**) or by the hydroxyl group (**PT1**). Our calculations reveal that the lowest energy pathway is **PT1**. The protonation pathways **PT1** and **PT2** in which the complex is ternary (Hantzsch ester also coordinating to the catalyst) could not be located. We do not exclude the possibility of the protonation happening through the ternary complex as being the correct pathway.

### **PT1**

(B3LYP/6-31G\*\*) Energy = -1238.006423

(B3LYP/6-31G\*\*) Free Energy = -1237.809521

M06-2X/6-31G\*\* Derived free energy = -1237.406021

M06-2X/6-31G\*\* Derived free energy in solution = -1237.419009

Number of Imaginary Frequencies = 1 (-793.21)

### B3LYP/6-31G\*\* Geometry

C	-4.58970	-0.41750	-0.98470	C	4.54630	0.22210	0.52720
C	-5.17300	0.30250	-0.01170	C	5.02700	-1.04290	0.82350
C	-4.62270	0.83210	1.23050	H	4.60190	-3.15950	0.77210
C	-3.46350	0.51110	1.81830	H	2.36060	-2.88790	-0.26400
H	-6.22190	0.51860	-0.19250	H	5.15890	1.08970	0.75140
H	-5.16060	-0.76070	-1.84000	H	6.00690	-1.16510	1.27260
H	-3.13010	0.95210	2.75080	C	3.48240	2.98150	0.02830
H	-5.22950	1.56630	1.75250	H	2.90860	3.87100	-0.24110
O	-2.57920	-0.44090	1.33600	H	3.68520	3.00760	1.10330
P	-2.03460	-0.30790	-0.19830	H	4.44650	3.02040	-0.48860
O	-3.28900	-0.84280	-1.09850	H	1.13400	2.67190	-1.06710
O	-1.52750	1.03270	-0.56500	N	1.56480	1.76660	-0.91050
C	2.72910	1.73020	-0.34360	O	-1.06900	-1.54360	-0.30400
C	4.23160	-2.16500	0.53930	H	-0.12800	-1.27720	-0.53290
C	2.97880	-2.02550	-0.03760	O	1.28450	-0.61060	-0.92480
C	2.48030	-0.74760	-0.35260	H	1.15150	0.53480	-1.04690
C	3.27740	0.40430	-0.05860				

**PT2**

(B3LYP/6-31G\*\*) Energy = -1238.003264

(B3LYP/6-31G\*\*) Free Energy = -1237.800497

M06-2X/6-31G\*\* Derived free energy = -1237.402541

M06-2X/6-31G\*\* Derived free energy in solution = -1237.417473

Number of Imaginary Frequencies = 1 (-65.01)

**B3LYP/6-31G\*\* Geometry**

O	-2.90240	-1.15240	-0.56640	C	-4.21750	0.55200	0.60700
P	-1.40270	-0.49360	-0.48420	H	-5.16710	0.65790	1.12340
O	-1.62370	1.06060	-0.95390	C	-3.39970	1.75750	0.54240
N	1.27000	-2.35500	-0.59290	H	-3.76250	2.60830	1.11170
O	-0.87660	-0.57890	0.92320	C	-2.26260	1.96940	-0.13490
C	3.25990	2.31440	-0.45180	H	-1.74940	2.92470	-0.11820
C	2.52030	2.03910	0.69500	C	-3.99140	-0.68150	0.12510
C	2.00570	0.75640	0.91610	H	-4.73180	-1.46610	0.23670
C	2.28580	-0.26550	-0.02130	H	0.38550	0.08280	1.68910
C	2.98750	0.04140	-1.20010	C	1.95880	-1.67810	0.26560
C	3.48000	1.32380	-1.41440	C	2.51550	-2.30310	1.50970
H	3.64720	3.31690	-0.60980	H	3.60950	-2.31560	1.45760
H	2.29690	2.80940	1.42540	H	2.23790	-1.67590	2.36120
H	3.17360	-0.74660	-1.92330	H	2.14440	-3.31920	1.66310
H	4.03640	1.54810	-2.31840	O	-0.62740	-1.14910	-1.61940
O	1.23160	0.52540	2.00190	H	0.45500	-1.80040	-1.22610
H	1.10820	-3.33450	-0.37220				

### Additional TS conformations with full catalyst system

#### Reaction 1

<b>TS Pathway</b>	(B3LYP/6-31G**: UFF) Energy	(B3LYP/6-31G**: UFF) Free Energy	M06-2X/6-31G** Derived free energy	M06-2X/6-31G** Derived free energy in solution
<b>NH-Type I E</b>	1868.150542	-1866.984959	-4601.392706	-4601.409224
	-1868.152359	-1866.988770	-4601.387724	-4601.404373
	-1868.150121	-1866.985315	-4601.393090	-4601.409608
<b>NH-Type II E</b>	-1868.149684	-1866.986855	-4601.401282	-4601.418356
	-1868.150092	-1866.987008	-4601.400675	-4601.417795
	-1868.152070	-1866.989922	-4601.399489	-4601.416789
	-1868.149647	-1866.986520	-4601.399184	-4601.416253
	-1868.151991	-1866.990083	-4601.398778	-4601.415989
	-1868.151934	-1866.990487	-4601.399013	-4601.415887
	-1868.149853	-1866.987204	-4601.398563	-4601.415660
	-1868.150516	-1866.988908	-4601.398462	-4601.415507
	-1868.151476	-1866.988932	-4601.397602	-4601.414807
	-1868.150775	-1866.987080	-4601.397752	-4601.414318
	-1868.151345	-1866.990100	-4601.397375	-4601.414184
	-1868.143480	-1866.981944	-4601.394818	-4601.414060
	-1868.145101	-1866.982240	-4601.395809	-4601.413499
	-1868.150692	-1866.989261	-4601.395544	-4601.412242
	-1868.150599	-1866.986582	-4601.394409	-4601.411563
	-1868.154250	-1866.988578	-4601.393526	-4601.409896
	-1868.145922	-1866.982974	-4601.391918	-4601.409806
-1868.147409	-1866.986899	-4601.391700	-4601.408816	

<b>NH-Type I Z</b>	-1868.147448	-1866.985457	-4601.398576	-4601.415469
	-1868.151368	-1866.986957	-4601.396481	-4601.415025
	-1868.149938	-1866.988260	-4061.396230	-4061.413128
	-1868.149852	-1866.987382	-4601.396005	-4601.412990
	-1868.142648	-1866.980464	-4601.394204	-4601.411499
	-1868.142628	-1866.980500	-4601.394138	-4601.411404
	-1868.147496	-1866.984329	-4601.393194	-4601.410871
	-1868.147270	-1866.985201	-4601.392668	-4601.410575
	-1868.146929	-1866.982491	-4601.390936	-4601.409891
	-1868.141523	-1866.979987	-4601.390600	-4601.408729
	-1868.145851	-1866.982705	-4601.390013	-4601.407796
	-1868.145308	-1866.982786	-4601.389885	-4601.407443
	-1868.146781	-1866.983672	-4601.389665	-4601.407430
	-1868.147627	-1866.986049	-4601.389118	-4601.407006
	-1868.140765	-1866.978259	-4601.386416	-4601.404094
	-1868.147264	-1866.984808	-4601.385785	-4601.403564
	-1868.132586	-1866.971987	-4601.379678	-4601.399710
<b>NH-Type II Z</b>	-1868.146577	-1866.982898	-4601.397008	-4601.414627
	-1868.147914	-1866.984073	-4601.395472	-4601.414129
	-1868.148139	-1866.983879	-4601.395722	-4601.413999
	-1868.146972	-1866.983204	-4601.395000	-4601.413360
	-1868.150790	-1866.986147	-4601.395436	-4601.412417
	-1868.143086	-1866.982277	-4601.393530	-4601.410797
	-1868.143887	-1866.984293	-4601.393563	-4601.411427
	-1868.136213	-1866.974127	-4601.387381	-4601.406287

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	-1868.134942	-1866.973300	-4601.387155	-4601.405910
	-1868.135663	-1866.973722	-4601.384124	-4601.405282
	-1868.143491	-1866.977736	-4601.388068	-4601.405014
<b>OOH-Type I E</b>	-1868.159400	-1866.997360	-4601.415196	-4601.433087
	-1868.159420	-1866.997323	-4601.415121	-4601.433061
	-1868.159360	-1866.997125	-4601.415146	-4601.433031
	-1868.159440	-1866.997317	-4601.414873	-4601.432962
	-1868.159432	-1866.997401	-4601.414940	-4601.432934
	-1868.159420	-1866.997144	-4601.414644	-4601.432815
	-1868.159381	-1866.997130	-4601.414669	-4601.432765
	-1868.159344	-1866.997114	-4601.414567	-4601.432676
	-1868.163725	-1866.999877	-4601.411439	-4601.430373
<b>OOH-Type II E</b>	-1868.170130	-1867.008353	-4601.418230	-4601.435231
	-1868.168401	-1867.006006	-4601.411663	-4601.428597
	-1868.108388	-1866.944478	-4601.409971	-4601.426910
<b>OOH-Type I Z</b>	-1868.124345	-1866.963805	-4601.383601	-4601.401342
	-1868.124362	-1866.963617	-4601.383391	-4601.401080
	-1868.131109	-1866.968818	-4601.381945	-4601.399685

## Reaction 2

<b>TS Pathway</b>	(B3LYP/6-31G**: UFF) Energy	(B3LYP/6-31G**: UFF) Free Energy	M06-2X/6-31G** Derived free energy	M06-2X/6-31G** Derived free energy in solution
<b>NH-Type I E</b>	-2290.933793	-2289.647256	-5023.894652	-5023.912270
	-2290.932086	-2289.643247	-5023.892803	-5023.910602
	-2290.934377	-2289.646145	-5023.892658	-5023.910372
	-2290.934373	-2289.646290	-5023.892667	-5023.910367
	-2290.934337	-2289.646005	-5023.892549	-5023.910250
	-2290.930371	-2289.643323	-5023.892404	-5023.910131
	-2290.930459	-2289.642950	-5023.892145	-5023.909810
	-2290.934466	-2289.645728	-5023.891879	-5063.909659
	-2290.930463	-2289.643117	-5023.891990	-5023.909525
	-2290.929030	-2289.641501	-5023.887706	-5023.905752
	-2290.932331	-2289.642642	-5023.887008	-5023.904491
	-2290.932702	-2289.643261	-5023.885989	-5023.903565
	-2290.928179	-2289.639535	-5023.881682	-5023.899471
	-2290.928158	-2289.639983	-5023.881697	-5023.899465
	-2290.907622	-2289.623460	-5023.865624	-5023.883544
	-2290.907631	-2289.623006	-5023.865089	-5023.883063
<b>NH-Type II E</b>	-2290.928229	-2289.640190	-5023.889940	-5023.907244
	-2290.928971	-2289.640739	-5023.887400	-5023.905086
	-2290.928627	-2289.640869	-5023.884617	-5023.902443
	-2290.928723	-2289.641048	-5023.884879	-5023.902642
	-2290.928713	-2289.640989	-5023.884630	-5023.902407
	-2290.925269	-2289.639124	-5023.882132	-5023.900745

	-2290.908095	-2289.620467	-5023.861031	-5023.878473
<b>NH-Type I Z</b>	-2290.939107	-2289.650540	-5023.897735	-5023.915497
	-2290.940608	-2289.650029	-5023.898169	-5023.915427
	-2290.936850	-2289.651469	-5023.898026	-5023.915361
	-2290.940583	-2289.650108	-5023.897956	-5023.915207
	-2290.940610	-2289.649933	-5023.897975	-5023.915195
	-2290.937176	-2289.649365	-5023.897049	-5023.914672
	-2290.937132	-2289.649383	-5023.897056	-5023.914666
	-2290.938328	-2289.650114	-5023.896330	-5023.914159
	-2290.936675	-2289.649694	-5023.895931	-5023.913399
	-2290.937065	-2289.649420	-5023.895992	-5023.913617
	-2290.936829	-2289.650209	-5023.896389	-5023.913749
	-2290.936985	-2289.649246	-5023.895784	-5023.913076
	-2290.938338	-2289.649859	-5023.895974	-5023.913763
	-2290.934576	-2289.648978	-5023.891739	-5023.909754
	-2290.934539	-2289.648654	-5023.890943	-5023.908883
	-2290.938931	-2289.648832	-5023.890408	-5023.908312
	-2290.938946	-2289.648848	-5023.890415	-5023.908294
	-2290.938919	-2289.648759	-5023.890238	-5023.908116
	-2290.938943	-2289.648807	-5023.890376	-5023.908256
	-2290.938967	-2289.648367	-5023.890091	-5023.907953
<b>NH-Type II Z</b>	-2290.931321	-2289.645119	-5023.890134	-5023.908446
	-2290.930664	-2289.644744	-5023.889153	-5023.907299
	-2290.931831	-2289.644621	-5023.886691	-5023.905153
	-2290.931921	-2289.643510	-5023.887358	-5023.905121

	-2290.931813	-2289.644435	-5023.886605	-5023.905084
	-2290.931792	-2289.644171	-5023.886206	-5023.904672
<b>OOH-Type I</b>	-2290.953732	-2289.667080	-5023.911612	-5023.930512
	-2290.953754	-2289.666955	-5023.911488	-5023.930374
	-2290.953698	-2289.667068	-5023.911415	-5023.930253
	-2290.937361	-2289.653751	-5023.896456	-5023.913867
<b>OOH-Type II E</b>	-2290.961578	-2289.674083	-5023.915796	-5023.933430
	-2290.960786	-2289.674337	-5023.914809	-5023.932541
	-2290.934960	-2289.646491	-5023.886858	-5023.904098
	-2290.934311	-2289.646631	-5023.884454	-5023.901532
<b>OOH-Type I Z</b>	-2290.935472	-2289.648868	-2289.648868	-5023.910932
	-2290.923155	-2289.638025	-5023.888658	-5023.908366
	-2290.903932	-2289.615328	-5023.864808	-5023.886517
<b>OOH-Type II Z</b>	-2290.902081	-2289.618163	-5023.856278	-5023.878037

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## Reaction 1

### NH-Type I E

C	-0.93350	-2.91520	-0.64080	C	-0.11270	3.13870	-2.22660
C	-3.65960	-3.53350	-0.20450	C	-1.18480	4.40680	0.54630
C	-3.22570	-2.27950	-0.01480	C	-1.20770	3.37670	1.47320
C	-1.77450	-1.96010	-0.16160	C	1.21640	3.35360	1.57470
H	-4.70610	-3.78220	-0.09000	C	1.29210	4.40110	0.68010
C	-2.72050	-4.60640	-0.57100	C	-2.41000	2.75370	2.12310
C	-1.41600	-4.32410	-0.77650	H	-3.25990	2.72330	1.44610
C	-0.48060	-5.44000	-1.09480	H	-2.15140	1.74460	2.44730
C	-0.93530	-6.69260	-1.21430	C	2.33120	2.61950	2.25370
C	-2.36780	-6.98310	-1.02030	H	2.31890	1.60370	1.84520
C	-3.21480	-5.99620	-0.71110	H	2.15010	2.55170	3.33090
H	0.57820	-5.25780	-1.22000	H	3.29690	3.07780	2.07540
H	-0.25070	-7.49880	-1.44480	C	2.48650	5.20750	0.34370
H	-2.72940	-7.99830	-1.12090	C	-2.35300	5.21150	0.12930
H	-4.26430	-6.21820	-0.56220	H	-4.40090	6.87270	0.80450
C	3.20680	-2.23600	-1.60380	H	-4.80270	5.78360	-0.53770
C	0.46450	-2.58840	-1.02080	H	4.40720	6.94540	0.96520
C	1.30630	-2.12740	-0.07710	H	5.43130	5.62330	1.61470
C	2.76710	-2.03270	-0.35260	O	-3.46500	5.01000	0.87430
H	4.25600	-2.14520	-1.84110	O	-2.31990	6.01420	-0.78980
C	0.95760	-2.78540	-2.41330	O	2.50500	5.99900	-0.58620
C	2.26910	-2.60230	-2.68500	O	3.53940	5.05830	1.17770
C	2.77010	-2.76670	-4.06910	Si	-4.45840	-0.93060	0.37680
C	1.92320	-3.06960	-5.05870	Si	4.00580	-1.68420	1.00980
C	0.48520	-3.24030	-4.77570	C	-3.85370	0.50590	4.80740
C	0.02430	-3.10400	-3.52700	C	-3.05390	-0.43640	4.29660
H	3.82290	-2.63480	-4.28590	C	-3.24570	-0.89660	2.90550
H	2.28930	-3.18430	-6.07080	C	-4.20320	-0.35220	2.13390
H	-0.19740	-3.46880	-5.58400	C	-5.11470	0.66020	2.72470
H	-1.03650	-3.21370	-3.34430	C	-4.94300	1.07060	3.98730
O	-1.37690	-0.64950	0.00250	H	-3.71280	0.84610	5.82500
P	-0.03850	-0.29810	0.94460	H	-2.25990	-0.85980	4.89800
O	0.79490	-1.70140	1.11950	H	-2.59280	-1.67120	2.52960
O	-0.44130	0.16360	2.32320	H	-5.94910	1.04600	2.15730
N	-0.76680	2.11630	-1.58570	H	-5.61340	1.80410	4.41590
H	-1.72300	2.29650	-1.30970	C	-8.79330	-2.60990	-0.19190

C	-8.34100	-2.35850	1.04230	H	2.49900	-3.78310	2.36890
C	-6.97590	-1.82680	1.23780	H	3.72760	0.25260	3.36500
C	-6.18720	-1.58500	0.17680	H	2.55700	0.11960	5.46140
C	-6.69090	-1.87420	-1.18750	C	5.90800	2.54800	0.40720
C	-7.92670	-2.35850	-1.36100	C	6.40100	1.71410	1.32890
H	-9.79240	-3.00050	-0.33590	C	5.78960	0.38450	1.52490
H	-8.97290	-2.54610	1.90070	C	4.73610	0.00740	0.78120
H	-6.62760	-1.65450	2.24660	C	4.19070	0.93730	-0.23720
H	-6.06030	-1.69830	-2.04990	C	4.74320	2.14500	-0.40550
H	-8.29280	-2.56920	-2.35740	H	6.36300	3.51720	0.25430
C	-4.12960	2.37450	-2.94030	H	7.25370	2.00810	1.92710
C	-4.75910	2.64650	-1.79260	H	6.20930	-0.28110	2.26930
C	-4.84360	1.62200	-0.73110	H	3.33680	0.65600	-0.83780
C	-4.26290	0.42170	-0.89600	H	4.33470	2.83410	-1.12930
C	-3.56890	0.12720	-2.17760	N	-0.02240	2.84420	1.87990
C	-3.50840	1.05180	-3.14360	H	-0.07080	1.88750	2.29970
H	-4.07410	3.12210	-3.72090	H	-2.71450	3.34210	2.99540
H	-5.22270	3.61220	-1.64510	C	4.67390	5.88970	0.87800
H	-5.39760	1.85870	0.16180	H	5.03450	5.69960	-0.13510
H	-3.12510	-0.84270	-2.35500	C	-4.59420	5.83190	0.53220
H	-3.00350	0.83230	-4.07540	H	-5.42890	5.43650	1.11040
C	7.63120	-4.64570	0.63830	C	0.08880	4.76430	-0.07380
C	6.74520	-4.80940	1.62680	H	0.15770	4.07010	-1.20300
C	5.60050	-3.88370	1.75840	H	0.11340	5.75050	-0.53150
C	5.43060	-2.88330	0.87590	O	0.74290	0.67870	0.08350
C	6.43420	-2.69400	-0.20190	H	-0.20910	1.55380	-0.88670
C	7.47190	-3.53160	-0.31610	C	-0.97820	4.01970	-3.11650
H	8.47020	-5.32260	0.54180	H	-1.86370	4.37960	-2.58930
H	6.86440	-5.62060	2.33340	H	-0.41480	4.88500	-3.46800
H	4.91570	-4.03680	2.57720	H	-1.28670	3.43620	-3.99190
H	6.34900	-1.86250	-0.88930	C	3.68370	2.24280	-4.05240
H	8.20360	-3.38650	-1.10030	C	2.77050	1.22020	-3.84410
C	1.83650	-1.96130	5.16270	C	1.54040	1.46730	-3.21390
C	1.83730	-3.01240	4.33550	C	1.23460	2.78520	-2.77710
C	2.54500	-2.93500	3.04110	C	2.17810	3.80210	-3.01080
C	3.19470	-1.81170	2.68700	C	3.38910	3.54750	-3.63960
C	3.20310	-0.65660	3.61850	H	4.63040	2.02330	-4.53750
C	2.55440	-0.72720	4.78720	H	2.97370	0.20450	-4.16450
H	1.31240	-2.01340	6.10820	H	1.96180	4.80630	-2.66010
H	1.31030	-3.91790	4.60700	H	4.10120	4.35160	-3.79220

O	0.70220	0.41030	-3.12790				
H	-0.08690	0.66510	-2.61340				
C	-1.18230	-2.70450	-0.95350	C	0.78480	3.31330	-2.34770
C	-3.93620	-3.24930	-0.58290	C	-0.84050	4.53820	0.17790
C	-3.45490	-2.03870	-0.26960	C	-1.14100	3.49900	1.04330
C	-1.99420	-1.75580	-0.40920	C	1.16390	3.37270	1.77110
H	-4.98590	-3.47830	-0.46240	C	1.51870	4.40040	0.92170
C	-3.04110	-4.31770	-1.05310	C	-2.49190	2.91280	1.33580
C	-1.72170	-4.07750	-1.20980	H	-3.15800	3.00810	0.48430
C	-0.82840	-5.20900	-1.59260	H	-2.36900	1.86290	1.60690
C	-1.33480	-6.42490	-1.82700	C	2.00310	2.68130	2.80640
C	-2.78350	-6.66260	-1.69420	H	1.61830	1.66950	2.94840
C	-3.59290	-5.66670	-1.32100	H	1.93150	3.21220	3.76260
H	0.24160	-5.07210	-1.66780	H	3.05220	2.65000	2.52890
H	-0.68020	-7.24170	-2.10250	C	2.80700	5.12180	0.91750
H	-3.18720	-7.64810	-1.88760	C	-1.82950	5.40420	-0.49570
H	-4.65450	-5.85190	-1.21310	H	-3.79240	7.21690	-0.43600
C	3.03250	-2.31430	-1.71560	H	-4.10550	6.00790	-1.69750
C	0.24250	-2.42360	-1.27150	H	5.44980	5.25120	1.07280
C	1.07710	-2.07710	-0.27300	H	4.74240	6.60250	1.98540
C	2.54930	-2.12990	-0.47820	O	-3.08930	5.29740	-0.01170
H	4.10250	-2.34020	-1.88730	O	-1.54130	6.18420	-1.39040
C	0.78310	-2.59850	-2.65050	O	3.11900	5.92510	0.05180
C	2.11850	-2.53270	-2.85510	O	3.60770	4.84830	1.97230
C	2.66800	-2.68020	-4.22230	Si	-4.61930	-0.73540	0.40250
C	1.84480	-2.85490	-5.26180	Si	3.75590	-2.01790	0.94120
C	0.38490	-2.89880	-5.05060	C	-9.02470	-2.32450	0.45250
C	-0.12090	-2.77430	-3.81820	C	-8.41370	-2.07380	-0.71130
H	3.73780	-2.64130	-4.38570	C	-7.02290	-1.57520	-0.72480
H	2.24680	-2.95840	-6.26130	C	-6.36570	-1.37250	0.42970
H	-0.27630	-3.02470	-5.89820	C	-7.04710	-1.65430	1.71670
H	-1.19480	-2.79040	-3.68640	C	-8.30780	-2.10520	1.72510
O	-1.56440	-0.47110	-0.15030	H	-10.04360	-2.68960	0.46430
P	-0.18970	-0.19420	0.74780	H	-8.93650	-2.23470	-1.64520
O	0.55670	-1.64710	0.91820	H	-6.54520	-1.37710	-1.67650
O	-0.55640	0.28810	2.13270	H	-6.53220	-1.50710	2.65640
N	-0.16960	2.37700	-2.02730	H	-8.80390	-2.31320	2.66430
H	-1.13000	2.68770	-2.08960	C	-4.72590	3.00840	-2.43200

C	-5.54990	2.93540	-1.38160	H	1.94820	-3.74620	2.41400
C	-5.51570	1.75490	-0.49370	H	3.81750	0.09100	3.16000
C	-4.63560	0.76220	-0.71270	H	2.65890	0.27650	5.26320
C	-3.75700	0.83180	-1.90900	C	6.38040	1.76560	0.09680
C	-3.79690	1.89880	-2.71630	C	6.95810	0.55930	0.12900
H	-4.75040	3.87130	-3.08460	C	6.14280	-0.64620	0.38910
H	-6.24510	3.74000	-1.18000	C	4.81990	-0.53430	0.59800
H	-6.22880	1.70030	0.31570	C	4.18240	0.79990	0.52360
H	-3.09810	0.01500	-2.16220	C	4.92470	1.89010	0.30400
H	-3.15860	1.94360	-3.58940	H	6.97460	2.65000	-0.09310
C	-3.32100	0.29940	4.79730	H	8.02400	0.46340	-0.03210
C	-2.77310	-0.74440	4.16670	H	6.63410	-1.60860	0.40280
C	-3.18650	-1.07670	2.78770	H	3.11470	0.89900	0.65880
C	-4.09870	-0.32210	2.14810	H	4.45730	2.86250	0.25700
C	-4.72850	0.81120	2.87090	N	-0.12660	2.91350	1.73530
C	-4.35290	1.10900	4.12090	H	-0.31070	1.94820	2.11570
H	-3.01630	0.54700	5.80580	H	-2.95840	3.43690	2.17710
H	-2.01960	-1.34400	4.66120	C	4.87910	5.51900	1.96510
H	-2.73250	-1.93490	2.31260	H	5.39220	5.17900	2.86430
H	-5.49710	1.40480	2.40260	C	-4.05520	6.17250	-0.61910
H	-4.81070	1.93980	4.64200	H	-5.00610	5.92820	-0.14670
C	6.29300	-5.94200	1.29890	C	0.56450	4.82600	-0.10680
C	6.53040	-4.90840	2.11450	H	0.85790	4.14330	-1.20150
C	5.72960	-3.67240	1.99560	H	0.75460	5.81320	-0.52290
C	4.77310	-3.57190	1.05700	O	0.63420	0.73860	-0.11820
C	4.49990	-4.73020	0.17020	H	0.04560	1.72160	-1.22300
C	5.22430	-5.85040	0.28390	C	0.35310	4.35300	-3.37330
H	6.87760	-6.84870	1.38540	H	-0.60650	4.80250	-3.11110
H	7.30870	-4.97510	2.86370	H	1.09410	5.14950	-3.45390
H	5.92990	-2.85070	2.67250	H	0.27580	3.86470	-4.35200
H	3.70590	-4.69100	-0.56210	C	4.81770	1.99130	-3.08130
H	5.02200	-6.69580	-0.36100	C	3.77280	1.08900	-3.20990
C	1.58260	-1.65900	5.07550	C	2.45090	1.47320	-2.93450
C	1.40540	-2.74420	4.31350	C	2.18350	2.80070	-2.50470
C	2.11170	-2.86420	3.02130	C	3.26520	3.69290	-2.38720
C	2.91210	-1.87310	2.59200	C	4.56780	3.30620	-2.67090
C	3.13610	-0.69230	3.46000	H	5.83250	1.66860	-3.29520
C	2.49930	-0.58920	4.63330	H	3.94150	0.06830	-3.53510
H	1.06210	-1.56660	6.01990	H	3.07550	4.70360	-2.03920
H	0.73850	-3.53270	4.63730	H	5.38140	4.01510	-2.55780

O	1.50340	0.53980	-3.17070			
H	0.63760	0.89060	-2.89020			
C	-0.89670	-2.92370	-0.69780	H	-1.71340	2.36150 -1.20840
C	-3.62850	-3.55400	-0.32100	C	-0.08440	3.18090 -2.10970
C	-3.20250	-2.30060	-0.11060	C	-1.15300	4.40430 0.67590
C	-1.74970	-1.97650	-0.22620	C	-1.23420	3.34480 1.56680
H	-4.67580	-3.80760	-0.22600	C	1.17910	3.26570 1.75490
C	-2.67900	-4.62060	-0.67950	C	1.31560	4.32690 0.88290
C	-1.37130	-4.33270	-0.85580	C	-2.47210	2.72720 2.15260
C	-0.42590	-5.44260	-1.16470	H	-3.30060	2.74170 1.44920
C	-0.87400	-6.69550	-1.30490	H	-2.24620	1.70100 2.44700
C	-2.30940	-6.99200	-1.14320	C	2.26200	2.51820 2.46700
C	-3.16570	-6.01050	-0.84240	H	2.29650	1.52300 2.01230
H	0.63470	-5.25580	-1.26600	H	2.01200	2.39460 3.52510
H	-0.18230	-7.49750	-1.52820	H	3.22330	3.01110 2.37060
H	-2.66560	-8.00730	-1.26050	C	2.60620	5.02720 0.69810
H	-4.21730	-6.23710	-0.71710	C	-2.28410	5.25570 0.25130
C	3.25490	-2.21920	-1.59080	H	-4.71950	5.85650 -0.50410
C	0.50500	-2.58450	-1.05270	H	-5.38850	5.52560 1.12970
C	1.32940	-2.12330	-0.09320	H	4.58120	5.92620 -0.83920
C	2.79420	-2.02110	-0.34630	H	3.55580	7.27220 -1.44000
H	4.30760	-2.12540	-1.81080	O	-3.43400	5.04260 0.93290
C	1.02140	-2.77290	-2.43830	O	-2.19350	6.10330 -0.62340
C	2.33660	-2.58540	-2.68790	O	3.60750	4.91370 1.38080
C	2.86140	-2.74540	-4.06360	O	2.55290	5.89240 -0.35170
C	2.03200	-3.04770	-5.06820	Si	-4.44600	-0.96090 0.28150
C	0.59000	-3.22260	-4.80970	Si	4.00960	-1.67080 1.03560
C	0.10790	-3.09070	-3.56860	C	-8.77740	-2.62770 -0.35530
H	3.91730	-2.61010	-4.26220	C	-7.99180	-2.37450 -1.40850
H	2.41540	-3.15870	-6.07420	C	-6.62630	-1.84840 -1.20410
H	-0.07840	-3.45070	-5.63000	C	-6.17020	-1.61330 0.03790
H	-0.95560	-3.20350	-3.40430	C	-7.04100	-1.90870 1.20210
O	-1.35670	-0.66770	-0.04430	C	-8.27720	-2.38690 1.01320
P	-0.05290	-0.32890	0.95030	H	-9.77770	-3.01370 -0.50320
O	0.80000	-1.72260	1.10510	H	-8.35420	-2.55450 -2.41230
O	-0.50420	0.08240	2.32960	H	-6.00410	-1.65720 -2.06960
N	-0.76170	2.16360	-1.48740	H	-6.68240	-1.75780 2.21100

H	-8.91060	-2.60600	1.86320	H	1.28290	-2.32840	6.08380
C	-4.04610	2.43600	-2.93460	H	1.33840	-4.15020	4.48400
C	-4.69580	2.67780	-1.79130	H	2.54360	-3.86970	2.26830
C	-4.80440	1.62330	-0.76210	H	3.66790	0.13450	3.48820
C	-4.22420	0.42610	-0.94990	H	2.48220	-0.13600	5.56270
C	-3.50600	0.16590	-2.22540	C	5.73750	2.65490	0.58180
C	-3.42430	1.11750	-3.16320	C	6.23900	1.82450	1.50250
H	-3.97340	3.20530	-3.69230	C	5.68540	0.46300	1.65000
H	-5.15670	3.64180	-1.62350	C	4.67170	0.05590	0.86780
H	-5.37460	1.83680	0.12630	C	4.12110	0.97990	-0.15290
H	-3.06120	-0.80020	-2.42090	C	4.62490	2.21310	-0.28180
H	-2.90170	0.92300	-4.09090	H	6.14120	3.65300	0.47120
C	-3.95230	0.36730	4.75840	H	7.05300	2.14640	2.13890
C	-3.13850	-0.56100	4.24430	H	6.11220	-0.19930	2.39330
C	-3.29600	-0.98800	2.83840	H	3.30480	0.67150	-0.79080
C	-4.23580	-0.42660	2.05750	H	4.21360	2.89530	-1.01030
C	-5.16430	0.56870	2.65090	N	-0.07790	2.77390	2.00050
C	-5.02360	0.94900	3.92660	H	-0.15540	1.80610	2.39080
H	-3.83650	0.68300	5.78700	H	-2.79130	3.28850	3.03740
H	-2.35810	-0.99760	4.85420	C	3.76960	6.61630	-0.59630
H	-2.63230	-1.75190	2.45940	H	4.05460	7.19960	0.28210
H	-5.98760	0.96440	2.07420	C	-4.53100	5.89860	0.57030
H	-5.70670	1.66960	4.35710	H	-4.31400	6.93310	0.84760
C	7.75470	-4.46760	0.59400	C	0.14850	4.74540	0.10080
C	6.86130	-4.71020	1.55950	H	0.21830	4.08340	-1.05350
C	5.67850	-3.83720	1.71280	H	0.19550	5.74470	-0.32370
C	5.48290	-2.80510	0.87320	O	0.73380	0.68730	0.14130
C	6.49320	-2.52880	-0.17910	H	-0.21270	1.57940	-0.79640
C	7.56480	-3.31930	-0.31330	C	-0.93170	4.10310	-2.97500
H	8.62130	-5.10620	0.48130	H	-1.81010	4.46670	-2.43920
H	7.00230	-5.54710	2.23120	H	-0.35340	4.96650	-3.30610
H	4.98630	-4.05420	2.51100	H	-1.25160	3.54860	-3.86490
H	6.38190	-1.67370	-0.83330	C	3.67100	2.23120	-3.99400
H	8.30040	-3.11200	-1.07980	C	2.74960	1.22070	-3.76890
C	1.81290	-2.21380	5.14720	C	1.53060	1.48200	-3.12170
C	1.84540	-3.21930	4.26560	C	1.24670	2.80390	-2.68170
C	2.56170	-3.05670	2.98380	C	2.19690	3.80880	-2.93880
C	3.18730	-1.90130	2.69580	C	3.39540	3.54150	-3.58490
C	3.16080	-0.79760	3.68700	H	4.60810	1.99930	-4.49170
C	2.50440	-0.94520	4.84420	H	2.93660	0.20210	-4.08950

H	1.98670	4.81650	-2.59520	H	-0.09780	0.69180	-2.50320
H	4.11270	4.33690	-3.75800				
O	0.68440	0.43380	-3.02600				

**NH-Type II E**

C	2.75280	2.28130	0.67570				
C	4.92130	0.65730	1.48930	O	-0.02380	1.66880	0.68600
C	4.06890	0.20620	0.55720	O	0.82500	-0.59580	1.36800
C	2.89100	1.03420	0.18250	N	-3.13570	-0.87740	-0.34650
H	5.77660	0.06090	1.78450	H	-3.56430	-0.13800	0.18270
C	4.70670	1.96800	2.13470	C	-3.91360	-1.95100	-0.69830
C	3.66930	2.74930	1.75710	C	-2.18150	-4.21260	0.94560
C	3.43810	4.03680	2.46650	C	-0.97350	-3.53670	1.07730
C	4.27190	4.43420	3.43460	C	-1.98820	-1.92380	2.56210
C	5.42150	3.59170	3.81590	C	-3.23070	-2.51210	2.40530
C	5.62660	2.42030	3.20400	C	0.34250	-3.90740	0.45900
H	2.58930	4.65970	2.21740	H	0.77370	-4.77830	0.96010
H	4.10010	5.37160	3.94770	H	0.21300	-4.16870	-0.59130
H	6.09320	3.92070	4.59830	C	-1.61310	-0.78170	3.46190
H	6.46750	1.80320	3.49530	H	-0.99430	-0.07000	2.90800
C	-0.21880	5.01590	-0.84130	H	-0.99850	-1.15980	4.28730
C	1.72470	3.17990	0.08620	H	-2.48550	-0.29990	3.88510
C	0.41030	2.82990	0.08320	C	-4.48380	-2.13330	3.10580
C	-0.60980	3.81740	-0.38440	C	-2.35330	-5.53010	0.31770
H	-0.94080	5.73270	-1.20880	H	-1.88720	-8.12290	-0.03340
C	2.14700	4.47390	-0.53490	H	-1.90080	-7.30140	-1.61300
C	1.20940	5.35770	-0.93800	H	-5.20520	-0.61260	5.86940
C	1.61090	6.65580	-1.52930	H	-6.16240	-0.51250	4.35400
C	2.90480	6.94930	-1.69180	O	-1.20630	-6.14650	-0.02090
C	3.93740	5.97420	-1.29670	O	-3.44730	-6.06730	0.14480
C	3.58430	4.80170	-0.75750	O	-5.58730	-2.42170	2.67660
H	0.85740	7.37110	-1.83500	O	-4.30910	-1.48180	4.27720
H	3.19700	7.89700	-2.12540	Si	4.40550	-1.44950	-0.23800
H	4.98270	6.20540	-1.45660	Si	-2.42650	3.36960	-0.46400
H	4.36110	4.09290	-0.50530	C	3.20480	-4.87360	2.74140
O	1.94100	0.53820	-0.67120	C	3.00030	-3.59560	3.08000
P	0.52970	0.21070	0.10650	C	3.38670	-2.51200	2.15280

C	3.93820	-2.80250	0.96100	H	-5.21710	0.62260	-3.60230
C	4.16600	-4.22310	0.59590	C	-4.87180	7.29050	-1.23470
C	3.81760	-5.20240	1.43920	C	-4.75210	6.38670	-2.21430
H	2.91950	-5.66800	3.41870	C	-3.98670	5.14310	-1.98650
H	2.54760	-3.35190	4.03230	C	-3.41660	4.91010	-0.79180
H	3.20370	-1.49010	2.45350	C	-3.54500	5.92010	0.28630
H	4.61510	-4.47390	-0.35700	C	-4.23640	7.04670	0.07580
H	3.98260	-6.23700	1.16810	H	-5.43060	8.20230	-1.40130
C	9.01490	-1.57410	-1.12460	H	-5.21280	6.56550	-3.17720
C	8.25310	-0.61330	-1.65820	H	-3.88440	4.44320	-2.80380
C	6.80310	-0.57570	-1.37680	H	-3.07730	5.75250	1.24840
C	6.23480	-1.51480	-0.60070	H	-4.32890	7.78280	0.86390
C	7.09340	-2.56210	0.00920	C	-4.02510	2.03450	3.74340
C	8.40770	-2.59110	-0.24450	C	-2.79550	2.54630	3.62670
H	10.07750	-1.60220	-1.32840	C	-2.27580	2.93050	2.29850
H	8.69690	0.14040	-2.29570	C	-3.02270	2.74850	1.19400
H	6.22040	0.23260	-1.79210	C	-4.39430	2.20010	1.33880
H	6.67700	-3.29910	0.67920	C	-4.86220	1.85120	2.54310
H	9.03100	-3.35360	0.20470	H	-4.40830	1.75600	4.71630
C	1.95400	-1.79690	-4.23400	H	-2.18010	2.68610	4.50590
C	1.86590	-2.76330	-3.31430	H	-1.30290	3.39870	2.24770
C	2.64600	-2.66970	-2.06400	H	-5.03610	2.08640	0.48150
C	3.45640	-1.62050	-1.84110	H	-5.86220	1.44920	2.64130
C	3.55220	-0.55510	-2.87210	N	-0.93440	-2.41270	1.83920
C	2.83640	-0.63770	-4.00050	H	-0.09890	-1.73810	1.71350
H	1.37820	-1.86120	-5.14810	H	1.02580	-3.06300	0.54460
H	1.22070	-3.61610	-3.48060	C	-5.52300	-1.14480	4.97350
H	2.53930	-3.46100	-1.34190	H	-6.07370	-2.05030	5.23770
H	4.16180	0.32010	-2.70170	C	-1.35300	-7.41970	-0.67540
H	2.89370	0.15130	-4.73920	H	-0.33730	-7.76490	-0.86530
C	-3.06570	0.50680	-4.13750	C	-3.38710	-3.54730	1.40200
C	-1.83460	0.91730	-3.81640	H	-3.83240	-2.82770	0.27180
C	-1.62770	1.79160	-2.64390	H	-4.28250	-4.15700	1.47600
C	-2.66900	2.16750	-1.87810	O	-0.41780	-0.36550	-0.90580
C	-4.03410	1.72200	-2.25690	H	-2.12640	-0.78410	-0.52470
C	-4.21880	0.93320	-3.32270	C	-5.40920	-1.62720	-0.66810
H	-3.21860	-0.13740	-4.99360	H	-6.00660	-2.52940	-0.77170
H	-0.98570	0.60580	-4.41140	H	-5.64010	-0.94250	-1.49080
H	-0.62270	2.12800	-2.43480	H	-5.66800	-1.14390	0.27810
H	-4.89730	2.06840	-1.71070	C	-2.51610	-4.31810	-4.03960



C	-3.57770	-4.76720	-3.25730	H	-4.09060	-5.69800	-3.47920
C	-4.01730	-4.01800	-2.16140	H	-1.78010	-1.46140	-2.37200
C	-3.40820	-2.78280	-1.84800	H	-1.04550	-2.76110	-4.31120
C	-2.31160	-2.37010	-2.62510	O	-5.05290	-4.49320	-1.39220
C	-1.87700	-3.12110	-3.71460	H	-4.69880	-5.21850	-0.83520
H	-2.18820	-4.90200	-4.89500				
C	2.77280	2.25070	0.65970	O	-0.00940	1.66490	0.66710
C	4.92270	0.60330	1.47500	O	0.81820	-0.61070	1.34280
C	4.06620	0.16150	0.54200	N	-3.14340	-0.83810	-0.32130
C	2.89860	1.00300	0.16500	H	-3.55570	-0.09260	0.21220
H	5.76990	-0.00330	1.77260	C	-3.94320	-1.89550	-0.67350
C	4.72240	1.91670	2.11960	C	-2.23550	-4.19550	0.93340
C	3.69340	2.70880	1.74190	C	-1.01500	-3.54030	1.05170
C	3.47540	3.99850	2.45160	C	-1.98100	-1.92170	2.56250
C	4.31340	4.38740	3.41950	C	-3.23490	-2.48880	2.41960
C	5.45440	3.53310	3.80060	C	0.28480	-3.92770	0.40980
C	5.64700	2.35950	3.18890	H	0.70630	-4.81350	0.89260
H	2.63270	4.62990	2.20300	H	0.13580	-4.17160	-0.64220
H	4.15120	5.32640	3.93280	C	-1.57540	-0.79410	3.46750
H	6.12970	3.85530	4.58270	H	-0.90700	-0.11740	2.92780
H	6.48150	1.73370	3.48020	H	-1.00760	-1.19740	4.31450
C	-0.17060	5.02020	-0.84690	H	-2.43440	-0.26650	3.86320
C	1.75400	3.16000	0.07100	C	-4.46840	-2.09440	3.14500
C	0.43630	2.82360	0.06800	C	-2.43980	-5.50470	0.29780
C	-0.57380	3.82450	-0.39280	H	-2.02580	-8.10160	-0.08170
H	-0.88550	5.74630	-1.21000	H	-2.05110	-7.26730	-1.65430
C	2.18950	4.45060	-0.54780	H	-5.10490	-0.57940	5.93270
C	1.26110	5.34600	-0.94650	H	-6.09710	-0.46610	4.44090
C	1.67640	6.64080	-1.53560	O	-1.30940	-6.13770	-0.06530
C	2.97330	6.91960	-1.70060	O	-3.54570	-6.02140	0.13890
C	3.99540	5.93160	-1.31030	O	-5.58490	-2.35760	2.73350
C	3.63000	4.76220	-0.77290	O	-4.25820	-1.45830	4.31910
H	0.93060	7.36570	-1.83760	Si	4.38110	-1.50080	-0.24790
H	3.27560	7.86480	-2.13270	Si	-2.39440	3.39730	-0.46780
H	5.04300	6.15090	-1.47220	C	3.09860	-4.89830	2.72790
H	4.39900	4.04380	-0.52390	C	2.91350	-3.61640	3.06260
O	1.94500	0.51850	-0.69130	C	3.32700	-2.54130	2.13720
P	0.52980	0.20300	0.08440	C	3.88160	-2.84340	0.94990

C	4.08870	-4.26830	0.58930	C	-4.80690	7.34020	-1.22870
C	3.71710	-5.23990	1.43160	C	-4.70800	6.43080	-2.20540
H	2.79330	-5.68650	3.40370	C	-3.95290	5.18030	-1.98090
H	2.45660	-3.36320	4.01050	C	-3.37060	4.94730	-0.79210
H	3.16110	-1.51590	2.43570	C	-3.47640	5.96300	0.28310
H	4.54210	-4.52840	-0.35900	C	-4.15870	7.09570	0.07550
H	3.86710	-6.27770	1.16390	H	-5.35840	8.25690	-1.39280
C	8.99560	-1.70790	-1.09010	H	-5.17840	6.60990	-3.16360
C	8.25400	-0.74190	-1.64240	H	-3.86840	4.47500	-2.79550
C	6.80210	-0.67860	-1.37600	H	-2.99960	5.79410	1.24050
C	6.21190	-1.59970	-0.59480	H	-4.23480	7.83600	0.86140
C	7.04790	-2.65330	0.03520	C	-3.94480	2.06670	3.75750
C	8.36400	-2.70540	-0.20470	C	-4.72250	1.90770	2.68200
H	10.05970	-1.75460	-1.28250	C	-4.23120	2.30670	1.34750
H	8.71580	-0.00240	-2.28390	C	-2.98390	2.78290	1.19360
H	6.23610	0.13350	-1.80660	C	-2.13230	2.96830	2.39680
H	6.61340	-3.37610	0.70930	C	-2.58860	2.62860	3.60830
H	8.97090	-3.47200	0.25950	H	-4.30620	1.78430	4.73760
C	1.94220	-1.79860	-4.25560	H	-5.71940	1.50020	2.78750
C	1.83890	-2.76890	-3.34160	H	-4.90580	2.22300	0.51210
C	2.61730	-2.69280	-2.08900	H	-1.14970	3.41140	2.31420
C	3.44060	-1.65540	-1.85790	H	-1.96730	2.77210	4.48280
C	3.55440	-0.58660	-2.88330	N	-0.94580	-2.42260	1.82110
C	2.84040	-0.65320	-4.01390	H	-0.10450	-1.75830	1.68640
H	1.36690	-1.84960	-5.17100	H	0.98510	-3.09750	0.49670
H	1.18180	-3.61130	-3.51390	C	-5.45060	-1.10670	5.04430
H	2.49800	-3.48640	-1.37140	H	-6.00600	-2.00550	5.32130
H	4.17530	0.27950	-2.70640	C	-1.48980	-7.40290	-0.72720
H	2.91030	0.13900	-4.74800	H	-0.48380	-7.76470	-0.93690
C	-3.07910	0.53460	-4.13350	C	-3.42320	-3.51340	1.41160
C	-1.84370	0.94140	-3.82450	H	-3.86980	-2.77870	0.29160
C	-1.62270	1.81580	-2.65460	H	-4.32780	-4.10850	1.49360
C	-2.65530	2.19480	-1.87860	O	-0.42440	-0.36040	-0.92870
C	-4.02530	1.75070	-2.24210	H	-2.13620	-0.75690	-0.51590
C	-4.22270	0.96290	-3.30640	C	-5.43260	-1.54620	-0.62580
H	-3.24240	-0.10930	-4.98790	H	-6.04650	-2.43720	-0.72970
H	-1.00180	0.62760	-4.42800	H	-5.66070	-0.85120	-1.44040
H	-0.61490	2.15020	-2.45600	H	-5.67260	-1.06590	0.32700
H	-4.88230	2.09420	-1.68390	C	-2.60890	-4.27370	-4.03360
H	-5.22420	0.65260	-3.57440	C	-3.67750	-4.70350	-3.25010

C	-4.09690	-3.95100	-2.14860	H	-4.21100	-5.62200	-3.47480
C	-3.46160	-2.72990	-1.83160	H	-1.80840	-1.43940	-2.35810
C	-2.35950	-2.33640	-2.61130	H	-1.10530	-2.74740	-4.30150
C	-1.94340	-3.09210	-3.70490	O	-5.13760	-4.41030	-1.37650
H	-2.29610	-4.86060	-4.89270	H	-4.79480	-5.14670	-0.82730
C	2.81010	2.20780	0.60930	P	0.58400	0.13220	0.04680
C	4.98470	0.58770	1.41450	O	0.04750	1.56680	0.68410
C	4.11790	0.12690	0.50050	O	0.83570	-0.76570	1.23800
C	2.94170	0.95680	0.12520	N	-3.12090	-0.73590	-0.18320
H	5.83830	-0.01050	1.71100	H	-3.32550	-0.29340	0.69860
C	4.78720	1.91080	2.04000	C	-3.94610	-1.75470	-0.58220
C	3.74600	2.68950	1.66780	C	-2.23350	-4.38720	0.84180
C	3.53260	3.99000	2.35920	C	-0.97410	-3.85750	1.03150
C	4.38550	4.40080	3.30470	C	-1.84510	-2.20090	2.56750
C	5.53880	3.56040	3.67950	C	-3.12980	-2.69310	2.40220
C	5.72800	2.37760	3.08460	C	0.30670	-4.38210	0.46270
H	2.68170	4.61210	2.11550	H	0.57440	-5.33460	0.92750
H	4.22650	5.34750	3.80470	H	0.19550	-4.56110	-0.60620
H	6.22600	3.90040	4.44340	C	-1.37700	-1.13340	3.51550
H	6.57190	1.76240	3.37110	H	-0.59100	-0.54580	3.03340
C	-0.21510	4.92390	-0.82390	H	-0.94950	-1.60060	4.41050
C	1.76210	3.09500	0.03820	H	-2.19300	-0.49730	3.83750
C	0.44960	2.74040	0.08190	C	-4.30680	-2.35610	3.23440
C	-0.59010	3.73350	-0.33230	C	-2.42450	-5.60800	0.03800
H	-0.95070	5.64420	-1.15620	H	-5.09390	-6.98520	-1.18070
C	2.16040	4.38110	-0.61180	H	-3.51820	-6.87700	-2.03010
C	1.20820	5.25870	-0.99230	H	-5.66290	-2.33960	5.52440
C	1.58730	6.54680	-1.61920	H	-4.73430	-0.91730	6.10310
C	2.87430	6.83660	-1.83530	O	-3.73670	-5.80780	-0.25260
C	3.92130	5.86790	-1.46210	O	-1.54710	-6.36650	-0.33430
C	3.58850	4.70480	-0.89080	O	-5.45100	-2.64520	2.92300
H	0.82290	7.25770	-1.90750	O	-4.01280	-1.73140	4.39810
H	3.15020	7.77670	-2.29520	Si	4.42440	-1.54920	-0.26150
H	4.96000	6.09640	-1.66320	Si	-2.41750	3.32540	-0.27040
H	4.37390	4.00030	-0.65300	C	3.13040	-4.88530	2.78050
O	1.99090	0.46380	-0.72840	C	2.96290	-3.59610	3.09580

C	3.38210	-2.54100	2.15010	H	-4.04690	4.50460	-2.58390
C	3.92690	-2.86840	0.96470	H	-5.29260	6.55180	-2.82080
C	4.11280	-4.30170	0.62520	C	-3.69790	1.84160	3.99870
C	3.73550	-5.25510	1.48570	C	-2.48440	2.37010	3.80950
H	2.81980	-5.65880	3.47070	C	-2.06910	2.80870	2.46140
H	2.51470	-3.32220	4.04210	C	-2.89420	2.65720	1.40930
H	3.22660	-1.50910	2.43170	C	-4.24800	2.09080	1.63600
H	4.55010	-4.58290	-0.32470	C	-4.62140	1.69370	2.85840
H	3.86830	-6.29890	1.23250	H	-4.00430	1.52200	4.98610
C	9.02200	-1.71470	-1.19680	H	-1.80550	2.48360	4.64470
C	8.46820	-2.66390	-0.43450	H	-1.10560	3.28710	2.35430
C	7.02240	-2.62150	-0.13070	H	-4.95000	1.99430	0.82480
C	6.25020	-1.64250	-0.63490	H	-5.60680	1.27470	3.01580
C	6.87940	-0.57800	-1.45530	C	-3.38070	0.52000	-3.91350
C	8.19010	-0.61610	-1.72450	C	-4.36700	0.93000	-3.10920
H	10.08100	-1.74370	-1.41840	C	-4.06800	1.80190	-1.95460
H	9.07780	-3.46510	-0.03700	C	-2.80280	2.17230	-1.68950
H	6.61460	-3.38850	0.50920	C	-1.71970	1.73750	-2.60810
H	6.29360	0.25460	-1.81580	C	-1.99300	0.94440	-3.65130
H	8.64610	0.16680	-2.31670	H	-3.59810	-0.11910	-4.75920
C	1.93550	-1.90650	-4.23180	H	-5.38710	0.62460	-3.30250
C	1.81410	-2.84210	-3.28470	H	-4.89280	2.16610	-1.36230
C	2.60660	-2.74660	-2.04280	H	-0.69850	2.05270	-2.44640
C	3.46530	-1.72940	-1.85660	H	-1.19790	0.61960	-4.31010
C	3.60090	-0.70020	-2.91860	N	-0.84540	-2.73770	1.80870
C	2.87160	-0.78210	-4.03860	H	-0.00270	-2.12750	1.67250
H	1.34900	-1.97130	-5.13910	H	1.10180	-3.65670	0.63590
H	1.13270	-3.67110	-3.42200	C	-5.14490	-1.42410	5.23030
H	2.46770	-3.50820	-1.29540	H	-5.84850	-0.77560	4.70350
H	4.25370	0.14850	-2.77940	C	-4.01120	-6.96290	-1.05880
H	2.95900	-0.01870	-4.80080	H	-3.66030	-7.87190	-0.56440
C	-4.84130	7.30420	-0.77890	C	-3.37830	-3.61420	1.29810
C	-4.19780	7.04800	0.36580	H	-3.69340	-2.81400	0.23580
C	-3.43610	5.79170	0.52180	H	-4.33110	-4.13370	1.34070
C	-3.39490	4.89550	-0.47880	O	-0.38120	-0.31620	-1.03140
C	-4.09760	5.19280	-1.75170	H	-2.15600	-0.63480	-0.50610
C	-4.78460	6.33350	-1.89040	C	-5.39700	-1.50350	-0.18300
H	-5.39890	8.22450	-0.89520	H	-6.00960	-2.39980	-0.28720
H	-4.23320	7.76010	1.18010	H	-5.81570	-0.70420	-0.80330
H	-2.91500	5.60840	1.45320	H	-5.45080	-1.19300	0.86170

C	-3.31750	-3.29760	-4.57740	H	-3.16330	-3.66270	-5.58870
C	-2.22870	-3.12560	-3.72920	H	-1.22170	-3.36090	-4.05460
C	-2.39110	-2.65320	-2.42040	H	-5.78010	-2.29570	-2.49060
C	-3.69140	-2.32950	-1.95160	H	-5.46390	-3.13780	-4.76670
C	-4.77690	-2.53380	-2.82250	O	-1.29840	-2.61830	-1.61270
C	-4.60250	-3.00650	-4.11950	H	-0.86140	-1.71690	-1.51180
C	2.73800	2.29480	0.66290	O	-0.03420	1.66040	0.65270
C	4.91250	0.68640	1.49010	O	0.83580	-0.59700	1.33770
C	4.07250	0.23160	0.54850	N	-3.11620	-0.88590	-0.35670
C	2.89080	1.05090	0.16650	H	-3.54360	-0.13670	0.15950
H	5.77010	0.09610	1.79100	C	-3.89680	-1.96160	-0.69700
C	4.68160	1.99340	2.13760	C	-2.17650	-4.21890	0.96710
C	3.64140	2.76730	1.75310	C	-0.96510	-3.54630	1.08470
C	3.39390	4.05130	2.46350	C	-1.96560	-1.91310	2.55640
C	4.21640	4.45300	3.43950	C	-3.21100	-2.49800	2.41200
C	5.36940	3.61870	3.82850	C	0.34510	-3.93060	0.46300
C	5.58880	2.45040	3.21560	H	0.77790	-4.79400	0.97570
H	2.54230	4.66810	2.20880	H	0.20630	-4.21020	-0.58130
H	4.03280	5.38780	3.95340	C	-1.58210	-0.76280	3.44180
H	6.03200	3.95130	4.61710	H	-0.97660	-0.05150	2.87280
H	6.43220	1.83940	3.51240	H	-0.95100	-1.13140	4.25900
C	-0.24260	5.01290	-0.86330	H	-2.45010	-0.28270	3.87600
C	1.70730	3.18620	0.06810	C	-4.45820	-2.10830	3.11700
C	0.39550	2.82740	0.05750	C	-2.35680	-5.54420	0.35840
C	-0.62860	3.81160	-0.40920	H	-1.91000	-8.14450	0.04870
H	-0.96760	5.72770	-1.22870	H	-1.91300	-7.34910	-1.54420
C	2.12470	4.48370	-0.54840	H	-5.15300	-0.58890	5.88820
C	1.18390	5.36250	-0.95490	H	-6.12160	-0.48640	4.38020
C	1.58100	6.66410	-1.54170	O	-1.21360	-6.17350	0.03050
C	2.87390	6.96550	-1.69680	O	-3.45410	-6.07680	0.19250
C	3.91030	5.99580	-1.29790	O	-5.56590	-2.38560	2.69140
C	3.56120	4.82040	-0.76260	O	-4.27230	-1.46250	4.28980
H	0.82490	7.37560	-1.84990	Si	4.43170	-1.41700	-0.25210
H	3.16300	7.91570	-2.12690	Si	-2.44450	3.36060	-0.47920
H	4.95500	6.23330	-1.45180	C	3.22000	-4.86800	2.69040
H	4.34070	4.11580	-0.50710	C	3.00750	-3.59350	3.03700
O	1.95030	0.54920	-0.69430	C	3.39560	-2.50130	2.12060
P	0.53810	0.20730	0.07550	C	3.95600	-2.78050	0.93030

C	4.19180	-4.19720	0.55590	C	-4.90970	7.27180	-1.23680
C	3.84220	-5.18430	1.38950	C	-4.79320	6.36770	-2.21650
H	2.93340	-5.66880	3.35960	C	-4.02050	5.12770	-1.99340
H	2.54730	-3.35900	3.98810	C	-3.44040	4.89840	-0.80280
H	3.20820	-1.48250	2.42880	C	-3.56470	5.90910	0.27510
H	4.64790	-4.43860	-0.39620	C	-4.26280	7.03240	0.06890
H	4.01310	-6.21620	1.11150	H	-5.47440	8.18060	-1.39980
C	9.05580	-1.50300	-1.06660	H	-5.26250	6.54330	-3.17590
C	8.29770	-0.53670	-1.59540	H	-3.92180	4.42710	-2.81050
C	6.84300	-0.51150	-1.33750	H	-3.08870	5.74470	1.23370
C	6.26690	-1.46790	-0.58850	H	-4.35260	7.76880	0.85690
C	7.12110	-2.52160	0.01660	C	-4.01480	2.04190	3.74290
C	8.43960	-2.53910	-0.21540	C	-2.78660	2.55480	3.61650
H	10.12180	-1.52190	-1.25270	C	-2.27500	2.93190	2.28330
H	8.74800	0.23090	-2.21140	C	-3.02780	2.74250	1.18410
H	6.26360	0.30280	-1.74640	C	-4.39670	2.19040	1.33910
H	6.69790	-3.27300	0.66590	C	-4.85770	1.84890	2.54820
H	9.05940	-3.30630	0.23050	H	-4.39240	1.76980	4.71970
C	1.98050	-1.76520	-4.24760	H	-2.16680	2.70120	4.49150
C	2.80280	-0.72880	-4.05350	H	-1.30350	3.40220	2.22470
C	3.59810	-0.63590	-2.81140	H	-5.04210	2.06860	0.48540
C	3.50220	-1.58880	-1.86650	H	-5.85620	1.44530	2.65410
C	2.59910	-2.74320	-2.10090	N	-0.91760	-2.41320	1.83220
C	1.87800	-2.82370	-3.22520	H	-0.08210	-1.74110	1.69400
H	1.39100	-1.83080	-5.15290	H	1.03150	-3.08670	0.52870
H	2.87790	0.05150	-4.79970	C	-5.47960	-1.12040	4.99500
H	4.20870	0.24160	-2.65890	H	-6.03140	-2.02380	5.26410
H	2.51010	-3.53140	-1.37260	C	-1.36850	-7.45610	-0.60340
H	1.22130	-3.66840	-3.38800	H	-0.35510	-7.81250	-0.78490
C	-3.10050	0.47320	-4.13000	C	-3.37660	-3.54120	1.41900
C	-1.86780	0.88520	-3.81690	H	-3.81780	-2.82720	0.28130
C	-1.65580	1.77010	-2.65330	H	-4.27620	-4.14380	1.49960
C	-2.69390	2.15330	-1.88710	O	-0.39970	-0.37690	-0.94100
C	-4.06110	1.70780	-2.25810	H	-2.10850	-0.79350	-0.54360
C	-4.25050	0.91040	-3.31670	C	-5.39190	-1.63470	-0.66750
H	-3.25700	-0.17950	-4.97900	H	-5.99110	-2.53710	-0.75780
H	-1.02120	0.56620	-4.41130	H	-5.62460	-0.96060	-1.49810
H	-0.64960	2.10620	-2.44970	H	-5.64690	-1.13890	0.27330
H	-4.92180	2.06080	-1.71180	C	-2.49810	-4.37550	-4.00490
H	-5.25030	0.60000	-3.59110	C	-3.56350	-4.81060	-3.21990

C	-4.00460	-4.04490	-2.13610	H	-4.07800	-5.74320	-3.43030
C	-3.39320	-2.80700	-1.83770	H	-1.76090	-1.49610	-2.37810
C	-2.29410	-2.40730	-2.61840	H	-1.02300	-2.82580	-4.29410
C	-1.85770	-3.17500	-3.69550	O	-5.04370	-4.50620	-1.36330
H	-2.16860	-4.97280	-4.85040	H	-4.69620	-5.23120	-0.80190

C	2.80290	2.20110	0.61640	H	6.18590	3.88840	4.48190
C	4.97290	0.58200	1.43480	H	6.54240	1.75310	3.40780
C	4.11360	0.12220	0.51320	C	-0.19530	4.92630	-0.85680
C	2.93800	0.95040	0.13250	C	1.76450	3.09140	0.03270
H	5.82670	-0.01450	1.73420	C	0.45050	2.74080	0.05860
C	4.76830	1.90260	2.06290	C	-0.58010	3.73560	-0.37390
C	3.72930	2.68110	1.68400	H	-0.92410	5.64860	-1.19930
C	3.50880	3.97970	2.37660	C	2.17540	4.37740	-0.61030
C	4.35380	4.38930	3.32980	C	1.23100	5.25840	-1.00220
C	5.50500	3.54940	3.71190	C	1.62240	6.54750	-1.61950
C	5.70020	2.36810	3.11600	C	2.91300	6.83480	-1.81590
H	2.65910	4.60130	2.12730	C	3.95200	5.86230	-1.43100
H	4.18990	5.33480	3.83050	C	3.60820	4.69820	-0.86840

H	0.86390	7.26120	-1.91660	H	2.87330	-5.69120	3.45360
H	3.19780	7.77580	-2.26860	H	2.54600	-3.36080	4.03780
H	4.99410	6.08860	-1.61670	H	3.23440	-1.53220	2.43450
H	4.38850	3.99080	-0.62250	H	4.58320	-4.57800	-0.34040
O	1.99070	0.45580	-0.72420	H	3.92070	-6.30900	1.20860
P	0.57960	0.12990	0.04620	C	9.03550	-1.66550	-1.19020
O	0.03460	1.57160	0.66030	C	8.48840	-2.62850	-0.44050
O	0.82690	-0.75100	1.25140	C	7.04230	-2.60070	-0.13680
N	-3.13730	-0.74070	-0.21440	C	6.26290	-1.62130	-0.62880
H	-3.36230	-0.26860	0.64680	C	6.88470	-0.54110	-1.43470
C	-3.95550	-1.76870	-0.60350	C	8.19570	-0.56600	-1.70370
C	-2.25710	-4.36780	0.90670	H	10.09460	-1.68400	-1.41210
C	-1.00110	-3.82990	1.09680	H	9.10370	-3.43040	-0.05360
C	-1.89460	-2.13430	2.57600	H	6.63980	-3.37930	0.49240
C	-3.17640	-2.63370	2.40850	H	6.29290	0.29230	-1.78480
C	0.28820	-4.36750	0.56020	H	8.64620	0.22790	-2.28530
H	0.56480	-5.29150	1.07530	C	1.92570	-1.94350	-4.20940
H	0.18400	-4.60450	-0.49770	C	2.78770	-0.93170	-4.06150
C	-1.44140	-1.03980	3.49970	C	3.60090	-0.82430	-2.83200
H	-0.65490	-0.45940	3.00980	C	3.47940	-1.73760	-1.85210
H	-1.01820	-1.48040	4.41010	C	2.52970	-2.86330	-2.03350
H	-2.26470	-0.40170	3.79820	C	1.79680	-2.95990	-3.14820
C	-4.36480	-2.27740	3.21590	H	1.32330	-2.02000	-5.10530
C	-2.43540	-5.61580	0.14310	H	2.88310	-0.18230	-4.83650
H	-5.08710	-7.05400	-1.04300	H	4.25050	0.03070	-2.71960
H	-3.50400	-6.97100	-1.88180	H	2.41720	-3.61800	-1.27420
H	-5.75360	-2.20390	5.48470	H	1.11120	-3.78710	-3.27370
H	-4.83680	-0.76450	6.03900	C	-4.80240	7.31860	-0.88860
O	-3.74420	-5.83390	-0.14970	C	-4.77280	6.42820	-1.88720
O	-1.55110	-6.38210	-0.19570	C	-4.02460	5.16320	-1.73100
O	-5.50420	-2.57740	2.89690	C	-3.38010	4.89720	-0.58180
O	-4.08850	-1.62130	4.36670	C	-3.40840	5.89270	0.51680
Si	4.43550	-1.54740	-0.25710	C	-4.08430	7.03880	0.37100
Si	-2.40820	3.32830	-0.34360	H	-5.34870	8.24590	-1.00270
C	3.17400	-4.91100	2.76650	H	-5.29430	6.63350	-2.81310
C	2.99410	-3.62520	3.08890	H	-3.99600	4.47470	-2.56360
C	3.40000	-2.56100	2.14740	H	-2.87950	5.69880	1.44150
C	3.94700	-2.87700	0.95990	H	-4.10370	7.76410	1.17410
C	4.14550	-4.30630	0.61210	C	-3.76830	1.93750	3.93100
C	3.77880	-5.26790	1.46790	C	-2.54480	2.44550	3.75010



C	-2.10310	2.85120	2.40020	H	-5.93080	-0.66290	4.62010
C	-2.91450	2.69080	1.33870	C	-4.00560	-7.02110	-0.91250
C	-4.27870	2.14620	1.55540	H	-3.65480	-7.90820	-0.37950
C	-4.67620	1.77890	2.77970	C	-3.40910	-3.58430	1.32620
H	-4.09420	1.64270	4.91980	H	-3.71150	-2.81130	0.24070
H	-1.87730	2.56670	4.59330	H	-4.36130	-4.10470	1.37070
H	-1.13220	3.31550	2.29960	O	-0.37890	-0.33640	-1.03020
H	-4.97050	2.04540	0.73590	H	-2.16760	-0.64500	-0.52380
H	-5.66990	1.37750	2.93030	C	-5.41220	-1.51190	-0.23010
C	-3.29050	0.45570	-3.95670	H	-6.02140	-2.41150	-0.32470
C	-4.29270	0.86850	-3.17380	H	-5.82340	-0.72670	-0.87310
C	-4.01990	1.76200	-2.02910	H	-5.48170	-1.18030	0.80700
C	-2.76260	2.15030	-1.75170	C	-3.26970	-3.38520	-4.55950
C	-1.66200	1.71340	-2.64850	C	-2.19300	-3.19530	-3.69980
C	-1.91150	0.90040	-3.68220	C	-2.37440	-2.70030	-2.40180
H	-3.48870	-0.19990	-4.79450	C	-3.68160	-2.37110	-1.95720
H	-5.30660	0.54900	-3.37670	C	-4.75480	-2.59360	-2.83890
H	-4.85680	2.12430	-1.45330	C	-4.56150	-3.08930	-4.12460
H	-0.64660	2.04240	-2.47780	H	-3.10060	-3.76810	-5.56180
H	-1.10350	0.57420	-4.32440	H	-1.18170	-3.43390	-4.00830
N	-0.88450	-2.68880	1.84440	H	-5.76310	-2.35250	-2.52520
H	-0.03780	-2.08340	1.70610	H	-5.41370	-3.23500	-4.78090
H	1.07470	-3.62520	0.69900	O	-1.29440	-2.64840	-1.57800
C	-5.23330	-1.29520	5.17410	H	-0.85600	-1.74630	-1.49240
C	2.92220	2.04250	0.69520	H	6.33660	3.39380	4.66370
C	5.00940	0.29010	1.45520	H	6.61070	1.29840	3.49140
C	4.13780	-0.08880	0.50880	C	0.05410	4.95700	-0.67610
C	3.01000	0.81250	0.15200	C	1.92560	3.00180	0.14750
H	5.83010	-0.35970	1.73570	C	0.59680	2.70500	0.14120
C	4.85860	1.58950	2.14090	C	-0.38610	3.76100	-0.25790
C	3.85830	2.43020	1.79150	H	-0.63910	5.72370	-0.99490
C	3.68750	3.70280	2.54380	C	2.39670	4.29910	-0.42860
C	4.53980	4.02900	3.52230	C	1.49450	5.23670	-0.78700
C	5.64950	3.12210	3.87280	C	1.94620	6.53670	-1.33690
C	5.79920	1.96310	3.22240	C	3.24980	6.77880	-1.50650
H	2.86810	4.37210	2.31800	C	4.24290	5.74600	-1.15970
H	4.41190	4.95580	4.06670	C	3.84460	4.57160	-0.65770

H	1.22150	7.29510	-1.60640	H	2.68220	-5.88140	3.33170
H	3.57860	7.72770	-1.91000	H	3.59850	-6.47670	1.16690
H	5.29550	5.93680	-1.32470	H	4.34720	-4.66680	-0.44730
H	4.59210	3.82100	-0.43990	H	3.20480	-1.69470	2.49630
O	2.04720	0.39940	-0.72900	H	2.48130	-3.42630	4.00080
P	0.63010	0.08740	0.03250	C	8.95040	-1.97760	-1.36790
O	0.12050	1.52750	0.68000	C	8.37770	-2.97400	-0.68380
O	0.85300	-0.82920	1.21450	C	6.94050	-2.91130	-0.34460
N	-3.05290	-0.54170	-0.13290	C	6.19430	-1.86430	-0.73930
H	-3.18970	-0.09450	0.76020	C	6.84550	-0.74980	-1.47180
C	-3.96630	-1.48820	-0.51180	C	8.14840	-0.80700	-1.77300
C	-2.42410	-4.23220	0.89710	H	10.00300	-2.02190	-1.61560
C	-1.13280	-3.77970	1.07320	H	8.96580	-3.82910	-0.37620
C	-1.88730	-2.08290	2.62550	H	6.51780	-3.72200	0.22770
C	-3.20450	-2.48990	2.47070	H	6.28270	0.13330	-1.73850
C	0.10980	-4.37860	0.49230	H	8.62080	0.01200	-2.29990
H	0.32860	-5.34200	0.96080	C	1.79910	-1.87280	-4.25000
H	-0.02300	-4.55780	-0.57410	C	1.62290	-2.80400	-3.30730
C	-1.35050	-1.05820	3.58200	C	2.44290	-2.78070	-2.07990
H	-0.65790	-0.39960	3.04840	C	3.38330	-1.83610	-1.90430
H	-0.77360	-1.56500	4.36470	C	3.58040	-0.81310	-2.96260
H	-2.14790	-0.50350	4.06260	C	2.82520	-0.82780	-4.06820
C	-4.27480	-2.02580	3.38280	H	1.19210	-1.88390	-5.14600
C	-2.69690	-5.44020	0.09880	H	0.87650	-3.57590	-3.43680
H	-3.88710	-6.64710	-1.95150	H	2.25300	-3.53110	-1.33190
H	-4.06820	-7.63130	-0.48290	H	4.30530	-0.02370	-2.83400
H	-6.66300	-0.97510	3.89620	H	2.95970	-0.06900	-4.82820
H	-7.48790	-2.46980	3.34230	C	-4.49960	7.48420	-0.85680
O	-4.02350	-5.56570	-0.17320	C	-3.91260	7.19850	0.31110
O	-1.87090	-6.24910	-0.28430	C	-3.19820	5.91710	0.48660
O	-4.13650	-1.37120	4.40070	C	-3.14280	5.02890	-0.52030
O	-5.50140	-2.44050	2.96300	C	-3.78360	5.35770	-1.81770
Si	4.37920	-1.74110	-0.32410	C	-4.42810	6.52080	-1.97380
Si	-2.22990	3.42470	-0.28460	H	-5.02280	8.42270	-0.98720
C	3.01140	-5.10860	2.64930	H	-3.95940	7.90470	1.12990
C	3.51730	-5.43680	1.45520	H	-2.72370	5.70860	1.43750
C	3.95800	-4.37970	0.52170	H	-3.72230	4.67350	-2.65250
C	3.86030	-3.08370	0.86670	H	-4.89150	6.76200	-2.92180
C	3.30180	-2.72860	2.19610	C	-3.75260	1.88990	3.88680
C	2.89670	-3.68870	3.03640	C	-2.49430	2.32100	3.75180

C	-2.00670	2.78500	2.43710	C	-4.37260	-6.70400	-0.97440
C	-2.81360	2.75670	1.36090	H	-5.45630	-6.66520	-1.08390
C	-4.22070	2.31310	1.53160	C	-3.51720	-3.39110	1.36460
C	-4.65820	1.88800	2.72300	H	-3.78480	-2.56860	0.30880
H	-4.11090	1.54880	4.84940	H	-4.49260	-3.86440	1.40320
H	-1.82950	2.33120	4.60580	O	-0.34010	-0.32580	-1.05600
H	-1.00120	3.17590	2.37560	H	-2.09490	-0.50780	-0.49100
H	-4.91150	2.33510	0.70530	C	-5.38090	-1.11600	-0.08020
H	-5.68210	1.55660	2.83960	H	-6.06820	-1.95950	-0.15720
C	-3.13020	0.66510	-3.98040	H	-5.74930	-0.29020	-0.69770
C	-4.13410	1.09630	-3.20980	H	-5.37550	-0.78370	0.95980
C	-3.85540	1.95560	-2.04100	C	-3.57210	-3.13570	-4.49420
C	-2.59240	2.29730	-1.73110	C	-2.45040	-3.03860	-3.67800
C	-1.48900	1.84570	-2.61710	C	-2.53580	-2.52700	-2.37630
C	-1.74360	1.06130	-3.67160	C	-3.79310	-2.09070	-1.88050
H	-3.33270	0.03130	-4.83390	C	-4.91460	-2.21830	-2.72060
H	-5.15370	0.81440	-3.43850	C	-4.81540	-2.72690	-4.01160
H	-4.69160	2.32910	-1.47210	H	-3.47600	-3.53240	-5.50080
H	-0.46750	2.13990	-2.42150	H	-1.47610	-3.36390	-4.02410
H	-0.93400	0.72290	-4.30540	H	-5.88550	-1.89070	-2.36930
N	-0.93040	-2.67370	1.85320	H	-5.70150	-2.79590	-4.63460
H	-0.05330	-2.11480	1.70990	O	-1.42010	-2.56610	-1.60270
H	0.94700	-3.69870	0.65230	H	-0.92520	-1.69430	-1.50640
C	-6.59460	-2.06270	3.81520				
H	-6.46450	-2.48080	4.81600				
C	2.63680	2.42780	0.66020	H	5.92330	4.26940	4.53670
C	4.90580	0.93580	1.44680	H	6.40620	2.17410	3.43370
C	4.07260	0.43160	0.52400	C	-0.47990	5.00570	-0.83740
C	2.83770	1.18760	0.17070	C	1.56050	3.27000	0.07390
H	5.79650	0.39880	1.73800	C	0.26550	2.85570	0.08510
C	4.62200	2.23230	2.09450	C	-0.80700	3.79150	-0.37140
C	3.53700	2.95080	1.72870	H	-1.23980	5.68480	-1.20000
C	3.23990	4.22480	2.43810	C	1.91260	4.58060	-0.55620
C	4.06100	4.67280	3.39490	C	0.92880	5.41600	-0.95210
C	5.26210	3.89950	3.76370	C	1.26060	6.72930	-1.55320
C	5.52710	2.74020	3.15160	C	2.53680	7.08440	-1.73140
H	2.35330	4.79660	2.19810	C	3.61980	6.16250	-1.34370
H	3.84120	5.60010	3.90820	C	3.32990	4.97680	-0.79590

H	0.47000	7.40590	-1.85350	H	3.21520	-5.55570	3.28150
H	2.77810	8.04310	-2.17240	H	2.62840	-3.28470	3.89790
H	4.65090	6.44330	-1.51620	H	3.19370	-1.35650	2.35860
H	4.14290	4.30770	-0.54950	H	4.93800	-4.18380	-0.42290
O	1.90680	0.63900	-0.67260	H	4.40780	-6.01050	1.06950
P	0.51470	0.24700	0.11060	C	9.10610	-1.54850	-1.00570
O	-0.10370	1.67600	0.69420	C	8.29380	-1.30530	-2.04040
O	0.84960	-0.54870	1.36820	C	6.83500	-1.19530	-1.82900
N	-3.09450	-0.99310	-0.27000	C	6.31710	-1.32400	-0.59490
H	-3.53780	-0.28170	0.28470	C	7.22380	-1.61310	0.54410
C	-3.84240	-2.08420	-0.63240	C	8.54410	-1.71500	0.34890
C	-1.99700	-4.30430	0.92820	H	10.17430	-1.62960	-1.15980
C	-0.81540	-3.58140	1.04620	H	8.70300	-1.18840	-3.03560
C	-1.86070	-2.04100	2.58620	H	6.20720	-1.00930	-2.68680
C	-3.08080	-2.67840	2.44540	H	6.82220	-1.75650	1.53930
C	0.49910	-3.88440	0.38920	H	9.20170	-1.92750	1.18190
H	0.35340	-4.14550	-0.65870	C	1.97510	-1.52910	-4.23910
H	1.14240	-3.00780	0.46180	C	2.77010	-0.47300	-4.03310
C	-1.51460	-0.90350	3.50350	C	3.59140	-0.39240	-2.80720
H	-0.88430	-0.18590	2.97120	C	3.54280	-1.37580	-1.89080
H	-0.92550	-1.28560	4.34580	C	2.67980	-2.55530	-2.14130
H	-2.40040	-0.42760	3.90590	C	1.93380	-2.62410	-3.25000
C	-4.32910	-2.36650	3.18570	H	1.36570	-1.58570	-5.13170
C	-2.13150	-5.61480	0.27650	H	2.80320	0.33130	-4.75650
H	-1.66180	-7.32720	-1.69950	H	4.19680	0.49000	-2.64020
H	-0.06080	-7.74270	-1.00470	H	2.64820	-3.37250	-1.43840
H	-6.03810	-0.83900	4.50540	H	1.30490	-3.48690	-3.42720
H	-5.85620	-2.38110	5.36720	C	-4.04940	1.82300	3.79780
O	-0.97000	-6.17870	-0.10150	C	-4.82730	1.63440	2.72740
O	-3.20780	-6.19080	0.11790	C	-4.36760	2.06800	1.39230
O	-5.43100	-2.69600	2.78300	C	-3.14530	2.60410	1.23180
O	-4.14780	-1.72510	4.36190	C	-2.29560	2.82500	2.43020
Si	4.48230	-1.20720	-0.28630	C	-2.72480	2.45430	3.64260
Si	-2.59830	3.25500	-0.43170	H	-4.38810	1.51530	4.77840
C	3.45470	-4.73360	2.61970	H	-5.80150	1.17620	2.83750
C	3.13140	-3.48050	2.95980	H	-5.04610	1.95950	0.56250
C	3.45670	-2.35960	2.05380	H	-1.33830	3.31980	2.34420
C	4.05980	-2.59530	0.87590	H	-2.10530	2.62410	4.51360
C	4.43160	-3.98380	0.51320	C	-3.07380	0.39380	-4.12780
C	4.14040	-4.99690	1.33830	C	-4.13080	0.66370	-3.35510

C	-3.98180	1.53720	-2.17270	H	-5.03230	-0.91370	5.99050
C	-2.77920	2.04180	-1.84410	C	-1.08380	-7.44290	-0.78000
C	-1.61020	1.73240	-2.70870	H	-1.57160	-8.18050	-0.13950
C	-1.75200	0.95430	-3.78850	C	-3.21810	-3.69890	1.42510
H	-3.18260	-0.24300	-4.99610	H	-3.71620	-2.97610	0.31940
H	-5.10140	0.25370	-3.60190	H	-4.08600	-4.34640	1.50570
H	-4.86920	1.79930	-1.61890	O	-0.41010	-0.37050	-0.89870
H	-0.63370	2.13820	-2.48610	H	-2.09510	-0.85590	-0.47440
H	-0.89660	0.72990	-4.41280	C	-5.34720	-1.81100	-0.57020
C	-5.28190	7.01050	-1.23990	H	-5.91690	-2.72880	-0.69270
C	-4.69250	6.84600	-0.05010	H	-5.61250	-1.10850	-1.36730
C	-3.84660	5.66070	0.19940	H	-5.60670	-1.36560	0.39440
C	-3.67270	4.73800	-0.76200	C	-2.41840	-4.33670	-4.04100
C	-4.31760	4.93320	-2.08410	C	-3.45220	-4.83660	-3.25210
C	-5.08180	6.00970	-2.30720	C	-3.89960	-4.12410	-2.13520
H	-5.90160	7.87850	-1.42450	C	-3.32880	-2.87450	-1.80740
H	-4.83390	7.58020	0.73250	C	-2.26000	-2.40870	-2.59330
H	-3.37360	5.54960	1.16740	C	-1.81560	-3.12460	-3.70240
H	-4.16460	4.22150	-2.88340	H	-2.08410	-4.89310	-4.91210
H	-5.54850	6.15370	-3.27310	H	-3.93680	-5.77990	-3.48440
N	-0.80430	-2.47180	1.83080	H	-1.75910	-1.48450	-2.33350
H	-0.00350	-1.75980	1.70050	H	-1.00480	-2.72570	-4.30300
H	0.98740	-4.73530	0.87250	O	-4.90470	-4.65020	-1.35840
C	-5.35350	-1.44950	5.09790	H	-4.51460	-5.37150	-0.82080
C	2.36120	2.68210	0.60270	H	5.40440	4.90750	4.47720
C	4.78240	1.46210	1.40640	H	6.12900	2.87860	3.38280
C	4.01630	0.86020	0.48400	C	-1.08080	4.85510	-0.81920
C	2.71100	1.47640	0.11120	C	1.17900	3.38090	0.03040
H	5.72080	1.02600	1.71460	C	-0.05300	2.80530	0.06040
C	4.35240	2.72420	2.04130	C	-1.24640	3.60980	-0.34900
C	3.19180	3.31000	1.67140	H	-1.92820	5.44250	-1.14620
C	2.74730	4.54320	2.37640	C	1.35200	4.72670	-0.59780
C	3.50930	5.08720	3.33230	C	0.26420	5.43350	-0.97070
C	4.79190	4.46060	3.70480	C	0.41810	6.77950	-1.57130
C	5.19070	3.33790	3.09740	C	1.63660	7.29150	-1.77120
H	1.80000	5.00670	2.13510	C	2.83340	6.51120	-1.40740
H	3.18200	5.98400	3.84250	C	2.70390	5.29720	-0.86020

H	-0.45630	7.35330	-1.85270	H	3.70490	-5.10520	3.40570
H	1.74810	8.27410	-2.21120	H	2.91730	-2.88010	3.96330
H	3.81800	6.91940	-1.59580	H	3.31260	-0.94940	2.37480
H	3.59810	4.73440	-0.62910	H	5.31330	-3.68050	-0.33010
O	1.86270	0.83510	-0.75210	H	4.94200	-5.50830	1.20830
P	0.52880	0.25870	0.00850	C	9.21290	-0.70430	-1.06490
O	-0.25140	1.57440	0.64940	C	8.74350	-0.82010	0.18200
O	0.92480	-0.58780	1.19800	C	7.28660	-0.83310	0.42640
N	-2.97770	-1.22830	-0.16190	C	6.42320	-0.71160	-0.59750
H	-3.24400	-0.81090	0.71560	C	6.95260	-0.60370	-1.98020
C	-3.63010	-2.37440	-0.53980	C	8.27360	-0.59610	-2.19850
C	-1.50680	-4.67350	0.87430	H	10.27990	-0.69630	-1.24620
C	-0.34870	-3.93940	1.02230	H	9.42940	-0.90730	1.01480
C	-1.44630	-2.43780	2.57920	H	6.93260	-0.95850	1.44180
C	-2.63700	-3.13290	2.44550	H	6.28440	-0.53770	-2.82530
C	0.99450	-4.22530	0.42090	H	8.65690	-0.51730	-3.20770
H	1.43820	-5.12020	0.86500	C	2.17120	-1.39140	-4.24630
H	0.89580	-4.39130	-0.65090	C	2.19990	-2.36150	-3.32570
C	-1.13770	-1.29940	3.50970	C	2.97960	-2.18280	-2.08460
H	-0.53010	-0.55970	2.98040	C	3.67330	-1.05170	-1.87540
H	-0.54730	-1.66940	4.35620	C	3.65270	0.01280	-2.91000
H	-2.03990	-0.85040	3.90800	C	2.93510	-0.14660	-4.02890
C	-3.84030	-2.97760	3.29550	H	1.59300	-1.51850	-5.15230
C	-1.64920	-5.93200	0.11570	H	1.64860	-3.27860	-3.48340
H	0.42200	-7.97390	-1.30420	H	2.96800	-2.97550	-1.35470
H	-1.08720	-8.46390	-0.46610	H	4.20020	0.93380	-2.75250
H	-5.16020	-3.20190	5.59440	H	2.91130	0.63680	-4.77530
H	-4.42880	-1.68010	6.20250	C	-6.06810	6.36200	-0.87530
O	-0.47580	-6.47390	-0.28700	C	-5.39760	6.23730	0.27580
O	-2.72770	-6.45080	-0.11560	C	-4.42410	5.13960	0.45050
O	-4.93700	-3.41340	2.98680	C	-4.21470	4.25580	-0.53990
O	-3.62040	-2.34680	4.47260	C	-4.95090	4.40810	-1.81940
Si	4.58720	-0.75490	-0.27620	C	-5.83050	5.40540	-1.97490
Si	-2.97480	2.88750	-0.30780	H	-6.78090	7.16600	-1.00530
C	3.87430	-4.28190	2.72410	H	-5.56610	6.94010	1.08150
C	3.44040	-3.05400	3.03190	H	-3.88600	5.06160	1.38710
C	3.66810	-1.93200	2.09770	H	-4.77280	3.73050	-2.64280
C	4.29440	-2.14310	0.92720	H	-6.36350	5.51850	-2.91010
C	4.78930	-3.50200	0.60070	C	-4.00210	1.18800	3.95090
C	4.58600	-4.51560	1.45120	C	-2.88630	1.90070	3.76590

C	-2.55010	2.41560	2.42300	H	-5.56630	-1.65870	4.81440
C	-3.34590	2.15120	1.37060	C	-0.59790	-7.68310	-1.05320
C	-4.59890	1.38630	1.59470	H	-1.18160	-7.50550	-1.95940
C	-4.90010	0.91900	2.81240	C	-2.75000	-4.09170	1.35490
H	-4.25080	0.81290	4.93490	H	-3.20790	-3.36410	0.28750
H	-2.22850	2.10570	4.60060	H	-3.59810	-4.76980	1.40310
H	-1.67130	3.03640	2.32080	O	-0.33680	-0.34700	-1.07610
H	-5.28670	1.20260	0.78630	H	-2.04740	-0.97620	-0.49910
H	-5.81090	0.35540	2.96810	C	-5.10010	-2.35430	-0.13170
C	-3.37130	-0.06150	-3.94430	H	-5.55770	-3.34100	-0.21160
C	-4.41990	0.15300	-3.14300	H	-5.64710	-1.64730	-0.76430
C	-4.29750	1.06970	-1.99090	H	-5.19710	-2.03500	0.90710
C	-3.12850	1.67890	-1.72520	C	-2.80220	-3.81660	-4.53710
C	-1.98080	1.46100	-2.64280	C	-1.74720	-3.44950	-3.70830
C	-2.09320	0.62630	-3.68330	C	-1.96890	-3.00650	-2.39810
H	-3.45900	-0.73430	-4.78730	C	-3.29750	-2.91260	-1.90810
H	-5.36110	-0.34510	-3.33600	C	-4.34340	-3.31350	-2.75890
H	-5.17760	1.26650	-1.39990	C	-4.11000	-3.75630	-4.05690
H	-1.04050	1.96930	-2.48210	H	-2.60290	-4.15450	-5.55000
H	-1.24930	0.46050	-4.34060	H	-0.72030	-3.50330	-4.05170
N	-0.39120	-2.80880	1.79590	H	-5.36690	-3.25920	-2.40930
H	0.33530	-2.06770	1.64110	H	-4.94540	-4.04560	-4.68650
H	1.65390	-3.37510	0.59320	O	-0.88550	-2.77530	-1.60820
C	-4.77540	-2.21720	5.32010	H	-0.59940	-1.81290	-1.53340
C	2.55950	2.43990	0.63400	H	5.70690	4.32150	4.60700
C	4.85500	1.00360	1.45160	H	6.27780	2.25950	3.48310
C	4.05560	0.49140	0.50410	C	-0.66830	4.90570	-0.81060
C	2.81780	1.22120	0.11980	C	1.44720	3.24260	0.06010
H	5.75370	0.47830	1.75300	C	0.17190	2.76850	0.06090
C	4.52060	2.28350	2.10810	C	-0.94360	3.67310	-0.35870
C	3.42090	2.97380	1.72990	H	-1.45870	5.56500	-1.14320
C	3.06970	4.22670	2.45220	C	1.74100	4.57770	-0.54600
C	3.85660	4.68470	3.43260	C	0.72160	5.37440	-0.93040
C	5.07380	3.94350	3.81470	C	0.99530	6.70980	-1.51140
C	5.38760	2.80270	3.19110	C	2.25490	7.12360	-1.68230
H	2.17050	4.77440	2.20310	C	3.37730	6.24520	-1.30520
H	3.59720	5.59630	3.95540	C	3.13950	5.04000	-0.77520

H	0.17590	7.35540	-1.80230	H	1.49930	-1.80030	-5.16830
H	2.45400	8.09850	-2.10820	H	2.92900	0.13850	-4.88640
H	4.39520	6.57450	-1.47010	H	4.26290	0.44110	-2.75910
H	3.98080	4.40460	-0.53410	H	2.66350	-3.32060	-1.32610
O	1.92970	0.66300	-0.76090	H	1.38930	-3.57710	-3.33720
P	0.55300	0.18110	-0.00960	C	3.59110	-4.65930	2.64660
O	-0.13830	1.54960	0.62760	C	3.30210	-3.40250	3.00250
O	0.88630	-0.69230	1.18110	C	3.60710	-2.28370	2.08650
N	-3.08470	-1.00890	-0.20540	C	4.17330	-2.52090	0.88970
H	-3.33260	-0.55910	0.66140	C	4.49210	-3.91850	0.50420
C	-3.81380	-2.11000	-0.57630	C	4.21540	-4.92960	1.33640
C	-1.90200	-4.54660	0.92810	H	3.36380	-5.47970	3.31480
C	-0.69000	-3.90590	1.07700	H	2.83870	-3.20210	3.95980
C	-1.68380	-2.27710	2.57310	H	3.35290	-1.28100	2.39970
C	-2.92530	-2.87670	2.43810	H	4.94380	-4.12720	-0.45760
C	0.63450	-4.31900	0.50990	H	4.44430	-5.94770	1.04940
H	0.99760	-5.23000	0.99300	C	9.12810	-0.78010	-1.20910
H	0.53690	-4.51730	-0.55640	C	8.67090	-1.82180	-0.50580
C	-1.29610	-1.14480	3.48110	C	7.22800	-1.94070	-0.20900
H	-0.60430	-0.48220	2.95350	C	6.36270	-1.01590	-0.66150
H	-0.77290	-1.54230	4.35870	C	6.88340	0.15170	-1.41550
H	-2.16310	-0.59980	3.83500	C	8.19150	0.25930	-1.67820
C	-4.11970	-2.61020	3.27240	H	10.18480	-0.69120	-1.42560
C	-2.13530	-5.81160	0.20410	H	9.35690	-2.58020	-0.15120
H	-0.21530	-8.07600	-1.08540	H	6.89770	-2.78080	0.38170
H	-1.78610	-8.39880	-0.27980	H	6.21760	0.94230	-1.73070
H	-5.45380	-2.70000	5.57490	H	8.56790	1.11650	-2.22150
H	-4.62520	-1.21600	6.15020	C	-5.51050	6.81430	-0.97130
O	-1.00390	-6.46580	-0.14960	C	-4.86730	6.64190	0.18920
O	-3.24910	-6.24260	-0.04040	C	-3.99140	5.46790	0.38290
O	-5.24470	-2.96620	2.96330	C	-3.84400	4.56330	-0.59990
O	-3.85920	-1.97470	4.43870	C	-4.54860	4.76770	-1.88970
Si	4.53610	-1.12500	-0.29650	C	-5.34000	5.83370	-2.06230
Si	-2.72610	3.09810	-0.34500	H	-6.15180	7.67420	-1.11520
C	2.08740	-1.68360	-4.26720	H	-4.98640	7.36180	0.98860
C	2.87760	-0.61580	-4.11200	H	-3.47350	5.35120	1.32690
C	3.67150	-0.45430	-2.87580	H	-4.41700	4.07170	-2.70650
C	3.60550	-1.37550	-1.89800	H	-5.85000	5.98450	-3.00500
C	2.73390	-2.56160	-2.08630	C	-3.91500	1.55870	3.92750
C	2.01790	-2.70660	-3.20680	C	-4.73120	1.34290	2.89090



C	-4.35410	1.81110	1.54160	H	-5.75690	-1.15270	4.75850
C	-3.16940	2.41100	1.33380	C	-1.21190	-7.68680	-0.87750
C	-2.27530	2.65730	2.49430	H	-1.75070	-7.49230	-1.80760
C	-2.62960	2.25290	3.72000	C	-3.10080	-3.84950	1.36780
H	-4.19310	1.22500	4.91850	H	-3.47570	-3.11570	0.27520
H	-5.67540	0.83550	3.03920	H	-4.00310	-4.45340	1.41830
H	-5.05830	1.66810	0.73940	O	-0.34900	-0.35980	-1.09860
H	-1.34550	3.19450	2.37000	H	-2.13200	-0.83730	-0.52930
H	-1.97790	2.44050	4.56350	C	-5.28370	-1.97940	-0.19010
C	-3.38810	0.14070	-3.93690	H	-5.80940	-2.93180	-0.26840
C	-2.17100	0.63750	-3.69620	H	-5.77040	-1.24210	-0.83680
C	-1.96190	1.57150	-2.57090	H	-5.37200	-1.64340	0.84430
C	-2.97940	1.89350	-1.75220	C	-3.02430	-3.63870	-4.54730
C	-4.33320	1.35740	-2.04560	C	-1.96060	-3.35430	-3.69740
C	-4.52360	0.52670	-3.07790	C	-2.17390	-2.89160	-2.39270
H	-3.54400	-0.54020	-4.76330	C	-3.50050	-2.68900	-1.93190
H	-1.33590	0.35750	-4.32530	C	-4.55770	-3.00840	-2.80270
H	-0.97150	1.97840	-2.42470	C	-4.33290	-3.47380	-4.09450
H	-5.18630	1.66550	-1.46080	H	-2.83140	-3.99400	-5.55550
H	-5.51320	0.14460	-3.29260	H	-0.93480	-3.49070	-4.02040
N	-0.65170	-2.75270	1.81690	H	-5.58060	-2.86970	-2.47530
H	0.13690	-2.07850	1.65380	H	-5.17500	-3.69780	-4.74150
H	1.35800	-3.51830	0.66360	O	-1.09570	-2.74230	-1.57660
C	-5.00470	-1.74930	5.27920	H	-0.72260	-1.80810	-1.52170
C	2.89820	2.06050	0.82020	H	6.53840	1.13850	3.62660
C	4.97250	0.26140	1.50370	C	0.09910	5.05820	-0.52890
C	4.11340	-0.05980	0.52520	C	1.92420	3.05920	0.30190
C	2.99110	0.86330	0.20780	C	0.59440	2.77360	0.22520
H	5.78860	-0.40550	1.75620	C	-0.36090	3.84100	-0.20620
C	4.81000	1.51540	2.26690	H	-0.57260	5.83370	-0.87010
C	3.81520	2.37710	1.95460	C	2.42460	4.38440	-0.18250
C	3.62970	3.59880	2.78350	C	1.54190	5.34470	-0.53060
C	4.46460	3.86190	3.79550	C	2.02040	6.67290	-0.98130
C	5.56900	2.93440	4.10660	C	3.33050	6.92020	-1.07370
C	5.73120	1.81920	3.38630	C	4.30480	5.86480	-0.74330
H	2.81360	4.28110	2.58600	C	3.88210	4.66450	-0.33060
H	4.32630	4.75220	4.39540	H	1.31000	7.44810	-1.24110
H	6.24190	3.15510	4.92510	H	3.67890	7.88990	-1.40500

H	5.36410	6.06020	-0.84990	H	6.23490	0.12120	-1.75330
H	4.61870	3.89940	-0.12790	H	6.55700	-3.72900	0.21430
O	2.02330	0.49070	-0.68650	H	8.89710	-3.82710	-0.31250
P	0.61130	0.14510	0.07730	C	1.71110	-1.61940	-4.27910
O	0.07710	1.58980	0.70940	C	2.64750	-0.68230	-4.09700
O	0.90320	-0.71840	1.30110	C	3.50980	-0.71870	-2.89700
N	-3.04640	-0.62330	-0.20180	C	3.36010	-1.69010	-1.97830
H	-3.34030	0.14210	0.37920	C	2.33140	-2.73700	-2.20250
C	-3.96930	-1.58020	-0.52700	C	1.55070	-2.70020	-3.28830
C	-2.43130	-4.02320	1.03090	H	1.07130	-1.58810	-5.15150
C	-1.15340	-3.48170	1.11240	H	2.76550	0.11450	-4.81990
C	-1.92230	-1.79650	2.65960	H	4.21600	0.08440	-2.74990
C	-3.22930	-2.24100	2.55140	H	2.19450	-3.53800	-1.49570
C	0.08960	-3.98460	0.43780	H	0.80260	-3.46660	-3.44270
H	0.44830	-4.89670	0.92270	C	3.04680	-5.20480	2.38820
H	-0.10810	-4.22830	-0.60600	C	3.54610	-5.45920	1.17340
C	-1.39890	-0.71760	3.56190	C	3.96830	-4.34620	0.29840
H	-0.85020	0.01900	2.96630	C	3.85640	-3.07320	0.71570
H	-0.67460	-1.15460	4.25840	C	3.30500	-2.79980	2.06700
H	-2.19510	-0.25810	4.13620	C	2.91850	-3.81040	2.85530
C	-4.31850	-1.69270	3.39760	H	2.73270	-6.01870	3.02860
C	-2.77130	-5.30760	0.40520	H	3.63780	-6.48030	0.82680
H	-1.06280	-7.74210	-0.86460	H	4.36080	-4.57360	-0.68510
H	-2.59900	-7.93710	0.04290	H	3.19970	-1.78580	2.42620
H	-6.62510	-0.42250	3.73010	H	2.50880	-3.60770	3.83630
H	-7.54150	-1.81970	3.07430	C	-4.46560	7.42150	-1.50570
O	-1.71410	-6.04350	0.01770	C	-4.00180	7.21730	-0.26740
O	-3.92420	-5.72110	0.27550	C	-3.28010	5.96940	0.05640
O	-4.19560	-1.06800	4.43480	C	-3.09010	5.03240	-0.88800
O	-5.53560	-1.98440	2.87160	C	-3.59940	5.26820	-2.26150
Si	4.36310	-1.66380	-0.39820	C	-4.25220	6.40060	-2.55140
Si	-2.17930	3.46630	-0.46490	H	-4.99410	8.33520	-1.74470
C	8.94710	-1.88820	-1.39500	H	-4.15430	7.96510	0.50010
C	8.22470	-0.83120	-1.78090	H	-2.90950	5.82470	1.06380
C	6.78280	-0.76410	-1.46550	H	-3.43790	4.53830	-3.04270
C	6.18120	-1.77100	-0.80810	H	-4.62030	6.57380	-3.55440
C	6.99750	-2.92820	-0.35970	C	-4.24140	2.06820	3.51530
C	8.30480	-2.98370	-0.64340	C	-2.94430	2.39200	3.51600
H	10.00390	-1.93810	-1.62340	C	-2.28310	2.80990	2.26300
H	8.69500	-0.02060	-2.32250	C	-2.97420	2.85400	1.11010

C	-4.42680	2.54580	1.13200	C	-2.02590	-7.29210	-0.62640
C	-5.02020	2.15530	2.26620	H	-2.60370	-7.11490	-1.53620
H	-4.72650	1.76090	4.43260	C	-3.54170	-3.24040	1.54640
H	-2.37440	2.34750	4.43500	H	-3.95700	-2.47750	0.44140
H	-1.24590	3.10740	2.30930	H	-4.48220	-3.77030	1.65790
H	-5.02770	2.66100	0.24430	O	-0.35580	-0.37150	-0.94860
H	-6.07880	1.92970	2.27610	H	-2.04740	-0.64250	-0.45390
C	-2.57290	0.68140	-4.23230	C	-5.40900	-1.07160	-0.43010
C	-1.37020	1.12120	-3.84890	H	-5.58870	-0.36260	-1.24510
C	-1.24110	1.97100	-2.64750	H	-5.55870	-0.55370	0.52170
C	-2.32370	2.28600	-1.91110	H	-6.11950	-1.89160	-0.50290
C	-3.65390	1.79190	-2.34780	C	-3.03590	-4.05200	-3.95030
C	-3.76950	1.03150	-3.44360	C	-4.09840	-4.38660	-3.11350
H	-2.66990	0.06010	-5.11310	C	-4.39010	-3.60430	-1.99210
H	-0.48890	0.86090	-4.42090	C	-3.62650	-2.45170	-1.70540
H	-0.25940	2.34590	-2.39760	C	-2.53480	-2.15510	-2.54030
H	-4.54630	2.06370	-1.80950	C	-2.24830	-2.93850	-3.65560
H	-4.74260	0.67850	-3.75960	H	-2.82330	-4.66010	-4.82500
N	-0.96040	-2.37970	1.88300	H	-4.72480	-5.25100	-3.31120
H	-0.07440	-1.78210	1.71330	H	-1.89380	-1.31130	-2.31530
H	0.86000	-3.21580	0.49550	H	-1.41580	-2.66790	-4.29670
C	-6.65910	-1.51020	3.63300	O	-5.42960	-3.96700	-1.16700
H	-6.65980	-1.95180	4.63210	H	-5.12490	-4.73020	-0.63120
C	2.71020	2.28370	0.72440	C	-0.37410	4.96270	-0.65770
C	4.92880	0.70400	1.49120	C	1.64350	3.16280	0.17460
C	4.10510	0.26620	0.52750	C	0.34470	2.75490	0.14440
C	2.90960	1.07370	0.16590	C	-0.71790	3.72870	-0.26010
H	5.79720	0.12140	1.77600	H	-1.12430	5.67190	-0.98000
C	4.65940	1.97620	2.19130	C	2.01170	4.50260	-0.37860
C	3.59550	2.73370	1.83900	C	1.03880	5.36500	-0.74090
C	3.30690	3.97600	2.60550	C	1.38680	6.70580	-1.26760
C	4.11550	4.35970	3.60020	C	2.66750	7.06000	-1.41240
C	5.29400	3.54570	3.95430	C	3.73930	6.11060	-1.06160
C	5.55050	2.41310	3.29090	C	3.43450	4.90010	-0.58060
H	2.43630	4.57630	2.37700	H	0.60450	7.40350	-1.54000
H	3.90190	5.26430	4.15480	H	2.92070	8.03880	-1.79890
H	5.94510	3.86370	4.75830	H	4.77430	6.39230	-1.20680
H	6.41230	1.81620	3.56260	H	4.23980	4.21280	-0.35970

O	1.99530	0.59210	-0.73250	H	8.65280	0.71790	-2.16000
P	0.60210	0.14970	0.00950	C	1.98280	-1.62300	-4.28180
O	-0.03850	1.53480	0.66270	C	2.86260	-0.63000	-4.11250
O	0.89660	-0.75390	1.18660	C	3.67780	-0.56350	-2.88150
N	-3.02960	-0.77460	-0.13410	C	3.54310	-1.49780	-1.92340
H	-3.19950	-0.32300	0.75080	C	2.57360	-2.60270	-2.12840
C	-3.87200	-1.79000	-0.50110	C	1.83630	-2.66010	-3.24320
C	-2.13820	-4.39190	0.92790	H	1.37830	-1.66860	-5.17840
C	-0.88560	-3.83240	1.06870	H	2.97040	0.13480	-4.87070
C	-1.75080	-2.18350	2.62020	H	4.34220	0.27710	-2.75080
C	-3.03390	-2.69410	2.49110	H	2.44550	-3.36900	-1.38300
C	0.40150	-4.31480	0.47120	H	1.13240	-3.46910	-3.38490
H	0.71960	-5.25050	0.93860	C	3.35210	-4.90870	2.52520
H	0.27340	-4.49490	-0.59490	C	3.15000	-3.64780	2.92390
C	-1.28330	-1.10570	3.55490	C	3.51540	-2.52270	2.03840
H	-0.69300	-0.37540	2.99230	C	4.04970	-2.75790	0.82660
H	-0.61520	-1.54400	4.30540	C	4.27000	-4.16020	0.39260
H	-2.11390	-0.64150	4.07390	C	3.93930	-5.17720	1.19750
C	-4.12550	-2.30890	3.41540	H	3.08060	-5.73350	3.17120
C	-2.46190	-5.62750	0.18950	H	2.71320	-3.44830	3.89380
H	-0.70360	-7.97650	-1.17790	H	3.33170	-1.51610	2.38660
H	-2.27030	-8.22430	-0.33900	H	4.69340	-4.36690	-0.58240
H	-6.57940	-1.43340	3.95840	H	4.09680	-6.19830	0.87550
H	-7.29760	-2.98200	3.40250	C	-5.12010	7.08500	-0.97310
O	-1.37910	-6.33970	-0.20130	C	-4.52900	6.86170	0.20630
O	-3.60450	-5.99050	-0.03440	C	-3.71330	5.64630	0.40720
O	-4.02130	-1.65360	4.43710	C	-3.56810	4.75570	-0.58860
O	-5.32330	-2.80270	3.00250	C	-4.21600	5.01510	-1.89810
Si	4.49210	-1.35180	-0.31980	C	-4.95270	6.11860	-2.07710
Si	-2.52590	3.23740	-0.32240	H	-5.71700	7.97540	-1.12240
C	9.09450	-1.25490	-1.23850	H	-4.64620	7.57070	1.01560
C	8.57400	-2.29690	-0.58120	H	-3.23700	5.48830	1.36700
C	7.12710	-2.33810	-0.28260	H	-4.08670	4.32870	-2.72340
C	6.32110	-1.34070	-0.68750	H	-5.42120	6.30950	-3.03400
C	6.91260	-0.17480	-1.39010	C	-3.99660	1.59590	3.82730
C	8.22430	-0.13790	-1.65450	C	-2.76680	2.10650	3.70870
H	10.15420	-1.22300	-1.45640	C	-2.29400	2.60540	2.40150
H	9.21150	-3.11280	-0.26560	C	-3.08530	2.53160	1.31590
H	6.74550	-3.18280	0.26950	C	-4.46480	2.00290	1.46930
H	6.29690	0.66980	-1.66540	C	-4.88800	1.54500	2.65380

H	-4.34380	1.22910	4.78450	H	-2.22040	-7.29820	-1.85490
H	-2.11370	2.15470	4.57050	C	-3.28510	-3.62900	1.40020
H	-1.31400	3.05750	2.35350	H	-3.61720	-2.84460	0.33390
H	-5.14880	1.99290	0.63700	H	-4.21550	-4.18720	1.44020
H	-5.89160	1.15330	2.75820	O	-0.31960	-0.33940	-1.08840
C	-3.11210	0.40130	-4.02380	H	-2.07920	-0.67530	-0.49630
C	-4.16070	0.72800	-3.26150	C	-5.30980	-1.51820	-0.07130
C	-3.98000	1.60980	-2.09020	H	-5.93360	-2.41010	-0.14210
C	-2.76080	2.07760	-1.76980	H	-5.73660	-0.72500	-0.69380
C	-1.61030	1.74180	-2.64750	H	-5.32760	-1.18130	0.96710
C	-1.77550	0.93650	-3.70410	C	-3.35310	-3.39740	-4.48570
H	-3.24240	-0.24880	-4.87900	C	-2.24040	-3.20310	-3.67430
H	-5.14460	0.34500	-3.49890	C	-2.36600	-2.70960	-2.36930
H	-4.85400	1.89370	-1.52720	C	-3.65410	-2.38700	-1.86610
H	-0.62560	2.13810	-2.44390	C	-4.76370	-2.61480	-2.70020
H	-0.93060	0.68290	-4.33150	C	-4.62540	-3.10760	-3.99360
N	-0.76320	-2.70410	1.83610	H	-3.22750	-3.77860	-5.49510
H	0.06670	-2.07890	1.67870	H	-1.24170	-3.43490	-4.02710
H	1.17210	-3.55840	0.62010	H	-5.75870	-2.38060	-2.34220
C	-6.43200	-2.51250	3.86890	H	-5.50550	-3.25840	-4.61070
H	-6.25960	-2.92630	4.86510	O	-1.24790	-2.65320	-1.59800
C	-1.67180	-7.53600	-0.94060	H	-0.81330	-1.74750	-1.52470
C	2.92600	2.11680	0.65550	C	0.09630	4.98850	-0.87910
C	5.03440	0.41210	1.45830	C	1.94230	3.05820	0.05640
C	4.15700	-0.01350	0.53680	C	0.61080	2.77880	0.06100
C	3.00500	0.86010	0.17470	C	-0.35670	3.81760	-0.40830
H	5.86610	-0.20840	1.75680	H	-0.58770	5.74160	-1.24640
C	4.87920	1.73520	2.09610	C	2.43050	4.32070	-0.58150
C	3.87150	2.55520	1.72290	C	1.54020	5.25020	-0.98870
C	3.70080	3.85730	2.42270	C	2.00840	6.51870	-1.59500
C	4.56030	4.22830	3.37870	C	3.31530	6.73940	-1.76780
C	5.67810	3.34220	3.75580	C	4.29550	5.71300	-1.36940
C	5.82810	2.15820	3.15230	C	3.88220	4.56700	-0.81650
H	2.87570	4.51250	2.17630	H	1.29330	7.27140	-1.90310
H	4.43260	5.17640	3.88510	H	3.65630	7.66550	-2.21230
H	6.37110	3.65000	4.52810	H	5.35080	5.88470	-1.53810
H	6.64610	1.50960	3.44040	H	4.62070	3.81890	-0.56270

O	2.02290	0.39990	-0.66230	H	1.00060	-3.62800	-3.40300
P	0.60490	0.15330	0.13240	C	2.96830	-5.07330	2.65120
O	0.11390	1.64830	0.67330	C	2.79310	-3.79070	2.98990
O	0.86280	-0.63500	1.40980	C	3.24840	-2.71640	2.08350
N	-3.08140	-0.65500	-0.24450	C	3.82110	-3.02200	0.90650
H	-3.36960	0.06770	0.39230	C	4.03130	-4.44470	0.54670
C	-4.00820	-1.59530	-0.59640	C	3.62200	-5.41610	1.37190
C	-2.39900	-4.03570	0.90040	H	2.63280	-5.86120	3.31290
C	-1.14430	-3.46670	1.04880	H	2.31430	-3.53660	3.92660
C	-2.00700	-1.84250	2.61420	H	3.10300	-1.68920	2.38660
C	-3.29350	-2.33230	2.45820	H	4.51320	-4.70340	-0.38790
C	0.12600	-3.94280	0.41180	H	3.77050	-6.45420	1.10470
H	0.47490	-4.86260	0.89070	C	8.94640	-2.54430	-1.03370
H	-0.03780	-4.18320	-0.63790	C	8.45140	-2.60260	0.20740
C	-1.53840	-0.76500	3.55100	C	7.01880	-2.33210	0.44660
H	-0.76490	-0.16940	3.05880	C	6.20650	-2.01020	-0.57580
H	-1.08530	-1.22580	4.43680	C	6.76050	-1.96600	-1.95260
H	-2.35720	-0.14110	3.88870	C	8.05860	-2.21520	-2.16610
C	-4.49440	-1.89340	3.20580	H	9.99530	-2.74350	-1.21110
C	-2.56010	-5.32020	0.19330	H	9.09810	-2.85030	1.03910
H	-5.14900	-7.19840	-0.33060	H	6.63760	-2.41260	1.45660
H	-3.83630	-6.92020	-1.52680	H	6.12790	-1.73930	-2.79740
H	-5.02480	-0.31790	5.98350	H	8.46000	-2.18160	-3.17080
H	-6.02240	-0.16280	4.49960	C	-2.98440	0.59050	-4.08520
O	-3.85860	-5.73030	0.18550	C	-4.00820	1.01880	-3.33990
O	-1.66960	-5.98670	-0.30410	C	-3.76360	1.90350	-2.18180
O	-5.63030	-2.11660	2.82030	C	-2.51100	2.26210	-1.84950
O	-4.24050	-1.25110	4.36960	C	-1.38080	1.78280	-2.68730
Si	4.39620	-1.69320	-0.26020	C	-1.60670	0.99130	-3.74270
Si	-2.19650	3.47530	-0.46080	H	-3.16250	-0.05590	-4.93470
C	1.88190	-1.75790	-4.22030	H	-5.01990	0.72690	-3.58950
C	2.78700	-0.79410	-4.01560	H	-4.61620	2.29270	-1.64840
C	3.60840	-0.79850	-2.78720	H	-0.36400	2.07230	-2.46390
C	3.44960	-1.76650	-1.86690	H	-0.77920	0.64130	-4.34660
C	2.46260	-2.84500	-2.11510	C	-4.42750	7.51550	-1.26580
C	1.71830	-2.83750	-3.22700	C	-4.36670	6.59390	-2.23420
H	1.27230	-1.75140	-5.11450	C	-3.66890	5.31290	-1.99620
H	2.90990	-0.00130	-4.74200	C	-3.10150	5.06450	-0.80330
H	4.30720	0.01240	-2.62190	C	-3.16400	6.09400	0.26210
H	2.33730	-3.64950	-1.40820	C	-3.79420	7.25430	0.04230

H	-4.93710	8.45450	-1.43970	H	-3.48210	-7.77570	-0.01250
H	-4.82610	6.78530	-3.19530	C	-3.55210	-3.31230	1.41280
H	-3.61340	4.59760	-2.80450	H	-3.97750	-2.54930	0.35420
H	-2.69740	5.91330	1.22230	H	-4.47930	-3.86860	1.50950
H	-3.83890	8.00440	0.82130	O	-0.37010	-0.40240	-0.86800
C	-3.82170	2.26400	3.77520	H	-2.07390	-0.67750	-0.46250
C	-2.56150	2.68930	3.63910	C	-5.43890	-1.07930	-0.43070
C	-2.03790	3.03940	2.30310	H	-6.17070	-1.87960	-0.47630
C	-2.81330	2.91230	1.21070	H	-5.64910	-0.35430	-1.22420
C	-4.21950	2.46590	1.37770	H	-5.53790	-0.57820	0.53580
C	-4.69040	2.14620	2.58920	C	-3.01350	-4.00300	-4.05700
H	-4.20720	2.01050	4.75400	C	-4.18470	-4.25420	-3.34690
H	-1.92320	2.78250	4.50810	C	-4.50690	-3.49390	-2.21920
H	-1.03480	3.43620	2.23710	C	-3.66760	-2.43900	-1.79350
H	-4.88340	2.40360	0.53130	C	-2.47550	-2.23220	-2.51090
H	-5.71480	1.81650	2.70410	C	-2.15320	-2.99310	-3.63240
N	-1.00310	-2.38190	1.86190	H	-2.77780	-4.59980	-4.93300
H	-0.12600	-1.77830	1.74980	H	-4.86310	-5.04390	-3.66420
H	0.88690	-3.16840	0.50740	H	-1.78250	-1.45940	-2.19940
C	-5.40530	-0.83320	5.10200	H	-1.23660	-2.78530	-4.17290
H	-6.00620	-1.69830	5.39130	O	-5.63630	-3.76650	-1.49720
C	-4.08750	-6.98650	-0.46450	H	-6.05120	-4.56330	-1.85160
C	2.92240	2.13130	0.67820	C	0.07210	5.00360	-0.81850
C	5.03070	0.41290	1.45120	C	1.93220	3.07780	0.09820
C	4.14020	-0.00550	0.53900	C	0.60160	2.79750	0.12020
C	2.98880	0.87520	0.19260	C	-0.37340	3.83150	-0.34320
H	5.86170	-0.21340	1.73930	H	-0.61730	5.75260	-1.18440
C	4.89060	1.73510	2.09420	C	2.41110	4.34210	-0.54280
C	3.88280	2.56160	1.73550	C	1.51440	5.27010	-0.93970
C	3.72720	3.86220	2.44150	C	1.97340	6.54040	-1.54930
C	4.60010	4.22580	3.38820	C	3.27800	6.76450	-1.73480
C	5.71770	3.33270	3.74910	C	4.26460	5.74010	-1.34740
C	5.85420	2.14980	3.14020	C	3.85970	4.59230	-0.79180
H	2.90260	4.52240	2.20720	H	1.25340	7.29160	-1.84960
H	4.48340	5.17280	3.89910	H	3.61230	7.69190	-2.18170
H	6.42150	3.63450	4.51400	H	5.31780	5.91460	-1.52630
H	6.67210	1.49600	3.41660	H	4.60260	3.84590	-0.54620

O	1.99570	0.42290	-0.63640	H	3.77990	-6.44490	1.13160
P	0.58360	0.17790	0.16830	C	8.88660	-2.54790	-1.14640
O	0.11780	1.66700	0.74240	C	8.42420	-2.59780	0.10750
O	0.85030	-0.63730	1.42870	C	6.99890	-2.32270	0.38260
N	-3.12570	-0.72160	-0.23160	C	6.16110	-2.00420	-0.62000
H	-3.49040	0.01560	0.34690	C	6.67880	-1.96950	-2.01100
C	-3.98620	-1.70800	-0.62750	C	7.97020	-2.22330	-2.25720
C	-2.35560	-4.08740	0.95160	H	9.93000	-2.75110	-1.35010
C	-1.10810	-3.49800	1.09370	H	9.09180	-2.84290	0.92340
C	-2.00370	-1.84820	2.60970	H	6.64370	-2.39910	1.40230
C	-3.28350	-2.35510	2.45280	H	6.02390	-1.74740	-2.84000
C	0.16760	-3.97120	0.46700	H	8.34500	-2.19730	-3.27230
H	0.53420	-4.86860	0.97370	C	1.81530	-1.71960	-4.20260
H	0.00760	-4.24560	-0.57560	C	1.67030	-2.70840	-3.31310
C	-1.55860	-0.74680	3.52840	C	2.48850	-2.72510	-2.08360
H	-1.06590	-1.18490	4.40460	C	3.38440	-1.75170	-1.85120
H	-2.39410	-0.15480	3.88050	C	3.55420	-0.66880	-2.85260
H	-0.81800	-0.12530	3.01790	C	2.80530	-0.65110	-3.96200
C	-4.49910	-1.92470	3.18460	H	1.21140	-1.70240	-5.10050
C	-2.50290	-5.37240	0.25280	H	0.94900	-3.49610	-3.48740
H	-5.12820	-7.11100	-0.58600	H	2.34100	-3.52940	-1.38120
H	-3.63630	-6.95630	-1.57020	H	4.27010	0.12480	-2.67810
H	-6.02340	-1.75710	5.36110	H	2.92170	0.14710	-4.68350
H	-5.08130	-0.34820	5.94990	C	-4.49510	7.47880	-1.24540
O	-3.82530	-5.71880	0.10160	C	-3.94410	7.25790	-0.04630
O	-1.60870	-6.09610	-0.13900	C	-3.22520	5.99420	0.21680
O	-5.62590	-2.17700	2.79040	C	-3.13010	5.05660	-0.74130
O	-4.26770	-1.26760	4.34230	C	-3.73030	5.31410	-2.07390
Si	4.35960	-1.68570	-0.26180	C	-4.37890	6.46140	-2.30940
Si	-2.21040	3.47550	-0.39710	H	-5.02150	8.40420	-1.44010
C	3.01380	-5.06160	2.69410	H	-4.02350	8.00400	0.73360
C	2.84030	-3.77860	3.03190	H	-2.77960	5.83910	1.19160
C	3.26690	-2.70560	2.11010	H	-3.63530	4.59040	-2.87140
C	3.81270	-3.01310	0.92090	H	-4.81250	6.65020	-3.28300
C	4.01730	-4.43630	0.55960	C	-3.83040	2.24140	3.83420
C	3.63460	-5.40630	1.39900	C	-2.57600	2.68440	3.70100
H	2.69970	-5.84850	3.36750	C	-2.05260	3.03690	2.36550
H	2.38470	-3.52310	3.97980	C	-2.82160	2.89350	1.27050
H	3.12310	-1.67780	2.41250	C	-4.22030	2.42310	1.43380
H	4.47510	-4.69650	-0.38660	C	-4.69150	2.10300	2.64490



H	-4.21620	1.98660	4.81250	H	-3.57290	-7.78890	0.00180
H	-1.94280	2.79160	4.57210	C	-3.51830	-3.36920	1.44020
H	-1.05650	3.45170	2.30170	H	-3.95080	-2.63860	0.32900
H	-4.87980	2.34560	0.58540	H	-4.43870	-3.93210	1.56330
H	-5.71120	1.75790	2.75690	O	-0.41080	-0.35070	-0.82660
C	-2.98170	0.67830	-4.09000	H	-2.11480	-0.68350	-0.42950
C	-4.00540	1.06350	-3.32140	C	-5.45150	-1.27180	-0.54370
C	-3.76480	1.91370	-2.13710	H	-6.12550	-2.10560	-0.72380
C	-2.51510	2.28000	-1.80230	H	-5.63120	-0.49910	-1.29850
C	-1.38370	1.84030	-2.66040	H	-5.66210	-0.85700	0.44550
C	-1.60670	1.08420	-3.74210	C	-2.92980	-3.82110	-4.25430
H	-3.15740	0.06010	-4.96080	C	-4.02920	-4.23110	-3.50430
H	-5.01490	0.76640	-3.57420	C	-4.33490	-3.60430	-2.29530
H	-4.61960	2.27950	-1.59120	C	-3.56970	-2.50640	-1.83710
H	-0.36890	2.13280	-2.43210	C	-2.42860	-2.15180	-2.58080
H	-0.77880	0.76470	-4.36200	C	-2.11600	-2.79500	-3.77590
N	-0.98650	-2.39260	1.87840	H	-2.70090	-4.31340	-5.19500
H	-0.11410	-1.77150	1.75790	H	-4.66680	-5.04760	-3.82750
H	0.91350	-3.18010	0.53680	H	-1.78020	-1.35400	-2.23880
C	-5.44610	-0.87680	5.07000	H	-1.24630	-2.47420	-4.33920
H	-6.07860	-0.22610	4.46250	O	-5.41810	-4.09050	-1.58950
C	-4.04690	-6.98120	-0.55890	H	-5.07710	-4.48740	-0.76870
C	-1.70890	2.75430	0.76510	C	2.40890	3.20900	1.91180
C	-4.43690	2.72260	0.01730	C	-0.29960	2.77250	1.23710
C	-3.72710	1.58580	-0.03150	C	0.67860	2.40100	0.38650
C	-2.27700	1.60140	0.32590	C	2.10080	2.70150	0.70830
H	-5.47960	2.73940	-0.26680	H	3.43570	3.45620	2.15530
C	-3.80130	3.99500	0.39790	C	0.05740	3.25460	2.60220
C	-2.49240	4.02760	0.72780	C	1.35630	3.45750	2.91700
C	-1.85440	5.34660	1.00350	C	1.72630	3.93590	4.26900
C	-2.58000	6.47020	0.97590	C	0.77900	4.14750	5.18940
C	-4.01820	6.41620	0.65660	C	-0.63860	3.89910	4.86310
C	-4.59730	5.24470	0.37550	C	-0.98320	3.47230	3.64260
H	-0.79550	5.41960	1.21030	H	2.76510	4.11400	4.51770
H	-2.11020	7.42480	1.17530	H	1.05000	4.49540	6.17780
H	-4.60010	7.32870	0.63850	H	-1.39860	4.05640	5.61750
H	-5.65150	5.21430	0.12910	H	-2.02610	3.27900	3.42820

O	-1.59020	0.40870	0.37910	H	-3.41900	-1.82980	3.87610
P	-0.22250	0.25860	-0.54580	C	-2.28650	-1.09710	-4.59530
O	0.34950	1.77900	-0.79070	C	-2.68830	-2.07060	-3.77010
O	-0.55600	-0.33190	-1.88920	C	-3.42140	-1.73690	-2.53080
N	3.08680	-2.10090	0.43570	C	-3.67090	-0.45510	-2.21560
H	3.81360	-2.08790	-0.26290	C	-3.24610	0.61770	-3.14920
C	3.03680	-3.18150	1.28090	C	-2.58610	0.31260	-4.27340
C	0.32120	-4.72850	0.10110	H	-1.74250	-1.33990	-5.49880
C	-0.41260	-3.65760	-0.37300	H	-2.46930	-3.10460	-4.00280
C	1.23690	-3.23760	-2.09810	H	-3.73850	-2.54360	-1.89000
C	2.05550	-4.23510	-1.59360	H	-3.45930	1.65450	-2.92170
C	-1.72580	-3.16990	0.15670	H	-2.26680	1.09770	-4.94650
H	-1.71150	-3.15920	1.24510	C	-9.09250	0.77270	-1.50590
H	-1.92480	-2.16140	-0.20200	C	-8.26620	0.49420	-2.52130
C	1.45850	-2.41140	-3.33240	C	-6.82960	0.25880	-2.26550
H	0.85080	-1.50600	-3.27950	C	-6.34720	0.32990	-1.01330
H	1.17130	-2.98400	-4.22080	C	-7.26850	0.63290	0.10830
H	2.50970	-2.15390	-3.44800	C	-8.56920	0.84430	-0.12670
C	3.33780	-4.67630	-2.18710	H	-10.14470	0.94460	-1.69240
C	-0.14660	-5.73180	1.08300	H	-8.64810	0.43970	-3.53260
H	-1.33370	-6.43050	3.36820	H	-6.18480	0.03080	-3.10310
H	-2.95060	-6.26280	2.61060	H	-6.89150	0.68650	1.12220
H	4.84480	-5.80540	-4.05990	H	-9.24020	1.06710	0.69270
H	4.74670	-4.33330	-5.08170	C	1.55340	1.87770	-4.80770
O	-1.43110	-5.56960	1.47120	C	2.25390	0.88980	-4.24110
O	0.55050	-6.64970	1.48210	C	2.84590	1.07240	-2.89820
O	4.16000	-5.33660	-1.57370	C	2.72290	2.24930	-2.25960
O	3.52020	-4.30060	-3.47310	C	1.94300	3.34010	-2.89650
Si	-4.55100	0.02390	-0.64540	C	1.38420	3.16010	-4.09900
Si	3.45570	2.52830	-0.56690	H	1.11410	1.74080	-5.78730
C	-4.52550	-3.31460	2.64770	H	2.38860	-0.04480	-4.76820
C	-5.13260	-3.53130	1.47550	H	3.35860	0.23720	-2.44280
C	-5.14820	-2.47430	0.44260	H	1.80160	4.28220	-2.38680
C	-4.52860	-1.30190	0.66210	H	0.80860	3.95490	-4.55550
C	-3.89400	-1.05370	1.98130	C	6.49760	-0.81980	0.69060
C	-3.88630	-2.01140	2.91690	C	6.52720	-0.32060	-0.54990
H	-4.50950	-4.08900	3.40360	C	5.56770	0.73010	-0.94820
H	-5.60930	-4.48270	1.27870	C	4.64080	1.17020	-0.07910
H	-5.66260	-2.66420	-0.49100	C	4.61640	0.61110	1.29500
H	-3.44460	-0.09750	2.20710	C	5.50220	-0.32310	1.66070

H	7.20000	-1.58870	0.98510	H	-1.81260	-7.53790	2.06080
H	7.25680	-0.68120	-1.26330	C	1.69460	-4.87200	-0.34230
H	5.63050	1.14170	-1.94780	H	2.42170	-4.14350	0.61580
H	3.89550	0.95750	2.01900	H	2.17070	-5.82460	-0.12740
H	5.48390	-0.72360	2.66600	O	0.74190	-0.53760	0.32130
C	5.67580	6.65940	-0.63390	H	2.26580	-1.52010	0.25300
C	6.38390	5.52780	-0.72310	C	4.40780	-3.83310	1.48520
C	5.69710	4.21920	-0.70410	H	4.91050	-3.97640	0.52540
C	4.35770	4.15820	-0.60630	H	4.31790	-4.80880	1.96280
C	3.58070	5.41810	-0.49670	H	5.02040	-3.19460	2.12890
C	4.20590	6.60130	-0.51150	C	0.86450	-3.17310	5.03040
H	6.17810	7.61800	-0.64690	C	1.07330	-1.96550	4.38140
H	7.46210	5.56770	-0.80920	C	1.70910	-1.89170	3.12770
H	6.29750	3.32470	-0.77360	C	2.18780	-3.09070	2.52800
H	2.50400	5.38900	-0.38790	C	1.94400	-4.30320	3.20570
H	3.63640	7.51780	-0.42680	C	1.29280	-4.36070	4.43020
N	0.08190	-2.94870	-1.43400	H	0.36080	-3.19160	5.99290
H	-0.35690	-2.02850	-1.67310	H	0.74340	-1.02620	4.81290
H	-2.53730	-3.83550	-0.15000	H	2.26330	-5.23250	2.74580
C	4.76540	-4.71620	-4.06190	H	1.13100	-5.31970	4.91230
H	5.61140	-4.30020	-3.50960	O	1.88300	-0.64760	2.62830
C	-1.90480	-6.51830	2.44110	H	1.42400	-0.53300	1.74980
C	2.87150	2.06000	0.73600	C	1.91240	3.03660	0.15530
C	4.91980	0.28160	1.53710	C	0.57940	2.76800	0.11350
C	4.06290	-0.08560	0.57280	C	-0.36640	3.82710	-0.35400
C	2.94580	0.82420	0.20350	H	-0.55990	5.77740	-1.13880
H	5.73330	-0.37360	1.82590	C	2.42770	4.31810	-0.42050
C	4.76820	1.58010	2.22440	C	1.55570	5.26660	-0.82380
C	3.78930	2.43560	1.85140	C	2.04980	6.55290	-1.36910
C	3.61900	3.71060	2.59940	C	3.36270	6.77210	-1.49020
C	4.45120	4.02370	3.59930	C	4.32430	5.72680	-1.09550
C	5.53810	3.10000	3.97680	C	3.88760	4.56440	-0.59770
C	5.68730	1.93940	3.32900	H	1.34880	7.32000	-1.67410
H	2.81590	4.39230	2.35260	H	3.72260	7.71140	-1.88990
H	4.32380	4.95220	4.14060	H	5.38550	5.89850	-1.22240
H	6.20890	3.36100	4.78510	H	4.61390	3.80410	-0.34550
H	6.48200	1.26270	3.61740	O	1.97760	0.40970	-0.67260
C	0.10770	5.00950	-0.77210	P	0.54620	0.14200	0.09060

O	0.05810	1.62200	0.67590	C	8.33880	-2.93370	-0.54810
O	0.79430	-0.69030	1.34600	C	6.89260	-2.87960	-0.24780
N	-3.15730	-0.67620	-0.30580	C	6.15190	-1.83470	-0.65820
H	-3.51600	0.10350	0.21740	C	6.81670	-0.71450	-1.36970
C	-4.03230	-1.66880	-0.66490	C	8.12770	-0.76390	-1.63540
C	-2.48360	-4.06550	0.96480	H	9.98390	-1.96940	-1.43120
C	-1.22390	-3.49090	1.09030	H	8.92280	-3.78680	-0.22750
C	-2.09650	-1.79710	2.57430	H	6.45890	-3.69420	0.31090
C	-3.38270	-2.28640	2.42870	H	6.25680	0.16600	-1.65090
C	0.05530	-3.97330	0.47150	H	8.60980	0.05910	-2.14710
H	-0.09930	-4.23590	-0.57490	C	1.80980	-1.78980	-4.25440
H	0.80650	-3.18710	0.54600	C	2.73000	-0.83920	-4.06010
C	-1.62950	-0.68340	3.46660	C	3.54650	-0.83860	-2.82820
H	-0.92620	-0.04960	2.91930	C	3.37030	-1.78870	-1.89240
H	-1.08350	-1.10650	4.31810	C	2.35890	-2.84940	-2.12790
H	-2.45860	-0.10520	3.85570	C	1.62020	-2.84710	-3.24330
C	-4.59260	-1.81220	3.14610	H	1.20480	-1.78700	-5.15190
C	-2.76720	-5.36450	0.33880	H	2.86990	-0.06020	-4.79830
H	-2.47520	-7.18020	-1.57820	H	4.24450	-0.02920	-2.67600
H	-0.95220	-7.76980	-0.83510	H	2.20350	-3.63440	-1.40700
H	-6.12930	-1.62940	5.31830	H	0.88530	-3.62440	-3.40720
H	-5.14750	-0.25750	5.92920	C	-3.93170	2.28360	3.71300
O	-1.67750	-6.07930	0.00420	C	-4.69850	2.18380	2.62270
O	-3.90310	-5.80540	0.16480	C	-4.15280	2.54390	1.29830
O	-5.72130	-2.00560	2.72950	C	-2.86890	2.92070	1.16860
O	-4.34880	-1.18930	4.32070	C	-2.02860	3.03930	2.38810
Si	4.32630	-1.72140	-0.28640	C	-2.53390	2.73950	3.59050
Si	-2.20280	3.49320	-0.47980	H	-4.33270	2.03300	4.68620
C	2.91730	-5.15300	2.59100	H	-5.72580	1.85470	2.70910
C	3.44230	-5.45470	1.39810	H	-4.81860	2.51940	0.45140
C	3.89400	-4.37710	0.49390	H	-1.01320	3.40410	2.32580
C	3.78330	-3.08900	0.86270	H	-1.92060	2.83570	4.47700
C	3.20340	-2.76320	2.19030	C	-2.87170	0.67190	-4.17660
C	2.79040	-3.74180	3.00500	C	-3.91460	1.04840	-3.42970
H	2.58110	-5.94090	3.25240	C	-3.70780	1.91030	-2.24740
H	3.53260	-6.48830	1.09010	C	-2.46950	2.29670	-1.89260
H	4.30590	-4.64310	-0.47180	C	-1.31720	1.87110	-2.72980
H	3.09960	-1.73600	2.51060	C	-1.50950	1.10270	-3.80870
H	2.36050	-3.50080	3.96860	H	-3.02230	0.04300	-5.04440
C	8.92460	-1.93160	-1.21240	H	-4.91470	0.73290	-3.69680

H	-4.57750	2.25880	-1.71390	H	-4.02710	-2.55560	0.29970
H	-0.31140	2.18330	-2.48760	H	-4.56970	-3.84320	1.51190
H	-0.66620	0.79280	-4.41260	O	-0.42440	-0.37680	-0.93050
C	-4.43150	7.51090	-1.40190	H	-2.14860	-0.66390	-0.51010
C	-3.90530	7.29420	-0.19100	C	-5.49160	-1.20890	-0.62520
C	-3.20350	6.02590	0.09510	H	-5.70290	-0.71740	0.32870
C	-3.09740	5.08120	-0.85480	H	-6.17000	-2.05060	-0.73960
C	-3.67220	5.33250	-2.19950	H	-5.65890	-0.49360	-1.43750
C	-4.30590	6.48380	-2.45560	C	-2.87680	-4.12770	-4.03200
H	-4.94530	8.43970	-1.61340	C	-3.96340	-4.48980	-3.23890
H	-3.99220	8.04700	0.58180	C	-4.32600	-3.71090	-2.13590
H	-2.77900	5.87310	1.07970	C	-3.61100	-2.53330	-1.82440
H	-3.57180	4.60010	-2.98840	C	-2.49410	-2.20880	-2.61420
H	-4.72110	6.66830	-3.43800	C	-2.13680	-2.98900	-3.71140
N	-1.08900	-2.37110	1.84840	H	-2.60850	-4.73370	-4.89290
H	-0.20670	-1.76290	1.70950	H	-4.55500	-5.37350	-3.45770
H	0.41500	-4.87100	0.98170	H	-1.88690	-1.34630	-2.36790
C	-5.52080	-0.76570	5.04080	H	-1.28600	-2.69650	-4.31790
H	-6.12630	-0.08980	4.43340	O	-5.39030	-4.09930	-1.35670
C	-1.93420	-7.33900	-0.64280	H	-5.09200	-4.85070	-0.80190
H	-2.52250	-7.99120	0.00580				
C	-3.62950	-3.30620	1.42900				
C	0.70960	-2.63600	1.24820	C	-1.48920	-1.86200	0.51740
C	3.35970	-3.52390	0.78460	C	-2.95120	-1.70610	0.73590
C	2.97090	-2.33350	0.30820	H	-4.50190	-1.65160	2.16180
C	1.58130	-1.84670	0.55670	C	-1.21310	-2.16040	2.93600
H	4.35250	-3.90340	0.58960	C	-2.53290	-1.94380	3.13770
C	2.41280	-4.40000	1.49010	C	-3.07360	-1.89010	4.51530
C	1.13220	-4.01130	1.66780	C	-2.25490	-2.02680	5.56410
C	0.16360	-4.98820	2.24600	C	-0.80830	-2.22770	5.35290
C	0.57230	-6.20000	2.63880	C	-0.31170	-2.28840	4.11210
C	1.98490	-6.59100	2.48660	H	-4.13280	-1.73450	4.67820
C	2.85680	-5.74270	1.93360	H	-2.65010	-1.98340	6.57080
H	-0.88590	-4.74570	2.33640	H	-0.14860	-2.31780	6.20620
H	-0.13690	-6.90350	3.05550	H	0.75440	-2.41550	3.97820
H	2.30990	-7.57190	2.80860	O	1.28560	-0.54390	0.21050
H	3.88970	-6.04340	1.80860	P	-0.07650	-0.19990	-0.66100
C	-3.43730	-1.75090	1.98530	O	-0.94480	-1.59360	-0.71110
C	-0.67870	-2.19080	1.54370	O	0.29250	0.18870	-2.06930

N	-1.96920	3.09020	1.50470	C	3.21130	-1.22350	-2.45330
H	-2.82300	3.55660	1.24110	C	2.29540	-2.30970	-2.88160
C	-1.00340	3.89210	2.06940	C	1.63250	-2.21600	-4.03980
C	1.17220	4.63910	-0.51530	H	1.25930	-0.94940	-5.82780
C	1.34230	3.47400	-1.23460	H	2.78220	0.81590	-5.15670
C	-1.02380	3.38100	-1.75570	H	4.07620	0.62930	-2.98970
C	-1.25200	4.54180	-1.02980	H	2.16080	-3.18800	-2.26310
C	2.61310	2.73100	-1.51000	H	0.97150	-3.01330	-4.35150
H	2.92940	2.89050	-2.54720	C	8.10680	-3.75860	-1.48880
H	3.41250	3.05520	-0.85580	C	7.24050	-3.63460	-2.50130
C	-2.02670	2.58610	-2.54260	C	5.97530	-2.89500	-2.30870
H	-1.59350	1.62270	-2.81240	C	5.68790	-2.34990	-1.11450
H	-2.31340	3.12610	-3.44940	C	6.65420	-2.48600	0.00200
H	-2.93680	2.42570	-1.96420	C	7.79960	-3.15520	-0.17620
C	-2.53600	5.26860	-0.96690	H	9.03360	-4.29960	-1.62920
C	2.24290	5.48320	0.06500	H	7.46430	-4.07500	-3.46430
H	5.45400	5.67300	-0.28790	H	5.29390	-2.80750	-3.14390
H	4.36440	7.07800	-0.04130	H	6.43560	-2.04560	0.96700
H	-4.53520	6.64740	-2.14210	H	8.50330	-3.25500	0.64000
H	-5.32900	5.10380	-2.59350	C	-1.87910	-2.32470	-4.73670
O	3.48730	5.21420	-0.38740	C	-2.39900	-1.12000	-4.48070
O	2.01640	6.37820	0.86270	C	-3.12910	-0.88150	-3.21900
O	-2.76540	6.15440	-0.15770	C	-3.27610	-1.86960	-2.31920
O	-3.44240	4.88580	-1.89510	C	-2.68780	-3.20140	-2.60840
Si	4.11580	-1.39740	-0.83590	C	-2.02700	-3.41490	-3.75290
Si	-4.14500	-1.57190	-0.69300	H	-1.34140	-2.50010	-5.65950
C	5.62820	2.63210	1.01060	H	-2.28280	-0.31520	-5.19510
C	4.68990	1.92470	1.64910	H	-3.52030	0.10690	-3.03540
C	4.18250	0.66430	1.06700	H	-2.76920	-4.00470	-1.89180
C	4.65100	0.23150	-0.11610	H	-1.59140	-4.38460	-3.95610
C	5.70300	1.01380	-0.81150	C	-6.26740	2.61460	-0.68090
C	6.16090	2.15340	-0.27960	C	-6.50190	1.74630	-1.67000
H	6.00480	3.55020	1.44210	C	-5.82630	0.43320	-1.67630
H	4.31400	2.26770	2.60100	C	-4.96550	0.10520	-0.69650
H	3.45040	0.09560	1.62310	C	-4.68860	1.08590	0.38230
H	6.11980	0.65810	-1.74520	C	-5.31770	2.26830	0.39430
H	6.92950	2.72080	-0.78810	H	-6.77170	3.57180	-0.66730
C	1.80800	-1.02790	-4.89820	H	-7.19490	1.99900	-2.46190
C	2.64820	-0.05450	-4.52770	H	-6.04230	-0.26100	-2.47920
C	3.39380	-0.16260	-3.25600	H	-3.98720	0.85450	1.17150

H	-5.13520	2.97490	1.19270	H	-0.44090	4.54130	1.06260
C	-7.26030	-5.00660	0.02860	H	-0.28960	6.10570	0.11280
C	-7.69290	-3.78200	-0.29150	O	-0.82720	0.84620	0.16020
C	-6.72450	-2.68920	-0.52110	H	-1.70150	2.29260	0.93110
C	-5.40350	-2.92260	-0.42920	C	-1.61810	5.06390	2.84280
C	-4.93390	-4.27860	-0.04960	H	-2.36580	5.57180	2.22880
C	-5.81350	-5.26470	0.16310	H	-0.86220	5.79450	3.12970
H	-7.96890	-5.80690	0.19860	H	-2.08800	4.68020	3.75440
H	-8.75380	-3.58790	-0.38260	C	2.23440	2.31600	4.45250
H	-7.10930	-1.71020	-0.76050	C	1.26080	1.44300	3.99270
H	-3.87840	-4.47410	0.08670	C	0.23920	1.86580	3.12360
H	-5.46700	-6.25000	0.44720	C	0.16950	3.23860	2.75690
N	0.23650	2.87450	-1.78000	C	1.20570	4.08940	3.19610
H	0.33440	1.87360	-2.08860	C	2.22500	3.64900	4.02840
H	2.42500	1.66290	-1.37860	H	3.01550	1.95540	5.11590
C	-4.68950	5.60170	-1.86530	H	1.25910	0.39540	4.27460
H	-5.13350	5.56520	-0.86850	H	1.20450	5.12550	2.87280
C	4.53360	6.02190	0.17940	H	2.99930	4.33850	4.34960
H	4.57710	5.88830	1.26270	O	-0.65690	0.92410	2.75760
C	-0.18090	5.07360	-0.20910	H	-0.73260	0.86850	1.76260
C	3.08420	1.76630	0.72160	H	0.01400	5.77180	-1.18600
C	4.96500	-0.18870	1.52040	C	2.85180	4.04250	-0.45990
C	4.06750	-0.48230	0.56780	C	2.07250	5.06520	-0.87160
C	3.03520	0.52370	0.20200	C	2.68460	6.29110	-1.43600
H	5.71850	-0.91360	1.80520	C	4.01180	6.38170	-1.56620
C	4.94210	1.12380	2.19720	C	4.87090	5.25370	-1.16290
C	4.04430	2.06410	1.82460	C	4.32750	4.14490	-0.64790
C	4.00240	3.35640	2.56080	H	2.05870	7.11810	-1.74770
C	4.87060	3.59900	3.54960	H	4.45780	7.27690	-1.97980
C	5.86970	2.58070	3.92640	H	5.94280	5.32090	-1.29740
C	5.90230	1.40520	3.28930	H	4.97910	3.32140	-0.39020
H	3.26460	4.10840	2.31410	O	2.02050	0.19260	-0.65720
H	4.83670	4.54050	4.08260	P	0.58040	0.07430	0.12660
H	6.57050	2.78500	4.72550	O	0.24060	1.60340	0.68950
H	6.63290	0.65940	3.57700	O	0.76280	-0.75970	1.39150
C	0.60690	4.94850	-0.81090	N	-3.20110	-0.42910	-0.30920
C	2.21930	2.82430	0.13620	H	-3.50150	0.36420	0.23120
C	0.86640	2.68480	0.10580	C	-4.14750	-1.34270	-0.68530
C	0.02420	3.82200	-0.37560	C	-2.80800	-3.83270	1.02390

C	-1.50350	-3.38290	1.16690	H	8.57280	-4.60020	-0.33940
C	-2.23020	-1.57300	2.58600	H	6.13530	-4.30080	0.24240
C	-3.55630	-1.94120	2.42770	H	6.24450	-0.40280	-1.65080
C	-0.27820	-4.03650	0.60470	H	8.57090	-0.70780	-2.18950
H	-0.03720	-4.94240	1.16870	C	1.60960	-2.00310	-4.22050
H	-0.44420	-4.34800	-0.42640	C	2.62320	-1.14760	-4.05160
C	-1.68060	-0.49120	3.47030	C	3.45100	-1.21130	-2.82910
H	-0.85980	0.01860	2.95900	C	3.19240	-2.12580	-1.87710
H	-1.26790	-0.94330	4.38010	C	2.07380	-3.07960	-2.08190
H	-2.45040	0.20860	3.77060	C	1.32500	-3.01900	-3.18900
C	-4.72430	-1.35890	3.13190	H	0.99850	-1.95340	-5.11230
C	-3.09070	-5.13060	0.39450	H	2.83270	-0.39880	-4.80440
H	-5.89050	-6.60230	-0.39450	H	4.23140	-0.47690	-2.69940
H	-4.36450	-6.71210	-1.33170	H	1.84710	-3.83120	-1.34440
H	-6.22750	-0.99160	5.30220	H	0.51110	-3.71800	-3.33060
H	-5.15510	0.33640	5.85450	C	-3.66170	2.70470	3.71970
O	-4.44270	-5.33250	0.23650	C	-4.43060	2.62990	2.62880
O	-2.28060	-5.97330	0.06250	C	-3.85400	2.90100	1.29640
O	-5.86850	-1.49730	2.73160	C	-2.54450	3.17320	1.16200
O	-4.43200	-0.70290	4.27640	C	-1.69930	3.25730	2.38090
Si	4.17620	-2.13690	-0.28750	C	-2.23040	3.03850	3.58970
Si	-1.83550	3.66250	-0.49400	H	-4.08480	2.52000	4.69820
C	2.54120	-5.43130	2.62960	H	-5.48170	2.38950	2.72000
C	3.00650	-5.77740	1.42420	H	-4.51770	2.90360	0.44780
C	3.52630	-4.74320	0.50610	H	-0.65630	3.53260	2.31150
C	3.53840	-3.45050	0.87520	H	-1.61280	3.11040	4.47560
C	3.01970	-3.07480	2.21480	C	-2.78560	0.88570	-4.16310
C	2.54560	-4.01390	3.04260	C	-3.78550	1.37700	-3.42430
H	2.15650	-6.18710	3.30190	C	-3.49300	2.22450	-2.24980
H	3.00030	-6.81510	1.11700	C	-2.22200	2.48290	-1.89400
H	3.88920	-5.04390	-0.46900	C	-1.11820	1.92840	-2.72090
H	3.00960	-2.04180	2.53350	C	-1.38680	1.17340	-3.79290
H	2.16140	-3.73640	4.01560	H	-2.99880	0.26870	-5.02630
C	8.72310	-2.73510	-1.29350	H	-4.81240	1.16640	-3.69310
C	8.06160	-3.69330	-0.63550	H	-4.32300	2.67040	-1.72510
C	6.63080	-3.51730	-0.30920	H	-0.08590	2.13460	-2.47670
C	5.97900	-2.40420	-0.68980	H	-0.57890	0.76940	-4.38950
C	6.72900	-1.33430	-1.39430	C	-3.63910	7.89690	-1.36900
C	8.02610	-1.49420	-1.68330	C	-3.64780	6.96700	-2.33130
H	9.77120	-2.86240	-1.53160	C	-3.08520	5.62520	-2.07140



C	-2.57070	5.33100	-0.86510	O	-0.44920	-0.36330	-0.87560
C	-2.55630	6.36870	0.19420	H	-2.18890	-0.49900	-0.49090
C	-3.06430	7.58370	-0.04540	C	-5.56470	-0.76490	-0.64580
H	-4.04950	8.88020	-1.55900	H	-5.75440	-0.30140	0.32600
H	-4.06460	7.19600	-3.30360	H	-6.31210	-1.53590	-0.81720
H	-3.08410	4.90160	-2.87430	H	-5.65300	-0.00270	-1.42710
H	-2.13190	6.14920	1.16590	C	-3.25340	-3.68130	-4.21650
H	-3.05290	8.33970	0.72900	C	-4.38740	-3.96780	-3.46070
N	-1.27070	-2.25800	1.89650	C	-4.64910	-3.26600	-2.28290
H	-0.33160	-1.74300	1.76100	C	-3.79550	-2.22000	-1.86080
H	0.55770	-3.33870	0.65830	C	-2.62650	-1.98940	-2.60920
C	-5.56810	-0.17940	4.98830	C	-2.36280	-2.70340	-3.77540
H	-6.13520	0.51100	4.36060	H	-3.05960	-4.23070	-5.13310
C	-4.80260	-6.60520	-0.33750	H	-5.08870	-4.74150	-3.75590
H	-4.45010	-7.41860	0.29940	H	-1.91610	-1.23590	-2.29150
C	-3.88880	-2.96330	1.45190	H	-1.46860	-2.47700	-4.34580
H	-4.21540	-2.23520	0.30210	O	-5.78100	-3.62050	-1.57510
H	-4.87020	-3.41050	1.57670	H	-5.49110	-4.02540	-0.73860
C	-1.59530	3.08250	-0.25100	C	0.99190	4.31940	2.24520
C	-4.26750	2.88970	-1.13460	C	1.10350	5.17670	3.44810
C	-3.64300	1.79660	-0.66920	C	0.00850	5.72070	3.98950
C	-2.19870	1.87440	-0.29860	C	-1.31630	5.46170	3.39490
H	-5.31600	2.86370	-1.39260	C	-1.42590	4.69440	2.30420
C	-3.54540	4.16800	-1.27370	H	2.07200	5.36430	3.89470
C	-2.26890	4.27190	-0.84680	H	0.09030	6.34520	4.86970
C	-1.55360	5.56690	-1.00860	H	-2.20140	5.88680	3.85040
C	-2.17990	6.62230	-1.54180	H	-2.41060	4.49930	1.90140
C	-3.58360	6.50730	-1.98190	O	-1.55680	0.76110	0.19310
C	-4.23180	5.34390	-1.85800	P	-0.19270	0.29650	-0.62140
H	-0.51930	5.66760	-0.70630	O	0.66900	1.65630	-0.99230
H	-1.65630	7.56250	-1.65780	O	-0.54180	-0.33540	-1.94770
H	-4.08510	7.36590	-2.40930	N	2.84980	-2.17310	0.74350
H	-5.26060	5.26580	-2.18670	H	3.71100	-2.08130	0.22730
C	2.20160	3.70540	1.66980	C	2.62840	-3.36720	1.39030
C	-0.30620	3.23230	0.46560	C	0.24680	-4.88840	-0.44030
C	0.78430	2.56160	0.03390	C	-0.49770	-3.80350	-0.87170
C	2.12140	2.88530	0.61000	C	1.32640	-3.07500	-2.28800
H	3.16350	3.94430	2.10880	C	2.16100	-4.04950	-1.76780
C	-0.21240	4.10400	1.67390	C	-1.91210	-3.47640	-0.50330

H	-2.61410	-4.07520	-1.09100	C	-3.28220	-1.22620	3.91430
H	-2.09210	-3.70250	0.54560	C	-3.52280	-2.12300	2.95130
C	1.56960	-2.14330	-3.43810	C	-3.96640	-1.67410	1.61510
H	1.35230	-1.11590	-3.13090	C	-4.11490	-0.36550	1.35490
H	0.85530	-2.38210	-4.23480	C	-3.85810	0.62310	2.43150
H	2.57030	-2.24410	-3.83570	C	-3.45860	0.21420	3.64170
C	3.56770	-4.31380	-2.16060	H	-2.96040	-1.55380	4.89430
C	-0.27490	-6.06910	0.28010	H	-3.39210	-3.17940	3.14800
H	-3.22940	-7.06340	1.15080	H	-4.17030	-2.41930	0.86350
H	-1.88600	-8.13610	0.63320	H	-3.98780	1.68140	2.24230
H	5.53260	-5.13160	-3.74380	H	-3.26620	0.93750	4.42340
H	5.42880	-3.62670	-4.71730	C	6.50830	6.05290	-0.28480
O	-1.61810	-6.07320	0.43460	C	5.34860	6.03970	-0.95020
O	0.43340	-6.98450	0.66570	C	4.47660	4.84820	-0.89560
O	4.33940	-4.92710	-1.44220	C	4.84880	3.76160	-0.19620
O	3.93440	-3.83840	-3.37060	C	6.12560	3.79690	0.56260
Si	-4.62860	0.24570	-0.32780	C	6.91140	4.87990	0.51440
Si	3.72760	2.26830	-0.11810	H	7.14730	6.92570	-0.32200
C	-3.97380	-2.92980	-3.70690	H	5.04430	6.90270	-1.52820
C	-3.28920	-1.78050	-3.73350	H	3.52950	4.88280	-1.41260
C	-3.50200	-0.76740	-2.67920	H	6.42770	2.96460	1.17960
C	-4.35150	-1.01150	-1.66800	H	7.83870	4.90340	1.07220
C	-5.13260	-2.27200	-1.66280	C	3.50450	0.75650	-4.55350
C	-4.95050	-3.18170	-2.62800	C	2.88480	1.88730	-4.20050
H	-3.81870	-3.67330	-4.47790	C	2.91750	2.34110	-2.79510
H	-2.57690	-1.59040	-4.52580	C	3.54080	1.60780	-1.85530
H	-2.96030	0.16600	-2.74010	C	4.16810	0.32050	-2.24710
H	-5.86010	-2.45900	-0.88300	C	4.18570	-0.05880	-3.52990
H	-5.51900	-4.10260	-2.62100	H	3.49320	0.42800	-5.58460
C	-9.23550	1.09810	-0.29800	H	2.37440	2.48280	-4.94630
C	-8.55980	1.10160	-1.45290	H	2.43200	3.27330	-2.54460
C	-7.10620	0.83690	-1.46090	H	4.62390	-0.32280	-1.51160
C	-6.45410	0.60120	-0.30960	H	4.67120	-0.98280	-3.81530
C	-7.21050	0.59020	0.96670	C	5.65150	-0.90320	2.75880
C	-8.52810	0.82790	0.96990	C	4.45280	-0.38410	3.04600
H	-10.30040	1.29100	-0.29040	C	3.83880	0.60920	2.14010
H	-9.07600	1.29710	-2.38390	C	4.47600	0.99240	1.02060
H	-6.57880	0.83610	-2.40700	C	5.81030	0.41770	0.71530
H	-6.70760	0.39300	1.90360	C	6.36310	-0.48310	1.53620
H	-9.07880	0.82170	1.90170	H	6.10150	-1.63170	3.42070

H	3.92760	-0.69340	3.94030	H	3.76160	-5.08570	2.11220
H	2.87250	1.01600	2.40120	H	4.37330	-3.51500	2.64670
H	6.34880	0.73300	-0.16960	H	4.63890	-4.06900	0.96680
H	7.33610	-0.89950	1.31000	C	-0.28020	-3.86100	4.57000
N	0.08430	-2.92480	-1.73590	C	0.04840	-2.57690	4.16360
H	-0.36200	-1.98290	-1.90180	C	0.92640	-2.33250	3.09080
H	-2.10110	-2.41900	-0.69100	C	1.53450	-3.43900	2.43420
C	5.31110	-4.06260	-3.72580	C	1.17160	-4.73190	2.86530
H	5.97680	-3.57490	-3.00970	C	0.27900	-4.95580	3.90510
C	-2.14910	-7.20610	1.14190	H	-0.97360	-4.00850	5.39340
H	-1.75800	-7.23560	2.16150	H	-0.36730	-1.70310	4.65370
C	1.67490	-4.86250	-0.66740	H	1.60040	-5.59090	2.36050
H	2.18840	-4.20540	0.49390	H	0.03560	-5.97200	4.19960
H	2.20600	-5.79160	-0.48210	O	1.18310	-1.03220	2.83150
O	0.57310	-0.55830	0.36920	H	0.92930	-0.77670	1.90290
H	2.07900	-1.56380	0.46310				
C	3.93470	-4.05500	1.80220				

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C	0.11270	-3.05670	1.08050	C	-2.72890	-1.72400	3.24700
C	2.53190	-4.42860	0.55800	C	-3.13910	-1.61610	4.66600
C	2.40460	-3.14720	0.18630	C	-2.30300	-1.99740	5.63800
C	1.10730	-2.43410	0.39190	C	-0.96540	-2.52160	5.30060
H	3.45980	-4.96250	0.40160	C	-0.58750	-2.62870	4.02150
C	1.40350	-5.15140	1.16640	H	-4.11700	-1.22730	4.92160
C	0.23930	-4.51110	1.40720	H	-2.60290	-1.91710	6.67490
C	-0.90810	-5.28960	1.95510	H	-0.28750	-2.81230	6.09270
C	-0.76930	-6.58790	2.24700	H	0.40410	-2.99820	3.79560
C	0.51920	-7.26600	2.01590	O	1.03810	-1.09860	0.05470
C	1.54860	-6.58810	1.49850	P	-0.25890	-0.52680	-0.82450
H	-1.87210	-4.82410	2.10910	O	-1.43740	-1.66990	-0.73060
H	-1.60670	-7.14760	2.64340	O	0.10030	-0.41960	-2.29140
H	0.62560	-8.31590	2.25680	N	1.10490	2.36210	1.23860
H	2.48900	-7.09540	1.32170	H	2.10730	2.31990	1.13460
C	-3.65590	-1.29550	2.17920	C	0.52610	3.57380	1.47320
C	-1.11280	-2.32640	1.49620	C	1.90260	3.75690	-1.45950
C	-1.90840	-1.79690	0.54860	C	1.72160	2.55780	-2.12830
C	-3.28260	-1.34500	0.89180	C	-0.65010	2.95470	-2.33460
H	-4.65440	-0.97140	2.44800	C	-0.53130	4.17540	-1.69540
C	-1.51530	-2.23040	2.92920	C	2.77740	1.57210	-2.52750

H	2.41280	0.56780	-2.29860	C	4.76780	1.58690	1.96020
H	2.93130	1.62210	-3.61180	C	5.30620	1.45130	0.74420
C	-1.90330	2.37160	-2.91330	C	5.02100	0.24670	-0.06330
H	-2.17470	2.89420	-3.83540	C	4.18400	-0.69880	0.39580
H	-2.74260	2.48780	-2.22890	C	3.60290	-0.54620	1.75480
H	-1.74100	1.31510	-3.12730	C	3.88540	0.53190	2.49530
C	-1.69680	5.06100	-1.56100	H	4.97860	2.46710	2.55390
C	3.25250	4.24430	-1.08710	H	5.95870	2.22020	0.35130
H	4.15310	6.54500	1.00960	H	5.50780	0.14880	-1.01910
H	5.01950	5.00330	0.70900	H	2.97120	-1.31730	2.17420
H	-3.46600	6.43440	-0.10950	H	3.46940	0.63120	3.48940
H	-2.21670	7.63200	0.37310	C	-8.43960	-3.24680	0.88880
O	3.16260	5.27050	-0.20500	C	-8.51460	-1.95790	0.53940
O	4.32270	3.81560	-1.47950	C	-7.29730	-1.22940	0.12470
O	-2.74180	4.99910	-2.17740	C	-6.11090	-1.86090	0.07600
O	-1.47900	6.02350	-0.60710	C	-6.03340	-3.28410	0.49150
Si	3.87010	-2.26680	-0.56950	C	-7.13680	-3.93960	0.87170
Si	-4.54770	-0.97500	-0.42980	H	-9.33030	-3.78060	1.19400
C	2.97960	-1.55050	-5.12490	H	-9.46730	-1.44460	0.56010
C	4.15770	-1.18270	-4.61010	H	-7.39220	-0.18590	-0.13190
C	4.44720	-1.41660	-3.18020	H	-5.08110	-3.79510	0.52290
C	3.52160	-1.97580	-2.38080	H	-7.07410	-4.97460	1.18200
C	2.23370	-2.41960	-2.97130	C	-2.99010	-2.68270	-4.51920
C	1.97490	-2.20840	-4.26760	C	-3.19880	-3.50340	-3.48440
H	2.76510	-1.37780	-6.17160	C	-3.71310	-2.96860	-2.20670
H	4.90180	-0.71140	-5.23900	C	-3.98010	-1.65700	-2.07420
H	5.42400	-1.15130	-2.80410	C	-3.75530	-0.75670	-3.23250
H	1.49060	-2.91810	-2.36510	C	-3.28220	-1.24260	-4.38660
H	1.03070	-2.52550	-4.69150	H	-2.60650	-3.07140	-5.45370
C	7.69520	-4.90940	-0.00080	H	-2.98170	-4.55970	-3.57670
C	7.16450	-4.77390	-1.22180	H	-3.82870	-3.64820	-1.37600
C	5.95860	-3.94220	-1.41820	H	-3.95580	0.30010	-3.15740
C	5.39620	-3.31120	-0.37330	H	-3.11080	-0.57980	-5.22500
C	5.98340	-3.47320	0.97860	C	-5.29100	3.65310	-0.65890
C	7.07390	-4.22940	1.15350	C	-5.91610	2.83240	-1.50960
H	8.57760	-5.51920	0.14420	C	-5.68190	1.37560	-1.43920
H	7.61560	-5.27510	-2.06840	C	-4.83220	0.86610	-0.53010
H	5.53710	-3.86900	-2.41100	C	-4.13570	1.78410	0.40460
H	5.53090	-2.98290	1.83140	C	-4.36040	3.10330	0.34590
H	7.50130	-4.34640	2.14100	H	-5.46300	4.72050	-0.70710

H	-6.59750	3.23260	-2.24900	H	-1.45360	4.45150	1.73020
H	-6.20670	0.72800	-2.13070	H	-1.18140	2.92700	2.58460
H	-3.44820	1.39790	1.14440	H	-1.41650	2.89810	0.83390
H	-3.86170	3.77250	1.03390	C	2.67320	6.15250	4.19870
N	0.46270	2.18590	-2.49480	C	1.74300	6.70520	3.32560
H	0.31180	1.14710	-2.65690	C	1.03540	5.89870	2.42470
H	3.72630	1.77800	-2.04580	C	1.26970	4.50470	2.39090
C	-2.55780	6.95920	-0.41260	C	2.20810	3.97460	3.29340
H	-2.75450	7.50670	-1.33650	C	2.90920	4.77590	4.18790
C	4.41550	5.79670	0.26320	H	3.20700	6.79630	4.89150
H	4.97460	6.24560	-0.56130	H	1.53790	7.77060	3.31670
C	0.73320	4.53010	-1.05890	H	2.34900	2.90030	3.30940
H	0.58450	4.23740	0.26280	H	3.61820	4.32850	4.87700
H	0.91310	5.59130	-0.90920	O	0.15010	6.55840	1.62910
O	-0.66600	0.73960	-0.09920	H	-0.24680	6.00790	0.93600
H	0.53840	1.63510	0.75730				
C	-0.98330	3.47120	1.65560				
C	2.94270	2.19250	-0.47140	C	0.53630	5.25980	-3.67130
C	5.40990	0.96350	0.14960	C	1.58950	5.29600	-4.49460
C	4.32410	0.19920	-0.04480	C	2.78470	4.48170	-4.20260
C	3.00510	0.84570	-0.32010	C	2.82500	3.71480	-3.10680
H	6.36720	0.52040	0.38590	H	-0.34050	5.85440	-3.89590
C	5.31870	2.43260	0.11080	H	1.56510	5.91660	-5.38100
C	4.13960	3.03090	-0.15970	H	3.62610	4.50020	-4.88330
C	4.05650	4.51760	-0.09960	H	3.70290	3.10970	-2.92280
C	5.14500	5.24690	0.17120	O	1.91640	0.05680	-0.61600
C	6.43680	4.58350	0.42690	P	0.55730	0.23820	0.33430
C	6.51980	3.24930	0.40460	O	0.54290	1.80680	0.83390
H	3.11550	5.02730	-0.25660	O	0.73630	-0.58870	1.59730
H	5.07820	6.32630	0.21500	N	-2.89340	-1.41900	-1.63970
H	7.31420	5.17920	0.64330	H	-3.00580	-1.63250	-2.61990
H	7.46940	2.76860	0.60470	C	-3.92960	-1.71070	-0.78110
C	-0.60660	4.35820	-1.56780	C	-1.76020	-3.97470	-0.52580
C	1.69000	2.84020	-0.93760	C	-0.63540	-3.27810	-0.09190
C	0.56390	2.69700	-0.20790	C	-1.61960	-2.96720	2.09300
C	-0.61890	3.55620	-0.49160	C	-2.75830	-3.64880	1.70870
H	-1.46090	4.98580	-1.79420	C	0.60370	-3.03740	-0.89810
C	1.67140	3.68570	-2.16700	H	0.35480	-2.60690	-1.86770
C	0.56860	4.41000	-2.45840	H	1.26970	-2.35090	-0.38340

C	-1.30970	-2.38830	3.44550	C	4.04430	-3.89100	-1.47460
H	-0.85780	-3.15250	4.08700	C	3.93290	-2.55360	-1.40210
H	-2.21260	-2.04730	3.94670	C	3.43650	-1.80400	-2.58330
H	-0.60460	-1.56110	3.33350	C	3.03010	-2.46080	-3.67680
C	-3.90370	-3.98410	2.58570	H	2.76330	-4.46220	-4.60720
C	-1.89590	-4.61660	-1.83970	H	3.65660	-5.69310	-2.71850
H	0.16740	-5.55680	-4.14620	H	4.45740	-4.45950	-0.65100
H	-1.34190	-6.42860	-3.71690	H	3.41460	-0.72390	-2.58300
H	-5.08760	-5.28580	4.57460	H	2.66510	-1.91240	-4.53550
H	-4.32200	-4.20740	5.78770	C	-5.76820	1.72990	-1.66160
O	-0.74130	-4.85270	-2.48340	C	-4.53910	1.63750	-2.18180
O	-2.98330	-4.94700	-2.31320	C	-3.38440	2.21880	-1.46500
O	-5.00450	-4.27590	2.15280	C	-3.56110	2.84570	-0.28780
O	-3.61690	-3.96120	3.90710	C	-4.92570	2.92540	0.29160
Si	4.48460	-1.65690	0.13380	C	-5.97030	2.40240	-0.36270
Si	-2.12020	3.61430	0.61920	H	-6.61320	1.30010	-2.18360
C	2.16740	-2.84170	4.03640	H	-4.38650	1.13170	-3.12640
C	2.86610	-1.70300	3.98190	H	-2.40310	2.12150	-1.90820
C	3.58970	-1.33730	2.74710	H	-5.08230	3.41030	1.24720
C	3.53540	-2.13410	1.66510	H	-6.96370	2.46330	0.06240
C	2.76520	-3.40020	1.73740	C	-2.89260	8.19100	1.35620
C	2.11570	-3.73180	2.86010	C	-1.74460	7.63000	1.74970
H	1.63800	-3.11200	4.94070	C	-1.50440	6.19110	1.51490
H	2.90480	-1.04770	4.84230	C	-2.44440	5.42860	0.92890
H	4.16120	-0.41780	2.73300	C	-3.70230	6.06870	0.46500
H	2.71540	-4.06660	0.89110	C	-3.91460	7.37400	0.67410
H	1.54720	-4.65160	2.90720	H	-3.06940	9.24530	1.52540
C	8.98750	-2.85730	0.59840	H	-0.98720	8.22880	2.23870
C	8.13960	-3.07740	1.61020	H	-0.55080	5.77810	1.80610
C	6.71600	-2.70170	1.48020	H	-4.44880	5.50200	-0.06980
C	6.26960	-2.13180	0.34800	H	-4.83000	7.83760	0.32950
C	7.21240	-1.89660	-0.77200	C	-1.38340	1.35820	4.67860
C	8.50070	-2.23900	-0.65140	C	-0.54800	2.32800	4.29230
H	10.02990	-3.13260	0.69260	C	-0.79300	3.05860	3.03130
H	8.49400	-3.53220	2.52620	C	-1.84710	2.74730	2.25520
H	6.05140	-2.89690	2.31050	C	-2.78050	1.68580	2.70710
H	6.86200	-1.44390	-1.69140	C	-2.55910	1.02840	3.85130
H	9.18810	-2.06460	-1.46900	H	-1.20140	0.81620	5.59750
C	3.09920	-3.93470	-3.72380	H	0.31670	2.57200	4.89570
C	3.59310	-4.61340	-2.68230	H	-0.07260	3.80120	2.72280

H	-3.65230	1.43560	2.12660	H	-4.36560	-1.36820	1.33020
H	-3.24590	0.25730	4.17530	H	-4.42200	0.07320	0.31340
N	-0.63770	-2.75700	1.15950	H	-2.85750	-0.62590	0.73540
H	0.06200	-1.96450	1.37670	C	-7.85330	-2.19280	-2.56930
H	1.11540	-3.98540	-1.07810	C	-6.72100	-2.59780	-3.26990
C	-4.71940	-4.27740	4.77560	C	-5.45240	-2.49380	-2.69580
H	-5.53840	-3.56850	4.63300	C	-5.28870	-1.93810	-1.40680
C	-0.85580	-5.45340	-3.78720	C	-6.45150	-1.57170	-0.70860
H	-1.43500	-4.81240	-4.45550	C	-7.71740	-1.68990	-1.27560
C	-2.93780	-3.96810	0.30520	H	-8.83440	-2.28060	-3.02640
H	-3.67260	-2.87000	-0.25370	H	-6.78880	-3.01070	-4.27100
H	-3.72120	-4.68200	0.06620	H	-6.36630	-1.16470	0.29160
O	-0.60680	-0.07020	-0.56770	H	-8.59090	-1.38090	-0.71000
H	-2.08200	-0.88530	-1.31290	O	-4.38000	-2.90160	-3.46160
C	-3.89280	-0.86400	0.48500	H	-3.95450	-3.68250	-3.04300
C	0.17110	-3.09000	1.01580	C	-2.95050	-1.70880	4.73170
C	2.59100	-4.44390	0.46060	C	-2.07790	-2.09850	5.66750
C	2.46050	-3.15400	0.11930	C	-0.75240	-2.61470	5.27440
C	1.15700	-2.45320	0.32930	C	-0.42220	-2.70560	3.98100
H	3.52270	-4.96970	0.30030	H	-3.91950	-1.32630	5.02780
C	1.46460	-5.18360	1.05190	H	-2.33940	-2.03120	6.71560
C	0.30160	-4.55000	1.31300	H	-0.04470	-2.91250	6.03730
C	-0.84070	-5.33930	1.85580	H	0.56150	-3.06920	3.71410
C	-0.69900	-6.64310	2.12050	O	1.08000	-1.11500	0.00500
C	0.58810	-7.31570	1.86520	P	-0.24710	-0.51760	-0.81210
C	1.61320	-6.62660	1.35400	O	-1.43350	-1.65620	-0.71700
H	-1.80290	-4.87630	2.02880	O	0.06850	-0.37700	-2.28690
H	-1.53260	-7.21090	2.51340	N	1.06050	2.42880	1.34600
H	0.69700	-8.36990	2.08450	H	2.06600	2.40830	1.26560
H	2.55290	-7.12920	1.16080	C	0.45660	3.64490	1.51370
C	-3.56110	-1.36640	2.26930	C	1.97280	3.75890	-1.33560
C	-1.03940	-2.36730	1.48110	C	1.80380	2.55300	-1.99680
C	-1.86890	-1.82610	0.56970	C	-0.54380	2.99890	-2.35550
C	-3.24260	-1.41340	0.96670	C	-0.43870	4.21500	-1.70850
H	-4.55210	-1.05560	2.57990	C	2.85310	1.52260	-2.28240
C	-1.39080	-2.29650	2.92870	H	2.59960	0.61380	-1.72740
C	-2.59260	-1.79850	3.29730	H	2.82870	1.25900	-3.34380

C	-1.75160	2.41820	-3.02820	C	5.12130	0.22990	0.02640
H	-1.77920	2.73050	-4.07840	C	4.23500	-0.69740	0.42710
H	-2.67630	2.75060	-2.56490	C	3.56580	-0.53030	1.74360
H	-1.67860	1.32990	-2.99490	C	3.80880	0.55020	2.49500
C	-1.53220	5.17690	-1.51250	H	4.92480	2.46850	2.62150
C	3.30860	4.24650	-0.90610	H	6.06620	2.18600	0.50210
H	4.10590	6.59930	1.17130	H	5.66780	0.12080	-0.89600
H	4.99560	5.06000	0.93000	H	2.89790	-1.29040	2.12400
H	-4.03200	5.96080	-1.20700	H	3.32290	0.66380	3.45540
H	-3.25380	7.06110	-2.36500	C	-8.16890	-4.01360	0.14560
O	3.18050	5.30380	-0.07020	C	-8.22890	-3.00640	-0.73310
O	4.39520	3.79880	-1.22610	C	-7.09470	-2.06830	-0.86220
O	-1.52220	6.01060	-0.60950	C	-6.00670	-2.20870	-0.08590
O	-2.53890	5.09990	-2.39880	C	-5.93700	-3.34170	0.87040
Si	3.93560	-2.24320	-0.58110	C	-6.96470	-4.19270	0.98130
Si	-4.57770	-1.03280	-0.28210	H	-8.99820	-4.70240	0.24080
C	3.14170	-1.37820	-5.12760	H	-9.10750	-2.87650	-1.35160
C	4.31900	-1.05400	-4.58210	H	-7.15830	-1.26570	-1.58690
C	4.57480	-1.33030	-3.15340	H	-5.05430	-3.50370	1.47250
C	3.62280	-1.89180	-2.38740	H	-6.91160	-5.02050	1.67670
C	2.33370	-2.28250	-3.01110	C	-3.21970	-1.61460	-4.72550
C	2.10390	-2.02940	-4.30530	C	-3.16440	-2.63830	-3.86580
H	2.95170	-1.17410	-6.17330	C	-3.60180	-2.45390	-2.46670
H	5.08640	-0.58630	-5.18510	C	-4.02520	-1.25090	-2.04260
H	5.54900	-1.09500	-2.75120	C	-4.11580	-0.12980	-3.00810
H	1.56770	-2.77830	-2.43190	C	-3.72970	-0.30290	-4.27840
H	1.15950	-2.30950	-4.75390	H	-2.89900	-1.74720	-5.75060
C	7.75540	-4.91380	-0.11010	H	-2.79760	-3.60280	-4.19200
C	7.21710	-4.31380	0.95790	H	-3.55640	-3.29610	-1.78700
C	6.01350	-3.47050	0.80500	H	-4.50090	0.83230	-2.70000
C	5.46010	-3.29400	-0.40680	H	-3.79230	0.51770	-4.98140
C	6.05330	-3.97290	-1.58500	C	-5.78510	3.40600	0.58730
C	7.14270	-4.73810	-1.44240	C	-6.69790	2.43770	0.72920
H	8.63640	-5.53270	0.00030	C	-6.33580	1.03090	0.45420
H	7.66120	-4.44490	1.93610	C	-5.09370	0.72170	0.04490
H	5.58820	-3.00070	1.68330	C	-4.08640	1.79680	-0.09890
H	5.60410	-3.87150	-2.56340	C	-4.41400	3.06830	0.15760
H	7.57240	-5.23670	-2.30150	H	-6.04760	4.43620	0.78980
C	4.74440	1.58730	2.01940	H	-7.70270	2.68160	1.04900
C	5.37180	1.43200	0.84920	H	-7.08480	0.26630	0.60290



H	-3.08180	1.55540	-0.41540	H	-1.55620	4.48810	1.62350
H	-3.67490	3.85000	0.05500	H	-1.26290	3.07180	2.64560
N	0.56280	2.20530	-2.43790	H	-1.45100	2.85270	0.90140
H	0.39600	1.16540	-2.60350	C	2.52100	6.31990	4.21130
H	3.84360	1.87350	-2.01490	C	1.60720	6.83970	3.30330
C	-3.61400	6.04140	-2.21200	C	0.91890	6.00730	2.40610
H	-4.35870	5.78040	-2.96270	C	1.16350	4.61280	2.42330
C	4.40780	5.84390	0.44760	C	2.08870	4.11550	3.35960
H	4.99980	6.28670	-0.35720	C	2.76680	4.94480	4.24540
C	0.79640	4.54730	-1.00770	H	3.03520	6.98770	4.89660
H	0.55280	4.25990	0.31360	H	1.39510	7.90280	3.25930
H	0.96930	5.60560	-0.83240	H	2.24140	3.04300	3.40620
O	-0.61890	0.73100	-0.04250	H	3.46470	4.52200	4.96090
H	0.53040	1.68350	0.85630	O	0.06470	6.65740	1.57940
C	-1.05660	3.52080	1.66870	H	-0.38540	6.12400	0.89860
C	0.78220	-2.77730	1.40850	C	-2.88620	-1.80300	4.74220
C	3.44260	-3.66560	1.01350	C	-2.03240	-1.87070	5.76960
C	3.04340	-2.51170	0.46200	C	-0.59250	-2.07920	5.52300
C	1.63490	-2.04430	0.63790	C	-0.13640	-2.21300	4.27220
H	4.45100	-4.02910	0.87300	H	-3.94060	-1.64310	4.93060
C	2.49820	-4.51000	1.75990	H	-2.39430	-1.76620	6.78420
C	1.21710	-4.11580	1.92170	H	0.09530	-2.11570	6.35790
C	0.25740	-5.05390	2.57340	H	0.92520	-2.34680	4.11090
C	0.67390	-6.23620	3.04080	O	1.30930	-0.79240	0.15600
C	2.08650	-6.63270	2.90030	P	-0.08530	-0.55460	-0.72110
C	2.95090	-5.81920	2.28630	O	-0.95150	-1.94310	-0.57220
H	-0.79130	-4.80580	2.66040	O	0.25250	-0.39970	-2.18900
H	-0.02870	-6.91200	3.51100	N	0.44760	2.60660	1.40000
H	2.41770	-7.58940	3.28280	H	1.44330	2.76790	1.38370
H	3.98410	-6.12360	2.17310	C	-0.37860	3.69130	1.51240
C	-3.33820	-1.84880	2.22280	C	1.20390	4.06710	-1.29470
C	-0.59290	-2.30290	1.71690	C	1.30020	2.84390	-1.93640
C	-1.44350	-2.07190	0.69870	C	-1.08410	2.77700	-2.32280
C	-2.89820	-1.91500	0.95740	C	-1.23810	4.01190	-1.72140
H	-4.39620	-1.73620	2.42930	C	2.54890	2.06340	-2.20710
C	-1.07730	-2.16440	3.12130	H	3.42030	2.54320	-1.77730
C	-2.39170	-1.94390	3.35330	H	2.41400	1.05140	-1.81520

C	-2.15770	1.93410	-2.94760	C	5.44860	0.95200	-0.48400
H	-2.42830	2.32940	-3.93170	C	4.52420	0.14870	0.07100
H	-3.06060	1.92930	-2.33800	C	3.82780	0.59810	1.30380
H	-1.78910	0.91410	-3.06000	C	4.07370	1.81040	1.81570
C	-2.50220	4.74700	-1.59290	H	5.23190	3.69100	1.57320
C	2.40140	4.82000	-0.84220	H	6.43080	2.94510	-0.39800
H	3.61140	7.17300	-0.27040	H	6.03460	0.62670	-1.33170
H	2.65180	7.28320	1.24620	H	3.14050	-0.05460	1.82130
H	-4.48950	6.21020	-2.78810	H	3.57120	2.13080	2.71910
H	-5.37730	4.67700	-3.05800	C	-6.05110	2.36820	-0.84750
O	2.04010	5.82400	-0.00830	C	-5.10180	2.15430	0.07040
O	3.56220	4.60830	-1.14310	C	-4.48330	0.81800	0.19950
O	-2.67590	5.61490	-0.73990	C	-4.87430	-0.18880	-0.60090
O	-3.44770	4.42960	-2.49290	C	-5.90730	0.06610	-1.63550
Si	4.23310	-1.56030	-0.62110	C	-6.46460	1.27680	-1.75010
Si	-4.14270	-1.89640	-0.43370	H	-6.52060	3.33900	-0.92970
C	2.44640	-1.58370	-4.96540	H	-4.79490	2.95610	0.72900
C	3.46430	-0.76800	-4.66960	H	-3.72510	0.67140	0.95570
C	4.03810	-0.76090	-3.30780	H	-6.21750	-0.72980	-2.30120
C	3.52370	-1.55020	-2.34940	H	-7.22090	1.45820	-2.50280
C	2.41630	-2.47830	-2.69710	C	-7.44950	-4.99880	0.78820
C	1.90460	-2.48860	-3.93380	C	-6.16050	-5.35430	0.78280
H	2.02390	-1.58820	-5.96180	C	-5.12360	-4.37460	0.39820
H	3.86860	-0.10830	-5.42630	C	-5.46650	-3.12730	0.03070
H	4.86690	-0.10180	-3.10490	C	-6.89810	-2.73350	0.06730
H	2.01350	-3.15910	-1.95990	C	-7.83490	-3.62250	0.42040
H	1.09460	-3.16260	-4.18070	H	-8.21040	-5.71450	1.07140
C	8.43710	-3.62300	-0.61090	H	-5.87310	-6.35940	1.06320
C	7.69580	-3.64260	-1.72500	H	-4.08740	-4.67690	0.44730
C	6.36660	-2.99630	-1.74290	H	-7.20270	-1.72640	-0.17160
C	5.89810	-2.38710	-0.64060	H	-8.87710	-3.33140	0.44820
C	6.72390	-2.36840	0.59060	C	-2.01130	-3.18200	-4.41910
C	7.92700	-2.95500	0.60360	C	-2.59290	-1.98120	-4.33310
H	9.41030	-4.09640	-0.59690	C	-3.28910	-1.58190	-3.09270
H	8.06730	-4.13250	-2.61570	C	-3.34750	-2.42000	-2.04290
H	5.78460	-3.03350	-2.65360	C	-2.70210	-3.75350	-2.15050
H	6.35540	-1.88190	1.48530	C	-2.06700	-4.11020	-3.27370
H	8.52840	-2.94170	1.50330	H	-1.49420	-3.47270	-5.32440
C	5.04580	2.70700	1.16270	H	-2.54730	-1.29460	-5.16850
C	5.70670	2.29520	0.07570	H	-3.72270	-0.59530	-3.04850

H	-2.70380	-4.43420	-1.31300	H	-2.08310	2.59520	0.77050
H	-1.58280	-5.07590	-3.34080	H	-2.51410	4.15230	1.54140
N	0.16440	2.23410	-2.38310	H	-2.01710	2.76730	2.52760
H	0.22560	1.18270	-2.53260	C	1.00280	6.73290	4.25810
H	2.69520	1.97100	-3.28880	C	0.04450	7.05800	3.30670
C	-4.66500	5.19680	-2.41840	C	-0.42810	6.10170	2.39360
H	-5.02460	5.25330	-1.39050	C	0.08320	4.78190	2.44050
C	3.11710	6.61160	0.52630	C	1.04850	4.48160	3.41960
H	3.85240	5.97000	1.01600	C	1.51190	5.43320	4.32070
C	-0.11510	4.60760	-1.01090	H	1.34620	7.49230	4.95480
H	-0.33260	4.30690	0.31170	H	-0.36930	8.05870	3.23870
H	-0.16500	5.68270	-0.86200	H	1.40840	3.46060	3.48730
O	-0.78700	0.60100	-0.03690	H	2.24810	5.16030	5.06990
H	0.09380	1.77150	0.89590	O	-1.35830	6.56700	1.52500
C	-1.84970	3.28970	1.58030	H	-1.65290	5.95800	0.82310
C	-0.36780	-3.19180	0.90260	C	-2.84290	-2.47540	5.48990
C	1.93530	-4.71820	0.30060	C	-1.55230	-3.08910	5.12210
C	1.94350	-3.39540	0.08180	C	-1.13790	-3.07270	3.85000
C	0.70980	-2.58880	0.33310	H	-4.54080	-1.43580	4.83260
H	2.81290	-5.31940	0.10410	H	-3.17300	-2.49460	6.52050
C	0.71970	-5.39590	0.77810	H	-0.93760	-3.54530	5.88720
C	-0.39150	-4.68000	1.05120	H	-0.17930	-3.51070	3.60470
C	-1.63030	-5.40350	1.45650	O	0.77440	-1.22030	0.17020
C	-1.62490	-6.73450	1.59210	P	-0.40980	-0.44030	-0.71060
C	-0.39360	-7.50140	1.32820	O	-1.70370	-1.45440	-0.76510
C	0.71720	-6.86920	0.93670	O	0.03560	-0.25870	-2.14870
H	-2.55390	-4.86830	1.63050	N	1.19070	2.23450	1.37370
H	-2.52810	-7.25400	1.88530	H	2.10270	1.80540	1.35150
H	-0.39510	-8.57770	1.44230	C	1.10530	3.55510	1.69650
H	1.61500	-7.44000	0.73440	C	2.41000	3.70540	-1.30510
C	-3.97720	-1.19670	2.11950	C	2.03200	2.52900	-1.93630
C	-1.53240	-2.39910	1.37250	C	-0.29020	3.20320	-1.92570
C	-2.23120	-1.67230	0.48000	C	0.03050	4.39380	-1.30320
C	-3.56490	-1.11760	0.84490	C	2.92050	1.43450	-2.45000
H	-4.92890	-0.78280	2.41830	H	3.24760	1.66620	-3.46990
C	-1.97840	-2.44560	2.79450	H	3.81340	1.31950	-1.84470
C	-3.14590	-1.86100	3.14360	C	-1.63630	2.76360	-2.42250
C	-3.59810	-1.89000	4.55390	H	-2.39590	2.89510	-1.65380

H	-1.58850	1.71270	-2.70530	C	3.35030	-1.03750	1.89650
H	-1.93850	3.36180	-3.28660	C	3.72500	-0.05590	2.72600
C	-0.88590	5.53920	-1.10680	H	5.01810	1.73780	2.95970
C	3.79430	4.13720	-1.05680	H	6.01940	1.56230	0.76050
H	6.72580	3.10620	-1.95010	H	5.39000	-0.33730	-0.77810
H	6.26750	4.83820	-1.85570	H	2.62980	-1.76740	2.23970
H	-2.54920	7.39740	-2.09170	H	3.29580	0.01070	3.71720
H	-3.90800	6.22800	-2.03460	C	-9.11070	-1.76260	0.30620
O	4.74630	3.41860	-1.67840	C	-8.41680	-2.27710	-0.71510
O	4.08460	5.10260	-0.35290	C	-7.02610	-1.84150	-0.96170
O	-0.57510	6.54080	-0.48610	C	-6.44380	-0.93910	-0.15280
O	-2.09330	5.39760	-1.70220	C	-7.22910	-0.35740	0.96490
Si	3.50930	-2.59330	-0.55200	C	-8.48950	-0.75120	1.18340
Si	-4.69550	-0.35240	-0.43630	H	-10.12940	-2.08030	0.48700
C	2.92990	-1.42130	-5.06170	H	-8.87240	-3.01390	-1.36400
C	1.91100	-1.94690	-4.37330	H	-6.50050	-2.26700	-1.80220
C	2.09300	-2.33190	-2.95840	H	-6.79460	0.40320	1.60080
C	3.27150	-2.12740	-2.34340	H	-9.05950	-0.32220	1.99740
C	4.40930	-1.58550	-3.12880	C	-3.18800	-1.57730	-4.70760
C	4.24390	-1.24570	-4.41310	C	-3.39570	-0.28650	-4.42400
H	2.79740	-1.13640	-6.09730	C	-3.89380	0.10900	-3.09020
H	0.94840	-2.08610	-4.84830	C	-4.13790	-0.82270	-2.15410
H	1.25270	-2.76490	-2.43520	C	-3.91720	-2.25430	-2.48100
H	5.39010	-1.49560	-2.68460	C	-3.46330	-2.60950	-3.68880
H	5.07710	-0.85660	-4.98360	H	-2.81820	-1.86740	-5.68250
C	7.04440	-5.64600	-0.18560	H	-3.19270	0.47270	-5.16820
C	6.54660	-5.05770	0.90820	H	-4.04100	1.15910	-2.88770
C	5.43250	-4.09450	0.78890	H	-4.10360	-3.01700	-1.73490
C	4.92140	-3.79660	-0.41770	H	-3.29300	-3.65300	-3.91990
C	5.46760	-4.46360	-1.62530	C	-4.91790	4.27320	0.24500
C	6.47560	-5.33760	-1.51310	C	-5.68400	3.69460	-0.68620
H	7.85990	-6.35240	-0.09980	C	-5.59470	2.23840	-0.91710
H	6.95820	-5.28580	1.88280	C	-4.72840	1.49260	-0.21090
H	5.03860	-3.63600	1.68740	C	-3.86660	2.14350	0.80660
H	5.04750	-4.26580	-2.60180	C	-3.96490	3.46070	1.02630
H	6.87060	-5.82700	-2.39390	H	-4.99580	5.33650	0.42880
C	4.72720	0.93710	2.29250	H	-6.38260	4.28880	-1.26070
C	5.27790	0.84140	1.07820	H	-6.25110	1.78210	-1.64790
C	4.88990	-0.25980	0.17290	H	-3.16180	1.56220	1.38550
C	3.94800	-1.14440	0.54060	H	-3.35110	3.93450	1.78050

N	0.71140	2.30440	-2.17190	H	-0.98140	3.67230	1.16870
H	0.42310	1.29830	-2.35640	H	-0.34580	5.13570	1.97100
H	2.34850	0.50640	-2.47320	C	3.89370	4.73800	4.78900
C	-2.96820	6.53110	-1.57370	C	3.65310	5.61070	3.73150
H	-3.11510	6.78900	-0.52320	C	2.78710	5.25840	2.69020
C	6.10280	3.84100	-1.44170	C	2.14210	4.00650	2.70560
H	6.31930	3.86110	-0.37200	C	2.40160	3.13830	3.78190
C	1.37550	4.58100	-0.77290	C	3.26660	3.49170	4.81350
H	1.33610	4.25890	0.55400	H	4.56860	5.02950	5.58860
H	1.64450	5.61860	-0.59890	H	4.12960	6.58430	3.68140
O	-0.73580	0.80170	0.08850	H	1.88900	2.18220	3.80730
H	0.42060	1.70870	0.91040	H	3.44060	2.80100	5.63290
C	-0.31380	4.04580	1.94890	O	2.57340	6.16760	1.68630
H	-0.66060	3.65260	2.90990	H	3.11430	5.90220	0.91170
C	-0.35870	-3.18860	0.91480	C	-1.54170	-3.06960	5.13460
C	1.94600	-4.71480	0.31740	C	-1.12710	-3.05670	3.86250
C	1.95140	-3.39340	0.09000	H	-4.53670	-1.42930	4.83800
C	0.71690	-2.58710	0.33970	H	-3.16490	-2.47590	6.53030
H	2.82430	-5.31570	0.12320	H	-0.92530	-3.52030	5.90170
C	0.73260	-5.39150	0.80160	H	-0.16680	-3.49180	3.61900
C	-0.37940	-4.67590	1.07200	O	0.78030	-1.21940	0.16980
C	-1.61630	-5.39940	1.48370	P	-0.40880	-0.44210	-0.70630
C	-1.60800	-6.72940	1.62810	O	-1.69940	-1.46030	-0.75860
C	-0.37560	-7.49560	1.36740	O	0.03120	-0.25950	-2.14590
C	0.73330	-6.86370	0.97000	N	1.17670	2.25200	1.38260
H	-2.54080	-4.86500	1.65530	H	2.08870	1.82280	1.35940
H	-2.50970	-7.24870	1.92610	C	1.09420	3.57460	1.69790
H	-0.37480	-8.57110	1.48870	C	2.39720	3.70560	-1.30340
H	1.63190	-7.43410	0.77010	C	2.01970	2.52610	-1.92930
C	-3.97370	-1.19880	2.12410	C	-0.30220	3.20120	-1.92630
C	-1.52440	-2.39580	1.38230	C	0.01740	4.39440	-1.30850
C	-2.22610	-1.67540	0.48700	C	2.90910	1.42740	-2.43270
C	-3.56140	-1.12320	0.84940	H	3.78960	1.30300	-1.81090
H	-4.92700	-0.78730	2.42070	H	2.33150	0.50340	-2.47010
C	-1.97000	-2.43730	2.80450	C	-1.64790	2.75860	-2.42220
C	-3.13990	-1.85580	3.15100	H	-1.94750	3.34910	-3.29260
C	-3.59210	-1.88100	4.56130	H	-2.40930	2.89820	-1.65680
C	-2.83480	-2.45960	5.49970	H	-1.60060	1.70520	-2.69550

C	-0.89960	5.54040	-1.11800	H	5.03010	1.75100	2.94170
C	3.78130	4.13660	-1.05430	H	6.05610	1.54460	0.75630
H	6.71340	3.07350	-1.90690	H	5.42430	-0.36150	-0.77340
H	6.26570	4.81000	-1.85300	H	2.62290	-1.74230	2.22950
H	-2.56130	7.39450	-2.11370	H	3.28810	0.04330	3.69740
H	-3.92020	6.22540	-2.05400	C	-9.10890	-1.77280	0.30850
O	4.73390	3.40410	-1.65880	C	-8.41400	-2.29210	-0.70970
O	4.07160	5.11170	-0.36370	C	-7.02280	-1.85830	-0.95650
O	-0.59000	6.54440	-0.50070	C	-6.44090	-0.95290	-0.15050
O	-2.10590	5.39640	-1.71510	C	-7.22710	-0.36630	0.96390
Si	3.51420	-2.59250	-0.55330	C	-8.48810	-0.75830	1.18240
Si	-4.69310	-0.36630	-0.43600	H	-10.12810	-2.08910	0.48920
C	2.90910	-1.42370	-5.06080	H	-8.86920	-3.03110	-1.35630
C	1.89530	-1.95240	-4.36730	H	-6.49660	-2.28710	-1.79500
C	2.08520	-2.33580	-2.95310	H	-6.79290	0.39660	1.59720
C	3.26580	-2.12670	-2.34350	H	-9.05890	-0.32540	1.99370
C	4.39790	-1.58120	-3.13460	C	-3.18160	-1.61590	-4.69890
C	4.22530	-1.24290	-4.41830	C	-3.39150	-0.32360	-4.42370
H	2.77090	-1.14030	-6.09610	C	-3.89070	0.07980	-3.09270
H	0.93100	-2.09530	-4.83790	C	-4.13420	-0.84630	-2.15080
H	1.24880	-2.77180	-2.42600	C	-3.91130	-2.27960	-2.46840
H	5.38040	-1.48740	-2.69540	C	-3.45610	-2.64200	-3.67370
H	5.05460	-0.85120	-4.99300	H	-2.81080	-1.91180	-5.67170
C	7.05170	-5.64530	-0.21340	H	-3.18930	0.43100	-5.17280
C	6.56230	-5.05690	0.88410	H	-4.03960	1.13080	-2.89700
C	5.44720	-4.09370	0.77320	H	-4.09710	-3.03780	-1.71770
C	4.92680	-3.79620	-0.42940	H	-3.28410	-3.68670	-3.89800
C	5.46380	-4.46320	-1.64110	C	-4.92480	4.26240	0.21980
C	6.47270	-5.33700	-1.53650	C	-5.68630	3.67780	-0.71150
H	7.86790	-6.35170	-0.13380	C	-5.59400	2.22050	-0.93420
H	6.98140	-5.28480	1.85560	C	-4.72900	1.47980	-0.22100
H	5.06030	-3.63480	1.67460	C	-3.87240	2.13740	0.79660
H	5.03640	-4.26530	-2.61440	C	-3.97380	3.45550	1.00920
H	6.86110	-5.82650	-2.42040	H	-5.00510	5.32650	0.39770
C	4.74020	0.94620	2.27880	H	-6.38350	4.26790	-1.29190
C	5.30430	0.83370	1.07210	H	-6.24710	1.75930	-1.66480
C	4.91560	-0.27170	0.17210	H	-3.16900	1.56020	1.38140
C	3.96060	-1.14350	0.53660	H	-3.36390	3.93420	1.76350
C	3.35140	-1.02060	1.88620	N	0.69980	2.30170	-2.16790
C	3.72580	-0.03490	2.71080	H	0.41220	1.29470	-2.35110

H	3.25810	1.66170	-3.44470	H	-0.35140	5.16070	1.96760
C	-2.98110	6.53030	-1.59280	C	3.90310	4.77420	4.76560
H	-3.12980	6.79270	-0.54360	C	3.65280	5.64210	3.70640
C	6.09090	3.82290	-1.41940	C	2.77950	5.28410	2.67330
H	6.29830	3.86420	-0.34860	C	2.13660	4.03110	2.69860
C	1.36220	4.58480	-0.77810	C	2.40580	3.16780	3.77650
H	1.32210	4.27170	0.54880	C	3.27820	3.52700	4.80000
H	1.63110	5.62350	-0.61150	H	4.58350	5.07020	5.55880
O	-0.73600	0.79880	0.09400	H	4.12730	6.61630	3.64860
H	0.40760	1.72420	0.92030	H	1.89460	2.21130	3.81040
C	-0.32280	4.07070	1.95120	H	3.45930	2.84020	5.62110
H	-0.66870	3.68360	2.91510	O	2.55690	6.18810	1.66670
H	-0.99310	3.69560	1.17420	H	3.09960	5.92390	0.89290
C	0.21800	-3.10980	1.00240	C	-0.92640	-2.84380	5.23020
C	2.72710	-4.32690	0.53490	C	-0.52900	-2.86210	3.95270
C	2.53590	-3.04940	0.17660	H	-4.13940	-1.70320	4.87530
C	1.19390	-2.41370	0.35740	H	-2.60990	-2.40280	6.61120
H	3.69480	-4.79610	0.42900	H	-0.24210	-3.13790	6.01560
C	1.61960	-5.13170	1.07330	H	0.48450	-3.16300	3.72220
C	0.41240	-4.56620	1.28350	O	1.06910	-1.07120	0.06130
C	-0.70990	-5.42500	1.75840	P	-0.25430	-0.50650	-0.77990
C	-0.50860	-6.72180	2.01840	O	-1.37740	-1.70730	-0.75610
C	0.82560	-7.31830	1.82380	O	0.08990	-0.30030	-2.24270
C	1.83430	-6.56740	1.37040	N	0.96890	2.41290	1.39680
H	-1.70460	-5.01880	1.88410	H	1.97450	2.39210	1.31810
H	-1.32790	-7.34000	2.36220	C	0.36240	3.61830	1.62950
H	0.98280	-8.36730	2.03930	C	1.76850	3.90620	-1.28260
H	2.80910	-7.01470	1.21970	C	1.60070	2.71030	-1.96080
C	-3.64120	-1.59280	2.14110	C	-0.78390	3.07520	-2.13160
C	-1.04290	-2.45680	1.43840	C	-0.67060	4.28730	-1.47880
C	-1.85330	-1.91820	0.50940	C	2.66930	1.75500	-2.40630
C	-3.24970	-1.54790	0.85880	H	3.45940	1.66870	-1.66610
H	-4.65530	-1.32500	2.41420	H	2.21770	0.78020	-2.58960
C	-1.46530	-2.45800	2.86950	C	-2.03340	2.46170	-2.69290
C	-2.70760	-2.03520	3.19670	H	-2.29210	2.92940	-3.64810
C	-3.13910	-2.02520	4.61350	H	-2.87980	2.60050	-2.02170
C	-2.29450	-2.41190	5.57580	H	-1.86560	1.39640	-2.85200

C	-1.77130	5.22450	-1.21520	H	4.81910	2.49620	2.97450
C	3.06140	4.54020	-0.93160	H	5.97270	2.36340	0.84780
H	5.51800	4.70190	-0.05550	H	5.62010	0.38100	-0.67430
H	6.17300	3.86590	-1.50560	H	2.86990	-1.26540	2.24460
H	-3.55070	7.07230	-2.20880	H	3.24520	0.61690	3.68840
H	-4.71790	5.73060	-2.42920	C	-5.54690	3.45110	-0.24920
O	4.15160	3.90800	-1.42520	C	-4.61360	2.94770	0.56600
O	3.13670	5.56150	-0.27290	C	-4.26210	1.51370	0.49490
O	-1.72400	6.05790	-0.31440	C	-4.88260	0.70790	-0.38450
O	-2.82090	5.12720	-2.04860	C	-5.89670	1.28170	-1.30380
Si	3.97820	-2.05800	-0.48380	C	-6.21030	2.58060	-1.23850
Si	-4.50860	-1.11850	-0.44990	H	-5.82230	4.49480	-0.18250
C	3.22740	-1.10970	-5.01630	H	-4.12690	3.58680	1.29070
C	4.37270	-0.73550	-4.43570	H	-3.51230	1.13200	1.17390
C	4.61210	-1.03390	-3.00840	H	-6.39430	0.64830	-2.02770
C	3.66860	-1.64980	-2.27510	H	-6.95440	2.99460	-1.90640
C	2.42020	-2.10210	-2.93940	C	-8.34210	-3.61080	0.62500
C	2.20890	-1.83700	-4.23440	C	-7.16500	-4.22300	0.45920
H	3.05040	-0.89170	-6.06150	C	-5.96160	-3.43540	0.12120
H	5.12750	-0.21390	-5.00980	C	-6.04200	-2.10330	-0.04360
H	5.56720	-0.76720	-2.58060	C	-7.34810	-1.42900	0.17100
H	1.67130	-2.65490	-2.39030	C	-8.43590	-2.14520	0.48150
H	1.29410	-2.16230	-4.71290	H	-9.22440	-4.18590	0.87480
C	7.92310	-4.58370	-0.40580	H	-7.09000	-5.29650	0.57550
C	6.96090	-4.86850	-1.29100	H	-5.01710	-3.95220	0.03790
C	5.71610	-4.07290	-1.31290	H	-7.43680	-0.35600	0.10040
C	5.54380	-3.06160	-0.44480	H	-9.38510	-1.64990	0.64020
C	6.61290	-2.75220	0.53600	C	-2.87890	-2.36900	-4.67660
C	7.74000	-3.47470	0.55240	C	-3.25800	-1.10570	-4.45770
H	8.83570	-5.16540	-0.38840	C	-3.78870	-0.70900	-3.13720
H	7.09210	-5.68160	-1.99320	C	-3.89810	-1.61160	-2.14680
H	4.94890	-4.31900	-2.03680	C	-3.47430	-3.01250	-2.40050
H	6.48930	-1.94970	1.25070	C	-2.99000	-3.36810	-3.59660
H	8.51850	-3.25050	1.27020	H	-2.48500	-2.65980	-5.64180
C	4.65380	1.65220	2.31740	H	-3.17160	-0.36840	-5.24540
C	5.28600	1.58140	1.14170	H	-4.06660	0.32250	-2.99080
C	5.06460	0.42570	0.24840	H	-3.51130	-3.74910	-1.61220
C	4.20710	-0.54940	0.59560	H	-2.66610	-4.38600	-3.77080
C	3.52390	-0.47110	1.91290	N	0.34110	2.32480	-2.31370
C	3.73760	0.57010	2.72580	H	0.20840	1.28550	-2.50000



H	3.13330	2.11450	-3.33110	H	-1.34020	2.95190	2.73620
C	-3.87180	6.09250	-1.84630	C	2.44010	6.15230	4.44710
H	-4.12500	6.17280	-0.78880	C	1.53550	6.72100	3.56120
C	5.40750	4.54460	-1.13020	C	0.84060	5.93680	2.62770
H	5.47160	5.51170	-1.63470	C	1.07400	4.54140	2.58150
C	0.59410	4.64110	-0.85330	C	1.98560	3.99240	3.50210
H	0.43700	4.29380	0.47300	C	2.66780	4.77380	4.42580
H	0.76410	5.69460	-0.64500	H	2.96260	6.78450	5.15930
O	-0.72010	0.69870	0.00800	H	1.34000	7.78810	3.55930
H	0.43460	1.67760	0.89990	H	2.11970	2.91690	3.50420
C	-1.14870	3.47800	1.79570	H	3.35680	4.31220	5.12580
H	-1.56040	2.87310	0.98480	O	-0.01100	6.62990	1.83260
H	-1.64770	4.44580	1.83550	H	-0.49270	6.12170	1.15600
C	0.76210	-2.88950	1.30290	C	-0.16680	-2.53170	4.19570
C	3.42210	-3.76300	0.87720	H	-3.96890	-1.97390	4.87670
C	3.03890	-2.56530	0.41420	H	-2.43430	-2.25220	6.72330
C	1.62840	-2.10780	0.59950	H	0.05410	-2.59370	6.28400
H	4.43190	-4.11950	0.72750	H	0.89430	-2.66380	4.03000
C	2.45990	-4.65900	1.53680	O	1.31420	-0.82280	0.20810
C	1.17990	-4.26760	1.71410	P	-0.06180	-0.51580	-0.67180
C	0.20390	-5.24550	2.27640	O	-0.95390	-1.89510	-0.61980
C	0.60380	-6.46640	2.64960	O	0.30040	-0.29560	-2.12770
C	2.01440	-6.86410	2.49340	N	0.42040	2.68830	1.49350
C	2.89410	-6.01140	1.95940	H	1.41110	2.87750	1.50390
H	-0.84340	-4.99390	2.37210	C	-0.44170	3.74600	1.61200
H	-0.11070	-7.17140	3.05470	C	1.14550	4.19660	-1.16470
H	2.33200	-7.85250	2.79950	C	1.28200	2.96070	-1.77510
H	3.92590	-6.31570	1.83430	C	-1.09120	2.85330	-2.22470
C	-3.35420	-1.98700	2.16370	C	-1.28590	4.08180	-1.62360
C	-0.60970	-2.42410	1.63880	C	2.54730	2.18750	-1.99840
C	-1.45230	-2.10850	0.63710	H	3.31810	2.47750	-1.29390
C	-2.90820	-1.96750	0.89870	H	2.32340	1.12270	-1.91080
H	-4.41300	-1.88760	2.37260	C	-2.13130	1.99050	-2.87900
C	-1.10070	-2.38690	3.04720	H	-2.39550	2.39070	-3.86270
C	-2.41410	-2.17070	3.28880	H	-3.04450	1.95620	-2.28540
C	-2.91510	-2.12960	4.68190	H	-1.73590	0.98120	-2.99700
C	-2.06780	-2.28340	5.70540	C	-2.57100	4.78560	-1.51560
C	-0.62850	-2.48760	5.45080	C	2.24290	5.08200	-0.70470

H	4.59150	5.65310	0.38610	H	6.07420	0.70680	-1.04360
H	5.45210	5.17000	-1.11390	H	3.07030	-0.19470	1.94660
H	-4.58430	6.18050	-2.79580	H	3.42240	1.94380	2.97870
H	-5.42800	4.61350	-3.00360	C	-6.05820	2.40790	-0.68280
O	3.47940	4.72100	-1.12060	C	-5.11080	2.14540	0.22410
O	2.04330	6.07810	-0.03330	C	-4.48740	0.80610	0.27920
O	-2.78120	5.64290	-0.66190	C	-4.87390	-0.15540	-0.57690
O	-3.48980	4.44550	-2.43540	C	-5.90540	0.15420	-1.59830
Si	4.25850	-1.52920	-0.55420	C	-6.46550	1.36810	-1.64690
Si	-4.14740	-1.87140	-0.49430	H	-6.53170	3.37990	-0.70970
C	2.63410	-1.22140	-4.95140	H	-4.81160	2.90860	0.93000
C	3.65890	-0.45350	-4.56550	H	-3.73200	0.61880	1.02940
C	4.18270	-0.55270	-3.18720	H	-6.21360	-0.60470	-2.30670
C	3.61640	-1.39220	-2.30340	H	-7.22100	1.58910	-2.38960
C	2.50200	-2.26700	-2.75210	C	-7.47510	-5.01270	0.56180
C	2.03470	-2.18010	-4.00340	C	-6.18910	-5.37780	0.53000
H	2.24810	-1.14780	-5.95980	C	-5.14570	-4.38630	0.19690
H	4.10530	0.24550	-5.26070	C	-5.47940	-3.11740	-0.09720
H	5.01820	0.07040	-2.91160	C	-6.90770	-2.71470	-0.03160
H	2.05670	-2.98490	-2.07730	C	-7.85050	-3.61470	0.27480
H	1.21750	-2.81370	-4.32340	H	-8.24070	-5.73710	0.80790
C	8.47370	-3.56860	-0.53060	H	-5.90900	-6.39950	0.75160
C	7.77610	-3.51020	-1.67130	H	-4.11210	-4.69950	0.22420
C	6.44400	-2.87040	-1.69400	H	-7.20500	-1.69310	-0.21080
C	5.92910	-2.34460	-0.56960	H	-8.89000	-3.31700	0.32430
C	6.70640	-2.41240	0.69110	C	-2.00380	-2.97610	-4.52760
C	7.91230	-2.99310	0.70830	C	-2.60260	-1.78790	-4.39650
H	9.44910	-4.03740	-0.51310	C	-3.30240	-1.44490	-3.14130
H	8.18530	-3.93230	-2.58010	C	-3.34700	-2.32190	-2.12330
H	5.89760	-2.84460	-2.62680	C	-2.68400	-3.64170	-2.28160
H	6.30000	-1.99410	1.60360	C	-2.04550	-3.94740	-3.41780
H	8.47830	-3.04300	1.62950	H	-1.48360	-3.22550	-5.44340
C	4.95370	2.62630	1.52270	H	-2.56810	-1.07010	-5.20580
C	5.66860	2.28390	0.44580	H	-3.75010	-0.46720	-3.06050
C	5.45050	0.97400	-0.20270	H	-2.67380	-4.35260	-1.46960
C	4.51210	0.13080	0.26270	H	-1.54790	-4.90290	-3.52130
C	3.76300	0.49760	1.49210	N	0.16850	2.33090	-2.24730
C	3.96690	1.68250	2.08050	H	0.24730	1.27950	-2.40290
H	5.11010	3.58590	1.99800	H	2.93070	2.37240	-3.00840
H	6.40700	2.96590	0.04500	C	-4.72970	5.17760	-2.38620

H	-5.08790	5.26320	-1.36020	C	0.77700	6.77600	4.44290
C	4.53930	5.60050	-0.70360	C	-0.18000	7.08290	3.48590
H	4.37710	6.60670	-1.09630	C	-0.59400	6.13160	2.54140
C	-0.18810	4.70070	-0.89780	C	-0.02640	4.83480	2.56350
H	-0.40730	4.37750	0.42830	C	0.93790	4.55190	3.54910
H	-0.25220	5.77340	-0.73240	C	1.34380	5.49940	4.48060
O	-0.75380	0.61530	0.05800	H	1.07800	7.53240	5.16200
H	0.09920	1.84260	0.98950	H	-0.63300	8.06730	3.43310
C	-1.89950	3.29490	1.66260	H	1.34090	3.54600	3.59940
H	-2.58950	4.13690	1.62030	H	2.08120	5.24110	5.23390
H	-2.05940	2.76480	2.60680	O	-1.53800	6.57420	1.67440
H	-2.10330	2.59590	0.84860	H	-1.77450	5.97910	0.94090
C	2.77420	2.22560	-0.62890	H	-0.78540	5.70230	-3.95920
C	5.32520	1.16750	-0.02940	H	1.03930	5.78700	-5.54220
C	4.28220	0.33400	-0.16430	H	3.15930	4.43100	-5.13000
C	2.92110	0.89110	-0.43400	H	3.37120	3.07360	-3.15460
H	6.31170	0.79130	0.20200	O	1.87440	0.03020	-0.67490
C	5.14660	2.62570	-0.12270	P	0.53460	0.16320	0.30830
C	3.92720	3.14370	-0.38000	O	0.44000	1.74200	0.76900
C	3.75740	4.62460	-0.36410	O	0.77760	-0.61870	1.58280
C	4.80750	5.42520	-0.14960	N	-2.79600	-1.50150	-1.74420
C	6.14320	4.84790	0.08830	H	-2.62480	-2.17350	-2.48450
C	6.30460	3.52100	0.10800	C	-3.85920	-1.78040	-0.92250
H	2.78370	5.07350	-0.50560	C	-1.62040	-4.06510	-0.53860
H	4.67740	6.49970	-0.13720	C	-0.49160	-3.41740	-0.07940
H	6.98920	5.50110	0.25880	C	-1.50680	-3.06740	2.08780
H	7.28620	3.10390	0.29610	C	-2.66520	-3.69620	1.67990
C	-0.88850	4.24390	-1.59280	C	0.78320	-3.22950	-0.84590
C	1.47020	2.78500	-1.06880	H	1.39510	-2.46020	-0.38090
C	0.38230	2.61080	-0.28940	H	1.33900	-4.17030	-0.87870
C	-0.83080	3.44540	-0.51490	C	-1.18050	-2.52640	3.45210
H	-1.75690	4.86930	-1.76600	H	-0.51990	-1.66190	3.34410
C	1.36540	3.60820	-2.30820	H	-0.65770	-3.28940	4.03980
C	0.23200	4.30210	-2.55090	H	-2.07570	-2.25290	4.00310
C	0.11620	5.13240	-3.77210	C	-3.82060	-4.00220	2.54200
C	1.12470	5.18100	-4.64950	C	-1.74160	-4.68840	-1.86980
C	2.35380	4.40110	-4.40770	H	0.36770	-5.98040	-3.96110
C	2.46930	3.65230	-3.30470	H	-1.29930	-6.58970	-3.69580

H	-5.42890	-3.57070	4.60990	H	1.84530	-4.53860	3.04610
H	-5.09770	-5.31130	4.47500	C	-2.58090	8.11180	1.71230
O	-0.57340	-5.13680	-2.38210	C	-3.67330	7.43470	1.34200
O	-2.80670	-4.79620	-2.45860	C	-3.58090	5.99470	1.02190
O	-4.94370	-4.20960	2.10470	C	-2.40480	5.35030	1.12250
O	-3.53860	-4.06340	3.86280	C	-1.19260	6.11730	1.50480
Si	4.55450	-1.49980	0.09840	C	-1.27830	7.42260	1.78850
Si	-2.23770	3.53680	0.71350	H	-2.64730	9.16670	1.94520
C	9.10900	-2.44650	0.64830	H	-4.62810	7.94000	1.27490
C	8.65520	-1.97670	-0.51950	H	-4.47740	5.48700	0.70350
C	7.21840	-1.67720	-0.68890	H	-0.22380	5.63710	1.52520
C	6.36270	-1.86730	0.32970	H	-0.39040	7.97940	2.05880
C	6.87020	-2.39560	1.61980	C	-1.30770	1.14650	4.65240
C	8.17270	-2.66780	1.76890	C	-0.52310	2.16600	4.28760
H	10.16120	-2.66690	0.77400	C	-0.82710	2.93320	3.06160
H	9.33900	-1.81530	-1.34280	C	-1.88100	2.60290	2.29370
H	6.86930	-1.30030	-1.64250	C	-2.75400	1.48030	2.71770
H	6.19730	-2.56690	2.44890	C	-2.48320	0.79420	3.83380
H	8.54280	-3.05260	2.71040	H	-1.08420	0.57970	5.54690
C	3.30650	-4.07840	-3.61300	H	0.34070	2.42710	4.88510
C	3.13960	-2.75140	-3.64460	H	-0.16030	3.73350	2.77900
C	3.54270	-1.92550	-2.48710	H	-3.61920	1.20530	2.13760
C	4.04700	-2.50560	-1.38400	H	-3.12860	-0.01860	4.13980
C	4.27570	-3.97110	-1.37690	C	-6.20250	1.98450	-1.27320
C	3.91520	-4.71630	-2.42900	C	-5.05970	1.96550	-1.96790
H	3.00750	-4.68480	-4.45810	C	-3.80250	2.42710	-1.34290
H	2.70420	-2.27960	-4.51590	C	-3.80360	2.89700	-0.08240
H	3.42240	-0.85430	-2.55400	C	-5.07670	2.91300	0.68160
H	4.74350	-4.44560	-0.52360	C	-6.21030	2.47770	0.11810
H	4.07770	-5.78630	-2.41830	H	-7.12190	1.64080	-1.72930
C	2.33990	-2.63230	4.07430	H	-5.05360	1.61530	-2.99100
C	2.96070	-1.45380	3.95670	H	-2.89370	2.37720	-1.92490
C	3.65490	-1.10530	2.70010	H	-5.09300	3.27380	1.70250
C	3.65040	-1.95910	1.66090	H	-7.13530	2.48840	0.67980
C	2.97090	-3.26980	1.80490	N	-0.50240	-2.88260	1.17550
C	2.34780	-3.58520	2.94700	H	0.18030	-2.09520	1.38760
H	1.83020	-2.88920	4.99370	H	0.58530	-2.93300	-1.87500
H	2.95580	-0.75260	4.78110	C	-4.66100	-4.34030	4.71840
H	4.16160	-0.15080	2.63410	H	-4.26000	-4.34250	5.73160
H	2.96860	-3.98250	0.99610	C	-0.65440	-5.70810	-3.69930

H	-1.05370	-4.98280	-4.41220	C	-6.75520	-2.05480	-3.39560
C	-2.85230	-3.97780	0.24710	C	-5.49640	-1.73590	-2.86780
H	-3.48720	-3.00280	-0.26220	C	-5.14840	-2.17610	-1.56550
H	-3.60100	-4.73760	0.02190	C	-6.09530	-2.91770	-0.83460
O	-0.63240	-0.22120	-0.56800	C	-7.33690	-3.23460	-1.36780
H	-1.95790	-1.04460	-1.33620	H	-8.63090	-3.04320	-3.08740
C	-3.93520	-0.91640	0.31850	H	-6.98990	-1.69500	-4.39160
H	-4.48570	-0.00250	0.08530	H	-5.83340	-3.27190	0.15840
H	-2.93200	-0.64960	0.65690	H	-8.04190	-3.82040	-0.78730
H	-4.48060	-1.42700	1.11470	O	-4.69050	-0.98060	-3.65940
C	-7.66340	-2.80060	-2.65740	H	-3.89290	-0.73890	-3.15310
C	0.76210	-2.88950	1.30290	H	-2.43430	-2.25220	6.72330
C	3.42210	-3.76300	0.87720	H	0.05410	-2.59370	6.28400
C	3.03890	-2.56530	0.41420	H	0.89430	-2.66380	4.03000
C	1.62840	-2.10780	0.59950	O	1.31420	-0.82280	0.20810
H	4.43190	-4.11950	0.72750	P	-0.06180	-0.51580	-0.67180
C	2.45990	-4.65900	1.53680	O	-0.95390	-1.89510	-0.61980
C	1.17990	-4.26760	1.71410	O	0.30040	-0.29560	-2.12770
C	0.20390	-5.24550	2.27640	N	0.42040	2.68830	1.49350
C	0.60380	-6.46640	2.64960	H	1.41110	2.87750	1.50390
C	2.01440	-6.86410	2.49340	C	-0.44170	3.74600	1.61200
C	2.89410	-6.01140	1.95940	C	1.14550	4.19660	-1.16470
H	-0.84340	-4.99390	2.37210	C	1.28200	2.96070	-1.77510
H	-0.11070	-7.17140	3.05470	C	-1.09120	2.85330	-2.22470
H	2.33200	-7.85250	2.79950	C	-1.28590	4.08180	-1.62360
H	3.92590	-6.31570	1.83430	C	2.54730	2.18750	-1.99840
C	-3.35420	-1.98700	2.16370	H	3.31810	2.47750	-1.29390
C	-0.60970	-2.42410	1.63880	H	2.32340	1.12270	-1.91080
C	-1.45230	-2.10850	0.63710	C	-2.13130	1.99050	-2.87900
C	-2.90820	-1.96750	0.89870	H	-2.39550	2.39070	-3.86270
H	-4.41300	-1.88760	2.37260	H	-3.04450	1.95620	-2.28540
C	-1.10070	-2.38690	3.04720	H	-1.73590	0.98120	-2.99700
C	-2.41410	-2.17070	3.28880	C	-2.57100	4.78560	-1.51560
C	-2.91510	-2.12960	4.68190	C	2.24290	5.08200	-0.70470
C	-2.06780	-2.28340	5.70540	H	4.59150	5.65310	0.38610
C	-0.62850	-2.48760	5.45080	H	5.45210	5.17000	-1.11390
C	-0.16680	-2.53170	4.19570	H	-4.58430	6.18050	-2.79580
H	-3.96890	-1.97390	4.87670	H	-5.42800	4.61350	-3.00360

O	3.47940	4.72100	-1.12060	C	-5.11080	2.14540	0.22410
O	2.04330	6.07810	-0.03330	C	-4.48740	0.80610	0.27920
O	-2.78120	5.64290	-0.66190	C	-4.87390	-0.15540	-0.57690
O	-3.48980	4.44550	-2.43540	C	-5.90540	0.15420	-1.59830
Si	4.25850	-1.52920	-0.55420	C	-6.46550	1.36810	-1.64690
Si	-4.14740	-1.87140	-0.49430	H	-6.53170	3.37990	-0.70970
C	2.63410	-1.22140	-4.95140	H	-4.81160	2.90860	0.93000
C	3.65890	-0.45350	-4.56550	H	-3.73200	0.61880	1.02940
C	4.18270	-0.55270	-3.18720	H	-6.21360	-0.60470	-2.30670
C	3.61640	-1.39220	-2.30340	H	-7.22100	1.58910	-2.38960
C	2.50200	-2.26700	-2.75210	C	-7.47510	-5.01270	0.56180
C	2.03470	-2.18010	-4.00340	C	-6.18910	-5.37780	0.53000
H	2.24810	-1.14780	-5.95980	C	-5.14570	-4.38630	0.19690
H	4.10530	0.24550	-5.26070	C	-5.47940	-3.11740	-0.09720
H	5.01820	0.07040	-2.91160	C	-6.90770	-2.71470	-0.03160
H	2.05670	-2.98490	-2.07730	C	-7.85050	-3.61470	0.27480
H	1.21750	-2.81370	-4.32340	H	-8.24070	-5.73710	0.80790
C	8.47370	-3.56860	-0.53060	H	-5.90900	-6.39950	0.75160
C	7.77610	-3.51020	-1.67130	H	-4.11210	-4.69950	0.22420
C	6.44400	-2.87040	-1.69400	H	-7.20500	-1.69310	-0.21080
C	5.92910	-2.34460	-0.56960	H	-8.89000	-3.31700	0.32430
C	6.70640	-2.41240	0.69110	C	-2.00380	-2.97610	-4.52760
C	7.91230	-2.99310	0.70830	C	-2.60260	-1.78790	-4.39650
H	9.44910	-4.03740	-0.51310	C	-3.30240	-1.44490	-3.14130
H	8.18530	-3.93230	-2.58010	C	-3.34700	-2.32190	-2.12330
H	5.89760	-2.84460	-2.62680	C	-2.68400	-3.64170	-2.28160
H	6.30000	-1.99410	1.60360	C	-2.04550	-3.94740	-3.41780
H	8.47830	-3.04300	1.62950	H	-1.48360	-3.22550	-5.44340
C	4.95370	2.62630	1.52270	H	-2.56810	-1.07010	-5.20580
C	5.66860	2.28390	0.44580	H	-3.75010	-0.46720	-3.06050
C	5.45050	0.97400	-0.20270	H	-2.67380	-4.35260	-1.46960
C	4.51210	0.13080	0.26270	H	-1.54790	-4.90290	-3.52130
C	3.76300	0.49760	1.49210	N	0.16850	2.33090	-2.24730
C	3.96690	1.68250	2.08050	H	0.24730	1.27950	-2.40290
H	5.11010	3.58590	1.99800	H	2.93070	2.37240	-3.00840
H	6.40700	2.96590	0.04500	C	-4.72970	5.17760	-2.38620
H	6.07420	0.70680	-1.04360	H	-5.08790	5.26320	-1.36020
H	3.07030	-0.19470	1.94660	C	4.53930	5.60050	-0.70360
H	3.42240	1.94380	2.97870	H	4.37710	6.60670	-1.09630
C	-6.05820	2.40790	-0.68280	C	-0.18810	4.70070	-0.89780

H	-0.40730	4.37750	0.42830	C	-0.59400	6.13160	2.54140
H	-0.25220	5.77340	-0.73240	C	-0.02640	4.83480	2.56350
O	-0.75380	0.61530	0.05800	C	0.93790	4.55190	3.54910
H	0.09920	1.84260	0.98950	C	1.34380	5.49940	4.48060
C	-1.89950	3.29490	1.66260	H	1.07800	7.53240	5.16200
H	-2.58950	4.13690	1.62030	H	-0.63300	8.06730	3.43310
H	-2.05940	2.76480	2.60680	H	1.34090	3.54600	3.59940
H	-2.10330	2.59590	0.84860	H	2.08120	5.24110	5.23390
C	0.77700	6.77600	4.44290	O	-1.53800	6.57420	1.67440
C	-0.18000	7.08290	3.48590	H	-1.77450	5.97910	0.94090

C	0.53550	-2.68290	1.51840	H	-2.49700	-0.79210	6.73970
C	3.11120	-3.81500	1.18970	H	-0.06070	-1.44550	6.36620
C	2.80810	-2.67190	0.56000	H	0.72070	-2.02600	4.16570
C	1.44220	-2.08070	0.69620	O	1.21760	-0.85250	0.10610
H	4.08650	-4.26800	1.08060	P	-0.17930	-0.55180	-0.74950
C	2.10730	-4.51770	2.00220	O	-1.12590	-1.88080	-0.53550
C	0.86630	-4.00460	2.14110	O	0.14520	-0.44890	-2.22470
C	-0.15630	-4.79770	2.88360	N	0.63410	2.50360	1.38170
C	0.16770	-5.96730	3.44650	H	1.63880	2.58710	1.34850
C	1.53870	-6.49400	3.32420	C	-0.09890	3.65260	1.52540
C	2.45740	-5.81200	2.63370	C	1.44160	3.96240	-1.32420
H	-1.17790	-4.45290	2.96420	C	1.43460	2.72860	-1.95360
H	-0.58000	-6.53720	3.98300	C	-0.95640	2.85530	-2.29770
H	1.79520	-7.43950	3.78430	C	-1.00590	4.08670	-1.67300
H	3.45940	-6.21150	2.53710	C	2.61120	1.84440	-2.24350
C	-3.48530	-1.31570	2.21760	H	3.42870	2.03300	-1.55630
C	-0.80260	-2.08900	1.77500	H	2.28840	0.80330	-2.18010
C	-1.63660	-1.89660	0.73500	C	-2.09980	2.10980	-2.92120
C	-3.07280	-1.59110	0.97040	H	-2.38470	2.57270	-3.87080
H	-4.52230	-1.06360	2.40640	H	-2.97680	2.12390	-2.27480
C	-1.26100	-1.75440	3.15410	H	-1.79850	1.07760	-3.09890
C	-2.54320	-1.37380	3.35420	C	-2.21430	4.90350	-1.49060
C	-3.00840	-1.01980	4.71490	C	2.64000	4.74180	-0.92940
C	-2.15690	-1.05310	5.74590	H	5.80720	4.56510	-1.56790
C	-0.74850	-1.43740	5.53060	H	4.86150	6.08900	-1.56870
C	-0.32000	-1.76510	4.30600	H	-4.15510	6.51140	-2.49340
H	-4.03890	-0.73050	4.87940	H	-5.12970	5.05470	-2.87230

O	3.80510	4.29260	-1.45130	C	-7.64670	-4.12390	-0.77550
O	2.57450	5.73510	-0.22840	C	-6.58870	-3.12310	-1.02460
O	-2.29920	5.76850	-0.62320	C	-5.66710	-2.85420	-0.08280
O	-3.21370	4.65520	-2.35360	C	-5.69130	-3.62680	1.18680
Si	4.08310	-1.87650	-0.55580	C	-6.64820	-4.53690	1.40700
Si	-4.32260	-1.60210	-0.42510	H	-8.45180	-5.52650	0.56590
C	2.38180	-1.79460	-4.93280	H	-8.39300	-4.31800	-1.53500
C	1.78120	-2.53490	-3.99540	H	-6.56000	-2.63790	-1.98930
C	2.31720	-2.56410	-2.61910	H	-4.93000	-3.48740	1.93820
C	3.39910	-1.83350	-2.29270	H	-6.65980	-5.10010	2.33130
C	4.08040	-1.04470	-3.34920	C	-2.22040	-3.00620	-4.36560
C	3.59180	-1.01980	-4.59550	C	-2.71580	-1.76550	-4.28850
H	1.98810	-1.76890	-5.94050	C	-3.40670	-1.31840	-3.06130
H	0.89790	-3.11020	-4.24030	C	-3.52940	-2.15000	-2.01440
H	1.81610	-3.18480	-1.88940	C	-3.00070	-3.53210	-2.11470
H	4.97260	-0.48110	-3.12720	C	-2.37360	-3.93410	-3.22690
H	4.08680	-0.43650	-5.36110	H	-1.70860	-3.33280	-5.26160
C	8.06770	-4.33870	-0.55380	H	-2.60450	-1.08330	-5.12130
C	7.69430	-3.66390	0.53980	H	-3.78990	-0.30960	-3.02090
C	6.43540	-2.89040	0.53830	H	-3.10460	-4.21560	-1.28100
C	5.65980	-2.86240	-0.55870	H	-1.97660	-4.93870	-3.29400
C	6.07830	-3.61280	-1.76780	C	-6.12390	2.71690	-0.84530
C	7.22010	-4.31200	-1.76310	C	-6.59350	1.72130	-1.60350
H	8.98970	-4.90560	-0.55460	C	-6.02530	0.36350	-1.47870
H	8.31320	-3.68230	1.42740	C	-5.04110	0.11470	-0.59720
H	6.15040	-2.34950	1.43240	C	-4.50890	1.23350	0.22240
H	5.46440	-3.60880	-2.65840	C	-5.02270	2.46390	0.10360
H	7.52400	-4.86160	-2.64460	H	-6.54760	3.70890	-0.92890
C	5.34750	2.31400	1.13750	H	-7.39510	1.90630	-2.30680
C	5.97530	1.80050	0.07450	H	-6.41240	-0.41300	-2.11930
C	5.56640	0.48690	-0.46410	H	-3.69400	1.07270	0.91230
C	4.53960	-0.18520	0.08540	H	-4.62880	3.27780	0.69840
C	3.86720	0.38070	1.28300	N	0.24600	2.21540	-2.38310
C	4.25110	1.56390	1.77760	H	0.21820	1.17030	-2.55120
H	5.65100	3.27170	1.53950	H	2.98120	2.02780	-3.25860
H	6.79010	2.34160	-0.38860	C	-4.38370	5.48290	-2.20400
H	6.13340	0.06780	-1.28300	H	-4.73170	5.47610	-1.17010
H	3.08460	-0.16450	1.78920	C	4.95860	5.09190	-1.13270
H	3.76860	1.96720	2.65820	H	5.07460	5.19250	-0.05200
C	-7.67920	-4.79110	0.38270	C	0.17670	4.58940	-0.99310



H	-0.02210	4.28080	0.34600	C	0.06930	6.03310	2.46980
H	0.22420	5.66110	-0.81670	C	0.46050	4.67310	2.47840
O	-0.79990	0.66160	-0.08660	C	1.38400	4.25590	3.45530
H	0.20500	1.71600	0.86250	C	1.92040	5.13390	4.38860
C	-1.59730	3.36840	1.61180	H	1.93790	7.18020	5.08100
H	-1.78640	2.81770	2.53860	H	0.29930	7.95140	3.37130
H	-1.90420	2.73370	0.77810	H	1.64690	3.20430	3.49390
H	-2.18830	4.28340	1.62740	H	2.62090	4.77370	5.13530
C	1.53180	6.47580	4.36070	O	-0.81230	6.60290	1.61180
C	0.61680	6.91500	3.41410	H	-1.17910	6.02850	0.91680
C	0.17740	-3.10990	1.07000	H	-0.33330	-3.19410	6.08080
C	2.65350	-4.36480	0.52150	H	0.41540	-3.20140	3.79400
C	2.47660	-3.07940	0.18630	O	1.05760	-1.06370	0.18980
C	1.15860	-2.41800	0.42950	P	-0.23250	-0.47240	-0.67970
H	3.60640	-4.85230	0.37280	O	-1.37990	-1.64960	-0.67600
C	1.54550	-5.15660	1.07900	O	0.12920	-0.26550	-2.13210
C	0.35180	-4.57440	1.32220	N	1.01480	2.40380	1.47970
C	-0.77580	-5.42320	1.80260	H	2.00680	2.41990	1.26920
C	-0.59150	-6.72750	2.03670	C	0.41230	3.61920	1.68590
C	0.72880	-7.34230	1.80780	C	1.80560	3.93160	-1.33550
C	1.74140	-6.60060	1.34820	C	1.57870	2.75600	-2.02450
H	-1.76160	-5.00430	1.95210	C	-0.81150	3.17660	-2.06900
H	-1.41480	-7.33830	2.38410	C	-0.64030	4.38960	-1.43570
H	0.87220	-8.39740	2.00240	C	2.59420	1.79600	-2.57360
H	2.70540	-7.06140	1.17150	H	2.81270	2.04690	-3.61830
C	-3.67920	-1.56940	2.19010	H	3.52950	1.83940	-2.02640
C	-1.07910	-2.44510	1.50680	C	-2.09420	2.53840	-2.51050
C	-1.87340	-1.87920	0.57920	H	-2.23420	1.64940	-1.88690
C	-3.27860	-1.51610	0.91070	H	-2.02390	2.20630	-3.55070
H	-4.68640	-1.29580	2.46530	H	-2.94400	3.20300	-2.39940
C	-1.51710	-2.46250	2.93160	C	-1.66270	5.42800	-1.20200
C	-2.75830	-2.03040	3.25060	C	3.11970	4.55080	-1.05620
C	-3.20360	-2.03200	4.66340	H	6.16640	4.00220	-1.99840
C	-2.37280	-2.43900	5.62950	H	5.43660	5.63920	-1.96140
C	-1.00630	-2.88260	5.29240	H	-3.28330	7.38430	-2.10110
C	-0.59650	-2.89070	4.01870	H	-4.54900	6.16680	-2.46300
H	-4.20280	-1.70220	4.91930	O	4.16060	4.00490	-1.73060
H	-2.69840	-2.43820	6.66170	O	3.25500	5.49890	-0.30190

O	-1.52510	6.31050	-0.36600	C	-6.15610	-1.87180	-0.09700
O	-2.74470	5.37030	-2.01110	C	-6.64510	-2.99920	-0.93090
Si	3.90360	-2.11080	-0.53560	C	-7.84070	-3.55060	-0.68730
Si	-4.50590	-1.06870	-0.43580	H	-9.65120	-3.48420	0.60080
C	3.02290	-1.20880	-5.05300	H	-8.88370	-1.61840	1.94590
C	4.19270	-0.84710	-4.51440	H	-6.64210	-0.53860	1.47330
C	4.47390	-1.13380	-3.09230	H	-6.05310	-3.38330	-1.74730
C	3.54420	-1.72470	-2.32190	H	-8.19440	-4.37200	-1.29700
C	2.26930	-2.16690	-2.94000	C	-2.68610	-2.47490	-4.52460
C	2.01940	-1.91190	-4.23020	C	-2.87090	-3.35430	-3.53370
H	2.81500	-0.99880	-6.09410	C	-3.47660	-2.91670	-2.25930
H	4.93620	-0.34370	-5.11860	C	-3.85050	-1.63590	-2.08840
H	5.44680	-0.87830	-2.69670	C	-3.65850	-0.67150	-3.19900
H	1.53020	-2.70040	-2.35900	C	-3.10110	-1.06890	-4.34930
H	1.08410	-2.22720	-4.67470	H	-2.23480	-2.79150	-5.45590
C	7.85290	-4.62840	-0.54320	H	-2.56600	-4.38520	-3.65820
C	6.85360	-4.94490	-1.37490	H	-3.57940	-3.63520	-1.45520
C	5.60690	-4.15220	-1.36950	H	-3.96080	0.35920	-3.09210
C	5.46880	-3.11390	-0.52760	H	-2.95560	-0.36110	-5.15510
C	6.58030	-2.76650	0.39110	C	-5.42130	3.51950	-0.44610
C	7.70940	-3.48620	0.38240	C	-4.47720	3.03830	0.37070
H	8.76710	-5.20770	-0.54620	C	-4.16240	1.59350	0.37100
H	6.95620	-5.78130	-2.05410	C	-4.82090	0.76120	-0.45240
H	4.81020	-4.42220	-2.05190	C	-5.86630	1.30110	-1.35430
H	6.48750	-1.93630	1.07840	C	-6.14620	2.60950	-1.35420
H	8.51930	-3.23420	1.05470	H	-5.66290	4.57370	-0.43720
C	4.64810	1.61960	2.21180	H	-3.95240	3.70560	1.04070
C	5.10310	1.62200	0.95460	H	-3.40590	1.22450	1.05020
C	4.86070	0.45970	0.07540	H	-6.40860	0.63780	-2.01660
C	4.15570	-0.59360	0.52070	H	-6.90900	3.00240	-2.01370
C	3.66360	-0.59280	1.92180	N	0.28740	2.38770	-2.28250
C	3.90110	0.45330	2.72130	H	0.13270	1.35840	-2.45410
H	4.82940	2.46870	2.85800	H	2.17380	0.78880	-2.54650
H	5.66160	2.46950	0.58240	C	-3.70940	6.41930	-1.81610
H	5.27530	0.47720	-0.91900	H	-4.02330	6.46950	-0.77170
H	3.12970	-1.44620	2.31820	C	5.43070	4.64260	-1.51220
H	3.55160	0.44310	3.74530	H	5.64100	4.73930	-0.44560
C	-8.68620	-3.03400	0.40660	C	0.65440	4.66510	-0.79750
C	-8.26240	-2.00540	1.14870	H	0.53300	4.30470	0.41540
C	-6.94580	-1.39140	0.88000	H	0.85500	5.71660	-0.60110

O	-0.68640	0.73720	0.11710	C	0.88430	5.97170	2.44290
H	0.45810	1.68110	0.96650	C	1.46210	6.89160	3.30640
C	-1.09870	3.55040	1.75150	H	2.72850	7.14580	5.03770
H	-1.38660	3.13210	2.72310	H	3.06040	4.69930	5.37590
H	-1.48000	2.88820	0.97250	H	0.25940	6.31830	1.62500
H	-1.53460	4.54570	1.66320	H	1.29630	7.95340	3.15850
C	2.26410	6.43620	4.35910	O	2.08320	2.83220	3.98600
C	2.46390	5.07630	4.55200	H	1.61000	2.28500	3.33080
C	1.88270	4.14090	3.68440				
C	1.09790	4.58930	2.59290				

C	0.69940	-2.76900	1.34060	H	-2.46410	-1.70010	6.71440
C	3.34170	-3.71000	0.94460	H	0.01600	-2.11580	6.29200
C	2.97280	-2.53610	0.41460	H	0.84360	-2.36630	4.04610
C	1.57280	-2.04380	0.58590	O	1.27850	-0.77890	0.11950
H	4.34420	-4.09090	0.80760	P	-0.10860	-0.49430	-0.75350
C	2.37340	-4.54670	1.66960	O	-1.00650	-1.86530	-0.63450
C	1.10160	-4.12440	1.83530	O	0.22620	-0.30700	-2.21530
C	0.11860	-5.04830	2.47220	N	0.42490	2.54210	1.51410
C	0.50510	-6.24810	2.92030	H	1.40420	2.77340	1.38420
C	1.90750	-6.67730	2.77390	C	-0.43060	3.61050	1.63640
C	2.79280	-5.87530	2.17480	C	1.20940	4.13150	-1.19000
H	-0.92350	-4.77490	2.56400	C	1.28230	2.93390	-1.87350
H	-0.21430	-6.91360	3.37970	C	-1.10770	2.94740	-2.27460
H	2.21430	-7.64830	3.14070	C	-1.23960	4.15210	-1.61600
H	3.81830	-6.20320	2.05790	C	2.51070	2.13260	-2.18980
C	-3.40110	-1.74650	2.15070	H	2.81850	2.30580	-3.22730
C	-0.66660	-2.26850	1.64940	H	3.34120	2.40150	-1.54680
C	-1.50780	-2.00600	0.63130	C	-2.18350	2.16510	-2.97360
C	-2.95910	-1.81470	0.88620	H	-1.83460	1.14490	-3.13830
H	-4.45670	-1.61000	2.35480	H	-2.42350	2.62140	-3.93880
C	-1.15130	-2.12730	3.05320	H	-3.10160	2.14580	-2.38780
C	-2.45990	-1.87200	3.28310	C	-2.46630	4.96190	-1.52950
C	-2.95320	-1.72100	4.67140	C	2.35370	4.95200	-0.73580
C	-2.10330	-1.81310	5.70020	H	5.50940	5.08500	-1.44610
C	-0.66900	-2.05990	5.45590	H	4.46020	6.52850	-1.26960
C	-0.21440	-2.20440	4.20570	H	-4.37000	6.46160	-2.74660
H	-4.00310	-1.53290	4.85820	H	-5.31760	4.97200	-3.05650

O	3.53450	4.65940	-1.33260	C	-6.28870	-5.17850	0.69890
O	2.23720	5.85040	0.07960	C	-5.22980	-4.21850	0.32490
O	-2.60180	5.88160	-0.73440	C	-5.54700	-2.97100	-0.06430
O	-3.42600	4.62970	-2.42300	C	-6.97320	-2.55700	-0.06570
Si	4.19830	-1.57490	-0.62020	C	-7.93010	-3.42820	0.27780
Si	-4.19670	-1.76370	-0.51110	H	-8.34940	-5.50590	0.94770
C	2.49810	-1.41400	-4.99540	H	-6.02190	-6.18370	0.99840
C	3.53450	-0.63970	-4.65590	H	-4.19890	-4.53430	0.40000
C	4.08210	-0.69220	-3.28430	H	-7.25790	-1.54950	-0.32690
C	3.52570	-1.49460	-2.36070	H	-8.96850	-3.12260	0.27760
C	2.39700	-2.37620	-2.75680	C	-2.03950	-3.07270	-4.47370
C	1.90890	-2.33250	-4.00240	C	-2.57370	-1.85060	-4.37980
H	2.09490	-1.37490	-5.99900	C	-3.27990	-1.44300	-3.14780
H	3.97330	0.02980	-5.38420	C	-3.39590	-2.29540	-2.11430
H	4.92610	-0.06510	-3.04600	C	-2.80240	-3.65200	-2.23020
H	1.95930	-3.06570	-2.04820	C	-2.15810	-4.01630	-3.34570
H	1.08300	-2.97240	-4.28470	H	-1.51500	-3.36990	-5.37260
C	8.36570	-3.71040	-0.58650	H	-2.48170	-1.15300	-5.20220
C	7.64680	-3.68540	-1.71510	H	-3.67180	-0.43970	-3.09440
C	6.32940	-3.01570	-1.74070	H	-2.85290	-4.34620	-1.40550
C	5.84910	-2.42980	-0.63080	H	-1.71310	-5.00020	-3.41930
C	6.65010	-2.46050	0.61650	C	-6.01890	2.53710	-0.94300
C	7.84260	-3.06820	0.63630	C	-5.11050	2.29550	0.00860
H	9.33030	-4.20090	-0.56680	C	-4.52170	0.94650	0.14640
H	8.02800	-4.15630	-2.61200	C	-4.89890	-0.04390	-0.68000
H	5.76520	-3.01690	-2.66330	C	-5.89250	0.23880	-1.74560
H	6.27200	-1.99310	1.51730	C	-6.42180	1.46140	-1.86900
H	8.42580	-3.09100	1.54780	H	-6.46390	3.51870	-1.03430
C	5.05710	2.61990	1.30630	H	-4.81390	3.08480	0.68650
C	5.73360	2.22630	0.22220	H	-3.79640	0.77700	0.92920
C	5.45800	0.90760	-0.38480	H	-6.19500	-0.54540	-2.42830
C	4.50360	0.10900	0.12460	H	-7.14780	1.66370	-2.64560
C	3.78690	0.53830	1.35310	N	0.12790	2.36350	-2.33020
C	4.04670	1.72890	1.90630	H	0.16450	1.32780	-2.52140
H	5.26090	3.58250	1.75650	H	2.26760	1.07300	-2.08510
H	6.48740	2.87080	-0.21090	C	-4.60290	5.45470	-2.39050
H	6.05860	0.59370	-1.22640	H	-4.99930	5.52550	-1.37610
H	3.07390	-0.11320	1.83580	C	4.63530	5.49990	-0.94500
H	3.53040	2.03370	2.80680	H	4.76850	5.49360	0.13840
C	-7.57240	-4.80470	0.67190	C	-0.11020	4.65920	-0.82800

H	-0.31440	4.29940	0.37660	C	0.74780	4.43290	3.73010
H	-0.12960	5.73130	-0.63700	C	-0.05340	4.69500	2.59050
O	-0.78280	0.65690	-0.02900	C	-0.57690	5.99030	2.42090
H	0.07850	1.73610	0.94140	C	-0.29590	7.00930	3.31930
C	-1.89650	3.24160	1.53940	H	0.74900	7.53160	5.13640
H	-2.19420	2.73810	2.46650	H	1.63900	5.23350	5.49790
H	-2.05580	2.54790	0.71210	H	-1.20150	6.19130	1.55460
H	-2.51150	4.13380	1.42040	H	-0.69870	8.00340	3.15710
C	0.51670	6.74230	4.42740	O	1.25100	3.20940	4.04030
C	1.02500	5.46760	4.63480	H	0.93790	2.56640	3.37530
C	0.59650	-2.96150	1.17110	H	0.17160	-2.55390	6.17090
C	3.18630	-4.00790	0.71450	H	0.88170	-2.73290	3.87890
C	2.88380	-2.77810	0.27590	O	1.26210	-0.94440	0.03940
C	1.50020	-2.23960	0.45180	P	-0.13730	-0.53380	-0.76080
H	4.17610	-4.42040	0.57510	O	-1.13140	-1.84290	-0.67650
C	2.16880	-4.84740	1.36480	O	0.15990	-0.31920	-2.23230
C	0.92400	-4.36710	1.56940	N	0.60710	2.60190	1.44820
C	-0.10700	-5.27380	2.15200	H	1.60680	2.73560	1.44950
C	0.21180	-6.52250	2.51140	C	-0.18920	3.70810	1.58720
C	1.58610	-7.02050	2.32080	C	1.39390	4.06460	-1.19510
C	2.51350	-6.23010	1.77170	C	1.42040	2.83420	-1.83260
H	-1.12970	-4.94500	2.27680	C	-0.94590	2.96830	-2.30640
H	-0.54190	-7.17540	2.93230	C	-1.03370	4.18760	-1.66410
H	1.83830	-8.03070	2.61630	C	2.61540	1.96070	-2.07710
H	3.51820	-6.60650	1.62430	H	3.10600	2.24550	-3.01430
C	-3.39110	-1.74370	2.22060	H	3.34910	2.06270	-1.28370
C	-0.72100	-2.39770	1.56330	C	-2.03200	2.23310	-3.03400
C	-1.58780	-2.03280	0.60000	H	-2.04920	2.53810	-4.08650
C	-3.01900	-1.80070	0.93290	H	-3.01470	2.44030	-2.61870
H	-4.42640	-1.55890	2.48360	H	-1.81840	1.16410	-2.99000
C	-1.13350	-2.30720	2.99420	C	-2.25470	4.99840	-1.53200
C	-2.40970	-1.97960	3.29900	C	2.57140	4.83310	-0.72760
C	-2.83070	-1.87330	4.71500	H	5.76720	4.62800	-1.19430
C	-1.94540	-2.07850	5.69640	H	4.82810	6.15480	-1.11000
C	-0.54360	-2.40610	5.37200	H	-4.14100	6.65890	-2.46450
C	-0.15480	-2.51050	4.09590	H	-5.02720	5.26930	-3.17410
H	-3.85640	-1.62750	4.96060	O	3.76230	4.35930	-1.16310
H	-2.25330	-1.99870	6.73090	O	2.47470	5.83120	-0.03680

O	-2.40950	5.81130	-0.62550	C	-5.62060	-2.96720	-0.19510
O	-3.18260	4.80400	-2.48440	C	-5.46290	-4.04440	0.81350
Si	4.20420	-1.76640	-0.58150	C	-6.38430	-5.01060	0.91560
Si	-4.33640	-1.63490	-0.38030	H	-8.30080	-5.79540	0.10640
C	2.87210	-1.11840	-5.03910	H	-8.54980	-4.05970	-1.56900
C	3.97390	-0.51630	-4.57870	H	-6.80070	-2.23150	-1.78710
C	4.40430	-0.72580	-3.18070	H	-4.59900	-4.07220	1.46230
C	3.68110	-1.50210	-2.35500	H	-6.26690	-5.79760	1.64920
C	2.47920	-2.19480	-2.88600	C	-2.66900	-2.18070	-4.72280
C	2.09400	-2.00600	-4.15410	C	-2.54580	-3.16610	-3.82620
H	2.55440	-0.96370	-6.06200	C	-3.08840	-2.99740	-2.46240
H	4.55150	0.12890	-5.22780	C	-3.67840	-1.84340	-2.10620
H	5.30760	-0.24160	-2.84610	C	-3.84640	-0.77100	-3.11550
H	1.90320	-2.86130	-2.25960	C	-3.36160	-0.93000	-4.35340
H	1.21280	-2.50690	-4.53420	H	-2.26940	-2.30080	-5.72140
C	8.29850	-4.03140	-0.39670	H	-2.04420	-4.08650	-4.09570
C	7.66560	-3.90930	-1.56970	H	-2.97820	-3.80580	-1.74970
C	6.37260	-3.19720	-1.64420	H	-4.36530	0.14380	-2.86550
C	5.82950	-2.66780	-0.53500	H	-3.47950	-0.14350	-5.08760
C	6.53400	-2.80820	0.76200	C	-6.15700	2.62830	0.27870
C	7.70430	-3.45460	0.82620	C	-4.86570	2.48550	-0.03860
H	9.24490	-4.55340	-0.34120	C	-4.30090	1.13840	-0.25370
H	8.09840	-4.33300	-2.46670	C	-5.07910	0.05080	-0.13990
H	5.87570	-3.12390	-2.60190	C	-6.50630	0.21260	0.23150
H	6.10300	-2.39010	1.66320	C	-7.01630	1.43580	0.42410
H	8.21710	-3.55710	1.77380	H	-6.57190	3.61520	0.43740
C	4.97260	2.24400	1.74250	H	-4.23100	3.35480	-0.13360
C	5.71230	1.93400	0.67270	H	-3.25460	1.04240	-0.50870
C	5.47180	0.67030	-0.05410	H	-7.14380	-0.65030	0.36250
C	4.48820	-0.16160	0.33160	H	-8.05710	1.55360	0.69660
C	3.70800	0.16700	1.55280	N	0.25760	2.32230	-2.32230
C	3.93520	1.30800	2.21450	H	0.23670	1.27190	-2.49510
H	5.14550	3.17040	2.27460	H	2.28330	0.92480	-2.15690
H	6.48960	2.60750	0.33660	C	-4.37970	5.59800	-2.36230
H	6.11610	0.42710	-0.88560	H	-4.85760	5.43430	-1.39480
H	2.97290	-0.52040	1.94350	C	4.90670	5.12680	-0.74950
H	3.36960	1.53940	3.10770	H	4.98840	5.14200	0.33970
C	-7.55740	-5.01370	0.01850	C	0.11250	4.68020	-0.91470
C	-7.69440	-4.05630	-0.90590	H	-0.13600	4.34200	0.41130
C	-6.67720	-2.99150	-1.02510	H	0.14660	5.74850	-0.71480

O	-0.70100	0.63380	0.01890	C	0.30920	4.75370	2.54930
H	0.23150	1.78190	0.93810	C	1.24500	4.38070	3.53260
C	-1.67130	3.34410	1.66150	C	1.72980	5.28070	4.47320
H	-2.31310	4.22220	1.59110	H	1.63900	7.32260	5.17340
H	-1.85620	2.85890	2.62520	H	-0.02290	8.01620	3.45280
H	-1.91770	2.63070	0.87310	H	1.56130	3.34410	3.57120
C	1.27430	6.60130	4.44780	H	2.44240	4.95290	5.22340
C	0.34560	6.99690	3.49550	O	-1.05090	6.62230	1.68050
C	-0.14860	6.09260	2.54280	H	-1.36260	6.04340	0.96280
C	-0.13430	-2.79770	1.42310	H	-0.48980	-1.77890	6.34170
C	2.18120	-4.37070	1.00360	H	0.16580	-2.36540	4.10280
C	2.09780	-3.15870	0.43720	O	0.87260	-1.03940	0.12460
C	0.86890	-2.32630	0.62880	P	-0.43830	-0.46320	-0.73970
H	3.04980	-4.99630	0.85410	O	-1.61320	-1.60240	-0.56810
C	1.06470	-4.91740	1.78830	O	-0.06750	-0.37300	-2.20330
C	-0.05880	-4.19120	1.96570	N	0.90840	2.22800	1.40740
C	-1.21360	-4.82060	2.67030	H	1.81230	1.78150	1.39270
C	-1.11530	-6.06060	3.16290	C	0.85930	3.56380	1.67650
C	0.13360	-6.82590	2.99970	C	2.27100	3.66630	-1.30490
C	1.16540	-6.28840	2.34200	C	1.93800	2.46830	-1.92120
H	-2.15260	-4.29580	2.77900	C	-0.39080	3.11460	-2.03800
H	-1.95780	-6.51090	3.67190	C	-0.11860	4.30900	-1.40030
H	0.20770	-7.82770	3.40250	C	2.85760	1.35740	-2.33280
H	2.07540	-6.86170	2.21430	H	3.76470	1.34930	-1.74000
C	-3.80090	-0.69690	2.24160	H	2.32100	0.41190	-2.23150
C	-1.33550	-1.97830	1.72660	C	-1.69970	2.65960	-2.61270
C	-2.11460	-1.56860	0.70670	H	-1.97940	3.28280	-3.46620
C	-3.45130	-0.97290	0.97540	H	-2.49490	2.74100	-1.87350
H	-4.75690	-0.23310	2.45530	H	-1.61040	1.62130	-2.92970
C	-1.71870	-1.64100	3.12800	C	-1.06400	5.43690	-1.23980
C	-2.89790	-1.02310	3.36370	C	3.63760	4.15050	-1.04930
C	-3.28650	-0.66800	4.74810	H	6.60250	3.27740	-2.00120
C	-2.46270	-0.93640	5.76700	H	6.04990	4.97750	-1.84730
C	-1.15960	-1.58120	5.51490	H	-3.40240	6.57510	-0.72220
C	-0.80220	-1.91120	4.26840	H	-2.70300	7.28580	-2.19130
H	-4.23790	-0.18770	4.94000	O	4.61690	3.46890	-1.67060
H	-2.74640	-0.67490	6.77830	O	3.88870	5.13490	-0.35750

O	-0.79570	6.44420	-0.60860	C	-6.25830	-1.50850	-0.14880
O	-2.24640	5.27190	-1.87680	C	-6.47680	-2.34830	1.05780
Si	3.48880	-2.58410	-0.67740	C	-7.62160	-3.02510	1.21300
Si	-4.65630	-0.58100	-0.40310	H	-9.59540	-3.50110	0.30890
C	1.79920	-2.08690	-5.03250	H	-9.23150	-2.18390	-1.69370
C	1.06060	-2.68640	-4.09310	H	-7.05210	-0.94730	-2.02890
C	1.59220	-2.84710	-2.72410	H	-5.71310	-2.44670	1.81340
C	2.81060	-2.37320	-2.40500	H	-7.77500	-3.63860	2.09150
C	3.63810	-1.74510	-3.46520	C	-2.93780	-2.09500	-4.48650
C	3.15390	-1.60150	-4.70520	C	-3.15910	-0.78740	-4.30790
H	1.40980	-1.96490	-6.03490	C	-3.72690	-0.29900	-3.03410
H	0.06960	-3.05060	-4.33100	C	-4.00820	-1.16230	-2.04540
H	0.97480	-3.35120	-1.99410	C	-3.78980	-2.61350	-2.26000
H	4.63610	-1.39710	-3.25140	C	-3.27390	-3.05340	-3.41430
H	3.75770	-1.13580	-5.47320	H	-2.51540	-2.45310	-5.41640
C	6.93340	-5.75760	-0.78900	H	-2.91500	-0.08290	-5.09240
C	6.70840	-5.04840	0.32310	H	-3.89360	0.76110	-2.91350
C	5.61920	-4.05070	0.35700	H	-4.02980	-3.32100	-1.47600
C	4.84970	-3.85150	-0.72670	H	-3.10160	-4.11120	-3.56460
C	5.10240	-4.64220	-1.95610	C	-5.40000	4.05950	-0.39210
C	6.09090	-5.54500	-1.98330	C	-6.11380	3.27090	-1.20170
H	7.73120	-6.48860	-0.81570	C	-5.87520	1.81310	-1.21590
H	7.32370	-5.20290	1.20000	C	-4.94730	1.26630	-0.41140
H	5.45300	-3.48570	1.26610	C	-4.13650	2.15600	0.46150
H	4.48850	-4.50440	-2.83580	C	-4.35510	3.47670	0.47080
H	6.27330	-6.12370	-2.87960	H	-5.58220	5.12590	-0.37320
C	5.56250	1.23900	1.08810	H	-6.87370	3.69770	-1.84340
C	6.05890	0.64820	-0.00370	H	-6.45980	1.20660	-1.88920
C	5.39990	-0.55100	-0.56140	H	-3.34910	1.75490	1.08350
C	4.27590	-1.03330	-0.00250	H	-3.76070	4.12260	1.10370
C	3.75580	-0.39450	1.23280	N	0.63390	2.22680	-2.22300
C	4.36700	0.68040	1.74640	H	0.36580	1.22600	-2.42720
H	6.04420	2.11620	1.50020	H	3.14750	1.47450	-3.38320
H	6.94630	1.04460	-0.47970	C	-3.15110	6.38400	-1.76790
H	5.85760	-1.04180	-1.40790	H	-4.03750	6.09440	-2.33160
H	2.90080	-0.80420	1.75010	C	5.95320	3.96220	-1.45720
H	3.99530	1.13400	2.65510	H	6.19800	3.96600	-0.39330
C	-8.67080	-2.95400	0.17810	C	1.20090	4.52500	-0.82100
C	-8.46990	-2.22700	-0.92580	H	1.11720	4.21590	0.51830
C	-7.20530	-1.48390	-1.10360	H	1.44250	5.56810	-0.64300



O	-0.85950	0.81930	-0.05110	C	2.21030	3.14860	3.73660
H	0.15810	1.72250	0.89070	C	3.10710	3.50710	4.73930
C	-0.54830	4.10240	1.90760	H	4.42270	5.05260	5.47520
H	-0.90410	3.75550	2.88320	H	3.90860	6.60870	3.58760
H	-1.22860	3.71830	1.14280	H	1.70970	2.18640	3.77660
H	-0.55140	5.19260	1.88670	H	3.31300	2.81670	5.55160
C	3.72400	4.75790	4.69750	O	2.29100	6.17580	1.63670
C	3.44150	5.63130	3.65070	H	2.87110	5.95080	0.87830
C	2.54450	5.27310	2.63880				
C	1.90920	4.01680	2.67100				

C	0.61030	-2.84420	1.27780	C	-0.62630	-2.12110	5.42820
C	3.21050	-3.88810	0.86570	C	-0.20940	-2.27620	4.16620
C	2.89350	-2.68740	0.36290	H	-3.94000	-1.40900	4.91510
C	1.51140	-2.14540	0.53200	H	-2.36950	-1.67880	6.73250
H	4.19970	-4.30340	0.73100	H	0.07390	-2.22320	6.24720
C	2.20460	-4.70010	1.56710	H	0.83430	-2.49310	3.98030
C	0.95320	-4.22520	1.74460	O	1.26920	-0.86600	0.07700
C	-0.06870	-5.11570	2.36720	P	-0.12170	-0.49710	-0.75630
C	0.26440	-6.34090	2.78900	O	-1.09410	-1.81940	-0.64700
C	1.64560	-6.83000	2.62850	O	0.19110	-0.30800	-2.22330
C	2.56500	-6.05620	2.04350	N	0.51410	2.57730	1.51900
H	-1.09650	-4.79570	2.47040	H	1.49690	2.79670	1.39340
H	-0.48290	-6.98230	3.23810	C	-0.33160	3.65960	1.59960
H	1.90940	-7.82110	2.97440	C	1.38420	4.07390	-1.17880
H	3.57470	-6.42700	1.91740	C	1.42830	2.86830	-1.85200
C	-3.41580	-1.63700	2.19310	C	-0.93380	3.00570	-2.37080
C	-0.72350	-2.28390	1.62050	C	-1.04000	4.21100	-1.70970
C	-1.57520	-1.97170	0.62510	C	2.62930	2.00700	-2.10890
C	-3.01530	-1.74280	0.91730	H	2.99790	2.16760	-3.12840
H	-4.45840	-1.45320	2.42590	H	3.43830	2.23380	-1.42370
C	-1.16740	-2.13640	3.03700	C	-1.98990	2.28360	-3.15640
C	-2.45420	-1.81340	3.30070	H	-1.77600	1.21370	-3.12700
C	-2.90620	-1.65070	4.70160	H	-1.96940	2.60980	-4.20240
C	-2.03900	-1.79970	5.70900	H	-2.98780	2.47950	-2.77400

C	-2.23510	5.07250	-1.66090	H	5.31330	3.32850	1.92980
C	2.54870	4.84020	-0.68450	H	6.58210	2.62700	-0.01420
H	5.72590	4.83470	-1.30780	H	6.11950	0.39000	-1.10030
H	4.73800	6.32110	-1.13330	H	3.03210	-0.30950	1.86040
H	-4.06180	6.69780	-2.73890	H	3.51190	1.80290	2.89220
H	-4.96720	5.28990	-3.38460	C	-7.50650	-5.02880	0.03170
O	3.73190	4.49640	-1.24840	C	-7.62970	-4.11100	-0.93410
O	2.44890	5.73880	0.13290	C	-6.61670	-3.04480	-1.07540
O	-2.38060	5.96120	-0.83340	C	-5.57830	-2.97930	-0.22510
O	-3.15420	4.82090	-2.62060	C	-5.43540	-4.01330	0.82980
Si	4.17630	-1.73590	-0.61040	C	-6.35280	-4.98080	0.95220
Si	-4.30190	-1.64300	-0.43300	H	-8.24710	-5.81110	0.13630
C	2.60600	-1.35280	-5.02060	H	-8.47110	-4.14730	-1.61390
C	3.69010	-0.66920	-4.63820	H	-6.72950	-2.31620	-1.86910
C	4.19670	-0.79430	-3.25560	H	-4.58540	-4.00800	1.49750
C	3.55850	-1.57370	-2.36570	H	-6.24630	-5.73610	1.72010
C	2.37610	-2.35620	-2.80990	C	-2.45730	-2.33560	-4.68320
C	1.92300	-2.24500	-4.06450	C	-2.38670	-3.29540	-3.75380
H	2.23260	-1.26000	-6.03220	C	-2.99170	-3.08230	-2.42280
H	4.19740	-0.01950	-5.33950	C	-3.58900	-1.91440	-2.12910
H	5.08030	-0.24020	-2.98220	C	-3.70000	-0.87130	-3.17670
H	1.86950	-3.02640	-2.12950	C	-3.15660	-1.06980	-4.38420
H	1.05610	-2.81080	-4.38110	H	-2.01010	-2.48730	-5.65700
C	8.27210	-4.00310	-0.52330	H	-1.87950	-4.22630	-3.97160
C	7.58200	-3.93270	-1.66790	H	-2.91640	-3.86760	-1.68050
C	6.28690	-3.22170	-1.71050	H	-4.22340	0.05370	-2.97990
C	5.79840	-2.64350	-0.60030	H	-3.23250	-0.30460	-5.14590
C	6.56670	-2.72580	0.66510	C	-6.18560	2.61990	0.01820
C	7.73930	-3.37040	0.70020	C	-4.89050	2.48140	-0.28510
H	9.22040	-4.52370	-0.49120	C	-4.30530	1.13390	-0.43480
H	7.97010	-4.39680	-2.56530	C	-5.06920	0.04180	-0.27780
H	5.74500	-3.18680	-2.64570	C	-6.50100	0.19980	0.07670
H	6.18120	-2.26550	1.56640	C	-7.02910	1.42310	0.21210
H	8.29900	-3.43000	1.62460	H	-6.61530	3.60700	0.12960
C	5.09840	2.38180	1.45190	H	-4.26790	3.35470	-0.41700
C	5.79820	1.99390	0.38050	H	-3.25630	1.04070	-0.67980
C	5.50510	0.69840	-0.26680	H	-7.12730	-0.66540	0.24270
C	4.51410	-0.08510	0.19400	H	-8.07310	1.53820	0.47340
C	3.77420	0.33410	1.41260	N	0.27000	2.35370	-2.35710
C	4.04720	1.50510	2.00030	H	0.25710	1.31330	-2.53680

H	2.33090	0.96030	-2.02010	H	-2.40450	4.19130	1.31790
C	-4.32820	5.65050	-2.57910	C	0.63310	6.85640	4.31170
H	-4.83460	5.55960	-1.61560	C	1.12370	5.58170	4.55860
C	4.85910	5.28100	-0.82120	C	0.83940	4.52540	3.68150
H	4.96520	5.25230	0.26490	C	0.04930	4.76480	2.52940
C	0.07740	4.66040	-0.86970	C	-0.45700	6.06090	2.31980
H	-0.19270	4.30550	0.32960	C	-0.16880	7.10160	3.19120
H	0.09970	5.73060	-0.66900	H	0.87120	7.66270	4.99950
O	-0.71100	0.67690	0.00220	H	1.72950	5.36460	5.43200
H	0.16680	1.76220	0.96160	H	-1.07260	6.24530	1.44350
C	-1.80190	3.30210	1.50550	H	-0.55810	8.09570	2.99810
H	-2.11860	2.86800	2.46110	O	1.32670	3.30520	4.02900
H	-1.95660	2.55580	0.72530	H	1.00830	2.64790	3.38060

C	0.31960	-2.93740	1.37840	C	-2.44540	-1.83750	5.72560
C	2.85870	-4.13520	1.00100	C	-1.04060	-2.22490	5.49330
C	2.61990	-2.92150	0.48580	C	-0.58120	-2.37310	4.24540
C	1.27670	-2.28650	0.65710	H	-4.28940	-1.32970	4.86670
H	3.81630	-4.61830	0.86490	H	-2.81090	-1.72210	6.73780
C	1.79980	-4.88130	1.69630	H	-0.38030	-2.38060	6.33670
C	0.57320	-4.33770	1.84630	H	0.45710	-2.63850	4.09590
C	-0.51030	-5.17230	2.44230	O	1.12340	-0.98480	0.22490
C	-0.25390	-6.41260	2.87330	P	-0.21580	-0.53200	-0.65690
C	1.10230	-6.97530	2.74730	O	-1.24940	-1.80920	-0.59120
C	2.07510	-6.25400	2.18230	O	0.16640	-0.35620	-2.11210
H	-1.52240	-4.79950	2.51740	N	0.77510	2.50040	1.40760
H	-1.04580	-7.01230	3.30330	H	1.62470	2.26660	1.88910
H	1.30400	-7.97840	3.10050	C	0.20650	3.74250	1.57180
H	3.06570	-6.67950	2.07950	C	1.75180	3.99610	-1.30010
C	-3.66460	-1.51260	2.16300	C	1.63320	2.73210	-1.85830
C	-0.99420	-2.30830	1.68230	C	-0.74970	3.02890	-2.15280
C	-1.78800	-1.93240	0.66080	C	-0.68810	4.28960	-1.58630
C	-3.21930	-1.59700	0.90020	C	2.72930	1.75030	-2.14810
H	-4.69100	-1.24840	2.36880	H	3.13030	1.91190	-3.15510
C	-1.48450	-2.16060	3.08270	H	3.54940	1.86220	-1.44810
C	-2.76210	-1.77680	3.30270	C	-1.94830	2.34360	-2.74390
C	-3.26170	-1.62090	4.68840	H	-1.72530	1.28490	-2.87460

H	-2.19950	2.78320	-3.71400	C	3.80600	0.03650	1.44000
H	-2.82160	2.45530	-2.10400	C	4.21360	1.18310	1.99860
C	-1.80060	5.25980	-1.51610	H	5.61610	2.89830	1.82670
C	3.02100	4.70630	-1.01750	H	6.73090	2.05700	-0.15560
H	6.13890	4.15320	-1.69710	H	6.03950	-0.15620	-1.16530
H	5.34380	5.76220	-1.70830	H	3.02750	-0.53240	1.92680
H	-3.63990	6.82850	-2.67300	H	3.75360	1.53640	2.91240
H	-4.75670	5.43270	-2.82090	C	-8.45240	-3.55820	0.33040
O	4.13040	4.07780	-1.47830	C	-7.61520	-4.03810	-0.59580
O	3.07270	5.78280	-0.45000	C	-6.34060	-3.34390	-0.87540
O	-1.75130	6.28580	-0.85870	C	-6.00480	-2.23750	-0.18870
O	-2.87820	4.92790	-2.26570	C	-6.95220	-1.69850	0.81950
Si	3.94620	-2.09810	-0.54650	C	-8.10760	-2.32710	1.06730
Si	-4.41340	-1.31940	-0.51870	H	-9.38650	-4.06520	0.53470
C	2.28910	-1.75030	-4.92830	H	-7.86950	-4.93630	-1.14370
C	3.41780	-1.11660	-4.59180	H	-5.69850	-3.75010	-1.64070
C	3.95070	-1.22930	-3.21810	H	-6.72740	-0.77980	1.34550
C	3.29100	-1.94240	-2.28910	H	-8.79730	-1.92760	1.79960
C	2.05750	-2.67190	-2.68250	C	-2.36690	-2.69800	-4.51190
C	1.58250	-2.57510	-3.93000	C	-2.51520	-3.56210	-3.50170
H	1.89690	-1.66720	-5.93360	C	-3.18730	-3.13660	-2.25670
H	3.94260	-0.51700	-5.32410	C	-3.65510	-1.88150	-2.13050
H	4.87070	-0.71880	-2.98330	C	-3.49910	-0.93480	-3.26180
H	1.53200	-3.29370	-1.97100	C	-2.88380	-1.32120	-4.38610
H	0.68160	-3.10510	-4.21050	H	-1.86770	-3.00520	-5.42180
C	7.85100	-4.68370	-0.51460	H	-2.13320	-4.57080	-3.58920
C	7.13420	-4.58640	-1.64070	H	-3.26170	-3.84000	-1.43650
C	5.89860	-3.77570	-1.66570	H	-3.87010	0.07680	-3.18900
C	5.49070	-3.13360	-0.55800	H	-2.76350	-0.62480	-5.20590
C	6.28840	-3.24600	0.68690	C	-5.68390	3.18350	-0.67030
C	7.40690	-3.98100	0.70610	C	-6.24810	2.29760	-1.49830
H	8.75590	-5.27710	-0.49550	C	-5.83260	0.88080	-1.45990
H	7.45740	-5.10150	-2.53600	C	-4.87380	0.47880	-0.60880
H	5.33380	-3.72030	-2.58620	C	-4.24300	1.46810	0.29880
H	5.96790	-2.73490	1.58630	C	-4.63260	2.74920	0.27070
H	7.98790	-4.06260	1.61560	H	-5.99910	4.21830	-0.68590
C	5.30450	1.96170	1.38260	H	-7.01920	2.61390	-2.18870
C	5.91760	1.49830	0.28870	H	-6.32120	0.17300	-2.11840
C	5.48770	0.22070	-0.31650	H	-3.47090	1.16430	0.99230
C	4.45120	-0.46370	0.19940	H	-4.18120	3.47120	0.93780

N	0.39660	2.28990	-2.21730	H	-1.62760	2.96480	0.81450
H	0.29400	1.24540	-2.37070	H	-1.75890	4.66190	1.37050
H	2.31540	0.74200	-2.09800	C	2.54640	6.25450	4.23230
C	-3.95470	5.87900	-2.23320	C	1.16080	6.36390	4.24040
H	-4.27990	6.05960	-1.20650	C	0.36810	5.58040	3.39100
C	5.36540	4.77350	-1.24490	C	0.96490	4.64690	2.51620
H	5.54610	4.89230	-0.17380	C	2.36930	4.57790	2.52240
C	0.54420	4.70660	-0.93860	C	3.15950	5.35420	3.36170
H	0.37870	4.37810	0.42260	H	3.13970	6.87410	4.89780
H	0.64860	5.77030	-0.74270	H	0.67230	7.06480	4.91460
O	-0.78860	0.66380	0.07220	H	2.85720	3.90870	1.82280
H	0.23720	1.73810	0.95960	H	4.24020	5.26600	3.32540
C	-1.31560	3.68850	1.57070	O	-0.99170	5.70440	3.41900
H	-1.67060	3.33260	2.54180	H	-1.22660	6.40840	4.03750

**NH-Type II Z**

C	3.11370	1.96160	0.28070	C	1.89770	5.60500	-2.97340
C	5.30600	0.42560	1.17690	C	3.14810	5.65280	-3.44490
C	4.29820	-0.17370	0.52410	C	4.16660	4.71530	-2.93500
C	3.08830	0.61730	0.14890	C	3.84700	3.82340	-1.99020
H	6.18640	-0.13290	1.46850	H	1.15330	6.29120	-3.35780
C	5.25050	1.86570	1.48870	H	3.41430	6.37380	-4.20710
C	4.21040	2.61080	1.05650	H	5.17190	4.74540	-3.33510
C	4.16390	4.05780	1.40250	H	4.60480	3.13120	-1.64810
C	5.15770	4.61770	2.10200	O	2.02890	0.00620	-0.48240
C	6.30430	3.80170	2.54490	P	0.57840	0.11070	0.32300
C	6.34850	2.49620	2.25770	O	0.40730	1.67020	0.84690
H	3.32380	4.67070	1.10340	O	0.67560	-0.68400	1.61810
H	5.11960	5.67020	2.35170	N	-3.28500	-0.63850	-0.30460
H	7.10630	4.26180	3.10750	H	-3.66700	-0.40990	0.60080
H	7.19090	1.90240	2.59030	C	-3.91740	-1.60540	-1.03510
C	0.14560	4.55560	-1.43540	C	-1.99020	-4.11440	-0.08910
C	2.07890	2.78500	-0.38950	C	-0.82640	-3.50860	0.34580
C	0.78010	2.64310	-0.04570	C	-1.98310	-2.51780	2.21960
C	-0.21900	3.63960	-0.52480	C	-3.19700	-3.03510	1.79370
H	-0.57380	5.27160	-1.81480	C	0.52040	-3.62290	-0.29960
C	2.46530	3.77540	-1.43710	H	0.98260	-4.58140	-0.04610
C	1.53220	4.61700	-1.93190	H	0.43530	-3.57930	-1.38410

C	-1.71400	-1.75130	3.48150	C	3.23760	-3.26440	-2.14790
H	-1.02140	-0.93330	3.26070	C	3.82730	-2.13250	-1.72940
H	-1.21130	-2.41380	4.19700	C	3.96470	-0.99700	-2.67680
H	-2.63110	-1.39690	3.93970	C	3.47610	-1.08910	-3.91930
C	-4.44750	-2.87820	2.57880	H	2.41000	-2.39890	-5.36470
C	-2.11810	-4.97270	-1.27230	H	2.20860	-4.27410	-3.84040
H	-1.44480	-5.78270	-3.70390	H	3.13300	-4.11670	-1.49770
H	-0.08810	-6.75720	-3.04780	H	4.45280	-0.08160	-2.36700
H	-6.99200	-2.19370	2.74860	H	3.57110	-0.25590	-4.60350
H	-7.50620	-3.65180	1.84240	C	-2.47550	1.62560	4.28570
O	-0.98650	-5.57510	-1.67390	C	-3.37300	1.39520	3.32140
O	-3.18890	-5.13880	-1.85500	C	-3.21750	2.03080	1.99750
O	-4.56590	-2.36540	3.67750	C	-2.17430	2.84000	1.74840
O	-5.50520	-3.38650	1.90150	C	-1.18400	3.09160	2.82580
Si	4.49890	-1.95560	0.00230	C	-1.32510	2.51190	4.02400
Si	-1.97910	3.68290	0.09400	H	-2.58650	1.15770	5.25520
C	2.32770	-4.76040	3.07480	H	-4.21580	0.74200	3.50780
C	2.29530	-3.43390	3.24290	H	-3.97000	1.84010	1.25040
C	3.00650	-2.55010	2.29650	H	-0.32110	3.71670	2.64070
C	3.65810	-3.06830	1.24150	H	-0.59220	2.68550	4.80120
C	3.72830	-4.54290	1.08900	C	-4.68900	1.81350	-3.24970
C	3.09260	-5.34260	1.95420	C	-5.25140	2.41140	-2.19390
H	1.80370	-5.40910	3.76460	C	-4.40320	2.97980	-1.12590
H	1.74100	-3.00380	4.06720	C	-3.06360	2.90380	-1.20970
H	2.97660	-1.48320	2.46620	C	-2.44760	2.22950	-2.37950
H	4.30980	-4.98220	0.28890	C	-3.21880	1.72390	-3.34910
H	3.14480	-6.41750	1.83970	H	-5.30880	1.39190	-4.03020
C	9.09370	-2.85750	-0.21750	H	-6.32900	2.47690	-2.11690
C	8.34250	-3.47810	0.69930	H	-4.87920	3.47700	-0.29000
C	6.89190	-3.20610	0.77730	H	-1.37290	2.13970	-2.46210
C	6.31800	-2.34380	-0.07970	H	-2.76690	1.23620	-4.20310
C	7.15920	-1.65100	-1.08580	C	-2.97750	8.23700	0.66130
C	8.47340	-1.89650	-1.15110	C	-3.60880	7.53470	-0.28560
H	10.15650	-3.05430	-0.27390	C	-3.30380	6.10090	-0.47310
H	8.79590	-4.17860	1.38870	C	-2.40590	5.48710	0.31860
H	6.31630	-3.70160	1.54590	C	-1.69310	6.28090	1.35010
H	6.71850	-0.93670	-1.76800	C	-1.96780	7.58070	1.51420
H	9.08530	-1.38820	-1.88500	H	-3.19840	9.28760	0.79830
C	2.80750	-2.32870	-4.36050	H	-4.34280	8.01560	-0.91930
C	2.69770	-3.36320	-3.51990	H	-3.80450	5.57460	-1.27150

H	-0.93460	5.82360	1.96720	H	-2.14600	-1.92590	-2.23460
H	-1.44320	8.15610	2.26600	H	-3.59510	-2.76020	-2.86370
N	-0.86850	-2.72350	1.45780	C	-8.23530	-1.45430	-1.00250
H	-0.08270	-1.99030	1.59110	C	-7.59340	-2.59580	-1.46600
H	1.16250	-2.81170	0.03840	C	-6.19340	-2.69060	-1.47220
C	-6.78140	-3.24600	2.54650	C	-5.41950	-1.59480	-1.01480
H	-6.79810	-3.80000	3.48810	C	-6.09870	-0.45980	-0.53720
C	-1.09400	-6.38300	-2.86180	C	-7.48580	-0.37560	-0.52640
H	-1.78970	-7.20880	-2.69920	H	-9.32040	-1.40770	-1.01220
C	-3.25430	-3.70560	0.50290	H	-8.15250	-3.45060	-1.83200
H	-3.69830	-2.76830	-0.36450	H	-5.51180	0.38750	-0.20340
H	-4.08840	-4.38760	0.36380	H	-7.97260	0.52540	-0.16750
O	-0.48030	-0.26560	-0.68080	O	-5.70890	-3.86680	-1.94280
H	-2.27130	-0.47340	-0.42890	H	-4.76430	-4.04860	-1.78170
C	-3.22850	-1.86210	-2.37180				
H	-3.43380	-1.01320	-3.02810				

C	2.94780	2.13010	0.67870	C	2.36190	4.31090	-0.55810
C	5.16160	0.46900	1.25150	C	1.44050	5.21840	-0.94480
C	4.20280	0.03360	0.42000	C	1.86060	6.47240	-1.61390
C	2.99700	0.87360	0.19480	C	3.15330	6.70000	-1.86600
H	6.05060	-0.12700	1.42190	C	4.16490	5.69470	-1.49360
C	5.03450	1.77670	1.92710	C	3.79550	4.56260	-0.88390
C	3.98060	2.57980	1.65640	H	1.12130	7.20850	-1.90460
C	3.85410	3.87660	2.37360	H	3.45890	7.61500	-2.35670
C	4.79300	4.25930	3.24670	H	5.20690	5.86950	-1.72880
C	5.95650	3.39140	3.51320	H	4.55550	3.82860	-0.65480
C	6.07080	2.21260	2.89120	O	1.94500	0.38950	-0.53680
H	2.99950	4.51860	2.20430	P	0.60180	0.15950	0.38720
H	4.69810	5.20410	3.76610	O	0.15220	1.66580	0.92350
H	6.71370	3.70900	4.21840	O	0.98240	-0.60370	1.65750
H	6.92430	1.57840	3.09640	N	-3.19190	-1.15610	-0.48950
C	0.00750	4.94250	-0.75760	H	-4.02770	-0.61950	-0.31160
C	1.92220	3.06390	0.14330	C	-3.32350	-2.39900	-1.07030
C	0.59620	2.77500	0.23580	C	-1.72960	-4.41570	1.11240
C	-0.40790	3.78200	-0.22890	C	-0.61620	-3.68180	1.46920
H	-0.70210	5.67430	-1.11950	C	-1.99060	-1.93540	2.39950

C	-3.14700	-2.64680	2.07970	H	5.89960	0.62780	-2.03580
C	0.82600	-4.07070	1.33290	H	8.10420	0.82520	-2.98640
H	1.16450	-4.56720	2.24940	C	1.28140	-1.93230	-3.93580
H	0.98500	-4.76330	0.51140	C	2.16730	-0.93070	-3.95220
C	-1.93000	-0.61610	3.11270	C	3.19540	-0.83290	-2.89490
H	-0.93810	-0.17580	3.00890	C	3.24520	-1.74340	-1.90590
H	-2.16580	-0.74460	4.17270	C	2.26480	-2.85730	-1.90490
H	-2.67210	0.06210	2.69620	C	1.33820	-2.94650	-2.86620
C	-4.50260	-2.26040	2.48970	H	0.52230	-2.00090	-4.70420
C	-1.71970	-5.76980	0.50970	H	2.12620	-0.18240	-4.73310
H	0.43630	-8.17970	0.36060	H	3.87110	0.00880	-2.91220
H	-1.33540	-8.39840	0.54530	H	2.28230	-3.60410	-1.12910
H	-6.44160	-1.91020	4.29210	H	0.62620	-3.76160	-2.85960
H	-5.74830	-0.32140	4.75680	C	-4.54380	7.41030	-1.05570
O	-0.57330	-6.46010	0.70470	C	-4.47890	6.47110	-2.00680
O	-2.67430	-6.23130	-0.08990	C	-3.76000	5.20540	-1.75120
O	-5.51740	-2.70680	1.95460	C	-3.17910	4.98730	-0.55880
O	-4.56620	-1.40520	3.52410	C	-3.24440	6.03700	0.48640
Si	4.47880	-1.56080	-0.51320	C	-3.89340	7.18380	0.25060
Si	-2.24620	3.41790	-0.19910	H	-5.06870	8.33820	-1.24250
C	4.17600	-5.21780	2.41370	H	-4.95030	6.63720	-2.96680
C	4.04110	-3.97440	2.88870	H	-3.69940	4.47600	-2.54680
C	4.13220	-2.81690	1.97430	H	-2.76500	5.88230	1.44490
C	4.36010	-3.00540	0.66240	H	-3.94050	7.94860	1.01490
C	4.51020	-4.38820	0.14450	C	-3.71870	2.35090	4.12710
C	4.41950	-5.43460	0.97400	C	-2.46410	2.77200	3.93490
H	4.10350	-6.06610	3.08170	C	-1.98650	3.07870	2.57050
H	3.85730	-3.81310	3.94300	C	-2.79380	2.90060	1.50860
H	4.00140	-1.82630	2.38590	C	-4.18670	2.44150	1.73430
H	4.68680	-4.55720	-0.91040	C	-4.62440	2.18860	2.97370
H	4.52430	-6.44170	0.59170	H	-4.07240	2.13010	5.12580
C	8.78940	-1.18400	-2.32980	H	-1.79850	2.89850	4.77870
C	8.44780	-2.29450	-1.66710	H	-0.99150	3.48550	2.45720
C	7.09430	-2.42660	-1.08810	H	-4.87160	2.33200	0.90990
C	6.19180	-1.44170	-1.24070	H	-5.64640	1.87200	3.13360
C	6.58830	-0.20230	-1.95510	C	-3.25410	0.29490	-3.56670
C	7.81660	-0.08350	-2.47340	C	-1.98160	0.62590	-3.32280
H	9.78090	-1.08570	-2.75270	C	-1.66090	1.61260	-2.27040
H	9.16240	-3.09930	-1.55240	C	-2.63870	2.15360	-1.52130
H	6.85890	-3.32740	-0.54330	C	-4.05070	1.80830	-1.82710



C	-4.33970	0.92790	-2.79380	C	-2.05630	-2.84530	-1.79770
H	-3.49070	-0.43250	-4.33240	H	-2.03260	-2.41070	-2.80160
H	-1.18270	0.16750	-3.89110	H	-1.17880	-2.47530	-1.26660
H	-0.62410	1.87410	-2.11670	H	-2.00650	-3.93280	-1.88650
H	-4.86070	2.29460	-1.30480	C	-6.99370	-3.10780	-3.28690
H	-5.37040	0.68370	-3.01640	C	-7.01370	-2.28620	-2.16380
N	-0.79410	-2.44350	2.03260	C	-5.85840	-2.08700	-1.40620
H	0.03120	-1.73950	1.98960	C	-4.63290	-2.68000	-1.78280
H	1.42250	-3.16650	1.19610	C	-4.64990	-3.52820	-2.90320
C	-5.89300	-1.03250	3.94450	C	-5.80630	-3.74300	-3.64850
H	-6.44310	-0.57220	3.12120	H	-7.89900	-3.25710	-3.86780
C	-0.54610	-7.77450	0.11990	H	-7.92070	-1.78560	-1.84120
H	-0.68590	-7.71790	-0.96200	H	-3.73500	-4.01730	-3.21360
C	-3.03900	-3.80090	1.22460	H	-5.77290	-4.39630	-4.51490
H	-3.32410	-3.24630	-0.09090	O	-5.95950	-1.25310	-0.30850
H	-3.89550	-4.46710	1.17350	H	-5.90460	-1.80460	0.50180
O	-0.45410	-0.43360	-0.49770				
H	-2.25960	-0.73120	-0.43540				
				C	2.34730	4.35180	-0.64290
C	2.99150	2.19670	0.61020	C	1.40470	5.24040	-1.02150
C	5.23750	0.57710	1.16870	C	1.79180	6.49380	-1.71130
C	4.27730	0.11370	0.35280	C	3.07570	6.73970	-1.98930
C	3.05030	0.93300	0.14490	C	4.11010	5.75470	-1.62580
H	6.12580	-0.00530	1.36190	C	3.77030	4.62300	-0.99840
C	5.10480	1.89500	1.82290	H	1.03530	7.21490	-1.99540
C	4.03520	2.67790	1.55970	H	3.35730	7.65460	-2.49430
C	3.90160	3.98330	2.26030	H	5.14460	5.94390	-1.88190
C	4.84990	4.39300	3.11080	H	4.54630	3.90380	-0.77610
C	6.03060	3.54630	3.36930	O	1.98790	0.42400	-0.55380
C	6.15120	2.36020	2.76280	P	0.66220	0.19070	0.39290
H	3.03450	4.60990	2.09760	O	0.21160	1.69760	0.92720
H	4.74980	5.34390	3.61810	O	1.06150	-0.56950	1.65760
H	6.79500	3.88530	4.05640	N	-3.13480	-1.09190	-0.41650
H	7.01720	1.74150	2.96250	H	-3.95960	-0.55200	-0.20170
C	-0.01960	4.94380	-0.80490	C	-3.29450	-2.32580	-1.00640
C	1.94100	3.10730	0.08300	C	-1.67920	-4.39530	1.10360
C	0.62180	2.80080	0.20930	C	-0.54740	-3.67850	1.44070
C	-0.40690	3.78450	-0.25260	C	-1.87050	-1.93360	2.43970
H	-0.74690	5.65810	-1.16640	C	-3.04340	-2.62710	2.14240

C	0.87620	-4.10340	1.25580	H	7.85470	-1.58200	-4.27680
H	1.23410	-4.60390	2.16300	C	1.20320	-2.03500	-3.79360
H	0.98270	-4.81240	0.43940	C	2.02610	-0.98090	-3.82960
C	-1.77600	-0.63260	3.18150	C	3.10070	-0.84600	-2.82410
H	-0.78770	-0.19260	3.04710	C	3.25300	-1.77410	-1.86210
H	-1.96800	-0.78800	4.24680	C	2.35650	-2.95510	-1.85100
H	-2.53310	0.05610	2.81300	C	1.38320	-3.07490	-2.76190
C	-4.38030	-2.24730	2.61480	H	0.40800	-2.13020	-4.52160
C	-1.58450	-5.75160	0.51620	H	1.89660	-0.21640	-4.58450
H	-3.79490	-7.57470	-1.00170	H	3.72790	0.03690	-2.84450
H	-2.04720	-7.52910	-1.40690	H	2.48290	-3.73210	-1.11450
H	-6.21280	-1.97110	4.56660	H	0.72820	-3.93640	-2.74630
H	-5.53130	-0.36240	4.97440	C	-3.65920	2.31840	4.14300
O	-2.76610	-6.12480	-0.03780	C	-2.42030	2.78000	3.94200
O	-0.60220	-6.47050	0.51050	C	-1.95490	3.08100	2.57210
O	-5.41720	-2.67160	2.10290	C	-2.75680	2.85740	1.51480
O	-4.40090	-1.43200	3.68160	C	-4.12920	2.34450	1.74880
Si	4.52360	-1.53390	-0.51270	C	-4.55760	2.09930	2.99290
Si	-2.23830	3.39190	-0.19620	H	-4.00470	2.10330	5.14580
C	4.30570	-5.02100	2.60520	H	-1.75970	2.94630	4.78300
C	4.00930	-3.77340	2.98780	H	-0.97680	3.52500	2.44980
C	4.06710	-2.66540	2.01170	H	-4.80680	2.18650	0.92610
C	4.41340	-2.90700	0.73550	H	-5.56600	1.74520	3.15870
C	4.75280	-4.28920	0.32120	C	-3.26150	0.28840	-3.57360
C	4.69660	-5.29110	1.20700	C	-1.98740	0.61610	-3.33290
H	4.25980	-5.83380	3.31840	C	-1.66080	1.59560	-2.27570
H	3.72070	-3.57330	4.01150	C	-2.63530	2.13460	-1.52110
H	3.81330	-1.66880	2.34570	C	-4.04910	1.79370	-1.82310
H	5.04440	-4.49390	-0.70150	C	-4.34320	0.91800	-2.79240
H	4.94050	-6.30040	0.90170	H	-3.50220	-0.43390	-4.34280
C	8.85560	-1.80840	-2.30690	H	-1.19150	0.15990	-3.90720
C	8.66580	-1.89450	-0.98600	H	-0.62290	1.85390	-2.12310
C	7.30120	-1.80740	-0.42670	H	-4.85600	2.27940	-1.29470
C	6.24260	-1.62230	-1.23570	H	-5.37500	0.67640	-3.01220
C	6.46130	-1.55060	-2.70310	C	-4.62120	7.33130	-1.07420
C	7.69910	-1.63420	-3.20690	C	-4.05340	7.14020	0.12220
H	9.85430	-1.87390	-2.71870	C	-3.30400	5.89670	0.39610
H	9.51080	-2.03120	-0.32370	C	-3.20030	4.94620	-0.54840
H	7.17410	-1.91730	0.64220	C	-3.81690	5.17210	-1.87910
H	5.63150	-1.44030	-3.38360	C	-4.49260	6.30150	-2.12480

H	-5.16960	8.24210	-1.27680	C	-2.04970	-2.78260	-1.76510
H	-4.14110	7.89590	0.89200	H	-2.04190	-2.34370	-2.76700
H	-2.84370	5.76730	1.36760	H	-1.15500	-2.42810	-1.25270
H	-3.71100	4.43930	-2.66720	H	-2.01460	-3.87010	-1.86300
H	-4.93810	6.46730	-3.09710	C	-7.03170	-2.95910	-3.13210
N	-0.69110	-2.44610	2.02430	C	-7.01500	-2.17450	-1.98270
H	0.13740	-1.74910	1.97500	C	-5.83590	-1.99940	-1.25620
H	1.48870	-3.21470	1.09370	C	-4.62430	-2.58250	-1.68970
C	-5.70820	-1.08390	4.17790	C	-4.67700	-3.39160	-2.83760
H	-6.31890	-0.64660	3.38590	C	-5.85680	-3.58110	-3.55300
C	-2.78750	-7.44350	-0.60810	H	-7.95490	-3.08820	-3.68910
H	-2.57030	-8.19530	0.15450	H	-7.91030	-1.68270	-1.61670
C	-2.97720	-3.76720	1.26220	H	-3.77120	-3.86420	-3.19700
H	-3.28700	-3.18500	-0.03280	H	-5.85120	-4.20130	-4.44400
H	-3.84940	-4.41270	1.23780	O	-5.89840	-1.19470	-0.13560
O	-0.40350	-0.40890	-0.47750	H	-5.81620	-1.76240	0.66160
H	-2.19470	-0.68040	-0.37310				
C	2.81260	2.36950	0.62580	C	1.04150	5.32020	-0.98520
C	5.15660	0.89610	1.18650	C	1.35060	6.60250	-1.66100
C	4.23720	0.38100	0.35500	C	2.61760	6.93360	-1.92840
C	2.96060	1.11950	0.14420	C	3.71150	6.01450	-1.56640
H	6.07970	0.37120	1.38150	C	3.44200	4.85730	-0.95150
C	4.92990	2.19330	1.85610	H	0.55070	7.27570	-1.94370
C	3.81280	2.90660	1.59170	H	2.84230	7.86940	-2.42360
C	3.58550	4.19080	2.30720	H	4.73320	6.27300	-1.81330
C	4.49570	4.65110	3.17320	H	4.26160	4.18810	-0.72980
C	5.72750	3.88130	3.43380	O	1.94180	0.55050	-0.57240
C	5.93320	2.71430	2.81320	P	0.62550	0.21560	0.35700
H	2.68020	4.76050	2.14300	O	0.06900	1.68070	0.90860
H	4.32730	5.58620	3.69160	O	1.06530	-0.53180	1.61680
H	6.46060	4.26090	4.13370	N	-3.08020	-1.28840	-0.44710
H	6.83650	2.15190	3.01450	H	-3.92820	-0.78810	-0.22710
C	-0.36170	4.93110	-0.77790	C	-3.18610	-2.52640	-1.04410
C	1.70820	3.21450	0.10030	C	-1.44330	-4.50170	1.04090
C	0.41100	2.82070	0.21260	C	-0.35810	-3.71470	1.37100
C	-0.67650	3.74370	-0.23940	C	-1.78620	-2.07260	2.40250
H	-1.13160	5.60280	-1.13250	C	-2.91380	-2.83740	2.10500
C	2.03740	4.49080	-0.60890	C	1.09420	-4.01920	1.15770

H	1.50500	-4.51970	2.04170	C	1.35180	-1.88360	-3.85410
H	1.24780	-4.68020	0.30970	C	2.11380	-0.78420	-3.86750
C	-1.77010	-0.77420	3.15480	C	3.16920	-0.60210	-2.84890
H	-0.81650	-0.26590	3.00980	C	3.36580	-1.53420	-1.89880
H	-1.93370	-0.95030	4.22170	C	2.54040	-2.76580	-1.91520
H	-2.57830	-0.13660	2.80390	C	1.58230	-2.92680	-2.83590
C	-4.26990	-2.54130	2.58520	H	0.56980	-2.01330	-4.59100
C	-1.38450	-5.83910	0.40470	H	1.94740	-0.01720	-4.61270
H	0.89010	-8.12290	0.10870	H	3.74190	0.31720	-2.84830
H	-0.85850	-8.44210	0.35660	H	2.70710	-3.54590	-1.19050
H	-6.11020	-2.39700	4.54940	H	0.97790	-3.82480	-2.83910
H	-5.51250	-0.76110	4.97970	C	-3.82400	2.04430	4.14820
O	-0.19550	-6.46950	0.53650	C	-2.61410	2.57810	3.94870
O	-2.33660	-6.33880	-0.16790	C	-2.17070	2.91800	2.58060
O	-5.28280	-3.00720	2.06420	C	-2.96170	2.65930	1.52310
O	-4.33030	-1.75200	3.67050	C	-4.30160	2.06580	1.75550
Si	4.59840	-1.23650	-0.52580	C	-4.71150	1.78450	2.99820
Si	-2.48060	3.24040	-0.18370	H	-4.15350	1.80010	5.14970
C	4.54840	-4.76620	2.55170	H	-1.96170	2.77410	4.78960
C	4.17530	-3.54230	2.94380	H	-1.22000	3.41840	2.46040
C	4.17800	-2.42230	1.97990	H	-4.97140	1.87690	0.93280
C	4.55190	-2.62890	0.70530	H	-5.69720	1.37090	3.16300
C	4.97630	-3.98430	0.28050	C	-3.32260	0.11470	-3.59020
C	4.96910	-4.99750	1.15510	C	-2.07000	0.51570	-3.34790
H	4.54270	-5.58800	3.25590	C	-1.80070	1.50240	-2.28130
H	3.86480	-3.37070	3.96630	C	-2.80410	1.97430	-1.51990
H	3.86360	-1.44590	2.32190	C	-4.19550	1.55160	-1.82280
H	5.29060	-4.16020	-0.74070	C	-4.43850	0.67020	-2.80090
H	5.27450	-5.98750	0.84220	H	-3.52120	-0.61260	-4.36660
C	8.96880	-1.21650	-2.24470	H	-1.24920	0.11400	-3.92790
C	8.76150	-1.34300	-0.92970	H	-0.77990	1.82170	-2.12800
C	7.38470	-1.34820	-0.39420	H	-5.02890	1.98190	-1.28750
C	6.33130	-1.20890	-1.21900	H	-5.45450	0.36950	-3.02170
C	6.57070	-1.09100	-2.68000	C	-5.09320	7.04170	-1.01550
C	7.81980	-1.08990	-3.16220	C	-4.50690	6.87490	0.17550
H	9.97670	-1.21400	-2.63910	C	-3.68590	5.67410	0.43500
H	9.60150	-1.44470	-0.25470	C	-3.53460	4.73810	-0.51740
H	7.24560	-1.48660	0.67000	C	-4.17280	4.93780	-1.84220
H	5.74750	-1.01320	-3.37300	C	-4.91360	6.02850	-2.07470
H	7.99070	-1.00360	-4.22750	H	-5.69390	7.92130	-1.20750

H	-4.63170	7.61900	0.95150	C	-1.92830	-2.91450	-1.82090
H	-3.21160	5.56450	1.40220	H	-1.95350	-2.46410	-2.81750
H	-4.03060	4.21830	-2.63670	H	-1.04650	-2.52130	-1.31410
H	-5.37470	6.17560	-3.04280	H	-1.84330	-3.99800	-1.93050
N	-0.57900	-2.50260	1.97440	C	-6.90570	-3.31710	-3.14830
H	0.20260	-1.75260	1.92550	C	-6.91580	-2.53280	-1.99860
H	1.63130	-3.07960	1.01650	C	-5.74120	-2.30980	-1.27840
C	-5.65290	-1.47930	4.17300	C	-4.50850	-2.84020	-1.71920
H	-6.28690	-1.06330	3.38800	C	-4.53390	-3.65240	-2.86560
C	-0.12150	-7.76630	-0.08280	C	-5.70850	-3.89070	-3.57450
H	-0.30770	-7.69140	-1.15660	H	-7.82590	-3.48530	-3.70000
C	-2.77760	-3.96080	1.21480	H	-7.82900	-2.07990	-1.62680
H	-3.12950	-3.38740	-0.08240	H	-3.61260	-4.09320	-3.22560
H	-3.60060	-4.66850	1.17240	H	-5.68230	-4.51410	-4.46290
O	-0.38660	-0.44520	-0.53170	O	-5.83200	-1.51300	-0.15280
H	-2.16250	-0.83000	-0.41550	H	-5.72730	-2.08470	0.63810

C	-2.88170	2.17890	0.56870	C	-0.40170	4.16480	2.66300
C	-5.40690	1.13890	-0.15890	C	-0.32660	4.94590	3.91930
C	-4.37220	0.30070	0.00610	C	-1.37190	4.97930	4.75310
C	-3.02200	0.84940	0.33920	C	-2.60170	4.23170	4.42780
H	-6.38460	0.76870	-0.43380	C	-2.68040	3.52730	3.29280
C	-5.23050	2.59470	-0.02730	H	0.57520	5.49180	4.16770
C	-4.02310	3.10430	0.29550	H	-1.31620	5.54920	5.67160
C	-3.85310	4.58470	0.32920	H	-3.43780	4.24860	5.11500
C	-4.89320	5.39210	0.09220	H	-3.58420	2.97100	3.08180
C	-6.21720	4.82300	-0.21970	O	-1.98570	-0.01870	0.60000
C	-6.37750	3.49740	-0.28310	P	-0.60650	0.13840	-0.32390
H	-2.88680	5.02820	0.52750	O	-0.49980	1.72620	-0.75110
H	-4.76320	6.46640	0.11690	O	-0.79080	-0.63160	-1.61630
H	-7.05520	5.48170	-0.40800	N	3.23380	-0.82170	0.04820
H	-7.35020	3.08670	-0.52430	H	3.59570	-0.87700	-0.89260
C	0.75920	4.12350	1.75320	C	3.77710	-1.65590	0.98700
C	-1.59530	2.72440	1.07250	C	1.51190	-4.05170	0.69320
C	-0.47780	2.56500	0.33250	C	0.40310	-3.41600	0.17090
C	0.73740	3.36900	0.64270	C	1.57700	-2.96910	-1.89670
H	1.62740	4.72890	1.98770	C	2.73500	-3.55360	-1.40570
C	-1.53420	3.50110	2.34430	C	-0.91690	-3.24970	0.85790

H	-1.50830	-2.48450	0.36130	C	-2.19850	-2.60660	-4.12750
H	-1.46360	-4.19710	0.85360	C	-2.24510	-3.48040	-3.11560
C	1.35310	-2.42370	-3.27690	C	-3.01240	-3.16000	-1.89400
H	0.67120	-1.57070	-3.21900	C	-3.65480	-1.98510	-1.78650
H	0.87870	-3.19580	-3.89500	C	-3.61540	-1.02980	-2.92120
H	2.28900	-2.16050	-3.75980	C	-2.92080	-1.32310	-4.02720
C	3.94270	-3.73420	-2.24890	H	-1.63170	-2.83760	-5.02000
C	1.60070	-4.63760	2.03730	H	-1.71410	-4.42080	-3.18540
H	-0.53770	-5.73080	4.20340	H	-3.03670	-3.88770	-1.09900
H	1.08750	-6.44760	3.94570	H	-4.14400	-0.08690	-2.85910
H	6.52650	-3.45210	-2.68020	H	-2.88670	-0.62080	-4.84990
H	6.93240	-4.70470	-1.46430	C	2.50900	8.10740	-1.39570
O	0.43040	-5.00780	2.58180	C	1.37100	7.44950	-1.63960
O	2.67180	-4.78560	2.62250	C	1.27860	6.00140	-1.36230
O	4.04460	-3.49380	-3.43880	C	2.34180	5.32740	-0.88830
O	4.97380	-4.21520	-1.51390	C	3.59040	6.07440	-0.58800
Si	-4.63870	-1.53050	-0.27350	C	3.66910	7.38790	-0.83550
Si	2.19590	3.50110	-0.52100	H	2.57790	9.16890	-1.59580
C	-9.16000	-2.46600	-1.06090	H	0.51340	7.97660	-2.03730
C	-8.76580	-2.00620	0.13230	H	0.33080	5.50840	-1.52290
C	-7.33920	-1.70940	0.37660	H	4.44090	5.58050	-0.14540
C	-6.43310	-1.89200	-0.59890	H	4.57920	7.92930	-0.61140
C	-6.87490	-2.40800	-1.91770	C	1.61460	1.11630	-4.53140
C	-8.16830	-2.67800	-2.13480	C	0.75400	2.08510	-4.20180
H	-10.20450	-2.68470	-1.24140	C	0.94220	2.84980	-2.95140
H	-9.49020	-1.85150	0.92140	C	1.96500	2.56600	-2.12490
H	-7.03860	-1.34120	1.35000	C	2.92040	1.49640	-2.50750
H	-6.16070	-2.57140	-2.71330	C	2.75570	0.81470	-3.64670
H	-8.49050	-3.05400	-3.09720	H	1.47640	0.55200	-5.44450
C	-3.57870	-4.10200	3.50160	H	-0.08600	2.30760	-4.84700
C	-3.41500	-2.77480	3.53900	H	0.21600	3.60790	-2.70210
C	-3.75880	-1.95180	2.36050	H	3.76190	1.25730	-1.87700
C	-4.20690	-2.53450	1.23460	H	3.46020	0.04040	-3.92140
C	-4.43110	-4.00070	1.21800	C	6.11660	2.07080	1.63230
C	-4.12390	-4.74330	2.28870	C	4.93380	1.91330	2.23630
H	-3.32300	-4.70610	4.36240	C	3.69050	2.33570	1.55710
H	-3.02580	-2.30060	4.43060	C	3.74190	2.89320	0.33470
H	-3.64090	-0.88050	2.43050	C	5.05640	3.03370	-0.34130
H	-4.85120	-4.47790	0.34170	C	6.18010	2.65100	0.27670
H	-4.28280	-5.81370	2.27150	H	7.02660	1.75890	2.12810

H	4.88540	1.47980	3.22670	C	3.11490	-1.48690	2.35210
H	2.74980	2.19040	2.06920	H	3.44500	-2.23520	3.06980
H	5.11190	3.45210	-1.33860	H	3.38380	-0.50030	2.73880
H	7.13630	2.75700	-0.21890	H	2.02720	-1.51090	2.24890
N	0.48480	-2.88090	-1.08300	C	8.07610	-2.05180	0.86820
H	-0.21070	-2.12150	-1.34960	C	7.32500	-2.95890	1.60540
H	-0.78150	-2.95410	1.89690	C	5.92510	-2.87530	1.64900
C	6.21310	-4.39100	-2.21940	C	5.26730	-1.83610	0.94580
H	6.10700	-5.15150	-2.99690	C	6.05320	-0.94490	0.19430
C	0.49560	-5.53020	3.92240	C	7.43910	-1.03770	0.14830
H	0.94470	-4.79870	4.59740	H	9.15880	-2.13770	0.85540
C	2.78180	-3.94310	-0.00640	H	7.79490	-3.76140	2.16420
H	3.38860	-2.90110	0.62880	H	5.55400	-0.13630	-0.32770
H	3.53720	-4.67800	0.25660	H	8.01340	-0.31740	-0.42530
O	0.52820	-0.25710	0.59350	O	5.32190	-3.83260	2.39750
H	2.24150	-0.54400	0.15200	H	4.35730	-3.92720	2.28930

C	3.02190	1.96220	0.77980	C	1.70620	5.16220	-0.78960
C	5.16190	0.23100	1.42680	C	2.20340	6.43310	-1.36750
C	4.26120	-0.14170	0.50510	C	3.51560	6.63260	-1.52490
C	3.09010	0.73300	0.23560	C	4.47260	5.58030	-1.13840
H	6.02420	-0.39230	1.63290	C	4.03310	4.43240	-0.61020
C	5.00540	1.50590	2.15750	H	1.50520	7.20500	-1.66710
C	3.98720	2.34230	1.85170	H	3.87780	7.56030	-1.94880
C	3.82850	3.60400	2.62280	H	5.53230	5.73430	-1.29690
C	4.70520	3.92340	3.58200	H	4.75610	3.66570	-0.36830
C	5.83110	3.02000	3.88920	O	2.09130	0.30950	-0.59830
C	5.97320	1.87210	3.21720	P	0.67870	0.05500	0.20430
H	2.99970	4.27070	2.42360	O	0.19210	1.54440	0.76600
H	4.58680	4.84260	4.14100	O	0.94020	-0.74800	1.47920
H	6.53790	3.28650	4.66440	N	-3.01390	-0.98640	-0.59480
H	6.79840	1.21150	3.45230	H	-3.64340	-0.28050	-0.24190
C	0.25730	4.92830	-0.69300	C	-3.55300	-2.12030	-1.14670
C	2.05620	2.94210	0.21570	C	-1.88840	-4.36850	0.77290
C	0.71910	2.68630	0.19890	C	-0.77310	-3.65330	1.16890
C	-0.22300	3.75850	-0.24740	C	-2.15030	-1.96470	2.20690
H	-0.40900	5.70870	-1.03510	C	-3.30160	-2.67650	1.89220
C	2.57480	4.20930	-0.39020	C	0.66470	-4.04280	1.00120

H	0.98750	-4.62330	1.87310	C	1.59010	-1.71410	-4.11410
H	0.81250	-4.66820	0.12590	C	2.56280	-0.79820	-4.05130
C	-2.08000	-0.68900	2.99110	C	3.52880	-0.81760	-2.93280
H	-1.26670	-0.73850	3.71910	C	3.44250	-1.75750	-1.97460
H	-3.02320	-0.47570	3.48600	C	2.37510	-2.78370	-2.06800
H	-1.84530	0.13840	2.31390	C	1.49390	-2.75720	-3.07510
C	-4.65240	-2.26230	2.32520	H	0.87420	-1.69370	-4.92550
C	-1.89450	-5.66120	0.05340	H	2.63450	-0.03000	-4.81040
H	0.27030	-8.01910	-0.42770	H	4.26900	-0.03360	-2.87980
H	-1.48970	-8.27800	-0.19090	H	2.28870	-3.55300	-1.32000
H	-7.32160	-2.49300	1.90180	H	0.70930	-3.50100	-3.13010
H	-7.33370	-3.98380	2.89380	C	-4.17090	7.61460	-0.96300
O	-0.73730	-6.35590	0.12950	C	-4.13540	6.71330	-1.95150
O	-2.87270	-6.07690	-0.54630	C	-3.48090	5.40530	-1.73930
O	-5.03180	-1.11360	2.54210	C	-2.93010	5.11080	-0.54920
O	-5.48080	-3.31760	2.43330	C	-2.96220	6.11860	0.53810
Si	4.56870	-1.69620	-0.48440	C	-3.55250	7.30370	0.34150
Si	-2.07540	3.48650	-0.24550	H	-4.64830	8.57350	-1.11800
C	3.89950	-5.48610	2.20050	H	-4.58310	6.94120	-2.91020
C	3.78910	-4.26530	2.73670	H	-3.44160	4.70730	-2.56390
C	3.99290	-3.06560	1.89820	H	-2.50530	5.90230	1.49560
C	4.30120	-3.19350	0.59560	H	-3.57520	8.03790	1.13640
C	4.42160	-4.55130	0.00900	C	-3.57060	2.29370	4.03930
C	4.22820	-5.63570	0.76910	C	-2.31890	2.73130	3.86630
H	3.74470	-6.36510	2.81260	C	-1.83590	3.07810	2.51380
H	3.54290	-4.15300	3.78460	C	-2.63830	2.92890	1.44370
H	3.88140	-2.09340	2.35690	C	-4.02780	2.45230	1.64820
H	4.66020	-4.67050	-1.04060	C	-4.46700	2.15030	2.87600
H	4.31220	-6.62430	0.33680	H	-3.92760	2.04220	5.02940
C	9.02490	-1.40280	-1.92420	H	-1.65930	2.84050	4.71730
C	8.58450	-2.53720	-1.36850	H	-0.83870	3.48400	2.41530
C	7.18360	-2.64350	-0.90950	H	-4.70650	2.36290	0.81690
C	6.33850	-1.60930	-1.06450	H	-5.48310	1.80620	3.01990
C	6.84250	-0.34630	-1.65930	C	-3.22580	0.55450	-3.73140
C	8.11310	-0.25140	-2.06940	C	-1.93850	0.79720	-3.46250
H	10.05110	-1.32350	-2.25910	C	-1.57130	1.71940	-2.36780
H	9.25350	-3.38010	-1.25290	C	-2.52400	2.29040	-1.60940
H	6.86600	-3.56650	-0.44980	C	-3.95040	2.03780	-1.93620
H	6.19620	0.51760	-1.73940	C	-4.28040	1.21220	-2.93690
H	8.47880	0.67390	-2.49560	H	-3.49690	-0.11870	-4.53410



H	-1.16200	0.31820	-4.04510	C	-2.66390	-2.73990	-2.23120
H	-0.52290	1.91600	-2.19650	H	-2.81000	-3.81830	-2.31890
H	-4.73560	2.54920	-1.39930	H	-2.86970	-2.27550	-3.19990
H	-5.32140	1.03520	-3.17460	H	-1.61800	-2.54510	-1.98150
N	-0.94740	-2.46240	1.81950	C	-7.84320	-2.27470	-1.85250
H	-0.10560	-1.77070	1.81070	C	-7.32180	-1.27170	-1.04200
H	1.27420	-3.13900	0.94500	C	-5.94770	-1.18900	-0.78890
C	-6.85500	-3.01770	2.73980	C	-5.05080	-2.11420	-1.37790
H	-6.92320	-2.40150	3.63800	C	-5.61080	-3.12110	-2.18580
C	-0.72510	-7.60440	-0.58450	C	-6.97790	-3.20740	-2.42590
H	-0.91160	-7.44170	-1.64850	H	-8.91170	-2.32290	-2.03990
C	-3.19370	-3.77600	0.97290	H	-7.96000	-0.51480	-0.59680
H	-3.47700	-3.05120	-0.26150	H	-4.95440	-3.85770	-2.63480
H	-4.04330	-4.44180	0.86540	H	-7.36360	-3.99770	-3.06230
O	-0.28810	-0.50020	-0.80000	O	-5.51790	-0.12400	-0.01440
H	-2.00880	-0.77750	-0.69290	H	-5.51430	-0.36000	0.93660

C	2.88700	2.23030	0.20150	C	0.93960	4.50990	-2.13530
C	5.29780	1.04760	1.06540	C	1.15420	5.44850	-3.26100
C	4.34320	0.28010	0.51670	C	2.37520	5.60150	-3.78470
C	3.02570	0.88670	0.15630	C	3.51180	4.82930	-3.24780
H	6.26540	0.63810	1.31600	C	3.32860	3.98420	-2.22690
C	5.06560	2.48370	1.30480	H	0.32320	6.01360	-3.66450
C	3.91900	3.06060	0.88660	H	2.53140	6.28640	-4.60810
C	3.69850	4.50860	1.15120	H	4.49370	4.94240	-3.68920
C	4.63960	5.23400	1.76640	H	4.17240	3.41210	-1.86460
C	5.90140	4.60090	2.19550	O	2.04270	0.10920	-0.41330
C	6.10400	3.29660	1.97980	P	0.57840	0.10260	0.37720
H	2.77350	4.98870	0.85950	O	0.25620	1.65070	0.86490
H	4.47520	6.28660	1.95720	O	0.71820	-0.66020	1.68590
H	6.65990	5.19420	2.68960	N	-3.17440	-0.95430	-0.31250
H	7.03070	2.83770	2.30140	H	-3.61160	-0.80100	0.58380
C	-0.41190	4.33840	-1.57140	C	-3.67760	-1.95080	-1.10450
C	1.74450	2.87800	-0.48630	C	-1.57560	-4.31930	-0.13310
C	0.48340	2.61600	-0.08220	C	-0.48330	-3.62350	0.34930
C	-0.63780	3.46360	-0.57850	C	-1.79550	-2.72350	2.17270
H	-1.21660	4.95480	-1.95520	C	-2.94150	-3.33660	1.69570
C	1.98010	3.82280	-1.61680	C	0.89520	-3.62730	-0.23640

H	1.43780	-4.52490	0.07560	C	3.18460	-1.96580	-4.35630
H	0.85530	-3.63210	-1.32390	C	3.06590	-2.98660	-3.49960
C	-1.60820	-1.95460	3.45010	C	3.56890	-2.85560	-2.11630
H	-1.02060	-1.05560	3.23750	C	4.13560	-1.70920	-1.70750
H	-1.01400	-2.56150	4.14380	C	4.28300	-0.58850	-2.66930
H	-2.55040	-1.70210	3.92170	C	3.82700	-0.70940	-3.92180
C	-4.28040	-3.38300	2.34500	H	2.81410	-2.05960	-5.36890
C	-1.58750	-5.17560	-1.32590	H	2.59680	-3.90950	-3.81540
H	0.63920	-6.82500	-2.99270	H	3.46440	-3.69710	-1.45070
H	-1.04860	-7.37810	-2.73450	H	4.75610	0.33580	-2.36190
H	-5.99020	-3.46100	4.36760	H	3.93000	0.11190	-4.61910
H	-5.76640	-1.70800	4.68240	C	-3.45950	7.96930	0.76180
O	-0.40010	-5.70280	-1.66840	C	-2.49500	7.41240	1.50170
O	-2.61310	-5.40310	-1.96380	C	-2.14560	5.98890	1.31450
O	-5.14930	-4.16140	1.99910	C	-2.80840	5.23590	0.41910
O	-4.47650	-2.46720	3.32060	C	-3.85540	5.87260	-0.42120
Si	4.74470	-1.48160	0.03780	C	-4.16580	7.16400	-0.25290
Si	-2.34930	3.44100	0.17160	H	-3.71540	9.01220	0.89650
C	2.85420	-4.51810	3.06120	H	-1.96680	8.00320	2.23890
C	2.65090	-3.20560	3.22220	H	-1.34250	5.57790	1.90600
C	3.26390	-2.24140	2.28530	H	-4.35750	5.31510	-1.19780
C	3.99020	-2.67830	1.24350	H	-4.92450	7.62550	-0.87190
C	4.25050	-4.13080	1.09790	C	-2.61120	1.31640	4.35340
C	3.70600	-5.00230	1.95610	C	-1.62320	2.18230	4.10490
H	2.40390	-5.22610	3.74480	C	-1.53540	2.84770	2.78880
H	2.03290	-2.84680	4.03510	C	-2.43330	2.57480	1.82500
H	3.10970	-1.18500	2.45350	C	-3.52220	1.60820	2.10980
H	4.88850	-4.49320	0.30190	C	-3.60820	1.01820	3.30750
H	3.89260	-6.06260	1.84540	H	-2.67830	0.82800	5.31680
C	9.35700	-2.29570	0.15170	H	-0.88640	2.39900	4.86740
C	8.67180	-2.15530	1.29240	H	-0.71690	3.53100	2.61160
C	7.21800	-1.89490	1.25540	H	-4.26390	1.37640	1.36240
C	6.57860	-1.78860	0.07800	H	-4.40940	0.32090	3.51180
C	7.34230	-1.95330	-1.18320	C	-5.35330	1.58950	-2.91980
C	8.65930	-2.19150	-1.14580	C	-4.03620	1.48750	-3.12960
H	10.42190	-2.48710	0.17690	C	-3.08210	2.04150	-2.14630
H	9.18030	-2.23320	2.24460	C	-3.53220	2.65910	-1.04050
H	6.68000	-1.79110	2.18970	C	-4.99520	2.75600	-0.80840
H	6.84640	-1.88080	-2.14140	C	-5.85630	2.25770	-1.70360
H	9.21620	-2.30940	-2.06640	H	-6.05200	1.18150	-3.63860

H	-3.66590	1.00400	-4.02410	H	-1.82720	-2.12330	-2.21110
H	-2.02300	1.94560	-2.34350	H	-3.20390	-2.96610	-2.98160
H	-5.37330	3.24350	0.08160	H	-3.09480	-1.20330	-3.01900
H	-6.92230	2.33400	-1.53350	C	-7.98600	-2.17920	-1.29770
N	-0.63510	-2.84720	1.45800	C	-7.22310	-3.23680	-1.77450
H	0.08170	-2.06140	1.62520	C	-5.82240	-3.21060	-1.70460
H	1.44030	-2.74520	0.09520	C	-5.17360	-2.07570	-1.15810
C	-5.78570	-2.48620	3.91990	C	-5.97410	-1.02830	-0.66810
H	-6.54900	-2.27320	3.16830	C	-7.36130	-1.06470	-0.73180
C	-0.39570	-6.51200	-2.86050	H	-9.06900	-2.22680	-1.36390
H	-0.73690	-5.93120	-3.72010	H	-7.68470	-4.11990	-2.20290
C	-2.88570	-4.01860	0.41310	H	-5.48020	-0.15070	-0.26900
H	-3.37890	-3.10430	-0.47260	H	-7.94460	-0.22760	-0.36200
H	-3.66990	-4.75580	0.25710	O	-5.20660	-4.31200	-2.20280
O	-0.42320	-0.38090	-0.63990	H	-4.26940	-4.43230	-1.96230
H	-2.17380	-0.70160	-0.38890				
C	-2.90130	-2.09040	-2.41100				
C	3.11150	1.92120	0.69260	C	1.80890	5.11650	-0.90280
C	5.20100	0.09920	1.24340	C	2.30980	6.34530	-1.56260
C	4.20290	-0.26460	0.42400	C	3.61430	6.48950	-1.81450
C	3.06480	0.66610	0.20350	C	4.55770	5.41660	-1.45260
H	6.04060	-0.56520	1.41190	C	4.11520	4.30630	-0.85160
C	5.17910	1.41260	1.91920	H	1.62010	7.13060	-1.84650
C	4.18340	2.29080	1.66200	H	3.97900	7.38650	-2.29830
C	4.15750	3.58970	2.38630	H	5.60850	5.52380	-1.68910
C	5.13000	3.89960	3.25150	H	4.82550	3.52160	-0.63160
C	6.23050	2.94890	3.50260	O	1.97100	0.26230	-0.51560
C	6.25340	1.76800	2.87470	P	0.63510	0.11940	0.43560
H	3.34970	4.29230	2.22880	O	0.28670	1.65600	0.96160
H	5.10840	4.84610	3.77610	O	0.98470	-0.66340	1.69690
H	7.01530	3.20750	4.20170	N	-3.19890	-0.80920	-0.37400
H	7.06050	1.07270	3.06910	H	-3.95450	-0.16000	-0.22850
C	0.36070	4.93070	-0.72360	C	-3.46050	-2.01100	-0.97860
C	2.14870	2.92800	0.17230	C	-2.06040	-4.24510	1.12530
C	0.80580	2.72930	0.26920	C	-0.87310	-3.64440	1.49290
C	-0.12920	3.79570	-0.20440	C	-2.04830	-1.80560	2.51880
H	-0.29980	5.70440	-1.09120	C	-3.27300	-2.38660	2.20970
C	2.66880	4.14730	-0.52370	C	0.50960	-4.19860	1.32770

H	0.78420	-4.78010	2.21500	C	1.07780	-2.06370	-3.86580
H	0.57730	-4.87200	0.47680	C	1.07320	-2.98020	-2.89260
C	-1.82540	-0.54140	3.29770	C	2.10520	-2.94500	-1.83670
H	-0.80510	-0.18540	3.15110	C	3.06400	-2.00280	-1.84980
H	-2.00600	-0.71190	4.36280	C	3.06970	-0.99830	-2.94380
H	-2.52800	0.22020	2.97040	C	2.12450	-1.02380	-3.89180
C	-4.57470	-1.97250	2.77000	H	0.31550	-2.08190	-4.63390
C	-2.07780	-5.58670	0.50260	H	0.30820	-3.74540	-2.87050
H	-2.64900	-7.25830	-1.48760	H	2.05530	-3.68200	-1.05360
H	-3.28310	-7.91190	0.03770	H	3.81350	-0.21640	-2.96620
H	-6.21150	-1.57300	4.84470	H	2.12140	-0.27810	-4.67620
H	-5.50610	0.05380	5.11610	C	-4.03690	7.65950	-1.05780
O	-3.27160	-5.82790	-0.09780	C	-3.98590	6.73980	-2.02850
O	-1.16680	-6.39480	0.49820	C	-3.34400	5.43240	-1.77820
O	-5.64370	-2.43030	2.39520	C	-2.82050	5.15650	-0.57120
O	-4.49320	-1.06710	3.77150	C	-2.86840	6.18530	0.49580
Si	4.33320	-1.89320	-0.48080	C	-3.44760	7.36980	0.26470
Si	-1.98240	3.53230	-0.21810	H	-4.50550	8.61790	-1.24070
C	3.78190	-5.44560	2.53990	H	-4.41200	6.95210	-3.00050
C	3.73660	-4.18410	2.98300	H	-3.29130	4.71970	-2.58930
C	3.90970	-3.05980	2.03960	H	-2.43260	5.98520	1.46640
C	4.12110	-3.29700	0.73270	H	-3.48220	8.11900	1.04500
C	4.16750	-4.69990	0.24980	C	-3.61860	2.54840	4.06520
C	4.00530	-5.71570	1.10600	C	-2.35370	2.95400	3.90980
H	3.65050	-6.26930	3.22940	C	-1.82050	3.21540	2.55650
H	3.56680	-3.98340	4.03280	C	-2.58940	3.01760	1.47000
H	3.84940	-2.05250	2.42620	C	-3.98930	2.56000	1.65340
H	4.32600	-4.90800	-0.80100	C	-4.47630	2.34510	2.88160
H	4.03570	-6.73710	0.74930	H	-4.01340	2.36320	5.05570
C	8.62620	-1.89480	-2.37630	H	-1.72190	3.10520	4.77530
C	8.21340	-2.95840	-1.67820	H	-0.81930	3.61460	2.46900
C	6.86470	-2.97130	-1.07360	H	-4.63880	2.41510	0.80590
C	6.03680	-1.92460	-1.23830	H	-5.50180	2.02510	3.00960
C	6.51390	-0.73770	-1.99100	C	-3.01300	0.55710	-3.70640
C	7.73780	-0.72680	-2.53280	C	-3.99680	1.13230	-3.00730
H	9.61430	-1.88370	-2.81790	C	-3.67600	2.06320	-1.90510
H	8.86650	-3.81240	-1.55350	C	-2.39670	2.31500	-1.57530
H	6.57220	-3.83680	-0.50010	C	-1.31210	1.69440	-2.37860
H	5.89050	0.14130	-2.08000	C	-1.60570	0.85700	-3.38060
H	8.08480	0.14430	-3.07350	H	-3.24570	-0.12360	-4.51460

H	-5.03030	0.91760	-3.24690	C	-2.24330	-2.60160	-1.67780
H	-4.49090	2.55920	-1.39960	H	-2.40870	-3.64420	-1.95950
H	-0.27460	1.91160	-2.16870	H	-1.96050	-1.99530	-2.54770
H	-0.81180	0.40250	-3.95870	H	-1.37260	-2.53750	-1.02490
N	-0.91290	-2.41320	2.09110	C	-7.48650	-2.16720	-2.58630
H	-0.03650	-1.79840	2.05120	C	-6.42090	-2.47750	-3.41730
H	1.21250	-3.36890	1.23230	C	-5.10180	-2.46700	-2.93940
C	-5.74820	-0.70400	4.37160	C	-4.83950	-2.13340	-1.58980
H	-6.43530	-0.30470	3.62260	C	-5.94590	-1.83380	-0.77170
C	-3.40230	-7.12230	-0.70810	C	-7.25010	-1.84450	-1.24740
H	-4.40470	-7.14410	-1.13430	H	-8.49850	-2.18300	-2.98000
C	-3.30300	-3.49520	1.27240	H	-6.56970	-2.72970	-4.46200
H	-3.52810	-2.90030	0.04730	H	-5.77720	-1.63100	0.27960
H	-4.22530	-4.06960	1.26060	H	-8.07220	-1.61940	-0.57610
O	-0.47410	-0.40180	-0.43670	O	-4.16480	-2.78350	-3.87920
H	-2.21870	-0.49360	-0.28250	H	-3.27680	-2.71420	-3.51280

C	2.99390	2.18230	0.63320	C	1.42230	5.25520	-0.95840
C	5.22770	0.53900	1.17170	C	1.81580	6.51560	-1.63120
C	4.26360	0.09220	0.35130	C	3.10130	6.76020	-1.90290
C	3.04480	0.92510	0.14980	C	4.13090	5.76670	-1.54950
H	6.10990	-0.05400	1.36060	C	3.78540	4.62850	-0.93730
C	5.10540	1.85010	1.84110	H	1.06270	7.24290	-1.90850
C	4.04090	2.64360	1.58880	H	3.38750	7.68020	-2.39610
C	3.91600	3.94000	2.30750	H	5.16680	5.95510	-1.80110
C	4.86680	4.33160	3.16370	H	4.55820	3.90360	-0.72300
C	6.04180	3.47360	3.41050	O	1.97570	0.43130	-0.54960
C	6.15470	2.29540	2.78740	P	0.66080	0.18980	0.40990
H	3.05300	4.57450	2.15360	O	0.20440	1.69550	0.94430
H	4.77270	5.27580	3.68430	O	1.06990	-0.57290	1.66490
H	6.80820	3.79780	4.10250	N	-3.09730	-0.98090	-0.33210
H	7.01650	1.66810	2.97880	H	-3.87770	-0.36680	-0.16800
C	-0.00380	4.95930	-0.75420	C	-3.31820	-2.18860	-0.94220
C	1.94720	3.10570	0.12050	C	-3.04820	-2.59470	2.23830
C	0.62580	2.80360	0.24000	C	-1.85530	-1.94180	2.52700
C	-0.39660	3.79350	-0.22040	C	-0.59430	-3.68610	1.44000
H	-0.72760	5.67790	-1.11420	C	-1.75030	-4.35810	1.09760
C	2.36050	4.35820	-0.58840	C	-1.69200	-0.68170	3.32680

H	-0.70070	-0.25830	3.16120	C	4.21580	-5.04630	2.58970
H	-2.44990	0.03990	3.03460	C	3.93870	-3.79510	2.97520
C	0.81450	-4.14730	1.22510	C	4.01400	-2.68580	2.00180
H	1.45090	-3.27240	1.08050	C	4.35630	-2.92970	0.72490
H	0.89160	-4.83470	0.38700	C	4.67390	-4.31620	0.30720
H	1.16860	-4.68420	2.11240	C	4.60220	-5.31910	1.19070
C	-1.70180	-5.69260	0.46080	H	4.15710	-5.85990	3.30090
C	-4.36010	-2.27190	2.83450	H	3.65320	-3.59300	3.99940
H	-5.95640	-2.03340	4.97320	H	3.77670	-1.68620	2.33870
H	-5.35890	-0.36530	5.25180	H	4.96210	-4.52300	-0.71600
H	-2.77630	-8.08060	0.00010	H	4.83000	-6.33140	0.88310
H	-3.97070	-7.37200	-1.13700	C	-4.60750	7.34120	-1.04460
O	-4.30920	-1.39350	3.86180	C	-4.06900	7.12550	0.16110
O	-5.40810	-2.77980	2.46570	C	-3.32010	5.87950	0.42550
O	-0.74580	-6.44610	0.42790	C	-3.18830	4.95110	-0.53720
O	-2.89270	-5.99860	-0.11580	C	-3.77170	5.20500	-1.87790
Si	4.48960	-1.55510	-0.51960	C	-4.44670	6.33660	-2.11480
Si	-2.22590	3.39370	-0.19870	H	-5.15540	8.25390	-1.24010
C	8.82370	-1.88340	-2.29860	H	-4.18000	7.86300	0.94550
C	8.62720	-1.97640	-0.97920	H	-2.88300	5.73100	1.40480
C	7.26180	-1.87210	-0.42470	H	-3.64130	4.49140	-2.67980
C	6.20960	-1.66510	-1.23670	H	-4.86790	6.52280	-3.09430
C	6.43530	-1.58560	-2.70250	C	-3.72050	2.27270	4.09980
C	7.67380	-1.68440	-3.20190	C	-2.49910	2.79110	3.93130
H	9.82310	-1.96130	-2.70680	C	-2.00400	3.09420	2.57230
H	9.46720	-2.13120	-0.31450	C	-2.76200	2.82290	1.49420
H	7.12870	-1.98700	0.64290	C	-4.10990	2.23510	1.69120
H	5.60990	-1.45680	-3.38520	C	-4.56500	1.98310	2.92450
H	7.83470	-1.62610	-4.27070	H	-4.08830	2.05740	5.09450
C	1.16240	-1.98840	-3.80280	H	-1.87650	3.00430	4.79050
C	2.00370	-0.94890	-3.83550	H	-1.04460	3.58380	2.47280
C	3.08100	-0.83620	-2.83000	H	-4.74660	2.02090	0.84870
C	3.21820	-1.77100	-1.87220	H	-5.55440	1.56790	3.06250
C	2.30170	-2.93660	-1.86550	C	-3.18210	0.37180	-3.66550
C	1.32480	-3.03510	-2.77510	C	-1.91290	0.68900	-3.38930
H	0.36510	-2.06700	-4.53050	C	-1.60630	1.63640	-2.29820
H	1.88690	-0.17930	-4.58740	C	-2.59580	2.16270	-1.55450
H	3.72200	0.03680	-2.84640	C	-4.00370	1.83210	-1.89310
H	2.41610	-3.71920	-1.13320	C	-4.27890	0.97810	-2.88690
H	0.65450	-3.88490	-2.76210	H	-3.40780	-0.32170	-4.46480

H	-1.10650	0.25090	-3.96290	C	-2.09170	-2.71140	-1.68060
H	-0.57110	1.88680	-2.11690	H	-1.88630	-2.10760	-2.57310
H	-4.82020	2.30550	-1.36720	H	-1.20310	-2.57610	-1.06360
H	-5.30620	0.74080	-3.13130	H	-2.19640	-3.76870	-1.93620
N	-0.69550	-2.46740	2.05690	C	-7.37680	-2.49290	-2.44400
H	0.13760	-1.79720	2.00920	C	-6.32450	-2.79360	-3.29500
H	-1.83260	-0.88530	4.39210	C	-4.99440	-2.73990	-2.85120
C	-2.96110	-7.29370	-0.73510	C	-4.70690	-2.36750	-1.51710
H	-2.22060	-7.37820	-1.53390	C	-5.80070	-2.08260	-0.67680
C	-5.56880	-1.12710	4.50170	C	-7.11550	-2.13750	-1.11790
H	-6.30350	-0.76710	3.77860	H	-8.39750	-2.54230	-2.81140
C	-3.03220	-3.68840	1.28440	H	-6.49270	-3.07200	-4.33000
H	-3.31780	-3.08810	0.07190	H	-5.61140	-1.85530	0.36590
H	-3.91850	-4.31700	1.28150	H	-7.92630	-1.92100	-0.43020
O	-0.41000	-0.40620	-0.46340	O	-4.07420	-3.05590	-3.80760
H	-2.13120	-0.61630	-0.26710	H	-3.17930	-2.95920	-3.46520

C	2.99360	2.07290	0.68380	C	1.56570	5.22450	-0.88890
C	5.14930	0.33060	1.23580	C	2.01700	6.47250	-1.54880
C	4.16660	-0.06980	0.41450	C	3.31300	6.66190	-1.81500
C	2.99360	0.81730	0.19400	C	4.29660	5.62040	-1.46800
H	6.01410	-0.30070	1.40340	C	3.89900	4.49320	-0.86710
C	5.07760	1.64160	1.91220	H	1.29790	7.23520	-1.82100
C	4.05050	2.48230	1.65380	H	3.64140	7.57270	-2.29880
C	3.97580	3.77940	2.37810	H	5.34060	5.76490	-1.71480
C	4.93540	4.12510	3.24430	H	4.63790	3.73250	-0.65640
C	6.07010	3.21590	3.49650	O	1.91870	0.37570	-0.53180
C	6.13730	2.03670	2.86860	P	0.58100	0.17870	0.41030
H	3.14260	4.45160	2.22020	O	0.18740	1.69690	0.96220
H	4.87800	5.07010	3.76890	O	0.95690	-0.60460	1.66640
H	6.84410	3.50350	4.19620	N	-3.20970	-1.06740	-0.50580
H	6.96940	1.37170	3.06380	H	-4.01520	-0.47900	-0.37010
C	0.12710	4.99130	-0.68770	C	-3.37340	-2.31400	-1.05760
C	1.99220	3.04320	0.16860	C	-1.89380	-4.35280	1.15840
C	0.65900	2.79670	0.27750	C	-0.75230	-3.65390	1.49400
C	-0.31780	3.83860	-0.16620	C	-2.05890	-1.85960	2.43980
H	-0.56370	5.74660	-1.03720	C	-3.24050	-2.53270	2.14590
C	2.46240	4.28330	-0.52530	C	0.67490	-4.09130	1.34020

H	0.99850	-4.63520	2.23450	C	1.15430	-1.97480	-3.91580
H	0.80560	-4.75740	0.49150	C	1.18220	-2.89970	-2.95090
C	-1.92830	-0.55200	3.16680	C	2.19590	-2.82310	-1.87950
H	-2.64740	0.16140	2.77060	C	3.11090	-1.83850	-1.87500
H	-0.91970	-0.15480	3.05050	C	3.08230	-0.82510	-2.96040
H	-2.15350	-0.68040	4.22890	C	2.14990	-0.88570	-3.91940
C	-4.57240	-2.17210	2.66850	H	0.40460	-2.02360	-4.69490
C	-1.93840	-5.71290	0.57730	H	0.45790	-3.70370	-2.94800
H	0.16090	-8.16890	0.36370	H	2.16940	-3.56660	-1.10120
H	-1.60440	-8.34970	0.63030	H	3.78900	-0.00910	-2.96740
H	-6.30470	-1.75480	4.62780	H	2.12100	-0.13390	-4.69750
H	-5.66020	-0.10370	4.90820	C	-3.65880	2.44300	4.18120
O	-0.79750	-6.42590	0.73260	C	-2.39530	2.83810	3.99200
O	-2.92520	-6.16430	0.02320	C	-1.91080	3.14430	2.62980
O	-5.60660	-2.71920	2.31470	C	-2.72210	2.99380	1.56660
O	-4.56430	-1.20340	3.61290	C	-4.12520	2.56380	1.78930
Si	4.36590	-1.68720	-0.49740	C	-4.56760	2.30800	3.02650
Si	-2.16280	3.52130	-0.13550	H	-4.01700	2.22220	5.17830
C	3.97170	-5.27820	2.50270	H	-1.72710	2.94360	4.83670
C	3.88250	-4.02220	2.95480	H	-0.90690	3.52960	2.51940
C	4.00270	-2.88600	2.01740	H	-4.81380	2.47770	0.96490
C	4.21060	-3.10650	0.70700	H	-5.59520	2.00800	3.18380
C	4.30730	-4.50350	0.21440	C	-3.17000	0.51710	-3.60670
C	4.19160	-5.53030	1.06500	C	-4.15600	1.04420	-2.87340
H	3.87850	-6.11080	3.18780	C	-3.84220	1.97750	-1.77090
H	3.71540	-3.83490	4.00750	C	-2.56590	2.28730	-1.48130
H	3.90860	-1.88430	2.41150	C	-1.48080	1.71960	-2.32280
H	4.46610	-4.69860	-0.83880	C	-1.76770	0.87310	-3.31930
H	4.25820	-6.54740	0.70120	H	-3.39790	-0.16170	-4.41750
C	8.66320	-1.50760	-2.37490	H	-5.18610	0.78890	-3.08600
C	8.28840	-2.59260	-1.68840	H	-4.66220	2.43220	-1.23690
C	6.93880	-2.66250	-1.08990	H	-0.44770	1.98150	-2.14450
C	6.07240	-1.64640	-1.24820	H	-0.97240	0.45500	-3.92280
C	6.50670	-0.43550	-1.98850	C	-4.38780	7.55530	-0.99800
C	7.73150	-0.37290	-2.52480	C	-3.81470	7.34260	0.19220
H	9.65190	-1.45480	-2.81210	C	-3.11500	6.06910	0.45990
H	8.97300	-3.42230	-1.56870	C	-3.06060	5.11430	-0.48430
H	6.67710	-3.54400	-0.52610	C	-3.68390	5.36300	-1.80780
H	5.85030	0.41970	-2.07280	C	-4.31490	6.51920	-2.04770
H	8.04710	0.51550	-3.05640	H	-4.90010	8.48790	-1.19600



H	-3.86190	8.10240	0.96150	C	-2.12170	-2.85080	-1.73090
H	-2.65040	5.92120	1.42690	H	-1.93770	-2.30530	-2.65680
H	-3.61930	4.62500	-2.59530	H	-1.25970	-2.68900	-1.08310
H	-4.76530	6.70160	-3.01480	H	-2.23030	-3.91130	-1.96400
N	-0.88290	-2.40630	2.04540	C	-7.33650	-2.78110	-2.77470
H	-0.04050	-1.73890	2.00100	C	-6.21980	-2.86980	-3.59890
H	1.30320	-3.20530	1.23150	C	-4.92620	-2.75400	-3.07530
C	-5.85070	-0.87640	4.16390	C	-4.73290	-2.54070	-1.69280
H	-6.52120	-0.50410	3.38570	C	-5.87890	-2.46440	-0.88720
C	-0.82310	-7.74570	0.16310	C	-7.16620	-2.57890	-1.40670
H	-1.01080	-7.69860	-0.91210	H	-8.32980	-2.87730	-3.20280
C	-3.18200	-3.68140	1.26450	H	-6.34050	-3.02930	-4.66880
H	-3.41760	-3.14860	-0.00940	H	-5.75960	-2.34530	0.18380
H	-4.05790	-4.32480	1.24980	H	-8.02250	-2.52460	-0.74280
O	-0.50760	-0.36940	-0.46630	O	-3.84370	-2.83340	-3.90660
H	-2.26140	-0.67220	-0.40950	H	-4.15710	-2.96020	-4.81150
C	2.59750	2.42680	-0.63040	C	-0.13940	4.00420	-2.74810
C	5.23160	1.73520	0.12390	C	-0.33530	4.69910	-4.04170
C	4.30600	0.77090	0.00700	C	0.68020	4.81040	-4.90510
C	2.89860	1.13360	-0.34790	C	1.99830	4.23530	-4.57470
H	6.24670	1.50100	0.41150	C	2.18560	3.61020	-3.40650
C	4.88220	3.15000	-0.07920	H	-1.30160	5.11800	-4.29360
C	3.62130	3.49490	-0.41350	H	0.53620	5.31670	-5.85070
C	3.27660	4.94160	-0.51860	H	2.81150	4.31390	-5.28460
C	4.21450	5.87760	-0.33380	H	3.15440	3.17910	-3.19090
C	5.59820	5.48640	-0.00860	O	1.97660	0.13280	-0.56730
C	5.91510	4.19410	0.11920	P	0.57740	0.16070	0.34320
H	2.26380	5.25770	-0.72770	O	0.31280	1.73780	0.74750
H	3.95750	6.92630	-0.41050	O	0.82050	-0.57640	1.64050
H	6.35290	6.24830	0.13740	N	-3.13430	-1.23430	-0.13500
H	6.93090	3.91440	0.37000	H	-3.40090	-1.51710	0.80600
C	-1.26810	3.87300	-1.80650	C	-3.50160	-2.08110	-1.15230
C	1.24770	2.79730	-1.12510	C	-0.94760	-4.30520	-0.76610
C	0.17320	2.54760	-0.34830	C	0.07110	-3.56420	-0.20490
C	-1.13390	3.19990	-0.65180	C	-1.24410	-3.16670	1.79410
H	-2.21000	4.32780	-2.07290	C	-2.32550	-3.81760	1.25100
C	1.07060	3.49880	-2.42760	C	1.40360	-3.28320	-0.82880

H	2.06560	-4.14680	-0.71740	C	4.23020	-3.83250	-3.30180
H	1.30030	-3.08940	-1.89450	C	3.87610	-2.54590	-3.39780
C	-1.10120	-2.64140	3.19410	C	4.05740	-1.63890	-2.24510
H	-0.61110	-1.66330	3.15830	C	4.55130	-2.10780	-1.08580
H	-0.44790	-3.31260	3.76340	C	4.98320	-3.52420	-1.00190
H	-2.05840	-2.56850	3.70200	C	4.82210	-4.34250	-2.04900
C	-3.62170	-4.06620	1.93930	H	4.09330	-4.49890	-4.14360
C	-0.89530	-4.98970	-2.06770	H	3.45080	-2.16720	-4.31810
H	1.49270	-5.98470	-4.01650	H	3.78360	-0.60020	-2.36010
H	-0.05230	-6.86490	-3.77610	H	5.43790	-3.90230	-0.09500
H	-5.35140	-3.97520	3.97220	H	5.13290	-5.37700	-1.98300
H	-5.54070	-2.19990	3.77960	C	-1.73150	0.75720	4.47260
O	0.35380	-5.24880	-2.51700	C	-0.95330	1.79440	4.14580
O	-1.89740	-5.31410	-2.69100	C	-1.22940	2.56860	2.91820
O	-4.28120	-5.07520	1.80380	C	-2.24790	2.22430	2.10960
O	-4.05280	-2.99410	2.65820	C	-3.11170	1.07920	2.48700
Si	4.79760	-0.99480	0.38450	C	-2.86830	0.38820	3.60670
Si	-2.58850	3.17850	0.53770	H	-1.52970	0.18610	5.36940
C	2.40880	-2.27370	4.21170	H	-0.11740	2.06670	4.77710
C	2.89600	-1.03310	4.10100	H	-0.58090	3.39930	2.66840
C	3.65070	-0.63960	2.89320	H	-3.95230	0.79940	1.87180
C	3.83590	-1.51740	1.89120	H	-3.50590	-0.44140	3.88150
C	3.30970	-2.89690	2.03090	C	-6.33950	1.53440	-1.73420
C	2.63090	-3.25210	3.12880	C	-6.48440	2.15420	-0.55720
H	1.85210	-2.56280	5.09360	C	-5.29610	2.63600	0.17710
H	2.73500	-0.31340	4.89310	C	-4.06550	2.45300	-0.33100
H	4.04140	0.36820	2.82900	C	-3.90960	1.74100	-1.62320
H	3.46700	-3.62850	1.25460	C	-4.98950	1.31460	-2.29060
H	2.24050	-4.25700	3.22440	H	-7.20850	1.18080	-2.27360
C	9.39240	-1.27850	1.24920	H	-7.47220	2.30930	-0.14310
C	8.52020	-1.53940	2.23020	H	-5.43650	3.16110	1.11390
C	7.06720	-1.45100	1.97380	H	-2.92610	1.55540	-2.03370
C	6.61680	-1.10120	0.75680	H	-4.87760	0.80040	-3.23580
C	7.58830	-0.82000	-0.32770	C	-3.80660	7.62200	1.47720
C	8.90340	-0.90240	-0.09260	C	-3.24000	6.87760	2.43260
H	10.45650	-1.34370	1.43610	C	-2.85790	5.47730	2.15410
H	8.87650	-1.81680	3.21380	C	-3.05620	4.94640	0.93380
H	6.38520	-1.67350	2.78270	C	-3.71560	5.77270	-0.10990
H	7.23680	-0.54380	-1.31420	C	-4.06450	7.03910	0.14690
H	9.61110	-0.69460	-0.88470	H	-4.08740	8.64730	1.68060

H	-3.05910	7.29920	3.41290	H	-3.22710	-1.02600	-2.99540
H	-2.42160	4.90530	2.95610	H	-1.71790	-1.56350	-2.23900
H	-3.95330	5.35030	-1.07600	H	-2.77720	-2.73250	-3.08660
H	-4.55220	7.63350	-0.61500	C	-7.55450	-3.50530	-1.46560
N	-0.11290	-3.01470	1.03320	C	-7.28600	-2.40320	-0.66620
H	0.49310	-2.20530	1.32060	C	-5.97580	-1.92290	-0.53040
H	1.85870	-2.41150	-0.36150	C	-4.91390	-2.55710	-1.22160
C	-5.35220	-3.14180	3.26650	C	-5.22070	-3.67140	-2.02960
H	-6.10760	-3.32030	2.49890	C	-6.51750	-4.14650	-2.15400
C	0.42860	-5.88440	-3.80350	H	-8.57450	-3.86730	-1.55390
H	-0.06010	-5.27320	-4.56590	H	-8.07320	-1.87940	-0.13430
C	-2.27560	-4.25200	-0.14930	H	-4.40940	-4.18980	-2.53280
H	-2.89280	-3.35380	-0.77400	H	-6.72030	-5.01420	-2.77270
H	-2.94030	-5.08220	-0.39190	O	-5.81320	-0.84060	0.27460
O	-0.51320	-0.34080	-0.58160	H	-4.91170	-0.49530	0.14150
H	-2.17530	-0.82810	-0.20150				
C	-2.75140	-1.84770	-2.45000				

### **OOH-Type I E**

O	1.92990	0.38960	-0.61940	H	-6.22390	-4.40270	0.00180
P	0.37720	0.23230	-0.08560	H	-4.26100	-3.93540	-2.91220
O	-0.08880	1.69210	0.55620	N	-4.28600	-3.07690	-2.37790
O	-0.43480	-0.08020	-1.31950	C	-1.85210	-4.68270	-0.72100
O	0.32030	-0.73860	1.07670	C	-0.86810	-3.75100	-0.43820
H	-3.47940	-2.46950	-2.47920	N	-0.93900	-3.05980	0.73580
C	-4.77170	-3.20010	-1.08510	H	-0.32100	-2.20720	0.85270
C	-4.31680	0.07180	1.67840	C	-1.84650	-3.29390	1.73220
C	-3.37210	-0.10380	0.67470	C	-1.62100	-2.49610	2.98700
C	-3.52560	-1.12750	-0.27530	H	-2.55740	-2.06050	3.33590
C	-4.65070	-1.99900	-0.20070	H	-1.25270	-3.14760	3.78500
C	-5.58420	-1.78490	0.82810	H	-0.89570	-1.70320	2.79890
C	-5.43630	-0.75900	1.75600	C	0.29490	-3.38760	-1.31270
H	-4.17010	0.85630	2.41180	H	0.88530	-4.27590	-1.53870
H	-2.51080	0.55160	0.61010	H	-0.05220	-2.97050	-2.26050
H	-6.44610	-2.43770	0.90340	H	0.91680	-2.63930	-0.82580
H	-6.18050	-0.61440	2.53240	C	-2.84990	-4.21820	1.50190
C	-6.03860	-4.04410	-1.01100	C	-1.94320	-5.50060	-1.94470
H	-6.89870	-3.46430	-1.36280	C	-3.90390	-4.60660	2.46380
H	-5.92520	-4.91830	-1.65820	H	-1.13630	-7.38840	-3.64220

H	-1.62990	-5.93980	-4.54490	C	4.46920	5.51860	-1.04630
C	-0.87720	-6.35160	-3.86830	C	3.93700	4.41050	-0.51820
H	0.11400	-6.29160	-4.31660	H	1.62960	7.25750	-1.84980
C	-4.67120	-4.62050	4.68900	H	4.03140	7.49330	-1.96370
H	-5.61360	-4.13140	4.43210	H	5.54400	5.62140	-1.12280
H	-4.82670	-5.70170	4.70130	H	4.60020	3.62240	-0.18780
H	-4.30920	-4.27300	5.65620	Si	-2.23890	3.84780	-0.38460
O	-2.96810	-6.07480	-2.28730	Si	4.33090	-1.64510	-0.14140
O	-4.91630	-5.20340	2.13340	C	-3.67620	0.69600	-3.54940
O	-3.64520	-4.26800	3.74560	C	-2.41890	1.15090	-3.57860
O	-0.79970	-5.57480	-2.66130	C	-1.96090	2.12930	-2.56980
O	-2.61600	-1.32870	-1.24390	C	-2.79390	2.54820	-1.60140
H	-1.77840	-0.73060	-1.21120	C	-4.19360	2.05480	-1.59030
C	-2.99460	-4.77810	0.17190	C	-4.60820	1.17520	-2.51050
H	-3.94470	-4.00200	-0.42670	H	-4.01190	-0.02410	-4.28420
H	-3.58750	-5.68690	0.09730	H	-1.73290	0.80250	-4.33960
C	2.79410	0.79520	0.36620	H	-0.94720	2.50130	-2.63570
C	2.69680	2.04170	0.86700	H	-4.88970	2.39010	-0.83830
C	4.68250	0.27940	1.83380	H	-5.62620	0.80790	-2.49120
C	3.90840	-0.09140	0.80270	C	-4.07110	7.98510	-1.59870
H	5.49400	-0.35420	2.16970	C	-4.21810	6.93480	-2.41500
C	1.83740	3.03410	0.17420	C	-3.64450	5.62320	-2.04690
C	0.50000	2.83420	0.05910	C	-2.97240	5.48100	-0.89170
C	-0.36640	3.96130	-0.41010	C	-2.81410	6.64840	0.00900
C	0.20320	5.08690	-0.86900	C	-3.33460	7.83470	-0.32760
H	-0.39800	5.90390	-1.24230	H	-4.49050	8.94590	-1.86790
C	4.46430	1.57450	2.50850	H	-4.75700	7.04310	-3.34730
C	3.52410	2.42880	2.04620	H	-3.77330	4.79300	-2.72760
C	3.30760	3.72000	2.75250	H	-2.27390	6.54600	0.94200
C	4.05900	4.04460	3.81110	H	-3.21690	8.68610	0.33030
C	5.10250	3.11870	4.29230	C	-3.93040	3.30740	3.96020
C	5.29410	1.94610	3.67790	C	-2.61510	3.19440	3.74600
H	2.53610	4.40490	2.42570	C	-2.06940	3.35190	2.38180
H	3.89860	4.98500	4.32240	C	-2.89280	3.56340	1.33970
H	5.70850	3.38940	5.14730	C	-4.34790	3.71700	1.59220
H	6.05860	1.26980	4.03950	C	-4.83750	3.59490	2.83210
C	2.45810	4.26010	-0.41180	H	-4.33060	3.19800	4.95980
C	1.66700	5.23840	-0.89900	H	-1.94560	2.99610	4.57300
C	2.26590	6.46480	-1.47610	H	-0.99870	3.32120	2.25800
C	3.59460	6.59800	-1.54040	H	-5.02000	3.97160	0.78440

H	-5.89760	3.71800	3.01240	H	3.02530	-0.64230	-5.68250
C	1.95660	-5.27970	1.64150	H	4.19060	1.03650	-4.37710
C	1.82570	-4.06550	2.18680	H	4.75610	0.60100	-1.95020
C	2.57610	-2.91920	1.63360	H	2.97780	-3.33210	-2.33550
C	3.38770	-3.08650	0.57520	H	2.40800	-2.87990	-4.62080
C	3.55970	-4.44500	0.00320	C	8.95690	-2.32580	0.26220
C	2.87380	-5.48050	0.50240	C	8.10870	-3.24300	0.74010
H	1.40020	-6.11780	2.04040	C	6.65010	-3.03910	0.61840
H	1.16220	-3.91750	3.02850	C	6.16620	-1.93910	0.01450
H	2.45260	-1.95080	2.09750	C	7.11440	-0.91870	-0.49690
H	4.24970	-4.60830	-0.81490	C	8.43500	-1.10450	-0.38150
H	2.99820	-6.46900	0.07990	H	10.02540	-2.47330	0.35210
C	3.28370	-0.83840	-4.64990	H	8.48860	-4.13620	1.21900
C	3.92830	0.08620	-3.93050	H	5.99270	-3.78690	1.03680
C	4.27340	-0.18190	-2.51940	H	6.74910	-0.00980	-0.95220
C	3.94520	-1.35450	-1.94670	H	9.12340	-0.35620	-0.75260
C	3.24160	-2.37800	-2.75800				
C	2.92490	-2.13070	-4.03490				
O	1.92520	0.40090	-0.62160	H	-6.20620	-4.42730	0.02500
P	0.37310	0.23700	-0.08730	H	-4.26180	-3.94930	-2.89930
O	-0.09690	1.69420	0.55730	N	-4.28730	-3.09130	-2.36420
O	-0.44040	-0.07690	-1.31970	C	-1.84010	-4.68580	-0.72520
O	0.32200	-0.73590	1.07370	C	-0.85990	-3.74870	-0.44710
H	-3.48460	-2.47980	-2.47000	N	-0.92760	-3.06000	0.72850
C	-4.76620	-3.21680	-1.06930	H	-0.31300	-2.20450	0.84420
C	-4.31550	0.05960	1.69000	C	-1.82660	-3.30190	1.73070
C	-3.37520	-0.11090	0.68130	C	-1.59830	-2.50480	2.98540
C	-3.52690	-1.13660	-0.26670	H	-2.53550	-2.07650	3.34140
C	-4.64610	-2.01520	-0.18550	H	-1.22010	-3.15510	3.77990
C	-5.57510	-1.80650	0.84860	H	-0.87980	-1.70650	2.79410
C	-5.42890	-0.77880	1.77470	C	0.29500	-3.37670	-1.32860
H	-4.17040	0.84630	2.42130	H	0.88800	-4.26140	-1.56180
H	-2.51840	0.55000	0.61130	H	-0.06070	-2.95810	-2.27250
H	-6.43220	-2.46490	0.92920	H	0.91670	-2.62700	-0.84370
H	-6.16960	-0.63860	2.55530	C	-2.82560	-4.23210	1.50540
C	-6.02860	-4.06720	-0.98860	C	-1.93460	-5.50200	-1.94990
H	-6.89360	-3.49160	-1.33500	C	-3.86960	-4.62970	2.47430
H	-5.91440	-4.94040	-1.63680	H	-1.12600	-7.38130	-3.65700

H	-1.63830	-5.93480	-4.55260	C	4.46030	5.53640	-1.01140
C	-0.87700	-6.34200	-3.88290	C	3.92830	4.42490	-0.49020
H	0.11010	-6.27320	-4.33910	H	1.62020	7.27210	-1.82020
C	-4.61490	-4.66010	4.70700	H	4.02190	7.51380	-1.92270
H	-5.56350	-4.17700	4.46130	H	5.53520	5.64200	-1.08260
H	-4.76220	-5.74240	4.71630	H	4.59190	3.63710	-0.16000
H	-4.24620	-4.31390	5.67210	Si	-2.24690	3.84580	-0.38830
O	-2.95800	-6.08230	-2.28630	Si	4.33080	-1.63270	-0.15150
O	-4.88210	-5.22970	2.15000	C	-3.65770	0.68920	-3.55980
O	-3.60070	-4.29620	3.75530	C	-2.40440	1.15510	-3.58830
O	-0.79590	-5.56710	-2.67490	C	-1.95460	2.13490	-2.57730
O	-2.62090	-1.33220	-1.24010	C	-2.79070	2.54370	-1.60730
H	-1.78580	-0.73140	-1.20920	C	-4.18610	2.03850	-1.59710
C	-2.97650	-4.78910	0.17480	C	-4.59360	1.15780	-2.51950
H	-3.93260	-4.01610	-0.41530	H	-3.98750	-0.03190	-4.29630
H	-3.56490	-5.70090	0.10170	H	-1.71560	0.81460	-4.35050
C	2.78810	0.80190	0.36710	H	-0.94410	2.51610	-2.64240
C	2.68810	2.04510	0.87560	H	-4.88470	2.36540	-0.84360
C	4.67010	0.27700	1.83970	H	-5.60820	0.78160	-2.50070
C	3.90090	-0.08730	0.80260	C	-4.09660	7.97190	-1.61370
H	5.48050	-0.35840	2.17500	C	-4.23320	6.92040	-2.43020
C	1.82890	3.04060	0.18680	C	-3.65290	5.61280	-2.05900
C	0.49210	2.83880	0.06610	C	-2.98470	5.47530	-0.90090
C	-0.37460	3.96540	-0.40340	C	-2.83750	6.64410	-0.00020
C	0.19440	5.09420	-0.85510	C	-3.36450	7.82690	-0.33940
H	-0.40720	5.91110	-1.22800	H	-4.52140	8.92980	-1.88480
C	4.44890	1.56790	2.52160	H	-4.76910	7.02480	-3.36470
C	3.51070	2.42510	2.06040	H	-3.77440	4.78130	-2.73950
C	3.29120	3.71180	2.77400	H	-2.30090	6.54550	0.93530
C	4.03810	4.02970	3.83770	H	-3.25530	8.67910	0.31870
C	5.07970	3.10090	4.31740	C	-3.95790	3.30640	3.94870
C	5.27390	1.93220	3.69660	C	-2.64140	3.19490	3.74080
H	2.52100	4.39860	2.44830	C	-2.08960	3.35110	2.37890
H	3.87550	4.96690	4.35430	C	-2.90850	3.56020	1.33270
H	5.68230	3.36630	5.17650	C	-4.36510	3.71080	1.57810
H	6.03700	1.25360	4.05700	C	-4.86030	3.58990	2.81590
C	2.44920	4.27060	-0.39100	H	-4.36260	3.19810	4.94660
C	1.65800	5.24910	-0.87750	H	-1.97550	2.99910	4.57120
C	2.25670	6.47930	-1.44690	H	-1.01830	3.32140	2.25980
C	3.58530	6.61580	-1.50490	H	-5.03400	3.96210	0.76640

H	-5.92150	3.71090	2.99090	C	2.92540	-2.09220	-4.04820
C	1.97000	-5.29170	1.59900	H	3.03230	-0.59540	-5.68780
C	1.83380	-4.08280	2.15450	H	4.20160	1.07270	-4.37220
C	2.57930	-2.92850	1.61110	H	4.76270	0.62260	-1.94710
C	3.39210	-3.08350	0.55180	H	2.97210	-3.30250	-2.35510
C	3.56960	-4.43640	-0.03200	H	2.40600	-2.83630	-4.63840
C	2.88800	-5.47900	0.45830	C	8.95870	-2.29700	0.26390
H	1.41730	-6.13560	1.99090	C	8.11270	-3.22410	0.72640
H	1.17000	-3.94490	2.99760	C	6.65360	-3.02570	0.60040
H	2.45160	-1.96450	2.08310	C	6.16710	-1.92080	0.00760
H	4.26000	-4.58960	-0.85160	C	7.11280	-0.88970	-0.48680
H	3.01650	-6.46330	0.02720	C	8.43380	-1.07040	-0.36720
C	3.28910	-0.79790	-4.65600	H	10.02740	-2.44040	0.35720
C	3.93590	0.12080	-3.93100	H	8.49460	-4.12120	1.19620
C	4.27890	-0.15600	-2.52110	H	5.99820	-3.78150	1.00710
C	3.94720	-1.33090	-1.95530	H	6.74550	0.02340	-0.93180
C	3.24030	-2.34750	-2.77250	H	9.12030	-0.31410	-0.72540
O	1.92130	0.36070	-0.60600	H	-6.27050	-4.34470	0.00090
P	0.36690	0.23700	-0.06570	H	-4.32890	-3.84180	-2.92110
O	-0.06550	1.70470	0.57870	N	-4.34710	-2.99090	-2.37460
O	-0.45670	-0.05720	-1.29630	C	-1.90620	-4.62990	-0.75650
O	0.29520	-0.73300	1.09650	C	-0.91610	-3.70900	-0.46040
H	-3.53880	-2.38550	-2.47320	N	-0.98110	-3.03640	0.72480
C	-4.82350	-3.13070	-1.08030	H	-0.35740	-2.18910	0.85410
C	-4.34060	0.10880	1.71760	C	-1.88650	-3.28270	1.71990
C	-3.40130	-0.06040	0.70750	C	-1.65770	-2.50270	2.98520
C	-3.56270	-1.07500	-0.25080	H	-2.59350	-2.07220	3.34230
C	-4.69100	-1.94260	-0.18020	H	-1.28770	-3.16490	3.77360
C	-5.61790	-1.73650	0.85620	H	-0.93290	-1.70720	2.80650
C	-5.46170	-0.72020	1.79330	C	0.24870	-3.34050	-1.33020
H	-4.18880	0.88680	2.45700	H	0.82570	-4.23160	-1.57780
H	-2.53760	0.59220	0.64460	H	-0.09540	-2.89690	-2.26690
H	-6.48150	-2.38730	0.92960	H	0.88230	-2.61200	-0.82890
H	-6.20110	-0.58140	2.57540	C	-2.89280	-4.20110	1.47880
C	-6.09240	-3.97180	-1.00800	C	-2.00700	-5.42270	-1.99590
H	-6.95350	-3.38440	-1.34430	C	-3.94110	-4.60510	2.44010
H	-5.98700	-4.83680	-1.66870	H	-1.21160	-7.27100	-3.74570

H	-1.71530	-5.80100	-4.60740	C	4.54940	5.44670	-1.05650
C	-0.95630	-6.22840	-3.94790	C	4.00060	4.34880	-0.52420
H	0.03090	-6.15550	-4.40320	H	1.73640	7.23370	-1.84860
C	-4.68680	-4.66890	4.67200	H	4.14140	7.42740	-1.97470
H	-5.63230	-4.17580	4.43470	H	5.62540	5.53070	-1.13820
H	-4.84080	-5.75030	4.66260	H	4.65150	3.54970	-0.19580
H	-4.31600	-4.34190	5.64300	Si	-2.18290	3.88400	-0.37390
O	-3.03500	-5.98830	-2.34330	Si	4.29640	-1.70950	-0.13950
O	-4.95830	-5.19130	2.10580	C	-3.64720	0.75820	-3.55240
O	-3.67010	-4.29520	3.72680	C	-2.38810	1.20800	-3.58370
O	-0.86910	-5.48190	-2.72280	C	-1.92200	2.17780	-2.57050
O	-2.65860	-1.27070	-1.22560	C	-2.74890	2.59330	-1.59540
H	-1.81370	-0.68410	-1.18760	C	-4.15050	2.10540	-1.58160
C	-3.04590	-4.73620	0.13930	C	-4.57280	1.23410	-2.50630
H	-3.99360	-3.94660	-0.43970	H	-3.98890	0.04430	-4.29050
H	-3.64200	-5.64180	0.05120	H	-1.70670	0.86190	-4.35000
C	2.79760	0.75380	0.37430	H	-0.90710	2.54640	-2.63850
C	2.72570	2.00380	0.87140	H	-4.84190	2.43720	-0.82380
C	4.68470	0.20950	1.83360	H	-5.59190	0.87040	-2.48480
C	3.89950	-0.15050	0.80710	C	-3.96020	8.04580	-1.58470
H	5.48760	-0.43640	2.16680	C	-4.12330	6.99750	-2.40050
C	1.88110	3.01010	0.18040	C	-3.56730	5.67820	-2.03330
C	0.54000	2.83380	0.07290	C	-2.89480	5.52690	-0.87950
C	-0.30920	3.97310	-0.39710	C	-2.71890	6.69200	0.02090
C	0.27710	5.08880	-0.85920	C	-3.22360	7.88530	-0.31480
H	-0.31220	5.91410	-1.23320	H	-4.36680	9.01230	-1.85310
C	4.49180	1.50940	2.50660	H	-4.66250	7.11320	-3.33180
C	3.56480	2.37890	2.04610	H	-3.70920	4.84970	-2.71350
C	3.37370	3.67520	2.75060	H	-2.17850	6.58200	0.95300
C	4.13520	3.98900	3.80520	H	-3.09290	8.73500	0.34280
C	5.16470	3.04620	4.28380	C	-3.88780	3.35240	3.96690
C	5.33310	1.86910	3.67130	C	-2.57280	3.23170	3.75570
H	2.61270	4.37250	2.42580	C	-2.02300	3.38730	2.39290
H	3.99330	4.93310	4.31510	C	-2.84280	3.60410	1.34900
H	5.77930	3.30820	5.13540	C	-4.29730	3.76680	1.59840
H	6.08750	1.18040	4.03100	C	-4.79050	3.64670	2.83710
C	2.51980	4.22430	-0.41040	H	-4.29100	3.24430	4.96540
C	1.74330	5.21560	-0.89500	H	-1.90630	3.02850	4.58390
C	2.36070	6.43060	-1.47680	H	-0.95210	3.35120	2.27170
C	3.69120	6.54050	-1.54780	H	-4.96590	4.02680	0.78930



H	-5.85020	3.77630	3.01500	C	2.91520	-2.15880	-4.04630
C	1.85840	-5.30830	1.62980	H	3.04400	-0.66200	-5.68440
C	1.74970	-4.09420	2.18010	H	4.21350	0.99830	-4.35930
C	2.51860	-2.95880	1.62980	H	4.75640	0.54260	-1.93100
C	3.32600	-3.13620	0.56990	H	2.94210	-3.37020	-2.35350
C	3.47460	-4.49570	-0.00650	H	2.39660	-2.89980	-4.64110
C	2.77070	-5.52080	0.48910	C	8.90720	-2.47970	0.27870
H	1.28850	-6.13820	2.02680	C	8.03990	-3.37890	0.75640
H	1.09140	-3.93830	3.02430	C	6.58580	-3.14710	0.62970
H	2.41290	-1.99010	2.09770	C	6.12520	-2.03950	0.02150
H	4.16300	-4.66860	-0.82390	C	7.09460	-1.03950	-0.49050
H	2.87830	-6.51000	0.06350	C	8.41100	-1.25050	-0.37050
C	3.29130	-0.86640	-4.65080	H	9.97230	-2.64760	0.37240
C	3.93820	0.04800	-3.92050	H	8.40080	-4.27790	1.23920
C	4.26890	-0.23150	-2.50820	H	5.91280	-3.88070	1.04850
C	3.92450	-1.40410	-1.94500	H	6.74820	-0.12550	-0.95060
C	3.21830	-2.41620	-2.76810	H	9.11490	-0.51710	-0.74200
O	1.89090	0.53880	-0.64320	H	-5.60040	-5.31530	-1.59510
P	0.35210	0.26930	-0.11450	H	-5.92430	-4.79810	0.05930
O	-0.21210	1.69050	0.53590	H	-3.99710	-4.25730	-2.86350
O	-0.44030	-0.09290	-1.34690	N	-4.07330	-3.39340	-2.34300
O	0.36670	-0.70970	1.04290	C	-1.55680	-4.81090	-0.69080
H	-3.30920	-2.73590	-2.45840	C	-0.63900	-3.80560	-0.43900
C	-4.55290	-3.52210	-1.04890	N	-0.73960	-3.10450	0.72660
C	-4.30390	-0.17990	1.65680	H	-0.17860	-2.21010	0.82520
C	-3.35910	-0.30360	0.64570	C	-1.61180	-3.38760	1.74170
C	-3.44720	-1.35050	-0.28720	C	-1.42230	-2.55970	2.98290
C	-4.50640	-2.29900	-0.18730	H	-2.38050	-2.18050	3.33880
C	-5.44290	-2.13510	0.84830	H	-1.00260	-3.17530	3.78410
C	-5.36020	-1.08710	1.75910	H	-0.75240	-1.72430	2.77530
H	-4.20680	0.62460	2.37620	C	0.47710	-3.36960	-1.34100
H	-2.54810	0.41090	0.56200	H	1.13050	-4.21330	-1.56410
H	-6.25530	-2.84610	0.94320	H	0.08260	-2.99840	-2.28930
H	-6.10530	-0.98410	2.54130	H	1.04690	-2.56670	-0.87800
C	-5.76550	-4.44140	-0.95880	C	-2.55200	-4.38220	1.54030
H	-6.66150	-3.92080	-1.31320	C	-1.60490	-5.65640	-1.89800

C	-3.56430	-4.82550	2.52310	C	1.90220	6.64440	-1.32150
H	-0.68610	-7.52140	-3.56380	C	3.22140	6.86020	-1.34570
H	-1.28380	-6.12910	-4.49160	C	4.14800	5.82210	-0.85800
C	-0.49960	-6.47460	-3.81380	C	3.67180	4.66860	-0.37560
H	0.48170	-6.35770	-4.27270	H	1.22800	7.40760	-1.69020
C	-4.29140	-4.86250	4.76190	H	3.61280	7.79250	-1.73170
H	-5.26900	-4.44250	4.51420	H	5.21600	5.99240	-0.90200
H	-4.37250	-5.95150	4.79220	H	4.37390	3.91340	-0.04900
H	-3.93850	-4.47670	5.71790	Si	-2.45930	3.73010	-0.41290
O	-2.59170	-6.30480	-2.21890	Si	4.39940	-1.37670	-0.18460
O	-4.54140	-5.48930	2.21580	C	-3.61440	0.49540	-3.60840
O	-3.30700	-4.45570	3.79650	C	-2.39950	1.05420	-3.62790
O	-0.46490	-5.66890	-2.62390	C	-2.03020	2.06070	-2.61050
O	-2.53300	-1.49680	-1.26260	C	-2.90010	2.40130	-1.64400
H	-1.74060	-0.84150	-1.23740	C	-4.25420	1.79420	-1.64460
C	-2.67760	-4.96880	0.22000	C	-4.58900	0.88890	-2.57250
H	-3.68180	-4.26220	-0.37650	H	-3.88480	-0.24570	-4.34920
H	-3.21120	-5.91500	0.16540	H	-1.68270	0.76910	-4.38690
C	2.72410	0.96350	0.36090	H	-1.05000	2.51550	-2.66650
C	2.54820	2.18490	0.90030	H	-4.97950	2.06500	-0.89380
C	4.59970	0.49510	1.85940	H	-5.57280	0.43790	-2.56130
C	3.87210	0.12090	0.79630	C	-4.52350	7.74420	-1.66660
H	5.43440	-0.10760	2.19550	C	-4.57880	6.69000	-2.48930
C	1.64380	3.14830	0.22440	C	-3.93110	5.41720	-2.10850
C	0.32230	2.87440	0.07590	C	-3.28270	5.31450	-0.93570
C	-0.59790	3.95890	-0.38970	C	-3.22680	6.48560	-0.02770
C	-0.08670	5.12750	-0.80740	C	-3.81460	7.63670	-0.37560
H	-0.72720	5.91620	-1.17610	H	-4.99730	8.67660	-1.94500
C	4.29840	1.75410	2.57000	H	-5.09750	6.76690	-3.43610
C	3.32690	2.57480	2.11120	H	-3.98710	4.58280	-2.79410
C	3.02550	3.82770	2.85440	H	-2.70760	6.41450	0.92000
C	3.73150	4.15280	3.94360	H	-3.77160	8.49090	0.28770
C	4.80940	3.26530	4.42160	C	-4.20740	3.07710	3.89290
C	5.07770	2.12650	3.77320	C	-2.88360	3.03840	3.70590
H	2.22790	4.48310	2.53000	C	-2.31960	3.22850	2.35320
H	3.50910	5.06490	4.48210	C	-3.13220	3.39760	1.29490
H	5.37820	3.53620	5.30170	C	-4.59870	3.46460	1.51660
H	5.86690	1.47790	4.13260	C	-5.10610	3.31250	2.74600
C	2.20260	4.42540	-0.31310	H	-4.62120	2.94360	4.88390
C	1.36550	5.36760	-0.79460	H	-2.22110	2.87670	4.54630

H	-1.24640	3.25600	2.25070	C	3.33630	-2.12090	-2.80860
H	-5.26740	3.67800	0.69390	C	3.00240	-1.86960	-4.08030
H	-6.17510	3.37210	2.90400	H	3.02220	-0.35250	-5.70450
C	2.29730	-5.21240	1.51760	H	4.10770	1.36160	-4.37640
C	2.07970	-4.02330	2.08990	H	4.70190	0.91750	-1.95850
C	2.74250	-2.81320	1.56100	H	3.12080	-3.09300	-2.40000
C	3.56160	-2.89750	0.49840	H	2.52030	-2.63400	-4.67620
C	3.82750	-4.22650	-0.10630	C	9.06240	-1.73130	0.22350
C	3.22130	-5.32020	0.37150	C	8.28230	-2.72710	0.65780
H	1.80530	-6.09760	1.89900	C	6.81310	-2.62630	0.53390
H	1.41000	-3.94290	2.93590	C	6.25150	-1.54180	-0.02950
H	2.54970	-1.86680	2.04640	C	7.12420	-0.43400	-0.49170
H	4.52130	-4.31990	-0.93210	C	8.45440	-0.52640	-0.37390
H	3.41420	-6.28700	-0.07490	H	10.13840	-1.80310	0.31540
C	3.29430	-0.55170	-4.67610	H	8.72500	-3.60860	1.10320
C	3.89500	0.39240	-3.94430	H	6.21170	-3.43670	0.91820
C	4.25890	0.11970	-2.53880	H	6.69510	0.46460	-0.90990
C	3.99260	-1.07680	-1.98380	H	9.08710	0.28570	-0.70800
O	1.89650	0.54470	-0.65000	H	-5.85790	-4.88200	-0.00350
P	0.35750	0.26650	-0.12660	H	-3.88980	-4.33500	-2.89750
O	-0.22450	1.68480	0.51390	N	-3.98650	-3.46860	-2.38460
O	-0.42210	-0.10850	-1.36380	C	-1.47870	-4.84600	-0.68290
O	0.37110	-0.70550	1.03630	C	-0.57780	-3.82710	-0.42510
H	-3.22880	-2.80220	-2.49130	N	-0.70620	-3.11720	0.73250
C	-4.48510	-3.59530	-1.09750	H	-0.15820	-2.21490	0.83100
C	-4.31390	-0.23930	1.59700	C	-1.59070	-3.40310	1.73600
C	-3.35170	-0.35840	0.60190	C	-1.43370	-2.56110	2.97220
C	-3.41620	-1.40790	-0.32990	H	-2.40240	-2.18660	3.30410
C	-4.46750	-2.36670	-0.24260	H	-1.02550	-3.16460	3.78830
C	-5.42220	-2.20750	0.77700	H	-0.76730	-1.72160	2.76970
C	-5.36400	-1.15520	1.68480	C	0.54670	-3.38450	-1.31320
H	-4.23530	0.56850	2.31530	H	1.21270	-4.22220	-1.52070
H	-2.54550	0.36280	0.52960	H	0.16210	-3.02420	-2.26980
H	-6.22910	-2.92600	0.86150	H	1.10050	-2.57210	-0.84730
H	-6.12300	-1.05610	2.45410	C	-2.51450	-4.41180	1.52830
C	-5.68750	-4.52920	-1.02110	C	-1.49550	-5.70320	-1.88280
H	-6.58410	-4.02170	-1.39260	C	-3.53660	-4.86060	2.49840
H	-5.50180	-5.40450	-1.64970	H	-0.52700	-7.57700	-3.51020

H	-1.11700	-6.19930	-4.46460	C	4.04390	5.85380	-1.03190
C	-0.34420	-6.53120	-3.76710	C	3.59320	4.70480	-0.51560
H	0.64540	-6.41060	-4.20680	H	1.08650	7.38200	-1.83950
C	-4.30070	-4.88920	4.72470	H	3.46460	7.79760	-1.93690
H	-5.27920	-4.48300	4.45850	H	5.10840	6.03760	-1.10020
H	-4.36890	-5.97880	4.76080	H	4.31130	3.96610	-0.18600
H	-3.96820	-4.49290	5.68370	Si	-2.52520	3.69180	-0.39120
O	-2.47020	-6.36310	-2.21690	Si	4.43330	-1.31580	-0.14560
O	-4.49930	-5.54070	2.18090	C	-3.76140	0.44140	-3.54160
O	-3.30580	-4.47630	3.77260	C	-2.53550	0.97500	-3.57430
O	-0.34080	-5.71310	-2.58520	C	-2.14040	1.98700	-2.57210
O	-2.48590	-1.54890	-1.29040	C	-2.99900	2.36010	-1.60760
H	-1.70350	-0.88040	-1.26060	C	-4.36560	1.78100	-1.59430
C	-2.61200	-5.01040	0.21110	C	-4.72290	0.86920	-2.50720
H	-3.61560	-4.31950	-0.40660	H	-4.05040	-0.30410	-4.27090
H	-3.13360	-5.96310	0.15580	H	-1.82830	0.66470	-4.33250
C	2.71990	1.00870	0.34480	H	-1.15120	2.41990	-2.63880
C	2.52560	2.24220	0.84920	H	-5.08270	2.07920	-0.84640
C	4.61950	0.62270	1.83740	H	-5.71600	0.43960	-2.48600
C	3.88820	0.20160	0.79450	C	-4.66310	7.69200	-1.56320
H	5.46900	0.04680	2.18350	C	-4.73840	6.63940	-2.38620
C	1.59900	3.17020	0.15390	C	-4.06670	5.37130	-2.03210
C	0.28080	2.87190	0.02980	C	-3.37700	5.27120	-0.88290
C	-0.66540	3.93740	-0.42890	C	-3.29770	6.44100	0.02500
C	-0.17940	5.10500	-0.87870	C	-3.90720	7.58780	-0.29880
H	-0.83890	5.87980	-1.24370	H	-5.15480	8.62080	-1.82180
C	4.30070	1.89650	2.51260	H	-5.29160	6.71380	-3.31350
C	3.30790	2.68310	2.04030	H	-4.13980	4.53820	-2.71760
C	2.98910	3.95170	2.74890	H	-2.74420	6.37230	0.95330
C	3.70050	4.32430	3.81920	H	-3.84760	8.44090	0.36460
C	4.80180	3.47390	4.31090	C	-4.13920	2.99630	3.96170
C	5.08580	2.32130	3.69460	C	-2.82110	2.97460	3.73620
H	2.17420	4.58050	2.41480	C	-2.29870	3.18460	2.36990
H	3.46540	5.24790	4.33240	C	-3.14320	3.35140	1.33650
H	5.37510	3.78340	5.17520	C	-4.60310	3.40540	1.60230
H	5.89230	1.70010	4.06400	C	-5.07290	3.23660	2.84440
C	2.12910	4.44340	-0.41970	H	-4.52270	2.84820	4.96280
C	1.26950	5.36370	-0.90380	H	-2.13280	2.81160	4.55540
C	1.77820	6.63600	-1.46830	H	-1.22960	3.22670	2.23790
C	3.09360	6.86870	-1.52340	H	-5.29760	3.62370	0.80280

H	-6.13720	3.28670	3.03440	C	3.08380	-1.90080	-4.04530
C	2.33330	-5.12200	1.62400	H	3.10050	-0.41410	-5.69740
C	2.10850	-3.92190	2.16980	H	4.14780	1.33950	-4.39040
C	2.77120	-2.72110	1.62000	H	4.72270	0.94850	-1.95830
C	3.59700	-2.82500	0.56440	H	3.20120	-3.09090	-2.34130
C	3.87310	-4.16590	-0.00860	H	2.61870	-2.68270	-4.63170
C	3.26670	-5.25120	0.48770	C	9.09380	-1.64480	0.30650
H	1.84050	-6.00040	2.01990	C	8.31290	-2.62850	0.76650
H	1.43230	-3.82560	3.00900	C	6.84440	-2.53570	0.62880
H	2.57300	-1.76530	2.08450	C	6.28440	-1.47090	0.02750
H	4.57490	-4.27490	-0.82570	C	7.15760	-0.37650	-0.46420
H	3.46660	-6.22680	0.06410	C	8.48720	-0.46150	-0.33380
C	3.36400	-0.59020	-4.66260	H	10.16920	-1.71080	0.40850
C	3.94360	0.37570	-3.94230	H	8.75450	-3.49420	1.24300
C	4.29590	0.13440	-2.52810	H	6.24210	-3.33510	1.03410
C	4.04050	-1.05540	-1.95380	H	6.72920	0.50640	-0.91550
C	3.40750	-2.12360	-2.76570	H	9.12040	0.34090	-0.68980
O	1.88930	0.57430	-0.64610	H	-5.77680	-4.97860	-0.03430
P	0.35550	0.27160	-0.12150	H	-3.78680	-4.40940	-2.90930
O	-0.25000	1.67990	0.51970	N	-3.90440	-3.54270	-2.40130
O	-0.41630	-0.11520	-1.36000	C	-1.39150	-4.87480	-0.67100
O	0.38430	-0.70020	1.04110	C	-0.50780	-3.84160	-0.41080
H	-3.15700	-2.86380	-2.50200	N	-0.65530	-3.12870	0.74250
C	-4.41400	-3.67350	-1.11870	H	-0.12140	-2.21800	0.84090
C	-4.32300	-0.30860	1.56810	C	-1.54430	-3.42250	1.73980
C	-3.34830	-0.41600	0.58380	C	-1.40880	-2.57320	2.97350
C	-3.38820	-1.46790	-0.34680	H	-2.38490	-2.20800	3.29420
C	-4.42600	-2.44180	-0.26810	H	-1.00180	-3.16830	3.79630
C	-5.39410	-2.29420	0.74050	H	-0.75010	-1.72710	2.77360
C	-5.36110	-1.23900	1.64630	C	0.61700	-3.38680	-1.29220
H	-4.26360	0.50140	2.28560	H	1.30020	-4.21420	-1.48480
H	-2.55200	0.31650	0.51880	H	0.23550	-3.04350	-2.25640
H	-6.19100	-3.02450	0.81780	H	1.15130	-2.56000	-0.82890
H	-6.12990	-1.14880	2.40680	C	-2.45260	-4.44460	1.52880
C	-5.60120	-4.62710	-1.05150	C	-1.38350	-5.73920	-1.86590
H	-6.50210	-4.13580	-1.43450	C	-3.47840	-4.90160	2.49120
H	-5.39450	-5.50160	-1.67470	H	-0.37220	-7.61120	-3.46850

H	-0.96490	-6.24670	-4.44020	C	3.94040	5.91000	-1.06950
C	-0.19800	-6.56510	-3.73010	C	3.51090	4.75820	-0.54140
H	0.79610	-6.43600	-4.15720	H	0.95440	7.38610	-1.86860
C	-4.26920	-4.92160	4.70820	H	3.32500	7.83750	-1.98550
H	-5.24900	-4.52810	4.42810	H	5.00140	6.10950	-1.14670
H	-4.32560	-6.01170	4.75060	H	4.24260	4.03320	-0.21110
H	-3.95220	-4.51530	5.66820	Si	-2.59000	3.64700	-0.38560
O	-2.34570	-6.41330	-2.20760	Si	4.45700	-1.24220	-0.13730
O	-4.42710	-5.59850	2.16830	C	-3.78310	0.37970	-3.53530
O	-3.26820	-4.50360	3.76470	C	-2.56270	0.92590	-3.56510
O	-0.22000	-5.73930	-2.55390	C	-2.18120	1.94370	-2.56360
O	-2.44600	-1.59740	-1.29710	C	-3.04660	2.30970	-1.60250
H	-1.67640	-0.91340	-1.26380	C	-4.40740	1.71700	-1.59280
C	-2.52970	-5.05170	0.21400	C	-4.75230	0.79970	-2.50500
H	-3.53950	-4.37930	-0.41620	H	-4.06200	-0.37010	-4.26420
H	-3.03690	-6.01220	0.15950	H	-1.84980	0.62150	-4.32040
C	2.70570	1.05630	0.34570	H	-1.19620	2.38630	-2.62780
C	2.49080	2.28830	0.84540	H	-5.13030	2.00980	-0.84820
C	4.61720	0.71130	1.83300	H	-5.74120	0.36030	-2.48650
C	3.88970	0.27210	0.79500	C	-4.78610	7.61750	-1.55180
H	5.47750	0.15190	2.17910	C	-4.84820	6.56430	-2.37520
C	1.54540	3.19650	0.14930	C	-4.15880	5.30530	-2.02270
C	0.23200	2.87500	0.03170	C	-3.46640	5.21400	-0.87440
C	-0.73420	3.92240	-0.42800	C	-3.40190	6.38440	0.03400
C	-0.26930	5.09570	-0.88570	C	-4.02730	7.52300	-0.28840
H	-0.94270	5.85740	-1.25250	H	-5.29050	8.53980	-1.80950
C	4.27930	1.98320	2.50240	H	-5.40340	6.63180	-3.30190
C	3.27070	2.74960	2.03040	H	-4.22080	4.47200	-2.70890
C	2.93420	4.01740	2.73240	H	-2.84620	6.32280	0.96150
C	3.64510	4.40920	3.79620	H	-3.97830	8.37650	0.37520
C	4.76290	3.58070	4.28770	C	-4.19060	2.92020	3.96720
C	5.06300	2.42890	3.67760	C	-2.87250	2.91820	3.74080
H	2.10730	4.63030	2.39830	C	-2.35400	3.13920	2.37470
H	3.39740	5.33230	4.30420	C	-3.20150	3.29610	1.34230
H	5.33550	3.90560	5.14680	C	-4.66180	3.32940	1.60930
H	5.88170	1.82380	4.04690	C	-5.12840	3.15070	2.85130
C	2.05170	4.47470	-0.43440	H	-4.57130	2.76400	4.96810
C	1.17490	5.37780	-0.91970	H	-2.18150	2.76290	4.55920
C	1.66010	6.65380	-1.49630	H	-1.28570	3.19700	2.24210
C	2.97130	6.90630	-1.56220	H	-5.35990	3.54020	0.81100

H	-6.19320	3.18560	3.04210	C	3.11740	-1.88600	-4.03110
C	2.42580	-5.07060	1.66440	H	3.09290	-0.40950	-5.69240
C	2.17720	-3.86990	2.19840	H	4.09860	1.37790	-4.39860
C	2.81950	-2.66230	1.63940	H	4.68870	1.01660	-1.96540
C	3.64930	-2.76040	0.58640	H	3.26890	-3.06230	-2.32020
C	3.95170	-4.10120	0.02650	H	2.67200	-2.68340	-4.61200
C	3.36450	-5.19300	0.53170	C	9.12400	-1.48280	0.30010
H	1.94830	-5.95440	2.06720	C	8.36260	-2.47420	0.77590
H	1.49670	-3.77830	3.03460	C	6.89220	-2.40960	0.64260
H	2.60260	-1.70620	2.09450	C	6.31110	-1.36280	0.02990
H	4.65740	-4.20480	-0.78790	C	7.16260	-0.25950	-0.47950
H	3.58370	-6.16860	0.11770	C	8.49390	-0.31900	-0.35330
C	3.36290	-0.57250	-4.65700	H	10.20080	-1.52810	0.39890
C	3.91950	0.41210	-3.94400	H	8.82140	-3.32550	1.26210
C	4.28040	0.18870	-2.52900	H	6.30550	-3.21400	1.06090
C	4.05480	-1.00300	-1.94640	H	6.71670	0.60930	-0.94120
C	3.44870	-2.09240	-2.75070	H	9.11130	0.48980	-0.72240
O	1.87060	0.62840	-0.64970	H	-5.63500	-5.14390	-0.01490
P	0.34500	0.28590	-0.12430	H	-3.67220	-4.52050	-2.89790
O	-0.29560	1.67710	0.51890	N	-3.81500	-3.65690	-2.39120
O	-0.42060	-0.12150	-1.36000	C	-1.26120	-4.90430	-0.67600
O	0.40270	-0.68530	1.03800	C	-0.40910	-3.84330	-0.42190
H	-3.09140	-2.95370	-2.49710	N	-0.57090	-3.13520	0.73230
C	-4.31710	-3.79980	-1.10740	H	-0.06220	-2.20920	0.82920
C	-4.32270	-0.42710	1.57110	C	-1.44300	-3.45640	1.73570
C	-3.35020	-0.50410	0.58180	C	-1.32840	-2.60080	2.96740
C	-3.35930	-1.55860	-0.34630	H	-2.31400	-2.26120	3.28780
C	-4.36380	-2.56660	-0.26010	H	-0.90540	-3.18260	3.79140
C	-5.33090	-2.44910	0.75350	H	-0.69340	-1.73750	2.76470
C	-5.32860	-1.39150	1.65690	C	0.69470	-3.35410	-1.31130
H	-4.28680	0.38600	2.28660	H	1.39420	-4.16350	-1.52010
H	-2.57900	0.25440	0.51080	H	0.29410	-3.00970	-2.26730
H	-6.10170	-3.20630	0.83660	H	1.21510	-2.51960	-0.84590
H	-6.09580	-1.32550	2.42150	C	-2.31880	-4.50780	1.53220
C	-5.47400	-4.78960	-1.03360	C	-1.23540	-5.76860	-1.87070
H	-6.39130	-4.32800	-1.41440	C	-3.32070	-4.99750	2.50350
H	-5.24240	-5.65920	-1.65500	H	-0.17960	-7.60610	-3.48380

H	-0.82730	-6.26260	-4.44960	C	3.78800	6.02420	-1.03570
C	-0.04290	-6.55500	-3.74740	C	3.38810	4.85640	-0.51960
H	0.94190	-6.39310	-4.18480	H	0.76580	7.42920	-1.82630
C	-4.08700	-5.04360	4.72910	H	3.12390	7.94380	-1.93400
H	-5.08320	-4.68640	4.45820	H	4.84360	6.25220	-1.10890
H	-4.10350	-6.13490	4.77480	H	4.13800	4.14760	-0.19520
H	-3.77520	-4.62370	5.68510	Si	-2.68180	3.58400	-0.38840
O	-2.17760	-6.47540	-2.20250	Si	4.48110	-1.12970	-0.14300
O	-4.24920	-5.72500	2.18960	C	-3.76540	0.29690	-3.55680
O	-3.11120	-4.59240	3.77490	C	-2.56250	0.88090	-3.58100
O	-0.08010	-5.72960	-2.57120	C	-2.21520	1.90510	-2.57350
O	-2.41760	-1.65680	-1.30150	C	-3.09390	2.23920	-1.61280
H	-1.66730	-0.95330	-1.26590	C	-4.43550	1.60450	-1.60930
C	-2.38640	-5.11760	0.21800	C	-4.74960	0.68150	-2.52680
H	-3.42020	-4.47880	-0.40460	H	-4.01930	-0.45730	-4.29020
H	-2.86210	-6.09430	0.16760	H	-1.83890	0.60290	-4.33620
C	2.67580	1.12670	0.34360	H	-1.24420	2.37840	-2.63320
C	2.43020	2.35100	0.84850	H	-5.16890	1.87110	-0.86510
C	4.59730	0.82530	1.82860	H	-5.72450	0.21160	-2.51310
C	3.87970	0.37090	0.79000	C	-4.98240	7.49580	-1.55130
H	5.47140	0.28630	2.17260	C	-5.00850	6.44540	-2.38020
C	1.46270	3.23870	0.15610	C	-4.28560	5.20500	-2.02880
C	0.15770	2.88520	0.03580	C	-3.59870	5.12800	-0.87620
C	-0.83410	3.91010	-0.41990	C	-3.57400	6.29520	0.03820
C	-0.39900	5.09860	-0.86730	C	-4.22990	7.41690	-0.28310
H	-1.09130	5.84510	-1.23030	H	-5.51160	8.40440	-1.80800
C	4.22710	2.08520	2.50330	H	-5.55900	6.50150	-3.31040
C	3.19810	2.82660	2.03570	H	-4.31900	4.37350	-2.71920
C	2.82760	4.08090	2.74490	H	-3.02320	6.24500	0.96930
C	3.52800	4.48600	3.81060	H	-4.21020	8.26810	0.38500
C	4.66840	3.68570	4.29700	C	-4.28510	2.80150	3.95350
C	4.99930	2.54570	3.68050	C	-2.96620	2.83380	3.73380
H	1.98400	4.67280	2.41480	C	-2.44670	3.07170	2.37100
H	3.25530	5.39900	4.32400	C	-3.29270	3.20970	1.33470
H	5.23240	4.02120	5.15770	C	-4.75470	3.20350	1.59400
H	5.83440	1.96120	4.04610	C	-5.22290	3.00990	2.83320
C	1.93660	4.53400	-0.41740	H	-4.66680	2.63290	4.95200
C	1.03740	5.41850	-0.89590	H	-2.27560	2.69420	4.55540
C	1.48980	6.71200	-1.45980	H	-1.37950	3.15760	2.24380
C	2.79400	6.99950	-1.52050	H	-5.45400	3.39710	0.79230



H	-6.28920	3.01610	3.01850	C	3.15990	-1.79600	-4.03910
C	2.53490	-4.99930	1.66540	H	3.10150	-0.31650	-5.69680
C	2.26650	-3.80420	2.20230	H	4.06410	1.49100	-4.39810
C	2.88110	-2.58370	1.64020	H	4.66160	1.13760	-1.96550
C	3.70650	-2.66460	0.58220	H	3.33970	-2.97290	-2.33140
C	4.03230	-3.99880	0.01980	H	2.73410	-2.60240	-4.62220
C	3.46910	-5.10230	0.52710	C	9.15300	-1.27360	0.28510
H	2.07720	-5.89250	2.07030	C	8.41380	-2.28380	0.75630
H	1.59030	-3.72670	3.04340	C	6.94200	-2.24910	0.62720
H	2.64810	-1.63270	2.09800	C	6.33750	-1.21080	0.02270
H	4.73640	-4.08820	-0.79770	C	7.16440	-0.08660	-0.48160
H	3.70520	-6.07310	0.11130	C	8.49710	-0.11890	-0.35890
C	3.37450	-0.47560	-4.66170	H	10.23090	-1.29720	0.38060
C	3.90740	0.52020	-3.94590	H	8.89160	-3.12870	1.23520
C	4.27260	0.30190	-2.53130	H	6.37350	-3.06890	1.04060
C	4.07450	-0.89620	-1.95160	H	6.69910	0.77560	-0.93660
C	3.49560	-1.99770	-2.75910	H	9.09650	0.70490	-0.72420
O	1.49360	-1.19300	0.55870	H	-3.37190	6.94290	0.89540
P	0.20460	-0.42310	-0.10990	H	-0.09800	6.02200	1.92000
O	-0.70970	-1.59520	-0.83270	N	-0.73380	5.25010	2.07030
O	-0.55360	0.20180	1.03610	C	0.07390	5.17000	-1.10650
O	0.66670	0.46500	-1.25480	C	0.59290	3.90060	-1.29350
H	-0.32690	4.32280	2.01650	N	-0.25540	2.88510	-1.60890
C	-1.97380	5.38220	1.46160	H	0.12640	1.89080	-1.54480
C	-4.68220	2.02890	1.54920	C	-1.58650	3.02850	-1.87550
C	-3.31660	1.79730	1.45140	C	-2.27040	1.76370	-2.30870
C	-2.40910	2.87210	1.45840	H	-3.08130	1.52830	-1.61680
C	-2.89330	4.20690	1.55160	H	-2.71580	1.88790	-3.29750
C	-4.28470	4.39930	1.63570	H	-1.56380	0.93350	-2.32520
C	-5.17570	3.33340	1.64870	C	2.03410	3.49040	-1.21800
H	-5.37090	1.18980	1.55110	H	2.53510	3.75570	-2.15450
H	-2.91070	0.79630	1.36430	H	2.56070	4.00990	-0.41970
H	-4.67480	5.40780	1.69920	H	2.09950	2.40980	-1.07930
H	-6.24180	3.51630	1.73590	C	-2.16090	4.27680	-1.72150
C	-2.55850	6.78110	1.60420	C	0.86440	6.36650	-0.75840
H	-2.92820	6.93490	2.62360	C	-3.58210	4.61370	-1.95540
H	-1.78040	7.51940	1.39640	H	2.62410	8.31650	-1.23110

H	2.93680	7.59380	0.36170	C	2.21820	-6.97120	0.04180
C	2.97640	7.42010	-0.71630	C	2.13210	-5.66650	-0.24110
H	3.99070	7.17110	-1.02720	H	-1.08660	-7.73090	0.51360
C	-5.70670	3.89990	-2.67950	H	1.07460	-8.80900	0.53670
H	-6.16990	4.05630	-1.70260	H	3.18620	-7.45330	0.09040
H	-5.86120	4.78880	-3.29500	H	3.04710	-5.11160	-0.39430
H	-6.12390	3.01780	-3.16480	Si	-3.36440	-2.89900	0.27640
O	0.38110	7.35980	-0.23320	Si	4.47630	-0.03190	0.62990
O	-4.06280	5.69450	-1.65560	C	-3.05030	-0.62140	4.37420
O	-4.30450	3.62500	-2.52520	C	-1.95660	-1.16370	3.82890
O	2.17490	6.28220	-1.07830	C	-2.05210	-1.89760	2.55010
O	-1.08350	2.65690	1.36200	C	-3.22920	-1.99460	1.90620
H	-0.85420	1.66320	1.25130	C	-4.44530	-1.42930	2.54310
C	-1.36750	5.34840	-1.14430	C	-4.35820	-0.77580	3.70840
H	-1.75250	5.37310	0.15880	H	-2.98160	-0.08150	5.30960
H	-1.72570	6.35800	-1.33480	H	-0.99780	-1.06340	4.32040
C	2.31140	-1.74190	-0.39220	H	-1.15080	-2.33410	2.14580
C	1.87510	-2.79280	-1.11520	H	-5.41670	-1.57040	2.09100
C	4.45250	-1.72700	-1.56920	H	-5.24810	-0.36860	4.17050
C	3.69690	-1.22920	-0.57820	C	-6.64190	-6.23660	0.53000
H	5.47480	-1.39150	-1.69950	C	-6.18930	-5.67080	1.65500
C	0.67420	-3.53830	-0.64810	C	-5.15830	-4.61380	1.59040
C	-0.52390	-2.91390	-0.47870	C	-4.68130	-4.20700	0.40140
C	-1.72330	-3.71930	-0.09610	C	-5.17750	-4.84730	-0.84050
C	-1.61010	-5.04250	0.08560	C	-6.10850	-5.80710	-0.77840
H	-2.46320	-5.63720	0.38330	H	-7.39550	-7.01210	0.57630
C	3.91110	-2.74750	-2.48960	H	-6.57450	-5.98810	2.61540
C	2.67760	-3.26050	-2.28200	H	-4.78850	-4.19510	2.51610
C	2.13500	-4.25720	-3.24310	H	-4.78720	-4.54410	-1.80370
C	2.87610	-4.66910	-4.27830	H	-6.46990	-6.27300	-1.68600
C	4.23450	-4.12840	-4.48000	C	-4.82040	-0.23850	-3.30420
C	4.72540	-3.21480	-3.63510	C	-3.81310	-1.10120	-3.47880
H	1.13490	-4.65220	-3.12040	C	-3.33130	-1.91750	-2.34500
H	2.47840	-5.39540	-4.97530	C	-3.88250	-1.78190	-1.12540
H	4.82940	-4.46860	-5.31770	C	-5.00440	-0.82840	-0.94460
H	5.72040	-2.81760	-3.79320	C	-5.44540	-0.09660	-1.97500
C	0.80340	-4.99130	-0.30730	H	-5.17500	0.36000	-4.13320
C	-0.30150	-5.70760	-0.00870	H	-3.35260	-1.20820	-4.45220
C	-0.19610	-7.15390	0.29680	H	-2.55310	-2.64570	-2.52920
C	0.99840	-7.75310	0.31110	H	-5.48830	-0.72440	0.01190

H	-6.26370	0.59830	-1.83710	C	1.75170	1.87020	3.12580
C	5.71140	3.99840	-1.43510	H	0.77510	1.02870	4.93590
C	5.27960	2.97760	-2.18430	H	1.92550	-1.10250	4.82350
C	4.87290	1.70790	-1.54580	H	3.56220	-1.57260	2.95220
C	4.95440	1.56380	-0.21160	H	2.78900	2.39460	1.39180
C	5.44360	2.69830	0.61100	H	1.23710	2.81980	3.18010
C	5.79580	3.85210	0.03120	C	8.28710	-2.25090	2.22740
H	5.99860	4.93210	-1.90100	C	8.37300	-0.96290	1.87570
H	5.21340	3.08360	-3.25940	C	7.18010	-0.24980	1.37260
H	4.50430	0.91250	-2.17620	C	5.99930	-0.88570	1.28050
H	5.51200	2.59920	1.68720	C	5.91690	-2.31940	1.65560
H	6.14600	4.67920	0.63500	C	7.00010	-2.96350	2.10640
C	1.48640	0.83550	4.14340	H	9.16050	-2.77420	2.59440
C	2.12220	-0.33940	4.08160	H	9.31710	-0.43990	1.95760
C	3.08590	-0.60440	2.99320	H	7.28610	0.78510	1.08470
C	3.33070	0.33110	2.05840	H	4.98480	-2.85970	1.54920
C	2.62140	1.63240	2.13670	H	6.93740	-4.01030	2.37450

### **OOH-Type II E**

O	2.15180	0.23500	-0.73910	H	-6.58930	-3.57790	-0.56080
P	0.65690	0.09470	-0.08160	H	-7.10760	-2.25020	0.48540
O	0.30080	1.57070	0.58960	H	-5.77080	-0.35400	0.71880
O	-0.25070	-0.20830	-1.24950	N	-5.26240	-0.52890	-0.13900
O	0.67080	-0.85640	1.09860	C	-2.97410	-3.93960	0.76110
H	-4.35130	-0.08630	-0.19690	C	-1.69340	-3.41750	0.77720
C	-5.27400	-1.85400	-0.55710	N	-1.44970	-2.31630	1.54240
C	-2.69890	-2.93850	-3.84280	H	-0.52430	-1.80310	1.40470
C	-2.24920	-2.03400	-2.89060	C	-2.34720	-1.72640	2.38370
C	-3.08870	-1.64610	-1.82880	C	-1.74590	-0.62490	3.20920
C	-4.39570	-2.19240	-1.71830	H	-0.83970	-0.99050	3.70050
C	-4.80700	-3.12000	-2.69250	H	-1.42450	0.19120	2.55410
C	-3.98410	-3.48510	-3.75170	H	-2.43690	-0.26170	3.96030
H	-2.04260	-3.21770	-4.66260	C	-0.49180	-3.93050	0.03740
H	-1.25670	-1.59950	-2.94330	H	-0.24950	-4.94760	0.35170
H	-5.79720	-3.55460	-2.62340	H	-0.69190	-3.96460	-1.03550
H	-4.34090	-4.18550	-4.50010	H	0.35620	-3.27270	0.22600
C	-6.65310	-2.49190	-0.47820	C	-3.65620	-2.17340	2.37440
H	-7.29390	-2.10180	-1.27620	C	-3.41500	-5.14120	0.02290

C	-4.76980	-1.64550	3.19440	C	2.61970	6.30580	-1.55940
H	-3.38560	-7.68900	-0.71420	C	3.94560	6.43270	-1.67280
H	-3.46910	-6.64960	-2.15590	C	4.83210	5.34190	-1.22780
C	-2.83280	-6.97640	-1.33040	C	4.31440	4.22990	-0.69340
H	-1.91440	-7.42530	-1.70800	H	1.97420	7.10610	-1.89970
C	-5.49310	-0.60300	5.18290	H	4.37100	7.33070	-2.10180
H	-6.06460	0.15050	4.63690	H	5.90360	5.43920	-1.34620
H	-6.16460	-1.41520	5.46980	H	4.98570	3.43390	-0.40140
H	-5.02130	-0.16610	6.06230	Si	-1.84500	3.61830	-0.48280
O	-4.58650	-5.47440	-0.06150	Si	4.22020	-2.10520	-0.18680
O	-5.93910	-1.71940	2.84340	C	-3.01480	0.97070	-4.18420
O	-4.41080	-1.10780	4.37940	C	-3.96990	1.44430	-3.37740
O	-2.41370	-5.84590	-0.54770	C	-3.60900	2.27530	-2.21020
O	-2.67290	-0.76460	-0.90240	C	-2.31870	2.52620	-1.92450
H	-1.69240	-0.49160	-1.05280	C	-1.26750	2.01720	-2.84150
C	-4.03930	-3.19780	1.41120	C	-1.59830	1.27750	-3.90710
H	-4.65400	-2.54370	0.38960	H	-3.27720	0.36090	-5.03900
H	-4.92950	-3.77460	1.65360	H	-5.01010	1.22460	-3.58010
C	3.09750	0.57500	0.19010	H	-4.40620	2.71070	-1.62670
C	3.11480	1.82650	0.69090	H	-0.22440	2.23740	-2.66080
C	4.97310	-0.10770	1.59750	H	-0.82750	0.90040	-4.56690
C	4.11390	-0.42210	0.61740	C	-3.71270	7.89020	-0.95280
H	5.70970	-0.82830	1.93260	C	-3.81420	7.01320	-1.95830
C	2.23590	2.86060	0.07790	C	-3.23210	5.66130	-1.82490
C	0.88910	2.68240	0.02880	C	-2.60760	5.30330	-0.68970
C	0.01690	3.79330	-0.45550	C	-2.48940	6.28390	0.41650
C	0.57190	4.92390	-0.91520	C	-3.01510	7.50850	0.29130
H	-0.04400	5.73030	-1.29100	H	-4.13750	8.88090	-1.05020
C	4.92650	1.22220	2.24010	H	-4.32070	7.29240	-2.87310
C	4.03770	2.15140	1.81810	H	-3.30800	4.98290	-2.66270
C	3.96940	3.45970	2.52340	H	-1.97310	6.01670	1.32950
C	4.80580	3.72760	3.53290	H	-2.92740	8.22270	1.09980
C	5.79530	2.72160	3.96370	C	-3.36990	2.34410	3.76530
C	5.85090	1.53190	3.35520	C	-4.10940	2.06390	2.68720
H	3.23770	4.20360	2.23760	C	-3.62080	2.42110	1.34030
H	4.75260	4.68070	4.04300	C	-2.41850	2.99950	1.18210
H	6.47040	2.94650	4.77930	C	-1.59760	3.29390	2.38450
H	6.57430	0.79550	3.68270	C	-2.04990	2.98460	3.60580
C	2.84020	4.08680	-0.52790	H	-3.73090	2.09060	4.75360
C	2.03580	5.07600	-0.97440	H	-5.07560	1.58990	2.79820

H	-4.27010	2.23630	0.50380	C	2.28040	-2.89330	-2.22570
H	-0.63630	3.78090	2.28580	C	1.66370	-2.76490	-3.40660
H	-1.45110	3.20690	4.47950	H	1.64820	-1.67920	-5.34520
C	1.96170	-5.25310	2.46360	H	3.56720	-0.29170	-4.82320
C	2.03920	-3.97930	2.86460	H	4.69810	-0.47520	-2.56900
C	2.76440	-2.98680	2.04460	H	1.90810	-3.62030	-1.52440
C	3.33900	-3.35350	0.88550	H	0.80700	-3.38350	-3.64210
C	3.25550	-4.77070	0.45260	C	8.78760	-3.11030	-0.59370
C	2.60280	-5.66870	1.20020	C	7.96750	-3.98790	-0.00530
H	1.42750	-5.98010	3.06140	C	6.52810	-3.68180	0.13150
H	1.56670	-3.67090	3.78820	C	6.02940	-2.53010	-0.35160
H	2.80940	-1.96520	2.39530	C	6.95190	-1.55080	-0.97870
H	3.71810	-5.08350	-0.47530	C	8.25600	-1.82870	-1.09630
H	2.53910	-6.70010	0.87850	H	9.84220	-3.33280	-0.69300
C	2.15000	-1.78060	-4.39170	H	8.35630	-4.92460	0.37290
C	3.21000	-1.01750	-4.10410	H	5.89930	-4.40280	0.63060
C	3.88410	-1.14710	-2.79530	H	6.58640	-0.59140	-1.31610
C	3.44650	-2.03820	-1.88800	H	8.92660	-1.10810	-1.54650

O	2.11910	0.38190	-0.66630	H	-3.09940	-7.06110	-1.81240
P	0.62330	0.08800	-0.06200	C	-2.48470	-7.28900	-0.93870
O	0.07150	1.52920	0.55300	H	-1.53640	-7.73240	-1.24140
O	-0.19930	-0.34380	-1.25230	C	-5.56990	-0.74950	5.14250
O	0.68850	-0.82720	1.14490	H	-6.16370	-0.03090	4.57380
H	-4.31640	-0.35530	-0.26630	H	-6.20970	-1.58690	5.42950
C	-5.16570	-2.17330	-0.56870	H	-5.13490	-0.27910	6.02350
C	-2.47660	-3.31920	-3.74130	O	-4.34160	-5.74770	0.11780
C	-2.08420	-2.35130	-2.82730	O	-5.92230	-1.91780	2.81250
C	-2.96250	-1.94300	-1.80560	O	-4.45080	-1.21760	4.36710
C	-4.25050	-2.53190	-1.69530	O	-2.13810	-6.08050	-0.24110
C	-4.60380	-3.52220	-2.63000	O	-2.60040	-1.00120	-0.91680
C	-3.74270	-3.90880	-3.65050	H	-1.63240	-0.68890	-1.07040
H	-1.79070	-3.61430	-4.53080	C	-3.92910	-3.38030	1.48510
H	-1.10860	-1.88060	-2.88010	H	-4.54840	-2.79820	0.41640
H	-5.57840	-3.99050	-2.56050	H	-4.80020	-3.98300	1.73300
H	-4.05550	-4.65960	-4.36910	C	2.99590	0.79460	0.29830
C	-6.52490	-2.85390	-0.49440	C	2.85210	2.02030	0.84130
H	-6.42200	-3.93980	-0.52100	C	4.86930	0.26890	1.77190
H	-7.01480	-2.58150	0.44340	C	4.11650	-0.08840	0.72050
H	-7.15580	-2.52650	-1.32760	H	5.68250	-0.36680	2.10290
H	-5.74580	-0.63900	0.62850	C	1.92250	2.98970	0.19800
N	-5.21100	-0.83070	-0.20940	C	0.60280	2.69670	0.05100
C	-2.81780	-4.10280	0.89500	C	-0.32880	3.74150	-0.47090
C	-1.56490	-3.51670	0.90170	C	0.15290	4.92940	-0.86270
N	-1.38880	-2.36700	1.61350	H	-0.50490	5.69000	-1.26180
H	-0.48550	-1.82040	1.47110	C	4.62580	1.54570	2.47510
C	-2.32930	-1.78380	2.41210	C	3.66680	2.39200	2.03440
C	-1.80400	-0.61380	3.19260	C	3.41220	3.65150	2.78420
H	-2.54810	-0.21770	3.87310	C	4.15060	3.96000	3.85660
H	-0.92530	-0.92200	3.76740	C	5.21680	3.04680	4.31120
H	-1.45770	0.16160	2.50220	C	5.44090	1.90030	3.65990
C	-0.32640	-4.00520	0.20730	H	2.62270	4.32540	2.47890
H	0.09300	-4.87040	0.73010	H	3.96230	4.87740	4.39930
H	-0.55390	-4.31890	-0.81030	H	5.81200	3.30450	5.17770
H	0.41330	-3.20540	0.19100	H	6.22060	1.23200	4.00360
C	-3.61390	-2.29590	2.40390	C	2.45440	4.28280	-0.33390
C	-3.18650	-5.36800	0.22590	C	1.59740	5.21090	-0.81260
C	-4.76490	-1.79060	3.18600	C	2.10720	6.50500	-1.32370
H	-3.03580	-7.96710	-0.28320	C	3.42080	6.75190	-1.33860

C	4.36890	5.73010	-0.85850	H	-4.66240	2.10890	0.27250
C	3.91790	4.56080	-0.39020	H	-1.05920	3.56340	2.19050
H	1.41740	7.25560	-1.68940	H	-1.97450	3.02800	4.34920
H	3.79220	7.69680	-1.71360	C	4.26570	-5.08910	3.00210
H	5.43300	5.92500	-0.89790	C	3.18930	-4.35010	2.71060
H	4.63700	3.81860	-0.07200	C	3.28400	-3.27060	1.70720
Si	-2.16130	3.40080	-0.63190	C	4.44130	-3.03640	1.06760
Si	4.54350	-1.66830	-0.18900	C	5.63660	-3.84610	1.40980
C	-2.78420	0.54680	-4.31390	C	5.55010	-4.82050	2.32430
C	-3.83630	0.92350	-3.57990	H	4.19940	-5.88020	3.73770
C	-3.64700	1.81200	-2.41470	H	2.24700	-4.54090	3.20780
C	-2.41490	2.21690	-2.05780	H	2.40660	-2.67950	1.49360
C	-1.25650	1.81310	-2.89540	H	6.58890	-3.65130	0.93720
C	-1.43220	1.01760	-3.95770	H	6.42310	-5.40930	2.57470
H	-2.92100	-0.10520	-5.16680	C	1.70750	-2.45380	-3.83880
H	-4.82980	0.58220	-3.84010	C	2.50810	-1.38230	-3.82610
H	-4.52450	2.16170	-1.89480	C	3.42110	-1.15410	-2.68680
H	-0.25860	2.15560	-2.65940	C	3.42870	-2.00170	-1.64310
H	-0.58290	0.71750	-4.55800	C	2.57120	-3.21090	-1.68510
C	-4.38290	7.44500	-1.44190	C	1.75040	-3.41900	-2.72260
C	-4.30890	6.52870	-2.41450	H	1.03270	-2.61950	-4.66870
C	-3.61280	5.24720	-2.17470	H	2.48260	-0.67540	-4.64520
C	-3.05870	4.99340	-0.97670	H	4.05450	-0.27540	-2.69060
C	-3.13700	6.01640	0.09390	H	2.60520	-3.93810	-0.88640
C	-3.76600	7.17700	-0.12730	H	1.12230	-4.29980	-2.75130
H	-4.89140	8.38420	-1.61710	C	8.81660	-1.47620	-2.09830
H	-4.75670	6.72470	-3.38010	C	8.34550	-0.41540	-1.43230
H	-3.54990	4.53490	-2.98520	C	7.00150	-0.46150	-0.81910
H	-2.68250	5.83100	1.05900	C	6.25370	-1.57450	-0.91360
H	-3.82190	7.92250	0.65530	C	6.77510	-2.74020	-1.66750
C	-3.87900	2.19710	3.56460	C	7.99120	-2.69410	-2.22480
C	-4.58260	1.92750	2.46040	H	9.80010	-1.44260	-2.54900
C	-4.03530	2.26860	1.13160	H	8.94630	0.48040	-1.34350
C	-2.80900	2.80600	1.01590	H	6.63710	0.41950	-0.31060
C	-2.03140	3.09340	2.24920	H	6.17350	-3.63510	-1.76880
C	-2.54110	2.80860	3.45360	H	8.37100	-3.54730	-2.77180
H	-4.28400	1.96180	4.53990				
H	-5.56380	1.47750	2.53740				

O	2.13470	0.36710	-0.68100	H	-3.18860	-7.00180	-1.87990
P	0.63620	0.07840	-0.07220	C	-2.57420	-7.25500	-1.01230
O	0.09380	1.52550	0.54850	H	-1.63040	-7.70180	-1.32630
O	-0.18920	-0.34380	-1.26370	C	-5.55050	-0.75220	5.17350
O	0.70010	-0.83550	1.13420	H	-6.13080	-0.01170	4.61810
H	-4.34900	-0.31720	-0.24860	H	-6.20490	-1.58270	5.44970
C	-5.20400	-2.13070	-0.56770	H	-5.10120	-0.30510	6.06030
C	-2.51960	-3.25530	-3.75180	O	-4.40990	-5.70860	0.07670
C	-2.11940	-2.30490	-2.82220	O	-5.93150	-1.88870	2.82940
C	-2.99770	-1.90440	-1.79820	O	-4.44370	-1.22940	4.38690
C	-4.29060	-2.48250	-1.69750	O	-2.21170	-6.06460	-0.29300
C	-4.65150	-3.45550	-2.64740	O	-2.63140	-0.97630	-0.89270
C	-3.79180	-3.83410	-3.67250	H	-1.66780	-0.66880	-1.05100
H	-1.83450	-3.54500	-4.54470	C	-3.96350	-3.36520	1.47680
H	-1.13840	-1.84330	-2.86550	H	-4.58490	-2.76460	0.42080
H	-5.63100	-3.91610	-2.58630	H	-4.83750	-3.96360	1.72830
H	-4.11050	-4.57100	-4.40380	C	3.01360	0.77920	0.28440
C	-6.56520	-2.80810	-0.49670	C	2.87650	2.00890	0.81950
H	-6.46610	-3.89480	-0.53450	C	4.88160	0.25090	1.76350
H	-7.05340	-2.54280	0.44530	C	4.12720	-0.10880	0.71410
H	-7.19760	-2.46970	-1.32570	H	5.68990	-0.38810	2.10010
H	-5.77270	-0.60670	0.64890	C	1.94880	2.97720	0.17240
N	-5.24630	-0.79050	-0.19810	C	0.62690	2.68980	0.03570
C	-2.86270	-4.09490	0.87300	C	-0.30330	3.73750	-0.48300
C	-1.60200	-3.52640	0.88320	C	0.18270	4.91900	-0.88910
N	-1.41090	-2.38680	1.60810	H	-0.47380	5.68170	-1.28630
H	-0.50580	-1.85580	1.47110	C	4.64750	1.53530	2.45620
C	-2.34040	-1.79810	2.41630	C	3.69450	2.38490	2.00880
C	-1.79530	-0.64000	3.20250	C	3.45010	3.65290	2.74730
H	-2.52620	-0.24880	3.90160	C	4.19190	3.96570	3.81610
H	-0.90650	-0.95780	3.75790	C	5.25140	3.04850	4.27820
H	-1.45930	0.14480	2.51600	C	5.46620	1.89440	3.63720
C	-0.36890	-4.02190	0.18250	H	2.66560	4.33010	2.43650
H	0.03770	-4.90310	0.69060	H	4.01120	4.88950	4.35040
H	-0.59790	-4.31340	-0.84230	H	5.84930	3.30970	5.14180
H	0.38480	-3.23330	0.18020	H	6.24120	1.22340	3.98640
C	-3.63030	-2.29510	2.40790	C	2.48440	4.26270	-0.37340
C	-3.24960	-5.34620	0.18760	C	1.62950	5.19150	-0.85440
C	-4.77120	-1.78300	3.20070	C	2.14340	6.47750	-1.38150
H	-3.13000	-7.93980	-0.36690	C	3.45830	6.71620	-1.40800



C	4.40380	5.69360	-0.92420	H	-4.63020	2.11940	0.31840
C	3.94910	4.53160	-0.44140	H	-1.00480	3.57410	2.19330
H	1.45550	7.22850	-1.74970	H	-1.89020	3.02930	4.36250
H	3.83270	7.65510	-1.79490	C	4.24100	-5.09300	3.03350
H	5.46860	5.88190	-0.97220	C	3.16670	-4.35680	2.72750
H	4.66570	3.78840	-0.11980	C	3.26890	-3.28600	1.71550
Si	-2.14120	3.41340	-0.61510	C	4.43100	-3.05680	1.08280
Si	4.54400	-1.69830	-0.18340	C	5.62360	-3.86360	1.44080
C	-2.85750	0.58220	-4.29700	C	5.53040	-4.83010	2.36300
C	-3.89380	0.97420	-3.54880	H	4.16920	-5.87770	3.77550
C	-3.67490	1.85510	-2.38300	H	2.22070	-4.54330	3.21920
C	-2.43170	2.23730	-2.03990	H	2.39260	-2.69800	1.48920
C	-1.29050	1.81490	-2.89170	H	6.57950	-3.67270	0.97390
C	-1.49310	1.02740	-3.95510	H	6.40150	-5.41660	2.62510
H	-3.01600	-0.06390	-5.15060	C	1.70840	-2.48630	-3.83340
H	-4.89630	0.65150	-3.79830	C	2.51720	-1.42090	-3.82610
H	-4.53990	2.21970	-1.85190	C	3.43040	-1.19260	-2.68690
H	-0.28390	2.13860	-2.66580	C	3.43000	-2.03370	-1.63790
H	-0.65650	0.71440	-4.56650	C	2.56420	-3.23720	-1.67420
C	-4.32910	7.48580	-1.37640	C	1.74350	-3.44550	-2.71190
C	-4.27850	6.57330	-2.35390	H	1.03330	-2.65190	-4.66300
C	-3.59390	5.28290	-2.12930	H	2.49790	-0.71860	-4.64940
C	-3.02720	5.01690	-0.93980	H	4.07010	-0.31850	-2.69500
C	-3.07930	6.03590	0.13630	H	2.59220	-3.96030	-0.87170
C	-3.69780	7.20470	-0.07140	H	1.11020	-4.32270	-2.73690
H	-4.82900	8.43160	-1.54060	C	8.82360	-1.55060	-2.08180
H	-4.73670	6.77900	-3.31270	C	8.35680	-0.48040	-1.42790
H	-3.54880	4.57440	-2.94420	C	7.01060	-0.51220	-0.81870
H	-2.61400	5.84100	1.09420	C	6.25640	-1.62150	-0.90470
H	-3.73450	7.94730	0.71520	C	6.77290	-2.79770	-1.64540
C	-3.80410	2.19840	3.60040	C	7.99110	-2.76460	-2.19900
C	-4.52220	1.93240	2.50470	H	9.80880	-1.52760	-2.52940
C	-3.99280	2.27840	1.16990	H	8.96290	0.41260	-1.34590
C	-2.76880	2.81760	1.03990	H	6.65010	0.37600	-0.32010
C	-1.97550	3.10230	2.26380	H	6.16620	-3.68990	-1.73970
C	-2.46840	2.81200	3.47380	H	8.36740	-3.62550	-2.73630
H	-4.19550	1.95790	4.58010				
H	-5.50160	1.48070	2.59290				

**OOH-Type I Z**

O	1.10910	-1.55820	0.97490	H	4.36530	7.27850	-2.20820
P	0.10240	-0.36930	0.42960	H	4.88300	6.38930	-0.75940
O	-1.19320	-1.10600	-0.31260	C	4.66880	6.30120	-1.82680
O	-0.30170	0.39290	1.65760	H	5.54000	5.93100	-2.36620
O	0.75790	0.39430	-0.72030	C	-4.66810	4.92970	-2.35230
H	2.11110	2.99920	0.96660	H	-4.99000	4.91030	-1.30900
C	0.19930	3.69200	1.04230	H	-4.64880	5.96580	-2.69710
C	1.28480	5.67540	4.70320	H	-5.33450	4.32990	-2.97150
C	1.02550	4.30980	4.68140	O	2.26170	6.60290	-0.79810
C	0.67480	3.66010	3.48750	O	-2.56470	5.89570	-1.08410
C	0.58200	4.43170	2.29850	O	-3.36890	4.32720	-2.49410
C	0.85370	5.80250	2.33950	O	3.63240	5.32810	-2.05780
C	1.20470	6.43190	3.53170	O	0.42740	2.33440	3.59200
H	1.55760	6.15020	5.64160	H	0.30850	1.82000	2.76140
H	1.08950	3.70540	5.58020	C	0.05680	4.98790	-1.30390
H	0.81120	6.37340	1.41710	H	0.08820	4.61170	0.04160
H	1.41730	7.49590	3.54310	H	-0.11120	6.04750	-1.13750
C	-1.23320	3.19430	1.02810	C	1.35020	-2.58000	0.09610
H	-1.90330	4.05530	1.06130	C	0.35770	-3.44200	-0.21060
H	-1.45890	2.57880	0.15980	C	2.94770	-3.84070	-1.25960
H	-1.39840	2.56570	1.90190	C	2.73560	-2.83080	-0.40090
H	0.98870	1.93930	0.15100	H	3.93210	-4.02820	-1.66000
N	1.17580	2.83380	0.63070	C	-0.95630	-3.33010	0.47210
C	1.38680	4.59800	-1.72020	C	-1.70570	-2.21260	0.32380
C	1.57760	3.29460	-2.13860	C	-3.16430	-2.27470	0.63340
N	0.47430	2.52710	-2.40410	C	-3.65560	-3.33880	1.28900
H	0.59810	1.51500	-2.28250	H	-4.70250	-3.39480	1.55440
C	-0.82830	2.96870	-2.34450	C	1.84050	-4.70680	-1.70420
C	-1.81910	1.91340	-2.73820	C	0.59580	-4.51810	-1.21670
H	-1.53600	0.97150	-2.25460	C	-0.51780	-5.36090	-1.73440
H	-2.82900	2.18240	-2.44900	C	-0.27780	-6.31980	-2.63610
H	-1.80020	1.75590	-3.82270	C	1.09230	-6.54210	-3.13520
C	2.87240	2.56190	-2.32390	C	2.09680	-5.77500	-2.69860
H	3.09920	2.45500	-3.39030	H	-1.53480	-5.20000	-1.40260
H	3.70370	3.07420	-1.84980	H	-1.09060	-6.92870	-3.01030
H	2.75700	1.56340	-1.89240	H	1.28000	-7.32130	-3.86260
C	-1.06150	4.24760	-1.89090	H	3.09850	-5.93770	-3.07670
C	2.44970	5.59890	-1.46160	C	-1.49250	-4.47930	1.25830
C	-2.38370	4.90530	-1.76950	C	-2.78320	-4.46970	1.65290

C	-3.33170	-5.60380	2.43260	H	-3.41050	1.46980	4.34810
C	-2.54480	-6.63250	2.76630	H	-3.47760	-0.53990	2.80840
C	-1.12540	-6.63840	2.36380	H	-4.66970	2.09460	-0.42430
C	-0.62310	-5.62060	1.65490	H	-4.73510	3.95780	1.08840
H	-4.37140	-5.60370	2.73570	C	5.70600	0.71540	-3.57100
H	-2.94550	-7.46020	3.33710	C	4.60050	-0.02980	-3.68630
H	-0.48950	-7.46590	2.65090	C	4.09360	-0.78920	-2.52420
H	0.42490	-5.63590	1.38570	C	4.74410	-0.73990	-1.34880
Si	-4.34060	-0.93230	0.06790	C	5.97540	0.07790	-1.23170
Si	4.19490	-1.76270	0.10560	C	6.42640	0.77230	-2.28330
C	-8.74900	-2.40800	0.64540	H	6.07430	1.27680	-4.41970
C	-8.31120	-1.35430	1.34480	H	4.07010	-0.07200	-4.62870
C	-6.92270	-0.87670	1.17570	H	3.19660	-1.37990	-2.64630
C	-6.09370	-1.50150	0.32190	H	6.51580	0.11520	-0.29400
C	-6.58640	-2.66530	-0.45380	H	7.32350	1.37110	-2.19460
C	-7.84440	-3.09490	-0.29840	C	3.23400	0.89620	3.85350
H	-9.76570	-2.75820	0.76880	C	3.65810	1.47350	2.72430
H	-8.97300	-0.84890	2.03630	C	3.92940	0.65160	1.52530
H	-6.59660	-0.02190	1.75180	C	3.78310	-0.68380	1.57330
H	-5.92830	-3.17420	-1.14730	C	3.29570	-1.31380	2.82660
H	-8.20180	-3.94590	-0.86380	C	3.03260	-0.56440	3.90360
C	-4.12270	-0.21370	-4.56690	H	3.03340	1.49860	4.73010
C	-5.01130	0.45240	-3.82210	H	3.80650	2.54500	2.68790
C	-5.07910	0.21850	-2.36490	H	4.25620	1.14910	0.62360
C	-4.22120	-0.62880	-1.76950	H	3.14100	-2.38480	2.87110
C	-3.27530	-1.40410	-2.61290	H	2.67370	-1.02740	4.81350
C	-3.22300	-1.19790	-3.93460	C	7.91940	-4.44870	1.11450
H	-4.07130	-0.04410	-5.63450	C	7.52790	-4.28550	-0.15330
H	-5.68300	1.16420	-4.28420	C	6.35620	-3.44100	-0.46370
H	-5.84400	0.72890	-1.79500	C	5.66040	-2.84700	0.52310
H	-2.64180	-2.16400	-2.18170	C	6.12000	-3.01400	1.92610
H	-2.53370	-1.76600	-4.54590	C	7.18520	-3.77630	2.20340
C	-4.07930	2.80200	2.86800	H	8.77890	-5.06520	1.34390
C	-3.69930	1.59930	3.31320	H	8.07020	-4.76880	-0.95560
C	-3.70390	0.43710	2.40100	H	6.08830	-3.29580	-1.50180
C	-4.05430	0.58520	1.11090	H	5.61590	-2.51790	2.73940
C	-4.42360	1.93410	0.61280	H	7.51700	-3.89420	3.22700
C	-4.45910	2.97670	1.45210				
H	-4.08760	3.65240	3.53720				

O	1.11720	-1.55740	0.99690	C	-2.37910	4.87610	-1.79470
P	0.11230	-0.36630	0.45310	H	4.35940	7.29020	-2.19110
O	-1.18630	-1.09970	-0.28830	H	4.86680	6.41610	-0.72950
O	-0.28930	0.39770	1.68060	C	4.66470	6.31800	-1.79840
O	0.76950	0.39470	-0.69740	H	5.54400	5.94890	-2.32540
H	2.10910	3.01440	0.98350	C	-4.65510	4.89010	-2.41110
C	0.19360	3.69810	1.04770	H	-4.99160	4.87630	-1.37240
C	1.25260	5.71610	4.69730	H	-4.63470	5.92410	-2.76230
C	1.01100	4.34720	4.68320	H	-5.31050	4.28390	-3.03580
C	0.66960	3.68610	3.49290	O	2.24540	6.61200	-0.79680
C	0.56810	4.44950	2.29930	O	-2.57380	5.86710	-1.11400
C	0.82200	5.82400	2.33260	O	-3.35180	4.29180	-2.53100
C	1.16370	6.46480	3.52140	O	3.63690	5.33660	-2.03270
H	1.51820	6.20000	5.63310	O	0.43990	2.35780	3.60470
H	1.08150	3.74910	5.58580	H	0.31820	1.83980	2.77700
H	0.77320	6.38900	1.40700	C	0.05690	4.97720	-1.30800
H	1.36260	7.53150	3.52670	H	0.08130	4.60960	0.03970
C	-1.23620	3.19290	1.03180	H	-0.11970	6.03670	-1.14930
H	-1.91020	4.05120	1.05800	C	1.35070	-2.58210	0.11930
H	-1.45570	2.57240	0.16530	C	0.35400	-3.44200	-0.17910
H	-1.40170	2.56780	1.90830	C	2.93660	-3.85140	-1.24220
H	0.99430	1.94360	0.17100	C	2.73210	-2.83720	-0.38660
N	1.17560	2.84160	0.64630	H	3.91780	-4.04200	-1.64890
C	1.39270	4.59440	-1.71170	C	-0.95760	-3.32110	0.50630
C	1.59570	3.29010	-2.12170	C	-1.70380	-2.20270	0.35070
N	0.50010	2.51390	-2.39300	C	-3.16410	-2.26200	0.65270
H	0.62910	1.50320	-2.26430	C	-3.65920	-3.32050	1.31470
C	-0.80600	2.94650	-2.34500	H	-4.70760	-3.37440	1.57430
C	-1.78610	1.88140	-2.73910	C	1.82470	-4.71670	-1.67630
H	-1.51010	0.95000	-2.23120	C	0.58330	-4.52250	-1.18260
H	-2.80230	2.15290	-2.47630	C	-0.53570	-5.36330	-1.69170
H	-1.74300	1.70240	-3.81950	C	-0.30360	-6.32590	-2.59150
C	2.89740	2.56580	-2.29230	C	1.06300	-6.55430	-3.09710
H	3.13440	2.45700	-3.35620	C	2.07220	-5.78900	-2.66840
H	3.72080	3.08560	-1.81290	H	-1.55050	-5.19790	-1.35540
H	2.78550	1.56810	-1.85820	H	-1.12040	-6.93330	-2.95940
C	-1.05170	4.22570	-1.89920	H	1.24430	-7.33650	-3.82290
C	2.44650	5.60420	-1.45050	H	3.07140	-5.95610	-3.05140

C	-1.49760	-4.46430	1.29810	C	-4.47330	2.99550	1.40140
C	-2.78920	-4.44970	1.68980	H	-4.13110	3.69350	3.48410
C	-3.34140	-5.57830	2.47480	H	-3.46680	1.51950	4.32820
C	-2.55720	-6.60680	2.81550	H	-3.51340	-0.50670	2.80940
C	-1.13700	-6.61780	2.41570	H	-4.65720	2.09330	-0.46820
C	-0.63130	-5.60500	1.70230	H	-4.74360	3.97270	1.02350
H	-4.38170	-5.57460	2.77570	C	5.67050	0.68810	-3.60710
H	-2.96060	-7.43070	3.39000	C	4.56170	-0.05470	-3.70550
H	-0.50340	-7.44520	2.70810	C	4.06620	-0.80610	-2.53340
H	0.41700	-5.62370	1.43450	C	4.73000	-0.75160	-1.36560
Si	-4.33790	-0.92840	0.06210	C	5.96390	0.06460	-1.26690
Si	4.19630	-1.76700	0.09990	C	6.40500	0.75140	-2.32770
C	-8.74950	-2.40600	0.60900	H	6.03060	1.24340	-4.46330
C	-8.32160	-1.34280	1.30000	H	4.02070	-0.10120	-4.64170
C	-6.93210	-0.86470	1.14080	H	3.16680	-1.39590	-2.64210
C	-6.09220	-1.49880	0.30470	H	6.51470	0.10660	-0.33540
C	-6.57380	-2.67340	-0.46160	H	7.30420	1.34890	-2.25260
C	-7.83290	-3.10340	-0.31530	C	3.26270	0.91010	3.84180
H	-9.76700	-2.75640	0.72500	C	3.68080	1.48160	2.70740
H	-8.99220	-0.82970	1.97710	C	3.94490	0.65380	1.51090
H	-6.61430	-0.00160	1.70920	C	3.79910	-0.68130	1.56650
H	-5.90690	-3.18990	-1.14090	C	3.32100	-1.30530	2.82640
H	-8.18220	-3.96210	-0.87380	C	3.06340	-0.55050	3.90080
C	-4.07700	-0.25850	-4.57800	H	3.06630	1.51700	4.71620
C	-4.97270	0.41510	-3.84850	H	3.82920	2.55290	2.66500
C	-5.05410	0.19640	-2.38960	H	4.26520	1.14690	0.60440
C	-4.20170	-0.64430	-1.77740	H	3.16740	-2.37620	2.87730
C	-3.24790	-1.42830	-2.60380	H	2.71060	-1.00920	4.81540
C	-3.18320	-1.23600	-3.92710	C	7.92690	-4.45510	1.07990
H	-4.01560	-0.10000	-5.64680	C	7.52680	-4.29010	-0.18500
H	-5.64010	1.12180	-4.32440	C	6.35340	-3.44470	-0.48630
H	-5.82430	0.71270	-1.83220	C	5.66510	-2.85100	0.50610
H	-2.61870	-2.18390	-2.15910	C	6.13390	-3.02020	1.90560
H	-2.48830	-1.81050	-4.52590	C	7.20040	-3.78380	2.17460
C	-4.11350	2.83590	2.82430	H	8.78750	-5.07250	1.30250
C	-3.74060	1.63810	3.28790	H	8.06320	-4.77280	-0.99170
C	-3.73300	0.46600	2.38830	H	6.07740	-3.29930	-1.52230
C	-4.06500	0.60030	1.09190	H	5.63500	-2.52540	2.72300
C	-4.42620	1.94390	0.57400	H	7.53880	-3.90370	3.19580

O	-1.44840	-1.34000	-0.83210	C	2.88990	4.42850	2.87020
P	-0.20100	-0.36440	-0.36380	H	-2.50500	8.25630	0.13780
O	0.88860	-1.32980	0.44790	H	-2.58600	7.26400	-1.33400
O	0.37520	0.18090	-1.63760	C	-2.87250	7.31700	-0.28130
O	-0.67120	0.62710	0.69750	H	-3.95400	7.24320	-0.17160
H	-0.55890	3.25700	-1.59080	C	4.58520	4.27250	4.49970
C	1.30150	3.30060	-0.75770	H	5.32100	3.96440	3.75420
C	2.84170	4.95500	-4.42350	H	4.66900	5.35070	4.65350
C	1.99420	3.85450	-4.45690	H	4.73640	3.73830	5.43710
C	1.47840	3.29930	-3.27480	O	-0.27120	6.91440	-0.12200
C	1.81630	3.90520	-2.03610	O	3.62570	5.12900	2.19860
C	2.69080	4.99920	-2.02500	O	3.25230	3.93080	4.07410
C	3.20500	5.53080	-3.20280	O	-2.33500	6.19730	0.44720
H	3.22960	5.35910	-5.35440	O	0.65600	2.23320	-3.42930
H	1.72030	3.37750	-5.39210	H	0.61270	1.59010	-2.67650
H	2.96060	5.44040	-1.06920	C	0.98340	4.92450	1.36380
H	3.87310	6.38520	-3.16990	H	1.37250	4.27040	0.16400
C	2.24470	2.28200	-0.13190	H	1.50820	5.85540	1.17350
H	3.20560	2.75140	0.08970	C	-2.01030	-2.04180	0.19990
H	1.83110	1.83590	0.77230	C	-1.31610	-3.04590	0.77190
H	2.38990	1.47160	-0.84910	C	-3.92700	-2.44340	1.66110
H	-0.34030	2.11260	-0.30640	C	-3.41730	-1.77730	0.61210
N	-0.02730	2.96990	-0.78310	H	-4.95200	-2.27410	1.97040
C	-0.44780	4.94860	1.19630	C	-0.04300	-3.49380	0.15030
C	-1.16030	3.82840	1.58690	C	0.99980	-2.63550	0.02290
N	-0.51780	2.89000	2.34710	C	2.34070	-3.16980	-0.36540
H	-0.87820	1.93570	2.27840	C	2.46740	-4.46060	-0.70870
C	0.75520	3.02130	2.86220	H	3.43010	-4.87680	-0.96600
C	1.13130	1.89900	3.78350	C	-3.11670	-3.43430	2.39570
H	2.11910	2.04180	4.20640	C	-1.86630	-3.72980	1.97750
H	0.40530	1.82470	4.60030	C	-1.05200	-4.70020	2.75820
H	1.09550	0.95500	3.22450	C	-1.56740	-5.30010	3.83740
C	-2.58880	3.48850	1.29020	C	-2.94540	-4.99540	4.26840
H	-3.22780	3.78490	2.12880	C	-3.68010	-4.10850	3.58820
H	-2.94720	3.99720	0.40080	H	-0.03280	-4.92290	2.47080
H	-2.66500	2.40680	1.15460	H	-0.97170	-6.00500	4.40290
C	1.50950	4.09190	2.44550	H	-3.35680	-5.48660	5.14070
C	-0.98540	6.10330	0.43540	H	-4.68810	-3.88470	3.91440

C	0.08960	-4.89900	-0.33870	H	4.13400	1.66820	-4.61230
C	1.29620	-5.35320	-0.73800	H	2.30030	0.08600	-4.49400
C	1.44880	-6.74980	-1.20890	H	2.17180	-1.58280	-2.59140
C	0.38700	-7.56040	-1.26420	H	5.85570	0.05450	-1.00990
C	-0.94300	-7.06320	-0.86540	H	5.96020	1.63960	-2.82900
C	-1.08910	-5.80530	-0.43370	C	-6.05530	2.86340	2.45060
H	2.42090	-7.11910	-1.51170	C	-5.30780	1.88000	2.96240
H	0.49880	-8.58000	-1.60970	C	-4.80630	0.79820	2.08960
H	-1.80280	-7.71730	-0.93280	C	-5.11460	0.77980	0.77940
H	-2.07870	-5.45700	-0.16980	C	-5.92350	1.89160	0.21750
Si	3.86900	-2.09740	-0.25540	C	-6.36820	2.87510	1.00910
Si	-4.53510	-0.60640	-0.33810	H	-6.41900	3.65890	3.08800
C	7.80170	-4.59230	-0.78590	H	-5.06450	1.87600	4.01700
C	6.96770	-4.42340	-1.81830	H	-4.18630	0.03670	2.53570
C	5.72670	-3.64020	-1.64680	H	-6.12880	1.94090	-0.84150
C	5.42230	-3.10450	-0.45200	H	-6.94610	3.68930	0.59140
C	6.35770	-3.28550	0.68570	C	-2.39650	1.02510	-4.17390
C	7.48310	-3.99310	0.52560	C	-2.64610	1.85630	-3.15580
H	8.71180	-5.16480	-0.90990	C	-3.31330	1.35600	-1.93610
H	7.20020	-4.85870	-2.78150	C	-3.68710	0.06870	-1.85020
H	5.06890	-3.50800	-2.49720	C	-3.41970	-0.84480	-2.98800
H	6.14400	-2.84870	1.65120	C	-2.80100	-0.39200	-4.08520
H	8.16430	-4.12520	1.35640	H	-1.90240	1.39000	-5.06500
C	3.94770	-0.21260	4.03260	H	-2.35900	2.89740	-3.22370
C	3.59950	-1.49290	3.86440	H	-3.48480	2.04330	-1.12240
C	3.56160	-2.07650	2.50780	H	-3.71300	-1.88570	-2.93040
C	3.86060	-1.32230	1.43570	H	-2.59940	-1.06190	-4.91090
C	4.22510	0.10060	1.62910	C	-8.22860	-2.99050	-1.99980
C	4.27530	0.62190	2.85970	C	-8.13330	-1.67230	-2.20170
H	3.98190	0.21670	5.02560	C	-6.97040	-0.92470	-1.68000
H	3.35420	-2.10650	4.72140	C	-6.01230	-1.55500	-0.97850
H	3.30370	-3.12250	2.39640	C	-6.11130	-3.02590	-0.78810
H	4.46600	0.72810	0.78710	C	-7.16360	-3.70120	-1.26670
H	4.55130	1.65790	2.99650	H	-9.07870	-3.54000	-2.38300
C	4.07680	0.96220	-3.79420	H	-8.90670	-1.14970	-2.74970
C	3.06570	0.08860	-3.72890	H	-6.90510	0.13080	-1.89200
C	2.98700	-0.87200	-2.60880	H	-5.32800	-3.57560	-0.28810
C	3.91750	-0.85930	-1.64040	H	-7.22880	-4.77300	-1.13040
C	5.06160	0.07860	-1.74530				
C	5.12760	0.95190	-2.75760				

## **Reaction 2**

### **NH-Type I E**

C	-3.26290	1.64140	0.89150	C	3.81670	-1.49080	0.81560
C	-5.68970	0.36850	0.20420	C	1.85890	-3.90060	-0.28380
C	-4.52970	-0.28110	0.02560	C	0.73890	-3.18890	-0.67870
C	-3.23890	0.40830	0.32730	C	1.94450	-2.26010	-2.55840
H	-6.63300	-0.10000	-0.03750	C	3.10750	-2.89810	-2.16420
C	-5.71250	1.74860	0.71680	C	-0.59760	-3.23210	-0.00980
C	-4.55870	2.37070	1.03830	H	-1.24630	-2.44450	-0.38500
C	-4.60880	3.78910	1.49430	H	-1.06320	-4.20680	-0.16710
C	-5.78210	4.41960	1.61960	C	1.73770	-1.46080	-3.81150
C	-7.03860	3.71880	1.29640	H	1.76290	-2.11850	-4.68560
C	-7.00720	2.45430	0.86370	H	0.77640	-0.94690	-3.76360
H	-3.70120	4.33390	1.71600	H	2.54570	-0.74110	-3.94560
H	-5.81210	5.45000	1.94980	C	4.30170	-2.89780	-3.03540
H	-7.98460	4.23390	1.40230	C	1.88430	-4.94730	0.75430
H	-7.93350	1.94880	0.62000	H	0.97140	-6.01460	3.09260
C	0.23800	3.86780	1.98490	H	-0.35370	-6.79690	2.17590
C	-2.00520	2.29880	1.31380	H	7.27350	-4.11010	-2.58170
C	-1.07540	2.57850	0.37960	H	6.40710	-4.10190	-4.15510
C	0.04700	3.49780	0.70780	O	0.67120	-5.41070	1.11890
H	1.03030	4.56120	2.24270	O	2.92230	-5.39320	1.22700
C	-1.76040	2.66790	2.73580	O	4.38450	-2.39870	-4.14310
C	-0.66690	3.39560	3.05160	O	5.33450	-3.55660	-2.44960
C	-0.38970	3.74400	4.46390	Si	-4.55640	-2.03010	-0.63410
C	-1.20910	3.32140	5.43300	Si	1.04390	4.36740	-0.60710
C	-2.39300	2.50630	5.09830	C	-2.20300	-1.94860	-4.68920
C	-2.65570	2.19300	3.82420	C	-3.02760	-0.94610	-4.36550
H	0.47940	4.33840	4.71710	C	-3.77650	-0.98530	-3.09190
H	-1.00400	3.57280	6.46560	C	-3.62780	-2.02160	-2.24820
H	-3.04460	2.15640	5.88850	C	-2.74060	-3.14620	-2.63220
H	-3.51930	1.58060	3.60030	C	-2.05770	-3.10480	-3.78290
O	-2.05820	-0.29220	0.20360	H	-1.64530	-1.91700	-5.61610
P	-0.83600	0.35880	-0.73890	H	-3.13840	-0.09810	-5.02890
O	-1.15960	1.97950	-0.85240	H	-4.43000	-0.15760	-2.84590
O	-0.90850	-0.25610	-2.11330	H	-2.63580	-4.00780	-1.99220
N	2.54410	-1.16740	1.23090	H	-1.40170	-3.92160	-4.05470



C	-8.93650	-3.51400	-1.37970	H	-0.88760	5.26890	-5.16620
C	-8.51310	-3.26570	-0.13490	H	-0.24580	5.87100	-2.79870
C	-7.13220	-2.79430	0.09700	H	1.28330	1.85630	-2.27030
C	-6.29860	-2.60410	-0.93980	H	0.70820	1.31620	-4.55430
C	-6.77100	-2.88860	-2.31700	C	5.62660	3.52160	-0.13370
C	-8.02240	-3.31800	-2.52310	C	5.17840	4.24750	-1.16440
H	-9.94750	-3.86020	-1.55130	C	3.72980	4.49150	-1.32350
H	-9.18030	-3.41040	0.70500	C	2.85610	3.98570	-0.43660
H	-6.80630	-2.60350	1.11220	C	3.35690	3.15560	0.68700
H	-6.11300	-2.75340	-3.16450	C	4.67150	2.94870	0.83540
H	-8.36700	-3.52460	-3.52810	H	6.68710	3.34050	-0.01600
C	-2.86010	-5.05170	2.52370	H	5.87560	4.66050	-1.88170
C	-2.85130	-3.74140	2.79170	H	3.38840	5.09920	-2.15250
C	-3.38840	-2.78050	1.80620	H	2.67100	2.70530	1.39070
C	-3.85880	-3.21370	0.62260	H	5.03790	2.34960	1.65720
C	-3.89540	-4.67040	0.34690	N	0.83610	-2.36650	-1.76280
C	-3.41490	-5.53950	1.24500	H	0.05880	-1.68670	-1.95430
H	-2.46870	-5.75640	3.24570	H	-0.48410	-3.09970	1.06670
H	-2.44860	-3.38120	3.72970	C	6.55370	-3.58130	-3.20530
H	-3.38990	-1.73160	2.06360	H	6.89700	-2.56440	-3.40670
H	-4.31720	-5.03890	-0.57970	C	0.67200	-6.43340	2.12850
H	-3.43810	-6.60180	1.03960	H	1.35670	-7.24000	1.86020
C	0.17160	8.88250	0.29820	C	3.15000	-3.56290	-0.86310
C	1.43860	8.45350	0.25740	H	3.65830	-2.67500	0.00490
C	1.73270	7.03470	-0.03450	H	3.91920	-4.32160	-0.75140
C	0.73000	6.17300	-0.27610	O	0.44200	0.16270	0.05190
C	-0.67270	6.65270	-0.21610	H	1.91500	-0.64180	0.60410
C	-0.93580	7.93690	0.05340	C	5.52050	0.86400	-2.41010
H	-0.04430	9.92080	0.51390	C	6.30810	-0.04870	-1.72810
H	2.25150	9.14390	0.44140	C	5.77630	-0.82820	-0.69230
H	2.76400	6.71320	-0.03900	C	4.42460	-0.65030	-0.27670
H	-1.49070	5.96400	-0.38880	C	3.65030	0.28540	-0.99850
H	-1.95990	8.28450	0.09570	C	4.18230	1.02610	-2.04800
C	-0.15550	3.30580	-5.01820	H	5.94670	1.45090	-3.21790
C	-0.41360	4.52660	-4.53710	H	7.35240	-0.20140	-1.97870
C	-0.04710	4.86830	-3.14680	H	2.61280	0.45760	-0.72900
C	0.52910	3.95010	-2.35050	H	3.56810	1.74500	-2.57540
C	0.82110	2.60410	-2.89660	O	6.65120	-1.73000	-0.17860
C	0.49620	2.29930	-4.15880	H	6.28070	-2.17840	0.59670
H	-0.42130	3.05430	-6.03670	C	0.51100	-1.69850	4.90630

C	0.34660	-0.54660	4.13500	C	6.12130	-1.18150	3.81580
C	1.03990	-0.39050	2.93880	C	5.24600	-0.88480	2.77470
C	1.91260	-1.39700	2.48700	C	4.75790	-1.90350	1.93970
C	2.06350	-2.56250	3.25200	C	5.15850	-3.22680	2.17460
C	1.37100	-2.69970	4.45620	C	6.04490	-3.51710	3.21670
H	-0.03000	-1.81750	5.84010	H	7.21560	-2.72960	4.84540
H	-0.32580	0.23980	4.46440	H	6.48800	-0.38230	4.45270
H	0.89150	0.48630	2.32110	H	4.93130	0.13840	2.60280
H	2.69780	-3.36830	2.91040	H	4.75520	-4.03380	1.57200
H	1.50280	-3.60720	5.03890	H	6.34480	-4.54660	3.38730
C	6.52850	-2.49950	4.03680				

C	3.91970	0.62310	0.55460	H	5.08470	5.41800	-2.79750
C	4.98840	-1.77670	1.58410	H	7.19840	4.35260	-3.28380
C	3.96700	-1.82240	0.71420	H	7.69450	2.01900	-2.38400
C	3.32660	-0.55070	0.26900	H	6.07870	0.86900	-1.02880
H	5.45970	-2.68840	1.93060	O	2.19180	-0.56640	-0.50460
C	5.52230	-0.48320	2.05090	P	0.88930	0.14080	0.24560
C	5.02800	0.67040	1.55170	O	1.29440	1.71260	0.61320
C	5.56950	1.96500	2.04630	O	0.69230	-0.52100	1.60030
C	6.55840	1.98300	2.94760	N	-3.31930	-0.62420	-1.23310
C	7.11310	0.71740	3.46550	C	-4.38210	-0.30020	-0.41740
C	6.62120	-0.45270	3.04380	C	-3.13450	-3.13520	0.47480
H	5.16390	2.90400	1.69270	C	-1.80810	-2.78090	0.65450
H	6.94940	2.92660	3.30540	C	-2.34870	-1.59150	2.69130
H	7.91550	0.73930	4.19160	C	-3.69000	-1.89520	2.54740
H	7.03020	-1.37750	3.43140	C	-0.66470	-3.20340	-0.21400
C	2.99320	4.38130	-1.29120	H	0.23700	-2.65670	0.04990
C	3.53280	1.83390	-0.20510	H	-0.50010	-4.27660	-0.10100
C	2.28090	2.34640	-0.11260	C	-1.70810	-0.89020	3.85440
C	2.04130	3.74330	-0.59260	H	-1.62370	-1.57700	4.70360
H	2.82970	5.37920	-1.67370	H	-0.71270	-0.54200	3.57250
C	4.55510	2.51820	-1.05240	H	-2.32440	-0.05720	4.18900
C	4.28750	3.73680	-1.56480	C	-4.66320	-1.61050	3.62100
C	5.29380	4.43220	-2.40110	C	-3.65250	-4.04820	-0.56000
C	6.46420	3.84500	-2.67150	H	-3.65830	-5.03480	-3.03810
C	6.75380	2.49820	-2.14470	H	-2.29860	-6.13130	-2.63350
C	5.85310	1.86580	-1.38400	H	-7.86220	-2.10080	3.79600

H	-6.71120	-2.07300	5.17370	C	-2.94690	2.63860	-2.78610
O	-2.70810	-4.76610	-1.20100	C	-3.26520	3.53840	-1.84930
O	-4.84530	-4.16100	-0.81080	C	-2.20850	4.14730	-1.01660
O	-4.41400	-1.14430	4.71850	C	-0.92380	3.78620	-1.17630
O	-5.92240	-1.95570	3.24330	C	-0.57870	2.79430	-2.22570
Si	3.48190	-3.48110	0.00740	C	-1.53650	2.26030	-2.99210
Si	0.43830	4.63490	-0.22760	H	-3.71850	2.19420	-3.40120
C	0.32550	-5.51360	2.82300	H	-4.29590	3.83390	-1.70520
C	0.74900	-4.27170	3.08290	H	-2.49460	4.90250	-0.30320
C	1.76330	-3.63820	2.21540	H	0.45010	2.51170	-2.40170
C	2.24930	-4.29490	1.14700	H	-1.27700	1.55890	-3.77350
C	1.79860	-5.68440	0.88530	C	0.74300	9.09260	-1.63680
C	0.88440	-6.25850	1.67710	C	1.45280	8.66890	-0.58450
H	-0.42180	-5.97660	3.45410	C	1.35440	7.26230	-0.14320
H	0.34190	-3.72320	3.92260	C	0.55140	6.40330	-0.79380
H	2.08270	-2.63240	2.44800	C	-0.22920	6.87740	-1.96290
H	2.21360	-6.24520	0.05760	C	-0.13730	8.15270	-2.36000
H	0.55560	-7.27090	1.48170	H	0.81420	10.12250	-1.96170
C	7.43000	-5.99840	-0.28440	H	2.10040	9.35500	-0.05420
C	6.46200	-6.38280	0.55500	H	1.93900	6.93760	0.70890
C	5.21320	-5.59890	0.65590	H	-0.86860	6.19900	-2.51100
C	5.03560	-4.50510	-0.10580	H	-0.70430	8.49740	-3.21520
C	6.12150	-4.07570	-1.02090	C	-0.36410	4.85400	4.39620
C	7.25320	-4.78550	-1.10680	C	-1.18890	5.46640	3.54050
H	8.34550	-6.57090	-0.35810	C	-0.92460	5.41030	2.08800
H	6.59200	-7.26770	1.16450	C	0.12570	4.71810	1.61210
H	4.46380	-5.91840	1.36510	C	1.06950	4.09360	2.57490
H	6.01330	-3.18120	-1.61790	C	0.82790	4.14690	3.89040
H	8.04390	-4.46850	-1.77450	H	-0.55810	4.89130	5.46030
C	1.88010	-2.94320	-4.37660	H	-2.05530	6.00000	3.90900
C	2.89530	-2.19450	-3.93350	H	-1.58630	5.94840	1.42590
C	3.40130	-2.37350	-2.55730	H	1.97470	3.61480	2.23380
C	2.83740	-3.27640	-1.73450	H	1.51820	3.69070	4.58820
C	1.72700	-4.11820	-2.24440	N	-1.48090	-1.97430	1.70350
C	1.26770	-3.95180	-3.49080	H	-0.52230	-1.49850	1.69280
H	1.50900	-2.81480	-5.38510	H	-0.89020	-3.02450	-1.26520
H	3.34760	-1.45450	-4.58080	C	-6.95210	-1.65260	4.19510
H	4.21730	-1.74670	-2.22220	H	-7.07230	-0.57060	4.28570
H	1.27640	-4.87410	-1.62270	C	-3.18460	-5.62500	-2.25090
H	0.45080	-4.56180	-3.85480	H	-3.90340	-6.34840	-1.85950

C	-4.14630	-2.45790	1.27570	C	-3.21070	-1.18380	-2.53350
H	-4.47440	-1.44170	0.51610	C	-4.25140	-1.76880	-3.27140
H	-5.10810	-2.96080	1.30950	C	-3.99800	-2.26920	-4.55010
O	-0.24050	0.09050	-0.75030	H	-2.54250	-2.59550	-6.11020
H	-2.39700	-0.37890	-0.87040	H	-0.68830	-1.56990	-4.78880
C	-3.50550	2.56920	2.70950	H	-1.10740	-0.68880	-2.52450
C	-4.77840	2.03080	2.60050	H	-5.24670	-1.85510	-2.86900
C	-5.08550	1.10620	1.59220	H	-4.81870	-2.71350	-5.10610
C	-4.10570	0.74010	0.62870	C	-8.33970	-0.12610	-2.16590
C	-2.82550	1.31810	0.76600	C	-7.48680	0.97860	-2.20330
C	-2.51960	2.20060	1.79040	C	-6.21780	0.90310	-1.63320
H	-3.28170	3.26650	3.51100	C	-5.77360	-0.28450	-1.03000
H	-5.56600	2.28560	3.30130	C	-6.63640	-1.39280	-0.99640
H	-2.02580	1.08820	0.06970	C	-7.91230	-1.30720	-1.55980
H	-1.50830	2.57730	1.86350	H	-9.33180	-0.06450	-2.60280
O	-6.35040	0.60920	1.65070	H	-7.81070	1.90430	-2.66890
H	-6.53420	0.02730	0.89850	H	-5.56880	1.76960	-1.64160
C	-2.72450	-2.20690	-5.11300	H	-6.29670	-2.33340	-0.57670
C	-1.68790	-1.63660	-4.37170	H	-8.56570	-2.17370	-1.52890
C	-1.91820	-1.13450	-3.09600				
C	-3.24730	1.69510	0.92240	C	0.11300	3.46440	0.73560
C	-5.70140	0.49490	0.19770	H	1.12420	4.50450	2.26790
C	-4.55770	-0.18290	0.01910	C	-1.71740	2.68770	2.76570
C	-3.25270	0.46560	0.34800	C	-0.60650	3.39010	3.07910
H	-6.65440	0.05660	-0.06220	C	-0.32080	3.73580	4.49050
C	-5.69240	1.86730	0.73100	C	-1.14990	3.33570	5.46100
C	-4.52540	2.45580	1.06840	C	-2.35290	2.54800	5.12880
C	-4.54330	3.86990	1.53990	C	-2.62330	2.23720	3.85570
C	-5.70120	4.52840	1.66440	H	0.56230	4.30990	4.74190
C	-6.97250	3.86360	1.32430	H	-0.93870	3.58520	6.49270
C	-6.96990	2.60390	0.87690	H	-3.01260	2.21620	5.92010
H	-3.62420	4.38970	1.77370	H	-3.50150	1.64520	3.63360
H	-5.70750	5.55550	2.00600	O	-2.09100	-0.26620	0.22990
H	-7.90600	4.40130	1.42950	P	-0.85210	0.35480	-0.70990
H	-7.90690	2.12510	0.62040	O	-1.13970	1.98180	-0.82200
C	0.31160	3.83450	2.01140	O	-0.93730	-0.25480	-2.08560
C	-1.97280	2.32200	1.34470	N	2.53840	-1.20440	1.23820
C	-1.03660	2.57760	0.40950	C	3.79400	-1.55830	0.79630

C	1.75800	-3.93920	-0.22130	H	-10.07830	-3.54610	-1.61160
C	0.64490	-3.21550	-0.61400	H	-8.57920	-3.24720	-3.49410
C	1.83960	-2.34320	-2.52920	H	-6.17870	-2.53380	-3.11700
C	2.99420	-3.00190	-2.14460	H	-6.95470	-2.44780	1.14620
C	-0.68530	-3.22600	0.06980	H	-9.23960	-3.13940	0.76600
H	-1.32390	-2.43160	-0.30830	C	-3.10370	-5.07150	2.43020
H	-1.17100	-4.19370	-0.07250	C	-3.05760	-3.76950	2.73350
C	1.62920	-1.55490	-3.78890	C	-3.53620	-2.76510	1.76110
H	1.56270	-2.23080	-4.64750	C	-3.99170	-3.15170	0.55600
H	0.70810	-0.97520	-3.70790	C	-4.06620	-4.59830	0.23840
H	2.47760	-0.89790	-3.97840	C	-3.63880	-5.50650	1.12440
C	4.17160	-3.04830	-3.03700	H	-2.75710	-5.80800	3.14320
C	1.78420	-4.95950	0.84280	H	-2.66920	-3.44820	3.69130
H	0.94220	-5.94220	3.22800	H	-3.50920	-1.72310	2.04500
H	-0.45940	-6.68990	2.40020	H	-4.47160	-4.92710	-0.71020
H	7.13310	-4.29020	-2.59910	H	-3.68990	-6.56150	0.88870
H	6.23200	-4.33880	-4.15200	C	0.49030	8.85320	0.24350
O	0.57080	-5.38140	1.25340	C	-0.55480	8.05240	0.00590
O	2.82340	-5.41830	1.30030	C	-0.34040	6.61520	-0.25980
O	4.24160	-2.58670	-4.16180	C	0.90420	6.10740	-0.28070
O	5.20460	-3.70530	-2.44950	C	2.05750	6.99750	0.00040
Si	-4.62660	-1.91560	-0.68090	C	1.85910	8.29890	0.24500
Si	1.15000	4.28730	-0.58200	H	0.33520	9.90620	0.43980
C	-2.21260	-1.83800	-4.70060	H	-1.55960	8.45470	0.00930
C	-3.04910	-0.83970	-4.39440	H	-1.20060	5.98110	-0.43810
C	-3.81500	-0.87680	-3.13080	H	3.06490	6.60690	0.02100
C	-3.67040	-1.90710	-2.27910	H	2.70090	8.94720	0.45130
C	-2.76380	-3.02400	-2.64030	C	-0.06780	3.23020	-4.98940
C	-2.06750	-2.98550	-3.78320	C	0.46730	2.29590	-4.19680
H	-1.64300	-1.80810	-5.62040	C	0.84640	2.63160	-2.80920
H	-3.15850	0.00240	-5.06530	C	0.64370	3.86800	-2.32720
H	-4.47970	-0.05400	-2.89880	C	0.07220	4.90650	-3.22150
H	-2.65490	-3.87740	-1.98980	C	-0.26950	4.60050	-4.47950
H	-1.39740	-3.79620	-4.03850	H	-0.34670	2.98640	-6.00630
C	-9.05410	-3.23750	-1.44720	H	0.62340	1.29370	-4.57130
C	-8.22650	-3.07220	-2.48590	H	1.26900	1.86090	-2.18280
C	-6.82770	-2.65160	-2.26040	H	-0.06730	5.92000	-2.87500
C	-6.38410	-2.42510	-1.01220	H	-0.68670	5.35920	-5.12900
C	-7.30370	-2.61820	0.13520	C	5.71130	3.31980	-0.14730
C	-8.56930	-3.00100	-0.07240	C	4.84620	2.82640	0.74600

C	3.39970	3.09860	0.60840	H	7.28290	-0.36770	-2.10080
C	2.95060	3.86080	-0.40350	H	2.58530	0.38240	-0.74990
C	3.91300	4.39310	-1.39810	H	3.51700	1.62920	-2.63780
C	5.22120	4.13750	-1.27470	O	6.60320	-1.85560	-0.25990
H	6.76960	3.11590	-0.04940	H	6.24400	-2.28820	0.52950
H	5.20500	2.22840	1.57170	C	0.60820	-1.62330	4.98300
H	2.72320	2.67520	1.33720	C	0.43090	-0.49010	4.18720
H	3.56110	4.99440	-2.22710	C	1.08860	-0.37200	2.96670
H	5.92200	4.52710	-2.00150	C	1.93720	-1.39900	2.51480
N	0.74270	-2.41430	-1.71420	C	2.09810	-2.54720	3.30370
H	-0.02070	-1.72020	-1.90590	C	1.44270	-2.64560	4.53210
H	-0.56030	-3.08350	1.14350	H	0.09650	-1.71190	5.93650
C	6.40640	-3.77920	-3.22950	H	-0.22330	0.31160	4.51660
H	6.75800	-2.77710	-3.48350	H	0.93060	0.49060	2.33160
C	0.57730	-6.37400	2.29270	H	2.71200	-3.36900	2.96270
H	1.21250	-7.21770	2.01640	H	1.58340	-3.53930	5.13380
C	3.04540	-3.64250	-0.83180	C	6.56960	-2.57430	3.96030
H	3.59150	-2.75210	0.00800	C	6.05640	-3.59210	3.15860
H	3.79810	-4.41760	-0.72030	C	5.14800	-3.29940	2.13620
O	0.41920	0.12650	0.08290	C	4.75510	-1.97360	1.90240
H	1.90210	-0.68140	0.61700	C	5.27150	-0.95520	2.72030
C	5.45850	0.72100	-2.50380	C	6.16890	-1.25400	3.74180
C	6.24750	-0.19440	-1.82750	H	7.27410	-2.80620	4.75330
C	5.72900	-0.94990	-0.76730	H	6.35010	-4.62340	3.32850
C	4.39020	-0.74500	-0.32300	H	4.72100	-4.10600	1.54980
C	3.61370	0.19210	-1.04050	H	4.95940	0.06910	2.55190
C	4.13200	0.90960	-2.11270	H	6.55740	-0.45460	4.36540
H	5.87400	1.28930	-3.33020				

C	-3.25200	1.69190	0.91810	C	-6.98020	3.85780	1.30400
C	-5.70290	0.48710	0.19070	C	-6.97530	2.59670	0.86060
C	-4.55790	-0.18950	0.01580	H	-3.63370	4.38810	1.76150
C	-3.25430	0.46180	0.34530	H	-5.71860	5.55300	1.98390
H	-6.65470	0.04670	-0.07000	H	-7.91440	4.39510	1.40460
C	-5.69680	1.86080	0.72050	H	-7.91100	2.11630	0.60280
C	-4.53120	2.45140	1.05940	C	0.29950	3.84000	2.01280
C	-4.55170	3.86680	1.52680	C	-1.97950	2.32110	1.34280
C	-5.71050	4.52480	1.64580	C	-1.04180	2.57770	0.40940

C	0.10470	3.46770	0.73700	Si	1.14340	4.29090	-0.57910
H	1.10990	4.51220	2.27040	C	-2.20810	-1.84730	-4.69910
C	-1.72840	2.68940	2.76390	C	-3.04290	-0.84780	-4.39230
C	-0.62020	3.39500	3.07900	C	-3.80960	-0.88490	-3.12920
C	-0.33900	3.74410	4.49040	C	-3.66710	-1.91620	-2.27830
C	-1.16960	3.34370	5.45950	C	-2.76300	-3.03470	-2.64060
C	-2.36970	2.55210	5.12560	C	-2.06600	-2.99630	-3.78310
C	-2.63590	2.23840	3.85230	H	-1.63780	-1.81740	-5.61840
H	0.54180	4.32110	4.74320	H	-3.15000	-0.00460	-5.06210
H	-0.96190	3.59580	6.49130	H	-4.47270	-0.06090	-2.89660
H	-3.03060	2.22020	5.91580	H	-2.65650	-3.88920	-1.99110
H	-3.51210	1.64390	3.62900	H	-1.39790	-3.80840	-4.03920
O	-2.09100	-0.26790	0.22970	C	-9.04720	-3.25930	-1.44300
P	-0.85190	0.35460	-0.70890	C	-8.22000	-3.09490	-2.48210
O	-1.14130	1.98120	-0.82210	C	-6.82230	-2.66980	-2.25760
O	-0.93540	-0.25490	-2.08480	C	-6.37960	-2.43820	-1.01010
N	2.54130	-1.20370	1.23930	C	-7.29890	-2.62990	0.13770
C	3.79720	-1.55650	0.79750	C	-8.56340	-3.01690	-0.06890
C	1.76220	-3.93630	-0.22570	H	-10.07050	-3.57150	-1.60650
C	0.64900	-3.21260	-0.61820	H	-8.57190	-3.27440	-3.48980
C	1.84490	-2.33640	-2.53080	H	-6.17340	-2.55290	-3.11450
C	2.99950	-2.99510	-2.14640	H	-6.95070	-2.45510	1.14820
C	-0.68170	-3.22470	0.06450	H	-9.23350	-3.15440	0.76980
H	-1.32110	-2.43120	-0.31430	C	-3.09270	-5.06820	2.43920
H	-1.16600	-4.19300	-0.07790	C	-3.04930	-3.76530	2.73890
C	1.63520	-1.54590	-3.78930	C	-3.53050	-2.76460	1.76390
H	1.57500	-2.21980	-4.64990	C	-3.98550	-3.15550	0.56000
H	0.71130	-0.97050	-3.70990	C	-4.05740	-4.60310	0.24660
H	2.48130	-0.88450	-3.97420	C	-3.62770	-5.50800	1.13490
C	4.17750	-3.03900	-3.03820	H	-2.74410	-5.80200	3.15400
C	1.78760	-4.95860	0.83640	H	-2.66110	-3.44050	3.69560
H	0.94220	-5.94690	3.21880	H	-3.50590	-1.72190	2.04530
H	-0.45740	-6.69360	2.38680	H	-4.46310	-4.93550	-0.70060
H	7.13790	-4.28470	-2.60310	H	-3.67700	-6.56370	0.90230
H	6.23790	-4.32540	-4.15680	C	0.47450	8.85670	0.23920
O	0.57380	-5.38160	1.24500	C	-0.56880	8.05390	0.00080
O	2.82630	-5.41840	1.29390	C	-0.35150	6.61660	-0.26240
O	4.24860	-2.57360	-4.16130	C	0.89390	6.11080	-0.28000
O	5.20980	-3.69850	-2.45220	C	2.04530	7.00320	0.00210
Si	-4.62320	-1.92390	-0.68000	C	1.84420	8.30470	0.24430

H	0.31730	9.90970	0.43360	O	0.41900	0.12770	0.08490
H	-1.57420	8.45450	0.00150	H	1.90520	-0.68050	0.61810
H	-1.21020	5.98090	-0.44180	C	5.46370	0.73170	-2.49520
H	3.05320	6.61430	0.02540	C	6.25200	-0.18660	-1.82190
H	2.68460	8.95470	0.45120	C	5.73260	-0.94530	-0.76440
C	-0.05740	3.23180	-4.99070	C	4.39390	-0.74080	-0.31970
C	0.47490	2.29780	-4.19580	C	3.61820	0.19900	-1.03440
C	0.84810	2.63380	-2.80660	C	4.13720	0.91980	-2.10410
C	0.64260	3.87010	-2.32560	H	5.88000	1.30260	-3.31950
C	0.07380	4.90810	-3.22230	H	7.28730	-0.35960	-2.09540
C	-0.26230	4.60190	-4.48160	H	2.58970	0.38910	-0.74350
H	-0.33160	2.98780	-6.00890	H	3.52260	1.64150	-2.62670
H	0.63350	1.29590	-4.56990	O	6.60590	-1.85350	-0.25980
H	1.26970	1.86350	-2.17880	H	6.24580	-2.28900	0.52760
H	-0.06780	5.92150	-2.87650	C	0.61210	-1.62110	4.98460
H	-0.67720	5.36030	-5.13290	C	0.43610	-0.48730	4.18930
C	5.70440	3.32880	-0.13040	C	1.09340	-0.36980	2.96860
C	4.83710	2.83370	0.75970	C	1.94020	-1.39800	2.51600
C	3.39070	3.10430	0.61760	C	2.09970	-2.54680	3.30420
C	2.94390	3.86670	-0.39520	C	1.44470	-2.64460	4.53290
C	3.90890	4.40080	-1.38640	H	0.10080	-1.70930	5.93830
C	5.21690	4.14670	-1.25890	H	-0.21680	0.31540	4.51930
H	6.76270	3.12610	-0.02920	H	0.93630	0.49330	2.33390
H	5.19370	2.23550	1.58620	H	2.71210	-3.36940	2.96240
H	2.71240	2.67960	1.34390	H	1.58420	-3.53870	5.13410
H	3.55890	5.00200	-2.21620	C	6.57380	-2.58290	3.95750
H	5.91970	4.53760	-1.98310	C	6.05690	-3.59840	3.15520
N	0.74730	-2.40950	-1.71690	C	5.14800	-3.30210	2.13440
H	-0.01680	-1.71560	-1.90820	C	4.75820	-1.97500	1.90250
H	-0.55780	-3.08170	1.13830	C	5.27840	-0.95890	2.72080
C	6.41210	-3.77020	-3.23170	C	6.17640	-1.26130	3.74080
H	6.76490	-2.76730	-3.48080	H	7.27880	-2.81750	4.74920
C	0.57930	-6.37660	2.28180	H	6.34820	-4.63060	3.32350
H	1.21560	-7.21920	2.00460	H	4.71840	-4.10700	1.54750
C	3.04990	-3.63800	-0.83470	H	4.96940	0.06660	2.55370
H	3.59510	-2.74910	0.00660	H	6.56800	-0.46360	4.36470
H	3.80280	-4.41310	-0.72420				



C	-3.22880	1.68340	0.94770	C	3.00590	-3.01020	-2.14190
C	-5.69670	0.50260	0.23850	C	-0.68950	-3.24570	0.04420
C	-4.55850	-0.17870	0.04040	H	-1.32510	-2.44890	-0.33430
C	-3.24650	0.45880	0.36290	H	-1.17290	-4.21250	-0.11350
H	-6.65450	0.07200	-0.01650	C	1.64660	-1.57030	-3.79760
C	-5.67510	1.86970	0.78430	H	1.57480	-2.24950	-4.65330
C	-4.50130	2.44980	1.11280	H	0.72870	-0.98480	-3.71910
C	-4.50690	3.86080	1.59420	H	2.49900	-0.91960	-3.99030
C	-5.66010	4.52360	1.73780	C	4.18880	-3.05740	-3.02720
C	-6.93850	3.86720	1.40840	C	1.78700	-4.95920	0.84650
C	-6.94720	2.61110	0.95110	H	0.92410	-5.93140	3.23240
H	-3.58290	4.37530	1.81960	H	-0.45470	-6.70410	2.38950
H	-5.65740	5.54830	2.08670	H	7.15470	-4.27840	-2.55850
H	-7.86810	4.40840	1.52890	H	6.26450	-4.34830	-4.11680
H	-7.88930	2.13860	0.70210	O	0.57350	-5.38770	1.24940
C	0.34320	3.81370	2.00850	O	2.82610	-5.40820	1.31370
C	-1.94720	2.30210	1.36080	O	4.26290	-2.60500	-4.15540
C	-1.02050	2.56020	0.41700	O	5.22180	-3.70360	-2.42780
C	0.13190	3.44640	0.73390	Si	-4.64250	-1.90060	-0.68280
H	1.15750	4.48430	2.25830	Si	1.15180	4.27500	-0.59320
C	-1.67850	2.66550	2.78000	C	-2.24530	-1.76550	-4.71050
C	-0.56480	3.36760	3.08410	C	-3.08020	-0.77160	-4.38630
C	-0.26760	3.71370	4.49300	C	-3.84190	-0.82770	-3.12100
C	-1.08970	3.31550	5.47020	C	-3.69500	-1.87100	-2.28560
C	-2.29610	2.52860	5.14800	C	-2.78920	-2.98200	-2.66580
C	-2.57610	2.21630	3.87730	C	-2.09720	-2.92670	-3.81070
H	0.61790	4.28720	4.73720	H	-1.67870	-1.72170	-5.63150
H	-0.87030	3.56560	6.50010	H	-3.19110	0.08100	-5.04360
H	-2.95000	2.19820	5.94470	H	-4.50490	-0.00780	-2.87390
H	-3.45620	1.62460	3.66250	H	-2.67710	-3.84420	-2.02740
O	-2.09110	-0.28020	0.22680	H	-1.42780	-3.73340	-4.08020
P	-0.85220	0.34150	-0.71200	C	-9.08280	-3.18400	-1.44170
O	-1.13740	1.96950	-0.81590	C	-8.26010	-3.00960	-2.48280
O	-0.93730	-0.26420	-2.08920	C	-6.85720	-2.60140	-2.25930
N	2.53540	-1.20350	1.23610	C	-6.40500	-2.39550	-1.01070
C	3.79230	-1.55510	0.79590	C	-7.31940	-2.59880	0.13910
C	1.76200	-3.94370	-0.22240	C	-8.58880	-2.97010	-0.06660
C	0.64800	-3.22710	-0.62530	H	-10.11010	-3.48350	-1.60460
C	1.85190	-2.35500	-2.53480	H	-8.61970	-3.16810	-3.49120

H	-6.21240	-2.47540	-3.11800	C	3.90280	4.38180	-1.44780
H	-6.96370	-2.44460	1.15040	C	5.21280	4.12840	-1.34170
H	-9.25540	-3.11540	0.77360	H	6.77950	3.11160	-0.13560
C	-3.11590	-5.10450	2.37640	H	5.23870	2.22480	1.50850
C	-3.06390	-3.80700	2.69750	H	2.75330	2.66920	1.30800
C	-3.54250	-2.78750	1.74090	H	3.53850	4.98020	-2.27350
C	-4.00450	-3.15590	0.53260	H	5.90300	4.51690	-2.07930
C	-4.08480	-4.59750	0.19490	N	0.75030	-2.42710	-1.72620
C	-3.65730	-5.51940	1.06670	H	-0.01320	-1.73450	-1.92070
H	-2.76960	-5.85190	3.07790	H	-0.57710	-3.11310	1.12040
H	-2.67090	-3.50020	3.65820	C	6.42920	-3.77830	-3.19900
H	-3.51110	-1.74970	2.03920	H	6.77670	-2.77670	-3.46060
H	-4.49500	-4.91170	-0.75660	C	0.57890	-6.37420	2.29470
H	-3.71300	-6.57090	0.81660	H	1.22990	-7.21030	2.03270
C	0.49550	8.83730	0.25430	C	3.05170	-3.64590	-0.82700
C	-0.55170	8.03460	0.03330	H	3.59470	-2.75100	0.01430
C	-0.33850	6.59860	-0.24010	H	3.80590	-4.41840	-0.70820
C	0.90670	6.09390	-0.28420	O	0.41980	0.10960	0.07870
C	2.06270	6.98620	-0.02160	H	1.89620	-0.68500	0.61360
C	1.86550	8.28650	0.22980	C	5.44790	0.70670	-2.52130
H	0.34140	9.88940	0.45620	C	6.24380	-0.19240	-1.83130
H	-1.55720	8.43430	0.05590	C	5.72910	-0.94100	-0.76440
H	-1.20020	5.96280	-0.40430	C	4.38660	-0.74490	-0.32720
H	3.07120	6.59810	-0.02040	C	3.60370	0.17670	-1.05760
H	2.70930	8.93640	0.42240	C	4.11850	0.88700	-2.13650
C	-0.13530	3.21990	-4.98110	H	5.86060	1.26920	-3.35310
C	0.42060	2.28770	-4.20050	H	7.28200	-0.35820	-2.09870
C	0.82400	2.62370	-2.81980	H	2.57250	0.36040	-0.77220
C	0.62230	3.85790	-2.33190	H	3.49810	1.59410	-2.67210
C	0.02810	4.89450	-3.21350	O	6.61090	-1.83190	-0.24390
C	-0.33550	4.58830	-4.46530	H	6.25290	-2.25970	0.54880
H	-0.43280	2.97580	-5.99270	C	0.60160	-1.63420	4.97770
H	0.57450	1.28660	-4.57900	C	0.42260	-0.50010	4.18370
H	1.26070	1.85400	-2.20180	C	1.08150	-0.37790	2.96440
H	-0.11170	5.90630	-2.86220	C	1.93360	-1.40160	2.51180
H	-0.76980	5.34540	-5.10530	C	2.09710	-2.55040	3.29930
C	5.71970	3.31440	-0.21900	C	1.44000	-2.65300	4.52650
C	4.86770	2.82160	0.68720	H	0.08850	-1.72580	5.93020
C	3.41910	3.09170	0.56890	H	-0.23400	0.29910	4.51400
C	2.95500	3.85070	-0.43860	H	0.92260	0.48560	2.33080

H	2.71400	-3.36980	2.95810	C	6.14810	-1.21420	3.75160
H	1.58270	-3.54730	5.12690	H	7.25970	-2.75090	4.77950
C	6.55880	-2.52980	3.98020	H	6.36210	-4.58420	3.35880
C	6.06030	-3.55660	3.18080	H	4.73950	-4.09100	1.56600
C	5.15600	-3.27780	2.15080	H	4.93370	0.09120	2.54690
C	4.75290	-1.95700	1.90730	H	6.52510	-0.40790	4.37350
C	5.25470	-0.92920	2.72280				
C	-3.38860	1.43220	0.90970	P	-0.89130	0.29930	-0.72270
C	-5.73150	0.01440	0.21390	O	-1.31630	1.89640	-0.84240
C	-4.53360	-0.56220	0.03470	O	-0.92630	-0.32220	-2.09540
C	-3.28840	0.20290	0.34500	N	2.59910	-0.98150	1.21420
H	-6.64380	-0.50960	-0.03310	C	3.88280	-1.22820	0.78510
C	-5.83990	1.38830	0.73210	C	2.07130	-3.79020	-0.24900
C	-4.72710	2.07970	1.05680	C	0.90480	-3.14580	-0.62990
C	-4.86520	3.49120	1.51560	C	2.01830	-2.16270	-2.53720
C	-6.07530	4.04800	1.64040	C	3.22340	-2.72860	-2.15980
C	-7.28570	3.27180	1.31380	C	-0.40970	-3.28640	0.06310
C	-7.17590	2.01260	0.87860	H	-1.12580	-2.55690	-0.30730
H	-3.99330	4.09070	1.73960	H	-0.79300	-4.30060	-0.06830
H	-6.16910	5.07400	1.97240	C	1.74170	-1.38640	-3.79120
H	-8.26180	3.72750	1.41940	H	1.75280	-2.05580	-4.65720
H	-8.06890	1.45160	0.63230	H	0.76680	-0.90250	-3.71350
C	-0.02870	3.87640	1.98330	H	2.52180	-0.64520	-3.96440
C	-2.17320	2.16910	1.32550	C	4.40350	-2.65560	-3.04560
C	-1.26670	2.50480	0.38660	C	2.03960	-4.84760	0.77680
C	-0.20220	3.49300	0.70770	H	2.79400	-7.24340	1.62280
H	0.72170	4.61650	2.23660	H	4.39450	-6.62270	2.14120
C	-1.94540	2.55590	2.74560	H	7.46990	-3.61290	-2.60650
C	-0.89820	3.35150	3.05490	H	6.58750	-3.70750	-4.16820
C	-0.63720	3.71990	4.46530	O	3.29730	-5.29010	1.08370
C	-1.42410	3.24880	5.43900	O	1.05110	-5.32580	1.30140
C	-2.55590	2.36010	5.11130	O	4.43780	-2.17420	-4.16350
C	-2.80410	2.02800	3.83900	O	5.49280	-3.21920	-2.45910
H	0.19370	4.36850	4.71330	Si	-4.45380	-2.30410	-0.63960
H	-1.23090	3.51510	6.47010	Si	0.73950	4.41520	-0.61270
H	-3.18080	1.97180	5.90520	C	-2.08360	-2.06110	-4.67910
H	-3.62870	1.36230	3.62020	C	-2.99580	-1.13150	-4.37300
O	-2.06660	-0.42320	0.22370	C	-3.74810	-1.22200	-3.10390

C	-3.51550	-2.23180	-2.24710	H	-2.45980	8.17420	0.09340
C	-2.52630	-3.27570	-2.60940	C	-0.41740	3.29200	-5.02000
C	-1.84190	-3.18810	-3.75670	C	-0.73550	4.49860	-4.53880
H	-1.52390	-1.99120	-5.60270	C	-0.38370	4.85910	-3.14940
H	-3.17640	-0.30480	-5.04770	C	0.23950	3.97140	-2.35400
H	-4.47430	-0.45290	-2.87170	C	0.59740	2.64170	-2.90030
H	-2.34680	-4.11480	-1.95590	C	0.28550	2.31980	-4.16140
H	-1.11160	-3.94490	-4.01260	H	-0.67220	3.02700	-6.03790
C	-8.75070	-4.02930	-1.34320	H	-1.24740	5.21580	-5.16730
C	-7.94960	-3.80770	-2.39210	H	-0.63130	5.85090	-2.80140
C	-6.59250	-3.25950	-2.18630	H	1.09790	1.91890	-2.27440
C	-6.16110	-2.97390	-0.94610	H	0.54560	1.34780	-4.55620
C	-7.05060	-3.22930	0.21280	C	5.36300	3.81150	-0.16470
C	-8.27840	-3.72730	0.02310	C	4.87170	4.51410	-1.19180
H	-9.74430	-4.43140	-1.49300	C	3.41140	4.68120	-1.34310
H	-8.29300	-4.03050	-3.39400	C	2.57020	4.12920	-0.45230
H	-5.96340	-3.09770	-3.05070	C	3.12010	3.32540	0.66760
H	-6.71050	-3.01130	1.21760	C	4.44470	3.18800	0.80860
H	-8.92700	-3.91090	0.86980	H	6.43220	3.68660	-0.05270
C	-2.59040	-5.25640	2.48710	H	5.54230	4.96420	-1.91210
C	-2.66710	-3.95210	2.77440	H	3.03400	5.27100	-2.16950
C	-3.26020	-3.01270	1.79990	H	2.46260	2.83970	1.37490
C	-3.69750	-3.45830	0.60840	H	4.84690	2.60890	1.62780
C	-3.64340	-4.91040	0.31300	N	0.93350	-2.32700	-1.71940
C	-3.11260	-5.76040	1.20090	H	0.11180	-1.70150	-1.90800
H	-2.15240	-5.94490	3.19800	H	-0.28410	-3.14340	1.13710
H	-2.28920	-3.58020	3.71810	C	6.70110	-3.15820	-3.23020
H	-3.32530	-1.96860	2.06920	H	6.95620	-2.12050	-3.45500
H	-4.03660	-5.29080	-0.62140	C	3.33880	-6.38210	2.01630
H	-3.06910	-6.81900	0.98060	H	2.89350	-6.09310	2.97110
C	-0.36140	8.88110	0.28950	C	3.33030	-3.37670	-0.85130
C	0.92580	8.51750	0.24660	H	3.79100	-2.44030	-0.01200
C	1.29150	7.11500	-0.04340	H	4.15220	-4.07930	-0.75960
C	0.33380	6.20240	-0.28090	O	0.39890	0.18810	0.06570
C	-1.09150	6.60970	-0.21790	H	1.92560	-0.50370	0.59390
C	-1.41940	7.87940	0.04950	C	5.38060	1.19830	-2.49070
H	-0.62980	9.90750	0.50340	C	6.24260	0.36330	-1.79980
H	1.70260	9.24920	0.42710	C	5.78240	-0.43710	-0.74570
H	2.33800	6.84710	-0.05020	C	4.42310	-0.36330	-0.32370
H	-1.87350	5.87960	-0.38740	C	3.57260	0.49690	-1.05450

C	4.03690	1.26110	-2.11900	H	0.87380	0.57570	2.33680
H	5.75290	1.80310	-3.31180	H	2.90360	-3.17000	2.87650
H	7.29440	0.29070	-2.05510	H	1.74920	-3.49290	5.02110
H	2.52690	0.59160	-0.77870	C	6.67030	-2.04750	3.99730
H	3.36500	1.92110	-2.65250	C	6.12050	-0.77580	3.81930
O	6.73470	-1.25110	-0.22150	C	5.22300	-0.53920	2.78160
H	6.41000	-1.71120	0.56670	C	4.85520	-1.57280	1.90520
C	0.66100	-1.63600	4.91880	C	5.39940	-2.85070	2.09820
C	0.41960	-0.49140	4.15670	C	6.30730	-3.08160	3.13670
C	1.08160	-0.29280	2.94910	H	7.37460	-2.22940	4.80330
C	2.00080	-1.24790	2.47940	H	6.39290	0.03500	4.48810
C	2.22870	-2.40540	3.23580	H	4.79350	0.44700	2.64730
C	1.56610	-2.58740	4.45000	H	5.10050	-3.66890	1.45260
H	0.14150	-1.79040	5.85950	H	6.72320	-4.07550	3.27170
H	-0.29080	0.25430	4.50110				
C	-3.38600	1.40040	0.95270	C	-0.60980	3.73210	4.46220
C	-5.72890	-0.02220	0.26400	C	-1.38030	3.26000	5.44850
C	-4.53050	-0.59280	0.07090	C	-2.50730	2.35810	5.14050
C	-3.28590	0.17280	0.38300	C	-2.76740	2.01480	3.87360
H	-6.64110	-0.54620	0.01650	H	0.21780	4.39010	4.69590
C	-5.83890	1.34670	0.79470	H	-1.17710	3.53490	6.47540
C	-4.72630	2.04140	1.11360	H	-3.11870	1.96920	5.94450
C	-4.86750	3.45040	1.57990	H	-3.58810	1.33980	3.66900
C	-6.07920	4.00030	1.71870	O	-2.06380	-0.45040	0.25260
C	-7.28860	3.21970	1.39990	P	-0.89570	0.27670	-0.69840
C	-7.17650	1.96340	0.95680	O	-1.33610	1.86870	-0.82430
H	-3.99710	4.05400	1.79760	O	-0.92820	-0.35010	-2.06870
H	-6.17510	5.02440	2.05600	N	2.62930	-0.94980	1.21530
H	-8.26600	3.66970	1.51690	C	3.90780	-1.19370	0.76920
H	-8.06890	1.39920	0.71580	C	2.09210	-3.77720	-0.20550
C	-0.03320	3.87850	1.97180	C	0.91880	-3.14740	-0.58990
C	-2.16960	2.14610	1.35180	C	2.01430	-2.18540	-2.51840
C	-1.27780	2.48500	0.40010	C	3.22390	-2.74320	-2.14360
C	-0.21890	3.48500	0.70110	C	-0.39350	-3.29170	0.10690
H	0.71260	4.62800	2.21040	H	-1.11580	-2.57110	-0.26900
C	-1.92730	2.54370	2.76650	H	-0.77020	-4.30950	-0.01730
C	-0.88420	3.35180	3.05760	C	1.72490	-1.42530	-3.77950

H	1.71340	-2.10810	-4.63500	C	-3.69740	-3.50010	0.59720
H	0.75590	-0.93100	-3.69270	C	-3.64220	-4.94650	0.27530
H	2.50900	-0.69480	-3.97740	C	-3.11750	-5.81300	1.15070
C	4.39460	-2.68460	-3.04280	H	-2.17040	-6.03480	3.15020
C	2.07370	-4.81640	0.83920	H	-2.30710	-3.67950	3.71180
H	2.85180	-7.19080	1.72520	H	-3.33000	-2.03630	2.08460
H	4.44870	-6.54680	2.22590	H	-4.02950	-5.30930	-0.66850
H	7.46930	-3.61990	-2.61540	H	-3.07330	-6.86750	0.91130
H	6.57040	-3.75400	-4.16480	C	-0.43510	8.86910	0.24270
O	3.33630	-5.24380	1.14780	C	0.85470	8.51800	0.17890
O	1.09150	-5.29230	1.37760	C	1.22910	7.11670	-0.10540
O	4.41530	-2.22770	-4.17130	C	0.27640	6.19260	-0.31660
O	5.49210	-3.23140	-2.45560	C	-1.15150	6.58610	-0.23080
Si	-4.45030	-2.32420	-0.63140	C	-1.48720	7.85490	0.03130
Si	0.69420	4.40680	-0.64000	H	-0.70980	9.89480	0.45250
C	-2.08060	-2.02950	-4.66750	H	1.62730	9.25900	0.33830
C	-3.00410	-1.11270	-4.35670	H	2.27800	6.85910	-0.13000
C	-3.75470	-1.21850	-3.08780	H	-1.92910	5.84680	-0.37930
C	-3.50920	-2.22930	-2.23580	H	-2.52960	8.13970	0.09190
C	-2.50370	-3.25670	-2.60100	C	-0.52590	3.23250	-5.01720
C	-1.82230	-3.15620	-3.74920	C	-0.85200	4.43850	-4.54000
H	-1.52250	-1.94860	-5.59120	C	-0.47960	4.81560	-3.16030
H	-3.19580	-0.28560	-5.02790	C	0.17090	3.94340	-2.36960
H	-4.49170	-0.46080	-2.85230	C	0.53790	2.61450	-2.91200
H	-2.30930	-4.09370	-1.94890	C	0.20680	2.27750	-4.16430
H	-1.08060	-3.90090	-4.00740	H	-0.79630	2.95520	-6.02790
C	-8.74600	-4.03890	-1.37100	H	-1.38590	5.14310	-5.16440
C	-7.94380	-3.79830	-2.41480	H	-0.73550	5.80630	-2.81530
C	-6.58720	-3.25330	-2.19760	H	1.05940	1.90370	-2.28950
C	-6.15750	-2.98890	-0.95200	H	0.47270	1.30550	-4.55570
C	-7.04820	-3.26570	0.20100	C	5.33010	3.84940	-0.26870
C	-8.27550	-3.76110	0.00100	C	4.81390	4.53420	-1.29550
H	-9.73920	-4.43880	-1.52920	C	3.34970	4.68740	-1.42160
H	-8.28580	-4.00350	-3.42090	C	2.52990	4.13980	-0.50840
H	-5.95720	-3.07670	-3.05830	C	3.10710	3.35600	0.61170
H	-6.70940	-3.06570	1.21000	C	4.43520	3.23170	0.72990
H	-8.92500	-3.96040	0.84350	H	6.40210	3.73470	-0.17510
C	-2.60290	-5.33290	2.44910	H	5.46710	4.98010	-2.03410
C	-2.67940	-4.03370	2.75910	H	2.95210	5.26300	-2.24850
C	-3.26530	-3.07600	1.79820	H	2.46690	2.87500	1.33780

H	4.85760	2.66810	1.54970	H	6.43150	-1.67030	0.51250
N	0.93650	-2.34300	-1.69030	C	0.78300	-1.52490	4.97910
H	0.11150	-1.72160	-1.87960	C	0.52270	-0.39630	4.19950
H	-0.26870	-3.13950	1.17960	C	1.15320	-0.22410	2.97120
C	6.69180	-3.18290	-3.24090	C	2.05940	-1.19000	2.49870
H	6.93980	-2.14960	-3.49230	C	2.30460	-2.33250	3.27220
C	3.39050	-6.31770	2.10050	C	1.67370	-2.48800	4.50680
H	2.94610	-6.01460	3.05140	H	0.28870	-1.65800	5.93650
C	3.34450	-3.36930	-0.82570	H	-0.17730	0.35750	4.54700
H	3.81120	-2.41850	-0.00690	H	0.93100	0.63190	2.34640
H	4.16900	-4.06830	-0.73020	H	2.96890	-3.10540	2.91080
O	0.39700	0.17870	0.08750	H	1.87060	-3.38160	5.09190
H	1.94090	-0.48930	0.59800	C	6.75460	-1.94670	3.94560
C	5.33840	1.19940	-2.56030	C	6.19850	-0.67970	3.75420
C	6.21540	0.37530	-1.87530	C	5.28220	-0.46410	2.72850
C	5.77660	-0.41450	-0.80430	C	4.90130	-1.51430	1.87780
C	4.42420	-0.34150	-0.36050	C	5.45230	-2.78720	2.08420
C	3.55780	0.50690	-1.08600	C	6.37910	-2.99710	3.11050
C	4.00090	1.26130	-2.16640	H	7.47350	-2.11230	4.74210
H	5.69410	1.79670	-3.39410	H	6.48060	0.14380	4.40300
H	7.26290	0.30390	-2.14800	H	4.84800	0.51850	2.58390
H	2.51640	0.59980	-0.79340	H	5.14390	-3.61780	1.45930
H	3.31780	1.91310	-2.69560	H	6.79980	-3.98740	3.25610
O	6.74110	-1.21800	-0.28630				
C	-3.26800	1.62590	0.96750	H	-7.93560	1.99660	0.70910
C	-5.71270	0.40110	0.25040	C	0.26470	3.83780	1.99550
C	-4.56250	-0.26140	0.05790	C	-1.99690	2.27270	1.37180
C	-3.26320	0.39800	0.38880	C	-1.07830	2.54010	0.42280
H	-6.66190	-0.04510	-0.00980	C	0.05570	3.45390	0.72540
C	-5.71690	1.76820	0.79660	H	1.06530	4.52820	2.23510
C	-4.55460	2.36970	1.12770	C	-1.72860	2.65270	2.78660
C	-4.58740	3.78110	1.60720	C	-0.62850	3.38080	3.07950
C	-5.75290	4.42300	1.74720	C	-0.33090	3.74260	4.48440
C	-7.01830	3.74290	1.41570	C	-1.13790	3.33180	5.46900
C	-7.00280	2.48650	0.95970	C	-2.32810	2.51590	5.15900
H	-3.67360	4.31300	1.83380	C	-2.60920	2.19030	3.89190
H	-5.76980	5.44800	2.09450	H	0.54320	4.33690	4.71970
H	-7.95790	4.26700	1.53370	H	-0.91780	3.59280	6.49600

H	-2.96950	2.17560	5.96170	H	-2.58490	-3.89120	-1.96810
H	-3.47750	1.57830	3.68570	H	-1.33090	-3.78190	-4.01780
O	-2.09520	-0.32240	0.26360	C	-9.02830	-3.33400	-1.47540
P	-0.86510	0.31210	-0.67810	C	-8.19760	-3.14630	-2.50770
O	-1.18400	1.93210	-0.80210	C	-6.80370	-2.71620	-2.26960
O	-0.93920	-0.30670	-2.05050	C	-6.36780	-2.50290	-1.01620
N	2.60830	-1.13800	1.24020	C	-7.29090	-2.72120	0.12380
C	3.85630	-1.48010	0.76880	C	-8.55200	-3.11270	-0.09510
C	1.82130	-3.90380	-0.15140	H	-10.04890	-3.64990	-1.64890
C	0.69120	-3.21170	-0.55250	H	-8.54400	-3.31050	-3.51990
C	1.85100	-2.36760	-2.50260	H	-6.15200	-2.58140	-3.12150
C	3.01710	-3.00740	-2.12100	H	-6.94830	-2.56220	1.13880
C	-0.63780	-3.23630	0.13430	H	-9.22480	-3.26930	0.73800
H	-1.29700	-2.47000	-0.26550	C	-3.09370	-5.18170	2.39720
H	-1.10010	-4.21930	0.01770	C	-3.05630	-3.88460	2.72240
C	1.61680	-1.60420	-3.77350	C	-3.53190	-2.86630	1.76300
H	2.46160	-0.95160	-3.99180	C	-3.97680	-3.23550	0.54870
H	1.53240	-2.29660	-4.61730	C	-4.03900	-4.67670	0.20540
H	0.69760	-1.02220	-3.68600	C	-3.61440	-5.59740	1.07950
C	4.18040	-3.06710	-3.03060	H	-2.75090	-5.92860	3.10110
C	1.88110	-4.88520	0.94750	H	-2.67850	-3.57760	3.68910
H	1.14830	-5.77500	3.38840	H	-3.51280	-1.82870	2.06360
H	-0.30740	-6.53040	2.66800	H	-4.43380	-4.99150	-0.75250
H	7.15860	-4.27480	-2.60820	H	-3.65760	-6.64850	0.82540
H	6.23180	-4.36910	-4.14370	C	0.28830	8.84540	0.18170
O	0.68260	-5.29210	1.41310	C	-0.74050	8.01510	-0.02360
O	2.93520	-5.32310	1.39150	C	-0.49420	6.58170	-0.28200
O	4.22780	-2.63800	-4.16930	C	0.76250	6.10660	-0.32750
O	5.22920	-3.69700	-2.44120	C	1.89830	7.02940	-0.08300
Si	-4.61550	-1.98400	-0.66920	C	1.67110	8.32750	0.15470
Si	1.04890	4.29090	-0.61690	H	0.10990	9.89560	0.37270
C	-2.18990	-1.84240	-4.67970	H	-1.75530	8.39070	0.00070
C	-3.04670	-0.86190	-4.37230	H	-1.34130	5.92350	-0.43390
C	-3.81480	-0.91830	-3.11070	H	2.91580	6.66550	-0.08450
C	-3.65130	-1.94800	-2.26180	H	2.50010	8.99990	0.33400
C	-2.71660	-3.04240	-2.62090	C	-0.22760	3.15990	-4.98930
C	-2.02090	-2.98780	-3.76360	C	0.34800	2.24780	-4.19920
H	-1.61910	-1.79840	-5.59820	C	0.74650	2.60750	-2.82300
H	-3.17180	-0.02030	-5.04120	C	0.52070	3.84280	-2.34850
H	-4.49810	-0.11080	-2.87850	C	-0.09620	4.85700	-3.24040



C	-0.45500	4.52950	-4.48820	C	4.40660	-0.67900	-0.38210
H	-0.52100	2.89860	-5.99780	C	3.59690	0.23850	-1.08790
H	0.52220	1.24600	-4.56680	C	4.07440	0.95030	-2.18260
H	1.20040	1.85400	-2.19750	H	5.77480	1.33670	-3.45560
H	-0.25600	5.86960	-2.90010	H	7.24010	-0.28850	-2.25030
H	-0.90550	5.27050	-5.13600	H	2.57430	0.41730	-0.77020
C	5.63780	3.42440	-0.27330	H	3.43580	1.65620	-2.69770
C	4.80380	2.92710	0.64690	O	6.63610	-1.75820	-0.36870
C	3.34930	3.16820	0.53940	H	6.30500	-2.18740	0.43480
C	2.86190	3.90830	-0.47120	C	0.83190	-1.45960	5.06900
C	3.79030	4.44710	-1.49420	C	0.60410	-0.35710	4.24340
C	5.10560	4.21760	-1.39910	C	1.20950	-0.27150	2.99360
H	6.70200	3.24300	-0.19730	C	2.05510	-1.30130	2.54270
H	5.19360	2.34920	1.47260	C	2.26390	-2.42080	3.36070
H	2.69820	2.74040	1.28850	C	1.66130	-2.48600	4.61810
H	3.40730	5.03070	-2.32210	H	0.36240	-1.52170	6.04600
H	5.78140	4.61110	-2.14710	H	-0.04800	0.44610	4.57300
N	0.76580	-2.43490	-1.67220	H	1.01330	0.56690	2.33680
H	-0.00780	-1.75220	-1.86690	H	2.87380	-3.24590	3.02050
H	-0.51760	-3.06090	1.20360	H	1.83940	-3.35670	5.24300
C	6.41830	-3.78450	-3.23920	C	6.74890	-2.39750	3.85760
H	6.75990	-2.78760	-3.52510	C	6.22170	-3.43720	3.09410
C	0.72730	-6.23910	2.49320	C	5.27550	-3.17580	2.09780
H	1.33270	-7.10600	2.22160	C	4.85810	-1.85970	1.85130
C	3.09560	-3.61110	-0.79240	C	5.38910	-0.81930	2.63100
H	3.64850	-2.69460	0.01060	C	6.32430	-1.08670	3.62700
H	3.85650	-4.37690	-0.67290	H	7.48300	-2.60480	4.63030
O	0.40980	0.10940	0.11590	H	6.53410	-4.46130	3.27400
H	1.94290	-0.64660	0.62430	H	4.83880	-3.99890	1.54260
C	5.39120	0.77340	-2.61050	H	5.05840	0.19750	2.45360
C	6.21130	-0.12440	-1.94790	H	6.72350	-0.27030	4.22110
C	5.73460	-0.87210	-0.86280				
C	-3.40830	1.37680	0.93570	H	-6.63810	-0.60830	-0.00640
C	-5.73270	-0.07330	0.24240	C	-5.85940	1.29820	0.76260
C	-4.52750	-0.63350	0.06080	C	-4.75580	2.00550	1.08450
C	-3.29240	0.14730	0.37360	C	-4.91350	3.41580	1.54140

C	-6.13130	3.95500	1.66850	C	2.10960	-4.78770	0.86400
C	-7.33110	3.16090	1.34600	H	2.88990	-7.15690	1.76050
C	-7.20390	1.90310	0.91160	H	4.49200	-6.51300	2.24450
H	-4.05030	4.02880	1.76170	H	7.48570	-3.61620	-2.62550
H	-6.23920	4.98010	1.99910	H	6.57840	-3.75590	-4.16940
H	-8.31340	3.60240	1.45350	O	3.37390	-5.21480	1.16640
H	-8.08920	1.32890	0.66790	O	1.13110	-5.25870	1.41320
C	-0.08680	3.89130	1.96680	O	4.42650	-2.22590	-4.17260
C	-2.20180	2.13560	1.33970	O	5.51020	-3.22240	-2.45720
C	-1.30690	2.47900	0.39270	Si	-4.42630	-2.37030	-0.62510
C	-0.26070	3.49120	0.69640	Si	0.64960	4.41800	-0.64290
H	0.64980	4.64940	2.20720	C	-2.05060	-2.08150	-4.65810
C	-1.97270	2.54080	2.75440	C	-2.98660	-1.17400	-4.35760
C	-0.93960	3.36030	3.04920	C	-3.73910	-1.27840	-3.08980
C	-0.67860	3.74900	4.45410	C	-3.48300	-2.27850	-2.22840
C	-1.45100	3.27290	5.43710	C	-2.46350	-3.29620	-2.58210
C	-2.56640	2.35810	5.12520	C	-1.78050	-3.19690	-3.72930
C	-2.81460	2.00740	3.85790	H	-1.49120	-2.00150	-5.58110
H	0.14050	4.41660	4.69070	H	-3.18730	-0.35540	-5.03650
H	-1.25780	3.55420	6.46410	H	-4.48640	-0.52810	-2.86280
H	-3.17930	1.96610	5.92650	H	-2.26010	-4.12480	-1.92210
H	-3.62700	1.32330	3.65040	H	-1.02850	-3.93420	-3.97920
O	-2.06280	-0.46340	0.25380	C	-8.70080	-4.14150	-1.35440
P	-0.89770	0.27040	-0.69650	C	-7.89870	-3.90430	-2.39920
O	-1.35120	1.85800	-0.82980	C	-6.54880	-3.34150	-2.18540
O	-0.92290	-0.36050	-2.06530	C	-6.12520	-3.05750	-0.94200
N	2.65000	-0.92310	1.21530	C	-7.01560	-3.33060	0.21210
C	3.92820	-1.16150	0.76610	C	-8.23680	-3.84200	0.01520
C	2.12160	-3.75590	-0.18800	H	-9.68900	-4.55440	-1.51020
C	0.94530	-3.13200	-0.57290	H	-8.23600	-4.12550	-3.40360
C	2.03190	-2.17810	-2.51060	H	-5.91860	-3.16830	-3.04660
C	3.24400	-2.73080	-2.13700	H	-6.68160	-3.11470	1.21950
C	-0.36400	-3.27610	0.12930	H	-8.88610	-4.03850	0.85850
H	-1.09340	-2.56780	-0.25550	C	-2.55110	-5.32900	2.48690
H	-0.73170	-4.29900	0.02270	C	-2.64540	-4.02840	2.78570
C	1.73660	-1.42500	-3.77470	C	-3.24060	-3.08650	1.81490
H	1.72710	-2.11150	-4.62730	C	-3.66300	-3.52630	0.61610
H	0.76560	-0.93480	-3.68850	C	-3.58840	-4.97460	0.30680
H	2.51710	-0.69170	-3.97700	C	-3.05540	-5.82670	1.19120
C	4.41050	-2.67720	-3.04170	H	-2.11170	-6.01920	3.19540

H	-2.28090	-3.66130	3.73650	C	6.70580	-3.18040	-3.24900
H	-3.32000	-2.04540	2.09240	H	6.95500	-2.14900	-3.50700
H	-3.96790	-5.35030	-0.63520	C	3.43330	-6.28240	2.12580
H	-2.99680	-6.88250	0.96090	H	2.99690	-5.97210	3.07810
C	-0.52740	8.87120	0.22370	C	3.37090	-3.34790	-0.81510
C	0.76610	8.53290	0.16480	H	3.83500	-2.39170	-0.00570
C	1.15550	7.13470	-0.11480	H	4.19750	-4.04430	-0.71850
C	0.21280	6.20050	-0.32670	O	0.39390	0.18420	0.09270
C	-1.21920	6.57990	-0.24650	H	1.95680	-0.47210	0.59680
C	-1.56850	7.84590	0.01150	C	5.33660	1.23370	-2.57040
H	-0.81320	9.89450	0.43020	C	6.21670	0.40410	-1.89590
H	1.53070	9.28200	0.32490	C	5.78430	-0.38700	-0.82330
H	2.20700	6.88750	-0.13520	C	4.43590	-0.31100	-0.36830
H	-1.98890	5.83240	-0.39540	C	3.56580	0.54160	-1.08420
H	-2.61390	8.12030	0.06820	C	4.00240	1.29830	-2.16550
C	-0.53910	3.21640	-5.02110	H	5.68740	1.83250	-3.40520
C	-0.88320	4.41920	-4.54810	H	7.26150	0.32990	-2.17800
C	-0.52070	4.80480	-3.16810	H	2.52690	0.63570	-0.78330
C	0.13870	3.94350	-2.37300	H	3.31680	1.95390	-2.68690
C	0.52540	2.61830	-2.91050	O	6.75000	-1.19490	-0.31440
C	0.20340	2.27370	-4.16310	H	6.44550	-1.64720	0.48640
H	-0.80220	2.93300	-6.03190	C	0.83420	-1.44920	5.00080
H	-1.42450	5.11490	-5.17620	C	0.56690	-0.33100	4.20870
H	-0.79140	5.79280	-2.82650	C	1.18710	-0.17500	2.97300
H	1.05430	1.91610	-2.28430	C	2.08940	-1.14710	2.50600
H	0.48400	1.30440	-4.55100	C	2.34070	-2.27990	3.29150
C	5.28810	3.89730	-0.25310	C	1.72050	-2.41900	4.53350
C	4.77060	4.57680	-1.28290	H	0.34840	-1.56950	5.96420
C	3.30580	4.71970	-1.41410	H	-0.13030	0.42740	4.55210
C	2.48680	4.16780	-0.50270	H	0.95920	0.67250	2.33860
C	3.06570	3.39060	0.62100	H	3.00160	-3.05760	2.93410
C	4.39410	3.27610	0.74410	H	1.92200	-3.30490	5.12850
H	6.36060	3.79020	-0.15560	C	6.79930	-1.89910	3.92480
H	5.42320	5.02560	-2.02020	C	6.24580	-0.63180	3.72840
H	2.90690	5.29020	-2.24380	C	5.32140	-0.42070	2.70900
H	2.42640	2.90750	1.34660	C	4.92930	-1.47590	1.86970
H	4.81750	2.71860	1.56740	C	5.47790	-2.74910	2.08120
N	0.95720	-2.33430	-1.67820	C	6.41290	-2.95440	3.10090
H	0.12850	-1.71810	-1.86960	H	7.52470	-2.06120	4.71610
H	-0.23780	-3.10550	1.19920	H	6.53660	0.19570	4.36830

H	4.89020	0.56240	2.56050	H	6.83160	-3.94510	3.25020
H	5.16160	-3.58350	1.46560				
C	-3.33770	1.50450	0.94410				
C	-5.71740	0.14740	0.25050	C	3.88130	-1.32820	0.81270
C	-4.53550	-0.46180	0.07370	C	1.98060	-3.85260	-0.14550
C	-3.27040	0.27040	0.38420	C	0.83520	-3.18120	-0.54240
H	-6.64320	-0.35140	0.00240	C	1.98150	-2.26390	-2.46820
C	-5.78950	1.52450	0.76610	C	3.16280	-2.87010	-2.08230
C	-4.65890	2.18740	1.08910	C	-0.48620	-3.27340	0.14550
C	-4.76040	3.60390	1.54250	H	-1.18240	-2.53480	-0.24390
C	-5.95550	4.19250	1.66480	H	-0.89390	-4.28030	0.03280
C	-7.18570	3.44710	1.34080	C	1.71230	-1.48630	-3.72630
C	-7.10870	2.18400	0.91000	H	1.69300	-2.15790	-4.59020
H	-3.87350	4.18180	1.76400	H	0.75060	-0.97770	-3.64080
H	-6.02260	5.22190	1.99270	H	2.50180	-0.75630	-3.90350
H	-8.14960	3.92840	1.44430	C	4.40470	-2.95130	-2.88220
H	-8.01590	1.64560	0.66520	C	1.91700	-4.88540	0.90450
C	0.08130	3.88190	1.98160	H	2.60790	-7.28090	1.80440
C	-2.10280	2.21470	1.35000	H	4.22080	-6.68800	2.31640
C	-1.19340	2.52190	0.40440	H	5.29490	-1.93920	-5.82270
C	-0.10670	3.48990	0.71070	H	6.34310	-1.90980	-4.36630
H	0.84810	4.60870	2.22390	O	3.16060	-5.35270	1.22580
C	-1.86010	2.61020	2.76530	O	0.91350	-5.32410	1.43520
C	-0.79450	3.38600	3.06230	O	5.41200	-3.51140	-2.48240
C	-0.51950	3.76250	4.46780	O	4.32620	-2.37270	-4.10120
C	-1.31260	3.31870	5.44930	Si	-4.50140	-2.20550	-0.60170
C	-2.46520	2.45200	5.13500	Si	0.84460	4.37900	-0.62530
C	-2.72580	2.11250	3.86720	C	-2.74180	-5.21570	2.52960
H	0.32660	4.39500	4.70610	C	-2.78440	-3.91040	2.81970
H	-1.10920	3.59090	6.47690	C	-3.34330	-2.95230	1.84320
H	-3.09540	2.08600	5.93520	C	-3.78410	-3.38310	0.64760
H	-3.56600	1.46350	3.65810	C	-3.76750	-4.83530	0.34840
O	-2.06600	-0.38870	0.26390	C	-3.26740	-5.70190	1.23800
P	-0.87080	0.29860	-0.68360	H	-2.32870	-5.91790	3.24210
O	-1.26130	1.90310	-0.81840	H	-2.40390	-3.55160	3.76740
O	-0.91560	-0.33260	-2.05200	H	-3.38080	-1.90710	2.11370
N	2.61140	-1.03660	1.25550	H	-4.16350	-5.20220	-0.59020

H	-3.25130	-6.76070	1.01500	H	-0.41510	9.90690	0.44120
C	-2.11060	-2.02900	-4.63140	H	1.90430	9.20490	0.35440
C	-3.00380	-1.07890	-4.33240	H	2.49190	6.78650	-0.10230
C	-3.76190	-1.14770	-3.06550	H	-1.73910	5.89370	-0.39860
C	-3.55370	-2.15840	-2.20360	H	-2.27960	8.20350	0.06240
C	-2.58330	-3.22320	-2.55640	C	-0.36790	3.22320	-5.00950
C	-1.89430	-3.15580	-3.70230	C	-0.65980	4.44140	-4.54110
H	-1.54680	-1.97540	-5.55370	C	-0.28950	4.81300	-3.15940
H	-3.16510	-0.25200	-5.01170	C	0.32470	3.92420	-2.35820
H	-4.47340	-0.36310	-2.83970	C	0.65430	2.58180	-2.89090
H	-2.42090	-4.06120	-1.89690	C	0.32510	2.24940	-4.14480
H	-1.17800	-3.92790	-3.95160	H	-0.63680	2.94990	-6.02160
C	-8.82400	-3.82240	-1.40750	H	-1.16440	5.15970	-5.17420
C	-8.42390	-3.56580	-0.15680	H	-0.51710	5.81300	-2.82140
C	-7.06150	-3.05220	0.09370	H	1.14650	1.85760	-2.25990
C	-6.22180	-2.83070	-0.93200	H	0.56340	1.26730	-4.52890
C	-6.66800	-3.12570	-2.31580	N	0.89220	-2.38170	-1.64520
C	-7.90250	-3.59370	-2.53880	H	0.09010	-1.73490	-1.84250
H	-9.82140	-4.19970	-1.59290	H	-0.36360	-3.11060	1.21710
H	-9.09630	-3.73460	0.67430	C	5.53260	-2.43170	-4.87990
H	-6.75390	-2.85600	1.11370	H	5.83070	-3.46860	-5.05120
H	-6.00410	-2.96860	-3.15480	C	3.17180	-6.42480	2.18200
H	-8.22770	-3.80830	-3.54860	H	2.72960	-6.10420	3.12820
C	5.45740	3.68120	-0.20710	C	3.24740	-3.49400	-0.76120
C	4.97310	4.38460	-1.23690	H	3.74350	-2.55290	0.04940
C	3.51560	4.58280	-1.37760	H	4.05640	-4.21350	-0.67220
C	2.67010	4.05820	-0.47450	O	0.41480	0.16440	0.10830
C	3.21150	3.25370	0.64890	H	1.94290	-0.55490	0.63390
C	4.53370	3.08820	0.78020	C	5.40250	1.02860	-2.50460
H	6.52440	3.53360	-0.10280	C	6.24670	0.16570	-1.82750
H	5.64720	4.81260	-1.96730	C	5.77880	-0.61460	-0.75950
H	3.14420	5.17200	-2.20720	C	4.42810	-0.49580	-0.31860
H	2.54930	2.79020	1.36670	C	3.59360	0.38620	-1.04210
H	4.93000	2.50880	1.60220	C	4.06600	1.13430	-2.11410
C	-0.16710	8.87350	0.23580	H	5.78290	1.62400	-3.32930
C	1.11280	8.48590	0.18720	H	7.29070	0.05350	-2.09940
C	1.45060	7.07400	-0.09060	H	2.55490	0.51320	-0.75310
C	0.47450	6.17690	-0.31140	H	3.40860	1.81700	-2.63720
C	-0.94250	6.61100	-0.24260	O	6.71650	-1.44030	-0.23930
C	-1.24510	7.88910	0.01400	H	6.37980	-1.92690	0.52700

C	0.71790	-1.54860	5.00520	C	6.70240	-2.17410	3.98790
C	1.59080	-2.53440	4.54650	C	6.18600	-0.89010	3.79840
C	2.23720	-2.40050	3.31740	C	5.27630	-0.64460	2.77350
C	2.02560	-1.25710	2.53520	C	4.86250	-1.68140	1.92230
C	1.13790	-0.26750	2.99440	C	5.37290	-2.97130	2.12660
C	0.49160	-0.41850	4.21730	C	6.29370	-3.21110	3.15170
H	0.21110	-1.66520	5.95820	H	7.41670	-2.36300	4.78330
H	1.76160	-3.42890	5.13820	H	6.49440	-0.07650	4.44790
H	2.88750	-3.19020	2.96730	H	4.87380	0.35150	2.62970
H	0.94120	0.59000	2.36310	H	5.03920	-3.79160	1.50120
H	-0.19410	0.35340	4.55370	H	6.68420	-4.21410	3.29470
C	-3.28490	1.79770	0.73490	H	0.61070	4.54640	4.36860
C	-5.76860	0.62340	0.07590	H	-0.92290	4.01530	6.16000
C	-4.65110	-0.11590	0.00890	H	-3.05760	2.70650	5.67630
C	-3.32860	0.51730	0.29310	H	-3.56840	1.99540	3.43390
H	-6.73340	0.19600	-0.15690	O	-2.19140	-0.25870	0.27810
C	-5.71430	2.04450	0.45930	P	-0.93060	0.20790	-0.72980
C	-4.53250	2.61780	0.77130	O	-1.14390	1.82950	-0.99420
C	-4.50230	4.07030	1.10350	O	-1.05690	-0.53800	-2.03350
C	-5.63390	4.78400	1.12540	N	2.78270	-0.78160	1.21390
C	-6.92270	4.14030	0.81090	C	3.92120	-1.36770	0.67880
C	-6.96240	2.84280	0.49110	C	1.58640	-3.80840	0.55410
H	-3.56840	4.57200	1.31760	C	0.47410	-3.19260	0.00820
H	-5.60560	5.83900	1.36570	C	1.60900	-2.91200	-2.11290
H	-7.83460	4.72290	0.83240	C	2.72360	-3.57770	-1.62600
H	-7.91170	2.37860	0.25400	C	-0.86340	-3.06310	0.66280
C	0.34580	3.88030	1.67950	H	-1.51560	-2.40470	0.09780
C	-1.99230	2.41200	1.11580	H	-1.32230	-4.05180	0.74920
C	-1.03270	2.53610	0.17750	C	1.38490	-2.42650	-3.51600
C	0.14560	3.40640	0.43840	H	1.12770	-3.26640	-4.17050
H	1.18180	4.53800	1.88810	H	0.56900	-1.69990	-3.52540
C	-1.73490	2.88670	2.50360	H	2.29440	-1.98340	-3.91820
C	-0.59620	3.56280	2.77080	C	3.75990	-4.09300	-2.54840
C	-0.29800	3.99760	4.15450	C	1.63060	-4.50100	1.85880
C	-1.14460	3.70380	5.14750	H	1.11230	-4.76200	4.44570
C	-2.38170	2.94950	4.86660	H	-0.55330	-5.32730	4.09710
C	-2.66400	2.56060	3.61770	H	6.25200	-6.10140	-2.04760

H	5.32790	-5.91820	-3.57640	C	5.71070	2.80130	-0.35970
O	0.43770	-4.64450	2.47220	C	4.81900	2.51770	0.59650
O	2.66570	-4.93410	2.34640	C	3.39930	2.88450	0.41950
O	3.81940	-3.89050	-3.74800	C	3.00030	3.52480	-0.69350
O	4.64230	-4.88850	-1.89450	C	3.99380	3.84050	-1.74760
Si	-4.77970	-1.92160	-0.46030	C	5.27750	3.49450	-1.58960
Si	1.23550	4.05900	-0.93100	H	6.74960	2.52600	-0.23300
C	-2.31210	-2.51030	-4.40380	H	5.13470	2.01920	1.50230
C	-3.15120	-1.47580	-4.27810	H	2.70140	2.62240	1.20090
C	-3.92840	-1.29980	-3.03340	H	3.68410	4.35030	-2.65140
C	-3.79210	-2.17140	-2.01900	H	6.00050	3.72150	-2.36210
C	-2.87110	-3.32460	-2.17230	C	0.92610	8.71140	-0.45120
C	-2.16860	-3.48120	-3.30110	C	-0.17960	7.97490	-0.60890
H	-1.73610	-2.63700	-5.31130	C	-0.07640	6.50960	-0.76620
H	-3.25750	-0.76170	-5.08430	C	1.12700	5.91050	-0.76580
H	-4.60020	-0.45420	-2.95160	C	2.34830	6.73140	-0.57640
H	-2.75330	-4.04680	-1.37920	C	2.25070	8.05880	-0.43050
H	-1.48960	-4.31760	-3.40640	H	0.85250	9.78490	-0.33450
C	-9.24620	-3.16310	-1.13740	H	-1.15200	8.44990	-0.62020
C	-8.39260	-3.18660	-2.16780	H	-0.98410	5.92950	-0.88170
C	-6.98130	-2.79400	-1.97120	H	3.32520	6.26980	-0.54740
C	-6.55210	-2.40240	-0.75930	H	3.14210	8.65690	-0.29190
C	-7.50080	-2.38820	0.38060	C	-0.05020	2.73930	-5.25230
C	-8.77780	-2.74620	0.19960	C	-0.16340	4.02200	-4.89020
H	-10.27960	-3.45120	-1.28050	C	0.23360	4.44750	-3.53110
H	-8.73320	-3.49470	-3.14790	C	0.69550	3.54740	-2.64460
H	-6.31160	-2.83300	-2.81880	C	0.83350	2.13350	-3.06360
H	-7.16400	-2.08520	1.36430	C	0.47580	1.74860	-4.29410
H	-9.46920	-2.73250	1.03210	H	-0.34010	2.42630	-6.24700
C	-3.44160	-4.65290	3.10340	H	-0.54420	4.75240	-5.59240
C	-3.88610	-5.20070	1.96670	H	0.14820	5.49410	-3.27940
C	-4.30550	-4.33760	0.84320	H	1.21020	1.40060	-2.36930
C	-4.21980	-3.00070	0.94690	H	0.57130	0.71150	-4.58840
C	-3.75320	-2.39910	2.22160	N	0.56780	-2.68660	-1.25850
C	-3.37720	-3.18410	3.23880	H	-0.16660	-2.01550	-1.58590
H	-3.13740	-5.28380	3.92830	H	-0.76710	-2.66720	1.67270
H	-3.94070	-6.27690	1.86760	C	5.71550	-5.40610	-2.69310
H	-4.68250	-4.80070	-0.06030	H	6.37700	-4.59540	-3.00640
H	-3.71550	-1.32610	2.34530	C	0.47760	-5.31020	3.74620
H	-3.03100	-2.74420	4.16510	H	0.86450	-6.32580	3.63670

C	2.84020	-3.78010	-0.18680	C	2.49960	-0.29180	2.52070
H	3.48500	-2.67850	0.29980	C	1.14200	-0.21890	2.89090
H	3.57110	-4.51680	0.13340	C	0.76790	0.35200	4.10280
O	0.33020	-0.01770	0.07610	H	1.43330	1.30060	5.92720
H	1.98720	-0.61000	0.58100	H	3.83650	1.18200	5.28140
C	5.11580	-0.10830	-3.28730	H	4.51060	0.22440	3.14400
C	5.81860	-1.11370	-2.64110	H	0.38800	-0.54780	2.18770
C	5.43260	-1.54800	-1.36830	H	-0.28770	0.41030	4.35350
C	4.33530	-0.93950	-0.70030	C	7.11780	-2.08280	3.51010
C	3.62750	0.05730	-1.39780	C	5.97760	-2.88590	3.52720
C	4.00830	0.47470	-2.66760	C	4.94980	-2.67620	2.60670
H	5.42720	0.21890	-4.27450	C	5.05290	-1.65560	1.65000
H	6.67490	-1.59500	-3.10060	C	6.21740	-0.86470	1.62620
H	2.77020	0.51330	-0.91840	C	7.23690	-1.07360	2.55210
H	3.46410	1.26330	-3.17210	H	7.91420	-2.24820	4.22950
O	6.17520	-2.57320	-0.86720	H	5.88170	-3.68350	4.25740
H	5.94200	-2.75410	0.05510	H	4.07570	-3.31710	2.62970
C	1.72820	0.85260	4.98310	H	6.31870	-0.08530	0.87930
C	3.07230	0.78270	4.62070	H	8.12470	-0.44920	2.52140
C	3.46270	0.22600	3.40260				
C	-3.25660	1.79440	0.80100	H	1.23340	4.52420	1.88210
C	-5.76400	0.65360	0.16900	C	-1.67050	2.86940	2.54830
C	-4.65460	-0.09350	0.06460	C	-0.52960	3.54940	2.79520
C	-3.32110	0.52050	0.34110	C	-0.21120	3.99000	4.17260
H	-6.73650	0.23980	-0.05600	C	-1.04120	3.69700	5.17970
C	-5.68950	2.06660	0.57760	C	-2.28000	2.93750	4.92100
C	-4.49620	2.62530	0.87230	C	-2.58060	2.54340	3.67790
C	-4.44650	4.07350	1.22140	H	0.69890	4.54240	4.37050
C	-5.57120	4.79580	1.27940	H	-0.80470	4.01270	6.18760
C	-6.87220	4.16670	0.98680	H	-2.94200	2.69460	5.74200
C	-6.92980	2.87440	0.64930	H	-3.48550	1.97420	3.51000
H	-3.50400	4.56590	1.41820	O	-2.19460	-0.27030	0.29900
H	-5.52840	5.84740	1.53200	P	-0.93170	0.19670	-0.70500
H	-7.77850	4.75620	1.03790	O	-1.14320	1.81860	-0.96150
H	-7.88820	2.42130	0.42770	O	-1.05650	-0.54080	-2.01400
C	0.39490	3.86510	1.68860	N	2.79410	-0.78550	1.22050
C	-1.95170	2.39450	1.16510	C	3.92800	-1.37440	0.67910
C	-1.00760	2.51850	0.21110	C	1.57280	-3.80080	0.55080
C	0.17780	3.38510	0.45280	C	0.46380	-3.19050	-0.00750



C	1.61420	-2.91510	-2.12030	H	-6.36510	-2.69860	-2.83320
C	2.72310	-3.58450	-1.62480	H	-7.17840	-2.09040	1.38040
C	-0.88340	-3.06760	0.62790	H	-9.49110	-2.70800	1.04470
H	-1.53220	-2.42090	0.04640	C	-3.48080	-4.79030	2.96890
H	-1.33570	-4.05940	0.71530	C	-3.39400	-3.46810	3.15420
C	1.40130	-2.42940	-3.52520	C	-3.80950	-2.54050	2.08130
H	1.14820	-3.26860	-4.18210	C	-4.24960	-3.02050	0.90480
H	0.58580	-1.70240	-3.54060	C	-4.37050	-4.48640	0.71770
H	2.31380	-1.98620	-3.92060	C	-3.99950	-5.32400	1.69370
C	3.76080	-4.10930	-2.53980	H	-3.17830	-5.47080	3.75410
C	1.60780	-4.47970	1.86290	H	-3.01760	-3.07440	4.08950
H	1.09110	-4.69680	4.45060	H	-3.74730	-1.47770	2.26690
H	-0.58800	-5.23080	4.11650	H	-4.76350	-4.88620	-0.20880
H	6.22790	-6.14420	-2.02330	H	-4.08480	-6.39370	1.55320
H	5.31900	-5.94480	-3.55900	C	0.83460	8.68010	-0.56710
O	0.41280	-4.59890	2.47740	C	-0.25330	7.91440	-0.70900
O	2.63720	-4.91900	2.35700	C	-0.11570	6.44860	-0.83040
O	3.82960	-3.90850	-3.73920	C	1.10120	5.87800	-0.81300
O	4.63190	-4.91210	-1.87950	C	2.30270	6.73110	-0.64060
Si	-4.80670	-1.88380	-0.45680	C	2.17400	8.05900	-0.52750
Si	1.25150	4.02780	-0.93440	H	0.73580	9.75410	-0.47680
C	-2.36340	-2.37170	-4.42860	H	-1.23650	8.36620	-0.73390
C	-3.19460	-1.33560	-4.26820	H	-1.00940	5.84500	-0.93430
C	-3.96570	-1.19200	-3.01550	H	3.28970	6.29260	-0.59760
C	-3.83210	-2.09540	-2.02890	H	3.05090	8.68090	-0.40140
C	-2.91960	-3.24950	-2.22040	C	-0.05710	2.62210	-5.21990
C	-2.22230	-3.37660	-3.35620	C	0.42570	1.73850	-4.34030
H	-1.79140	-2.47440	-5.34160	C	0.83870	2.18670	-2.99540
H	-3.29850	-0.59620	-5.05160	C	0.71620	3.47350	-2.63480
H	-4.63000	-0.34380	-2.90460	C	0.20170	4.45260	-3.62560
H	-2.80200	-3.99450	-1.44860	C	-0.16830	4.04630	-4.84700
H	-1.54870	-4.21330	-3.48910	H	-0.36140	2.29710	-6.20640
C	-9.28880	-3.06400	-1.14030	H	0.51280	0.69400	-4.60970
C	-8.44370	-3.05810	-2.17790	H	1.21990	1.45630	-2.30070
C	-7.02770	-2.68380	-1.97920	H	0.12690	5.50170	-3.37950
C	-6.58560	-2.33810	-0.75800	H	-0.54360	4.76200	-5.56690
C	-7.52530	-2.35620	0.38940	C	5.74800	2.83450	-0.38480
C	-8.80650	-2.69780	0.20650	C	4.86600	2.53890	0.57660
H	-10.32560	-3.33900	-1.28490	C	3.44110	2.89150	0.41020
H	-8.79460	-3.32900	-3.16530	C	3.02780	3.53020	-0.69840

C	4.01120	3.86010	-1.75780	H	2.77930	0.51650	-0.89990
C	5.29940	3.52710	-1.60950	H	3.46030	1.27460	-3.15590
H	6.79050	2.56910	-0.26630	O	6.16750	-2.58650	-0.88630
H	5.19310	2.03940	1.47800	H	5.93670	-2.77260	0.03550
H	2.75020	2.61540	1.19310	C	1.79020	0.87800	4.98960
H	3.69000	4.36850	-2.65840	C	3.12880	0.81000	4.60750
H	6.01470	3.76410	-2.38620	C	3.50220	0.24400	3.38840
N	0.56750	-2.68700	-1.27440	C	2.52730	-0.28490	2.52620
H	-0.16430	-2.01210	-1.60330	C	1.17530	-0.21300	2.91560
H	-0.80680	-2.66010	1.63460	C	0.81820	0.36680	4.12840
C	5.70530	-5.44030	-2.67090	H	1.50810	1.33290	5.93430
H	6.37920	-4.63650	-2.97560	H	3.90160	1.21770	5.25290
C	0.44210	-5.24290	3.76260	H	4.54590	0.24300	3.11330
H	0.80580	-6.26880	3.66990	H	0.41230	-0.55130	2.22660
C	2.83100	-3.78130	-0.18410	H	-0.23340	0.42340	4.39550
H	3.48120	-2.68370	0.29950	C	7.13490	-2.12320	3.48970
H	3.55550	-4.52150	0.14290	C	5.98630	-2.91400	3.51400
O	0.32830	-0.03580	0.10080	C	4.95450	-2.69220	2.60080
H	1.99240	-0.61800	0.59420	C	5.06200	-1.67180	1.64440
C	5.10620	-0.10350	-3.28750	C	6.23400	-0.89210	1.61450
C	5.80790	-1.11580	-2.65080	C	7.25770	-1.11320	2.53300
C	5.42730	-1.55500	-1.37800	H	7.93470	-2.29850	4.20300
C	4.33730	-0.94440	-0.70050	H	5.88690	-3.71150	4.24380
C	3.63070	0.05970	-1.38840	H	4.07370	-3.32380	2.62880
C	4.00510	0.48190	-2.65840	H	6.33710	-0.11070	0.86960
H	5.41360	0.22710	-4.27490	H	8.15160	-0.49790	2.49760
H	6.65850	-1.59940	-3.11840				
C	-3.26220	1.79770	0.80760	H	-3.53710	4.57310	1.39240
C	-5.75860	0.62090	0.20040	H	-5.57430	5.83720	1.48330
C	-4.64240	-0.11780	0.11090	H	-7.81280	4.71770	0.99980
C	-3.31440	0.51600	0.36870	H	-7.89920	2.37290	0.42470
H	-6.72750	0.19330	-0.01370	C	0.38220	3.90120	1.64850
C	-5.69760	2.04180	0.58310	C	-1.96200	2.41720	1.15360
C	-4.51000	2.61640	0.86980	C	-1.02780	2.54200	0.19010
C	-4.47460	4.06950	1.19940	C	0.15280	3.41870	0.41580
C	-5.60630	4.78180	1.24500	H	1.21960	4.56480	1.83130
C	-6.90080	4.13620	0.95910	C	-1.67130	2.90130	2.53160
C	-6.94560	2.83850	0.64110	C	-0.52970	3.58500	2.76550

C	-0.19910	4.03060	4.13840	C	-4.19910	-3.01230	1.03440
C	-1.01880	3.73890	5.15430	C	-4.29880	-4.48480	0.89240
C	-2.25860	2.97630	4.90980	C	-3.90500	-5.28690	1.88920
C	-2.57030	2.57790	3.67090	H	-3.05830	-5.35840	3.94390
H	0.71170	4.58540	4.32590	H	-2.94240	-2.95070	4.20920
H	-0.77320	4.05790	6.15890	H	-3.71170	-1.42180	2.34660
H	-2.91230	2.73490	5.73790	H	-4.69320	-4.91820	-0.01820
H	-3.47600	2.00680	3.51350	H	-3.97350	-6.36150	1.78120
O	-2.17720	-0.25940	0.32600	C	-2.36660	-2.49980	-4.33660
P	-0.93730	0.21010	-0.70330	C	-3.20670	-1.46780	-4.19750
O	-1.16510	1.82820	-0.97440	C	-3.96670	-1.29580	-2.94160
O	-1.07680	-0.54510	-2.00060	C	-3.81410	-2.16900	-1.93090
N	2.74300	-0.77320	1.24200	C	-2.89250	-3.31940	-2.09890
C	3.89090	-1.35290	0.72000	C	-2.20530	-3.47230	-3.23770
C	1.58740	-3.83810	0.58140	H	-1.80290	-2.62320	-5.25220
C	0.47350	-3.21120	0.04790	H	-3.32580	-0.75230	-5.00070
C	1.60070	-2.88780	-2.07100	H	-4.63900	-0.45180	-2.84870
C	2.72110	-3.54870	-1.59150	H	-2.76290	-4.04270	-1.30900
C	-0.85430	-3.10710	0.72070	H	-1.52610	-4.30690	-3.35410
H	-1.51130	-2.42440	0.19010	C	-9.23460	-3.19830	-1.04820
H	-1.30980	-4.09980	0.77880	C	-8.82300	-2.81960	0.16730
C	1.35350	-2.37300	-3.46210	C	-7.41820	-2.41490	0.38020
H	1.08160	-3.19730	-4.12970	C	-6.55030	-2.41330	-0.64610
H	0.53640	-1.64770	-3.44040	C	-7.01000	-2.84520	-1.98910
H	2.25120	-1.90850	-3.86660	C	-8.28320	-3.21450	-2.17760
C	3.81280	-4.11490	-2.41540	H	-10.26310	-3.49610	-1.20590
C	1.48690	-4.58110	1.85530	H	-9.51740	-2.80970	0.99750
H	1.98070	-6.77240	3.27150	H	-7.10260	-2.11800	1.37300
H	3.67520	-6.26290	3.56240	H	-6.32530	-2.87070	-2.82530
H	4.47640	-4.17700	-5.58140	H	-8.61790	-3.52940	-3.15760
H	5.70340	-4.02410	-4.28090	C	0.83810	8.72240	-0.53480
O	2.68750	-5.11030	2.22520	C	-0.26020	7.96930	-0.66370
O	0.47920	-4.75560	2.51530	C	-0.13970	6.50450	-0.81220
O	4.71940	-4.78030	-1.94550	C	1.07170	5.92190	-0.83310
O	3.69240	-3.87720	-3.74150	C	2.28510	6.76130	-0.67520
Si	-4.77830	-1.92410	-0.35800	C	2.17180	8.08830	-0.53700
Si	1.20070	4.07030	-0.98550	H	0.75180	9.79560	-0.42450
C	-3.38280	-4.70700	3.14290	H	-1.23930	8.43070	-0.65790
C	-3.31970	-3.37860	3.28940	H	-1.04150	5.91110	-0.90360
C	-3.75890	-2.49040	2.19300	H	3.26870	6.31390	-0.66270

H	3.05740	8.69980	-0.42130	C	3.98520	0.46790	-2.63940
C	-0.17730	2.68930	-5.25880	H	5.44770	0.25580	-4.21360
C	-0.30060	3.97370	-4.90600	H	6.72720	-1.51770	-3.00340
C	0.12570	4.41850	-3.56210	H	2.71500	0.48220	-0.91430
C	0.62420	3.53410	-2.67960	H	3.42640	1.23670	-3.15840
C	0.77330	2.11830	-3.08870	O	6.22030	-2.49270	-0.78390
C	0.38910	1.71620	-4.30570	H	5.91440	-2.76480	0.09200
H	-0.48890	2.36230	-6.24230	C	1.63950	0.86300	4.99560
H	-0.71100	4.69140	-5.60460	C	2.98500	0.83220	4.63320
H	0.03110	5.46610	-3.31800	C	3.39150	0.27450	3.42100
H	1.17840	1.39790	-2.39690	C	2.44460	-0.28220	2.54520
H	0.49210	0.67790	-4.59290	C	1.08610	-0.24890	2.91600
C	5.69230	2.84670	-0.45880	C	0.69480	0.32190	4.12250
C	5.28790	3.46130	-1.57630	H	1.33090	1.31080	5.93540
C	3.86760	3.83380	-1.74430	H	3.73650	1.26260	5.28900
C	2.97440	3.55000	-0.78150	H	4.43900	0.30090	3.16130
C	3.42720	2.85460	0.44940	H	0.34180	-0.61350	2.22080
C	4.71760	2.53510	0.60500	H	-0.36130	0.34550	4.37530
H	6.73120	2.57060	-0.33460	C	7.01980	-2.04080	3.63050
H	5.99940	3.68700	-2.35980	C	7.16900	-1.04630	2.66160
H	3.56290	4.34470	-2.64940	C	6.17400	-0.84270	1.70810
H	2.72570	2.59160	1.22770	C	5.00600	-1.62620	1.71360
H	5.04790	2.03770	1.50610	C	4.87210	-2.62940	2.68320
N	0.56070	-2.68300	-1.20840	C	5.87300	-2.83470	3.63310
H	-0.18290	-2.01910	-1.52780	H	7.79690	-2.20090	4.37180
H	-0.74170	-2.76600	1.74920	H	8.06180	-0.42870	2.64470
C	4.73240	-4.44250	-4.55590	H	6.29720	-0.07200	0.95520
H	4.76910	-5.52770	-4.43640	H	3.98640	-3.25320	2.69080
C	2.65140	-5.92140	3.41140	H	5.75340	-3.61620	4.37720
H	2.30520	-5.33910	4.26830				
C	2.83830	-3.77860	-0.15610				
H	3.47330	-2.66310	0.34570				
H	3.59560	-4.50850	0.11620				
O	0.33960	0.00050	0.08080				
H	1.95030	-0.60560	0.60350				
C	5.12420	-0.08110	-3.23330				
C	5.84350	-1.06240	-2.56900				
C	5.44560	-1.50630	-1.30070				
C	4.31950	-0.92400	-0.65580				
C	3.59380	0.04590	-1.37400				

C	-3.25350	1.79360	0.82150	C	-0.86470	-3.12500	0.67610
C	-5.76170	0.63340	0.23020	H	-1.51910	-2.43800	0.14780
C	-4.65000	-0.10990	0.12430	H	-1.31880	-4.11900	0.71930
C	-3.31630	0.51470	0.37570	C	1.37010	-2.33860	-3.48090
H	-6.73450	0.21220	0.02140	H	1.12410	-3.15970	-4.16210
C	-5.68980	2.05150	0.62120	H	0.53810	-1.63080	-3.46020
C	-4.49650	2.61880	0.89840	H	2.26280	-1.85040	-3.86840
C	-4.45030	4.07040	1.23360	C	3.83800	-4.06570	-2.43260
C	-5.57790	4.78800	1.29480	C	1.47320	-4.60340	1.81230
C	-6.87860	4.15010	1.02010	H	1.95650	-6.81240	3.20330
C	-6.93320	2.85420	0.69630	H	3.64960	-6.30820	3.51150
H	-3.50840	4.56870	1.41790	H	4.54570	-4.05520	-5.58960
H	-5.53800	5.84210	1.53720	H	5.75230	-3.91920	-4.26840
H	-7.78710	4.73580	1.07350	O	2.67130	-5.13760	2.18310
H	-7.89130	2.39440	0.48790	O	0.46140	-4.78580	2.46390
C	0.40380	3.87880	1.65190	O	4.74390	-4.73310	-1.96400
C	-1.94790	2.40400	1.16390	O	3.73290	-3.80260	-3.75520
C	-1.01740	2.52780	0.19660	Si	-4.79780	-1.90970	-0.36470
C	0.16820	3.39850	0.41970	Si	1.20960	4.05230	-0.98520
H	1.24330	4.54030	1.83220	C	-3.38660	-4.74310	3.08880
C	-1.64970	2.88480	2.54160	C	-3.31860	-3.41690	3.25260
C	-0.50520	3.56480	2.77180	C	-3.76230	-2.51280	2.17120
C	-0.16920	4.01030	4.14340	C	-4.21190	-3.01790	1.00880
C	-0.98700	3.72230	5.16190	C	-4.31710	-4.48810	0.84780
C	-2.22970	2.96320	4.92150	C	-3.91890	-5.30460	1.83100
C	-2.54610	2.56450	3.68390	H	-3.05850	-5.40620	3.87870
H	0.74390	4.56230	4.32790	H	-2.93380	-3.00260	4.17550
H	-0.73750	4.04140	6.16550	H	-3.71110	-1.44640	2.33860
H	-2.88180	2.72440	5.75170	H	-4.71930	-4.90810	-0.06570
H	-3.45380	1.99590	3.52960	H	-3.99150	-6.37750	1.70910
O	-2.18470	-0.26850	0.32140	C	-2.40800	-2.43380	-4.36360
P	-0.94170	0.20040	-0.70440	C	-3.24600	-1.40280	-4.20580
O	-1.16330	1.81970	-0.97010	C	-4.00030	-1.24820	-2.94430
O	-1.08290	-0.54830	-2.00560	C	-3.84520	-2.13660	-1.94730
N	2.74030	-0.78060	1.24590	C	-2.92650	-3.28600	-2.13640
C	3.89350	-1.36020	0.73550	C	-2.24370	-3.42280	-3.27990
C	1.58170	-3.84500	0.54840	H	-1.84840	-2.54460	-5.28330
C	0.46890	-3.21770	0.01280	H	-3.36730	-0.67520	-4.99770
C	1.61090	-2.86530	-2.09310	H	-4.66990	-0.40390	-2.83560
C	2.73250	-3.52260	-1.61150	H	-2.79500	-4.02140	-1.35780

H	-1.56640	-4.25670	-3.41150	H	6.75420	2.59670	-0.35100
C	-9.26390	-3.15950	-1.03570	H	6.00790	3.71210	-2.37150
C	-8.84180	-2.79630	0.18090	H	3.56530	4.34970	-2.65350
C	-7.43400	-2.39870	0.38770	H	2.75260	2.58160	1.22190
C	-6.57400	-2.38800	-0.64510	H	5.08030	2.04460	1.49230
C	-7.04550	-2.80220	-1.98960	N	0.56210	-2.67770	-1.23760
C	-8.32120	-3.16520	-2.17260	H	-0.18390	-2.01440	-1.55500
H	-10.29450	-3.45230	-1.18880	H	-0.76080	-2.79480	1.70900
H	-9.52970	-2.79410	1.01650	C	4.78960	-4.34060	-4.56650
H	-7.10970	-2.11490	1.38160	H	4.83490	-5.42780	-4.47000
H	-6.36710	-2.81980	-2.83120	C	2.62700	-5.96390	3.35840
H	-8.66450	-3.46750	-3.15350	H	2.27570	-5.39240	4.22060
C	0.80800	8.70180	-0.54230	C	2.83860	-3.77240	-0.17830
C	-0.28400	7.93900	-0.66690	H	3.47120	-2.66660	0.34330
C	-0.15110	6.47510	-0.81320	H	3.59480	-4.50520	0.08950
C	1.06530	5.90300	-0.83650	O	0.33400	-0.01720	0.07950
C	2.27170	6.75310	-0.68300	H	1.95120	-0.61550	0.60240
C	2.14730	8.07940	-0.54700	C	5.18110	-0.06290	-3.19190
H	0.71270	9.77440	-0.43360	C	5.89770	-1.04160	-2.52080
H	-1.26710	8.39170	-0.65920	C	5.48240	-1.49700	-1.26210
H	-1.04800	5.87360	-0.90090	C	4.34350	-0.92430	-0.63100
H	3.25920	6.31430	-0.67200	C	3.62170	0.04330	-1.35630
H	3.02770	8.69870	-0.43460	C	4.02770	0.47330	-2.61420
C	-0.17040	2.64930	-5.25040	H	5.51810	0.28170	-4.16500
C	-0.30370	3.93330	-4.90010	H	6.79200	-1.48750	-2.94320
C	0.12370	4.38490	-3.55890	H	2.73460	0.47230	-0.90600
C	0.63270	3.50690	-2.67610	H	3.46910	1.23900	-3.13840
C	0.79220	2.09120	-3.08210	O	6.25390	-2.48320	-0.74070
C	0.40810	1.68340	-4.29720	H	5.93160	-2.76750	0.12540
H	-0.48280	2.31710	-6.23200	C	1.62500	0.86660	4.99050
H	-0.72320	4.64560	-5.59880	C	2.96970	0.85130	4.62400
H	0.02090	5.43220	-3.31700	C	3.37880	0.29070	3.41410
H	1.20450	1.37540	-2.38980	C	2.43630	-0.28480	2.54600
H	0.51940	0.64590	-4.58320	C	1.07880	-0.26630	2.92010
C	5.71270	2.86500	-0.47150	C	0.68440	0.30770	4.12410
C	5.30040	3.47910	-1.58640	H	1.31370	1.31670	5.92830
C	3.87660	3.84000	-1.75000	H	3.71770	1.29600	5.27430
C	2.98830	3.54700	-0.78540	H	4.42490	0.32810	3.14960
C	3.45010	2.85260	0.44280	H	0.33730	-0.64550	2.22960
C	4.74340	2.54280	0.59410	H	-0.37110	0.31990	4.38060

C	6.96970	-2.09300	3.69130	H	7.73360	-2.26570	4.44350
C	7.14430	-1.09490	2.73040	H	8.04370	-0.48670	2.73110
C	6.16630	-0.87520	1.76290	H	6.30920	-0.10030	1.01770
C	4.99060	-1.64720	1.74500	H	3.93850	-3.26730	2.69840
C	4.83070	-2.65290	2.70810	H	5.67430	-3.65770	4.41070
C	5.81420	-2.87390	3.67240				
C	4.21210	0.71140	-0.58010	P	1.22180	0.30980	0.37150
C	5.74190	-1.54930	0.17210	O	1.96500	1.69690	0.72370
C	4.40950	-1.65930	0.06990	O	0.69920	-0.35020	1.59040
C	3.59350	-0.46350	-0.29230	N	-3.42830	-0.27900	-1.30120
H	6.34770	-2.39490	0.46660	C	-4.71580	-0.48000	-0.81570
C	6.41010	-0.25310	-0.03640	C	-3.20140	-3.21560	0.28890
C	5.68600	0.83970	-0.36230	C	-1.93520	-2.70520	0.50150
C	6.37670	2.15680	-0.45890	C	-2.75130	-1.36360	2.35850
C	7.69920	2.24400	-0.27620	C	-4.04010	-1.81350	2.13920
C	8.48530	1.03690	0.03820	C	-0.69780	-3.06050	-0.26600
C	7.87510	-0.14630	0.15890	H	0.15860	-2.48560	0.08610
H	5.81970	3.06160	-0.66070	H	-0.48250	-4.12280	-0.15960
H	8.19480	3.20370	-0.34670	C	-2.26710	-0.47070	3.46300
H	9.55520	1.11410	0.18260	H	-2.35700	-0.97520	4.42890
H	8.45730	-1.02640	0.40260	H	-1.22500	-0.19450	3.29540
C	2.16650	4.26850	-1.90530	H	-2.87890	0.43030	3.51010
C	3.43870	1.87020	-1.10730	C	-5.21220	-1.56180	3.01230
C	2.42220	2.37920	-0.37690	C	-3.54220	-4.31920	-0.64160
C	1.80180	3.68170	-0.75570	H	-3.30680	-5.67170	-2.92020
H	1.72100	5.20130	-2.21510	H	-1.81710	-6.47550	-2.32990
C	3.79050	2.50200	-2.41280	H	-5.67250	0.01810	5.79620
C	3.18050	3.65040	-2.78240	H	-6.80160	0.03210	4.40160
C	3.52090	4.29010	-4.07460	O	-2.47220	-4.97860	-1.13790
C	4.41420	3.72190	-4.89160	O	-4.68830	-4.62900	-0.91440
C	5.05690	2.44910	-4.51360	O	-6.32520	-1.98740	2.76290
C	4.76010	1.86620	-3.34640	O	-4.93280	-0.84530	4.12340
H	3.04650	5.21990	-4.36310	Si	3.58390	-3.27920	0.51690
H	4.66130	4.18940	-5.83600	Si	0.53130	4.51170	0.34710
H	5.76260	1.98290	-5.18900	C	1.04010	-5.05100	-3.00690
H	5.22600	0.92130	-3.10050	C	1.61080	-3.84930	-3.14500
O	2.24180	-0.62420	-0.49650	C	2.43790	-3.29150	-2.05470

C	2.58680	-3.96740	-0.90160	H	1.80570	8.89470	2.45640
C	1.99980	-5.32480	-0.78070	C	0.98610	2.69660	4.64920
C	1.26020	-5.83300	-1.77440	C	2.02610	3.29650	4.05950
H	0.42860	-5.45760	-3.80200	C	1.87440	3.88520	2.71310
H	1.46410	-3.27960	-4.05330	C	0.69170	3.82790	2.07510
H	2.91320	-2.33580	-2.21320	C	-0.45120	3.14700	2.72940
H	2.17600	-5.91820	0.10710	C	-0.31300	2.62110	3.95270
H	0.82850	-6.82090	-1.67980	H	1.09560	2.26140	5.63410
C	0.96570	-2.41650	4.31700	H	2.98180	3.34800	4.56460
C	2.07010	-1.69920	4.08310	H	2.73550	4.34350	2.24220
C	2.90190	-1.98650	2.89560	H	-1.39910	3.05930	2.22310
C	2.54670	-2.95720	2.03410	H	-1.15090	2.13390	4.43280
C	1.34600	-3.77720	2.32750	C	-3.77720	3.91150	-1.39470
C	0.59170	-3.51180	3.40140	C	-3.59560	4.63440	-0.28370
H	0.34820	-2.19980	5.17900	C	-2.23770	4.81000	0.27220
H	2.34890	-0.89680	4.75390	C	-1.18060	4.23700	-0.32760
H	3.78620	-1.38580	2.72710	C	-1.38590	3.45300	-1.56950
H	1.06350	-4.59160	1.68030	C	-2.61780	3.29920	-2.07290
H	-0.29220	-4.10290	3.60360	H	-4.77200	3.77390	-1.79820
C	6.76660	-6.56840	1.50140	H	-4.44360	5.08500	0.21550
C	6.65860	-6.08880	0.25670	H	-2.11010	5.40770	1.16640
C	5.65540	-5.04870	-0.05110	H	-0.54420	3.00960	-2.08360
C	4.85200	-4.57660	0.91680	H	-2.76840	2.73050	-2.98110
C	4.97300	-5.11450	2.29370	N	-1.77090	-1.77890	1.49570
C	5.88220	-6.05810	2.56870	H	-0.84920	-1.33620	1.59240
H	7.50060	-7.33070	1.72850	H	-0.84810	-2.87670	-1.33310
H	7.30480	-6.46170	-0.52730	C	-6.06750	-0.55450	4.95710
H	5.58040	-4.67440	-1.06490	H	-6.53520	-1.47790	5.30670
H	4.33260	-4.75000	3.08570	C	-2.77910	-6.05180	-2.04310
H	5.97160	-6.44970	3.57380	H	-3.40100	-6.80330	-1.55180
C	1.08050	9.17660	0.37590	C	-4.31350	-2.59500	0.95330
C	0.59910	8.56000	-0.70860	H	-4.70560	-1.53870	-0.08930
C	0.43010	7.09240	-0.71210	H	-5.26500	-3.11330	0.93000
C	0.77780	6.36280	0.36320	O	0.15990	0.73150	-0.73210
C	1.28740	7.05930	1.57210	H	-0.25240	0.03030	-1.27600
C	1.43470	8.39020	1.57340	C	-5.85690	2.38950	2.24270
H	1.20310	10.25200	0.38120	C	-4.51910	2.25110	1.89930
H	0.32920	9.13460	-1.58520	C	-4.11920	1.33910	0.90410
H	0.00450	6.62340	-1.58990	C	-5.09920	0.54730	0.24210
H	1.53440	6.50970	2.46710	C	-6.44090	0.70390	0.62560



C	-6.82970	1.61180	1.60550	H	-1.41690	0.67550	-2.57630
H	-6.14350	3.11100	3.00350	H	-4.22450	-2.57560	-2.68840
H	-3.75360	2.85780	2.37040	H	-2.97310	-3.57640	-4.52750
H	-7.19570	0.09670	0.13810	C	-7.88070	-1.03010	-3.73410
H	-7.87900	1.71510	1.86390	C	-7.69410	-1.99170	-2.74250
O	-2.81140	1.24550	0.61310	C	-6.67520	-1.84140	-1.79740
H	-2.78800	0.65810	-0.23470	C	-5.83110	-0.72730	-1.83450
C	-1.41710	-2.08750	-4.55720	C	-6.02570	0.23580	-2.83620
C	-0.98220	-0.89270	-3.98290	C	-7.04000	0.08510	-3.77860
C	-1.69390	-0.30980	-2.93470	H	-8.67220	-1.14780	-4.46880
C	-2.87380	-0.89890	-2.39680	H	-8.33680	-2.86660	-2.70160
C	-3.31960	-2.09050	-3.02930	H	-6.52470	-2.61130	-1.04820
C	-2.59910	-2.66070	-4.07500	H	-5.37320	1.10310	-2.86760
H	-0.86640	-2.54950	-5.37030	H	-7.17600	0.83990	-4.54830
H	-0.09260	-0.39520	-4.36190				

C	4.17190	0.79250	-0.64510	C	3.27400	4.32780	-4.13720
C	5.78180	-1.41120	0.10790	C	4.15680	3.77910	-4.97870
C	4.45150	-1.56170	0.03330	C	4.84860	2.52870	-4.61250
C	3.59440	-0.39720	-0.33370	C	4.60610	1.94640	-3.43260
H	6.41760	-2.23320	0.40560	H	2.76320	5.24080	-4.41700
C	6.40800	-0.10020	-0.13570	H	4.35950	4.24590	-5.93390
C	5.64580	0.96640	-0.46140	H	5.54620	2.07830	-5.30670
C	6.29650	2.30090	-0.59290	H	5.10750	1.01780	-3.19460
C	7.61970	2.42810	-0.44190	O	2.24500	-0.60110	-0.51300
C	8.44670	1.24870	-0.12730	P	1.21430	0.30710	0.37010
C	7.87330	0.05090	0.02520	O	1.92950	1.71240	0.71090
H	5.71000	3.18670	-0.79500	O	0.72550	-0.36690	1.59540
H	8.08610	3.40010	-0.53830	N	-3.40890	-0.32460	-1.29980
H	9.51690	1.35830	-0.00830	C	-4.69380	-0.54990	-0.81780
H	8.48550	-0.80850	0.26900	C	-3.14690	-3.28230	0.26340
C	1.99090	4.28380	-1.92500	C	-1.88650	-2.75780	0.47610
C	3.35190	1.92600	-1.15570	C	-2.71390	-1.44300	2.34700
C	2.34280	2.40890	-0.39840	C	-3.99820	-1.90480	2.12530
C	1.67810	3.69370	-0.76190	C	-0.64810	-3.09230	-0.29910
H	1.51070	5.20250	-2.22500	H	0.20110	-2.50230	0.04600
C	3.64750	2.56040	-2.47360	H	-0.41320	-4.15050	-0.19230
C	2.99360	3.68840	-2.83050	C	-2.23640	-0.55900	3.46140

H	-2.31310	-1.07950	4.42010	C	4.99430	-4.44270	0.94250
H	-1.19950	-0.26520	3.29220	C	5.14800	-4.94500	2.32970
H	-2.86090	0.33200	3.52580	C	6.09040	-5.85210	2.61520
C	-5.17110	-1.67420	3.00300	H	7.73990	-7.09080	1.78500
C	-3.47520	-4.38690	-0.67040	H	7.49020	-6.28150	-0.48770
H	-3.20770	-5.74330	-2.94840	H	5.70260	-4.56360	-1.04510
H	-1.72380	-6.54090	-2.33480	H	4.50460	-4.58390	3.12070
H	-5.64040	-0.13480	5.80800	H	6.20360	-6.21740	3.62770
H	-6.76940	-0.10700	4.41370	C	0.92120	9.16720	0.43260
O	-2.39760	-5.03990	-1.15860	C	0.42120	8.55440	-0.64560
O	-4.61760	-4.70440	-0.95030	C	0.26720	7.08520	-0.65750
O	-6.28100	-2.10540	2.74940	C	0.64720	6.35050	0.40340
O	-4.89600	-0.97040	4.12330	C	1.17690	7.04260	1.60610
Si	3.68190	-3.19450	0.52880	C	1.31080	8.37490	1.61510
Si	0.42210	4.49680	0.37660	H	1.03300	10.24370	0.44400
C	1.15310	-5.12730	-2.91900	H	0.12530	9.13320	-1.51100
C	1.68790	-3.91380	-3.09390	H	-0.17420	6.61920	-1.52890
C	2.50740	-3.30390	-2.02600	H	1.44950	6.48870	2.49090
C	2.68560	-3.94490	-0.85730	H	1.69670	8.87600	2.49350
C	2.13270	-5.31170	-0.69200	C	0.98520	2.64300	4.64950
C	1.40100	-5.86770	-1.66600	C	2.00460	3.26570	4.04780
H	0.54820	-5.57260	-3.69810	C	1.81870	3.86800	2.71170
H	1.51820	-3.37330	-4.01600	C	0.62530	3.79980	2.09500
H	2.95400	-2.33920	-2.21300	C	-0.49490	3.09510	2.76290
H	2.32460	-5.87120	0.21470	C	-0.32580	2.55680	3.97680
H	0.99290	-6.86190	-1.53910	H	1.11990	2.19740	5.62660
C	1.09850	-2.29340	4.34190	H	2.96900	3.32520	4.53530
C	2.22520	-1.60960	4.11350	H	2.66430	4.34330	2.22970
C	3.04600	-1.91170	2.92200	H	-1.45060	3.00010	2.27350
C	2.65890	-2.86240	2.05230	H	-1.14730	2.05150	4.46670
C	1.43030	-3.64300	2.33610	C	-3.91100	3.84900	-1.28500
C	0.68700	-3.36540	3.41460	C	-3.71720	4.57380	-0.17720
H	0.48950	-2.06600	5.20720	C	-2.35130	4.76420	0.35410
H	2.53090	-0.82400	4.79240	C	-1.29900	4.20470	-0.26650
H	3.94900	-1.33830	2.75630	C	-1.51840	3.41850	-1.50450
H	1.12030	-4.43990	1.67970	C	-2.75760	3.24920	-1.98430
H	-0.21670	-3.92800	3.61070	H	-4.91160	3.69920	-1.66950
C	6.97880	-6.35830	1.54920	H	-4.56090	5.01400	0.33820
C	6.84100	-5.91160	0.29530	H	-2.21400	5.36170	1.24700
C	5.80100	-4.91190	-0.02420	H	-0.68140	2.98490	-2.03390

H	-2.91840	2.67630	-2.88820	H	-2.77940	0.59880	-0.20800
N	-1.73100	-1.83710	1.47690	C	-1.36830	-2.09790	-4.55720
H	-0.81550	-1.38230	1.57550	C	-0.95700	-0.89280	-3.98740
H	-0.80890	-2.91320	-1.36540	C	-1.67910	-0.32020	-2.94030
C	-6.03230	-0.69760	4.96090	C	-2.84570	-0.93170	-2.39840
H	-6.49500	-1.62830	5.29730	C	-3.27040	-2.13180	-3.02930
C	-2.69050	-6.11800	-2.06260	C	-2.53970	-2.69150	-4.07360
H	-3.31730	-6.86840	-1.57590	H	-0.80860	-2.55220	-5.36850
C	-4.26520	-2.67780	0.93210	H	-0.07780	-0.37900	-4.36910
H	-4.66970	-1.61770	-0.10270	H	-1.42120	0.67140	-2.58540
H	-5.21140	-3.20580	0.90540	H	-4.16640	-2.63200	-2.68680
O	0.12510	0.70380	-0.71620	H	-2.89680	-3.61520	-4.52350
H	-0.25340	0.00080	-1.28250	C	-7.84280	-1.10270	-3.75210
C	-5.87950	2.25800	2.28020	C	-7.65250	-2.07070	-2.76730
C	-4.53790	2.13240	1.94690	C	-6.63810	-1.92020	-1.81730
C	-4.12450	1.24310	0.93700	C	-5.80270	-0.79940	-1.84260
C	-5.09390	0.45780	0.25240	C	-6.00100	0.17010	-2.83750
C	-6.43980	0.60030	0.62640	C	-7.01060	0.01920	-3.78480
C	-6.84240	1.48810	1.61910	H	-8.63060	-1.22060	-4.49070
H	-6.17650	2.96350	3.05190	H	-8.28860	-2.95070	-2.73580
H	-3.78080	2.73440	2.43690	H	-6.48460	-2.69440	-1.07310
H	-7.18690	-0.00150	0.12100	H	-5.35490	1.04250	-2.85940
H	-7.89440	1.58170	1.86920	H	-7.14950	0.77900	-4.54900
O	-2.81400	1.16470	0.65280				

**NH-Type II E**

C	-0.22220	-3.45360	0.89380	H	-2.44700	-7.42920	2.08090
C	2.10260	-5.02030	0.55640	H	-0.30310	-8.78600	1.83610
C	2.13830	-3.71270	0.25960	H	1.74380	-7.70610	1.14400
C	0.88460	-2.89560	0.32410	C	-3.97010	-1.57020	1.76930
H	2.99060	-5.63270	0.49480	C	-1.42030	-2.65500	1.24130
C	0.85730	-5.66280	0.99460	C	-2.13260	-2.09490	0.24980
C	-0.25880	-4.92590	1.16220	C	-3.52100	-1.61580	0.50470
C	-1.51980	-5.61700	1.56110	H	-4.96170	-1.20360	1.98960
C	-1.52830	-6.93450	1.79320	C	-1.91180	-2.56980	2.64430
C	-0.29080	-7.72100	1.64350	C	-3.12820	-2.03660	2.88950
C	0.84010	-7.12080	1.26010	C	-3.62540	-1.93270	4.28080
H	-2.44880	-5.07090	1.65250	C	-2.86180	-2.34330	5.29940

C	-1.52060	-2.90240	5.04050	C	6.52110	-5.72450	1.22350
C	-1.06690	-3.00910	3.78630	H	7.90140	-6.98520	0.02000
H	-4.60610	-1.51810	4.47850	H	7.17160	-6.11400	-2.12210
H	-3.22350	-2.26270	6.31620	H	5.35840	-4.34880	-2.23470
H	-0.90230	-3.22060	5.87000	H	5.12290	-4.42590	2.09260
H	-0.07500	-3.40750	3.61650	H	6.84660	-6.11780	2.17780
O	0.95540	-1.56570	-0.05700	C	5.07630	0.13970	3.13530
P	-0.32710	-0.80860	-0.87670	C	5.96340	-0.29280	2.23270
O	-1.53870	-1.92390	-0.97210	C	5.55160	-1.25900	1.19290
O	0.12020	-0.51820	-2.29060	C	4.28250	-1.70110	1.13820
N	0.36640	2.77520	1.36120	C	3.31860	-1.25470	2.17690
C	1.39990	3.68030	1.20770	C	3.69210	-0.37100	3.11050
C	1.88770	3.90540	-2.10760	H	5.37330	0.85570	3.89050
C	1.56670	2.63920	-2.56350	H	6.98140	0.07380	2.25300
C	-0.76800	2.98190	-2.00810	H	6.29220	-1.60160	0.48270
C	-0.49360	4.24640	-1.51900	H	2.30960	-1.63570	2.19890
C	2.46800	1.64760	-3.24020	H	2.98350	-0.03920	3.85850
H	3.47050	1.67620	-2.81860	C	3.70160	-1.26830	-4.54260
H	2.55800	1.88100	-4.30660	C	4.74770	-1.01000	-3.74990
C	-2.09600	2.30770	-2.14760	C	4.76620	-1.51220	-2.36050
H	-2.18720	1.89780	-3.15720	C	3.72220	-2.20500	-1.87470
H	-2.92000	2.98430	-1.95600	C	2.56610	-2.48880	-2.76100
H	-2.11320	1.47400	-1.43660	C	2.55880	-2.04600	-4.02430
C	-1.47330	5.27340	-1.09700	H	3.68760	-0.90330	-5.56130
C	3.16780	4.61330	-2.31640	H	5.58620	-0.43860	-4.12630
H	5.81490	4.77600	-2.37940	H	5.64380	-1.33080	-1.75690
H	5.86630	3.99250	-3.99310	H	1.72820	-3.07160	-2.40400
H	-4.57410	5.91930	-1.73690	H	1.71520	-2.25700	-4.66880
H	-3.86350	6.05540	-0.09560	C	-2.72840	-2.10780	-5.04190
O	4.04220	3.96290	-3.12080	C	-2.87340	-3.07790	-4.13250
O	3.41100	5.70650	-1.83370	C	-3.51250	-2.78450	-2.83340
O	-1.15890	6.22940	-0.40410	C	-3.94850	-1.54290	-2.55440
O	-2.72660	5.11380	-1.57180	C	-3.80240	-0.47870	-3.57650
Si	3.78930	-2.94260	-0.16490	C	-3.21870	-0.74590	-4.75120
Si	-4.68920	-1.15390	-0.88570	H	-2.25540	-2.31910	-5.99210
C	7.13050	-6.22680	-0.02430	H	-2.51480	-4.07730	-4.34200
C	6.72770	-5.74560	-1.20630	H	-3.59080	-3.57680	-2.09900
C	5.67430	-4.71060	-1.26580	H	-4.16410	0.52070	-3.38480
C	5.11890	-4.24670	-0.13330	H	-3.10860	0.03480	-5.49270
C	5.56750	-4.78660	1.17340	C	-5.90630	3.35480	-0.57760

C	-4.92100	2.88380	0.19520	H	1.11410	6.45260	0.90400
C	-4.51480	1.46650	0.09710	H	1.32390	8.16920	2.66030
C	-5.12560	0.64880	-0.77650	C	-3.20950	3.01540	3.60240
C	-6.21380	1.17790	-1.63310	C	-2.65990	4.18240	3.07260
C	-6.58210	2.46100	-1.53870	C	-1.49160	4.14380	2.31130
H	-6.21030	4.39030	-0.50050	C	-0.84280	2.92020	2.08880
H	-4.42040	3.54060	0.89250	C	-1.41130	1.73960	2.60040
H	-3.71730	1.10960	0.73290	C	-2.58180	1.79420	3.34980
H	-6.71710	0.52660	-2.33690	H	-4.12070	3.05430	4.19160
H	-7.37730	2.84560	-2.16400	H	-3.14650	5.13930	3.23970
C	-8.76150	-3.41200	-0.27030	H	-1.10710	5.05780	1.88180
C	-7.92980	-3.80600	-1.24070	H	-0.94250	0.78990	2.37300
C	-6.64690	-3.10250	-1.44990	H	-3.00690	0.87450	3.73900
C	-6.29780	-2.07440	-0.65610	C	5.40260	2.37590	0.11980
C	-7.24000	-1.62810	0.40130	C	5.18070	3.62610	0.69880
C	-8.40280	-2.26480	0.58570	C	3.88670	4.00640	1.03470
H	-9.70140	-3.92630	-0.11680	C	2.77640	3.15810	0.85280
H	-8.19400	-4.64210	-1.87530	C	3.03200	1.89080	0.27700
H	-6.00920	-3.43960	-2.25120	C	4.32810	1.52480	-0.10090
H	-7.00720	-0.76830	1.01530	H	6.40300	2.06380	-0.16500
H	-9.08860	-1.93220	1.35410	H	6.00500	4.30830	0.87740
N	0.28180	2.20250	-2.41420	H	3.72620	4.99140	1.45270
H	0.11470	1.16800	-2.51790	H	4.47000	0.56600	-0.58300
H	2.03650	0.65070	-3.13410	O	1.97940	1.06940	0.06680
C	-3.66770	6.12410	-1.16850	H	2.19220	0.12980	-0.06990
H	-3.28380	7.11980	-1.39790	C	1.67550	4.42570	3.57640
C	5.29250	4.63860	-3.32870	H	1.77430	3.37420	3.82840
H	5.13080	5.61620	-3.78860				
C	0.89740	4.63120	-1.32250				
H	1.15980	4.33280	-0.02230				
H	1.08330	5.69850	-1.24350				
O	-0.74610	0.33280	0.01430				
H	0.44190	1.87420	0.87850				
C	1.65360	6.74770	4.24650				
C	1.77620	5.39470	4.57130				
C	1.44390	4.79540	2.24240				
C	1.32290	6.15040	1.92260				
C	1.42660	7.12060	2.92280				
H	1.73280	7.50420	5.02170				
H	1.95160	5.09300	5.59970				

C	0.49920	3.40270	0.86830	C	-2.57650	-1.51760	-3.23840
C	-1.69490	5.14740	0.53150	H	-3.57860	-1.45910	-2.81880
C	-1.83460	3.84590	0.23810	H	-2.68430	-1.76370	-4.30030
C	-0.64950	2.93250	0.30230	C	1.91810	-2.52020	-2.10720
H	-2.53210	5.82770	0.47100	H	2.04670	-2.12880	-3.11980
C	-0.40030	5.69140	0.96080	H	2.68340	-3.26010	-1.90590
C	0.65490	4.86920	1.12610	H	1.99920	-1.68500	-1.40180
C	1.97060	5.46060	1.50850	C	1.06030	-5.42140	-1.05340
C	2.08570	6.77480	1.73090	C	-3.51070	-4.40630	-2.27540
C	0.91310	7.65600	1.58660	H	-6.15930	-4.37510	-2.34500
C	-0.26520	7.14510	1.21640	H	-6.15190	-3.59680	-3.96230
H	2.85460	4.84350	1.59400	H	4.06610	-6.36250	-1.77300
H	3.04360	7.19700	2.00620	H	3.41030	-6.39290	-0.10370
H	1.01160	8.71790	1.77160	O	-4.33080	-3.69910	-3.08890
H	-1.12050	7.79970	1.10330	O	-3.83900	-5.47180	-1.78130
C	4.10540	1.26060	1.73750	O	0.67930	-6.33460	-0.33670
C	1.63000	2.51270	1.21820	O	2.31000	-5.38190	-1.56190
C	2.28950	1.88990	0.22790	Si	-3.54160	3.20670	-0.18230
C	3.63540	1.30790	0.48090	Si	4.76450	0.77430	-0.90500
H	5.08760	0.84970	1.94060	C	-6.61120	6.74660	-0.06010
C	2.12930	2.40980	2.61840	C	-6.24670	6.22970	-1.23950
C	3.31090	1.80010	2.85920	C	-5.27920	5.11370	-1.29300
C	3.81840	1.68800	4.24600	C	-4.76390	4.61180	-0.15760
C	3.09730	2.16690	5.26570	C	-5.16960	5.19140	1.14610
C	1.79280	2.80940	5.01270	C	-6.04530	6.20270	1.19080
C	1.33060	2.92400	3.76220	H	-7.31900	7.56440	-0.02020
H	4.77200	1.21280	4.43950	H	-6.65850	6.62850	-2.15750
H	3.46650	2.08090	6.27950	H	-4.99170	4.72370	-2.25980
H	1.20830	3.18330	5.84350	H	-4.75630	4.80040	2.06750
H	0.36550	3.38510	3.59660	H	-6.33940	6.62510	2.14290
O	-0.82670	1.61140	-0.07510	C	-5.06420	0.24530	3.12830
P	0.38940	0.75060	-0.89380	C	-5.91520	0.74320	2.22470
O	1.68590	1.76610	-0.99520	C	-5.42970	1.67090	1.18170
O	-0.08240	0.48500	-2.30420	C	-4.13000	2.01230	1.12520
N	-0.57260	-2.72880	1.37350	C	-3.20310	1.49430	2.16460
C	-1.67110	-3.55670	1.23930	C	-3.64410	0.64550	3.10110
C	-2.18000	-3.79720	-2.07040	H	-5.41590	-0.44280	3.88590
C	-1.75890	-2.56600	-2.54130	H	-6.95890	0.45780	2.24670
C	0.53970	-3.08480	-1.97240	H	-6.14170	2.06850	0.47090
C	0.16510	-4.32020	-1.47600	H	-2.16720	1.79460	2.18440

H	-2.96310	0.26090	3.84940	H	9.70850	3.61250	0.04710
C	-3.58310	1.49300	-4.54580	H	7.60980	4.82080	-0.07290
C	-4.64710	1.32570	-3.75260	H	5.44060	3.57650	-0.44700
C	-4.62790	1.84270	-2.36870	H	7.69240	-0.12550	-0.60310
C	-3.53340	2.45630	-1.88780	H	9.73420	1.07420	-0.21410
C	-2.35840	2.64150	-2.77550	N	-0.44460	-2.22890	-2.38810
C	-2.38420	2.18580	-4.03390	H	-0.19720	-1.21310	-2.50450
H	-3.59630	1.11690	-5.56050	H	-2.06720	-0.55610	-3.15020
H	-5.52710	0.81710	-4.12430	C	3.16720	-6.46720	-1.16660
H	-5.51720	1.73550	-1.76450	H	2.68290	-7.42690	-1.35560
H	-1.47850	3.16200	-2.42330	C	-5.62800	-4.28070	-3.29460
H	-1.52640	2.32430	-4.67930	H	-5.53940	-5.26980	-3.75020
C	2.92600	1.96050	-5.06270	C	-1.25130	-4.58900	-1.27360
C	3.20640	2.90690	-4.16070	H	-1.48570	-4.24920	0.02410
C	3.80590	2.53800	-2.86170	H	-1.52320	-5.63630	-1.17820
C	4.07380	1.25140	-2.57460	O	0.71940	-0.41570	0.00310
C	3.77390	0.21120	-3.58930	H	-0.57970	-1.83180	0.87720
C	3.22560	0.54720	-4.76320	C	-2.13370	-6.53680	4.34000
H	2.48120	2.22810	-6.01230	C	-2.15720	-5.17220	4.63770
H	2.98570	3.94440	-4.37570	C	-1.79270	-4.64480	2.29640
H	3.97910	3.31980	-2.13820	C	-1.77060	-6.01100	2.00380
H	3.98840	-0.82710	-3.39310	C	-1.93980	-6.95130	3.02340
H	3.00250	-0.21680	-5.49680	H	-2.26320	-7.27000	5.13070
C	5.56060	-3.84370	-0.67250	H	-2.30550	-4.83810	5.66040
C	4.73130	-3.26950	0.20570	H	-1.58800	-6.34740	0.99060
C	4.46090	-1.81860	0.13100	H	-1.91310	-8.00960	2.78190
C	5.04870	-1.06770	-0.81680	C	2.97670	-3.20430	3.61890
C	5.95070	-1.71750	-1.79990	C	2.35060	-4.33270	3.09040
C	6.19320	-3.03150	-1.72960	C	1.18770	-4.21690	2.32870
H	5.76920	-4.90340	-0.61090	C	0.62360	-2.95270	2.10310
H	4.26040	-3.86670	0.97390	C	1.26970	-1.81210	2.61300
H	3.78390	-1.38320	0.85090	C	2.43260	-1.94400	3.36450
H	6.42100	-1.12860	-2.57760	H	3.88290	-3.30320	4.20880
H	6.85450	-3.50130	-2.44600	H	2.77200	-5.31960	3.25940
C	8.78370	3.08010	-0.13400	H	0.74130	-5.10360	1.90120
C	7.62630	3.74620	-0.20110	H	0.86470	-0.83370	2.38470
C	6.36490	3.01670	-0.44500	H	2.91770	-1.05450	3.75380
C	6.37110	1.68360	-0.62350	C	-5.56970	-1.98100	0.13150
C	7.65800	0.94940	-0.51850	C	-5.43840	-3.23620	0.72720
C	8.79880	1.61310	-0.29280	C	-4.17520	-3.70420	1.06980

C	-3.00660	-2.94110	0.87680	H	-4.50980	-0.25170	-0.59250
C	-3.17010	-1.66700	0.28290	O	-2.06090	-0.92730	0.06190
C	-4.43660	-1.21280	-0.09970	H	-2.20450	0.02310	-0.08790
H	-6.54510	-1.60140	-0.15780	C	-1.99170	-4.23290	3.62330
H	-6.30980	-3.85460	0.91460	H	-2.01330	-3.17230	3.85450
H	-4.08650	-4.69210	1.50220				
C	1.72980	-3.06440	0.81770	P	0.37900	-0.71420	-0.83660
C	4.51970	-3.28200	0.43070	O	-0.21730	-2.25070	-0.97070
C	3.90660	-2.11320	0.19430	O	0.60080	-0.22280	-2.24680
C	2.41530	-2.01920	0.28130	N	-1.46310	2.46320	1.22330
H	5.59370	-3.37480	0.35140	C	-0.97580	3.75230	1.15030
C	3.74980	-4.47030	0.82540	C	-0.62750	4.38470	-2.16620
C	2.41760	-4.37850	1.01640	C	-0.11920	3.17600	-2.61100
C	1.65700	-5.61180	1.36970	C	-2.19340	2.05170	-2.06090
C	2.29320	-6.77650	1.53860	C	-2.73810	3.23150	-1.58630
C	3.75500	-6.85450	1.36430	C	1.18940	2.94310	-3.30580
C	4.44670	-5.76320	1.02160	H	1.07800	3.12640	-4.38080
H	0.58100	-5.58960	1.47750	H	1.48840	1.90340	-3.15700
H	1.73480	-7.66820	1.79300	C	-2.85860	0.71810	-2.19660
H	4.26440	-7.79890	1.50610	H	-2.65580	0.31790	-3.19300
H	5.51930	-5.82950	0.88740	H	-3.93000	0.77940	-2.04260
C	-2.43270	-3.33770	1.75860	H	-2.40930	0.04070	-1.46280
C	0.30410	-2.94970	1.20250	C	-4.14580	3.47800	-1.20670
C	-0.61270	-2.75610	0.23990	C	0.05770	5.66180	-2.45840
C	-2.03860	-3.10430	0.49620	H	0.17140	8.19450	-3.14100
H	-3.46330	-3.57150	1.98090	H	-0.67750	8.71230	-1.64590
C	-0.13890	-3.18750	2.60410	H	-7.01530	2.23830	-2.02580
C	-1.45460	-3.34630	2.86540	H	-6.60990	2.79380	-0.36770
C	-1.91180	-3.57380	4.25570	O	-0.59940	6.70750	-1.89420
C	-1.02700	-3.59430	5.25870	O	1.06180	5.80550	-3.13290
C	0.40910	-3.39260	4.98340	O	-4.47790	4.41620	-0.49430
C	0.83280	-3.19780	3.72910	O	-5.05290	2.64360	-1.75430
H	-2.96430	-3.71880	4.46530	Si	4.95050	-0.60620	-0.17310
H	-1.36200	-3.75590	6.27510	Si	-3.25580	-3.40230	-0.89630
H	1.11830	-3.39780	5.80100	C	9.49920	-1.72140	-0.10330
H	1.88770	-3.03780	3.54690	C	8.91150	-1.42070	-1.26750
O	1.82250	-0.80460	-0.00700	C	7.47620	-1.06980	-1.30500



C	6.75640	-1.05170	-0.17050	H	-2.65020	-1.71720	-5.58220
C	7.41310	-1.38620	1.11640	C	-6.82600	-0.39860	-0.56300
C	8.71300	-1.70370	1.14680	C	-6.87140	-1.39900	-1.44940
H	10.55020	-1.97840	-0.07500	C	-5.73020	-2.32800	-1.57420
H	9.48580	-1.43400	-2.18480	C	-4.63820	-2.16550	-0.80850
H	7.02400	-0.83830	-2.25970	C	-4.58670	-1.04460	0.16000
H	6.84250	-1.37690	2.03680	C	-5.62480	-0.20740	0.27370
H	9.19070	-1.94830	2.08670	H	-7.66750	0.27370	-0.45920
C	4.41380	2.62110	3.19590	H	-7.74970	-1.53940	-2.06590
C	5.36740	2.76620	2.26960	H	-5.79870	-3.15170	-2.27420
C	5.54790	1.73750	1.22420	H	-3.70840	-0.88760	0.76960
C	4.74500	0.65940	1.18390	H	-5.58600	0.61610	0.97180
C	3.72360	0.48140	2.24860	C	-5.32620	-7.56190	-0.20540
C	3.55950	1.41800	3.19080	C	-4.40150	-7.43730	-1.16350
H	4.27510	3.37750	3.95730	C	-3.74390	-6.13420	-1.39560
H	6.00250	3.64250	2.27670	C	-4.05690	-5.06970	-0.63560
H	6.33740	1.87240	0.49790	C	-5.10190	-5.21270	0.40990
H	3.10820	-0.40410	2.28610	C	-5.69830	-6.39330	0.61500
H	2.80890	1.28880	3.95990	H	-5.80880	-8.51570	-0.03540
C	3.86980	0.98990	-4.45160	H	-4.13210	-8.29110	-1.77180
C	4.61570	1.73780	-3.63110	H	-3.01300	-6.06910	-2.18550
C	4.94860	1.24660	-2.27810	H	-5.40820	-4.35830	0.99890
C	4.48370	0.05920	-1.85250	H	-6.46320	-6.49090	1.37440
C	3.66050	-0.76630	-2.77130	N	-0.88160	2.05290	-2.45100
C	3.37030	-0.32380	-4.00090	H	-0.39160	1.12440	-2.54240
H	3.62550	1.34830	-5.44310	H	1.95550	3.62360	-2.94340
H	4.98050	2.70300	-3.95750	C	-6.42490	2.93720	-1.43480
H	5.57740	1.85850	-1.65000	H	-6.66670	3.96790	-1.70150
H	3.29740	-1.73740	-2.46320	C	0.01460	7.99070	-2.07950
H	2.76930	-0.92830	-4.66780	H	0.97430	8.02910	-1.55960
C	-1.09210	-3.21250	-5.05870	C	-1.85480	4.37510	-1.37840
C	-0.64560	-4.04180	-4.10910	H	-1.48470	4.26680	-0.08460
C	-1.33900	-4.11710	-2.80700	H	-2.36180	5.33130	-1.29720
C	-2.41600	-3.34860	-2.56350	O	-0.53520	0.09960	0.06210
C	-2.91690	-2.44830	-3.62990	H	-0.97100	1.71430	0.71180
C	-2.28550	-2.38040	-4.80850	C	-2.32420	6.45040	4.25100
H	-0.58300	-3.15220	-6.01180	C	-2.94620	6.48510	3.00400
H	0.22890	-4.65370	-4.28890	C	-1.49240	4.71120	2.21120
H	-0.94610	-4.77770	-2.04380	C	-0.86870	4.68430	3.47030
H	-3.79260	-1.83690	-3.46780	C	-1.28720	5.54350	4.48300

H	-2.64310	7.12570	5.03920	C	3.14740	4.17540	-0.11310
H	-3.75790	7.18160	2.81710	C	2.55270	2.91530	-0.02510
H	-0.05290	3.98990	3.64540	C	1.25630	2.79030	0.44670
H	-0.79810	5.50950	5.45180	C	0.47650	3.90970	0.79420
C	-4.30370	0.73590	3.83580	C	1.09060	5.18740	0.68000
C	-4.58650	1.96510	3.24170	C	2.42300	5.29810	0.25710
C	-3.68260	2.55770	2.35880	H	4.16770	4.28110	-0.46980
C	-2.45880	1.93080	2.08880	H	3.07100	2.02150	-0.33630
C	-2.18330	0.67910	2.66740	H	0.84770	1.79100	0.52770
C	-3.10280	0.09200	3.53140	H	2.85000	6.29390	0.20480
H	-5.01500	0.27780	4.51630	O	0.48030	6.37580	0.93480
H	-5.52870	2.46540	3.44640	H	-0.40260	6.23950	1.31060
H	-3.94490	3.48240	1.86460	C	-2.53920	5.61660	1.98690
H	-1.25820	0.17570	2.40990	H	-3.05470	5.62020	1.03210
H	-2.87580	-0.87180	3.97550				
C	-1.99390	2.89260	0.83890	C	1.60370	3.68970	4.27020
C	-4.79020	2.87290	0.43710	C	0.72280	3.63350	5.27540
C	-4.07930	1.75980	0.20580	C	-0.69310	3.31780	5.00260
C	-2.58610	1.79250	0.30130	C	-1.10310	3.09550	3.74840
H	-5.86770	2.87460	0.35130	H	2.64150	3.91870	4.47800
C	-4.12590	4.12200	0.83610	H	1.04650	3.81680	6.29180
C	-2.79180	4.14320	1.03490	H	-1.39820	3.26200	5.82180
C	-2.14050	5.43610	1.39370	H	-2.14220	2.85190	3.56780
C	-2.87410	6.54260	1.55880	O	-1.88940	0.63320	0.01900
C	-4.33610	6.49680	1.37530	P	-0.44960	0.67020	-0.82180
C	-4.93090	5.35120	1.02820	O	0.01010	2.25320	-0.95580
H	-1.06730	5.50490	1.50870	O	-0.64040	0.16720	-2.23260
H	-2.39470	7.47810	1.81720	N	1.71820	-2.32810	1.21160
H	-4.92440	7.39470	1.51390	C	1.34570	-3.65570	1.14790
H	-6.00440	5.32660	0.88720	C	0.97690	-4.31580	-2.15880
C	2.13430	3.51300	1.77000	C	0.35590	-3.15790	-2.59530
C	-0.56280	2.90130	1.22000	C	2.33450	-1.85330	-2.09340
C	0.36420	2.78930	0.25430	C	2.99140	-2.97940	-1.63030
C	1.75570	3.25740	0.50720	C	-0.98280	-3.04330	-3.26070
H	3.14180	3.83320	1.99000	H	-0.88330	-3.23840	-4.33470
C	-0.13690	3.16910	2.62120	H	-1.36060	-2.02840	-3.12170
C	1.16250	3.43300	2.87990	C	2.87450	-0.46490	-2.24030

H	2.61220	-0.08050	-3.22910	C	-4.45070	-0.45980	-1.83720
H	3.95040	-0.43040	-2.11190	C	-3.72480	0.44310	-2.76510
H	2.38500	0.16800	-1.49260	C	-3.40460	0.03010	-3.99760
C	4.42370	-3.09910	-1.28330	H	-3.50550	-1.66150	-5.43620
C	0.39420	-5.64800	-2.42630	H	-4.69390	-3.14640	-3.93240
H	0.44730	-8.17910	-3.08790	H	-5.35000	-2.36210	-1.61990
H	1.41790	-8.62180	-1.64330	H	-3.45880	1.44650	-2.46120
H	7.14990	-1.60090	-2.15960	H	-2.87530	0.69130	-4.67150
H	6.83570	-2.20940	-0.50020	C	0.73930	3.34510	-5.02930
O	1.15390	-6.63110	-1.87800	C	0.23710	4.12730	-4.06760
O	-0.61430	-5.87990	-3.06880	C	0.93740	4.24970	-2.77280
O	4.85500	-4.00380	-0.58070	C	2.07800	3.57250	-2.54880
O	5.23960	-2.18670	-1.85000	C	2.63780	2.72310	-3.62770
Si	-4.98960	0.16980	-0.16620	C	1.99990	2.61190	-4.79950
Si	2.92920	3.68140	-0.89040	H	0.22560	3.25010	-5.97710
C	-9.61630	0.90150	-0.16530	H	-0.68690	4.66620	-4.23240
C	-8.98880	0.64670	-1.31970	H	0.49980	4.86880	-1.99910
C	-7.52880	0.41680	-1.33510	H	3.56190	2.18330	-3.48000
C	-6.82640	0.46320	-0.19040	H	2.40810	1.98600	-5.58240
C	-7.52730	0.74610	1.08540	C	6.75340	0.99870	-0.65560
C	-8.84960	0.95390	1.09580	C	6.70080	2.01780	-1.52000
H	-10.68530	1.06990	-0.15320	C	5.48150	2.84580	-1.61260
H	-9.54870	0.60870	-2.24510	C	4.41770	2.57310	-0.83840
H	-7.04530	0.22000	-2.28230	C	4.47620	1.43300	0.10650
H	-6.97130	0.78770	2.01380	C	5.58410	0.68660	0.18970
H	-9.35960	1.16120	2.02760	H	7.65110	0.39980	-0.57600
C	-4.23460	-2.97890	3.23420	H	7.55570	2.24680	-2.14280
C	-5.16070	-3.20850	2.29700	H	5.46830	3.68520	-2.29700
C	-5.41030	-2.20620	1.24040	H	3.62240	1.18850	0.72190
C	-4.69730	-1.06670	1.20090	H	5.62570	-0.15210	0.86910
C	-3.70670	-0.79840	2.27560	C	4.62560	8.00030	-0.15730
C	-3.48000	-1.71080	3.22850	C	3.71260	7.80490	-1.11490
H	-4.04540	-3.71540	4.00430	C	3.17260	6.45120	-1.36070
H	-5.72280	-4.13330	2.30420	C	3.58110	5.41020	-0.61350
H	-6.17720	-2.40980	0.50590	C	4.61350	5.63340	0.43040
H	-3.16400	0.13350	2.31130	C	5.10310	6.85990	0.64810
H	-2.75200	-1.51540	4.00530	H	5.02190	8.99120	0.02290
C	-3.77300	-1.32840	-4.44190	H	3.36630	8.63830	-1.71240
C	-4.42660	-2.14810	-3.61120	H	2.44810	6.33040	-2.15000
C	-4.79250	-1.69090	-2.25470	H	4.99750	4.80270	1.00770

H	5.85930	7.01640	1.40650	C	3.95940	-2.22450	2.30170
N	1.02070	-1.97190	-2.45590	C	2.67930	-1.70920	2.05810
H	0.44930	-1.08960	-2.53930	C	2.30400	-0.48840	2.64640
H	-1.68300	-3.77560	-2.86740	C	3.18460	0.17780	3.49350
C	6.63950	-2.35730	-1.56460	H	5.12530	0.16260	4.43920
H	6.96800	-3.35850	-1.85030	H	5.81130	-1.96860	3.35280
C	0.64380	-7.96260	-2.03570	H	4.29260	-3.12130	1.79870
H	-0.27860	-8.08310	-1.46360	H	1.33230	-0.06980	2.40950
C	2.21760	-4.19610	-1.40140	H	2.88170	1.11720	3.94460
H	1.86860	-4.12180	-0.10130	C	-2.75550	-4.44460	-0.00770
H	2.80930	-5.10330	-1.33260	C	-2.27120	-3.13670	0.05930
O	0.53890	-0.06390	0.06660	C	-0.97890	-2.89670	0.49680
H	1.14970	-1.62750	0.71170	C	-0.09510	-3.94200	0.82810
C	3.01150	-6.22420	4.20430	C	-0.59830	-5.26910	0.73520
C	3.59830	-6.20540	2.94000	C	-1.92640	-5.49740	0.34770
C	1.97370	-4.56500	2.19240	H	-3.77120	-4.64150	-0.33750
C	1.38690	-4.59120	3.46900	H	-2.87250	-2.29330	-0.24440
C	1.90690	-5.41040	4.46760	H	-0.65730	-1.86510	0.56310
H	3.41040	-6.86880	4.98170	H	-2.26650	-6.52670	0.31080
H	4.46170	-6.82880	2.72870	O	0.11880	-6.39890	0.97820
H	0.51970	-3.96960	3.66850	H	0.99840	-6.18500	1.32440
H	1.44490	-5.41830	5.45020	C	3.08880	-5.37590	1.93660
C	4.44410	-0.35640	3.77170	H	3.57610	-5.33490	0.96800
C	4.82400	-1.55470	3.16850				
C	1.97190	-2.90940	0.83340	H	5.96720	-5.36810	0.90130
C	4.76910	-2.90940	0.43720	C	-2.15710	-3.51550	1.76340
C	4.06590	-1.79240	0.20100	C	0.54090	-2.90800	1.21490
C	2.57220	-1.81440	0.29400	C	-0.38560	-2.79160	0.24930
H	5.84670	-2.91840	0.35390	C	-1.77830	-3.25660	0.50130
C	4.09600	-4.15270	0.83910	H	-3.16560	-3.83300	1.98290
C	2.76130	-4.16480	1.03460	C	0.11400	-3.17570	2.61580
C	2.10130	-5.45260	1.39620	C	-1.18580	-3.43850	2.87380
C	2.82780	-6.56270	1.56870	C	-1.62780	-3.69510	4.26380
C	4.29070	-6.52630	1.38980	C	-0.74740	-3.64030	5.26950
C	4.89310	-5.38580	1.03890	C	0.66900	-3.32590	4.99740
H	1.02730	-5.51500	1.50750	C	1.07980	-3.10350	3.74350
H	2.34220	-7.49420	1.82960	H	-2.66600	-3.92320	4.47110
H	4.87330	-7.42690	1.53460	H	-1.07170	-3.82370	6.28570

H	1.37380	-3.27110	5.81700	H	6.95800	-0.83710	2.01660
H	2.11910	-2.86080	3.56340	H	9.34330	-1.22840	2.03900
O	1.88500	-0.65010	0.00790	C	4.23740	2.94880	3.22190
P	0.43940	-0.67500	-0.82360	C	5.16710	3.17260	2.28700
O	-0.02970	-2.25490	-0.96000	C	5.41590	2.16690	1.23340
O	0.62430	-0.16770	-2.23350	C	4.69830	1.03040	1.19410
N	-1.68750	2.34600	1.21830	C	3.70380	0.76820	2.26680
C	-1.30160	3.66920	1.14960	C	3.47800	1.68360	3.21700
C	-0.96830	4.32440	-2.16380	H	4.04880	3.68770	3.98980
C	-0.36090	3.15990	-2.60170	H	5.73290	4.09520	2.29380
C	-2.34350	1.87300	-2.06940	H	6.18570	2.36590	0.50060
C	-2.98630	3.00610	-1.60390	H	3.15780	-0.16170	2.30350
C	0.96820	3.03210	-3.28410	H	2.74720	1.49250	3.99230
H	0.85540	3.22200	-4.35780	C	3.77080	1.30150	-4.44270
H	1.34130	2.01550	-3.14480	C	4.44170	2.11190	-3.61660
C	-2.89660	0.48890	-2.20600	C	4.81180	1.64910	-2.26330
H	-2.65450	0.10350	-3.19950	C	4.45590	0.42280	-1.84330
H	-3.97040	0.46300	-2.05960	C	3.71270	-0.47050	-2.76690
H	-2.39940	-0.14800	-1.46690	C	3.38890	-0.05260	-3.99670
C	-4.41250	3.13820	-1.23680	H	3.49990	1.63890	-5.43460
C	-0.38140	5.65150	-2.44790	H	4.71940	3.10690	-3.93920
H	-0.42690	8.17710	-3.13000	H	5.38150	2.31310	-1.63170
H	-1.38310	8.63700	-1.68120	H	3.43650	-1.47080	-2.46190
H	-7.16320	1.65610	-2.06140	H	2.84660	-0.70670	-4.66730
H	-6.81440	2.25320	-0.40490	C	-0.78280	-3.29310	-5.04060
O	-1.13090	6.64300	-1.90080	C	-0.27810	-4.08500	-4.08820
O	0.62190	5.87280	-3.10200	C	-0.97450	-4.21950	-2.79250
O	-4.82660	4.05080	-0.53400	C	-2.11310	-3.54250	-2.55770
O	-5.24350	2.22710	-1.78320	C	-2.67690	-2.68440	-3.62740
Si	4.98780	-0.20930	-0.17090	C	-2.04280	-2.56240	-4.80010
Si	-2.95740	-3.66430	-0.89650	H	-0.27160	-3.18880	-5.98880
C	9.60920	-0.97390	-0.15350	H	0.64550	-4.62220	-4.26080
C	8.98730	-0.71630	-1.31030	H	-0.53480	-4.84620	-2.02610
C	7.52920	-0.47550	-1.33100	H	-3.60110	-2.14700	-3.47220
C	6.82270	-0.51480	-0.18860	H	-2.45370	-1.92970	-5.57620
C	7.51740	-0.80090	1.09000	C	-6.76890	-0.96800	-0.60950
C	8.83790	-1.01870	1.10520	C	-6.72480	-1.97600	-1.48740
H	10.67690	-1.15050	-0.13760	C	-5.50970	-2.80840	-1.59630
H	9.55060	-0.68400	-2.23390	C	-4.44090	-2.55010	-0.82420
H	7.05010	-0.27700	-2.28010	C	-4.49000	-1.42170	0.13560

C	-5.59430	-0.67200	0.23450	C	-1.29730	4.61200	3.46780
H	-7.66350	-0.36620	-0.51790	C	-1.79230	5.44070	4.47140
H	-7.58350	-2.19300	-2.10920	H	-3.27110	6.91780	5.00350
H	-5.50370	-3.63930	-2.29110	H	-4.35900	6.88070	2.76790
H	-3.63240	-1.18840	0.75000	H	-0.43350	3.98220	3.65580
H	-5.62890	0.15740	0.92590	H	-1.31430	5.44760	5.44630
C	-4.66400	-7.98620	-0.20520	C	-4.41480	0.39960	3.79650
C	-3.75560	-7.78220	-1.16530	C	-4.78510	1.60470	3.20080
C	-3.21240	-6.42740	-1.39760	C	-3.91980	2.26720	2.32920
C	-3.61330	-5.39410	-0.63560	C	-2.64840	1.73680	2.07200
C	-4.64070	-5.62660	0.41120	C	-2.28340	0.50910	2.65240
C	-5.13320	-6.85400	0.61670	C	-3.16440	-0.14920	3.50520
H	-5.06280	-8.97780	-0.03500	H	-5.09630	-0.11330	4.46830
H	-3.41550	-8.60930	-1.77490	H	-5.76520	2.03040	3.39590
H	-2.49200	-6.29950	-2.18950	H	-4.24610	3.17050	1.83340
H	-5.01900	-4.80170	1.00040	H	-1.31940	0.07900	2.40490
H	-5.88590	-7.01720	1.37710	H	-2.86910	-1.09400	3.95000
N	-1.03280	1.97950	-2.44760	C	2.79240	4.41120	-0.05980
H	-0.46890	1.09300	-2.53330	C	2.29830	3.10810	0.02640
H	1.67840	3.76200	-2.90440	C	1.00920	2.88310	0.48070
C	-6.63690	2.40590	-1.47200	C	0.13790	3.93910	0.81080
H	-6.96360	3.41080	-1.74620	C	0.65090	5.26080	0.69950
C	-0.61560	7.97050	-2.07440	C	1.97610	5.47460	0.29420
H	0.31230	8.09120	-1.51110	H	3.80590	4.59630	-0.40310
C	-2.19980	4.21730	-1.38960	H	2.88910	2.25660	-0.27460
H	-1.83530	4.14200	-0.09370	H	0.67980	1.85490	0.56140
H	-2.78320	5.12950	-1.31600	H	2.32400	6.50060	0.24240
O	-0.53950	0.06220	0.07320	O	-0.05500	6.39830	0.93950
H	-1.12990	1.63950	0.71430	H	-0.93010	6.19480	1.30300
C	-2.89200	6.26550	4.22250	C	-3.01490	5.40950	1.95980
C	-3.49930	6.24830	2.96790	H	-3.51740	5.37080	0.99880
C	-1.90480	4.58730	2.20090				
C	-2.04790	2.86690	0.86640	C	-2.87460	4.10060	1.04740
C	-4.84860	2.76600	0.50880	C	-2.25160	5.41670	1.36920
C	-4.11260	1.66580	0.29420	C	-3.01080	6.50790	1.52010
C	-2.61980	1.73950	0.36660	C	-4.47360	6.42140	1.35770
H	-5.92670	2.73850	0.43740	C	-5.04380	5.25360	1.04470
C	-4.21060	4.04090	0.86890	H	-1.17900	5.51440	1.46880

H	-2.55210	7.46060	1.75170	H	6.97020	-3.67130	-1.43210
H	-5.08250	7.30720	1.48440	O	-0.32870	-5.91250	-3.01590
H	-6.11820	5.19900	0.91940	O	1.48430	-6.60590	-1.86240
C	2.08380	3.58690	1.71640	O	5.27090	-1.77470	-1.91460
C	-0.61080	2.91820	1.22140	O	5.00700	-3.66340	-0.71720
C	0.30250	2.80490	0.24260	Si	-4.98420	0.04300	-0.02980
C	1.68880	3.30490	0.46450	Si	2.82330	3.74070	-0.96160
H	3.08760	3.93280	1.91390	C	-9.63380	0.61510	-0.04590
C	-0.16730	3.21910	2.61050	C	-8.94810	0.71860	1.09860
C	1.13200	3.50750	2.84360	C	-7.48120	0.54170	1.10120
C	1.59160	3.79320	4.22220	C	-6.82920	0.27850	-0.04410
C	0.72810	3.74070	5.24260	C	-7.59450	0.16660	-1.31000
C	-0.68720	3.40000	4.99820	C	-8.92380	0.32630	-1.30830
C	-1.11400	3.15060	3.75470	H	-10.70850	0.74380	-0.04950
H	2.62900	4.04120	4.40930	H	-9.46600	0.93090	2.02490
H	1.06540	3.94550	6.25040	H	-6.94390	0.62760	2.03770
H	-1.37810	3.34780	5.82970	H	-7.08780	-0.03620	-2.24390
H	-2.15220	2.88910	3.59550	H	-9.48140	0.24720	-2.23260
O	-1.89500	0.59290	0.10710	C	-4.12830	-3.05750	3.38940
P	-0.48620	0.65030	-0.78500	C	-3.46800	-1.89450	3.37280
O	-0.06070	2.24020	-0.95270	C	-3.74710	-0.89850	2.31770
O	-0.72210	0.12800	-2.18240	C	-4.64170	-1.16690	1.34920
N	1.85820	-2.24600	1.23590	C	-5.40230	-2.44030	1.40280
C	1.54480	-3.58620	1.14570	C	-5.15290	-3.33730	2.36460
C	1.16190	-4.27320	-2.13980	H	-3.92180	-3.78950	4.15930
C	0.42200	-3.18190	-2.55960	H	-2.72270	-1.68240	4.12840
C	2.30800	-1.71150	-2.17430	H	-3.20720	0.03510	2.34530
C	3.07380	-2.76170	-1.69920	H	-6.17920	-2.64460	0.67860
C	-0.95860	-3.17490	-3.14970	H	-5.70890	-4.26510	2.39950
H	-0.91810	-3.43840	-4.21220	C	-3.81030	-1.49040	-4.30250
H	-1.37880	-2.17240	-3.05060	C	-4.39460	-2.32400	-3.43470
C	2.74570	-0.29970	-2.40530	C	-4.74280	-1.85590	-2.07740
H	2.33060	0.05530	-3.35150	C	-4.45490	-0.59920	-1.69740
H	3.82750	-0.21650	-2.41900	C	-3.80460	0.31860	-2.66560
H	2.32750	0.32130	-1.60650	C	-3.49980	-0.10520	-3.89830
C	4.53110	-2.63580	-1.47860	H	-3.55560	-1.83170	-5.29740
C	0.80180	-5.69640	-2.30520	H	-4.61840	-3.34190	-3.72620
H	-0.84730	-7.75620	-2.18630	H	-5.24470	-2.54030	-1.41150
H	-1.62340	-7.28890	-3.73660	H	-3.58180	1.34080	-2.39040
H	6.64570	-4.50420	0.12350	H	-3.02560	0.56690	-4.60180

C	0.44550	3.52360	-5.00380	C	2.41460	-4.03590	-1.42800
C	-0.01320	4.27230	-3.99480	H	2.08390	-3.99320	-0.13300
C	0.74690	4.35610	-2.73120	H	3.06140	-4.90770	-1.38840
C	1.89920	3.67750	-2.58300	O	0.54560	-0.05250	0.07860
C	2.40950	2.86490	-3.71360	H	1.26090	-1.56330	0.74450
C	1.71740	2.78860	-4.85700	C	3.36960	-6.17350	4.09460
H	-0.11200	3.45690	-5.92900	C	3.86430	-6.17590	2.79160
H	-0.94530	4.81230	-4.09860	C	2.23270	-4.49490	2.15170
H	0.34510	4.94940	-1.91880	C	1.73850	-4.50180	3.46600
H	3.34000	2.32360	-3.62710	C	2.30780	-5.32990	4.43000
H	2.08960	2.18930	-5.67780	H	3.80540	-6.82590	4.84500
C	6.60820	0.98800	-0.93360	H	4.68940	-6.82800	2.52180
C	6.52350	2.00260	-1.80140	H	0.90430	-3.85680	3.72340
C	5.32150	2.86130	-1.82040	H	1.91640	-5.32230	5.44270
C	4.30130	2.61620	-0.98120	C	4.58920	-0.18220	3.71520
C	4.40050	1.49020	-0.02350	C	4.96960	-1.40090	3.15490
C	5.49530	0.72070	-0.00110	C	4.10280	-2.10390	2.31780
H	7.48780	0.35770	-0.91660	C	2.82180	-1.59980	2.05460
H	7.33710	2.20050	-2.48710	C	2.44430	-0.36160	2.60470
H	5.28170	3.69350	-2.51250	C	3.32580	0.33630	3.42460
H	3.58550	1.27580	0.65100	H	5.27210	0.36300	4.35940
H	5.56430	-0.10820	0.68840	H	5.95790	-1.80600	3.35240
C	4.59340	8.02740	-0.22230	H	4.42920	-3.02470	1.85680
C	3.63630	7.85940	-1.14130	H	1.47050	0.04590	2.35630
C	3.07170	6.51600	-1.38830	H	3.02180	1.29040	3.84280
C	3.50360	5.45690	-0.68080	C	-2.58040	-4.49650	0.14980
C	4.58290	5.64980	0.32060	C	-2.12730	-3.17590	0.19660
C	5.09420	6.86720	0.53960	C	-0.82090	-2.90480	0.56670
H	5.00770	9.01080	-0.04130	C	0.10860	-3.92490	0.85480
H	3.27220	8.70760	-1.70660	C	-0.36300	-5.26620	0.77910
H	2.31000	6.41690	-2.14520	C	-1.70470	-5.52630	0.45380
H	4.98020	4.80440	0.86710	H	-3.60790	-4.71930	-0.12320
H	5.88370	7.00200	1.26770	H	-2.76540	-2.34680	-0.06940
N	0.99440	-1.94380	-2.47320	H	-0.52700	-1.86450	0.61870
H	0.35980	-1.10340	-2.54170	H	-2.01610	-6.56540	0.43490
H	-1.60230	-3.89830	-2.65490	O	0.37570	-6.38150	0.99580
C	6.42560	-3.62790	-0.48630	H	1.29560	-6.16770	1.20760
H	6.70370	-2.71140	0.03910	C	3.30490	-5.33630	1.82350
C	-0.69590	-7.29370	-3.16430	H	3.71280	-5.32350	0.81900
H	0.08230	-7.84420	-3.69810				



C	0.59450	3.43640	0.51800	C	0.63030	-3.19050	-1.94080
C	-1.62370	5.12680	0.08430	C	0.28570	-4.33200	-1.24690
C	-1.76700	3.79880	-0.04490	C	-2.57260	-1.82470	-3.25680
C	-0.57010	2.90850	0.06730	H	-2.63210	-2.12780	-4.30810
H	-2.47020	5.79170	-0.01640	H	-2.13910	-0.82460	-3.19940
C	-0.30800	5.71840	0.37560	C	2.00240	-2.68090	-2.25460
C	0.75880	4.91980	0.58570	H	2.11800	-2.57840	-3.33890
C	2.08830	5.54450	0.83530	H	2.77290	-3.34900	-1.88580
C	2.21130	6.87560	0.89180	H	2.12750	-1.69370	-1.80220
C	1.03110	7.73800	0.69550	C	1.21540	-5.36560	-0.72230
C	-0.16340	7.19130	0.44640	C	-3.33690	-4.69710	-2.07430
H	2.97290	4.93400	0.95890	H	-5.97370	-4.92430	-2.28950
H	3.17970	7.32410	1.07210	H	-5.93400	-4.23990	-3.94730
H	1.13660	8.81400	0.74590	H	4.13750	-6.46930	-1.55710
H	-1.02430	7.83080	0.29590	H	3.44270	-6.49130	0.10130
C	4.12360	1.30330	1.68220	O	-4.17340	-4.11380	-2.96030
C	1.69900	2.56390	0.98240	O	-3.57350	-5.76900	-1.54850
C	2.31010	1.74520	0.10500	O	0.91650	-6.11710	0.18910
C	3.65570	1.19230	0.42910	O	2.38560	-5.46890	-1.38860
H	5.08520	0.89140	1.95150	Si	-3.48040	3.09560	-0.31190
C	2.21340	2.66600	2.37810	Si	4.78000	0.46920	-0.88090
C	3.36640	2.04490	2.70790	C	-6.63750	6.54580	-0.04720
C	3.88990	2.13440	4.09070	C	-6.38710	5.97150	-1.22990
C	3.21150	2.81260	5.02290	C	-5.39300	4.88230	-1.32990
C	1.93450	3.46740	4.67880	C	-4.73950	4.46270	-0.23330
C	1.45630	3.39540	3.43110	C	-5.01890	5.10530	1.07360
H	4.82190	1.64920	4.35230	C	-5.91890	6.09210	1.16050
H	3.59260	2.87530	6.03400	H	-7.36480	7.34390	0.02670
H	1.38010	3.99730	5.44260	H	-6.91120	6.30410	-2.11660
H	0.50730	3.86330	3.20430	H	-5.20010	4.44500	-2.29980
O	-0.73210	1.54760	-0.08310	H	-4.49370	4.77990	1.96310
P	0.29930	0.72030	-1.05040	H	-6.12130	6.56040	2.11510
O	1.73260	1.49450	-1.11460	C	-4.63950	0.17430	3.18150
O	-0.16800	0.48570	-2.44480	C	-5.54060	0.50150	2.24960
N	-0.93140	-1.99650	1.37100	C	-5.17620	1.43170	1.16030
C	-1.76210	-3.12900	1.32560	C	-3.93160	1.93270	1.07890
C	-2.06720	-3.95710	-1.86530	C	-2.95990	1.61780	2.15830
C	-1.70400	-2.77330	-2.48560	C	-3.29250	0.77390	3.14340

H	-4.90060	-0.51540	3.97350	C	6.94770	2.16800	-1.47860
H	-6.53460	0.07480	2.28220	C	6.48480	1.20170	-0.66600
H	-5.93340	1.69870	0.43810	C	7.36630	0.67890	0.40880
H	-1.98420	2.07820	2.17750	C	8.59510	1.18050	0.58100
H	-2.58200	0.54450	3.92690	H	10.07940	2.65950	-0.16050
C	-3.74020	1.18070	-4.59160	H	8.66350	3.50610	-1.93700
C	-2.62720	1.81670	-4.21090	H	6.34900	2.56280	-2.28400
C	-2.53470	2.40290	-2.85760	H	7.02770	-0.12260	1.05270
C	-3.55850	2.28740	-1.99350	H	9.23490	0.79420	1.36390
C	-4.79920	1.60440	-2.43560	N	-0.38800	-2.40240	-2.41900
C	-4.88040	1.07290	-3.66140	H	-0.16390	-1.43870	-2.70230
H	-3.80830	0.74730	-5.58090	H	-3.58300	-1.81010	-2.85630
H	-1.78990	1.90090	-4.89150	C	3.22670	-6.55950	-0.96640
H	-1.63370	2.93790	-2.59290	H	2.73310	-7.51350	-1.16540
H	-5.65900	1.55280	-1.78610	C	-5.39340	-4.83240	-3.20930
H	-5.78840	0.57720	-3.97950	H	-5.17830	-5.83010	-3.59890
C	3.13930	1.34230	-5.19170	C	-1.11210	-4.58640	-0.98380
C	3.29270	2.34330	-4.31790	H	-1.36660	-3.91230	0.37730
C	3.82880	2.07160	-2.96840	H	-1.37700	-5.57920	-0.63780
C	4.15600	0.81830	-2.60560	O	0.60030	-0.57430	-0.21370
C	4.00720	-0.28080	-3.58970	H	-0.13240	-1.12630	0.27720
C	3.51870	-0.03260	-4.81110	C	-1.94450	-5.50400	4.95500
H	2.74260	1.53830	-6.17940	C	-2.39160	-4.18010	4.93140
H	3.01750	3.35290	-4.59400	C	-1.78380	-4.00010	2.58590
H	3.92300	2.89310	-2.26880	C	-1.33510	-5.32270	2.61740
H	4.29340	-1.29040	-3.33410	C	-1.41720	-6.07020	3.79650
H	3.40660	-0.83840	-5.52500	H	-2.00660	-6.08560	5.87040
C	5.39650	-4.08400	-0.01440	H	-2.80330	-3.72670	5.82870
C	6.14260	-3.47010	-0.93870	H	-0.89310	-5.76970	1.73350
C	5.92020	-2.04170	-1.23820	H	-1.06120	-7.09650	3.80310
C	4.96350	-1.35550	-0.59110	C	2.19260	-1.48750	4.19460
C	4.11980	-2.04820	0.41380	C	2.04930	-2.71610	3.54910
C	4.32620	-3.34350	0.68320	C	1.02980	-2.92360	2.62070
H	5.57540	-5.12420	0.22270	C	0.11070	-1.89950	2.32240
H	6.92450	-4.01270	-1.45390	C	0.29000	-0.65310	2.95360
H	6.55990	-1.55240	-1.96240	C	1.30260	-0.45750	3.88730
H	3.32800	-1.51830	0.92680	H	2.98420	-1.33410	4.92200
H	3.70710	-3.85590	1.40650	H	2.74070	-3.52590	3.76650
C	9.08570	2.25500	-0.30350	H	0.95140	-3.88050	2.11820
C	8.30420	2.72150	-1.28370	H	-0.39110	0.15370	2.70550

H	1.38520	0.50140	4.38970	H	-6.19180	-4.52190	0.73200
C	-5.83340	-2.55970	-0.10850	H	-3.87750	-4.80780	1.49720
C	-5.46800	-3.73170	0.56060	H	-5.15280	-0.63670	-0.81460
C	-4.15910	-3.88540	1.00320	O	-2.72410	-0.67730	-0.03430
C	-3.18450	-2.88660	0.82640	H	-1.95990	-0.85850	0.57950
C	-3.57990	-1.70230	0.16260	C	-2.31620	-3.43750	3.75680
C	-4.89350	-1.55930	-0.31160	H	-2.67080	-2.41150	3.73930
H	-6.85090	-2.42150	-0.46360				

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C	-3.03920	1.88070	0.96350	H	-3.20510	1.73050	3.67380
C	-5.59700	0.86510	0.32340	O	-2.04580	-0.13230	0.17640
C	-4.51030	0.11550	0.08570	P	-0.79970	0.43410	-0.78960
C	-3.15080	0.67050	0.36210	O	-0.97000	2.08030	-0.84350
H	-6.58800	0.49460	0.10290	O	-0.96650	-0.12700	-2.17700
C	-5.47200	2.22290	0.87920	N	2.43070	-1.36870	1.22480
C	-4.25460	2.72190	1.18070	C	3.65850	-1.79630	0.75940
C	-4.15510	4.12020	1.68710	C	1.50370	-4.02990	-0.44320
C	-5.25860	4.85310	1.87440	C	0.43220	-3.24450	-0.82100
C	-6.58560	4.28630	1.57070	C	1.68850	-2.36230	-2.69210
C	-6.68840	3.04130	1.09460	C	2.81560	-3.06550	-2.30230
H	-3.19320	4.56800	1.89700	C	-0.90170	-3.20960	-0.14770
H	-5.18000	5.86860	2.24100	H	-1.47780	-2.34780	-0.47600
H	-7.47450	4.88380	1.72680	H	-1.45250	-4.12970	-0.35410
H	-7.66570	2.63440	0.86630	C	1.52190	-1.54460	-3.93940
C	0.69870	3.71370	2.00450	H	1.45050	-2.20300	-4.81120
C	-1.71140	2.40170	1.36040	H	0.61580	-0.94100	-3.86310
C	-0.79010	2.62620	0.40290	H	2.39130	-0.90970	-4.10680
C	0.42940	3.41530	0.72280	C	4.01180	-3.11640	-3.16730
H	1.56460	4.31460	2.25760	C	1.47150	-5.09510	0.57840
C	-1.38200	2.68430	2.78500	H	0.50250	-6.11180	2.91320
C	-0.21190	3.28860	3.08630	H	-0.87590	-6.80310	2.00160
C	0.14750	3.54690	4.49950	H	6.88360	-4.56970	-2.78320
C	-0.67340	3.16060	5.48250	H	6.01930	-4.35720	-4.34190
C	-1.94110	2.47610	5.16220	O	0.23120	-5.47980	0.94640
C	-2.27910	2.24780	3.88790	O	2.48310	-5.61210	1.02860
H	1.07790	4.04510	4.74190	O	4.12890	-2.60580	-4.26690
H	-0.40860	3.34570	6.51540	O	5.00890	-3.83750	-2.58950
H	-2.59420	2.15380	5.96280	Si	-4.72350	-1.60380	-0.61440

Si	1.46430	4.23120	-0.59710	H	1.04040	9.83020	0.73610
C	-9.24190	-2.63840	-1.28760	H	-0.95640	8.51550	0.32830
C	-8.76710	-2.47500	-0.04730	H	-0.76880	6.05220	-0.25630
C	-7.34240	-2.14460	0.16220	H	3.54380	6.40540	0.02050
C	-6.51950	-1.99830	-0.89020	H	3.34180	8.73650	0.58310
C	-7.04980	-2.18760	-2.26250	C	0.03890	3.40450	-4.99050
C	-8.34100	-2.48930	-2.44850	C	-0.10890	4.62610	-4.46670
H	-10.28510	-2.88140	-1.44290	C	0.33060	4.89720	-3.08200
H	-9.42460	-2.58550	0.80520	C	0.86140	3.91420	-2.33300
H	-6.97540	-2.02130	1.17390	C	1.03220	2.56790	-2.92660
H	-6.40250	-2.08450	-3.12280	C	0.64240	2.32660	-4.18410
H	-8.72790	-2.62650	-3.45000	H	-0.28070	3.20450	-6.00500
C	-3.24960	-4.85330	2.42770	H	-0.54720	5.42030	-5.05710
C	-3.11590	-3.55700	2.72860	H	0.22010	5.90070	-2.69920
C	-3.57940	-2.52450	1.77880	H	1.45990	1.77060	-2.33850
C	-4.11300	-2.88080	0.59620	H	0.76730	1.34300	-4.61450
C	-4.28910	-4.32020	0.28510	C	5.96360	2.96950	-0.29440
C	-3.87170	-5.25360	1.14960	C	5.55230	3.76630	-1.28720
H	-2.91120	-5.61000	3.12330	C	4.12610	4.13540	-1.39740
H	-2.66680	-3.26100	3.66770	C	3.23600	3.67560	-0.50200
H	-3.47590	-1.48690	2.06080	C	3.69120	2.75780	0.57190
H	-4.76100	-4.62360	-0.64090	C	4.98690	2.43540	0.67520
H	-3.99600	-6.30340	0.91790	H	7.00800	2.69840	-0.21140
C	-2.50290	-1.59560	-4.74130	H	6.26420	4.14850	-2.00710
C	-2.43460	-2.68000	-3.96070	H	3.81760	4.80410	-2.19170
C	-3.14470	-2.70660	-2.66500	H	2.98600	2.33600	1.27440
C	-3.84030	-1.63440	-2.25200	H	5.32170	1.76850	1.45780
C	-3.93180	-0.44440	-3.13320	N	0.57910	-2.41140	-1.89490
C	-3.29610	-0.42650	-4.31140	H	-0.14860	-1.67920	-2.06930
H	-1.97820	-1.57260	-5.68760	H	-0.77480	-3.14470	0.93280
H	-1.85310	-3.53790	-4.27250	C	6.21730	-3.92630	-3.35770
H	-3.08340	-3.59930	-2.06350	H	6.65840	-2.93510	-3.48720
H	-4.50860	0.41870	-2.82540	C	0.17120	-6.50680	1.94970
H	-3.35720	0.44610	-4.94870	H	0.80090	-7.35420	1.67260
C	1.12250	8.78180	0.48000	C	2.81740	-3.74840	-1.00760
C	0.02110	8.05660	0.25490	H	3.36800	-2.93440	-0.13000
C	0.13590	6.62530	-0.09190	H	3.53270	-4.56090	-0.91580
C	1.34510	6.04750	-0.19960	O	0.47500	0.09420	-0.04150
C	2.56180	6.85360	0.06830	H	1.84170	-0.76860	0.62070
C	2.45380	8.14980	0.38660	C	6.48740	-3.22830	3.69230

C	5.92040	-1.96470	3.81350	H	-0.44090	-2.61450	5.52780
C	4.97920	-1.51880	2.87850	H	1.36440	-4.15770	4.78370
C	4.60340	-2.35380	1.80120	H	2.69210	-3.66380	2.78650
C	5.18800	-3.62280	1.70190	H	0.48010	-0.01690	2.21970
C	6.12040	-4.06620	2.63660	H	-0.87730	-0.53230	4.22470
H	7.21290	-3.56180	4.42840	C	5.59790	0.40200	-2.41650
H	6.18480	-1.29760	4.62700	C	4.22960	0.55800	-2.20530
H	4.88670	-4.28040	0.89590	C	3.58170	-0.12090	-1.17090
H	6.54940	-5.05830	2.54300	C	4.31030	-0.97210	-0.31810
O	4.48330	-0.26710	3.06560	C	5.69400	-1.11750	-0.54170
H	3.75170	-0.10760	2.45070	C	6.33060	-0.43230	-1.57090
C	0.15510	-2.37890	4.65150	H	6.08980	0.93610	-3.22360
C	1.16680	-3.24280	4.23220	H	3.66470	1.21810	-2.85360
C	1.93870	-2.95800	3.10460	H	2.51710	0.03840	-1.02590
C	1.70600	-1.77570	2.38580	H	6.27490	-1.76690	0.10070
C	0.68160	-0.90570	2.80500	H	7.40160	-0.54800	-1.70810
C	-0.08600	-1.21250	3.92380				
C	-3.19410	1.75950	0.89040	C	-0.49790	3.31080	3.08170
C	-5.67590	0.59370	0.21210	C	-0.19000	3.58940	4.50330
C	-4.54400	-0.09700	0.00890	C	-1.02030	3.17040	5.46470
C	-3.22440	0.53920	0.30150	C	-2.24720	2.42980	5.11230
H	-6.63980	0.16330	-0.01990	C	-2.53880	2.18270	3.83000
C	-5.63900	1.96430	0.74930	H	0.71060	4.12860	4.76940
C	-4.45830	2.53410	1.07060	H	-0.79280	3.37020	6.50380
C	-4.44770	3.94050	1.56340	H	-2.90770	2.08160	5.89570
C	-5.59430	4.61250	1.71870	H	-3.43470	1.62400	3.59290
C	-6.88060	3.96940	1.39270	O	-2.07080	-0.19910	0.14930
C	-6.90350	2.71570	0.92890	P	-0.84870	0.42670	-0.81450
H	-3.51680	4.44250	1.79010	O	-1.09590	2.06350	-0.86610
H	-5.58050	5.63420	2.07610	O	-0.99050	-0.14310	-2.20200
H	-7.80460	4.51780	1.52290	N	2.49360	-1.25130	1.23050
H	-7.85150	2.25240	0.68480	C	3.75520	-1.59090	0.78610
C	0.42430	3.77000	2.02440	C	1.70680	-3.86110	-0.38920
C	-1.90650	2.35140	1.31850	C	0.58470	-3.14900	-0.77990
C	-0.97010	2.61410	0.38530	C	1.77840	-2.23650	-2.67520
C	0.20520	3.45580	0.73680	C	2.94290	-2.87180	-2.28350
H	1.25820	4.40550	2.30000	C	-0.73970	-3.17160	-0.08810
C	-1.63100	2.65430	2.75050	H	-1.37380	-2.36170	-0.43960

H	-1.23260	-4.13220	-0.25300	C	-2.24670	-2.85890	-3.93930
C	1.56270	-1.43870	-3.92740	C	-2.97020	-2.89470	-2.65120
H	0.61960	-0.89400	-3.85790	C	-3.74220	-1.86050	-2.27940
H	2.39010	-0.74910	-4.09200	C	-3.90180	-0.70600	-3.19730
H	1.54090	-2.10390	-4.79660	C	-3.25280	-0.68000	-4.36810
C	4.13220	-2.87600	-3.16590	H	-1.84250	-1.77470	-5.69360
C	1.74060	-4.83740	0.70730	H	-1.60480	-3.68440	-4.21830
H	0.81930	-5.72380	3.11340	H	-2.85650	-3.76270	-2.02160
H	-0.45800	-6.63400	2.24560	H	-4.53910	0.12490	-2.92200
H	6.17040	-4.05760	-4.37010	H	-3.36370	0.16730	-5.03220
H	6.76290	-2.61690	-3.51190	C	0.77160	8.84270	0.50760
O	0.54880	-5.31640	1.08820	C	-0.30520	8.09000	0.25540
O	2.78770	-5.22280	1.22940	C	-0.14610	6.66140	-0.08510
O	4.21620	-2.34700	-4.25970	C	1.07950	6.11350	-0.15980
O	5.14970	-3.57870	-2.61270	C	2.26840	6.95000	0.13850
Si	-4.64760	-1.84100	-0.65310	C	2.12010	8.24350	0.45080
Si	1.25440	4.30080	-0.55350	H	0.65710	9.88930	0.75860
C	-9.10670	-3.13040	-1.27170	H	-1.29520	8.52490	0.30170
C	-8.30920	-2.98320	-2.33640	H	-1.03160	6.06610	-0.27260
C	-6.90040	-2.57370	-2.15700	H	3.26210	6.52630	0.11750
C	-6.41750	-2.34050	-0.92480	H	2.98800	8.85240	0.66920
C	-7.30400	-2.51230	0.25140	C	-0.01600	3.45190	-4.99060
C	-8.57890	-2.88480	0.08560	C	-0.21250	4.66710	-4.46770
H	-10.13830	-3.43070	-1.40220	C	0.17690	4.94430	-3.06920
H	-8.69370	-3.16450	-3.33170	C	0.71090	3.97300	-2.30730
H	-6.27640	-2.46740	-3.03370	C	0.93580	2.63440	-2.89990
H	-6.92350	-2.33460	1.24970	C	0.59110	2.38740	-4.16930
H	-9.22530	-3.00770	0.94490	H	-0.29860	3.24750	-6.01510
C	-3.02590	-4.92990	2.47930	H	-0.65360	5.45170	-5.06880
C	-2.96830	-3.62150	2.75070	H	0.02810	5.94310	-2.68730
C	-3.48190	-2.63940	1.77370	H	1.36800	1.84700	-2.30220
C	-3.98120	-3.05240	0.59450	H	0.75570	1.40920	-4.59850
C	-4.07100	-4.50610	0.31500	C	5.77190	3.14870	-0.10930
C	-3.61100	-5.39410	1.20530	C	5.37240	3.93280	-1.11710
H	-2.65210	-5.65000	3.19530	C	3.94170	4.26770	-1.27210
H	-2.54390	-3.27870	3.68550	C	3.03590	3.78930	-0.40260
H	-3.44190	-1.59170	2.03330	C	3.48020	2.88800	0.68970
H	-4.51360	-4.85680	-0.60880	C	4.77940	2.59750	0.83420
H	-3.67260	-6.45430	0.99690	H	6.81920	2.90140	0.00560
C	-2.37720	-1.80510	-4.75320	H	6.09650	4.32800	-1.81750

H	3.64170	4.92550	-2.07870	H	4.40380	-4.55390	1.07110
H	2.76480	2.45270	1.37330	C	0.30840	-2.12940	4.75350
H	5.10560	1.94420	1.63170	C	-0.03650	-1.06870	3.91440
N	0.67270	-2.34310	-1.87450	C	0.70710	-0.79670	2.77060
H	-0.09460	-1.65350	-2.05870	C	1.81730	-1.59610	2.43140
H	-0.60660	-3.05550	0.98760	C	2.15890	-2.66860	3.27190
C	6.35740	-3.62350	-3.38500	C	1.40830	-2.92040	4.42140
H	7.04560	-4.24520	-2.81310	H	-0.27020	-2.33720	5.64840
C	0.55740	-6.24470	2.18980	H	-0.89330	-0.44270	4.14650
H	1.27230	-7.04870	2.00830	H	0.42470	0.00880	2.10420
C	2.99330	-3.54980	-0.99140	H	2.99060	-3.31570	3.03830
H	3.54910	-2.71440	-0.08610	H	1.69670	-3.74900	5.06250
H	3.76420	-4.30970	-0.91100	C	5.56680	0.67290	-2.42660
O	0.43750	0.14050	-0.06690	C	4.20020	0.79190	-2.18600
H	1.89170	-0.67960	0.62090	C	3.59120	0.09200	-1.14080
C	6.73080	-2.34710	3.83650	C	4.35850	-0.74150	-0.30770
C	6.47710	-3.34440	2.90240	C	5.73850	-0.85500	-0.56410
C	5.48680	-3.18480	1.92160	C	6.33670	-0.14980	-1.60290
C	4.74900	-1.98600	1.86810	H	6.02800	1.22380	-3.24040
C	5.00750	-0.99890	2.83590	H	3.60550	1.44160	-2.81800
C	5.98210	-1.16820	3.81220	H	2.52650	0.22520	-0.97300
H	7.50090	-2.49360	4.58830	H	6.34880	-1.49600	0.05920
H	7.02820	-4.27900	2.90630	H	7.40660	-0.24180	-1.76520
H	4.42810	-0.08190	2.80690				
H	6.15950	-0.38390	4.54120				
O	5.32400	-4.21060	1.03260				
C	-3.38560	1.47630	0.98200	H	-8.32960	3.63060	1.45110
C	-5.68380	-0.00590	0.27090	H	-8.06440	1.35580	0.68320
C	-4.46930	-0.54480	0.08800	C	-0.19290	4.11940	2.07200
C	-3.24540	0.25200	0.41370	C	-2.19750	2.24710	1.41790
H	-6.58010	-0.55270	0.01500	C	-1.28620	2.60990	0.49510
C	-5.83480	1.36190	0.79030	C	-0.31150	3.69260	0.80440
C	-4.74420	2.08720	1.11500	H	0.52370	4.88440	2.33170
C	-4.92760	3.49940	1.55710	C	-2.03310	2.69030	2.82990
C	-6.15460	4.02010	1.67360	C	-1.05710	3.57230	3.13770
C	-7.33970	3.20430	1.35240	C	-0.86490	4.00530	4.54100
C	-7.18980	1.94590	0.92790	C	-1.64260	3.50870	5.50960
H	-4.07620	4.13010	1.77240	C	-2.69420	2.52550	5.18390
H	-6.28060	5.04660	1.99310	C	-2.88010	2.13400	3.91800

H	-0.09240	4.72280	4.78800	H	-8.17020	-3.94640	-3.43510
H	-1.49990	3.82310	6.53540	H	-5.86160	-2.97230	-3.06390
H	-3.31090	2.11740	5.97420	H	-6.56940	-3.12320	1.20940
H	-3.64570	1.40080	3.70000	H	-8.76730	-4.05730	0.83430
O	-2.00500	-0.34210	0.31010	C	-2.42370	-5.25320	2.42850
P	-0.83680	0.40860	-0.62820	C	-2.51310	-3.95550	2.73920
O	-1.28280	1.99160	-0.73010	C	-3.12240	-3.00560	1.78540
O	-0.88730	-0.17160	-2.02150	C	-3.56400	-3.43460	0.58910
N	2.66580	-1.17100	1.27530	C	-3.49610	-4.88130	0.26830
C	3.94730	-1.36300	0.79840	C	-2.94710	-5.74020	1.13650
C	2.09550	-3.70960	-0.54320	H	-1.97740	-5.94940	3.12660
C	0.92020	-3.05180	-0.86530	H	-2.13860	-3.59780	3.68930
C	2.00920	-1.91470	-2.69920	H	-3.19900	-1.96810	2.07530
C	3.22470	-2.48800	-2.36800	H	-3.89580	-5.25150	-0.66720
C	-0.38600	-3.22050	-0.16030	H	-2.89310	-6.79430	0.89760
H	-1.08600	-2.44320	-0.45590	C	-2.07010	-1.81760	-4.70250
H	-0.80280	-4.20490	-0.38150	C	-1.88810	-2.91890	-3.96470
C	1.71120	-1.03960	-3.88260	C	-2.61330	-3.08420	-2.68760
H	0.79380	-0.47470	-3.70080	C	-3.43360	-2.11730	-2.24500
H	2.54420	-0.37140	-4.09120	C	-3.65450	-0.91240	-3.08310
H	1.57720	-1.65820	-4.77720	C	-3.00520	-0.77020	-4.24540
C	4.40270	-2.33730	-3.25290	H	-1.53420	-1.69250	-5.63440
C	2.21640	-4.75880	0.47630	H	-1.20350	-3.68830	-4.29740
H	1.38920	-5.88670	2.81290	H	-2.45980	-3.98930	-2.12200
H	0.17240	-6.82350	1.88850	H	-4.33590	-0.13730	-2.75610
H	6.52450	-3.27040	-4.51930	H	-3.15880	0.11500	-4.84910
H	7.00380	-1.82670	-3.59810	C	0.48940	9.18370	0.05810
O	1.06850	-5.35630	0.82410	C	-0.20650	8.61460	-0.93230
O	3.29500	-5.09830	0.96540	C	-0.15040	7.15150	-1.13360
O	4.43000	-1.75530	-4.32260	C	0.58620	6.38070	-0.31390
O	5.48620	-2.96320	-2.73420	C	1.37320	7.02430	0.76830
Si	-4.34850	-2.26590	-0.62990	C	1.32300	8.35000	0.94570
Si	0.69130	4.53020	-0.53590	H	0.44920	10.25510	0.20580
C	-8.60820	-4.06070	-1.38310	H	-0.81320	9.22460	-1.58910
C	-7.82250	-3.76710	-2.42600	H	-0.71460	6.72890	-1.94990
C	-6.47690	-3.19750	-2.20370	H	2.01090	6.42960	1.40940
C	-6.04010	-2.96650	-0.95390	H	1.90190	8.81510	1.73310
C	-6.91310	-3.29950	0.19770	C	-0.93540	3.13050	-4.70950
C	-8.13060	-3.81650	-0.00710	C	-1.76320	3.69930	-3.82590
H	-9.59360	-4.47810	-1.54520	C	-1.24310	4.18370	-2.53040



C	0.06110	4.04920	-2.22760	H	6.32190	-0.23860	4.59700
C	0.97680	3.45990	-3.23110	O	5.72910	-3.85930	0.83060
C	0.50350	3.01340	-4.40100	H	4.84120	-4.28100	0.85170
H	-1.31580	2.76450	-5.65440	C	0.60630	-2.53070	4.71940
H	-2.81810	3.78990	-4.04990	C	0.15090	-1.44860	3.96420
H	-1.93840	4.59750	-1.81030	C	0.85300	-1.01780	2.84300
H	2.03340	3.40250	-3.03390	C	2.03410	-1.67510	2.44380
H	1.17650	2.57890	-5.12890	C	2.48610	-2.77130	3.19700
C	5.22250	3.59520	0.17400	C	1.77460	-3.18280	4.32490
C	4.85660	4.44410	-0.79340	H	0.05970	-2.86230	5.59680
C	3.42470	4.71180	-1.04120	H	-0.76150	-0.92980	4.24420
C	2.48350	4.08710	-0.31390	H	0.48620	-0.19310	2.24290
C	2.89530	3.12730	0.74060	H	3.37400	-3.31360	2.91080
C	4.19410	2.90700	0.97910	H	2.14870	-4.02600	4.89920
H	6.27070	3.39950	0.35880	C	5.48820	1.23140	-2.29890
H	5.60850	4.94440	-1.38960	C	4.11600	1.15750	-2.07590
H	3.14950	5.43640	-1.79760	C	3.59220	0.36130	-1.05630
H	2.15510	2.59780	1.32520	C	4.45300	-0.39080	-0.23650
H	4.49430	2.21000	1.74940	C	5.83890	-0.31200	-0.47470
N	0.93010	-2.15850	-1.89270	C	6.35090	0.49930	-1.48180
H	0.10660	-1.50470	-2.00500	H	5.88010	1.85620	-3.09540
H	-0.24610	-3.16420	0.91960	H	3.43920	1.71280	-2.71010
C	6.68500	-2.86860	-3.51590	H	2.51680	0.36510	-0.90070
H	7.42940	-3.45570	-2.97890	H	6.52150	-0.88670	0.13820
C	1.15640	-6.35790	1.85550	H	7.42550	0.55560	-1.62800
H	1.92560	-7.09260	1.61240				
C	3.34510	-3.24780	-1.12550				
H	3.83100	-2.43550	-0.16540				
H	4.17720	-3.94440	-1.10360				
O	0.45870	0.27360	0.14250				
H	2.02370	-0.57830	0.73320				
C	7.03490	-2.09270	3.74230				
C	6.84330	-3.03710	2.74100				
C	5.82310	-2.89000	1.78910				
C	4.98820	-1.75550	1.83550				
C	5.18750	-0.82240	2.86890				
C	6.19290	-0.98070	3.81560				
H	7.83010	-2.22920	4.46930				
H	7.46850	-3.92080	2.66710				
H	4.53910	0.04650	2.91460				

C	-3.20250	1.76080	0.87440	C	-0.73350	-3.16840	-0.10570
C	-5.67800	0.58340	0.19390	H	-1.36740	-2.35810	-0.45640
C	-4.54300	-0.10460	-0.00180	H	-1.22520	-4.12900	-0.27340
C	-3.22640	0.53800	0.29060	C	1.57980	-1.41520	-3.92950
H	-6.63960	0.14810	-0.03850	H	0.63090	-0.88000	-3.86540
C	-5.64740	1.95730	0.72310	H	2.40190	-0.71600	-4.08070
C	-4.46970	2.53240	1.04580	H	1.57400	-2.07390	-4.80390
C	-4.46500	3.94140	1.53110	C	4.14750	-2.85310	-3.16700
C	-5.61400	4.61090	1.67800	C	1.74200	-4.84210	0.68440
C	-6.89720	3.96230	1.35020	H	0.80630	-5.74410	3.08060
C	-6.91470	2.70600	0.89330	H	-0.46390	-6.65050	2.19840
H	-3.53630	4.44690	1.75890	H	6.19090	-4.02200	-4.37340
H	-5.60470	5.63440	2.03010	H	6.78000	-2.58930	-3.49960
H	-7.82330	4.50870	1.47360	O	0.54840	-5.32360	1.05650
H	-7.86030	2.23850	0.64780	O	2.78660	-5.23150	1.20860
C	0.40410	3.78110	2.02730	O	4.23500	-2.31560	-4.25640
C	-1.91920	2.35670	1.30900	O	5.16350	-3.55930	-2.61550
C	-0.97740	2.61920	0.38140	Si	-4.63880	-1.85290	-0.65300
C	0.19380	3.46430	0.73890	Si	1.24990	4.30990	-0.54510
H	1.23490	4.41860	2.30730	C	-9.09140	-3.17120	-1.25740
C	-1.65370	2.66300	2.74220	C	-8.29600	-3.02660	-2.32410
C	-0.52430	3.32280	3.07950	C	-6.88940	-2.60740	-2.14920
C	-0.22700	3.60620	4.50240	C	-6.40640	-2.36300	-0.91930
C	-1.06310	3.18820	5.45930	C	-7.29070	-2.53150	0.25920
C	-2.28570	2.44360	5.10040	C	-8.56350	-2.91280	0.09750
C	-2.56770	2.19200	3.81690	H	-10.12120	-3.47880	-1.38460
H	0.67040	4.14830	4.77330	H	-8.68060	-3.21730	-3.31760
H	-0.84350	3.39170	6.49940	H	-6.26700	-2.50360	-3.02740
H	-2.95080	2.09590	5.88030	H	-6.91010	-2.34440	1.25570
H	-3.46050	1.63040	3.57520	H	-9.20810	-3.03350	0.95840
O	-2.06940	-0.19640	0.14540	C	-2.99850	-4.91600	2.49560
P	-0.84600	0.43050	-0.81610	C	-2.94820	-3.60590	2.75980
O	-1.09460	2.06710	-0.87020	C	-3.46760	-2.63190	1.77770
O	-0.98510	-0.13940	-2.20410	C	-3.96540	-3.05400	0.60110
N	2.49330	-1.25660	1.23140	C	-4.04850	-4.50990	0.33040
C	3.75660	-1.59450	0.79070	C	-3.58260	-5.39040	1.22510
C	1.71290	-3.85830	-0.40540	H	-2.62000	-5.63000	3.21520
C	0.59210	-3.14320	-0.79490	H	-2.52550	-3.25560	3.69260
C	1.79130	-2.21970	-2.68100	H	-3.43340	-1.58280	2.03180
C	2.95500	-2.85630	-2.28900	H	-4.49130	-4.86830	-0.59030

H	-3.63940	-6.45210	1.02290	H	6.81060	2.91230	0.05680
C	-2.37550	-1.82810	-4.75720	H	6.10290	4.34520	-1.76730
C	-2.24830	-2.88230	-3.94330	H	3.64990	4.94180	-2.04780
C	-2.97030	-2.91480	-2.65430	H	2.74490	2.45670	1.38810
C	-3.73600	-1.87660	-2.28070	H	5.08340	1.94770	1.66430
C	-3.89240	-0.72190	-3.19900	N	0.68300	-2.33120	-1.88460
C	-3.24560	-0.69920	-4.37100	H	-0.08480	-1.64100	-2.06740
H	-1.84250	-1.80050	-5.69870	H	-0.60220	-3.05470	0.97050
H	-1.61080	-3.71080	-4.22330	C	6.37410	-3.59700	-3.38360
H	-2.86060	-3.78390	-2.02550	H	7.06020	-4.22390	-2.81480
H	-4.52600	0.11170	-2.92330	C	0.55130	-6.25930	2.15180
H	-3.35460	0.14800	-5.03560	H	1.26850	-7.06110	1.96960
C	0.75170	8.85070	0.51400	C	3.00140	-3.54270	-1.00110
C	-0.32190	8.09620	0.25400	H	3.55360	-2.71320	-0.08950
C	-0.15780	6.66800	-0.08560	H	3.77220	-4.30290	-0.92330
C	1.06930	6.12230	-0.15190	O	0.43910	0.14590	-0.06580
C	2.25450	6.96070	0.15520	H	1.89450	-0.68140	0.62230
C	2.10160	8.25400	0.46670	C	6.71570	-2.37830	3.85090
H	0.63350	9.89700	0.76430	C	6.46500	-3.36810	2.90790
H	-1.31310	8.52920	0.29330	C	5.48060	-3.19890	1.92270
H	-1.04080	6.07100	-0.27970	C	4.74530	-1.99830	1.87410
H	3.24900	6.53880	0.14130	C	5.00140	-1.01850	2.85000
H	2.96680	8.86430	0.69150	C	5.97020	-1.19730	3.83040
C	0.01010	3.46400	-4.99140	H	7.48100	-2.53220	4.60590
C	-0.18970	4.67870	-4.46900	H	7.01390	-4.30390	2.90790
C	0.19000	4.95470	-3.06760	H	4.42480	-0.09960	2.82420
C	0.71830	3.98260	-2.30260	H	6.14560	-0.41860	4.56590
C	0.94680	2.64420	-2.89450	O	5.32140	-4.21740	1.02470
C	0.61090	2.39860	-4.16660	H	4.40180	-4.56300	1.05900
H	-0.26520	3.26060	-6.01810	C	0.29690	-2.14470	4.74450
H	-0.62590	5.46410	-5.07260	C	-0.04180	-1.07770	3.91080
H	0.03930	5.95330	-2.68630	C	0.70510	-0.80280	2.76980
H	1.37520	1.85620	-2.29480	C	1.81250	-1.60520	2.42860
H	0.77830	1.42100	-4.59580	C	2.14760	-2.68410	3.26350
C	5.76420	3.15930	-0.06630	C	1.39360	-2.93900	4.41000
C	5.37300	3.94690	-1.07460	H	-0.28440	-2.35500	5.63710
C	3.94350	4.28150	-1.24090	H	-0.89610	-0.44910	4.14480
C	3.03050	3.79970	-0.38090	H	0.42750	0.00750	2.10720
C	3.46590	2.89470	0.71210	H	2.97710	-3.33340	3.02760
C	4.76390	2.60410	0.86660	H	1.67670	-3.77270	5.04690

C	5.58320	0.69200	-2.39720	H	3.62420	1.46690	-2.78940
C	4.21570	0.81070	-2.16110	H	2.53670	0.23700	-0.95940
C	3.60180	0.10310	-1.12410	H	6.35240	-1.49940	0.07300
C	4.36480	-0.73830	-0.29500	H	7.41910	-0.23110	-1.73660
C	5.74550	-0.85200	-0.54730				
C	6.34870	-0.13880	-1.57770				
H	6.04840	1.24940	-3.20440				
C	-3.18550	1.76360	0.89740	P	-0.84770	0.42570	-0.81420
C	-5.67140	0.60650	0.21850	O	-1.09070	2.06340	-0.86320
C	-4.54170	-0.08760	0.01440	O	-0.99200	-0.14330	-2.20160
C	-3.22000	0.54410	0.30720	N	2.48200	-1.26050	1.23040
H	-6.63650	0.17940	-0.01420	C	3.74530	-1.59650	0.78780
C	-5.62980	1.97690	0.75610	C	1.70360	-3.86900	-0.39420
C	-4.44710	2.54240	1.07790	C	0.58180	-3.15720	-0.78630
C	-4.43140	3.94920	1.56960	C	1.77890	-2.24160	-2.67790
C	-5.57530	4.62590	1.72290	C	2.94290	-2.87690	-2.28450
C	-6.86390	3.98760	1.39620	C	-0.74470	-3.18270	-0.09870
C	-6.89140	2.73340	0.93380	H	-1.37600	-2.36890	-0.44650
H	-3.49870	4.44770	1.79660	H	-1.23900	-4.14100	-0.27310
H	-5.55780	5.64790	2.07910	C	1.56480	-1.44350	-3.93010
H	-7.78580	4.53990	1.52460	H	0.62240	-0.89740	-3.86110
H	-7.84090	2.27370	0.68900	H	2.39320	-0.75500	-4.09480
C	0.43910	3.76570	2.02530	H	1.54210	-2.10880	-4.79930
C	-1.89570	2.35170	1.32350	C	4.13410	-2.88010	-3.16450
C	-0.96060	2.61250	0.38860	C	1.73620	-4.84690	0.70120
C	0.21700	3.45220	0.73800	H	0.80970	-5.73930	3.10240
H	1.27430	4.40000	2.29950	H	-0.46290	-6.65130	2.22950
C	-1.61740	2.65490	2.75510	H	6.17830	-4.05930	-4.36240
C	-0.48240	3.30910	3.08430	H	6.76490	-2.61610	-3.50420
C	-0.17240	3.58920	4.50510	O	0.54440	-5.32960	1.07700
C	-1.00290	3.17410	5.46810	O	2.78260	-5.23020	1.22590
C	-2.23200	2.43620	5.11800	O	4.21950	-2.35190	-4.25850
C	-2.52540	2.18750	3.83640	O	5.15150	-3.58060	-2.60840
H	0.72980	4.12660	4.76950	Si	-4.65000	-1.82950	-0.65210
H	-0.77400	3.37520	6.50660	Si	1.26370	4.29800	-0.55350
H	-2.89290	2.09140	5.90270	C	-9.11060	-3.11290	-1.27160
H	-3.42320	1.63110	3.60110	C	-8.31290	-2.96540	-2.33610
O	-2.06890	-0.19740	0.15220	C	-6.90390	-2.55680	-2.15630

C	-6.42080	-2.32500	-0.92390	H	2.99970	8.84470	0.68350
C	-7.30760	-2.49660	0.25210	C	-0.01900	3.45700	-4.98840
C	-8.58270	-2.86830	0.08590	C	-0.20770	4.67320	-4.46500
H	-10.14220	-3.41290	-1.40240	C	0.18590	4.94800	-3.06720
H	-8.69730	-3.14610	-3.33160	C	0.71640	3.97370	-2.30660
H	-6.27970	-2.45090	-3.03290	C	0.93340	2.63420	-2.90010
H	-6.92710	-2.31970	1.25050	C	0.58410	2.38910	-4.16860
H	-9.22920	-2.99130	0.94510	H	-0.30480	3.25440	-6.01240
C	-3.02880	-4.93140	2.46800	H	-0.64550	5.46040	-5.06510
C	-2.96970	-3.62410	2.74410	H	0.04320	5.94740	-2.68470
C	-3.48300	-2.63780	1.77100	H	1.36290	1.84450	-2.30360
C	-3.98430	-3.04610	0.59100	H	0.74200	1.40990	-4.59810
C	-4.07680	-4.49870	0.30690	C	5.78170	3.14450	-0.11970
C	-3.61650	-5.39040	1.19340	C	5.38030	3.93020	-1.12550
H	-2.65460	-5.65450	3.18080	C	3.94940	4.26560	-1.27720
H	-2.54400	-3.28510	3.67970	C	3.04520	3.78590	-0.40680
H	-3.44110	-1.59110	2.03410	C	3.49160	2.88290	0.68340
H	-4.52170	-4.84570	-0.61720	C	4.79100	2.59180	0.82480
H	-3.68000	-6.44980	0.98140	H	6.82920	2.89690	-0.00740
C	-2.38870	-1.78650	-4.75720	H	6.10310	4.32640	-1.82680
C	-2.26070	-2.84410	-3.94780	H	3.64790	4.92480	-2.08210
C	-2.98100	-2.88190	-2.65790	H	2.77740	2.44670	1.36770
C	-3.74710	-1.84560	-2.27980	H	5.11860	1.93690	1.62030
C	-3.90380	-0.68670	-3.19260	N	0.67180	-2.34900	-1.87920
C	-3.25800	-0.65890	-4.36510	H	-0.09490	-1.65920	-2.06290
H	-1.85660	-1.75490	-5.69900	H	-0.61500	-3.07530	0.97820
H	-1.62350	-3.67150	-4.23190	C	6.36150	-3.62350	-3.37740
H	-2.87020	-3.75340	-2.03260	H	7.04960	-4.24280	-2.80270
H	-4.53660	0.14610	-2.91240	C	0.55180	-6.25960	2.17740
H	-3.36690	0.19150	-5.02560	H	1.26900	-7.06160	1.99680
C	0.78350	8.83700	0.52080	C	2.99110	-3.55570	-0.99290
C	-0.29370	8.08590	0.26550	H	3.54380	-2.71940	-0.08430
C	-0.13530	6.65840	-0.07970	H	3.76300	-4.31440	-0.91050
C	1.08990	6.11000	-0.15580	O	0.43900	0.13650	-0.06870
C	2.27930	6.94460	0.14580	H	1.88080	-0.68750	0.62110
C	2.13160	8.23720	0.46250	C	6.71700	-2.33840	3.84480
H	0.66950	9.88270	0.77550	C	6.46770	-3.33870	2.91260
H	-1.28350	8.52120	0.31290	C	5.47870	-3.18410	1.92950
H	-1.02110	6.06410	-0.26930	C	4.73830	-1.98720	1.87190
H	3.27260	6.52030	0.12370	C	4.99220	-0.99700	2.83770

C	5.96540	-1.16150	3.81630	H	0.39500	-0.02280	2.09260
H	7.48600	-2.48110	4.59840	H	2.98840	-3.32230	3.04000
H	7.02110	-4.27180	2.92010	H	1.68530	-3.77140	5.05410
H	4.41070	-0.08150	2.80500	C	5.55860	0.66720	-2.42440
H	6.13930	-0.37500	4.54380	C	4.19160	0.78470	-2.18610
O	5.32000	-4.21240	1.04280	C	3.58180	0.08550	-1.14070
H	4.39950	-4.55520	1.07650	C	4.34900	-0.74560	-0.30510
C	0.28240	-2.16590	4.73800	C	5.72960	-0.85700	-0.55900
C	-0.06740	-1.10750	3.89800	C	6.32850	-0.15270	-1.59790
C	0.68130	-0.82620	2.75980	H	6.02030	1.21730	-3.23860
C	1.80200	-1.61370	2.42660	H	3.59700	1.43230	-2.82030
C	2.14860	-2.68380	3.26830	H	2.51670	0.21730	-0.97470
C	1.39270	-2.94490	4.41230	H	6.34000	-1.49600	0.06650
H	-0.30030	-2.38120	5.62840	H	7.39880	-0.24320	-1.75820
H	-0.93250	-0.49090	4.12440				
C	3.13530	1.76990	-0.97640	C	0.85490	3.15130	-5.50890
C	5.65350	0.66940	-0.32060	C	2.09720	2.42520	-5.18100
C	4.54130	-0.04540	-0.09380	C	2.41540	2.17880	-3.90490
C	3.20250	0.55430	-0.37860	H	-0.87500	4.08570	-4.77960
H	6.63020	0.26650	-0.09360	H	0.60610	3.35090	-6.54320
C	5.57720	2.03230	-0.87250	H	2.74740	2.08690	-5.97730
C	4.37920	2.57200	-1.18100	H	3.32230	1.63070	-3.68540
C	4.32950	3.97480	-1.68240	O	2.07010	-0.21230	-0.20190
C	5.45800	4.67170	-1.85910	P	0.83880	0.39120	0.75860
C	6.76330	4.06030	-1.54840	O	1.06370	2.03100	0.81520
C	6.82150	2.81090	-1.07620	O	0.97760	-0.17670	2.14640
H	3.38450	4.45500	-1.89720	N	-2.49470	-1.22620	-1.25430
H	5.41560	5.69050	-2.22230	C	-3.72540	-1.62750	-0.77160
H	7.67250	4.62860	-1.69600	C	-1.61770	-3.98550	0.33000
H	7.78330	2.37120	-0.84270	C	-0.51760	-3.24740	0.72380
C	-0.53670	3.71980	-2.04130	C	-1.73460	-2.35580	2.61900
C	1.82840	2.33540	-1.38200	C	-2.88070	-3.02250	2.22430
C	0.90570	2.58260	-0.43150	C	0.81390	-3.27740	0.05120
C	-0.29230	3.40150	-0.75940	H	1.42910	-2.44000	0.37270
H	-1.38660	4.34090	-2.30000	H	1.31770	-4.22420	0.26060
C	1.52170	2.63660	-2.80790	C	-1.51920	-1.54890	3.86900
C	0.37420	3.27900	-3.11650	H	-1.40790	-2.21330	4.73210
C	0.03700	3.55730	-4.53140	H	-0.61580	-0.94520	3.76160

H	-2.37460	-0.90510	4.06860	C	8.26380	-2.77500	2.47120
C	-4.13360	-3.14340	3.00080	H	10.20600	-3.22120	1.48460
C	-1.49310	-5.03660	-0.69840	H	9.37870	-2.89140	-0.77120
H	-2.14100	-7.46360	-1.59540	H	6.95160	-2.25240	-1.16340
H	-3.71750	-6.85740	-2.20200	H	6.33120	-2.31530	3.12670
H	-5.09280	-2.22200	5.94990	H	8.63570	-2.92790	3.47610
H	-6.12180	-2.20460	4.47950	C	0.00340	3.32090	4.95820
O	-2.71200	-5.52980	-1.05410	C	-0.52630	2.34960	4.20740
O	-0.45790	-5.46000	-1.17820	C	-0.94730	2.63360	2.82030
O	-5.12530	-3.70940	2.57090	C	-0.78870	3.85940	2.29750
O	-4.08590	-2.59610	4.23610	C	-0.22280	4.93880	3.14520
Si	4.69440	-1.77270	0.60250	C	0.15730	4.67990	4.40280
Si	-1.34380	4.20980	0.55340	H	0.31300	3.11540	5.97470
C	3.13390	-4.97130	-2.44910	H	-0.64740	1.35540	4.61500
C	3.04870	-3.67130	-2.75310	H	-1.36550	1.83540	2.22730
C	3.54410	-2.65430	-1.80230	H	-0.11730	5.94400	2.76390
C	4.05770	-3.02800	-0.61630	H	0.57090	5.46820	5.01850
C	4.18450	-4.47210	-0.30380	C	-5.86260	3.03370	0.18880
C	3.73950	-5.39150	-1.16950	C	-4.97950	2.52750	-0.67930
H	2.76670	-5.71690	-3.14230	C	-3.54470	2.86290	-0.55920
H	2.61060	-3.36050	-3.69280	C	-3.12470	3.69120	0.41280
H	3.47570	-1.61360	-2.08390	C	-4.10460	4.22470	1.38920
H	4.64090	-4.79020	0.62510	C	-5.40250	3.91680	1.27900
H	3.82750	-6.44460	-0.93630	H	-6.91230	2.78440	0.10380
C	2.42780	-1.71230	4.70370	H	-5.31520	1.87030	-1.46970
C	2.31580	-2.78120	3.90680	H	-2.85340	2.43420	-1.27090
C	3.03830	-2.82430	2.61840	H	-3.77450	4.87290	2.19140
C	3.79160	-1.78260	2.22940	H	-6.11680	4.31010	1.99040
C	3.92940	-0.61000	3.12770	C	-0.81900	8.76530	-0.40590
C	3.28120	-0.57710	4.29890	C	-2.04960	8.24200	-0.35530
H	1.89380	-1.67690	5.64430	C	-2.23430	6.80850	-0.04590
H	1.68950	-3.61380	4.19980	C	-1.16830	6.02860	0.20220
H	2.94020	-3.70450	2.00340	C	0.19360	6.61220	0.13070
H	4.55050	0.22830	2.83800	C	0.35770	7.90940	-0.15460
H	3.37650	0.28300	4.94880	H	-0.68310	9.81440	-0.63460
C	9.17220	-2.94650	1.31930	H	-2.91310	8.86650	-0.54440
C	8.71570	-2.76440	0.07480	H	-3.23790	6.40890	-0.03520
C	7.30390	-2.39050	-0.14840	H	1.06200	5.98950	0.30830
C	6.47460	-2.22290	0.89580	H	1.35240	8.33310	-0.20500
C	6.98430	-2.43380	2.27290	N	-0.63240	-2.42620	1.80970

H	0.12020	-1.72450	1.99310	C	-0.26730	-2.32780	-4.68380
H	0.68820	-3.22820	-1.03020	C	0.01680	-1.16730	-3.96230
C	-5.30090	-2.70650	4.99620	C	-0.73640	-0.82830	-2.84320
H	-5.56600	-3.75540	5.14740	C	-1.78910	-1.66010	-2.41840
C	-2.67590	-6.60390	-2.00660	C	-2.06890	-2.83240	-3.13480
H	-2.17640	-6.28750	-2.92500	C	-1.30990	-3.15180	-4.26110
C	-2.91460	-3.66960	0.91040	H	0.32140	-2.59180	-5.55670
H	-3.44720	-2.80140	0.07410	H	0.83240	-0.51830	-4.26710
H	-3.67680	-4.43910	0.82750	H	-0.49990	0.05350	-2.26080
O	-0.44520	0.09770	0.00680	H	-2.85490	-3.50040	-2.81230
H	-1.87300	-0.66320	-0.64700	H	-1.53460	-4.06480	-4.80470
C	-6.65380	-2.94890	-3.66020	C	-5.51730	0.58750	2.48110
C	-5.99270	-1.73850	-3.83140	C	-6.29970	-0.19980	1.63550
C	-5.02400	-1.32180	-2.91010	C	-5.71170	-0.89150	0.58190
C	-4.70820	-2.13980	-1.80020	C	-4.32710	-0.80560	0.33810
C	-5.39850	-3.34960	-1.64390	C	-3.54650	-0.00750	1.19610
C	-6.36060	-3.76170	-2.56220	C	-4.14580	0.68270	2.25220
H	-7.40080	-3.25760	-4.38550	H	-5.97300	1.13420	3.30130
H	-6.20560	-1.08780	-4.67280	H	-7.37150	-0.27530	1.79080
H	-5.17810	-3.97250	-0.78530	H	-6.33400	-1.50210	-0.05900
H	-6.87840	-4.70430	-2.41810	H	-2.47780	0.10110	1.03740
O	-4.44730	-0.11470	-3.14400	H	-3.54060	1.30500	2.90170
H	-3.71620	0.02620	-2.52340				
C	3.13800	1.76740	-0.97170	C	-0.53370	3.71560	-2.04090
C	5.65570	0.66470	-0.31820	C	1.83170	2.33300	-1.37870
C	4.54310	-0.04960	-0.09160	C	0.90770	2.57980	-0.42930
C	3.20460	0.55140	-0.37450	C	-0.29040	3.39780	-0.75870
H	6.63220	0.26090	-0.09220	H	-1.38350	4.33650	-2.30050
C	5.58000	2.02830	-0.86830	C	1.52670	2.63450	-2.80490
C	4.38210	2.56910	-1.17550	C	0.37880	3.27570	-3.11490
C	4.33300	3.97240	-1.67540	C	0.04330	3.55430	-4.53000
C	5.46170	4.66870	-1.85220	C	0.86330	3.15060	-5.50660
C	6.76680	4.05630	-1.54280	C	2.10640	2.42630	-5.17730
C	6.82460	2.80650	-1.07180	C	2.42290	2.17910	-3.90100
H	3.38810	4.45330	-1.88920	H	-0.86930	4.08140	-4.77910
H	5.41960	5.68790	-2.21450	H	0.61580	3.35060	-6.54100
H	7.67630	4.62430	-1.69040	H	2.75850	2.09000	-5.97290
H	7.78630	2.36600	-0.83920	H	3.33040	1.63240	-3.68050



O	2.07170	-0.21460	-0.19800	C	2.44270	-1.71110	4.71120
P	0.83960	0.38920	0.76150	C	2.32780	-2.78120	3.91640
O	1.06450	2.02890	0.81780	C	3.04630	-2.82660	2.62580
O	0.97880	-0.17740	2.15010	C	3.79870	-1.78570	2.23290
N	-2.49950	-1.22370	-1.25370	C	3.93980	-0.61180	3.12900
C	-3.72940	-1.62850	-0.77270	C	3.29520	-0.57680	4.30200
C	-1.61720	-3.97900	0.33580	H	1.91180	-1.67400	5.65360
C	-0.51900	-3.23940	0.73250	H	1.70240	-3.61330	4.21290
C	-1.74190	-2.34780	2.62360	H	2.94550	-3.70750	2.01210
C	-2.88610	-3.01640	2.22680	H	4.56050	0.22560	2.83630
C	0.81400	-3.26740	0.06310	H	3.39300	0.28420	4.95040
H	1.43020	-2.43380	0.39200	C	9.17400	-2.96030	1.29970
H	1.31520	-4.21680	0.26660	C	8.71290	-2.77520	0.05730
C	-1.53130	-1.53830	3.87280	C	7.30090	-2.39830	-0.15950
H	-1.43130	-2.20000	4.73920	C	6.47610	-2.23110	0.88840
H	-0.62350	-0.94030	3.77030	C	6.99100	-2.44500	2.26300
H	-2.38430	-0.88840	4.06330	C	8.27060	-2.78890	2.45560
C	-4.14080	-3.13740	3.00040	H	10.20790	-3.23740	1.46040
C	-1.48810	-5.02870	-0.69320	H	9.37220	-2.90210	-0.79160
H	-2.12470	-7.45750	-1.59190	H	6.94480	-2.25790	-1.17280
H	-3.70390	-6.85840	-2.19860	H	6.34140	-2.32630	3.11960
H	-5.11200	-2.20190	5.94110	H	8.64630	-2.94400	3.45880
H	-6.13650	-2.19980	4.46750	C	0.00000	3.31790	4.95880
O	-2.70500	-5.52680	-1.04970	C	-0.53250	2.34770	4.20860
O	-0.45130	-5.44750	-1.17370	C	-0.95160	2.63160	2.82080
O	-5.12970	-3.70820	2.57040	C	-0.78900	3.85660	2.29730
O	-4.09820	-2.58390	4.23300	C	-0.22000	4.93490	3.14430
Si	4.69560	-1.77760	0.60270	C	0.15870	4.67590	4.40230
Si	-1.34190	4.20790	0.55280	H	0.30830	3.11230	5.97570
C	3.11930	-4.97240	-2.44500	H	-0.65720	1.35440	4.61720
C	3.03680	-3.67220	-2.74880	H	-1.37190	1.83410	2.22830
C	3.53740	-2.65650	-1.79940	H	-0.11100	5.93940	2.76230
C	4.05280	-3.03150	-0.61460	H	0.57450	5.46330	5.01750
C	4.17690	-4.47590	-0.30240	C	-5.86290	3.04100	0.18470
C	3.72730	-5.39410	-1.16690	C	-4.98030	2.53360	-0.68310
H	2.74810	-5.71710	-3.13700	C	-3.54490	2.86620	-0.56220
H	2.59680	-3.36030	-3.68720	C	-3.12380	3.69330	0.41040
H	3.47130	-1.61570	-2.08100	C	-4.10330	4.22850	1.38630
H	4.63520	-4.79510	0.62520	C	-5.40160	3.92300	1.27530
H	3.81340	-6.44750	-0.93400	H	-6.91300	2.79360	0.09940

H	-5.31680	1.87710	-1.47380	C	-5.39070	-3.36170	-1.64550
H	-2.85410	2.43610	-1.27350	C	-6.34920	-3.78100	-2.56440
H	-3.77230	4.87580	2.18890	H	-7.39150	-3.28510	-4.38870
H	-6.11550	4.31740	1.98670	H	-6.21220	-1.10640	-4.67520
C	-0.80440	8.76190	-0.40620	H	-5.16650	-3.98320	-0.78700
C	-2.03650	8.24220	-0.35510	H	-6.86020	-4.72730	-2.42040
C	-2.22520	6.80910	-0.04600	O	-4.46250	-0.12000	-3.14490
C	-1.16140	6.02610	0.20140	H	-3.73290	0.02660	-2.52390
C	0.20220	6.60570	0.12920	C	-0.27710	-2.29730	-4.69440
C	0.37000	7.90250	-0.15590	C	-0.00210	-1.13430	-3.97340
H	-0.66550	9.81070	-0.63460	C	-0.75320	-0.80500	-2.85000
H	-2.89830	8.86930	-0.54350	C	-1.79440	-1.64900	-2.42100
H	-3.23000	6.41250	-0.03460	C	-2.06450	-2.82390	-3.13660
H	1.06890	5.98040	0.30600	C	-1.30770	-3.13380	-4.26710
H	1.36580	8.32320	-0.20680	H	0.30990	-2.55360	-5.57080
N	-0.63720	-2.41850	1.81800	H	0.80410	-0.47570	-4.28230
H	0.11540	-1.71640	2.00280	H	-0.52390	0.07900	-2.26790
H	0.69070	-3.20950	-1.01820	H	-2.84150	-3.50070	-2.81050
C	-5.31490	-2.69410	4.99030	H	-1.52470	-4.04880	-4.81030
H	-5.57580	-3.74320	5.14830	C	-5.53210	0.59010	2.47120
C	-2.66370	-6.60010	-2.00270	C	-6.31100	-0.20280	1.62750
H	-2.16530	-6.28090	-2.92090	C	-5.71960	-0.89650	0.57720
C	-2.91590	-3.66570	0.91370	C	-4.33500	-0.80660	0.33470
H	-3.44910	-2.80090	0.07610	C	-3.55800	-0.00330	1.19090
H	-3.67570	-4.43760	0.83120	C	-4.16060	0.68880	2.24380
O	-0.44440	0.09490	0.00990	H	-5.99080	1.13860	3.28860
H	-1.87890	-0.66100	-0.64520	H	-7.38280	-0.28130	1.78190
C	-6.64740	-2.97070	-3.66290	H	-6.33890	-1.51170	-0.06220
C	-5.99510	-1.75540	-3.83360	H	-2.48930	0.10790	1.03340
C	-5.03020	-1.33160	-2.91150	H	-3.55790	1.31570	2.89130
C	-4.70890	-2.14710	-1.80150				
C	2.98190	2.01890	-0.94220	C	4.16550	2.91330	-1.11890
C	5.56400	1.10380	-0.24960	C	4.01940	4.31230	-1.61170
C	4.50460	0.30590	-0.04830	C	5.09500	5.09380	-1.76160
C	3.13010	0.80720	-0.35160	C	6.43680	4.58000	-1.42980
H	6.56400	0.77260	-0.00860	C	6.58050	3.33440	-0.96590
C	5.39510	2.46240	-0.79200	H	3.04490	4.72130	-1.84170

H	4.98260	6.10950	-2.11840	H	-5.99960	-2.58100	4.45360
H	7.30300	5.21670	-1.55530	O	0.01440	-5.50410	-0.99670
H	7.56830	2.96660	-0.71690	O	-2.22880	-5.74220	-1.08730
C	-0.80890	3.69350	-2.06040	O	-4.87550	-4.06290	2.60110
C	1.64270	2.48690	-1.36740	O	-3.93810	-2.82640	4.23990
C	0.68710	2.65650	-0.43220	Si	4.77400	-1.41230	0.63600
C	-0.56240	3.38730	-0.77600	Si	-1.69080	4.11270	0.52250
H	-1.69800	4.25160	-2.33040	C	3.47950	-4.68510	-2.46280
C	1.33830	2.77360	-2.79670	C	3.29860	-3.39200	-2.75270
C	0.15080	3.32980	-3.12180	C	3.70770	-2.35200	-1.78620
C	-0.18160	3.59310	-4.54060	C	4.23820	-2.69920	-0.59950
C	0.68160	3.25800	-5.50600	C	4.46900	-4.13360	-0.30120
C	1.96910	2.62460	-5.16050	C	4.10110	-5.07370	-1.18090
C	2.28260	2.39260	-3.88060	H	3.17980	-5.44740	-3.17000
H	-1.12640	4.05340	-4.80160	H	2.85000	-3.10410	-3.69450
H	0.43660	3.44680	-6.54310	H	3.56660	-1.31650	-2.05930
H	2.65700	2.34300	-5.94730	H	4.94070	-4.42770	0.62790
H	3.22460	1.91320	-3.64840	H	4.26470	-6.12010	-0.95830
O	2.05500	-0.04240	-0.20170	C	2.48310	-1.54970	4.72240
P	0.77160	0.45950	0.74980	C	2.47690	-2.62700	3.92910
O	0.86510	2.11140	0.81450	C	3.21010	-2.60700	2.64620
O	0.94630	-0.09600	2.13890	C	3.86330	-1.49990	2.25670
N	-2.37420	-1.50100	-1.27180	C	3.88700	-0.31760	3.15250
C	-3.58300	-1.97610	-0.80370	C	3.23100	-0.34170	4.31950
C	-1.32980	-4.11670	0.38900	H	1.94120	-1.56100	5.65910
C	-0.29850	-3.27950	0.76740	H	1.92870	-3.51330	4.22100
C	-1.60080	-2.45200	2.63750	H	3.19970	-3.49490	2.03460
C	-2.68720	-3.21420	2.24900	H	4.43000	0.57370	2.86450
C	1.03290	-3.17850	0.09520	H	3.24220	0.52510	4.96740
H	1.57140	-2.29670	0.43370	C	9.31680	-2.27180	1.38660
H	1.62240	-4.07670	0.29010	C	8.86030	-2.10950	0.13930
C	-1.46260	-1.60270	3.87020	C	7.42770	-1.83420	-0.09470
H	-1.35220	-2.23610	4.75600	C	6.57880	-1.73700	0.94260
H	-0.58630	-0.95930	3.77350	C	7.08930	-1.92460	2.32280
H	-2.35300	-0.99350	4.02240	C	8.38770	-2.17650	2.53080
C	-3.93420	-3.41120	3.02030	H	10.36570	-2.47460	1.55980
C	-1.24490	-5.17910	-0.63290	H	9.53860	-2.18070	-0.70110
H	-0.24340	-6.16010	-2.95800	H	7.07600	-1.71120	-1.11180
H	1.18760	-6.76010	-2.06230	H	6.42140	-1.86050	3.17100
H	-4.98810	-2.47470	5.93250	H	8.75990	-2.31250	3.53800

C	-0.36420	3.32520	4.95390	C	-2.65320	-3.89490	0.95320
C	-0.79540	2.31560	4.19080	H	-3.24220	-3.10530	0.08250
C	-1.20780	2.56710	2.79470	H	-3.34180	-4.73270	0.87370
C	-1.13980	3.80330	2.27640	O	-0.47550	0.06270	-0.01560
C	-0.68340	4.92350	3.13780	H	-1.81190	-0.87370	-0.67120
C	-0.31070	4.69340	4.40310	C	-6.35820	-3.53010	-3.72430
H	-0.06160	3.14330	5.97700	C	-5.83040	-2.25120	-3.86070
H	-0.84410	1.31460	4.59590	C	-4.90740	-1.76330	-2.92880
H	-1.54740	1.73840	2.19290	C	-4.50780	-2.57320	-1.84070
H	-0.65370	5.93530	2.76130	C	-5.05480	-3.85770	-1.72470
H	0.02240	5.51160	5.02860	C	-5.97040	-4.34160	-2.65570
C	-6.10370	2.60510	0.09580	H	-7.07100	-3.89540	-4.45780
C	-5.17420	2.16830	-0.76160	H	-6.11330	-1.60310	-4.68330
C	-3.77000	2.60950	-0.62270	H	-4.74330	-4.49170	-0.90400
C	-3.42540	3.46370	0.35650	H	-6.37170	-5.34360	-2.54720
C	-4.45470	3.92060	1.32080	O	-4.45290	-0.49770	-3.13070
C	-5.72460	3.51750	1.19300	H	-3.73240	-0.30330	-2.51290
H	-7.13080	2.27880	-0.00320	C	-0.05380	-2.44030	-4.68910
H	-5.45020	1.49060	-1.55780	C	0.14540	-1.26490	-3.96310
H	-3.03960	2.23610	-1.32640	C	-0.63630	-0.98190	-2.84750
H	-4.18420	4.59000	2.12790	C	-1.63250	-1.88510	-2.43040
H	-6.47530	3.85520	1.89560	C	-1.82370	-3.07550	-3.14810
C	-1.57620	8.70070	-0.42870	C	-1.03810	-3.33640	-4.27200
C	-0.44390	8.03590	-0.17250	H	0.55320	-2.65790	-5.56260
C	-0.48710	6.59120	0.13260	H	0.91450	-0.55870	-4.26200
C	-1.66290	5.94050	0.17110	H	-0.46600	-0.08570	-2.26340
C	-2.91310	6.67990	-0.13210	H	-2.55480	-3.80530	-2.83230
C	-2.86980	7.98850	-0.41210	H	-1.20340	-4.25830	-4.82240
H	-1.54660	9.75900	-0.65370	C	-5.60840	0.16810	2.35710
H	0.50630	8.55390	-0.18940	C	-6.30200	-0.71960	1.53370
H	0.44210	6.06840	0.32540	C	-5.63760	-1.38820	0.51150
H	-3.86690	6.17240	-0.14120	C	-4.26530	-1.17590	0.27500
H	-3.78210	8.52680	-0.63430	C	-3.57400	-0.27830	1.11070
N	-0.48850	-2.45190	1.83850	C	-4.24940	0.38570	2.13750
H	0.20250	-1.68590	2.01100	H	-6.12380	0.69720	3.15330
H	0.90310	-3.10590	-0.98480	H	-7.36310	-0.89370	1.68360
C	-5.14920	-3.00340	4.99320	H	-6.18830	-2.08160	-0.11060
H	-5.33730	-4.06390	5.17600	H	-2.51870	-0.07130	0.95840
C	0.12480	-6.52900	-1.99760	H	-3.71490	1.08590	2.76950
H	-0.44720	-7.41300	-1.70940				

C	-3.42920	1.43930	0.99260	C	2.07590	-1.78880	-2.69350
C	-5.68950	-0.10300	0.28710	C	3.29660	-2.35620	-2.36890
C	-4.46180	-0.61000	0.10100	C	-0.32640	-3.21460	-0.22960
C	-3.25730	0.21580	0.42970	H	-1.03240	-2.43560	-0.50610
H	-6.57200	-0.67130	0.02960	H	-0.72910	-4.19540	-0.48820
C	-5.87520	1.26160	0.80280	C	1.77970	-0.87600	-3.84860
C	-4.80330	2.01730	1.11970	H	0.83890	-0.35000	-3.67080
C	-5.02310	3.42920	1.54700	H	2.59440	-0.17150	-4.00550
C	-6.26290	3.91850	1.66230	H	1.69420	-1.45980	-4.77190
C	-7.42690	3.06870	1.35290	C	4.47920	-2.16150	-3.23830
C	-7.24480	1.81100	0.93890	C	2.28360	-4.75620	0.36400
H	-4.18850	4.08540	1.75110	H	1.44050	-6.00880	2.62800
H	-6.41510	4.94480	1.97090	H	0.24100	-6.90680	1.64490
H	-8.42750	3.46960	1.45060	H	6.61640	-3.03740	-4.52340
H	-8.10420	1.19610	0.70170	H	7.07480	-1.61630	-3.55760
C	-0.32040	4.18760	2.06090	O	1.13760	-5.38290	0.66410
C	-2.26220	2.24320	1.42640	O	3.35800	-5.10770	0.85440
C	-1.35530	2.61690	0.50400	O	4.50740	-1.54070	-4.28600
C	-0.40960	3.72780	0.80250	O	5.56580	-2.79520	-2.73550
H	0.37610	4.97290	2.31340	Si	-4.30070	-2.31860	-0.63820
C	-2.12410	2.71880	2.83080	Si	0.61830	4.53200	-0.53880
C	-1.18230	3.64040	3.12850	C	-8.51170	-4.22410	-1.39410
C	-1.02260	4.11330	4.52300	C	-7.73890	-3.89740	-2.43680
C	-1.79560	3.61440	5.49410	C	-6.40950	-3.29120	-2.21370
C	-2.80830	2.58750	5.18030	C	-5.97460	-3.06020	-0.96330
C	-2.96430	2.15900	3.92240	C	-6.83350	-3.42890	0.18800
H	-0.27830	4.86290	4.76140	C	-8.03630	-3.97900	-0.01750
H	-1.67730	3.95870	6.51330	H	-9.48490	-4.66890	-1.55670
H	-3.42050	2.17730	5.97310	H	-8.08490	-4.07760	-3.44640
H	-3.70100	1.39420	3.71330	H	-5.80390	-3.04050	-3.07390
O	-2.00230	-0.35060	0.33430	H	-6.49120	-3.25240	1.20030
P	-0.84750	0.42060	-0.60350	H	-8.66250	-4.24620	0.82380
O	-1.33640	1.98930	-0.71580	C	-2.29680	-5.29610	2.37820
O	-0.88360	-0.16480	-1.99640	C	-2.42070	-4.00560	2.70660
N	2.67620	-1.13020	1.27650	C	-3.05230	-3.05840	1.76490
C	3.97000	-1.32320	0.83460	C	-3.48290	-3.48250	0.56300
C	2.16440	-3.66160	-0.60650	C	-3.38000	-4.92290	0.22370
C	0.98420	-3.00620	-0.91600	C	-2.80830	-5.77890	1.08000

H	-1.83290	-5.98990	3.06710	C	3.36480	4.70610	-0.97020
H	-2.05900	-3.65200	3.66290	C	2.40360	4.09330	-0.25940
H	-3.15600	-2.02730	2.06900	C	2.78550	3.15290	0.82400
H	-3.77290	-5.29150	-0.71520	C	4.07670	2.94310	1.10850
H	-2.72850	-6.82820	0.82750	H	6.17000	3.43960	0.55030
C	-2.05320	-1.75260	-4.71390	H	5.55780	4.94650	-1.24880
C	-1.86040	-2.87150	-4.00590	H	3.11090	5.41410	-1.74950
C	-2.57710	-3.07430	-2.72940	H	2.02930	2.62880	1.39270
C	-3.39910	-2.12350	-2.25630	H	4.35440	2.25870	1.89880
C	-3.63390	-0.89970	-3.06300	N	0.99210	-2.07520	-1.90880
C	-2.99260	-0.72360	-4.22510	H	0.15420	-1.43210	-2.00900
H	-1.52380	-1.60030	-5.64540	H	-0.19600	-3.19360	0.85290
H	-1.17360	-3.62810	-4.36250	C	6.76740	-2.66340	-3.50780
H	-2.41510	-3.99280	-2.18840	H	7.51580	-3.25790	-2.98470
H	-4.31860	-0.13770	-2.71300	C	1.22180	-6.43330	1.64570
H	-3.15570	0.17560	-4.80520	H	1.99940	-7.14960	1.37580
C	0.42090	9.20430	-0.11110	C	3.41430	-3.15790	-1.15240
C	-0.23940	8.60500	-1.10790	H	3.87400	-2.37150	-0.15890
C	-0.18530	7.13540	-1.25600	H	4.25820	-3.84050	-1.14430
C	0.51160	6.38930	-0.38060	O	0.45330	0.32160	0.16310
C	1.26120	7.06610	0.70790	H	2.05060	-0.52000	0.73480
C	1.21360	8.39750	0.83680	C	6.93050	-2.17050	3.87700
H	0.38290	10.28050	-0.00270	C	6.78430	-3.07270	2.82980
H	-0.81490	9.19500	-1.80940	C	5.80850	-2.88390	1.83980
H	-0.71700	6.68860	-2.08110	C	4.96910	-1.75360	1.89780
H	1.87190	6.49130	1.39170	C	5.12400	-0.86160	2.97440
H	1.76600	8.88680	1.62850	C	6.08740	-1.05990	3.95660
C	-0.92280	2.96360	-4.68360	H	7.69220	-2.33800	4.63290
C	-1.76270	3.59210	-3.85330	H	7.41380	-3.95240	2.74650
C	-1.26820	4.13240	-2.56960	H	4.47620	0.00750	3.02550
C	0.02510	3.99190	-2.22580	H	6.18310	-0.34940	4.77150
C	0.95450	3.33300	-3.17070	O	5.76220	-3.80620	0.83160
C	0.50450	2.83560	-4.32910	H	4.88820	-4.25640	0.81530
H	-1.28510	2.55540	-5.61820	C	0.55380	-2.55880	4.65320
H	-2.80950	3.68900	-4.11030	C	0.14690	-1.42220	3.95260
H	-1.97510	4.58980	-1.88830	C	0.86700	-0.96910	2.85140
H	2.00150	3.26050	-2.93570	C	2.01640	-1.65890	2.41930
H	1.18760	2.34840	-5.01300	C	2.41680	-2.81170	3.11430
C	5.12740	3.62490	0.32690	C	1.68900	-3.24580	4.22280
C	4.78920	4.45280	-0.66870	H	-0.00680	-2.90740	5.51520

H	-0.74150	-0.87800	4.26000	C	6.48120	0.55820	-1.30590
H	0.53570	-0.10340	2.29030	H	6.09040	1.94210	-2.91810
H	3.27800	-3.37930	2.79640	H	3.64110	1.81620	-2.64410
H	2.02300	-4.13350	4.75300	H	2.62310	0.44730	-0.89060
C	5.66030	1.30830	-2.14880	H	6.56950	-0.85380	0.29670
C	4.27910	1.24220	-1.98750	H	7.56160	0.60830	-1.40330
C	3.70400	0.43690	-1.00270				
C	4.52340	-0.33560	-0.15930				
C	5.91890	-0.26380	-0.33560				
C	3.14500	1.79810	-0.98070	O	2.08940	-0.19850	-0.23320
C	5.66580	0.71510	-0.30460	P	0.85350	0.38600	0.73270
C	4.55800	-0.01280	-0.09830	O	1.06790	2.02650	0.80730
C	3.21740	0.57750	-0.39360	O	1.00030	-0.19160	2.11590
H	6.64350	0.31990	-0.06870	N	-2.51630	-1.22740	-1.25360
C	5.58310	2.08180	-0.84630	C	-3.73270	-1.64230	-0.74640
C	4.38380	2.61250	-1.16610	C	-1.57870	-3.99290	0.27960
C	4.32720	4.01820	-1.65850	C	-0.47690	-3.25200	0.66390
C	5.45090	4.72740	-1.81440	C	-1.66490	-2.40000	2.59630
C	6.75790	4.12670	-1.48970	C	-2.81270	-3.07050	2.21380
C	6.82210	2.87430	-1.02670	C	0.84160	-3.25960	-0.03500
H	3.38060	4.49040	-1.88350	H	1.46060	-2.42870	0.29570
H	5.40340	5.74830	-2.17090	H	1.35250	-4.20960	0.13970
H	7.66330	4.70530	-1.61990	C	-1.43280	-1.60720	3.85250
H	7.78490	2.44240	-0.78290	H	-1.28500	-2.28200	4.70210
C	-0.54510	3.72320	-2.03490	H	-0.54460	-0.98390	3.73070
C	1.83510	2.35950	-1.38420	H	-2.29530	-0.98410	4.08380
C	0.90870	2.59040	-0.43320	C	-4.05130	-3.20870	3.00970
C	-0.29670	3.40060	-0.75490	C	-1.46660	-5.02570	-0.76840
H	-1.40140	4.33710	-2.28930	H	-2.11460	-7.44560	-1.68840
C	1.52670	2.66880	-2.80770	H	-3.70760	-6.84200	-2.25290
C	0.37150	3.29980	-3.11260	H	-4.95700	-2.34710	5.99380
C	0.03210	3.58410	-4.52570	H	-6.01150	-2.29300	4.54250
C	0.85570	3.19520	-5.50540	O	-2.68850	-5.52500	-1.10520
C	2.10660	2.48220	-5.18170	O	-0.43830	-5.43110	-1.27770
C	2.42680	2.23020	-3.90720	O	-5.05010	-3.76710	2.58600
H	-0.88610	4.10300	-4.77090	O	-3.98200	-2.68630	4.25460
H	0.60530	3.39920	-6.53840	Si	4.72000	-1.74570	0.58350
H	2.76190	2.15830	-5.97990	Si	-1.35280	4.19290	0.56540
H	3.34070	1.69260	-3.69070	C	3.20980	-4.93290	-2.50490

C	3.11490	-3.63130	-2.79890	H	-1.33010	1.80960	2.22350
C	3.59640	-2.61780	-1.83730	H	-0.15800	5.93630	2.79090
C	4.10530	-2.99660	-0.65100	H	0.53440	5.45740	5.04290
C	4.24180	-4.44200	-0.34860	C	-5.85900	2.96460	0.23480
C	3.81080	-5.35820	-1.22470	C	-4.97880	2.47650	-0.64640
H	2.85310	-5.67610	-3.20610	C	-3.54680	2.82810	-0.53840
H	2.67870	-3.31650	-3.73830	C	-3.12740	3.65410	0.43570
H	3.52100	-1.57550	-2.11080	C	-4.10390	4.16880	1.42560
H	4.69320	-4.76340	0.58160	C	-5.39880	3.84550	1.32640
H	3.90580	-6.41230	-0.99900	H	-6.90650	2.70330	0.15830
C	2.42950	-1.75650	4.67170	H	-5.31540	1.82270	-1.43900
C	2.31740	-2.80900	3.85330	H	-2.85720	2.41400	-1.26050
C	3.04450	-2.82840	2.56690	H	-3.77380	4.81580	2.22870
C	3.80420	-1.78220	2.20270	H	-6.11060	4.22500	2.04780
C	3.94050	-0.62740	3.12390	C	-0.97220	8.76680	-0.38210
C	3.28710	-0.61560	4.29260	C	0.12140	8.03300	-0.14670
H	1.89170	-1.73810	5.61070	C	-0.00530	6.59310	0.15810
H	1.68740	-3.64520	4.12730	C	-1.21810	6.01620	0.21710
H	2.94520	-3.69560	1.93370	C	-2.42560	6.83180	-0.06260
H	4.56490	0.21460	2.85300	C	-2.30670	8.13570	-0.34260
H	3.38160	0.23150	4.95940	H	-0.88140	9.82160	-0.60720
C	9.20320	-2.88080	1.33100	H	1.10120	8.49140	-0.18050
C	8.75710	-2.68820	0.08430	H	0.89320	6.01360	0.33320
C	7.34330	-2.32770	-0.14860	H	-3.40900	6.38400	-0.05450
C	6.50180	-2.18230	0.88910	H	-3.18810	8.72960	-0.54780
C	7.00000	-2.40580	2.26860	N	-0.57800	-2.44970	1.76510
C	8.28130	-2.73480	2.47560	H	0.17070	-1.74250	1.94570
H	10.23840	-3.14550	1.50350	H	0.69540	-3.18210	-1.11240
H	9.43010	-2.79650	-0.75640	C	-5.18370	-2.80940	5.03330
H	6.99980	-2.18020	-1.16520	H	-5.45030	-3.86050	5.16580
H	6.33710	-2.30660	3.11720	C	-2.66410	-6.58370	-2.07490
H	8.64460	-2.89670	3.48230	H	-2.18600	-6.24930	-2.99840
C	0.00830	3.30020	4.96620	C	-2.86640	-3.69790	0.89110
C	-0.50170	2.32450	4.20760	H	-3.42390	-2.82230	0.08130
C	-0.92600	2.61080	2.82210	H	-3.62240	-4.47380	0.81120
C	-0.78890	3.84260	2.30740	O	-0.42830	0.08820	-0.02050
C	-0.24480	4.92640	3.16400	H	-1.88620	-0.66580	-0.65490
C	0.13740	4.66580	4.42060	C	-6.72930	-2.98020	-3.55760
H	0.32010	3.09330	5.98180	C	-6.07130	-1.77210	-3.75440
H	-0.60460	1.32490	4.60740	C	-5.08000	-1.34870	-2.86050



C	-4.73680	-2.15820	-1.75250	H	0.72100	-0.44640	-4.34520
C	-5.42520	-3.36570	-1.56990	H	-0.55710	0.08240	-2.29230
C	-6.41020	-3.78420	-2.46040	H	-2.89500	-3.48570	-2.82930
H	-7.49450	-3.29360	-4.26160	H	-1.62800	-4.00740	-4.86790
H	-6.30470	-1.12740	-4.59500	C	-5.46010	0.53860	2.56410
H	-5.18820	-3.97980	-0.70950	C	-6.25940	-0.23990	1.72650
H	-6.92570	-4.72450	-2.29490	C	-5.69270	-0.92120	0.65460
O	-4.51000	-0.14350	-3.11940	C	-4.31300	-0.83380	0.38450
H	-3.76760	0.00660	-2.51480	C	-3.51540	-0.04420	1.23470
C	-0.37360	-2.26050	-4.75700	C	-4.09340	0.63550	2.30920
C	-0.07890	-1.10830	-4.02640	H	-5.89900	1.07730	3.39870
C	-0.80240	-0.79310	-2.88090	H	-7.32810	-0.31650	1.90190
C	-1.83560	-1.64080	-2.43970	H	-6.32810	-1.52450	0.02000
C	-2.12480	-2.80560	-3.16450	H	-2.44990	0.06570	1.05610
C	-1.39570	-3.10080	-4.31690	H	-3.47560	1.25030	2.95370
H	0.19110	-2.50530	-5.65110				
C	-3.27890	1.57060	1.04430	C	-0.54770	3.93020	4.56230
C	-5.66450	0.21870	0.36120	C	-1.30990	3.44260	5.54780
C	-4.48260	-0.37080	0.12810	C	-2.40480	2.50150	5.24060
C	-3.21350	0.35600	0.44200	C	-2.64580	2.14020	3.97500
H	-6.59260	-0.27720	0.11490	H	0.25670	4.61660	4.79560
C	-5.73550	1.57630	0.92270	H	-1.12300	3.73340	6.57350
C	-4.60290	2.24070	1.23340	H	-3.00870	2.09980	6.04400
C	-4.70670	3.64800	1.71600	H	-3.44290	1.43750	3.76970
C	-5.90380	4.22170	1.88300	O	-2.00760	-0.29560	0.28670
C	-7.13480	3.47080	1.57740	P	-0.82310	0.42460	-0.65510
C	-7.05690	2.21870	1.11610	O	-1.21090	2.02460	-0.72420
H	-3.82110	4.23340	1.92020	O	-0.90630	-0.13840	-2.05310
H	-5.97180	5.24420	2.23160	N	2.57200	-1.26240	1.26360
H	-8.10020	3.93990	1.71680	C	3.85510	-1.49980	0.81180
H	-7.96510	1.67700	0.88270	C	1.95700	-3.78980	-0.58130
C	0.04800	4.06390	2.07440	C	0.80420	-3.10020	-0.91740
C	-2.04410	2.27840	1.45600	C	1.95540	-1.97020	-2.71710
C	-1.15060	2.62320	0.50940	C	3.14980	-2.57870	-2.37040
C	-0.12400	3.66140	0.80470	C	-0.52090	-3.24720	-0.24280
H	0.80190	4.79580	2.32370	H	-1.18590	-2.43330	-0.52170
C	-1.81640	2.68770	2.86910	H	-0.97070	-4.20570	-0.51040
C	-0.80080	3.52960	3.15900	C	1.70130	-1.07390	-3.89480

H	0.79780	-0.48460	-3.72030	C	-3.56690	-1.90960	-2.27250
H	2.55610	-0.42770	-4.08340	C	-3.75780	-0.67460	-3.07340
H	1.56330	-1.67860	-4.79830	C	-3.11890	-0.52090	-4.24000
C	4.34650	-2.45090	-3.23380	H	-1.69900	-1.45260	-5.67520
C	2.03220	-4.85780	0.42370	H	-1.41580	-3.49410	-4.39750
H	1.11960	-6.00830	2.71910	H	-2.64950	-3.81290	-2.21140
H	-0.08450	-6.90950	1.74400	H	-4.40820	0.11320	-2.71500
H	6.47250	-3.42460	-4.46590	H	-3.25010	0.38590	-4.81630
H	6.96290	-1.99580	-3.52700	C	0.78610	9.13460	0.03320
O	0.86430	-5.43840	0.73170	C	0.07410	8.57940	-0.95340
O	3.09120	-5.22640	0.93330	C	0.09570	7.11480	-1.15100
O	4.40580	-1.86390	-4.29930	C	0.81580	6.32890	-0.33090
O	5.40550	-3.10490	-2.69980	C	1.62130	6.95710	0.74680
Si	-4.46110	-2.07010	-0.64730	C	1.60290	8.28410	0.92040
Si	0.87970	4.47580	-0.55030	H	0.77170	10.20720	0.17780
C	-8.81750	-3.62860	-1.37250	H	-0.51990	9.20160	-1.61040
C	-8.03730	-3.33980	-2.42090	H	-0.47930	6.70410	-1.96570
C	-6.66120	-2.84440	-2.20740	H	2.24900	6.35030	1.38600
C	-6.19080	-2.67610	-0.95980	H	2.19610	8.73790	1.70380
C	-7.05800	-3.00380	0.19770	C	-0.80440	3.09650	-4.70860
C	-8.30320	-3.45330	0.00080	C	-1.61140	3.69760	-3.82720
H	-9.82510	-3.99160	-1.52810	C	-1.07210	4.17730	-2.53760
H	-8.41190	-3.46880	-3.42810	C	0.22820	4.00450	-2.23720
H	-6.05100	-2.62180	-3.07200	C	1.12240	3.38180	-3.24000
H	-6.68750	-2.87780	1.20750	C	0.63170	2.94020	-4.40460
H	-8.93560	-3.69000	0.84670	H	-1.19940	2.73350	-5.64860
C	-2.64020	-5.24410	2.28280	H	-2.66410	3.81720	-4.04790
C	-2.66570	-3.95480	2.63760	H	-1.75240	4.61640	-1.81820
C	-3.23800	-2.94570	1.72250	H	2.17770	3.29610	-3.04660
C	-3.71240	-3.31340	0.51850	H	1.28880	2.48080	-5.13160
C	-3.71410	-4.74960	0.14810	C	5.39940	3.46030	0.12490
C	-3.19720	-5.66200	0.98070	C	5.04090	4.31560	-0.83970
H	-2.22140	-5.98360	2.95270	C	3.61190	4.60710	-1.07760
H	-2.26700	-3.64750	3.59530	C	2.66550	3.99820	-0.34370
H	-3.26260	-1.91580	2.04730	C	3.06890	3.02890	0.70580
H	-4.13910	-5.06870	-0.79510	C	4.36550	2.78660	0.93510
H	-3.19420	-6.70870	0.70570	H	6.44560	3.24770	0.30240
C	-2.22570	-1.58570	-4.73920	H	5.79680	4.80450	-1.44030
C	-2.07000	-2.71220	-4.03410	H	3.34370	5.33730	-1.83110
C	-2.78250	-2.88890	-2.75140	H	2.32430	2.50780	1.29220

H	4.65930	2.08050	1.70020	H	4.66180	-4.43940	0.87410
N	0.85580	-2.19490	-1.93330	C	0.39970	-2.57840	4.65480
H	0.05320	-1.51940	-2.05100	C	0.00770	-1.46280	3.91300
H	-0.39930	-3.23700	0.84030	C	0.74650	-1.04690	2.80990
C	6.62130	-3.03120	-3.45750	C	1.90060	-1.75290	2.41510
H	7.34260	-3.63630	-2.90900	C	2.28830	-2.88210	3.15510
C	0.90710	-6.45910	1.74720	C	1.54130	-3.27890	4.26520
H	1.67170	-7.20140	1.51320	H	-0.17560	-2.89900	5.51790
C	3.22840	-3.35420	-1.13500	H	-0.88340	-0.90620	4.18910
H	3.72080	-2.56170	-0.15210	H	0.42860	-0.19600	2.21930
H	4.04320	-4.07070	-1.10350	H	3.15360	-3.46140	2.87150
O	0.47550	0.23780	0.09950	H	1.86590	-4.14910	4.82930
H	1.95920	-0.64630	0.71170	C	5.56170	1.03400	-2.24940
C	6.83960	-2.32430	3.83450	C	4.18250	1.00620	-2.06230
C	6.64720	-3.26200	2.82680	C	3.60610	0.23300	-1.05310
C	5.65860	-3.08270	1.84760	C	4.41980	-0.54440	-0.20940
C	4.85700	-1.92440	1.87440	C	5.81310	-0.51220	-0.41140
C	5.05680	-0.99720	2.91310	C	6.37800	0.27810	-1.40670
C	6.03090	-1.18670	3.88630	H	5.99440	1.64220	-3.03760
H	7.61000	-2.48540	4.58300	H	3.54200	1.58000	-2.71720
H	7.24770	-4.16370	2.76870	H	2.52820	0.27290	-0.92310
H	4.43540	-0.10770	2.93990	H	6.46010	-1.10720	0.22040
H	6.16200	-0.44890	4.67150	H	7.45750	0.29930	-1.52400
O	5.56230	-4.04570	0.88250				
C	-3.38900	1.43160	0.99840	H	-8.06840	1.28670	0.71930
C	-5.68210	-0.06110	0.29130	C	-0.22770	4.11130	2.08340
C	-4.46530	-0.59260	0.10260	C	-2.20390	2.20710	1.43490
C	-3.24520	0.20830	0.42900	C	-1.29550	2.57720	0.51210
H	-6.57600	-0.61190	0.03560	C	-0.34120	3.67950	0.81690
C	-5.83830	1.30500	0.81450	H	0.47270	4.89280	2.33940
C	-4.75020	2.03610	1.13480	C	-2.04570	2.65670	2.84560
C	-4.93920	3.44770	1.57700	C	-1.08250	3.55340	3.15110
C	-6.16830	3.96150	1.70030	C	-0.89970	3.99650	4.55250
C	-7.35050	3.13890	1.38560	C	-1.67290	3.49430	5.52190
C	-7.19580	1.88150	0.95940	C	-2.70940	2.49430	5.19900
H	-4.09030	4.08370	1.78670	C	-2.88660	2.09350	3.93470
H	-6.29840	4.98740	2.02000	H	-0.13860	4.72690	4.79740
H	-8.34220	3.55960	1.49010	H	-1.53760	3.81660	6.54620

H	-3.32220	2.08160	5.98990	H	-6.54820	-3.18870	1.20640
H	-3.64110	1.34830	3.71850	H	-8.73470	-4.14780	0.82700
O	-2.00400	-0.38300	0.32590	C	-2.38460	-5.31120	2.39750
P	-0.83480	0.37220	-0.60480	C	-2.48190	-4.01710	2.72110
O	-1.28160	1.95510	-0.71130	C	-3.09760	-3.06140	1.77720
O	-0.87350	-0.20630	-1.99900	C	-3.53820	-3.48150	0.57760
N	2.68940	-1.18480	1.28830	C	-3.46150	-4.92440	0.24230
C	3.96690	-1.32570	0.78330	C	-2.90650	-5.78850	1.10140
C	2.15260	-3.70390	-0.53550	H	-1.93390	-6.01150	3.08850
C	0.96300	-3.07290	-0.85900	H	-2.10930	-3.66690	3.67470
C	2.02320	-1.93060	-2.70750	H	-3.18070	-2.02720	2.07740
C	3.25040	-2.47850	-2.37800	H	-3.86010	-5.28780	-0.69630
C	-0.34010	-3.26360	-0.15260	H	-2.84680	-6.83990	0.85220
H	-1.05140	-2.49540	-0.44620	C	-2.06080	-1.81170	-4.69890
H	-0.74390	-4.25270	-0.37890	C	-1.86430	-2.91350	-3.96570
C	1.70160	-1.07300	-3.89730	C	-2.58580	-3.09280	-2.68840
H	0.78740	-0.50610	-3.70510	C	-3.42010	-2.13940	-2.24260
H	2.52980	-0.40870	-4.13390	C	-3.65550	-0.93320	-3.07490
H	1.54670	-1.70620	-4.77850	C	-3.00800	-0.77750	-4.23640
C	4.42440	-2.30680	-3.26460	H	-1.52760	-1.67640	-5.63090
C	2.30080	-4.73800	0.49590	H	-1.17050	-3.67300	-4.30220
H	1.53750	-5.85540	2.84890	H	-2.41870	-3.99750	-2.12560
H	0.30360	-6.80940	1.96480	H	-4.34630	-0.16810	-2.74410
H	6.58350	-3.19510	-4.50660	H	-3.17250	0.10850	-4.83600
H	7.00360	-1.71470	-3.61550	C	0.29610	9.18880	0.10450
O	1.16700	-5.35160	0.86130	C	-0.40550	8.60430	-0.87280
O	3.38970	-5.05060	0.97950	C	-0.30800	7.14500	-1.08590
O	4.43620	-1.74220	-4.34380	C	0.47390	6.39320	-0.29090
O	5.52600	-2.88830	-2.73250	C	1.26480	7.05410	0.77780
Si	-4.33380	-2.30720	-0.62870	C	1.17650	8.37630	0.96620
Si	0.62900	4.54820	-0.52770	H	0.22530	10.25740	0.26100
C	-8.57490	-4.14130	-1.39040	H	-1.04740	9.19870	-1.51010
C	-7.79250	-3.83410	-2.43190	H	-0.88030	6.70920	-1.88960
C	-6.45380	-3.24960	-2.20690	H	1.93350	6.47500	1.40140
C	-6.02010	-3.01840	-0.95610	H	1.75770	8.85430	1.74420
C	-6.88970	-3.36520	0.19380	C	-0.99250	3.15880	-4.70730
C	-8.10080	-3.89610	-0.01330	C	-1.83240	3.66890	-3.79970
H	-9.55480	-4.57060	-1.55420	C	-1.31570	4.15060	-2.50200
H	-8.13750	-4.01450	-3.44170	C	-0.00280	4.06830	-2.21920
H	-5.84000	-3.01570	-3.06610	C	0.92510	3.54830	-3.25010

C	0.45520	3.10560	-4.42290	C	5.04840	-1.67710	1.79260
H	-1.36980	2.79510	-5.65420	C	5.25300	-0.72280	2.80550
H	-2.89380	3.71390	-4.00640	C	6.29250	-0.83680	3.72100
H	-2.01850	4.51940	-1.76480	H	7.98710	-2.02650	4.33720
H	1.98750	3.54300	-3.07310	H	7.61380	-3.75870	2.57720
H	1.13690	2.72300	-5.17150	H	4.58140	0.12780	2.85840
C	5.18690	3.70980	0.13380	H	6.42480	-0.07910	4.48670
C	4.79390	4.56600	-0.81640	O	5.81000	-3.78250	0.80500
C	3.35430	4.80590	-1.04760	H	4.92380	-4.20630	0.84260
C	2.43350	4.14860	-0.32300	C	0.71920	-2.66640	4.73550
C	2.87570	3.18350	0.71420	C	0.18320	-1.63630	3.96050
C	4.18110	2.98740	0.93730	C	0.85620	-1.16560	2.83780
H	6.24080	3.53440	0.30650	C	2.09230	-1.72750	2.45700
H	5.52930	5.09230	-1.41080	C	2.62610	-2.77210	3.23030
H	3.05670	5.53570	-1.79050	C	1.94040	-3.22490	4.35870
H	2.15230	2.62960	1.29740	H	0.19450	-3.02890	5.61400
H	4.50340	2.28580	1.69430	H	-0.77120	-1.19020	4.22550
N	0.95230	-2.18750	-1.89320	H	0.42740	-0.38160	2.22350
H	0.12170	-1.54240	-1.99900	H	3.55780	-3.24440	2.96160
H	-0.20110	-3.20990	0.92740	H	2.37820	-4.02630	4.94750
C	6.72400	-2.76580	-3.51160	C	5.32670	1.34380	-2.33660
H	7.48720	-3.31290	-2.95900	C	3.96490	1.21520	-2.07800
C	1.28420	-6.33950	1.90340	C	3.50030	0.39280	-1.05100
H	2.05110	-7.07360	1.65080	C	4.40990	-0.32960	-0.25860
C	3.39050	-3.22600	-1.13020	C	5.78500	-0.19580	-0.53200
H	3.86950	-2.39850	-0.18020	C	6.23810	0.64060	-1.54710
H	4.23400	-3.90870	-1.10770	H	5.67360	1.98790	-3.13870
O	0.45260	0.23860	0.17960	H	3.24660	1.74440	-2.68880
H	2.02030	-0.60700	0.76320	H	2.43000	0.35430	-0.86890
C	7.16430	-1.92490	3.63560	H	6.50540	-0.74620	0.05960
C	6.96680	-2.89140	2.65670	H	7.30550	0.73980	-1.72100
C	5.91110	-2.79000	1.73770				
C	2.94990	2.03360	-0.94770	C	4.12080	2.94070	-1.14220
C	5.54860	1.15620	-0.26950	C	3.95330	4.33320	-1.64650
C	4.50090	0.34710	-0.05280	C	5.01820	5.12560	-1.81470
C	3.11780	0.82890	-0.34820	C	6.36900	4.63080	-1.49120
H	6.55460	0.83910	-0.03450	C	6.53180	3.39180	-1.01610
C	5.35860	2.50770	-0.82230	H	2.97190	4.72860	-1.87080

H	4.89030	6.13630	-2.18050	H	-5.99290	-2.65500	4.43380
H	7.22640	5.27620	-1.63190	O	0.07430	-5.49560	-0.99860
H	7.52620	3.03800	-0.77320	O	-2.16730	-5.74090	-1.11240
C	-0.86800	3.65300	-2.05260	O	-4.84510	-4.11500	2.57720
C	1.60220	2.48140	-1.36700	O	-3.92820	-2.87970	4.22860
C	0.65170	2.64770	-0.42620	Si	4.79630	-1.36290	0.64020
C	-0.60920	3.36030	-0.76750	Si	-1.73630	4.08420	0.53260
H	-1.76490	4.19940	-2.32100	C	3.53110	-4.66720	-2.43690
C	1.28410	2.75150	-2.79660	C	3.33170	-3.37800	-2.73200
C	0.08760	3.28990	-3.11790	C	3.73040	-2.32820	-1.77180
C	-0.25960	3.53380	-4.53660	C	4.26970	-2.66280	-0.58540
C	0.59980	3.19870	-5.50540	C	4.51920	-4.09270	-0.28060
C	1.89820	2.58590	-5.16360	C	4.16110	-5.04160	-1.15480
C	2.22490	2.37170	-3.88390	H	3.24000	-5.43660	-3.13990
H	-1.21230	3.97910	-4.79480	H	2.87600	-3.10050	-3.67350
H	0.34380	3.37260	-6.54250	H	3.57510	-1.29600	-2.04950
H	2.58330	2.30470	-5.95290	H	4.99690	-4.37610	0.64870
H	3.17480	1.90690	-3.65430	H	4.33900	-6.08470	-0.92780
O	2.05510	-0.03310	-0.18200	C	2.52520	-1.50090	4.73730
P	0.76920	0.46100	0.77030	C	2.52470	-2.58200	3.94910
O	0.84480	2.11440	0.82350	C	3.25230	-2.56200	2.66300
O	0.95140	-0.08740	2.16090	C	3.89510	-1.45150	2.26590
N	-2.35170	-1.50580	-1.26810	C	3.91220	-0.26460	3.15590
C	-3.55720	-1.99620	-0.80760	C	3.26110	-0.28860	4.32560
C	-1.28820	-4.12390	0.38490	H	1.98730	-1.51230	5.67630
C	-0.26500	-3.28280	0.77580	H	1.98540	-3.47160	4.24760
C	-1.58580	-2.47350	2.64070	H	3.24630	-3.45250	2.05510
C	-2.66360	-3.24270	2.24140	H	4.44660	0.62980	2.86140
C	1.07120	-3.17060	0.11530	H	3.26780	0.58140	4.96930
H	1.60000	-2.28540	0.46020	C	9.35500	-2.15520	1.36740
H	1.66620	-4.06450	0.31380	C	8.88830	-2.00910	0.12190
C	-1.46290	-1.62770	3.87740	C	7.45050	-1.75550	-0.10470
H	-1.34910	-2.26320	4.76120	C	6.60710	-1.66200	0.93740
H	-0.59330	-0.97400	3.78720	C	7.12890	-1.83180	2.31560
H	-2.36070	-1.02910	4.02790	C	8.43220	-2.06390	2.51700
C	-3.91260	-3.45640	3.00520	H	10.40780	-2.34190	1.53520
C	-1.18960	-5.17800	-0.64450	H	9.56200	-2.07730	-0.72230
H	-0.14070	-6.12380	-2.97360	H	7.09060	-1.64480	-1.12030
H	1.26030	-6.75170	-2.05040	H	6.46570	-1.77030	3.16770
H	-4.98980	-2.55040	5.91840	H	8.81280	-2.18690	3.52270

C	-0.37730	3.31830	4.95760	C	-2.61660	-3.91600	0.94240
C	-0.80940	2.30420	4.20090	H	-3.20860	-3.12670	0.07100
C	-1.23300	2.54940	2.80710	H	-3.29820	-4.75860	0.85410
C	-1.17460	3.78420	2.28450	O	-0.47570	0.04840	0.00940
C	-0.71760	4.90930	3.13900	H	-1.79440	-0.88150	-0.65920
C	-0.33460	4.68510	4.40220	C	-6.30540	-3.54440	-3.75640
H	-0.06600	3.14100	5.97890	C	-5.79000	-2.25870	-3.87580
H	-0.84990	1.30400	4.60920	C	-4.87570	-1.77270	-2.93440
H	-1.57200	1.71700	2.21010	C	-4.47270	-2.59120	-1.85410
H	-0.69540	5.92000	2.75880	C	-5.00670	-3.88250	-1.75540
H	-0.00080	5.50670	5.02270	C	-5.91350	-4.36460	-2.69590
C	-6.14350	2.55280	0.13160	H	-7.01140	-3.90820	-4.49710
C	-5.21600	2.11840	-0.72920	H	-6.07600	-1.60390	-4.69200
C	-3.81330	2.56660	-0.59790	H	-4.69100	-4.52310	-0.94140
C	-3.46810	3.42490	0.37740	H	-6.30490	-5.37190	-2.60110
C	-4.49490	3.87870	1.34580	O	-4.43260	-0.50040	-3.11980
C	-5.76340	3.46910	1.22520	H	-3.71560	-0.30720	-2.49750
H	-7.16940	2.22130	0.03820	C	-0.01210	-2.39520	-4.68580
H	-5.49240	1.43700	-1.52210	C	0.16890	-1.22080	-3.95350
H	-3.08460	2.19440	-1.30390	C	-0.61920	-0.95440	-2.83850
H	-4.22370	4.55100	2.15030	C	-1.60370	-1.87330	-2.42790
H	-6.51230	3.80450	1.93080	C	-1.77730	-3.06210	-3.15260
C	-1.65140	8.66750	-0.44410	C	-0.98530	-3.30660	-4.27580
C	-0.51430	8.01030	-0.18910	H	0.60010	-2.60000	-5.55860
C	-0.54820	6.56730	0.12500	H	0.92890	-0.50270	-4.24730
C	-1.72020	5.91050	0.17290	H	-0.46330	-0.05860	-2.24990
C	-2.97590	6.64140	-0.12830	H	-2.49960	-3.80310	-2.84270
C	-2.94100	7.94850	-0.41660	H	-1.13690	-4.22770	-4.83150
H	-1.62850	9.72440	-0.67610	C	-5.61480	0.10290	2.36300
H	0.43300	8.53330	-0.21410	C	-6.29660	-0.78540	1.53040
H	0.38480	6.05070	0.31590	C	-5.62220	-1.43920	0.50520
H	-3.92710	6.12880	-0.12930	C	-4.25150	-1.21100	0.27480
H	-3.85730	8.48050	-0.63760	C	-3.57210	-0.31330	1.11990
N	-0.46810	-2.46170	1.84970	C	-4.25740	0.33610	2.14950
H	0.21630	-1.69240	2.02940	H	-6.13830	0.62050	3.16140
H	0.94990	-3.09630	-0.96540	H	-7.35630	-0.97140	1.67540
C	-5.14130	-3.07360	4.97450	H	-6.16370	-2.13350	-0.12410
H	-5.32040	-4.13720	5.14860	H	-2.51850	-0.09490	0.97230
C	0.19890	-6.50950	-2.00920	H	-3.73190	1.03700	2.78840
H	-0.39010	-7.39020	-1.74670				

C	3.06310	1.80260	-1.07220	C	-2.86070	-3.12110	2.28970
C	5.59300	0.74080	-0.39110	C	0.82530	-3.29630	0.08580
C	4.48790	0.02090	-0.14910	H	1.40290	-2.42380	0.38400
C	3.14350	0.59520	-0.45720	H	1.37550	-4.20780	0.33190
H	6.57290	0.35580	-0.14800	C	-1.50830	-1.59880	3.90230
C	5.50400	2.09060	-0.97020	H	-1.21110	-2.24800	4.73390
C	4.30070	2.61510	-1.28450	H	-0.70880	-0.87540	3.72190
C	4.23970	4.01390	-1.79780	H	-2.41960	-1.08570	4.19920
C	5.36200	4.71770	-1.98470	C	-4.11740	-3.23770	3.06210
C	6.67260	4.12000	-1.67180	C	-1.58520	-5.16070	-0.61030
C	6.74160	2.87700	-1.18530	H	-0.66720	-6.22350	-2.93450
H	3.29150	4.48790	-2.01070	H	0.73420	-6.89880	-2.04530
H	5.31030	5.73320	-2.35620	H	-5.06060	-2.40350	6.04230
H	7.57690	4.69400	-1.82770	H	-6.07690	-2.27120	4.56880
H	7.70740	2.44800	-0.94810	O	-0.35090	-5.56120	-0.98500
C	-0.55020	3.86190	-2.10690	O	-2.60580	-5.67510	-1.03770
C	1.75270	2.36190	-1.47850	O	-5.12210	-3.76050	2.60950
C	0.83800	2.62580	-0.52600	O	-4.05820	-2.73990	4.31770
C	-0.30120	3.53720	-0.82770	Si	4.65470	-1.67290	0.62020
H	-1.38470	4.49760	-2.36270	Si	-1.31540	4.34040	0.52850
C	1.45360	2.69450	-2.89810	C	9.13700	-2.71980	1.48860
C	0.33310	3.38940	-3.19290	C	8.70370	-2.61440	0.22700
C	0.00280	3.69940	-4.60300	C	7.29000	-2.28190	-0.04460
C	0.79990	3.27260	-5.58890	C	6.43560	-2.07590	0.97210
C	2.01200	2.49070	-5.27530	C	6.91990	-2.20150	2.36860
C	2.32340	2.21360	-4.00380	C	8.20130	-2.50500	2.61100
H	-0.88690	4.26920	-4.84080	H	10.17220	-2.96360	1.68940
H	0.55630	3.49630	-6.61950	H	9.38690	-2.77270	-0.59730
H	2.64540	2.13700	-6.07850	H	6.95690	-2.20440	-1.07240
H	3.20780	1.62630	-3.79330	H	6.24670	-2.04890	3.20130
O	2.02630	-0.19270	-0.28020	H	8.55470	-2.59490	3.63000
P	0.74860	0.40020	0.62230	C	3.21010	-4.97250	-2.38180
O	0.95870	2.03440	0.70700	C	3.73590	-5.32150	-1.20200
O	0.83320	-0.15980	2.01930	C	4.19480	-4.28070	-0.25810
N	-2.52600	-1.43460	-1.29850	C	4.06180	-2.97950	-0.56670
C	-3.74070	-1.77870	-0.72970	C	3.50820	-2.60110	-1.89220
C	-1.59240	-4.07990	0.39750	C	3.09940	-3.54680	-2.74700
C	-0.50720	-3.30790	0.76300	H	2.87330	-5.73310	-3.07400
C	-1.72600	-2.42360	2.66390	H	3.82460	-6.36650	-0.93500



H	4.63660	-4.58580	0.68220	C	-3.46470	2.70450	-0.55460
H	3.43450	-1.56370	-2.18550	C	-4.75200	2.36560	-0.69900
H	2.69280	-3.26930	-3.71080	H	-6.82360	2.71940	0.02380
C	2.30630	-1.48310	4.67230	H	-6.19550	4.40780	1.64720
C	2.26040	-2.60070	3.93800	H	-3.76830	5.11920	1.87770
C	3.00650	-2.68270	2.66480	H	-2.71650	2.20640	-1.15670
C	3.71660	-1.62980	2.22740	H	-5.03820	1.60590	-1.41290
C	3.78100	-0.40140	3.05760	N	-0.63510	-2.46950	1.83600
C	3.11000	-0.33210	4.21410	H	0.08330	-1.71840	1.97470
H	1.75420	-1.41960	5.60100	H	0.70120	-3.27640	-0.99620
H	1.66960	-3.44450	4.27000	C	-5.28260	-2.83290	5.06550
H	2.96000	-3.60040	2.10010	H	-5.59420	-3.87510	5.16460
H	4.36570	0.44860	2.72910	C	-0.31220	-6.60350	-1.97360
H	3.15010	0.56880	4.81260	H	-0.93350	-7.44760	-1.66830
C	-1.50050	8.97740	-0.20510	C	-2.88910	-3.77750	0.98290
C	-2.20280	8.14350	-0.97930	H	-3.44420	-2.92130	0.13620
C	-2.14200	6.68630	-0.74390	H	-3.63300	-4.56430	0.88850
C	-1.36950	6.18470	0.23660	O	-0.48940	0.08910	-0.19290
C	-0.61010	7.12060	1.10480	H	-1.89080	-0.81500	-0.76760
C	-0.67030	8.44100	0.89070	C	-6.89680	-3.10080	-3.36290
H	-1.54490	10.04530	-0.37510	C	-6.17210	-1.95210	-3.65800
H	-2.81950	8.53390	-1.77850	C	-5.12720	-1.53780	-2.82350
H	-2.74880	6.03920	-1.36300	C	-4.80090	-2.29570	-1.67390
H	-0.00810	6.75540	1.92220	C	-5.55580	-3.44270	-1.39190
H	-0.11560	9.12000	1.52540	C	-6.59260	-3.85270	-2.22530
C	0.58510	3.32760	4.69880	H	-7.70160	-3.40950	-4.02350
C	1.32990	3.89610	3.74420	H	-6.39170	-1.34910	-4.53260
C	0.72180	4.25330	2.44590	H	-5.32970	-4.01440	-0.49960
C	-0.57770	3.99710	2.20950	H	-7.15530	-4.74910	-1.98730
C	-1.40480	3.40930	3.28940	O	-4.48970	-0.39150	-3.17880
C	-0.85140	3.08190	4.46360	H	-3.72050	-0.25390	-2.60470
H	1.03040	3.05650	5.64730	C	-0.42760	-2.89230	-4.67800
H	2.38240	4.08200	3.91450	C	-1.54590	-3.59010	-4.22130
H	1.35070	4.68050	1.67440	C	-2.26490	-3.15540	-3.10650
H	-2.46260	3.25770	3.14650	C	-1.86580	-1.98930	-2.43610
H	-1.45880	2.64980	5.24840	C	-0.73420	-1.28530	-2.89280
C	-5.78680	3.00960	0.13360	C	-0.02490	-1.74040	-3.99970
C	-5.43940	3.93790	1.03180	H	0.12350	-3.24300	-5.54520
C	-4.02390	4.33520	1.17550	H	-1.87330	-4.49050	-4.73330
C	-3.07580	3.74920	0.42480	H	-3.10390	-3.73860	-2.75720

H	-0.40680	-0.40790	-2.34680	C	-6.10860	-0.09860	1.73220
H	0.84990	-1.18710	-4.32890	H	-5.60830	1.20280	3.38190
C	-5.23150	0.61820	2.54780	H	-3.16870	1.12240	2.90160
C	-3.86630	0.58580	2.27180	H	-2.30260	-0.12150	1.00300
C	-3.36950	-0.15380	1.19940	H	-6.31650	-1.40760	0.05410
C	-4.24340	-0.88910	0.37680	H	-7.17750	-0.07390	1.92110
C	-5.62100	-0.85040	0.66760				
C	3.02630	1.83040	-1.07320	P	0.74670	0.41120	0.65360
C	5.57670	0.81740	-0.39550	O	0.93510	2.04880	0.72030
C	4.48530	0.07970	-0.14480	O	0.84900	-0.14000	2.05230
C	3.12970	0.63010	-0.44790	N	-2.50700	-1.44210	-1.28620
H	6.56420	0.44990	-0.15630	C	-3.71570	-1.81880	-0.72560
C	5.46190	2.16140	-0.98360	C	-1.52710	-4.08770	0.38310
C	4.24860	2.66170	-1.29880	C	-0.45350	-3.30340	0.75610
C	4.16120	4.05400	-1.82560	C	-1.68530	-2.45410	2.66490
C	5.27030	4.77590	-2.02210	C	-2.80890	-3.16620	2.28500
C	6.59220	4.20470	-1.70680	C	0.87720	-3.26480	0.07670
C	6.68470	2.96760	-1.20930	H	1.44610	-2.39140	0.38790
H	3.20410	4.50840	-2.04130	H	1.43770	-4.17470	0.30400
H	5.19960	5.78650	-2.40340	C	-1.48100	-1.63450	3.90910
H	7.48570	4.79330	-1.87040	H	-1.17490	-2.28440	4.73680
H	7.65850	2.55810	-0.97100	H	-0.69240	-0.89780	3.73430
C	-0.63030	3.81480	-2.10210	H	-2.40040	-1.13740	4.20840
C	1.70450	2.36490	-1.47510	C	-4.06180	-3.31230	3.05880
C	0.79380	2.62480	-0.51790	C	-1.50620	-5.15130	-0.64250
C	-0.36440	3.51130	-0.82090	H	-0.55610	-6.15220	-2.99010
H	-1.47830	4.43180	-2.35870	H	0.83100	-6.84880	-2.09540
C	1.38730	2.67310	-2.89610	H	-5.01500	-2.51660	6.04630
C	0.25180	3.34350	-3.18990	H	-6.03800	-2.39980	4.57610
C	-0.09680	3.62730	-4.60120	O	-0.26730	-5.53110	-1.02340
C	0.69880	3.20050	-5.58840	O	-2.52090	-5.66960	-1.07950
C	1.92750	2.44500	-5.27510	O	-5.05660	-3.85240	2.60490
C	2.25570	2.19220	-4.00280	O	-4.00990	-2.82140	4.31750
H	-0.99870	4.17770	-4.83870	Si	4.68560	-1.61160	0.62140
H	0.44190	3.40490	-6.61970	Si	-1.37900	4.31320	0.53590
H	2.55980	2.09090	-6.07910	C	9.18810	-2.58890	1.46950
H	3.15240	1.62390	-3.79210	C	8.74860	-2.48480	0.20990
O	2.02560	-0.17220	-0.25500	C	7.32880	-2.17360	-0.05530

C	6.47490	-1.98550	0.96530	H	-0.24740	9.11590	1.50400
C	6.96620	-2.10970	2.35950	C	0.56640	3.34720	4.69700
C	8.25300	-2.39390	2.59600	C	1.29250	3.93330	3.73860
H	10.22770	-2.81730	1.66560	C	0.66960	4.27440	2.44300
H	9.43130	-2.62880	-0.61750	C	-0.62480	3.98760	2.21330
H	6.99080	-2.09760	-1.08160	C	-1.43110	3.37690	3.29620
H	6.29370	-1.97200	3.19530	C	-0.86430	3.06420	4.46800
H	8.61140	-2.48310	3.61340	H	1.02260	3.08830	5.64370
C	3.28660	-4.92540	-2.38610	H	2.34070	4.14570	3.90400
C	3.82070	-5.26940	-1.20850	H	1.28440	4.71550	1.66790
C	4.26450	-4.22420	-0.26230	H	-2.48450	3.19490	3.15680
C	4.11040	-2.92450	-0.56710	H	-1.45650	2.61540	5.25500
C	3.54710	-2.55110	-1.89010	C	-5.84080	2.93730	0.19260
C	3.15060	-3.50060	-2.74640	C	-5.49190	3.86810	1.08750
H	2.96160	-5.68930	-3.08030	C	-4.07880	4.27970	1.21410
H	3.92750	-6.31360	-0.94520	C	-3.13410	3.70390	0.45140
H	4.71260	-4.52470	0.67650	C	-3.52430	2.65640	-0.52440
H	3.45480	-1.51420	-2.17980	C	-4.80990	2.30490	-0.65370
H	2.73500	-3.22660	-3.70740	H	-6.87590	2.63670	0.09530
C	2.34970	-1.47040	4.68210	H	-6.24490	4.32970	1.71290
C	2.30820	-2.58210	3.93870	H	-3.82250	5.06540	1.91420
C	3.05080	-2.64910	2.66260	H	-2.77860	2.16630	-1.13600
C	3.75330	-1.58830	2.23200	H	-5.09740	1.54340	-1.36490
C	3.81260	-0.36640	3.07170	N	-0.59320	-2.47790	1.83770
C	3.14500	-0.31070	4.23090	H	0.11580	-1.72150	1.98680
H	1.80020	-1.41790	5.61300	H	0.74920	-3.22560	-1.00450
H	1.72360	-3.43220	4.26550	C	-5.22990	-2.94580	5.06790
H	3.00820	-3.56230	2.09030	H	-5.51760	-3.99530	5.16240
H	4.39100	0.48990	2.74820	C	-0.21570	-6.55310	-2.03240
H	3.18180	0.58540	4.83690	H	-0.84270	-7.40210	-1.75370
C	-1.62390	8.94220	-0.23040	C	-2.82750	-3.81330	0.97340
C	-2.31290	8.09360	-1.00040	H	-3.39900	-2.96190	0.13170
C	-2.23360	6.63910	-0.75420	H	-3.55810	-4.61190	0.87470
C	-1.45690	6.15480	0.23170	O	-0.49380	0.07910	-0.14960
C	-0.71350	7.10710	1.09590	H	-1.88390	-0.82150	-0.74240
C	-0.79040	8.42500	0.87200	C	-6.83050	-3.18380	-3.38640
H	-1.68190	10.00830	-0.40830	C	-6.13740	-2.01070	-3.66060
H	-2.93240	8.47000	-1.80410	C	-5.10560	-1.58190	-2.81710
H	-2.83100	5.97990	-1.36940	C	-4.76060	-2.34930	-1.67950
H	-0.11060	6.75630	1.91890	C	-5.48310	-3.52180	-1.41900

C	-6.50690	-3.94630	-2.26130	H	-3.02490	-3.73360	-2.78880
H	-7.62550	-3.50340	-4.05370	H	-0.41800	-0.34100	-2.31420
H	-6.37220	-1.39930	-4.52540	H	0.85820	-1.04630	-4.31170
H	-5.24110	-4.10370	-0.53770	C	-5.27250	0.51240	2.56880
H	-7.04420	-4.86230	-2.03990	C	-3.90640	0.51750	2.29560
O	-4.49900	-0.41300	-3.15230	C	-3.38820	-0.20060	1.21840
H	-3.73370	-0.26430	-2.57600	C	-4.24160	-0.95140	0.38810
C	-0.37370	-2.77790	-4.69400	C	-5.62020	-0.95080	0.67640
C	-1.47250	-3.51440	-4.25060	C	-6.12930	-0.22030	1.74580
C	-2.20200	-3.12140	-3.12710	H	-5.66600	1.08050	3.40650
C	-1.83410	-1.95800	-2.43450	H	-3.22520	1.06850	2.93120
C	-0.72210	-1.21530	-2.87790	H	-2.32190	-0.13990	1.02490
C	-0.00130	-1.62930	-3.99340	H	-6.29960	-1.52180	0.05740
H	0.18580	-3.09670	-5.56810	H	-7.19880	-0.22530	1.93290
H	-1.77590	-4.41300	-4.78040				
C	3.09810	1.84780	-0.95350	C	2.07420	2.45830	-5.16770
C	5.63840	0.81310	-0.27710	C	2.38790	2.22280	-3.88850
C	4.54280	0.07140	-0.05540	H	-0.93570	4.05610	-4.79420
C	3.19250	0.63730	-0.35020	H	0.57390	3.34730	-6.54420
H	6.62310	0.43580	-0.04070	H	2.73770	2.13170	-5.95800
C	5.53160	2.17210	-0.83410	H	3.30480	1.69520	-3.66020
C	4.32240	2.68020	-1.15320	O	2.07880	-0.15560	-0.17850
C	4.24040	4.07950	-1.66010	P	0.83350	0.42100	0.78350
C	5.35180	4.80470	-1.83020	O	1.00900	2.06750	0.82520
C	6.66990	4.22830	-1.50670	O	0.99710	-0.13480	2.17400
C	6.75680	2.98220	-1.03040	N	-2.43000	-1.39120	-1.26200
H	3.28500	4.53420	-1.88410	C	-3.68470	-1.75440	-0.81890
H	5.28600	5.82090	-2.19720	C	-1.58260	-3.96250	0.36580
H	7.56520	4.81980	-1.64850	C	-0.48370	-3.21520	0.75700
H	7.72770	2.56840	-0.78750	C	-1.71550	-2.31740	2.63970
C	-0.60830	3.70920	-2.05220	C	-2.85400	-2.99820	2.25150
C	1.77940	2.37650	-1.37040	C	0.84740	-3.20470	0.07610
C	0.84380	2.60490	-0.42720	H	1.45510	-2.37360	0.42610
C	-0.36790	3.40000	-0.76710	H	1.36700	-4.14880	0.25390
H	-1.46660	4.31500	-2.31970	C	-1.51260	-1.48210	3.87290
C	1.47640	2.66490	-2.79970	H	-1.46230	-2.12110	4.76000
C	0.31810	3.28190	-3.11910	H	-0.58550	-0.91350	3.78060
C	-0.01440	3.54820	-4.53740	H	-2.35020	-0.80050	4.01760
C	0.81920	3.15650	-5.50750	C	-4.09390	-3.13580	3.05440

C	-1.58340	-4.94120	-0.72980	H	3.29530	0.25300	5.05150
H	-0.63770	-5.81140	-3.12220	H	4.54350	0.23850	2.84230
H	0.67190	-6.67730	-2.25650	H	2.93970	-3.71120	2.06480
H	-5.06180	-2.07360	5.95230	H	1.74610	-3.66800	4.15180
H	-6.10960	-2.20850	4.50120	C	-1.03040	8.76790	-0.44700
O	-0.37700	-5.39410	-1.09730	C	0.05580	8.03320	-0.18180
O	-2.61590	-5.34770	-1.26250	C	-0.08140	6.59610	0.13150
O	-5.05330	-3.78680	2.68380	C	-1.29670	6.02250	0.16890
O	-4.05920	-2.50180	4.24850	C	-2.49550	6.83900	-0.14440
Si	4.73050	-1.64870	0.65010	C	-2.36700	8.14040	-0.43210
Si	-1.44220	4.20200	0.53140	H	-0.93190	9.82060	-0.67790
C	9.23540	-2.73110	1.34390	H	1.03730	8.48900	-0.19730
C	8.77090	-2.54850	0.10240	H	0.81150	6.01600	0.33170
C	7.35030	-2.20450	-0.11320	H	-3.48030	6.39440	-0.15480
C	6.52100	-2.06390	0.93490	H	-3.24200	8.73480	-0.66160
C	7.03960	-2.27640	2.30850	C	-0.15330	3.36000	4.96460
C	8.32700	-2.59060	2.50000	C	-0.63270	2.37050	4.20400
H	10.27560	-2.98380	1.50380	C	-1.03360	2.63810	2.80760
H	9.43390	-2.65290	-0.74660	C	-0.90660	3.86840	2.28620
H	6.99180	-2.06520	-1.12580	C	-0.39660	4.96730	3.14490
H	6.38670	-2.18170	3.16530	C	-0.03480	4.72280	4.41060
H	8.70510	-2.74460	3.50240	H	0.14100	3.16620	5.98790
C	3.21630	-4.84600	-2.42690	H	-0.72830	1.37370	4.61140
C	3.75440	-5.23350	-1.26480	H	-1.41250	1.82480	2.20830
C	4.23440	-4.22450	-0.29720	H	-0.31920	5.97590	2.76620
C	4.10890	-2.91400	-0.56610	H	0.33700	5.52560	5.03410
C	3.54190	-2.49260	-1.87310	C	-5.93520	2.96530	0.05450
C	3.11240	-3.40930	-2.74890	C	-5.55740	3.75850	1.06360
H	2.86540	-5.58320	-3.13700	C	-4.13470	4.12220	1.22660
H	3.83830	-6.28650	-1.02980	C	-3.21420	3.66190	0.36260
H	4.68590	-4.56020	0.62800	C	-3.63460	2.75340	-0.73350
H	3.47550	-1.44690	-2.13690	C	-4.92670	2.43520	-0.88410
H	2.69470	-3.10010	-3.69830	H	-6.97660	2.69670	-0.06590
C	2.45450	-1.64880	4.75030	H	-6.29320	4.13910	1.75990
C	3.21670	-0.60690	4.39910	H	-3.85230	4.78400	2.03620
C	3.94070	-0.62020	3.11070	H	-2.90690	2.33230	-1.41290
C	3.83260	-1.67320	2.28150	H	-5.23530	1.77540	-1.68330
C	3.01280	-2.83840	2.69400	N	-0.60310	-2.40110	1.84230
C	2.35260	-2.82090	3.85860	H	0.14210	-1.68990	2.02190
H	1.91510	-1.63690	5.68840	H	0.72010	-3.10210	-1.00160

C	-5.25530	-2.62990	5.03530	C	-0.63270	-0.92640	-2.78730
H	-5.45950	-3.67990	5.25720	C	-1.74420	-1.72930	-2.45960
C	-0.35610	-6.32250	-2.19910	C	-2.07630	-2.79940	-3.30720
H	-1.04320	-7.15010	-2.01560	C	-1.31670	-3.04430	-4.45230
C	-2.87780	-3.68610	0.96330	H	0.36890	-2.45190	-5.66500
H	-3.45730	-2.87360	0.05140	H	0.97730	-0.56300	-4.14930
H	-3.63640	-4.46240	0.89980	H	-0.35690	-0.12290	-2.11570
O	-0.43920	0.07660	0.03730	H	-2.90720	-3.45030	-3.08300
H	-1.84150	-0.80490	-0.65310	H	-1.59850	-3.87130	-5.09830
C	-6.65190	-2.52900	-3.87060	C	-5.56260	0.48980	2.37090
C	-6.37080	-3.53790	-2.95730	C	-4.20590	0.66980	2.11130
C	-5.37910	-3.37520	-1.97750	C	-3.57380	-0.02570	1.07640
C	-4.67210	-2.15910	-1.90350	C	-4.30860	-0.91630	0.27450
C	-4.95660	-1.16020	-2.85190	C	-5.67600	-1.09780	0.55570
C	-5.93050	-1.33350	-3.82790	C	-6.29750	-0.39810	1.58400
H	-7.42230	-2.67910	-4.62130	H	-6.04370	1.04490	3.17090
H	-6.90020	-4.48460	-2.97660	H	-3.63870	1.36820	2.71630
H	-4.39870	-0.23050	-2.80630	H	-2.51880	0.15560	0.89260
H	-6.12880	-0.54010	-4.54140	H	-6.25830	-1.79360	-0.03460
O	-5.19000	-4.41410	-1.11310	H	-7.35680	-0.54940	1.76800
H	-4.25390	-4.71050	-1.12170				
C	-0.21670	-2.24920	-4.77350				
C	0.11960	-1.19150	-3.92700				
C	3.13360	1.84620	-0.90050	C	1.82820	2.39720	-1.33100
C	5.65060	0.76140	-0.21610	C	0.87940	2.62210	-0.40060
C	4.54190	0.03180	-0.02090	C	-0.32340	3.42510	-0.75140
C	3.20280	0.62500	-0.31600	H	-1.39650	4.35640	-2.31190
H	6.62720	0.36390	0.02060	C	1.54980	2.70280	-2.76180
C	5.56980	2.13240	-0.74750	C	0.39800	3.32580	-3.09340
C	4.37180	2.66380	-1.07120	C	0.08880	3.60720	-4.51410
C	4.31590	4.07210	-1.55550	C	0.93730	3.22410	-5.47460
C	5.43970	4.78350	-1.70110	C	2.18560	2.52030	-5.12200
C	6.74560	4.18230	-1.37290	C	2.47810	2.27060	-3.84050
C	6.80880	2.92730	-0.91650	H	-0.82740	4.11940	-4.78040
H	3.36960	4.54390	-1.78310	H	0.70910	3.42600	-6.51320
H	5.39290	5.80630	-2.05220	H	2.86120	2.20070	-5.90490
H	7.65100	4.76260	-1.49520	H	3.39010	1.73870	-3.60340
H	7.77080	2.49490	-0.67040	O	2.07460	-0.15250	-0.16950
C	-0.54430	3.74540	-2.03720	P	0.82850	0.42810	0.78980

O	1.02140	2.07160	0.84870	C	4.17660	-4.25060	-0.38270
O	0.98110	-0.13940	2.17730	C	4.06780	-2.93140	-0.61380
N	-2.45540	-1.35560	-1.26110	C	3.50880	-2.46580	-1.90940
C	-3.70700	-1.73340	-0.82270	C	3.06660	-3.35130	-2.81050
C	-1.59630	-3.94270	0.33970	H	2.79150	-5.50960	-3.26060
C	-0.50160	-3.19090	0.73400	H	3.75430	-6.28550	-1.17430
C	-1.73400	-2.31500	2.62620	H	4.62260	-4.61860	0.53280
C	-2.86940	-2.99900	2.23500	H	3.45770	-1.41260	-2.14440
C	0.82480	-3.16410	0.04540	H	2.65260	-3.00950	-3.75040
H	1.43740	-2.34530	0.41390	C	2.39920	-1.78390	4.72710
H	1.34140	-4.11480	0.19100	C	3.16130	-0.73460	4.39850
C	-1.53360	-1.48770	3.86520	C	3.89320	-0.72430	3.11460
H	-1.48320	-2.13210	4.74830	C	3.79190	-1.76280	2.26650
H	-0.60740	-0.91700	3.77750	C	2.97510	-2.93810	2.65570
H	-2.37270	-0.80850	4.01340	C	2.30700	-2.94160	3.81590
C	-4.10600	-3.15150	3.04000	H	1.85360	-1.78910	5.66170
C	-1.59100	-4.91370	-0.76230	H	3.23340	0.11450	5.06570
H	-0.62150	-5.75640	-3.16470	H	4.49540	0.14030	2.86480
H	0.67340	-6.63550	-2.29080	H	2.91020	-3.80130	2.01250
H	-5.07710	-2.11040	5.94450	H	1.70200	-3.79570	4.09160
H	-6.12830	-2.25430	4.49680	C	-0.96840	8.79000	-0.41550
O	-0.38160	-5.35490	-1.13430	C	0.11240	8.04880	-0.14660
O	-2.62060	-5.32510	-1.29750	C	-0.03420	6.61160	0.16170
O	-5.05960	-3.81150	2.67000	C	-1.25270	6.04430	0.19050
O	-4.07520	-2.52030	4.23580	C	-2.44560	6.86820	-0.12570
Si	4.69940	-1.70880	0.64100	C	-2.30850	8.16970	-0.40900
Si	-1.40920	4.22230	0.54010	H	-0.86300	9.84270	-0.64340
C	9.18050	-2.88660	1.33420	H	1.09650	8.49920	-0.15620
C	8.72780	-2.66310	0.09500	H	0.85470	6.02590	0.36320
C	7.31510	-2.28770	-0.12030	H	-3.43260	6.42890	-0.14190
C	6.48140	-2.15970	0.92590	H	-3.17910	8.76950	-0.64110
C	6.98700	-2.41680	2.29670	C	-0.16620	3.33890	4.97810
C	8.26720	-2.75950	2.48790	C	-0.65910	2.36160	4.21020
H	10.21480	-3.16280	1.49370	C	-1.04520	2.64240	2.81220
H	9.39440	-2.75790	-0.75240	C	-0.89190	3.87250	2.29710
H	6.96570	-2.11640	-1.13120	C	-0.36700	4.95800	3.16370
H	6.33020	-2.33210	3.15170	C	-0.01820	4.70140	4.43070
H	8.63580	-2.94640	3.48820	H	0.11730	3.13540	6.00260
C	3.15170	-4.79760	-2.52960	H	-0.77660	1.36530	4.61290
C	3.68440	-5.22520	-1.37910	H	-1.43580	1.83870	2.20720

H	-0.26740	5.96620	2.78940	C	-5.94900	-1.32760	-3.83870
H	0.36480	5.49440	5.05990	H	-7.42370	-2.68720	-4.64090
C	-5.89800	2.98640	0.02550	H	-6.89020	-4.48920	-2.99540
C	-5.52800	3.77620	1.04000	H	-4.43090	-0.21170	-2.81200
C	-4.10710	4.14230	1.21280	H	-6.15240	-0.53520	-4.55200
C	-3.18050	3.68730	0.35250	O	-5.19160	-4.40290	-1.12320
C	-3.59250	2.78390	-0.75080	H	-4.25670	-4.70330	-1.14270
C	-4.88310	2.46400	-0.91050	C	-0.27800	-2.08540	-4.82140
H	-6.93800	2.71550	-0.10180	C	0.02450	-1.01610	-3.97670
H	-6.26850	4.15160	1.73410	C	-0.71560	-0.79340	-2.81990
H	-3.83050	4.79940	2.02820	C	-1.77840	-1.65200	-2.47490
H	-2.85990	2.36900	-1.42880	C	-2.07670	-2.73300	-3.32040
H	-5.18600	1.80930	-1.71570	C	-1.33090	-2.93540	-4.48250
N	-0.62260	-2.38670	1.82610	H	0.29780	-2.25480	-5.72610
H	0.12180	-1.67490	2.01210	H	0.84430	-0.34480	-4.21520
H	0.68970	-3.02930	-1.02810	H	-0.46690	0.02020	-2.14990
C	-5.26670	-2.66620	5.02640	H	-2.87060	-3.42360	-3.07970
H	-5.45650	-3.71950	5.24570	H	-1.58480	-3.77210	-5.12750
C	-0.35330	-6.27570	-2.24200	C	-5.59660	0.48930	2.37400
H	-1.04660	-7.10080	-2.07250	C	-4.24380	0.68740	2.10610
C	-2.89200	-3.67670	0.94090	C	-3.60860	-0.00330	1.07020
H	-3.47320	-2.85980	0.03950	C	-4.33560	-0.90730	0.27630
H	-3.64710	-4.45600	0.87350	C	-5.69780	-1.10920	0.56740
O	-0.44410	0.10220	0.03530	C	-6.32310	-0.41390	1.59650
H	-1.86800	-0.77630	-0.64480	H	-6.08120	1.04090	3.17430
C	-6.65810	-2.53030	-3.88660	H	-3.68210	1.39680	2.70370
C	-6.37050	-3.53710	-2.97340	H	-2.55730	0.19210	0.88000
C	-5.38500	-3.36560	-1.98900	H	-6.27250	-1.81760	-0.01570
C	-4.68930	-2.14300	-1.91050	H	-7.37860	-0.58060	1.78870
C	-4.98050	-1.14600	-2.85880				
C	3.09810	1.84780	-0.95350	C	5.35180	4.80470	-1.83020
C	5.63840	0.81310	-0.27710	C	6.66990	4.22830	-1.50670
C	4.54280	0.07140	-0.05540	C	6.75680	2.98220	-1.03040
C	3.19250	0.63730	-0.35020	H	3.28500	4.53420	-1.88410
H	6.62310	0.43580	-0.04070	H	5.28600	5.82090	-2.19720
C	5.53160	2.17210	-0.83410	H	7.56520	4.81980	-1.64850
C	4.32240	2.68020	-1.15320	H	7.72770	2.56840	-0.78750
C	4.24040	4.07950	-1.66010	C	-0.60830	3.70920	-2.05220



C	1.77940	2.37650	-1.37040	O	-4.05920	-2.50180	4.24850
C	0.84380	2.60490	-0.42720	Si	4.73050	-1.64870	0.65010
C	-0.36790	3.40000	-0.76710	Si	-1.44220	4.20200	0.53140
H	-1.46660	4.31500	-2.31970	C	9.23540	-2.73110	1.34390
C	1.47640	2.66490	-2.79970	C	8.77090	-2.54850	0.10240
C	0.31810	3.28190	-3.11910	C	7.35030	-2.20450	-0.11320
C	-0.01440	3.54820	-4.53740	C	6.52100	-2.06390	0.93490
C	0.81920	3.15650	-5.50750	C	7.03960	-2.27640	2.30850
C	2.07420	2.45830	-5.16770	C	8.32700	-2.59060	2.50000
C	2.38790	2.22280	-3.88850	H	10.27560	-2.98380	1.50380
H	-0.93570	4.05610	-4.79420	H	9.43390	-2.65290	-0.74660
H	0.57390	3.34730	-6.54420	H	6.99180	-2.06520	-1.12580
H	2.73770	2.13170	-5.95800	H	6.38670	-2.18170	3.16530
H	3.30480	1.69520	-3.66020	H	8.70510	-2.74460	3.50240
O	2.07880	-0.15560	-0.17850	C	3.21630	-4.84600	-2.42690
P	0.83350	0.42100	0.78350	C	3.75440	-5.23350	-1.26480
O	1.00900	2.06750	0.82520	C	4.23440	-4.22450	-0.29720
O	0.99710	-0.13480	2.17400	C	4.10890	-2.91400	-0.56610
N	-2.43000	-1.39120	-1.26200	C	3.54190	-2.49260	-1.87310
C	-3.68470	-1.75440	-0.81890	C	3.11240	-3.40930	-2.74890
C	-1.58260	-3.96250	0.36580	H	2.86540	-5.58320	-3.13700
C	-0.48370	-3.21520	0.75700	H	3.83830	-6.28650	-1.02980
C	-1.71550	-2.31740	2.63970	H	4.68590	-4.56020	0.62800
C	-2.85400	-2.99820	2.25150	H	3.47550	-1.44690	-2.13690
C	0.84740	-3.20470	0.07610	H	2.69470	-3.10010	-3.69830
H	1.45510	-2.37360	0.42610	C	2.45450	-1.64880	4.75030
H	1.36700	-4.14880	0.25390	C	3.21670	-0.60690	4.39910
C	-1.51260	-1.48210	3.87290	C	3.94070	-0.62020	3.11070
H	-1.46230	-2.12110	4.76000	C	3.83260	-1.67320	2.28150
H	-0.58550	-0.91350	3.78060	C	3.01280	-2.83840	2.69400
H	-2.35020	-0.80050	4.01760	C	2.35260	-2.82090	3.85860
C	-4.09390	-3.13580	3.05440	H	1.91510	-1.63690	5.68840
C	-1.58340	-4.94120	-0.72980	H	3.29530	0.25300	5.05150
H	-0.63770	-5.81140	-3.12220	H	4.54350	0.23850	2.84230
H	0.67190	-6.67730	-2.25650	H	2.93970	-3.71120	2.06480
H	-5.06180	-2.07360	5.95230	H	1.74610	-3.66800	4.15180
H	-6.10960	-2.20850	4.50120	C	-1.03040	8.76790	-0.44700
O	-0.37700	-5.39410	-1.09730	C	0.05580	8.03320	-0.18180
O	-2.61590	-5.34770	-1.26250	C	-0.08140	6.59610	0.13150
O	-5.05330	-3.78680	2.68380	C	-1.29670	6.02250	0.16890

C	-2.49550	6.83900	-0.14440	O	-0.43920	0.07660	0.03730
C	-2.36700	8.14040	-0.43210	H	-1.84150	-0.80490	-0.65310
H	-0.93190	9.82060	-0.67790	C	-6.65190	-2.52900	-3.87060
H	1.03730	8.48900	-0.19730	C	-6.37080	-3.53790	-2.95730
H	0.81150	6.01600	0.33170	C	-5.37910	-3.37520	-1.97750
H	-3.48030	6.39440	-0.15480	C	-4.67210	-2.15910	-1.90350
H	-3.24200	8.73480	-0.66160	C	-4.95660	-1.16020	-2.85190
C	-0.15330	3.36000	4.96460	C	-5.93050	-1.33350	-3.82790
C	-0.63270	2.37050	4.20400	H	-7.42230	-2.67910	-4.62130
C	-1.03360	2.63810	2.80760	H	-6.90020	-4.48460	-2.97660
C	-0.90660	3.86840	2.28620	H	-4.39870	-0.23050	-2.80630
C	-0.39660	4.96730	3.14490	H	-6.12880	-0.54010	-4.54140
C	-0.03480	4.72280	4.41060	O	-5.19000	-4.41410	-1.11310
H	0.14100	3.16620	5.98790	H	-4.25390	-4.71050	-1.12170
H	-0.72830	1.37370	4.61140	C	-0.21670	-2.24920	-4.77350
H	-1.41250	1.82480	2.20830	C	0.11960	-1.19150	-3.92700
H	-0.31920	5.97590	2.76620	C	-0.63270	-0.92640	-2.78730
H	0.33700	5.52560	5.03410	C	-1.74420	-1.72930	-2.45960
C	-5.93520	2.96530	0.05450	C	-2.07630	-2.79940	-3.30720
C	-5.55740	3.75850	1.06360	C	-1.31670	-3.04430	-4.45230
C	-4.13470	4.12220	1.22660	H	0.36890	-2.45190	-5.66500
C	-3.21420	3.66190	0.36260	H	0.97730	-0.56300	-4.14930
C	-3.63460	2.75340	-0.73350	H	-0.35690	-0.12290	-2.11570
C	-4.92670	2.43520	-0.88410	H	-2.90720	-3.45030	-3.08300
H	-6.97660	2.69670	-0.06590	H	-1.59850	-3.87130	-5.09830
H	-6.29320	4.13910	1.75990	C	-5.56260	0.48980	2.37090
H	-3.85230	4.78400	2.03620	C	-4.20590	0.66980	2.11130
H	-2.90690	2.33230	-1.41290	C	-3.57380	-0.02570	1.07640
H	-5.23530	1.77540	-1.68330	C	-4.30860	-0.91630	0.27450
N	-0.60310	-2.40110	1.84230	C	-5.67600	-1.09780	0.55570
H	0.14210	-1.68990	2.02190	C	-6.29750	-0.39810	1.58400
H	0.72010	-3.10210	-1.00160	H	-6.04370	1.04490	3.17090
C	-5.25530	-2.62990	5.03530	H	-3.63870	1.36820	2.71630
H	-5.45950	-3.67990	5.25720	H	-2.51880	0.15560	0.89260
C	-0.35610	-6.32250	-2.19910	H	-6.25830	-1.79360	-0.03460
H	-1.04320	-7.15010	-2.01560	H	-7.35680	-0.54940	1.76800
C	-2.87780	-3.68610	0.96330				
H	-3.45730	-2.87360	0.05140				
H	-3.63640	-4.46240	0.89980				

C	3.09810	1.84780	-0.95350	C	0.84740	-3.20470	0.07610
C	5.63840	0.81310	-0.27710	H	1.45510	-2.37360	0.42610
C	4.54280	0.07140	-0.05540	H	1.36700	-4.14880	0.25390
C	3.19250	0.63730	-0.35020	C	-1.51260	-1.48210	3.87290
H	6.62310	0.43580	-0.04070	H	-1.46230	-2.12110	4.76000
C	5.53160	2.17210	-0.83410	H	-0.58550	-0.91350	3.78060
C	4.32240	2.68020	-1.15320	H	-2.35020	-0.80050	4.01760
C	4.24040	4.07950	-1.66010	C	-4.09390	-3.13580	3.05440
C	5.35180	4.80470	-1.83020	C	-1.58340	-4.94120	-0.72980
C	6.66990	4.22830	-1.50670	H	-0.63770	-5.81140	-3.12220
C	6.75680	2.98220	-1.03040	H	0.67190	-6.67730	-2.25650
H	3.28500	4.53420	-1.88410	H	-5.06180	-2.07360	5.95230
H	5.28600	5.82090	-2.19720	H	-6.10960	-2.20850	4.50120
H	7.56520	4.81980	-1.64850	O	-0.37700	-5.39410	-1.09730
H	7.72770	2.56840	-0.78750	O	-2.61590	-5.34770	-1.26250
C	-0.60830	3.70920	-2.05220	O	-5.05330	-3.78680	2.68380
C	1.77940	2.37650	-1.37040	O	-4.05920	-2.50180	4.24850
C	0.84380	2.60490	-0.42720	Si	4.73050	-1.64870	0.65010
C	-0.36790	3.40000	-0.76710	Si	-1.44220	4.20200	0.53140
H	-1.46660	4.31500	-2.31970	C	9.23540	-2.73110	1.34390
C	1.47640	2.66490	-2.79970	C	8.77090	-2.54850	0.10240
C	0.31810	3.28190	-3.11910	C	7.35030	-2.20450	-0.11320
C	-0.01440	3.54820	-4.53740	C	6.52100	-2.06390	0.93490
C	0.81920	3.15650	-5.50750	C	7.03960	-2.27640	2.30850
C	2.07420	2.45830	-5.16770	C	8.32700	-2.59060	2.50000
C	2.38790	2.22280	-3.88850	H	10.27560	-2.98380	1.50380
H	-0.93570	4.05610	-4.79420	H	9.43390	-2.65290	-0.74660
H	0.57390	3.34730	-6.54420	H	6.99180	-2.06520	-1.12580
H	2.73770	2.13170	-5.95800	H	6.38670	-2.18170	3.16530
H	3.30480	1.69520	-3.66020	H	8.70510	-2.74460	3.50240
O	2.07880	-0.15560	-0.17850	C	3.21630	-4.84600	-2.42690
P	0.83350	0.42100	0.78350	C	3.75440	-5.23350	-1.26480
O	1.00900	2.06750	0.82520	C	4.23440	-4.22450	-0.29720
O	0.99710	-0.13480	2.17400	C	4.10890	-2.91400	-0.56610
N	-2.43000	-1.39120	-1.26200	C	3.54190	-2.49260	-1.87310
C	-3.68470	-1.75440	-0.81890	C	3.11240	-3.40930	-2.74890
C	-1.58260	-3.96250	0.36580	H	2.86540	-5.58320	-3.13700
C	-0.48370	-3.21520	0.75700	H	3.83830	-6.28650	-1.02980
C	-1.71550	-2.31740	2.63970	H	4.68590	-4.56020	0.62800
C	-2.85400	-2.99820	2.25150	H	3.47550	-1.44690	-2.13690

H	2.69470	-3.10010	-3.69830	H	-6.97660	2.69670	-0.06590
C	2.45450	-1.64880	4.75030	H	-6.29320	4.13910	1.75990
C	3.21670	-0.60690	4.39910	H	-3.85230	4.78400	2.03620
C	3.94070	-0.62020	3.11070	H	-2.90690	2.33230	-1.41290
C	3.83260	-1.67320	2.28150	H	-5.23530	1.77540	-1.68330
C	3.01280	-2.83840	2.69400	N	-0.60310	-2.40110	1.84230
C	2.35260	-2.82090	3.85860	H	0.14210	-1.68990	2.02190
H	1.91510	-1.63690	5.68840	H	0.72010	-3.10210	-1.00160
H	3.29530	0.25300	5.05150	C	-5.25530	-2.62990	5.03530
H	4.54350	0.23850	2.84230	H	-5.45950	-3.67990	5.25720
H	2.93970	-3.71120	2.06480	C	-0.35610	-6.32250	-2.19910
H	1.74610	-3.66800	4.15180	H	-1.04320	-7.15010	-2.01560
C	-1.03040	8.76790	-0.44700	C	-2.87780	-3.68610	0.96330
C	0.05580	8.03320	-0.18180	H	-3.45730	-2.87360	0.05140
C	-0.08140	6.59610	0.13150	H	-3.63640	-4.46240	0.89980
C	-1.29670	6.02250	0.16890	O	-0.43920	0.07660	0.03730
C	-2.49550	6.83900	-0.14440	H	-1.84150	-0.80490	-0.65310
C	-2.36700	8.14040	-0.43210	C	-6.65190	-2.52900	-3.87060
H	-0.93190	9.82060	-0.67790	C	-6.37080	-3.53790	-2.95730
H	1.03730	8.48900	-0.19730	C	-5.37910	-3.37520	-1.97750
H	0.81150	6.01600	0.33170	C	-4.67210	-2.15910	-1.90350
H	-3.48030	6.39440	-0.15480	C	-4.95660	-1.16020	-2.85190
H	-3.24200	8.73480	-0.66160	C	-5.93050	-1.33350	-3.82790
C	-0.15330	3.36000	4.96460	H	-7.42230	-2.67910	-4.62130
C	-0.63270	2.37050	4.20400	H	-6.90020	-4.48460	-2.97660
C	-1.03360	2.63810	2.80760	H	-4.39870	-0.23050	-2.80630
C	-0.90660	3.86840	2.28620	H	-6.12880	-0.54010	-4.54140
C	-0.39660	4.96730	3.14490	O	-5.19000	-4.41410	-1.11310
C	-0.03480	4.72280	4.41060	H	-4.25390	-4.71050	-1.12170
H	0.14100	3.16620	5.98790	C	-0.21670	-2.24920	-4.77350
H	-0.72830	1.37370	4.61140	C	0.11960	-1.19150	-3.92700
H	-1.41250	1.82480	2.20830	C	-0.63270	-0.92640	-2.78730
H	-0.31920	5.97590	2.76620	C	-1.74420	-1.72930	-2.45960
H	0.33700	5.52560	5.03410	C	-2.07630	-2.79940	-3.30720
C	-5.93520	2.96530	0.05450	C	-1.31670	-3.04430	-4.45230
C	-5.55740	3.75850	1.06360	H	0.36890	-2.45190	-5.66500
C	-4.13470	4.12220	1.22660	H	0.97730	-0.56300	-4.14930
C	-3.21420	3.66190	0.36260	H	-0.35690	-0.12290	-2.11570
C	-3.63460	2.75340	-0.73350	H	-2.90720	-3.45030	-3.08300
C	-4.92670	2.43520	-0.88410	H	-1.59850	-3.87130	-5.09830

C	-5.56260	0.48980	2.37090	H	-6.04370	1.04490	3.17090
C	-4.20590	0.66980	2.11130	H	-3.63870	1.36820	2.71630
C	-3.57380	-0.02570	1.07640	H	-2.51880	0.15560	0.89260
C	-4.30860	-0.91630	0.27450	H	-6.25830	-1.79360	-0.03460
C	-5.67600	-1.09780	0.55570	H	-7.35680	-0.54940	1.76800
C	-6.29750	-0.39810	1.58400				
C	3.09810	1.84780	-0.95350	O	0.99710	-0.13480	2.17400
C	5.63840	0.81310	-0.27710	N	-2.43000	-1.39120	-1.26200
C	4.54280	0.07140	-0.05540	C	-3.68470	-1.75440	-0.81890
C	3.19250	0.63730	-0.35020	C	-1.58260	-3.96250	0.36580
H	6.62310	0.43580	-0.04070	C	-0.48370	-3.21520	0.75700
C	5.53160	2.17210	-0.83410	C	-1.71550	-2.31740	2.63970
C	4.32240	2.68020	-1.15320	C	-2.85400	-2.99820	2.25150
C	4.24040	4.07950	-1.66010	C	0.84740	-3.20470	0.07610
C	5.35180	4.80470	-1.83020	H	1.45510	-2.37360	0.42610
C	6.66990	4.22830	-1.50670	H	1.36700	-4.14880	0.25390
C	6.75680	2.98220	-1.03040	C	-1.51260	-1.48210	3.87290
H	3.28500	4.53420	-1.88410	H	-1.46230	-2.12110	4.76000
H	5.28600	5.82090	-2.19720	H	-0.58550	-0.91350	3.78060
H	7.56520	4.81980	-1.64850	H	-2.35020	-0.80050	4.01760
H	7.72770	2.56840	-0.78750	C	-4.09390	-3.13580	3.05440
C	-0.60830	3.70920	-2.05220	C	-1.58340	-4.94120	-0.72980
C	1.77940	2.37650	-1.37040	H	-0.63770	-5.81140	-3.12220
C	0.84380	2.60490	-0.42720	H	0.67190	-6.67730	-2.25650
C	-0.36790	3.40000	-0.76710	H	-5.06180	-2.07360	5.95230
H	-1.46660	4.31500	-2.31970	H	-6.10960	-2.20850	4.50120
C	1.47640	2.66490	-2.79970	O	-0.37700	-5.39410	-1.09730
C	0.31810	3.28190	-3.11910	O	-2.61590	-5.34770	-1.26250
C	-0.01440	3.54820	-4.53740	O	-5.05330	-3.78680	2.68380
C	0.81920	3.15650	-5.50750	O	-4.05920	-2.50180	4.24850
C	2.07420	2.45830	-5.16770	Si	4.73050	-1.64870	0.65010
C	2.38790	2.22280	-3.88850	Si	-1.44220	4.20200	0.53140
H	-0.93570	4.05610	-4.79420	C	9.23540	-2.73110	1.34390
H	0.57390	3.34730	-6.54420	C	8.77090	-2.54850	0.10240
H	2.73770	2.13170	-5.95800	C	7.35030	-2.20450	-0.11320
H	3.30480	1.69520	-3.66020	C	6.52100	-2.06390	0.93490
O	2.07880	-0.15560	-0.17850	C	7.03960	-2.27640	2.30850
P	0.83350	0.42100	0.78350	C	8.32700	-2.59060	2.50000
O	1.00900	2.06750	0.82520	H	10.27560	-2.98380	1.50380

H	9.43390	-2.65290	-0.74660	C	-0.90660	3.86840	2.28620
H	6.99180	-2.06520	-1.12580	C	-0.39660	4.96730	3.14490
H	6.38670	-2.18170	3.16530	C	-0.03480	4.72280	4.41060
H	8.70510	-2.74460	3.50240	H	0.14100	3.16620	5.98790
C	3.21630	-4.84600	-2.42690	H	-0.72830	1.37370	4.61140
C	3.75440	-5.23350	-1.26480	H	-1.41250	1.82480	2.20830
C	4.23440	-4.22450	-0.29720	H	-0.31920	5.97590	2.76620
C	4.10890	-2.91400	-0.56610	H	0.33700	5.52560	5.03410
C	3.54190	-2.49260	-1.87310	C	-5.93520	2.96530	0.05450
C	3.11240	-3.40930	-2.74890	C	-5.55740	3.75850	1.06360
H	2.86540	-5.58320	-3.13700	C	-4.13470	4.12220	1.22660
H	3.83830	-6.28650	-1.02980	C	-3.21420	3.66190	0.36260
H	4.68590	-4.56020	0.62800	C	-3.63460	2.75340	-0.73350
H	3.47550	-1.44690	-2.13690	C	-4.92670	2.43520	-0.88410
H	2.69470	-3.10010	-3.69830	H	-6.97660	2.69670	-0.06590
C	2.45450	-1.64880	4.75030	H	-6.29320	4.13910	1.75990
C	3.21670	-0.60690	4.39910	H	-3.85230	4.78400	2.03620
C	3.94070	-0.62020	3.11070	H	-2.90690	2.33230	-1.41290
C	3.83260	-1.67320	2.28150	H	-5.23530	1.77540	-1.68330
C	3.01280	-2.83840	2.69400	N	-0.60310	-2.40110	1.84230
C	2.35260	-2.82090	3.85860	H	0.14210	-1.68990	2.02190
H	1.91510	-1.63690	5.68840	H	0.72010	-3.10210	-1.00160
H	3.29530	0.25300	5.05150	C	-5.25530	-2.62990	5.03530
H	4.54350	0.23850	2.84230	H	-5.45950	-3.67990	5.25720
H	2.93970	-3.71120	2.06480	C	-0.35610	-6.32250	-2.19910
H	1.74610	-3.66800	4.15180	H	-1.04320	-7.15010	-2.01560
C	-1.03040	8.76790	-0.44700	C	-2.87780	-3.68610	0.96330
C	0.05580	8.03320	-0.18180	H	-3.45730	-2.87360	0.05140
C	-0.08140	6.59610	0.13150	H	-3.63640	-4.46240	0.89980
C	-1.29670	6.02250	0.16890	O	-0.43920	0.07660	0.03730
C	-2.49550	6.83900	-0.14440	H	-1.84150	-0.80490	-0.65310
C	-2.36700	8.14040	-0.43210	C	-6.65190	-2.52900	-3.87060
H	-0.93190	9.82060	-0.67790	C	-6.37080	-3.53790	-2.95730
H	1.03730	8.48900	-0.19730	C	-5.37910	-3.37520	-1.97750
H	0.81150	6.01600	0.33170	C	-4.67210	-2.15910	-1.90350
H	-3.48030	6.39440	-0.15480	C	-4.95660	-1.16020	-2.85190
H	-3.24200	8.73480	-0.66160	C	-5.93050	-1.33350	-3.82790
C	-0.15330	3.36000	4.96460	H	-7.42230	-2.67910	-4.62130
C	-0.63270	2.37050	4.20400	H	-6.90020	-4.48460	-2.97660
C	-1.03360	2.63810	2.80760	H	-4.39870	-0.23050	-2.80630

H	-6.12880	-0.54010	-4.54140	H	-1.59850	-3.87130	-5.09830
O	-5.19000	-4.41410	-1.11310	C	-5.56260	0.48980	2.37090
H	-4.25390	-4.71050	-1.12170	C	-4.20590	0.66980	2.11130
C	-0.21670	-2.24920	-4.77350	C	-3.57380	-0.02570	1.07640
C	0.11960	-1.19150	-3.92700	C	-4.30860	-0.91630	0.27450
C	-0.63270	-0.92640	-2.78730	C	-5.67600	-1.09780	0.55570
C	-1.74420	-1.72930	-2.45960	C	-6.29750	-0.39810	1.58400
C	-2.07630	-2.79940	-3.30720	H	-6.04370	1.04490	3.17090
C	-1.31670	-3.04430	-4.45230	H	-3.63870	1.36820	2.71630
H	0.36890	-2.45190	-5.66500	H	-2.51880	0.15560	0.89260
H	0.97730	-0.56300	-4.14930	H	-6.25830	-1.79360	-0.03460
H	-0.35690	-0.12290	-2.11570	H	-7.35680	-0.54940	1.76800
H	-2.90720	-3.45030	-3.08300				

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C	0.90980	-3.24300	0.87520	C	-0.48910	-3.10340	5.02940
C	3.55870	-4.16120	0.52440	C	-0.01710	-3.04640	3.77860
C	3.25560	-2.88580	0.24250	H	-3.84500	-2.69410	4.45560
C	1.83600	-2.42200	0.31170	H	-2.31290	-3.02490	6.29660
H	4.57610	-4.52020	0.45980	H	0.19090	-3.24020	5.86020
C	2.51510	-5.10710	0.94690	H	1.04910	-3.13010	3.61110
C	1.24690	-4.68020	1.11990	O	1.56860	-1.11030	-0.02590
C	0.19970	-5.67460	1.49340	P	0.19260	-0.68780	-0.86070
C	0.52360	-6.95610	1.69930	O	-0.76980	-2.02750	-0.96290
C	1.92090	-7.40110	1.54700	O	0.52400	-0.31740	-2.28750
C	2.86560	-6.52700	1.18580	N	-0.80250	2.78830	1.27280
H	-0.83770	-5.38260	1.58420	C	-0.06090	3.94340	1.16370
H	-0.24180	-7.67310	1.96710	C	0.48150	4.43560	-2.15500
H	2.17710	-8.43850	1.71910	C	0.69930	3.15590	-2.63000
H	3.88830	-6.86270	1.06680	C	-1.58730	2.53040	-2.12320
C	-3.20750	-2.53600	1.74840	C	-1.85240	3.79580	-1.63570
C	-0.44490	-2.76500	1.23740	C	1.93370	2.61260	-3.29240
C	-1.28030	-2.38520	0.25640	H	2.83470	3.03310	-2.85240
C	-2.74860	-2.40460	0.49300	H	1.93590	2.86520	-4.35830
H	-4.27310	-2.57900	1.94160	C	-2.56770	1.40890	-2.29240
C	-0.94810	-2.85600	2.63590	H	-3.24920	1.62230	-3.12060
C	-2.27040	-2.71570	2.87580	H	-3.16860	1.28970	-1.39350
C	-2.78390	-2.79100	4.26260	H	-2.03250	0.48190	-2.49220
C	-1.93780	-2.97380	5.28260	C	-3.18010	4.33280	-1.28280

C	1.39030	5.59150	-2.30600	H	5.45460	1.41930	-4.02720
H	3.78140	6.75420	-2.30000	H	5.82430	0.52080	-1.69190
H	4.12230	6.14200	-3.95170	H	2.76570	-2.45820	-2.44010
H	-6.22360	3.56960	-2.04690	H	2.45330	-1.60720	-4.67050
H	-5.73640	4.09290	-0.40100	C	-1.81370	-2.85660	-5.06710
O	2.45170	5.36730	-3.11540	C	-1.59680	-3.78240	-4.12700
O	1.18770	6.66970	-1.77280	C	-2.28900	-3.69220	-2.82490
O	-3.32730	5.36670	-0.64850	C	-3.13540	-2.67810	-2.57100
O	-4.22230	3.61640	-1.75760	C	-3.38110	-1.66470	-3.62730
Si	4.63620	-1.69350	-0.16730	C	-2.75050	-1.74720	-4.80510
Si	-3.97610	-2.53990	-0.90840	H	-1.30390	-2.91840	-6.01980
C	8.75840	-3.91590	-0.07910	H	-0.90830	-4.59620	-4.31460
C	8.25220	-3.51020	-1.24980	H	-2.07040	-4.43770	-2.07550
C	6.95220	-2.80830	-1.29230	H	-4.05430	-0.83880	-3.45400
C	6.27390	-2.57540	-0.15600	H	-2.92410	-0.99880	-5.56750
C	6.84010	-3.02670	1.13810	C	-7.01150	1.03630	-0.82110
C	8.01750	-3.66250	1.17310	C	-6.02140	0.98290	0.07660
H	9.70990	-4.43070	-0.04720	C	-5.05030	-0.12940	0.04280
H	8.79300	-3.69610	-2.16870	C	-5.15570	-1.09440	-0.88560
H	6.56130	-2.49890	-2.25210	C	-6.24360	-1.01540	-1.89200
H	6.30140	-2.84610	2.06010	C	-7.12260	-0.00680	-1.85930
H	8.42880	-3.99270	2.11810	H	-7.72840	1.84650	-0.79250
C	4.95640	1.64530	3.11970	H	-5.93350	1.75120	0.83300
C	5.91810	1.50960	2.20030	H	-4.26010	-0.14610	0.77660
C	5.81980	0.44910	1.17590	H	-6.33330	-1.77710	-2.65650
C	4.75820	-0.37620	1.14960	H	-7.91690	0.04600	-2.59250
C	3.72020	-0.24890	2.20550	C	-6.21360	-6.56790	-0.00620
C	3.80910	0.71740	3.12760	C	-6.92340	-5.46450	-0.26630
H	5.02260	2.42700	3.86520	C	-6.23410	-4.18870	-0.55230
H	6.76540	2.18280	2.19740	C	-4.89070	-4.13290	-0.57640
H	6.62010	0.35100	0.45500	C	-4.11200	-5.35680	-0.25840
H	2.88870	-0.93460	2.25350	C	-4.73920	-6.50880	0.00690
H	3.04660	0.81240	3.89000	H	-6.71770	-7.50200	0.20570
C	3.97400	0.00310	-4.49050	H	-8.00510	-5.50260	-0.26610
C	4.87080	0.57660	-3.68060	H	-6.83870	-3.31420	-0.73250
C	5.07140	0.05810	-2.31170	H	-3.03240	-5.32140	-0.20420
C	4.33850	-0.97510	-1.86230	H	-4.16730	-7.39580	0.24730
C	3.34860	-1.60840	-2.76890	N	-0.31230	2.24000	-2.51830
C	3.17660	-1.14330	-4.01240	H	-0.05070	1.22400	-2.60960
H	3.82630	0.38150	-5.49360	H	1.93940	1.52550	-3.18980



C	-5.51910	4.16660	-1.46920	C	-4.17320	3.25940	2.85220
H	-5.56590	5.21520	-1.76920	C	-3.01610	3.56380	2.13410
C	3.34720	6.48070	-3.26450	C	-2.03590	2.57850	1.95350
H	2.82120	7.34660	-3.67290	C	-2.24890	1.28460	2.46180
C	-0.73600	4.70270	-1.39080	C	-3.40710	0.99950	3.17810
H	-0.43320	4.52790	-0.12320	H	-5.27480	1.76120	3.94600
H	-1.00370	5.75460	-1.33000	H	-4.92510	4.03130	2.98820
O	-0.47080	0.36100	0.01170	H	-2.89510	4.54730	1.70310
H	-0.50390	1.94040	0.75690	H	-1.50610	0.51750	2.27130
C	-0.71140	7.01540	4.12680	H	-3.55770	0.00010	3.57370
C	-0.26370	5.75270	4.49930	C	4.10300	3.58470	0.06010
C	-0.07930	4.75680	3.53430	C	3.58710	4.79730	0.52070
C	-0.35160	5.03060	2.17510	C	2.24560	4.89770	0.88140
C	-0.80000	6.30960	1.82430	C	1.39740	3.77640	0.82320
C	-0.98310	7.29990	2.78700	C	1.93280	2.55510	0.38190
H	-0.85090	7.77860	4.88690	C	3.26530	2.47320	-0.01320
H	-0.04730	5.50710	5.53350	H	5.14480	3.50600	-0.23670
H	-1.02130	6.52580	0.78620	H	4.22490	5.67320	0.59250
H	-1.33650	8.28180	2.49050	H	1.85140	5.85400	1.20300
O	0.37820	3.55470	3.97930	H	1.32690	1.65780	0.33170
H	0.36790	2.90640	3.26070	H	3.62990	1.52710	-0.38950
C	-4.37260	1.98630	3.38560				
C	1.70880	-2.99680	0.90990	C	0.27110	-2.87720	1.24890
C	4.50730	-3.21660	0.58420	C	-0.61760	-2.70370	0.25600
C	3.89690	-2.05530	0.30710	C	-2.04950	-3.05270	0.47660
C	2.40570	-1.96160	0.37010	H	-3.51850	-3.48140	1.92910
H	5.58240	-3.31010	0.52270	C	-0.21430	-3.07610	2.64220
C	3.73140	-4.39630	0.99460	C	-1.53840	-3.22110	2.86860
C	2.39490	-4.30350	1.15520	C	-2.03800	-3.40130	4.25110
C	1.62970	-5.52940	1.52360	C	-1.18340	-3.39520	5.28020
C	2.26460	-6.68820	1.73320	C	0.26160	-3.21030	5.04180
C	3.72970	-6.76710	1.59020	C	0.72350	-3.05680	3.79540
C	4.42640	-5.68270	1.23580	H	-3.09700	-3.53500	4.43370
H	0.55180	-5.50690	1.60980	H	-1.54930	-3.52330	6.29070
H	1.70280	-7.57470	1.99810	H	0.94630	-3.19430	5.87990
H	4.23770	-7.70680	1.76430	H	1.78430	-2.90830	3.63990
H	5.50150	-5.74990	1.12450	O	1.81770	-0.75230	0.05900
C	-2.48270	-3.24780	1.73250	P	0.41080	-0.68170	-0.82850

O	-0.19000	-2.21670	-0.95150	C	5.53740	1.82390	1.22680
O	0.69790	-0.23180	-2.24090	C	4.72270	0.75410	1.20770
N	-1.45360	2.45160	1.28290	C	3.68660	0.61840	2.26420
C	-1.03560	3.75210	1.10260	C	3.52230	1.58330	3.17740
C	-0.65630	4.32050	-2.21890	H	4.25300	3.55470	3.89780
C	-0.06680	3.15230	-2.66690	H	6.00300	3.75200	2.23120
C	-2.11080	1.91910	-2.25090	H	6.33750	1.92840	0.50660
C	-2.73390	3.04940	-1.75780	H	3.06130	-0.25900	2.32030
C	1.28940	2.97280	-3.28810	H	2.76100	1.48480	3.94050
H	1.23810	3.15570	-4.36720	C	3.91090	0.88280	-4.44620
H	1.61300	1.94230	-3.12610	C	4.61910	1.67440	-3.63320
C	-2.71960	0.57190	-2.48130	C	4.93100	1.23470	-2.25750
H	-2.36290	0.17170	-3.43330	C	4.48500	0.05010	-1.80510
H	-3.80360	0.62180	-2.48090	C	3.70510	-0.82470	-2.71580
H	-2.37200	-0.09810	-1.68810	C	3.43300	-0.42820	-3.96520
C	-4.19270	3.10570	-1.51600	H	3.68180	1.20350	-5.45410
C	-0.11580	5.68670	-2.36040	H	4.96830	2.63760	-3.98200
H	1.83810	7.49430	-2.33990	H	5.53070	1.88110	-1.63530
H	2.35710	6.99990	-3.98440	H	3.35820	-1.79420	-2.38440
H	-6.01930	5.24020	0.10250	H	2.86270	-1.06830	-4.62600
H	-6.48830	4.42430	-1.42590	C	-0.80720	-3.51550	-4.97880
O	0.97300	5.77900	-3.15830	C	-0.42980	-4.28640	-3.95310
O	-0.62530	6.66180	-1.83020	C	-1.20050	-4.27010	-2.69310
O	-5.03820	2.33680	-1.93380	C	-2.28030	-3.47780	-2.56520
O	-4.52190	4.18910	-0.76020	C	-2.70260	-2.64110	-3.71430
Si	4.94000	-0.55820	-0.10170	C	-2.00090	-2.65580	-4.85440
Si	-3.21240	-3.41470	-0.94850	H	-0.24120	-3.52190	-5.90130
C	9.48770	-1.67310	0.02380	H	0.44500	-4.91760	-4.04040
C	8.90540	-1.40820	-1.15170	H	-0.86290	-4.88390	-1.86680
C	7.47090	-1.05670	-1.20630	H	-3.57550	-2.00890	-3.64410
C	6.74620	-1.00230	-0.07590	H	-2.30810	-2.03880	-5.68890
C	7.39700	-1.29650	1.22360	C	-6.70980	-0.30540	-1.00790
C	8.69640	-1.61470	1.26940	C	-6.72710	-1.34850	-1.84580
H	10.53810	-1.93100	0.06450	C	-5.61500	-2.32140	-1.83910
H	9.48340	-1.45140	-2.06580	C	-4.57420	-2.15300	-1.00640
H	7.02310	-0.85500	-2.16990	C	-4.55940	-0.99400	-0.08470
H	6.82250	-1.25730	2.14080	C	-5.57350	-0.12100	-0.08360
H	9.16980	-1.83030	2.21850	H	-7.52350	0.40820	-1.00980
C	4.39140	2.77560	3.15950	H	-7.55800	-1.48570	-2.52550
C	5.35740	2.88350	2.24090	H	-5.65840	-3.17360	-2.50620

H	-3.72260	-0.83890	0.57810	C	-2.58570	1.96720	1.99470
H	-5.55650	0.73190	0.58020	C	-2.47360	0.66900	2.52310
C	-5.39170	-7.49150	-0.11930	C	-3.51420	0.12960	3.27290
C	-4.42070	-7.43830	-1.03760	H	-5.48330	0.44640	4.09800
C	-3.72790	-6.16200	-1.31260	H	-5.69760	2.72530	3.12620
C	-4.05640	-5.05000	-0.63120	H	-3.87910	3.68130	1.76800
C	-5.15160	-5.11420	0.36950	H	-1.57800	0.09320	2.31470
C	-5.77920	-6.27080	0.61370	H	-3.41720	-0.87320	3.67600
H	-5.89990	-8.42560	0.08210	C	3.09550	4.38790	-0.00110
H	-4.13940	-8.33060	-1.58190	C	2.55720	3.10220	-0.02010
H	-2.95890	-6.15470	-2.06860	C	1.24020	2.87320	0.36590
H	-5.46690	-4.22180	0.89410	C	0.41450	3.94380	0.74560
H	-6.58000	-6.31150	1.34080	C	0.95990	5.24130	0.74730
N	-0.78340	1.99260	-2.57380	C	2.28970	5.45690	0.39300
H	-0.25310	1.08410	-2.64140	H	4.12950	4.55330	-0.28960
H	2.01660	3.66280	-2.86880	H	3.14610	2.25750	-0.34840
C	-5.92670	4.33260	-0.49350	H	0.87510	1.85330	0.35840
H	-6.29930	3.46700	0.05930	H	0.34110	6.08610	1.02270
C	1.51040	7.10280	-3.30590	H	2.69170	6.46530	0.42230
H	0.76120	7.77850	-3.72460				
C	-1.91420	4.22910	-1.47540				
H	-1.57940	4.15120	-0.20910	C	0.90980	-3.24300	0.87520
H	-2.45640	5.16920	-1.42800	C	3.55870	-4.16120	0.52440
O	-0.52730	0.16100	0.01760	C	3.25560	-2.88580	0.24250
H	-0.96210	1.69040	0.77910	C	1.83600	-2.42200	0.31170
C	-2.42260	6.72030	3.91880	H	4.57610	-4.52020	0.45980
C	-1.74120	5.59080	4.35790	C	2.51510	-5.10710	0.94690
C	-1.31130	4.62320	3.44300	C	1.24690	-4.68020	1.11990
C	-1.58200	4.78390	2.06500	C	0.19970	-5.67460	1.49340
C	-2.25740	5.93740	1.64590	C	0.52360	-6.95610	1.69930
C	-2.68100	6.90130	2.55830	C	1.92090	-7.40110	1.54700
H	-2.74890	7.46260	4.64120	C	2.86560	-6.52700	1.18580
H	-1.52170	5.43100	5.40820	H	-0.83770	-5.38260	1.58420
H	-2.44070	6.08630	0.58860	H	-0.24180	-7.67310	1.96710
H	-3.20210	7.78590	2.20720	H	2.17710	-8.43850	1.71910
O	-0.62680	3.56600	3.95570	H	3.88830	-6.86270	1.06680
H	-0.46080	2.90730	3.26600	C	-3.20750	-2.53600	1.74840
C	-4.67530	0.86790	3.50830	C	-0.44490	-2.76500	1.23740
C	-4.79210	2.14740	2.96590	C	-1.28030	-2.38520	0.25640
C	-3.76250	2.69920	2.20320	C	-2.74860	-2.40460	0.49300

H	-4.27310	-2.57900	1.94160	C	8.75840	-3.91590	-0.07910
C	-0.94810	-2.85600	2.63590	C	8.25220	-3.51020	-1.24980
C	-2.27040	-2.71570	2.87580	C	6.95220	-2.80830	-1.29230
C	-2.78390	-2.79100	4.26260	C	6.27390	-2.57540	-0.15600
C	-1.93780	-2.97380	5.28260	C	6.84010	-3.02670	1.13810
C	-0.48910	-3.10340	5.02940	C	8.01750	-3.66250	1.17310
C	-0.01710	-3.04640	3.77860	H	9.70990	-4.43070	-0.04720
H	-3.84500	-2.69410	4.45560	H	8.79300	-3.69610	-2.16870
H	-2.31290	-3.02490	6.29660	H	6.56130	-2.49890	-2.25210
H	0.19090	-3.24020	5.86020	H	6.30140	-2.84610	2.06010
H	1.04910	-3.13010	3.61110	H	8.42880	-3.99270	2.11810
O	1.56860	-1.11030	-0.02590	C	4.95640	1.64530	3.11970
P	0.19260	-0.68780	-0.86070	C	5.91810	1.50960	2.20030
O	-0.76980	-2.02750	-0.96290	C	5.81980	0.44910	1.17590
O	0.52400	-0.31740	-2.28750	C	4.75820	-0.37620	1.14960
N	-0.80250	2.78830	1.27280	C	3.72020	-0.24890	2.20550
C	-0.06090	3.94340	1.16370	C	3.80910	0.71740	3.12760
C	0.48150	4.43560	-2.15500	H	5.02260	2.42700	3.86520
C	0.69930	3.15590	-2.63000	H	6.76540	2.18280	2.19740
C	-1.58730	2.53040	-2.12320	H	6.62010	0.35100	0.45500
C	-1.85240	3.79580	-1.63570	H	2.88870	-0.93460	2.25350
C	1.93370	2.61260	-3.29240	H	3.04660	0.81240	3.89000
H	2.83470	3.03310	-2.85240	C	3.97400	0.00310	-4.49050
H	1.93590	2.86520	-4.35830	C	4.87080	0.57660	-3.68060
C	-2.56770	1.40890	-2.29240	C	5.07140	0.05810	-2.31170
H	-3.24920	1.62230	-3.12060	C	4.33850	-0.97510	-1.86230
H	-3.16860	1.28970	-1.39350	C	3.34860	-1.60840	-2.76890
H	-2.03250	0.48190	-2.49220	C	3.17660	-1.14330	-4.01240
C	-3.18010	4.33280	-1.28280	H	3.82630	0.38150	-5.49360
C	1.39030	5.59150	-2.30600	H	5.45460	1.41930	-4.02720
H	3.78140	6.75420	-2.30000	H	5.82430	0.52080	-1.69190
H	4.12230	6.14200	-3.95170	H	2.76570	-2.45820	-2.44010
H	-6.22360	3.56960	-2.04690	H	2.45330	-1.60720	-4.67050
H	-5.73640	4.09290	-0.40100	C	-1.81370	-2.85660	-5.06710
O	2.45170	5.36730	-3.11540	C	-1.59680	-3.78240	-4.12700
O	1.18770	6.66970	-1.77280	C	-2.28900	-3.69220	-2.82490
O	-3.32730	5.36670	-0.64850	C	-3.13540	-2.67810	-2.57100
O	-4.22230	3.61640	-1.75760	C	-3.38110	-1.66470	-3.62730
Si	4.63620	-1.69350	-0.16730	C	-2.75050	-1.74720	-4.80510
Si	-3.97610	-2.53990	-0.90840	H	-1.30390	-2.91840	-6.01980

H	-0.90830	-4.59620	-4.31460	H	-0.50390	1.94040	0.75690
H	-2.07040	-4.43770	-2.07550	C	-0.71140	7.01540	4.12680
H	-4.05430	-0.83880	-3.45400	C	-0.26370	5.75270	4.49930
H	-2.92410	-0.99880	-5.56750	C	-0.07930	4.75680	3.53430
C	-7.01150	1.03630	-0.82110	C	-0.35160	5.03060	2.17510
C	-6.02140	0.98290	0.07660	C	-0.80000	6.30960	1.82430
C	-5.05030	-0.12940	0.04280	C	-0.98310	7.29990	2.78700
C	-5.15570	-1.09440	-0.88560	H	-0.85090	7.77860	4.88690
C	-6.24360	-1.01540	-1.89200	H	-0.04730	5.50710	5.53350
C	-7.12260	-0.00680	-1.85930	H	-1.02130	6.52580	0.78620
H	-7.72840	1.84650	-0.79250	H	-1.33650	8.28180	2.49050
H	-5.93350	1.75120	0.83300	O	0.37820	3.55470	3.97930
H	-4.26010	-0.14610	0.77660	H	0.36790	2.90640	3.26070
H	-6.33330	-1.77710	-2.65650	C	-4.37260	1.98630	3.38560
H	-7.91690	0.04600	-2.59250	C	-4.17320	3.25940	2.85220
C	-6.21360	-6.56790	-0.00620	C	-3.01610	3.56380	2.13410
C	-6.92340	-5.46450	-0.26630	C	-2.03590	2.57850	1.95350
C	-6.23410	-4.18870	-0.55230	C	-2.24890	1.28460	2.46180
C	-4.89070	-4.13290	-0.57640	C	-3.40710	0.99950	3.17810
C	-4.11200	-5.35680	-0.25840	H	-5.27480	1.76120	3.94600
C	-4.73920	-6.50880	0.00690	H	-4.92510	4.03130	2.98820
H	-6.71770	-7.50200	0.20570	H	-2.89510	4.54730	1.70310
H	-8.00510	-5.50260	-0.26610	H	-1.50610	0.51750	2.27130
H	-6.83870	-3.31420	-0.73250	H	-3.55770	0.00010	3.57370
H	-3.03240	-5.32140	-0.20420	C	4.10300	3.58470	0.06010
H	-4.16730	-7.39580	0.24730	C	3.58710	4.79730	0.52070
N	-0.31230	2.24000	-2.51830	C	2.24560	4.89770	0.88140
H	-0.05070	1.22400	-2.60960	C	1.39740	3.77640	0.82320
H	1.93940	1.52550	-3.18980	C	1.93280	2.55510	0.38190
C	-5.51910	4.16660	-1.46920	C	3.26530	2.47320	-0.01320
H	-5.56590	5.21520	-1.76920	H	5.14480	3.50600	-0.23670
C	3.34720	6.48070	-3.26450	H	4.22490	5.67320	0.59250
H	2.82120	7.34660	-3.67290	H	1.85140	5.85400	1.20300
C	-0.73600	4.70270	-1.39080	H	1.32690	1.65780	0.33170
H	-0.43320	4.52790	-0.12320	H	3.62990	1.52710	-0.38950
H	-1.00370	5.75460	-1.33000				
O	-0.47080	0.36100	0.01170				

C	-3.09100	1.48680	0.91290	C	0.66860	-3.12480	-3.30340
C	-5.51830	0.07200	0.60910	H	0.84650	-3.26790	-4.37490
C	-4.35760	-0.53180	0.31590	H	-0.18910	-2.46030	-3.17820
C	-3.08010	0.24260	0.36390	C	2.55890	1.13900	-2.39220
H	-6.45470	-0.46540	0.55830	H	3.48070	1.71100	-2.42250
C	-5.54970	1.48370	1.02060	H	1.93360	1.48230	-1.56120
C	-4.39720	2.16970	1.16950	H	1.99180	1.27610	-3.31480
C	-4.46380	3.61510	1.53130	C	5.19570	-0.10430	-1.39670
C	-5.64400	4.20590	1.75000	C	3.26780	-4.56050	-2.21900
C	-6.89390	3.43430	1.62330	H	2.53980	-7.11260	-2.17360
C	-6.85150	2.14500	1.27300	H	2.11550	-7.05820	-3.91720
H	-3.56490	4.21230	1.60350	H	7.92620	-0.87390	0.16490
H	-5.68540	5.25600	2.00940	H	7.82700	0.13780	-1.31510
H	-7.84530	3.91720	1.80550	O	2.54700	-5.25060	-3.11890
H	-7.77410	1.58670	1.17300	O	4.10770	-5.10710	-1.50590
C	0.18390	4.11520	1.71670	O	5.43710	1.02690	-1.77440
C	-1.83910	2.20580	1.24820	O	6.08890	-0.82680	-0.67510
C	-1.01660	2.57350	0.25140	Si	-4.35880	-2.35660	-0.09430
C	-0.04910	3.68280	0.46720	Si	0.65260	4.67210	-0.95210
H	0.87200	4.93340	1.89500	C	-8.72500	-4.04030	0.10360
C	-1.55390	2.65600	2.63930	C	-8.11450	-3.92750	-1.08200
C	-0.56320	3.54900	2.85830	C	-6.73710	-3.39700	-1.15960
C	-0.26120	3.99730	4.23690	C	-6.09330	-3.02590	-0.04000
C	-0.94990	3.50040	5.27050	C	-6.77470	-3.15390	1.27080
C	-2.01530	2.50470	5.04060	C	-8.02220	-3.63420	1.33750
C	-2.30230	2.10130	3.79740	H	-9.73390	-4.42800	0.16120
H	0.52070	4.72560	4.41300	H	-8.62820	-4.22350	-1.98750
H	-0.72630	3.82540	6.27840	H	-6.26970	-3.30790	-2.13080
H	-2.56070	2.09810	5.88250	H	-6.26610	-2.85620	2.17950
H	-3.07740	1.36070	3.64790	H	-8.51890	-3.72550	2.29480
O	-1.91520	-0.41500	0.02540	C	-1.98400	-4.77960	3.15380
P	-0.71670	0.33740	-0.84730	C	-2.72630	-5.41910	2.24370
O	-1.10030	1.94110	-0.96120	C	-3.47460	-4.65230	1.22600
O	-0.68970	-0.18290	-2.26690	C	-3.40680	-3.30950	1.19850
N	2.61900	-1.21200	1.31550	C	-2.61960	-2.60670	2.24490
C	3.01200	-2.52350	1.14630	C	-1.93540	-3.30490	3.15940
C	3.00330	-3.11720	-2.17430	H	-1.42800	-5.34010	3.89400
C	1.86930	-2.49010	-2.66110	H	-2.77180	-6.50040	2.24300
C	2.82770	-0.31800	-2.19150	H	-4.08330	-5.19440	0.51530
C	3.97130	-0.89480	-1.67190	H	-2.59740	-1.52930	2.29470

H	-1.35800	-2.78930	3.91590	H	-0.80640	10.12510	0.28360
C	-2.71670	-2.95060	-4.44900	H	1.48910	9.60110	-0.29360
C	-2.85790	-4.00710	-3.64100	H	2.16420	7.22660	-0.81350
C	-3.36400	-3.82510	-2.26480	H	-1.93300	5.99300	-0.11300
C	-3.66000	-2.59670	-1.80660	H	-2.55180	8.26510	0.38490
C	-3.50920	-1.43090	-2.71270	N	1.79620	-1.13210	-2.57420
C	-3.06100	-1.60020	-3.96270	H	0.83890	-0.69020	-2.65590
H	-2.34590	-3.08230	-5.45710	H	0.44960	-4.09790	-2.87020
H	-2.60440	-4.99830	-3.99390	C	7.32540	-0.15360	-0.38940
H	-3.49350	-4.69910	-1.64490	H	7.14050	0.74160	0.20910
H	-3.76900	-0.43590	-2.37740	C	2.77810	-6.67160	-3.14380
H	-2.95060	-0.74740	-4.62020	H	3.82110	-6.88460	-3.38710
C	-1.38800	3.42630	-4.99740	C	3.98560	-2.33300	-1.42840
C	-2.13220	3.86530	-3.97700	H	3.67090	-2.51600	-0.13200
C	-1.48740	4.27320	-2.71200	H	4.97640	-2.77080	-1.36060
C	-0.15120	4.20190	-2.57240	O	0.53080	0.16680	-0.00060
C	0.66640	3.72850	-3.71690	H	1.75730	-0.89130	0.85110
C	0.07950	3.35700	-4.86120	C	5.74070	-3.93180	4.20360
H	-1.85870	3.12250	-5.92340	C	6.05150	-4.18050	2.87410
H	-3.20910	3.91540	-4.07230	C	5.19600	-3.77630	1.83530
H	-2.11770	4.59020	-1.89490	C	4.02260	-3.05570	2.14730
H	1.74080	3.66740	-3.64080	C	3.71010	-2.85320	3.50530
H	0.68000	3.00460	-5.68990	C	4.54820	-3.27930	4.52700
C	5.31650	4.16510	-1.07010	H	6.41670	-4.26310	4.98650
C	4.70670	4.93610	-1.97730	H	6.95380	-4.71300	2.59270
C	3.23760	5.09100	-1.94960	H	2.79040	-2.33220	3.75020
C	2.50470	4.45520	-1.01900	H	4.27640	-3.09870	5.56200
C	3.18770	3.58960	-0.02790	O	5.62160	-4.08900	0.58010
C	4.51920	3.45780	-0.04900	H	4.91560	-4.38010	-0.03320
H	6.39250	4.05000	-1.08790	C	4.33890	1.97370	3.48610
H	5.28800	5.45190	-2.73050	C	5.16890	0.97850	2.96920
H	2.76520	5.73040	-2.68500	C	4.64290	-0.08090	2.23100
H	2.61530	3.04890	0.70880	C	3.25990	-0.15820	2.01070
H	5.01420	2.81920	0.66970	C	2.42460	0.85760	2.50980
C	-0.52300	9.10690	0.05050	C	2.96560	1.90860	3.24410
C	0.74330	8.81710	-0.26750	H	4.75710	2.79400	4.06100
C	1.12970	7.42590	-0.58330	H	6.24110	1.02320	3.13750
C	0.20830	6.44610	-0.57500	H	5.30040	-0.83730	1.82590
C	-1.18890	6.77340	-0.19310	H	1.36140	0.81310	2.29910
C	-1.53410	8.03320	0.09840	H	2.30960	2.68370	3.62750

C	-0.09240	-5.36470	0.10620	H	-0.86360	-6.08000	-0.16470
C	-0.30600	-3.99820	-0.06760	H	-1.23470	-3.62730	-0.48060
C	0.67350	-3.07300	0.28280	H	0.45260	-2.02100	0.14680
C	1.90540	-3.49720	0.80560	H	3.03450	-5.24020	1.41150
C	2.10610	-4.87730	0.98800	H	1.29580	-6.85710	0.81640
C	1.11730	-5.79890	0.64940				
C	1.01300	-3.25790	0.82870	O	0.48390	-0.32930	-2.32610
C	3.69790	-4.06270	0.47790	N	-0.84900	2.68320	1.30550
C	3.34200	-2.80060	0.19800	C	-0.13180	3.85420	1.18460
C	1.90260	-2.39730	0.26370	C	0.32340	4.40010	-2.13500
H	4.72990	-4.37810	0.41640	C	0.52070	3.12400	-2.63200
C	2.69560	-5.05240	0.89870	C	-1.76990	2.52320	-2.10110
C	1.41090	-4.67960	1.07260	C	-2.01150	3.78320	-1.59020
C	0.40770	-5.71680	1.45010	C	1.73030	2.58380	-3.34090
C	0.78650	-6.98280	1.65900	H	1.69680	2.85540	-4.40180
C	2.20120	-7.36810	1.50510	H	1.73530	1.49520	-3.25570
C	3.10690	-6.45540	1.13990	C	-2.74020	1.39620	-2.26960
H	-0.64100	-5.46850	1.54250	H	-2.68400	1.02070	-3.29510
H	0.05300	-7.73100	1.93060	H	-3.75760	1.70250	-2.05490
H	2.50190	-8.39310	1.67960	H	-2.44130	0.58820	-1.59380
H	4.14300	-6.74720	1.02030	C	-3.31760	4.36130	-1.20230
C	-3.12010	-2.65720	1.74170	C	1.22890	5.55600	-2.30650
C	-0.35760	-2.83650	1.20060	H	2.62710	7.31220	-3.70170
C	-1.21220	-2.48320	0.22680	H	3.62710	6.70930	-2.36200
C	-2.67690	-2.51910	0.48190	H	-5.89070	4.25570	-0.38520
H	-4.18330	-2.70160	1.94770	H	-5.62610	5.47450	-1.65210
C	-0.84530	-2.94280	2.60410	O	2.26880	5.33120	-3.14310
C	-2.16800	-2.83110	2.85770	O	1.04050	6.63440	-1.76870
C	-2.66610	-2.92500	4.24910	O	-3.40740	5.33180	-0.46610
C	-1.80640	-3.09400	5.26000	O	-4.39930	3.78870	-1.77300
C	-0.35780	-3.18930	4.99240	Si	4.67770	-1.55170	-0.19370
C	0.10070	-3.11620	3.73740	Si	-3.92010	-2.61860	-0.90720
H	-3.72720	-2.85270	4.45300	C	8.89230	-3.58860	-0.01990
H	-2.17040	-3.15850	6.27720	C	8.38830	-3.21530	-1.20220
H	0.33330	-3.31380	5.81610	C	7.05850	-2.57400	-1.27250
H	1.16700	-3.17410	3.56020	C	6.35100	-2.36330	-0.14960
O	1.57840	-1.09800	-0.07670	C	6.91430	-2.78020	1.15730
P	0.17910	-0.73240	-0.90420	C	8.11880	-3.36080	1.21740
O	-0.72200	-2.11350	-0.99750	H	9.86600	-4.05820	0.03240



H	8.95310	-3.38240	-2.11020	C	-5.02240	-1.11480	-0.89410
H	6.67060	-2.28970	-2.24120	C	-6.12440	-1.00140	-1.88140
H	6.35200	-2.61810	2.06860	C	-6.94840	0.05260	-1.85610
H	8.52830	-3.66500	2.17190	H	-7.43770	1.95610	-0.82000
C	4.80520	1.80440	3.09050	H	-5.61330	1.80810	0.76810
C	5.78430	1.70960	2.18450	H	-4.04300	-0.17830	0.72660
C	5.74740	0.64330	1.16190	H	-6.27020	-1.77570	-2.62430
C	4.72500	-0.22960	1.12440	H	-7.75400	0.13020	-2.57450
C	3.67010	-0.14820	2.16830	C	-6.42370	-6.47960	0.03840
C	3.70210	0.82440	3.08750	C	-5.08930	-6.53910	-0.02340
H	4.82540	2.59090	3.83360	C	-4.30690	-5.32240	-0.32280
H	6.59970	2.42120	2.18990	C	-4.92740	-4.15220	-0.55740
H	6.55950	0.58170	0.45060	C	-6.40810	-4.09030	-0.45750
H	2.87150	-0.87220	2.20990	C	-7.11390	-5.19410	-0.18140
H	2.92650	0.88630	3.84010	H	-6.99850	-7.36950	0.26010
C	3.98810	0.14540	-4.51440	H	-4.57880	-7.47770	0.14970
C	4.89520	0.71330	-3.71220	H	-3.22850	-5.39230	-0.31860
C	5.11210	0.18630	-2.34920	H	-6.93480	-3.15760	-0.58590
C	4.38140	-0.84690	-1.89550	H	-8.19260	-5.14440	-0.10650
C	3.38480	-1.47820	-2.79610	N	-0.49600	2.21780	-2.50360
C	3.19920	-1.00640	-4.03510	H	-0.24100	1.20560	-2.61680
H	3.82780	0.53050	-5.51300	H	2.64650	2.99550	-2.92520
H	5.47440	1.55870	-4.06030	C	-5.65770	4.40360	-1.44230
H	5.86950	0.64760	-1.73370	H	-6.39630	3.90940	-2.07230
H	2.80780	-2.33170	-2.46720	C	3.16240	6.44260	-3.31420
H	2.47060	-1.46840	-4.68860	H	3.91510	6.10500	-4.02650
C	-1.74110	-3.03950	-5.04920	C	-0.87240	4.66320	-1.33960
C	-1.54440	-3.95380	-4.09360	H	-0.54980	4.44950	-0.07110
C	-2.24580	-3.83470	-2.79880	H	-1.11630	5.71770	-1.24240
C	-3.08350	-2.80750	-2.56810	O	-0.53350	0.27690	-0.01980
C	-3.30720	-1.80790	-3.64170	H	-0.55790	1.84870	0.76450
C	-2.66730	-1.91570	-4.81250	C	-0.67630	6.85300	4.24150
H	-1.22350	-3.12170	-5.99610	C	-0.19060	5.59010	4.56260
H	-0.86330	-4.77780	-4.26230	C	-0.04550	4.61680	3.56850
H	-2.03280	-4.56510	-2.03330	C	-0.39480	4.91440	2.23210
H	-3.98110	-0.97920	-3.49150	C	-0.88410	6.19120	1.93340
H	-2.82860	-1.17940	-5.58920	C	-1.02810	7.15910	2.92530
C	-6.76170	1.11180	-0.84540	H	-0.78340	7.59880	5.02370
C	-5.75740	1.02740	0.03390	H	0.08670	5.32740	5.57800
C	-4.84640	-0.13540	0.00830	H	-1.17290	6.42070	0.91480

H	-1.41340	8.14060	2.66990	H	-4.92420	3.85680	3.17250
O	0.45380	3.41340	3.96190	C	3.99120	3.58170	-0.07920
H	0.40500	2.77730	3.23390	C	3.47660	4.77760	0.42430
C	-4.33740	1.81330	3.52460	C	2.14920	4.85030	0.83930
C	-3.36840	0.84020	3.27320	C	1.31680	3.71680	0.79380
C	-2.23550	1.14830	2.52630	C	1.85260	2.51170	0.31400
C	-2.05520	2.44950	2.02480	C	3.16840	2.45860	-0.13610
C	-3.04040	3.42080	2.24890	H	5.02090	3.52380	-0.42000
C	-4.16850	3.09540	3.00260	H	4.10350	5.66200	0.48670
H	-5.21860	1.57090	4.11060	H	1.75310	5.79450	1.19260
H	-3.49590	-0.16570	3.65990	H	1.26020	1.60540	0.27580
H	-1.49020	0.39230	2.30400	H	3.52980	1.52390	-0.53990
H	-2.94560	4.41020	1.82480				
C	0.99770	-3.28490	0.79970	C	0.09620	-3.17880	3.71280
C	3.68010	-4.09640	0.44620	H	-3.72800	-2.90670	4.44450
C	3.32950	-2.82970	0.18020	H	-2.16710	-3.24640	6.25920
C	1.89160	-2.42180	0.24610	H	0.33430	-3.40760	5.78770
H	4.71120	-4.41490	0.38410	H	1.16160	-3.23930	3.53150
C	2.67270	-5.08720	0.85190	O	1.57380	-1.11680	-0.07820
C	1.38900	-4.71120	1.02680	P	0.17700	-0.73230	-0.90100
C	0.38060	-5.74850	1.38970	O	-0.73680	-2.10470	-1.00570
C	0.75360	-7.01840	1.58480	O	0.48260	-0.31910	-2.32000
C	2.16710	-7.40780	1.42990	N	-0.81770	2.69100	1.30760
C	3.07750	-6.49470	1.07760	C	-0.09830	3.85980	1.18350
H	-0.66730	-5.49670	1.48260	C	0.32150	4.41710	-2.13800
H	0.01640	-7.76670	1.84600	C	0.51550	3.13950	-2.63260
H	2.46320	-8.43600	1.59330	C	-1.76820	2.53810	-2.07350
H	4.11270	-6.78940	0.95740	C	-2.00480	3.79860	-1.56200
C	-3.12830	-2.67570	1.73470	C	1.71800	2.59930	-3.35340
C	-0.36890	-2.85990	1.18150	H	1.66910	2.86250	-4.41580
C	-1.22460	-2.48680	0.21580	H	1.72920	1.51130	-3.26030
C	-2.68870	-2.52030	0.47550	C	-2.74120	1.41260	-2.23320
H	-4.19090	-2.71750	1.94380	H	-2.70030	1.04470	-3.26210
C	-0.85250	-2.98430	2.58510	H	-3.75520	1.71860	-2.00190
C	-2.17370	-2.87030	2.84470	H	-2.43350	0.60000	-1.56710
C	-2.66790	-2.98160	4.23620	C	-3.30630	4.37560	-1.15710
C	-1.80600	-3.16930	5.24180	C	1.21880	5.57610	-2.33050
C	-0.35870	-3.26790	4.96810	H	2.56770	7.33580	-3.76810

H	3.60550	6.74770	-2.45090	H	2.79560	-2.32640	-2.47490
H	-5.86930	4.27380	-0.31330	H	2.46430	-1.43870	-4.68720
H	-5.61820	5.49350	-1.58190	C	-1.80790	-2.95280	-5.08030
O	2.23920	5.35480	-3.19170	C	-1.59430	-3.87540	-4.13650
O	1.03840	6.65470	-1.79040	C	-2.27980	-3.77270	-2.83170
O	-3.38730	5.34280	-0.41560	C	-3.11890	-2.75170	-2.57960
O	-4.39450	3.80660	-1.71880	C	-3.36200	-1.74340	-3.64070
Si	4.67040	-1.58070	-0.19240	C	-2.73680	-1.83630	-4.82060
Si	-3.93990	-2.58690	-0.90820	H	-1.30240	-3.02310	-6.03470
C	8.87660	-3.63260	0.00550	H	-0.91170	-4.69440	-4.32230
C	8.38490	-3.24890	-1.17860	H	-2.05370	-4.50990	-2.07650
C	7.05820	-2.60200	-1.25650	H	-4.03890	-0.92030	-3.47430
C	6.34150	-2.39630	-0.13860	H	-2.91230	-1.09350	-5.58810
C	6.89100	-2.82470	1.17040	C	-6.75700	1.15910	-0.74060
C	8.09260	-3.41070	1.23730	C	-5.73920	1.05450	0.12080
H	9.84790	-4.10660	0.06340	C	-4.83540	-0.11250	0.06090
H	8.95730	-3.41190	-2.08260	C	-5.03100	-1.07550	-0.85530
H	6.67980	-2.31020	-2.22670	C	-6.14690	-0.93830	-1.82380
H	6.32090	-2.66720	2.07760	C	-6.96470	0.11930	-1.76700
H	8.49200	-3.72360	2.19330	H	-7.42840	2.00600	-0.68920
C	4.76540	1.76730	3.10170	H	-5.57950	1.82150	0.86620
C	5.75080	1.67800	2.20190	H	-4.02180	-0.17200	0.76670
C	5.72580	0.61220	1.17840	H	-6.30860	-1.69860	-2.57780
C	4.70740	-0.26500	1.13290	H	-7.78080	0.21390	-2.47140
C	3.64700	-0.19120	2.17180	C	-6.46270	-6.45050	-0.02490
C	3.66820	0.78090	3.09190	C	-5.12980	-6.51880	-0.10510
H	4.77690	2.55340	3.84550	C	-4.34120	-5.30100	-0.38340
H	6.56240	2.39380	2.21290	C	-4.95500	-4.12030	-0.58050
H	6.54240	0.55570	0.47190	C	-6.43380	-4.04930	-0.45930
H	2.85380	-0.92110	2.21030	C	-7.14510	-5.15430	-0.20260
H	2.88880	0.83690	3.84100	H	-7.04200	-7.34120	0.18100
C	4.00070	0.15570	-4.50100	H	-4.62490	-7.46560	0.03700
C	4.91700	0.70460	-3.69600	H	-3.26360	-5.37980	-0.39580
C	5.13020	0.16250	-2.33840	H	-6.95440	-3.10950	-0.55600
C	4.38700	-0.86490	-1.89190	H	-8.22230	-5.09790	-0.11230
C	3.38190	-1.47660	-2.79670	N	-0.49800	2.23210	-2.48850
C	3.19950	-0.99120	-4.03080	H	-0.24400	1.21980	-2.60250
H	3.84280	0.55210	-5.49560	H	2.63790	3.01820	-2.95310
H	5.50560	1.54610	-4.03760	C	-5.64850	4.42250	-1.37290
H	5.89380	0.60960	-1.72020	H	-6.39470	3.92970	-1.99500

C	3.11960	6.47230	-3.38990	C	-2.17370	1.14600	2.54950
H	3.85700	6.13740	-4.11920	C	-2.00670	2.45080	2.05260
C	-0.86350	4.67940	-1.32650	C	-2.98910	3.41840	2.30370
H	-0.52640	4.46250	-0.06220	C	-4.10010	3.08560	3.07930
H	-1.10630	5.73380	-1.22510	H	-5.12350	1.55150	4.19900
O	-0.52480	0.27580	-0.00690	H	-3.40650	-0.17850	3.70040
H	-0.53440	1.85760	0.76080	H	-1.43170	0.39320	2.30640
C	-0.59440	6.85320	4.25410	H	-2.90560	4.41080	1.88390
C	-0.08530	5.59610	4.56170	H	-4.85360	3.84410	3.27040
C	0.04390	4.62450	3.56390	C	4.01110	3.57650	-0.12210
C	-0.34400	4.91810	2.23740	C	3.49760	4.77980	0.36470
C	-0.85760	6.18850	1.95250	C	2.17440	4.85540	0.79250
C	-0.98600	7.15480	2.94820	C	1.34560	3.71860	0.77590
H	-0.68880	7.59790	5.03900	C	1.87950	2.50710	0.31050
H	0.22220	5.33680	5.56920	C	3.19100	2.45030	-0.15180
H	-1.17960	6.41310	0.94280	H	5.03750	3.51560	-0.47200
H	-1.39040	8.13130	2.70370	H	4.12190	5.66740	0.40410
O	0.56530	3.42610	3.94390	H	1.77800	5.80450	1.13230
H	0.50820	2.79010	3.21670	H	1.28940	1.59850	0.29280
C	-4.25530	1.79960	3.59620	H	3.55130	1.51030	-0.54370
C	-3.28990	0.83040	3.31780				

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C	-3.76350	1.60070	0.99610	C	-5.66020	-2.04100	-0.35550
C	-2.86820	4.22350	1.55850	C	-4.38900	0.34750	0.48690
C	-2.27880	3.52070	0.57920	C	-3.66540	-0.79840	0.35200
C	-2.70500	2.11520	0.33760	C	-4.34750	-2.05330	-0.08630
H	-2.60490	5.26190	1.72230	H	-6.16490	-2.93520	-0.69600
C	-3.90640	3.60580	2.40960	C	-5.82500	0.36510	0.06130
C	-4.34030	2.35170	2.14830	C	-6.43100	-0.78910	-0.29280
C	-5.35610	1.73470	3.04240	C	-7.86010	-0.79410	-0.68540
C	-5.86260	2.42850	4.06840	C	-8.55170	0.34880	-0.72190
C	-5.40830	3.80860	4.32720	C	-7.88870	1.62240	-0.38910
C	-4.47870	4.36710	3.54400	C	-6.60070	1.63610	-0.02780
H	-5.68880	0.71800	2.87890	H	-8.34930	-1.72400	-0.94780
H	-6.60230	1.97650	4.71650	H	-9.59470	0.34430	-1.01100
H	-5.82490	4.36480	5.15700	H	-8.44430	2.54910	-0.45370
H	-4.14530	5.37770	3.74430	H	-6.13240	2.58940	0.17350

O	-2.04710	1.34480	-0.58220	H	-0.31550	4.69060	2.38600
P	-1.22290	0.11920	0.13790	H	1.68220	5.46630	3.47950
O	-2.36080	-0.88590	0.78500	C	-3.35290	8.21860	-2.04370
O	-0.43190	0.63100	1.32530	C	-2.05930	8.30430	-1.71230
N	4.52930	-0.06720	-1.18530	C	-1.33080	7.10430	-1.24990
C	4.85760	-1.35080	-0.78010	C	-1.96090	5.91990	-1.16890
C	4.30380	0.39230	2.00950	C	-3.39770	5.83450	-1.53000
C	2.98270	0.79340	1.92580	C	-4.05520	6.92360	-1.94550
C	2.22220	-1.48360	2.24200	H	-3.88730	9.09710	-2.38140
C	3.52410	-1.94710	2.27220	H	-1.54320	9.25320	-1.78110
C	2.46560	2.19550	1.79140	H	-0.28830	7.20530	-0.98420
H	1.40370	2.17510	1.54120	H	-3.92420	4.89110	-1.45370
H	2.60500	2.73810	2.73050	H	-5.10350	6.85860	-2.20710
C	0.96800	-2.27650	2.47470	C	-0.07820	1.60880	-4.20870
H	0.08790	-1.64520	2.34830	C	-1.17220	2.37690	-4.23810
H	0.91490	-3.11320	1.77730	C	-1.48260	3.26800	-3.10140
H	0.97020	-2.69570	3.48330	C	-0.66500	3.31970	-2.03550
C	3.94080	-3.33960	2.53290	C	0.54180	2.45540	-2.00510
C	5.46720	1.28730	2.17800	C	0.81780	1.64790	-3.03770
H	5.81690	4.47230	2.64040	H	0.14830	0.95180	-5.03850
H	6.84830	3.19240	3.36130	H	-1.83550	2.34400	-5.09270
H	3.66610	-5.97220	2.16810	H	-2.38390	3.86150	-3.14500
H	4.09990	-5.61890	3.85710	H	1.19240	2.45390	-1.14040
O	5.14620	2.59450	2.30780	H	1.68960	1.00900	-3.01490
O	6.61690	0.88310	2.22900	C	-0.83730	-2.99950	-4.30510
O	5.09700	-3.71850	2.42360	C	-0.83740	-4.18740	-3.69120
O	2.93820	-4.16430	2.90740	C	-1.64190	-4.38980	-2.46830
Si	-1.08370	4.39150	-0.56800	C	-2.35460	-3.37640	-1.94550
Si	-3.37320	-3.62210	-0.39790	C	-2.38710	-2.07630	-2.66360
C	2.83880	5.76750	1.60640	C	-1.66050	-1.89690	-3.77330
C	2.80500	5.67940	0.27220	H	-0.24580	-2.84830	-5.19870
C	1.57180	5.23440	-0.40880	H	-0.24520	-5.00280	-4.08600
C	0.48620	4.88950	0.30640	H	-1.66380	-5.37430	-2.02680
C	0.53660	4.97480	1.78680	H	-2.99570	-1.25960	-2.30290
C	1.64720	5.40470	2.39960	H	-1.68340	-0.94600	-4.28890
H	3.73980	6.09650	2.10730	C	-6.36930	-7.16990	-1.02620
H	3.67830	5.93970	-0.31180	C	-6.16930	-6.66530	0.19680
H	1.55650	5.20310	-1.49110	C	-5.22320	-5.54700	0.39080

C	-4.55120	-5.03900	-0.65620	C	6.64890	3.56090	-1.61560
C	-4.78910	-5.59250	-2.01230	C	7.30790	2.44550	-1.09840
C	-5.64900	-6.60420	-2.18470	C	6.65060	1.22650	-0.92750
H	-7.06250	-7.98850	-1.17020	C	5.30010	1.10510	-1.29430
H	-6.69980	-7.07460	1.04670	C	4.63560	2.23700	-1.80890
H	-5.08240	-5.14800	1.38760	C	5.30030	3.44790	-1.96230
H	-4.28730	-5.17490	-2.87420	H	7.17450	4.50190	-1.74450
H	-5.82530	-7.00440	-3.17470	H	8.35320	2.51590	-0.81160
C	-0.95620	-4.90250	3.41950	H	7.18160	0.39650	-0.48640
C	-1.88820	-3.94730	3.50570	H	3.59200	2.15770	-2.09310
C	-2.62500	-3.51930	2.29840	H	4.76100	4.30240	-2.36040
C	-2.34760	-4.06510	1.10030	C	8.80180	-2.76100	-1.83960
C	-1.31590	-5.12930	1.01770	C	8.33560	-2.94200	-0.53780
C	-0.65720	-5.52250	2.11480	C	7.07000	-2.48030	-0.16900
H	-0.41610	-5.21820	4.30270	C	6.26040	-1.82480	-1.10460
H	-2.11040	-3.49050	4.46130	C	6.72910	-1.65860	-2.41730
H	-3.41320	-2.78750	2.41140	C	7.99120	-2.12230	-2.78060
H	-1.09420	-5.61270	0.08180	H	9.78740	-3.11920	-2.12190
H	0.09350	-6.29930	2.04820	H	8.95390	-3.44610	0.19870
N	2.00920	-0.15880	1.98500	H	6.70700	-2.65670	0.83770
H	1.01740	0.14570	1.78400	H	6.09920	-1.16400	-3.14960
H	3.02140	2.73800	1.02590	H	8.34060	-1.98510	-3.79970
C	3.31170	-5.53700	3.10550	O	1.99710	-0.77180	-0.98710
H	2.40500	-6.03950	3.44180	H	0.95700	-0.66750	-1.00510
C	6.25780	3.48680	2.49070	C	4.60820	-1.03050	1.93070
H	6.89680	3.48450	1.60530	H	4.86370	-1.26770	0.64430
O	-0.48010	-0.58500	-0.97720	H	5.58870	-1.30680	2.31050
C	1.81530	-4.41260	-1.15640				
C	1.42940	-3.08190	-1.12680				
C	2.38890	-2.05670	-1.01960				
C	3.77500	-2.37930	-0.94370	C	-3.73480	1.65160	1.00230
C	4.12130	-3.74790	-0.96740	C	-2.79100	4.26080	1.54920
C	3.17050	-4.75240	-1.07550	C	-2.21600	3.54220	0.57290
H	1.06080	-5.18840	-1.24670	C	-2.66840	2.14340	0.33920
H	0.38850	-2.78560	-1.18010	H	-2.50860	5.29510	1.70680
H	5.16620	-4.02300	-0.90720	C	-3.83850	3.66650	2.40530
H	3.48380	-5.79090	-1.10740	C	-4.29530	2.41890	2.15180
H	3.52270	0.07250	-1.27760	C	-5.32030	1.82530	3.05110

C	-5.81270	2.53400	4.07370	H	0.93960	-2.77460	3.43880
C	-5.33340	3.90730	4.32370	C	3.90130	-3.42160	2.48490
C	-4.39520	4.44440	3.53600	C	5.46760	1.19710	2.22580
H	-5.67140	0.81380	2.89390	H	5.83640	4.36640	2.77350
H	-6.55930	2.09910	4.72560	H	6.85630	3.05960	3.46180
H	-5.73870	4.47580	5.15070	H	3.60210	-6.04630	2.07130
H	-4.04340	5.45010	3.72970	H	4.04290	-5.72470	3.76470
C	-5.70170	-1.95760	-0.33780	O	5.15550	2.50350	2.38370
C	-4.38530	0.40860	0.49890	O	6.61380	0.78300	2.27500
C	-3.68350	-0.75090	0.36460	O	5.05440	-3.80840	2.37050
C	-4.38860	-1.99290	-0.07260	O	2.89120	-4.24470	2.84240
H	-6.22290	-2.84280	-0.67700	Si	-1.00700	4.38560	-0.58020
C	-5.82190	0.45170	0.07700	Si	-3.44090	-3.57670	-0.38920
C	-6.44990	-0.69200	-0.27310	C	2.93910	5.71150	1.58330
C	-7.88030	-0.67160	-0.66010	C	2.90210	5.61880	0.24960
C	-8.55130	0.48370	-0.69590	C	1.66170	5.18830	-0.42800
C	-7.86390	1.74560	-0.36850	C	0.57190	4.86280	0.29000
C	-6.57440	1.73650	-0.01240	C	0.62570	4.95380	1.77000
H	-8.38740	-1.59290	-0.91870	C	1.74360	5.36920	2.37960
H	-9.59540	0.49760	-0.98060	H	3.84550	6.03000	2.08150
H	-8.40260	2.68220	-0.43300	H	3.77790	5.86540	-0.33650
H	-6.08800	2.68170	0.18450	H	1.64470	5.15260	-1.51010
O	-2.02640	1.35690	-0.57830	H	-0.22960	4.68460	2.37160
P	-1.22460	0.11890	0.14600	H	1.78110	5.43470	3.45920
O	-2.38050	-0.86280	0.79630	C	-3.21140	8.24040	-2.08240
O	-0.42540	0.62000	1.33240	C	-1.91650	8.30660	-1.75190
N	4.52020	-0.09580	-1.17650	C	-1.20840	7.09790	-1.28040
C	4.84230	-1.38670	-0.78960	C	-1.85860	5.92490	-1.19030
C	4.29810	0.31560	2.03110	C	-3.29680	5.86150	-1.55030
C	2.98100	0.72990	1.94860	C	-3.93580	6.95840	-1.97410
C	2.19970	-1.54510	2.22420	H	-3.73080	9.12530	-2.42700
C	3.49730	-2.02100	2.24890	H	-1.38420	9.24590	-1.82810
C	2.47690	2.13840	1.83310	H	-0.16420	7.18310	-1.01620
H	1.41780	2.13070	1.57060	H	-3.83940	4.92790	-1.46670
H	2.60930	2.66460	2.78250	H	-4.98500	6.90930	-2.23510
C	0.93820	-2.33060	2.44110	C	-0.04620	1.57390	-4.21080
H	0.06390	-1.68800	2.33320	C	-1.13020	2.35600	-4.24110
H	0.87480	-3.14900	1.72300	C	-1.42710	3.25500	-3.10710

C	-0.60770	3.29900	-2.04210	H	-3.48190	-2.76540	2.42480
C	0.58660	2.41800	-2.00980	H	-1.15640	-5.56830	0.07360
C	0.85140	1.60470	-3.04080	H	0.01340	-6.28630	2.03910
H	0.17060	0.91150	-5.03870	N	1.99920	-0.21450	1.98850
H	-1.79500	2.32920	-5.09480	H	1.01090	0.10320	1.78930
H	-2.31960	3.86150	-3.15230	H	3.04570	2.68840	1.08280
H	1.23740	2.40990	-1.14510	C	3.25360	-5.62380	3.01670
H	1.71560	0.95560	-3.01810	H	2.34360	-6.12420	3.34690
C	-0.90950	-2.99200	-4.30490	C	6.27180	3.38290	2.59740
C	-0.92740	-4.18060	-3.69250	H	6.91510	3.40230	1.71540
C	-1.73030	-4.37080	-2.46660	O	-0.49340	-0.60230	-0.96590
C	-2.42370	-3.34620	-1.93990	C	1.78880	-4.43000	-1.22850
C	-2.43670	-2.04460	-2.65610	C	1.40800	-3.09860	-1.17400
C	-1.71160	-1.87620	-3.76840	C	2.37160	-2.07970	-1.04400
H	-0.31910	-2.84970	-5.20070	C	3.75650	-2.40870	-0.97290
H	-0.35080	-5.00540	-4.09060	C	4.09740	-3.77780	-1.02380
H	-1.76820	-5.35570	-2.02650	C	3.14270	-4.77630	-1.15260
H	-3.02980	-1.21810	-2.29200	H	1.03070	-5.20070	-1.33410
H	-1.72070	-0.92450	-4.28290	H	0.36830	-2.79750	-1.22420
C	-6.49690	-7.07520	-1.00320	H	5.14120	-4.05830	-0.96900
C	-6.28430	-6.57280	0.21860	H	3.45230	-5.81510	-1.20460
C	-5.31940	-5.47000	0.40810	H	3.51480	0.05010	-1.27030
C	-4.64280	-4.97420	-0.64180	C	6.66500	3.52420	-1.54480
C	-4.89460	-5.52490	-1.99640	C	7.30720	2.40350	-1.01780
C	-5.77160	-6.52240	-2.16470	C	6.64070	1.18680	-0.86810
H	-7.20390	-7.88260	-1.14380	C	5.29830	1.07360	-1.26550
H	-6.81830	-6.97270	1.07090	C	4.65100	2.21020	-1.79100
H	-5.16880	-5.07240	1.40400	C	5.32460	3.41860	-1.92390
H	-4.38920	-5.11630	-2.86050	H	7.19730	4.46360	-1.65680
H	-5.95810	-6.92060	-3.15380	H	8.34590	2.46790	-0.70680
C	-1.03960	-4.90300	3.42150	H	7.15730	0.35210	-0.41850
C	-1.96640	-3.94320	3.51360	H	3.61460	2.13610	-2.10170
C	-2.69610	-3.49920	2.30770	H	4.79900	4.27690	-2.33200
C	-2.41660	-4.03430	1.10520	C	8.79180	-2.78070	-1.85220
C	-1.38630	-5.09930	1.01500	C	8.31440	-2.99270	-0.55920
C	-0.73610	-5.50890	2.11110	C	7.04650	-2.53790	-0.18980
H	-0.50570	-5.23130	4.30380	C	6.24570	-1.85840	-1.11580
H	-2.19110	-3.49590	4.47310	C	6.72550	-1.66130	-2.42010



C	7.99000	-2.11810	-2.78410	C	-6.60720	1.62910	0.03450
H	9.77950	-3.13310	-2.13470	H	-8.36850	-1.73260	-0.85500
H	8.92590	-3.51520	0.17010	H	-9.61840	0.33380	-0.88950
H	6.67520	-2.73710	0.80970	H	-8.46040	2.53970	-0.35290
H	6.10290	-1.14760	-3.14540	H	-6.13650	2.58300	0.22730
H	8.34830	-1.95620	-3.79650	O	-2.05650	1.34160	-0.59160
O	1.98470	-0.79430	-0.98530	P	-1.22240	0.11960	0.12300
H	0.94530	-0.68690	-1.00000	O	-2.35200	-0.89210	0.77400
C	4.59020	-1.10810	1.92600	O	-0.43150	0.63730	1.30810
H	4.84530	-1.32490	0.63610	N	4.53500	-0.07470	-1.18730
H	5.56740	-1.40010	2.30250	C	4.86080	-1.35620	-0.77400
				C	4.29490	0.39660	2.01000
				C	2.97460	0.79850	1.91910
C	-3.75260	1.59630	1.00900	C	2.21100	-1.47740	2.23660
C	-2.84960	4.21830	1.56270	C	3.51230	-1.94200	2.27400
C	-2.27170	3.51640	0.57610	C	2.45850	2.20050	1.77920
C	-2.70360	2.11200	0.33600	H	1.39790	2.17960	1.52390
H	-2.58440	5.25650	1.72420	H	2.59330	2.74510	2.71770
C	-3.87590	3.59950	2.42690	C	0.95490	-2.26860	2.46420
C	-4.31260	2.34540	2.17070	H	0.07610	-1.63610	2.33550
C	-5.31370	1.72630	3.07970	H	0.90260	-3.10460	1.76570
C	-5.80540	2.41860	4.11390	H	0.95330	-2.68880	3.47240
C	-5.34890	3.79900	4.36700	C	3.92600	-3.33450	2.53890
C	-4.43190	4.35920	3.57040	C	5.45760	1.29150	2.18340
H	-5.64740	0.70930	2.92050	H	5.80320	4.47770	2.64150
H	-6.53440	1.96490	4.77290	H	6.82920	3.20010	3.37390
H	-5.75340	4.35390	5.20350	H	3.65100	-5.96700	2.17370
H	-4.09640	5.36990	3.76660	H	4.07380	-5.61360	3.86550
C	-5.66730	-2.04610	-0.31750	O	5.13560	2.59890	2.30890
C	-4.38480	0.34300	0.50800	O	6.60700	0.88760	2.24200
C	-3.66280	-0.80240	0.36030	O	5.08250	-3.71480	2.43740
C	-4.35000	-2.05640	-0.07170	O	2.92020	-4.15800	2.90760
H	-6.17590	-2.94020	-0.65230	Si	-1.08800	4.38930	-0.58130
C	-5.82810	0.35910	0.10710	Si	-3.37470	-3.61910	-0.40870
C	-6.43900	-0.79560	-0.23720	C	2.84840	5.78490	1.55590
C	-7.87550	-0.80220	-0.60120	C	2.80260	5.69490	0.22220
C	-8.56970	0.33960	-0.62180	C	1.56460	5.24470	-0.44680
C	-7.90220	1.61380	-0.30080	C	0.48680	4.89710	0.27890

C	0.55050	4.98530	1.75870	H	-3.03720	-1.23850	-2.29960
C	1.66530	5.41970	2.36050	H	-1.73830	-0.89320	-4.28840
H	3.75300	6.11760	2.04790	C	-6.35560	-7.17440	-1.06240
H	3.66960	5.95730	-0.37020	C	-6.15300	-6.68200	0.16510
H	1.53980	5.21130	-1.52880	C	-5.21230	-5.56060	0.36710
H	-0.29470	4.69860	2.36630	C	-4.54820	-5.03730	-0.67740
H	1.71010	5.48310	3.44000	C	-4.78850	-5.57760	-2.03820
C	-3.39400	8.20270	-2.03570	C	-5.64350	-6.59210	-2.21780
C	-2.10130	8.29910	-1.70400	H	-7.04470	-7.99540	-1.21220
C	-1.36070	7.10350	-1.24930	H	-6.67710	-7.10370	1.01290
C	-1.97890	5.91220	-1.17650	H	-5.06850	-5.17210	1.36760
C	-3.41490	5.81490	-1.53770	H	-4.29210	-5.14840	-2.89750
C	-4.08340	6.90020	-1.94590	H	-5.82160	-6.98290	-3.21130
H	-3.93730	9.07810	-2.36740	C	-0.93150	-4.93080	3.38200
H	-1.59480	9.25360	-1.76630	C	-1.85850	-3.97200	3.48110
H	-0.31960	7.21340	-0.98180	C	-2.60330	-3.53410	2.28230
H	-3.93210	4.86600	-1.46690	C	-2.33930	-4.07540	1.07900
H	-5.13100	6.82650	-2.20740	C	-1.31450	-5.14520	0.98270
C	-0.07780	1.61080	-4.22380	C	-0.64730	-5.54610	2.07180
C	-1.16770	2.38450	-4.25770	H	-0.38510	-5.25320	4.25880
C	-1.48060	3.27380	-3.12020	H	-2.07010	-3.51880	4.44080
C	-0.67000	3.31710	-2.04860	H	-3.38620	-2.79840	2.40600
C	0.53300	2.44770	-2.01410	H	-1.10560	-5.62750	0.04330
C	0.81130	1.64200	-3.04740	H	0.09820	-6.32690	1.99510
H	0.15030	0.95510	-5.05410	N	2.00050	-0.15310	1.97600
H	-1.82590	2.35780	-5.11640	H	1.00930	0.15200	1.77000
H	-2.37760	3.87340	-3.16840	H	3.01780	2.74160	1.01520
H	1.17950	2.44200	-1.14620	C	3.29090	-5.53110	3.10860
H	1.68040	0.99940	-3.02150	H	2.38130	-6.03240	3.43890
C	-0.86450	-2.93490	-4.32290	C	6.24550	3.49190	2.49780
C	-0.84700	-4.12740	-3.71840	H	6.89140	3.48740	1.61760
C	-1.64430	-4.34970	-2.49410	O	-0.47820	-0.58180	-0.99280
C	-2.36670	-3.34940	-1.95970	C	1.81830	-4.41610	-1.16750
C	-2.41920	-2.04440	-2.66810	C	1.43320	-3.08510	-1.13790
C	-1.70010	-1.84740	-3.77960	C	2.39280	-2.06090	-1.02460
H	-0.27850	-2.76900	-5.21750	C	3.77850	-2.38440	-0.94170
H	-0.24580	-4.93190	-4.12160	C	4.12380	-3.75320	-0.96480
H	-1.65210	-5.33800	-2.06090	C	3.17280	-4.75690	-1.07950

H	1.06360	-5.19120	-1.26350	C	-1.39520	2.46400	0.22600
H	0.39290	-2.78780	-1.19650	H	0.60020	4.89500	1.60450
H	5.16820	-4.02910	-0.89970	C	-1.03130	3.84940	2.65040
H	3.48560	-5.79560	-1.11110	C	-2.08710	3.01680	2.51110
H	3.52900	0.06430	-1.28660	C	-2.95690	2.74540	3.68660
C	6.65170	3.55470	-1.61690	C	-2.71760	3.34870	4.85670
C	7.30750	2.44380	-1.08580	C	-1.58160	4.28080	4.99230
C	6.65090	1.22440	-0.91490	C	-0.77990	4.51760	3.94820
C	5.30480	1.09830	-1.29540	H	-3.78420	2.05190	3.61230
C	4.64330	2.22550	-1.82420	H	-3.35270	3.14900	5.71010
C	5.30720	3.43670	-1.97780	H	-1.39610	4.76800	5.94080
H	7.17670	4.49600	-1.74560	H	0.05500	5.19880	4.05660
H	8.34940	2.51830	-0.78800	C	-5.96200	0.10050	0.56780
H	7.17850	0.39800	-0.46290	C	-3.55820	1.56050	0.93440
H	3.60290	2.14170	-2.11940	C	-3.51560	0.24340	0.58730
H	4.77070	4.28780	-2.38700	C	-4.78320	-0.51960	0.42930
C	8.81730	-2.76790	-1.78670	H	-6.89000	-0.43470	0.42340
C	8.33480	-2.94890	-0.49090	C	-4.88230	2.25650	1.00130
C	7.06480	-2.48720	-0.13800	C	-6.02160	1.54390	0.85530
C	6.26680	-1.83130	-1.08330	C	-7.33930	2.21660	0.93830
C	6.75170	-1.66550	-2.39010	C	-7.40950	3.53710	1.13280
C	8.01830	-2.12930	-2.73770	C	-6.17380	4.33200	1.25150
H	9.80650	-3.12570	-2.05650	C	-4.97940	3.73340	1.18340
H	8.94370	-3.45300	0.25350	H	-8.25130	1.64110	0.83900
H	6.68950	-2.66400	0.86420	H	-8.37250	4.02760	1.19120
H	6.13120	-1.17070	-3.13040	H	-6.23650	5.40480	1.38160
H	8.38050	-1.99200	-3.75230	H	-4.09050	4.34630	1.24370
O	2.00140	-0.77560	-0.99360	O	-1.42470	1.59330	-0.82840
H	0.96230	-0.67010	-1.01590	P	-1.05180	0.07040	-0.31970
C	4.59840	-1.02670	1.93510	O	-2.34520	-0.47740	0.54110
H	4.85780	-1.26680	0.65070	O	0.07300	0.10840	0.70020
H	5.57720	-1.30280	2.31950	N	3.74500	-0.50340	-0.17550
				C	4.35150	-1.66450	-0.62880
				C	3.36490	-2.36340	2.47940
				C	2.14460	-1.71800	2.53450
C	-2.31670	2.33970	1.20400	C	1.20350	-3.27430	0.92410
C	-0.14500	4.12300	1.50040	C	2.40900	-3.94340	0.83000
C	-0.31090	3.48170	0.33300	C	1.73600	-0.58700	3.43650

H	1.40000	-0.98680	4.40010	H	-0.94010	4.49390	-3.77390
H	2.56400	0.08990	3.63020	H	-1.35890	3.08330	-5.67670
C	-0.10220	-3.66040	0.29080	C	5.20120	4.72040	-0.29640
H	-0.86220	-2.89900	0.46730	C	4.82190	3.76900	-1.15550
H	0.01460	-3.80710	-0.78290	C	3.38900	3.57090	-1.45750
H	-0.45040	-4.61000	0.70550	C	2.45130	4.31430	-0.84070
C	2.64720	-5.22190	0.12540	C	2.88800	5.39930	0.07510
C	4.53200	-2.08300	3.34350	C	4.18760	5.58500	0.33730
H	4.96680	-0.51380	6.13840	H	6.24990	4.86370	-0.07100
H	5.89680	-1.95070	5.59670	H	5.56300	3.13650	-1.62710
H	2.41580	-6.84300	-1.95700	H	3.13130	2.81500	-2.17870
H	2.18940	-7.77260	-0.45750	H	2.16430	6.07370	0.51120
O	4.24530	-1.37170	4.45470	H	4.49950	6.37970	1.00250
O	5.65700	-2.47840	3.08600	C	-2.38840	-2.34320	-4.14880
O	3.75100	-5.72940	0.02650	C	-3.31760	-1.41130	-3.90880
O	1.53240	-5.78990	-0.38840	C	-4.06540	-1.42230	-2.63410
Si	0.62290	4.09170	-1.18220	C	-3.80640	-2.35690	-1.70280
Si	-4.72150	-2.31680	-0.08100	C	-2.77800	-3.38960	-1.97900
C	-0.98070	8.36820	-2.22410	C	-2.11310	-3.38580	-3.14050
C	0.12980	7.90480	-2.80960	H	-1.83570	-2.33380	-5.07920
C	0.63300	6.55530	-2.47950	H	-3.51990	-0.64380	-4.64470
C	-0.01720	5.79040	-1.58640	H	-4.81120	-0.65670	-2.46010
C	-1.25340	6.30630	-0.94700	H	-2.55490	-4.15620	-1.25400
C	-1.70700	7.52880	-1.25010	H	-1.36670	-4.14380	-3.34010
H	-1.35090	9.35620	-2.46540	C	-9.01760	-4.10180	-0.60410
H	0.66210	8.51690	-3.52610	C	-8.58930	-3.72470	0.60630
H	1.53100	6.19650	-2.96730	C	-7.23350	-3.16010	0.76900
H	-1.80670	5.69860	-0.24370	C	-6.42910	-3.01520	-0.29730
H	-2.61090	7.90280	-0.78660	C	-6.90550	-3.44260	-1.63510
C	-0.18420	1.35790	-4.91710	C	-8.13390	-3.95580	-1.77860
C	0.56340	0.90330	-3.90660	H	-10.01030	-4.51580	-0.72510
C	0.81410	1.75740	-2.72670	H	-9.23420	-3.83240	1.46880
C	0.32000	3.00550	-2.67270	H	-6.90250	-2.86380	1.75690
C	-0.50810	3.50320	-3.80090	H	-6.26820	-3.34560	-2.50360
C	-0.74870	2.72010	-4.85990	H	-8.48190	-4.26690	-2.75510
H	-0.37550	0.73000	-5.77760	C	-2.54580	-4.94080	3.13870
H	0.98170	-0.09240	-3.95040	C	-3.08910	-5.51370	2.05880
H	1.38670	1.35520	-1.90180	C	-3.79280	-4.68650	1.05690

C	-3.87330	-3.35430	1.21260	C	4.72900	2.63080	2.48060
C	-3.31020	-2.73240	2.43730	C	5.71380	1.70610	2.13470
C	-2.66990	-3.48370	3.34130	C	5.44370	0.64660	1.26690
H	-2.02500	-5.54420	3.87080	C	4.15780	0.50550	0.71690
H	-3.00730	-6.58280	1.91180	C	3.16060	1.43910	1.07090
H	-4.22670	-5.17070	0.19070	C	3.44770	2.48130	1.94490
H	-3.41890	-1.67280	2.61920	H	4.95420	3.45250	3.15330
H	-2.25430	-3.02730	4.23040	H	6.71700	1.80310	2.54060
N	1.15120	-2.14280	1.69390	H	6.22590	-0.06200	1.04160
H	0.43210	-1.42560	1.46000	H	2.15170	1.31430	0.68480
H	0.91360	-0.03620	2.97500	H	2.66070	3.18200	2.20770
C	1.74920	-7.01410	-1.10910	C	8.62110	-1.42240	-1.25240
H	0.76350	-7.32790	-1.45240	C	8.12240	-2.34170	-0.33070
C	5.37680	-1.04420	5.27930	C	6.74710	-2.43680	-0.09970
H	6.07290	-0.40550	4.73080	C	5.86120	-1.60800	-0.79270
O	-0.86320	-0.77800	-1.55880	C	6.36780	-0.68560	-1.72270
C	2.41890	-3.81980	-3.86040	C	7.73830	-0.59220	-1.94830
C	1.69120	-2.86910	-3.16020	H	9.69040	-1.34980	-1.42750
C	2.27600	-2.16450	-2.09290	H	8.80080	-2.98630	0.21990
C	3.63870	-2.38920	-1.74530	H	6.37600	-3.12920	0.64550
C	4.33590	-3.37710	-2.46940	H	5.67960	-0.04170	-2.26180
C	3.74740	-4.08600	-3.50820	H	8.11700	0.12810	-2.66740
H	1.95160	-4.35300	-4.68360	O	1.57210	-1.27410	-1.38980
H	0.66450	-2.63610	-3.42030	H	0.56280	-1.14040	-1.60460
H	5.36630	-3.58610	-2.20830	C	3.59490	-3.32610	1.41310
H	4.32290	-4.83160	-4.04660	H	4.14670	-2.59140	0.40340
H	2.75400	-0.45570	-0.42370	H	4.43430	-4.00070	1.55600

**OOH-Type II E**

C	4.36840	1.01730	-0.25300	C	6.35420	2.62670	0.24570
C	5.99010	-1.15630	0.54690	C	7.62700	2.81120	0.61460
C	4.69880	-1.37040	0.25290	C	8.47260	1.65480	0.96430
C	3.82380	-0.22030	-0.11790	C	7.96420	0.41880	0.92830
H	6.63290	-1.97020	0.85210	H	5.74770	3.49290	0.01820
C	6.55450	0.20410	0.52540	H	8.03710	3.81150	0.66790
C	5.78200	1.25300	0.17030				

H	9.50200	1.81080	1.25990	O	-1.93770	-4.36660	-2.53480
H	8.58800	-0.42470	1.19710	O	-4.14910	-4.36950	-2.08850
C	2.11930	4.39810	-1.70760	O	-5.80760	-3.00180	2.21230
C	3.56780	2.13770	-0.81420	O	-4.41230	-2.24360	3.81500
C	2.42300	2.49800	-0.19830	Si	3.99970	-3.09770	0.41700
C	1.68580	3.71440	-0.63840	Si	0.17380	4.32840	0.26550
H	1.58830	5.28020	-2.04600	C	1.07290	-2.97050	4.07300
C	4.00860	2.87000	-2.03900	C	0.74860	-3.69870	2.99860
C	3.31500	3.95540	-2.45110	C	1.65250	-3.73980	1.83050
C	3.74150	4.69520	-3.66150	C	2.80080	-3.04290	1.83900
C	4.79920	4.27900	-4.36580	C	3.15540	-2.24090	3.03560
C	5.53920	3.07400	-3.94580	C	2.33360	-2.20370	4.09120
C	5.16490	2.40170	-2.85120	H	0.41280	-2.94090	4.93000
H	3.19700	5.57490	-3.98170	H	-0.17790	-4.25800	2.98100
H	5.10930	4.81920	-5.25090	H	1.37020	-4.34680	0.98550
H	6.38060	2.72920	-4.53310	H	4.08160	-1.68100	3.06250
H	5.70780	1.50730	-2.57670	H	2.59300	-1.61520	4.96160
O	2.52980	-0.47500	-0.51290	C	7.43480	-6.14840	1.31840
P	1.30310	0.31560	0.27130	C	6.49340	-5.92440	2.24290
O	1.93900	1.72540	0.82670	C	5.40310	-4.96340	1.97360
O	0.83200	-0.47500	1.46380	C	5.35700	-4.30720	0.80180
N	-4.64590	0.29540	0.01460	C	6.39890	-4.56440	-0.22110
C	-4.86010	-0.64440	-0.98210	C	7.38440	-5.43590	0.02560
C	-2.70780	-3.22500	-0.59030	H	8.23360	-6.85190	1.51490
C	-1.46690	-2.72540	-0.23940	H	6.52780	-6.44650	3.19030
C	-2.33340	-1.93680	1.88430	H	4.65310	-4.80400	2.73600
C	-3.58620	-2.44390	1.58990	H	6.36790	-4.04530	-1.17110
C	-0.19170	-2.86810	-1.01860	H	8.14580	-5.62090	-0.72100
H	0.63690	-2.38710	-0.50220	C	2.06480	-4.70230	-3.54210
H	0.03400	-3.92500	-1.16560	C	2.56440	-3.46180	-3.50770
C	-1.89990	-1.29500	3.17120	C	3.19330	-2.94950	-2.27220
H	-0.94460	-0.78490	3.03420	C	3.23230	-3.71180	-1.16560
H	-2.66130	-0.59900	3.51990	C	2.71740	-5.10200	-1.22590
H	-1.79480	-2.05290	3.95300	C	2.15800	-5.56750	-2.34960
C	-4.70930	-2.58490	2.54160	H	1.60150	-5.07750	-4.44540
C	-3.01410	-4.02860	-1.79240	H	2.50730	-2.82900	-4.38380
H	-1.25540	-5.30690	-4.18890	H	3.62020	-1.95780	-2.28710
H	-2.73490	-6.04550	-3.49070	H	2.79620	-5.75000	-0.36210
H	-5.06750	-2.12060	5.72390	H	1.77710	-6.57970	-2.38830
H	-6.29620	-1.66890	4.49880	C	0.58670	8.99450	0.58620

C	1.62230	8.20430	0.88890	C	-2.07480	-0.69020	-4.29390
C	1.48820	6.73650	0.78790	C	-1.65640	-0.19450	-3.06900
C	0.32340	6.18340	0.40570	C	-2.54120	-0.15200	-1.97180
C	-0.81550	7.06910	0.05430	C	-3.87840	-0.61830	-2.11760
C	-0.68950	8.39910	0.14450	C	-4.25820	-1.12390	-3.37920
H	0.68360	10.07010	0.65810	C	-3.38360	-1.15900	-4.45540
H	2.56210	8.63800	1.20540	H	-1.37960	-0.70590	-5.12880
H	2.35250	6.12310	1.00410	H	-0.64860	0.17690	-2.92080
H	-1.75440	6.65730	-0.28300	H	-5.26790	-1.48880	-3.51320
H	-1.52160	9.04210	-0.11200	H	-3.72210	-1.53860	-5.41410
C	-0.01030	2.57550	4.61520	H	-3.69480	0.66390	0.01320
C	0.99780	3.37770	4.25760	C	-6.83930	1.57760	3.38730
C	1.06130	3.91910	2.88460	C	-7.28810	0.47230	2.66390
C	0.11160	3.60760	1.98500	C	-6.59390	0.00330	1.54800
C	-0.97390	2.67510	2.37590	C	-5.42390	0.65830	1.12920
C	-1.04490	2.21080	3.62890	C	-4.96870	1.76750	1.86840
H	-0.06320	2.18310	5.62240	C	-5.66540	2.21790	2.98340
H	1.76430	3.63970	4.97540	H	-7.39180	1.93290	4.25150
H	1.88520	4.56710	2.62600	H	-8.19350	-0.04540	2.96760
H	-1.70590	2.34910	1.65330	H	-6.94870	-0.87830	1.03540
H	-1.85440	1.55830	3.92110	H	-4.06690	2.28020	1.55330
C	-3.67540	3.27480	-2.20770	H	-5.29020	3.07670	3.53220
C	-3.78960	3.77770	-0.97400	C	-8.95830	-1.19650	-2.22830
C	-2.57870	4.11180	-0.19550	C	-8.42930	0.08360	-2.04940
C	-1.35630	3.89020	-0.70970	C	-7.11100	0.24340	-1.62950
C	-1.23840	3.32920	-2.07860	C	-6.30310	-0.87730	-1.38060
C	-2.33800	3.05530	-2.79210	C	-6.83130	-2.15800	-1.58110
H	-4.56080	3.02350	-2.77720	C	-8.15490	-2.31320	-1.99900
H	-4.76880	3.93850	-0.54190	H	-9.98790	-1.32100	-2.55070
H	-2.69450	4.53520	0.79450	H	-9.04300	0.95970	-2.23720
H	-0.26810	3.14090	-2.51610	H	-6.69970	1.23820	-1.49200
H	-2.24970	2.65260	-3.79270	H	-6.20630	-3.03280	-1.43950
N	-1.35280	-2.03690	0.93810	H	-8.55350	-3.31230	-2.14630
H	-0.45440	-1.52980	1.13170	O	-2.13650	0.34280	-0.79010
H	-0.29410	-2.42300	-2.00950	H	-1.10180	0.51220	-0.76890
C	-5.49540	-2.36680	4.75230	C	-3.86450	-2.89930	0.23550
H	-5.89160	-3.38460	4.75100	H	-4.46610	-1.87460	-0.39080
C	-2.22440	-5.11000	-3.73040	H	-4.70200	-3.58680	0.15150
H	-2.85460	-4.52090	-4.40030				
O	0.31190	0.61120	-0.84510				

				C	-3.54160	-2.50390	1.50280
C	4.40850	0.98180	-0.22440	C	-0.18570	-2.83340	-1.15970
C	6.01190	-1.21500	0.54740	H	0.66250	-2.38940	-0.64190
C	4.72560	-1.41850	0.22470	H	0.00770	-3.88940	-1.35540
C	3.85830	-0.25650	-0.12600	C	-1.84070	-1.44100	3.12660
H	6.64840	-2.03820	0.84030	H	-0.88830	-0.92110	3.00740
C	6.57940	0.14410	0.56970	H	-2.60040	-0.76790	3.52080
C	5.81600	1.20320	0.22550	H	-1.72610	-2.23950	3.86530
C	6.39090	2.57290	0.34000	C	-4.65600	-2.69240	2.45510
C	7.65770	2.74510	0.73460	C	-2.87660	-3.89920	-1.99230
C	8.49380	1.57850	1.07320	H	-4.15130	-4.30360	-4.28720
C	7.98270	0.34520	1.00100	H	-3.91220	-5.85250	-3.44900
H	5.79090	3.44580	0.12040	H	-4.97380	-2.43520	5.66520
H	8.06990	3.74260	0.81650	H	-6.21640	-1.89780	4.49020
H	9.51840	1.72460	1.38980	O	-4.18870	-4.19750	-2.20530
H	8.59940	-0.50610	1.26140	O	-2.00250	-4.23250	-2.77140
C	2.18690	4.39400	-1.64760	O	-5.76230	-3.07760	2.11090
C	3.61950	2.11600	-0.77380	O	-4.34410	-2.43500	3.74400
C	2.46680	2.46750	-0.16760	Si	4.02400	-3.14960	0.31460
C	1.73710	3.69220	-0.59710	Si	0.21450	4.29330	0.29770
H	1.66230	5.28310	-1.97760	C	1.09040	-3.18940	3.96540
C	4.07860	2.86900	-1.97900	C	0.75320	-3.84220	2.84730
C	3.39240	3.96250	-2.38180	C	1.65550	-3.82430	1.67760
C	3.83690	4.72270	-3.57300	C	2.81680	-3.15110	1.72960
C	4.90370	4.31700	-4.26970	C	3.18300	-2.42850	2.97240
C	5.63600	3.10350	-3.86060	C	2.36240	-2.44410	4.02920
C	5.24560	2.41300	-2.78310	H	0.43230	-3.20470	4.82430
H	3.29820	5.60880	-3.88520	H	-0.18170	-4.38530	2.79640
H	5.22700	4.87210	-5.14080	H	1.36270	-4.37370	0.79750
H	6.48480	2.76760	-4.44210	H	4.11820	-1.88630	3.03280
H	5.78320	1.51290	-2.51690	H	2.63130	-1.91500	4.93410
O	2.56750	-0.49490	-0.54090	C	7.41440	-6.26200	1.18330
P	1.33880	0.27830	0.25560	C	7.40910	-5.57540	0.03470
O	1.96920	1.67970	0.83920	C	6.33860	-4.59360	-0.23580
O	0.86740	-0.53320	1.43420	C	5.37110	-4.38020	0.67180
N	-4.58100	0.33980	0.12410	C	5.37750	-5.14980	1.94010
C	-4.84970	-0.53850	-0.91400	C	6.34820	-6.04000	2.18100
C	-2.69300	-3.15880	-0.72810	H	8.19770	-6.98170	1.38300
C	-1.44360	-2.69350	-0.35590	H	8.18840	-5.73740	-0.69870
C	-2.28520	-2.01430	1.81130	H	6.34970	-4.04880	-1.17200



H	4.60170	-5.00180	2.67890	C	-2.27370	3.12630	-2.82020
H	6.35320	-6.60080	3.10670	H	-4.49630	3.06860	-2.81290
C	2.13300	-4.53600	-3.74760	H	-4.71980	3.87890	-0.53870
C	2.17740	-5.37280	-2.70500	H	-2.65550	4.45020	0.82390
C	2.78450	-4.93600	-1.43060	H	-0.20530	3.21720	-2.53250
C	3.27210	-3.68990	-1.30230	H	-2.17850	2.76900	-3.83730
C	3.26830	-2.78690	-2.48030	N	-1.31290	-2.06800	0.85260
C	2.71570	-3.18450	-3.63300	H	-0.40940	-1.57460	1.06400
H	1.68390	-4.85210	-4.68020	H	-0.29770	-2.35920	-2.13600
H	1.76170	-6.36850	-2.78940	C	-5.41580	-2.61460	4.68520
H	2.82150	-5.63470	-0.60420	H	-5.81740	-3.62820	4.62220
H	3.72790	-1.81060	-2.42960	C	-4.45410	-4.90420	-3.42630
H	2.71160	-2.52320	-4.48980	H	-5.53020	-5.07710	-3.43800
C	0.61770	8.95290	0.70060	O	0.34790	0.59200	-0.85680
C	1.65410	8.15980	0.99280	C	-2.16740	-0.53880	-4.30320
C	1.52330	6.69360	0.86680	C	-1.69900	-0.10160	-3.07480
C	0.36080	6.14510	0.47170	C	-2.55260	-0.06370	-1.95310
C	-0.77950	7.03400	0.13360	C	-3.90790	-0.48160	-2.07780
C	-0.65650	8.36250	0.24620	C	-4.34180	-0.92310	-3.34650
H	0.71220	10.02730	0.79080	C	-3.49850	-0.94870	-4.44670
H	2.59210	8.58990	1.31930	H	-1.49450	-0.55620	-5.15570
H	2.38770	6.07760	1.07620	H	-0.67430	0.22720	-2.94200
H	-1.71750	6.62530	-0.21090	H	-5.37020	-1.23990	-3.46400
H	-1.48950	9.00790	-0.00070	H	-3.87410	-1.27850	-5.41000
C	-0.05840	2.47720	4.61520	H	-3.62330	0.69140	0.10920
C	0.93810	3.31200	4.30200	C	-6.68860	1.54490	3.57940
C	1.03440	3.87030	2.93750	C	-7.15390	0.45480	2.84320
C	0.12580	3.54220	2.00240	C	-6.48890	0.01480	1.69830
C	-0.94130	2.57010	2.34300	C	-5.33280	0.68340	1.26290
C	-1.04430	2.09120	3.58810	C	-4.86460	1.78080	2.01060
H	-0.13660	2.07360	5.61640	C	-5.53130	2.20170	3.15540
H	1.66940	3.58970	5.04990	H	-7.21690	1.87670	4.46770
H	1.84390	4.54960	2.71650	H	-8.04920	-0.07300	3.15970
H	-1.63250	2.22650	1.58870	H	-6.85470	-0.85570	1.17450
H	-1.84320	1.41120	3.84340	H	-3.97950	2.31070	1.67760
C	-3.61520	3.30510	-2.23050	H	-5.14610	3.05140	3.71130
C	-3.73800	3.75030	-0.97560	C	-9.00780	-0.90480	-2.02960
C	-2.53270	4.06640	-0.18130	C	-8.41050	0.34880	-1.88090
C	-1.30670	3.87770	-0.70000	C	-7.07310	0.44700	-1.50470
C	-1.17890	3.37690	-2.09090	C	-6.31290	-0.70950	-1.27080

C	-6.91260	-1.96250	-1.43550	C	-1.70040	2.03660	4.20640
C	-8.25480	-2.05770	-1.80930	H	1.66720	3.88330	4.89920
H	-10.05200	-0.98110	-2.31770	H	0.31490	3.09450	6.74190
H	-8.98650	1.25240	-2.05760	H	-1.87770	1.87090	6.29320
H	-6.60890	1.42140	-1.38990	H	-2.62800	1.50650	4.03270
H	-6.33260	-2.86420	-1.27990	O	-1.98340	-0.08160	0.25640
H	-8.71000	-3.03690	-1.92470	P	-0.70780	0.44660	-0.67890
O	-2.10330	0.38090	-0.76820	O	-0.74350	2.09110	-0.61130
H	-1.06220	0.52370	-0.76500	O	-0.90840	-0.00690	-2.09810
C	-3.84090	-2.88100	0.12730	N	3.25520	-1.27440	0.58600
H	-4.45840	-1.81530	-0.41290	C	3.06560	-2.46300	1.27040
H	-4.68040	-3.56320	0.03100	C	0.96540	-4.36310	-0.68850
				C	0.02710	-3.44470	-1.11950
				C	1.68590	-2.31480	-2.47340
				C	2.67580	-3.15730	-1.99840
C	-2.70920	1.93010	1.32250	C	-1.42610	-3.43670	-0.77730
C	-5.39330	1.25080	0.75170	H	-1.82420	-2.42790	-0.88360
C	-4.40610	0.45120	0.32370	H	-1.97970	-4.12240	-1.42560
C	-2.97980	0.81200	0.59860	C	1.78820	-1.27570	-3.55500
H	-6.42780	1.01990	0.54210	H	0.96070	-0.56880	-3.45940
C	-5.09910	2.49930	1.46910	H	2.73940	-0.75070	-3.51330
C	-3.82090	2.85230	1.71790	H	1.73140	-1.75700	-4.53760
C	-3.55540	4.18220	2.34060	C	4.05840	-3.23760	-2.51860
C	-4.56820	4.98010	2.69760	C	0.66960	-5.64650	-0.01740
C	-5.96100	4.55950	2.46330	H	-0.69370	-7.17600	1.71360
C	-6.21450	3.38740	1.87370	H	-2.03640	-7.33650	0.53650
H	-2.54540	4.53570	2.49280	H	5.60020	-2.01800	-5.08610
H	-4.36750	5.94450	3.14630	H	6.29580	-2.09550	-3.43440
H	-6.77610	5.20820	2.75700	O	-0.64490	-5.96650	0.01260
H	-7.24010	3.09110	1.69120	O	1.53360	-6.38190	0.43110
C	1.11720	3.62190	2.18110	O	4.93210	-3.89880	-1.98040
C	-1.31480	2.30270	1.65660	O	4.27120	-2.54410	-3.65540
C	-0.45500	2.55010	0.64950	Si	-4.84780	-1.05180	-0.69280
C	0.77790	3.34240	0.91060	Si	1.80070	4.07870	-0.47610
H	1.99780	4.21620	2.39520	C	-2.70060	-0.50260	-4.82400
C	-0.88650	2.52840	3.06410	C	-2.85160	-1.73270	-4.31910
C	0.28660	3.15100	3.30720	C	-3.53850	-1.92400	-3.02440
C	0.73330	3.37210	4.70170	C	-3.98530	-0.86370	-2.33240
C	-0.01330	2.93610	5.72280	C	-3.83860	0.49560	-2.91120
C	-1.28490	2.23260	5.46310	C	-3.22790	0.66520	-4.09040

H	-2.19480	-0.36080	-5.77020	C	1.94790	2.70920	-2.91590
H	-2.46900	-2.59080	-4.85620	C	1.20680	3.52290	-2.14890
H	-3.66730	-2.92780	-2.65270	C	-0.10720	3.99770	-2.64870
H	-4.22040	1.35910	-2.38150	C	-0.57120	3.57470	-3.83090
H	-3.11470	1.65790	-4.50630	H	-0.14300	2.30980	-5.60870
C	-9.47430	-1.32680	-1.37210	H	2.03660	1.58360	-4.83100
C	-8.67050	-1.05480	-2.40700	H	2.91720	2.37170	-2.58790
C	-7.20910	-0.96160	-2.20680	H	-0.70530	4.67240	-2.04880
C	-6.68260	-1.14290	-0.98360	H	-1.53710	3.90890	-4.18670
C	-7.57820	-1.44990	0.15800	C	6.34990	3.16440	0.26170
C	-8.90100	-1.53510	-0.02710	C	5.42240	2.56770	1.01750
H	-10.54450	-1.39560	-1.51800	C	3.98810	2.80650	0.75680
H	-9.08860	-0.90310	-3.39370	C	3.60350	3.64780	-0.22110
H	-6.58270	-0.74360	-3.06090	C	4.63990	4.26670	-1.08450
H	-7.16500	-1.60410	1.14720	C	5.93880	4.04130	-0.85140
H	-9.55320	-1.75740	0.80750	H	7.40090	2.98650	0.44870
C	-3.91500	-4.99260	1.66580	H	5.71970	1.90630	1.82090
C	-3.59810	-3.80890	2.20230	H	3.26830	2.28990	1.37390
C	-3.87160	-2.56070	1.45930	H	4.35920	4.89260	-1.91740
C	-4.42880	-2.60870	0.23580	H	6.69090	4.49310	-1.48500
C	-4.81070	-3.92300	-0.33620	N	0.43290	-2.43110	-1.93890
C	-4.55660	-5.05190	0.33730	H	-0.21820	-1.63350	-2.11400
H	-3.71080	-5.90710	2.20730	H	-1.56520	-3.77340	0.24600
H	-3.13890	-3.76280	3.18040	C	5.62260	-2.57400	-4.14910
H	-3.61840	-1.61920	1.92570	H	5.94650	-3.60310	-4.31810
H	-5.30820	-3.97650	-1.29600	C	-0.96020	-7.21230	0.65440
H	-4.83240	-6.00980	-0.08400	H	-0.42190	-8.03690	0.18240
C	1.26560	8.74540	-0.50330	O	0.56320	-0.05370	0.00280
C	1.91250	8.13460	-1.50160	C	-0.29960	-3.01610	3.94090
C	2.07900	6.66670	-1.48790	C	0.04560	-1.72530	3.56630
C	1.60360	5.93540	-0.46440	C	1.09070	-1.47210	2.66180
C	0.86220	6.62030	0.62640	C	1.82580	-2.56640	2.13060
C	0.70860	7.95020	0.60800	C	1.46140	-3.86620	2.53900
H	1.14050	9.82040	-0.51290	C	0.41160	-4.09990	3.41730
H	2.31200	8.71350	-2.32420	H	-1.11490	-3.17800	4.64040
H	2.56400	6.19650	-2.33150	H	-0.48150	-0.86150	3.95780
H	0.42370	6.06060	1.43810	H	2.03150	-4.70880	2.16310
H	0.16600	8.44530	1.40310	H	0.16540	-5.11690	3.70680
C	0.23640	2.65300	-4.65490	H	2.38890	-0.81390	0.30570
C	1.43850	2.25190	-4.22530	C	6.53290	0.36520	-1.52500

C	5.21090	0.62370	-1.89650	H	-4.50250	5.95200	2.87530
C	4.15680	0.08140	-1.16970	H	-6.89210	5.14930	2.49950
C	4.39770	-0.75080	-0.06050	H	-7.30310	2.97880	1.52320
C	5.72580	-0.95930	0.34630	C	0.99980	3.76630	2.05210
C	6.77410	-0.41050	-0.39220	C	-1.36330	2.31270	1.57130
H	7.35670	0.79020	-2.08990	C	-0.50540	2.54920	0.56050
H	5.00430	1.25260	-2.75680	C	0.68930	3.40370	0.79640
H	3.12800	0.28710	-1.44570	H	1.84060	4.42340	2.24160
H	5.95130	-1.53220	1.23130	C	-0.95400	2.61310	2.97040
H	7.79330	-0.58900	-0.06250	C	0.18700	3.30010	3.19340
C	6.47970	-4.22010	3.27180	C	0.61160	3.60110	4.57970
C	6.19740	-4.58640	1.95660	C	-0.12240	3.17450	5.61390
C	5.10290	-4.03570	1.28620	C	-1.35830	2.40230	5.37680
C	4.27240	-3.11530	1.93420	C	-1.75420	2.13380	4.12710
C	4.55540	-2.75660	3.26260	H	1.51900	4.16370	4.76080
C	5.65680	-3.29740	3.92200	H	0.18960	3.39150	6.62730
H	7.33270	-4.64980	3.78890	H	-1.94100	2.04990	6.21800
H	6.83190	-5.30050	1.44020	H	-2.65560	1.55560	3.96980
H	4.93220	-4.29320	0.24810	O	-1.96670	-0.12980	0.24760
H	3.91200	-2.04710	3.77250	P	-0.70110	0.39890	-0.70140
H	5.86640	-3.00360	4.94640	O	-0.77390	2.04310	-0.68700
O	1.38020	-0.17330	2.39780	O	-0.88530	-0.10380	-2.10610
H	1.02150	0.03020	1.47990	N	3.30140	-1.18750	0.57880
C	2.37070	-4.05340	-0.88680	C	3.16140	-2.35300	1.30990
H	2.75860	-3.37690	0.25300	C	1.08720	-4.36620	-0.55820
H	3.04560	-4.89610	-0.76660	C	0.13300	-3.47730	-1.01480
				C	1.76630	-2.37410	-2.42150
				C	2.77070	-3.18600	-1.92460
C	-2.74640	1.89760	1.24180	C	-1.31750	-3.47910	-0.66040
C	-5.41040	1.13910	0.67780	H	-1.73840	-2.48640	-0.81650
C	-4.40270	0.34500	0.28870	H	-1.86110	-4.21100	-1.26470
C	-2.98660	0.74940	0.55590	C	1.84970	-1.36850	-3.53610
H	-6.43810	0.87660	0.47180	H	1.01490	-0.66790	-3.45730
C	-5.14860	2.42210	1.34540	H	2.79520	-0.83170	-3.51560
C	-3.88030	2.81140	1.59060	H	1.79180	-1.88030	-4.50300
C	-3.64760	4.17270	2.15610	C	4.15260	-3.26420	-2.44680
C	-4.67960	4.96450	2.46880	C	0.81380	-5.63090	0.15580
C	-6.06130	4.50530	2.24160	H	-0.51990	-7.12730	1.94060
C	-6.28550	3.30360	1.70160	H	-1.86460	-7.34210	0.77450
H	-2.64650	4.55420	2.29950	H	6.36250	-2.12080	-3.41990

H	6.04330	-3.67170	-4.23780	C	0.93920	8.78560	-0.02940
O	-0.49600	-5.96750	0.20480	C	-0.09330	7.93620	-0.01070
O	1.69080	-6.34060	0.62080	C	0.13540	6.48880	-0.19730
O	5.04020	-3.88260	-1.88140	C	1.37700	6.01520	-0.40790
O	4.34760	-2.62050	-3.61560	C	2.52010	6.96350	-0.40110
Si	-4.80390	-1.21130	-0.66210	C	2.30940	8.27450	-0.22730
Si	1.64130	4.17760	-0.60880	H	0.77400	9.84620	0.10940
C	-2.66890	-0.78420	-4.81390	H	-1.09850	8.30610	0.14500
C	-2.79390	-1.99570	-4.25950	H	-0.71380	5.82080	-0.13550
C	-3.47710	-2.14900	-2.95800	H	3.53330	6.61390	-0.52170
C	-3.94520	-1.07110	-2.30850	H	3.14480	8.96270	-0.22170
C	-3.82790	0.26630	-2.94220	C	-0.03400	2.64640	-4.71980
C	-3.22130	0.40090	-4.12810	C	-0.74740	3.51290	-3.99260
H	-2.16590	-0.67020	-5.76540	C	-0.20900	4.02990	-2.71710
H	-2.39300	-2.86660	-4.76160	C	0.99710	3.63000	-2.27500
H	-3.58500	-3.13940	-2.54600	C	1.78900	2.68700	-3.10050
H	-4.22830	1.14230	-2.44780	C	1.29980	2.21970	-4.25520
H	-3.13010	1.37800	-4.58420	H	-0.43170	2.25800	-5.64840
C	-9.42040	-1.64100	-1.32890	H	-1.72720	3.82630	-4.32910
C	-8.62230	-1.39850	-2.37550	H	-0.82530	4.69700	-2.13450
C	-7.16430	-1.25660	-2.17930	H	2.76270	2.36310	-2.77310
C	-6.63530	-1.36410	-0.94850	H	1.88020	1.52620	-4.85000
C	-7.52440	-1.63860	0.20630	C	6.22780	3.31920	-0.13330
C	-8.84420	-1.76780	0.02490	C	5.78010	4.01380	-1.18530
H	-10.48810	-1.74560	-1.47190	C	4.33070	4.24170	-1.35920
H	-9.04250	-1.30660	-3.36870	C	3.45490	3.76270	-0.45900
H	-6.54240	-1.06410	-3.04280	C	3.95570	2.93830	0.67020
H	-7.10910	-1.73300	1.20200	C	5.27010	2.74230	0.83070
H	-9.49190	-1.96600	0.86910	H	7.28930	3.15350	-0.00270
C	-3.76210	-5.01770	1.86600	H	6.47870	4.42060	-1.90470
C	-3.47910	-3.80320	2.35000	H	3.99120	4.83170	-2.20160
C	-3.78830	-2.59710	1.55380	H	3.27010	2.47460	1.36470
C	-4.34300	-2.71410	0.33380	H	5.63290	2.13830	1.65230
C	-4.68770	-4.06240	-0.17970	N	0.51820	-2.48860	-1.87390
C	-4.40160	-5.15310	0.54210	H	-0.14750	-1.70940	-2.07390
H	-3.53240	-5.90150	2.44690	H	-1.44130	-3.76240	0.38120
H	-3.02210	-3.70130	3.32500	C	5.69820	-2.64340	-4.11160
H	-3.56270	-1.62950	1.97910	H	5.66240	-2.12830	-5.07130
H	-5.18390	-4.17180	-1.13540	C	-0.79000	-7.19840	0.88400
H	-4.65030	-6.13590	0.16350	H	-0.24130	-8.02840	0.43380

O	0.57890	-0.04860	0.00040	H	6.03160	-1.45080	1.07330
C	-0.16100	-2.92510	4.02970	H	3.06460	0.37560	-1.44260
C	0.14090	-1.63650	3.61190	H	4.86880	1.31560	-2.86880
C	1.17160	-1.38010	2.69200	C	6.63790	-3.91000	3.36770
C	1.93560	-2.46730	2.18840	C	5.82770	-2.93260	3.95100
C	1.61760	-3.76390	2.64310	C	4.70890	-2.45570	3.27230
C	0.58190	-4.00200	3.53680	C	4.39480	-2.93570	1.98990
H	-0.96620	-3.09020	4.73990	C	5.21230	-3.90990	1.40810
H	-0.40990	-0.77750	3.98070	C	6.32520	-4.39540	2.09900
H	2.21090	-4.59990	2.28940	H	7.50490	-4.28950	3.90060
H	0.37110	-5.01630	3.86130	H	6.06130	-2.54610	4.93870
H	2.41630	-0.75660	0.30960	H	4.07490	-1.70310	3.73000
C	6.46080	0.43560	-1.71660	H	5.01820	-4.25930	0.40180
C	6.76340	-0.33100	-0.59300	H	6.94980	-5.15240	1.63430
C	5.75690	-0.87450	0.20520	O	1.42300	-0.08180	2.38760
C	4.40830	-0.66270	-0.12570	H	1.04340	0.08840	1.47130
C	4.10660	0.16540	-1.22410	C	2.48710	-4.04350	-0.77710
C	5.12020	0.69380	-2.01540	H	2.87240	-3.32080	0.32710
H	7.25210	0.85380	-2.33080	H	3.17290	-4.87370	-0.63470
H	7.79900	-0.51160	-0.32010				

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C	3.34720	1.42700	-0.96870	C	1.22900	2.53630	-0.50660
C	5.64130	-0.06120	-0.25280	C	0.28200	3.64380	-0.80100
C	4.42690	-0.61270	-0.11270	H	-0.48390	4.93060	-2.28700
C	3.20560	0.18520	-0.43980	C	2.04220	2.69910	-2.81430
H	6.53530	-0.61000	0.00720	C	1.08090	3.60030	-3.11630
C	5.79250	1.32490	-0.72270	C	0.93850	4.09520	-4.50480
C	4.70330	2.05300	-1.04680	C	1.74620	3.63610	-5.46740
C	4.88390	3.48310	-1.42910	C	2.78060	2.63200	-5.15000
C	6.10820	4.01800	-1.49640	C	2.92130	2.18400	-3.89700
C	7.29300	3.20010	-1.17930	H	0.18000	4.82970	-4.74550
C	7.14490	1.92510	-0.80640	H	1.64100	3.99700	-6.48240
H	4.03190	4.11520	-1.63810	H	3.42180	2.25490	-5.93620
H	6.23210	5.05740	-1.77210	H	3.67550	1.43720	-3.68520
H	8.28090	3.63820	-1.23810	O	1.97120	-0.42500	-0.37850
H	8.01900	1.33360	-0.56340	P	0.76260	0.29390	0.52450
C	0.19730	4.12070	-2.05300	O	1.18340	1.87920	0.69710
C	2.16470	2.20140	-1.41520	O	0.74810	-0.31280	1.90680

N	-2.80320	-1.10320	-1.35330	C	6.39430	-3.34500	2.31020
C	-4.03560	-1.25720	-0.74100	C	7.60060	-3.87200	2.55430
C	-2.19480	-3.82600	0.36310	H	9.49100	-4.60140	1.63860
C	-1.01440	-3.19740	0.70790	H	8.80860	-4.15050	-0.64470
C	-2.07810	-2.15680	2.62180	H	6.51980	-3.15750	-1.12370
C	-3.29860	-2.70480	2.27110	H	5.73480	-3.12840	3.13970
C	0.29770	-3.35590	0.00920	H	7.90780	-4.07740	3.57170
H	0.99520	-2.58150	0.32060	C	2.39280	-5.27230	-2.57840
H	0.71580	-4.34170	0.22390	C	2.49130	-3.96930	-2.86340
C	-1.73740	-1.36140	3.85190	C	3.09550	-3.04030	-1.88580
H	-1.52400	-2.03910	4.68630	C	3.52380	-3.49410	-0.69400
H	-0.84830	-0.75590	3.65890	C	3.44940	-4.94680	-0.40310
H	-2.56630	-0.72510	4.15280	C	2.90470	-5.78650	-1.29250
C	-4.54890	-2.64870	3.05820	H	1.94850	-5.95290	-3.29300
C	-2.34000	-4.90790	-0.63200	H	2.12610	-3.59170	-3.80960
H	-0.26690	-6.89400	-2.12420	H	3.17910	-1.99760	-2.15440
H	-1.95930	-7.27750	-1.66290	H	3.84110	-5.33710	0.52760
H	-5.32730	-1.69740	6.05120	H	2.84570	-6.84500	-1.07500
H	-6.33390	-1.42680	4.59000	C	1.01400	3.27860	4.76210
O	-1.16940	-5.44760	-1.03740	C	-0.30310	3.24680	4.53390
O	-3.42360	-5.30740	-1.02590	C	-0.83820	3.65840	3.21960
O	-5.62380	-3.02150	2.61710	C	-0.01010	4.05970	2.24040
O	-4.40390	-2.17290	4.31540	C	1.45060	4.10850	2.51080
Si	4.29280	-2.35140	0.56040	C	1.93340	3.73140	3.70090
Si	-0.65970	4.52380	0.54720	H	1.40790	2.97160	5.72220
C	1.93260	-1.99380	4.59470	H	-0.98070	2.91490	5.30990
C	1.77330	-3.08250	3.83360	H	-1.90430	3.62980	3.07410
C	2.52160	-3.21730	2.56640	H	2.14350	4.40030	1.73500
C	3.34330	-2.23670	2.15770	H	3.00000	3.74610	3.88400
C	3.53560	-1.04410	3.02000	C	-5.24080	3.67230	-0.00740
C	2.86390	-0.92870	4.17240	C	-4.82660	4.49030	0.96630
H	1.38010	-1.89130	5.51970	C	-3.38350	4.73960	1.15930
H	1.09010	-3.86400	4.14010	C	-2.47770	4.14220	0.36520
H	2.38410	-4.11240	1.98100	C	-2.94430	3.21390	-0.69530
H	4.21540	-0.25680	2.71980	C	-4.25390	3.00230	-0.87620
H	2.99800	-0.05300	4.79430	H	-6.29750	3.48820	-0.15090
C	8.51650	-4.17620	1.43620	H	-5.54750	4.97620	1.61080
C	8.13990	-3.92730	0.17650	H	-3.07220	5.43240	1.93120
C	6.80860	-3.34800	-0.09730	H	-2.23570	2.69910	-1.32990
C	5.97360	-3.06190	0.91610	H	-4.59450	2.32980	-1.65070

C	0.13790	9.09480	-0.19130	H	0.49940	-1.43960	-4.45470
C	1.15800	8.26030	0.03390	C	-5.02480	1.38590	2.53590
C	0.90260	6.82370	0.26570	C	-3.69190	1.16280	2.19650
C	-0.35440	6.34640	0.27340	C	-3.35460	0.33880	1.12410
C	-1.47880	7.27640	-0.00610	C	-4.35950	-0.28790	0.36380
C	-1.24360	8.57700	-0.21990	C	-5.70310	-0.05330	0.71530
H	0.32320	10.14720	-0.36320	C	-6.03040	0.77910	1.78160
H	2.17360	8.63450	0.04430	H	-5.27730	2.03370	3.37020
H	1.74940	6.16940	0.40640	H	-2.89600	1.61370	2.77480
H	-2.49510	6.91790	-0.06350	H	-2.30330	0.21940	0.88170
H	-2.06510	9.25070	-0.42740	H	-6.49770	-0.52170	0.14980
N	-1.01660	-2.34490	1.77640	H	-7.07540	0.95330	2.01930
H	-0.20280	-1.68480	1.89200	O	-4.66870	0.11310	-3.24550
H	0.16500	-3.29190	-1.07060	H	-3.86700	0.16860	-2.70350
C	-5.61940	-2.09290	5.07860	C	-3.43220	-3.35140	0.96470
H	-6.07230	-3.08130	5.18510	H	-3.87460	-2.42960	0.13600
C	-1.27630	-6.49950	-2.00990	H	-4.27260	-4.03560	0.88160
H	-1.63860	-6.09940	-2.95960				
O	-0.48650	0.17110	-0.32270				
C	-7.44550	-2.22200	-3.21000				
C	-6.57320	-1.20860	-3.58840	C	-3.32790	1.51950	-0.96380
C	-5.45010	-0.90840	-2.80760	C	-5.01560	-0.56620	-1.81920
C	-5.19500	-1.64620	-1.62760	C	-4.09260	-0.79930	-0.87030
C	-6.10050	-2.65250	-1.25980	C	-3.08550	0.25580	-0.57120
C	-7.21470	-2.94860	-2.03910	H	-5.75630	-1.31610	-2.06710
H	-8.30890	-2.44400	-3.83040	C	-5.10500	0.75560	-2.47190
H	-6.73390	-0.62620	-4.48930	C	-4.32650	1.77110	-2.03950
H	-5.93300	-3.19970	-0.33960	C	-4.45020	3.10730	-2.67820
H	-7.89330	-3.73780	-1.73380	C	-5.34410	3.30680	-3.65390
H	-2.07540	-0.56550	-0.85740	C	-6.20860	2.19860	-4.10640
C	-1.03700	-2.92850	-4.74220	C	-6.09620	0.98800	-3.54750
C	-2.23860	-3.43590	-4.24780	H	-3.81470	3.92620	-2.36610
C	-2.85350	-2.87620	-3.12690	H	-5.43250	4.28060	-4.11790
C	-2.26100	-1.77570	-2.48950	H	-6.93230	2.36830	-4.89300
C	-1.04410	-1.26510	-2.98180	H	-6.73350	0.17980	-3.88400
C	-0.44250	-1.84360	-4.09530	C	-1.80730	4.99330	1.06110
H	-0.56890	-3.37430	-5.61450	C	-2.75960	2.63650	-0.17230
H	-2.71450	-4.28250	-4.73440	C	-1.41980	2.85150	-0.08180
H	-3.76430	-3.31710	-2.74970	C	-0.93300	4.13400	0.51720
H	-0.57060	-0.44060	-2.45970	H	-1.47840	5.93100	1.48600



C	-3.70470	3.54310	0.55290	C	-1.82680	-5.66050	-0.40440
C	-3.24110	4.67620	1.11840	C	-2.46450	-4.46450	0.18610
C	-4.16670	5.59560	1.82130	C	-3.30240	-3.71260	-0.54660
C	-5.46410	5.29200	1.92720	C	-3.53650	-4.06130	-1.96870
C	-5.97550	4.03290	1.35640	C	-2.95510	-5.14220	-2.50290
C	-5.14800	3.20110	0.71360	H	-1.60690	-6.86450	-2.11380
H	-3.79530	6.51590	2.25470	H	-1.16620	-6.27070	0.19820
H	-6.13930	5.96280	2.44270	H	-2.26420	-4.23360	1.21880
H	-7.02090	3.77700	1.47150	H	-4.19450	-3.45390	-2.57710
H	-5.54430	2.26840	0.33560	H	-3.13540	-5.40030	-3.53830
O	-1.97230	-0.02740	0.18060	C	-8.82300	-3.48500	0.21160
P	-0.57100	0.38460	-0.59990	C	-8.43870	-2.26030	0.58910
O	-0.48930	2.03670	-0.69050	C	-7.00580	-1.90090	0.58700
O	-0.64380	-0.07670	-2.05010	C	-6.08330	-2.79660	0.19610
N	2.60070	-1.89090	1.03270	C	-6.51420	-4.15770	-0.20790
C	3.94870	-1.84110	0.73580	C	-7.81360	-4.48060	-0.20230
C	2.63450	-3.39510	-1.95430	H	-9.87240	-3.75010	0.21260
C	1.45740	-2.72090	-2.21700	H	-9.17600	-1.52970	0.89590
C	2.67540	-0.74790	-2.91290	H	-6.71440	-0.90430	0.89640
C	3.88340	-1.36800	-2.64350	H	-5.78740	-4.90380	-0.49760
C	0.06590	-3.26720	-2.09610	H	-8.12750	-5.47430	-0.49470
H	-0.66530	-2.46600	-2.20490	C	-3.57310	-1.70990	4.80400
H	-0.11150	-4.03850	-2.84920	C	-3.53780	-0.65100	3.98780
C	2.45370	0.61260	-3.51880	C	-3.76160	-0.82470	2.53770
H	2.65900	0.58780	-4.59370	C	-3.94570	-2.05230	2.02000
H	1.41790	0.92250	-3.36360	C	-4.03700	-3.21340	2.94090
H	3.12740	1.34950	-3.08390	C	-3.85200	-3.05170	4.25670
C	5.22440	-0.85390	-2.99610	H	-3.41360	-1.58350	5.86700
C	2.75580	-4.82320	-1.60330	H	-3.35310	0.33750	4.38830
H	0.78990	-7.38810	-1.71160	H	-3.81170	0.06040	1.92470
H	2.57420	-7.40280	-1.90270	H	-4.26710	-4.19840	2.55490
H	6.31910	1.72330	-4.61950	H	-3.91530	-3.90220	4.92300
H	7.07650	1.03130	-3.14690	C	2.52290	4.56480	-3.91890
O	1.62580	-5.54530	-1.76830	C	3.33090	4.88680	-2.90330
O	3.79940	-5.32000	-1.20700	C	2.80530	4.92770	-1.52310
O	6.25640	-1.42230	-2.68330	C	1.52290	4.61140	-1.27230
O	5.21200	0.29060	-3.71850	C	0.61970	4.31380	-2.41350
Si	-4.28470	-2.32220	0.20290	C	1.09810	4.27850	-3.66320
Si	0.88200	4.59730	0.48390	H	2.90750	4.52810	-4.92990
C	-2.06740	-5.98730	-1.67960	H	4.37410	5.10800	-3.08810

H	3.48060	5.19450	-0.72360	H	5.73220	-3.18710	4.81220
H	-0.43510	4.14390	-2.25530	H	5.75910	-3.75960	-0.10370
H	0.43750	4.05760	-4.49160	H	7.34230	-5.05450	1.27080
C	3.33700	1.70610	3.24830	H	1.98870	-1.12530	0.70990
C	3.91790	2.79090	2.72580	C	0.24310	-4.81620	2.97200
C	3.14430	3.69730	1.85210	C	1.44150	-5.20290	2.37190
C	1.86000	3.42860	1.55880	C	2.24530	-4.27690	1.70550
C	1.21140	2.24640	2.17930	C	1.84480	-2.93400	1.64070
C	1.91580	1.42420	2.96710	C	0.62280	-2.54590	2.21990
H	3.90370	1.04200	3.88690	C	-0.15980	-3.48260	2.88640
H	4.95800	3.00410	2.93560	H	-0.37140	-5.54390	3.49290
H	3.63150	4.58190	1.46730	H	1.76620	-6.23840	2.42200
H	0.16400	2.04160	2.01480	H	3.16300	-4.60580	1.23870
H	1.44140	0.55890	3.41160	H	0.29330	-1.51720	2.12190
C	1.44330	8.83360	2.40460	H	-1.09160	-3.16100	3.33890
C	1.51960	8.69570	1.07560	C	5.64480	1.99180	-0.31090
C	1.34400	7.36490	0.45690	C	4.28050	1.76200	-0.47020
C	1.11260	6.28810	1.22660	C	3.70810	0.54600	-0.10470
C	1.02330	6.44830	2.69830	C	4.51070	-0.48520	0.41450
C	1.18130	7.65510	3.25530	C	5.89140	-0.24990	0.55880
H	1.57100	9.80780	2.85850	C	6.44800	0.97800	0.21500
H	1.70860	9.55850	0.45020	H	6.07450	2.95090	-0.58480
H	1.39440	7.28280	-0.62040	H	3.63480	2.53080	-0.86970
H	0.82700	5.58990	3.32850	H	2.63310	0.43520	-0.20580
H	1.11550	7.77060	4.32940	H	6.53200	-1.03220	0.94490
N	1.52230	-1.41860	-2.62050	H	7.51260	1.13840	0.35520
H	0.61890	-0.85830	-2.54300	O	4.03810	-1.73550	3.62870
H	-0.05020	-3.73220	-1.11820	H	3.36680	-1.38200	3.02680
C	6.50870	0.81140	-4.05330	C	3.88150	-2.63890	-1.91800
H	7.06820	0.09330	-4.65740	H	4.06290	-2.35530	-0.64350
C	1.72790	-6.93110	-1.39990	H	4.78600	-3.22710	-2.05290
H	1.85530	-7.02690	-0.31890				
O	0.55640	-0.11530	0.26380				
C	6.64950	-4.20690	3.13510	C	-3.04410	1.12190	-1.27630
C	5.75760	-3.32640	3.73670	C	-4.28580	-1.23810	-2.17700
C	4.85860	-2.58770	2.95900	C	-3.74010	-1.18940	-0.95050
C	4.85300	-2.73650	1.55260	C	-2.92260	-0.01020	-0.56420
C	5.76340	-3.62790	0.97070	H	-4.89690	-2.08250	-2.47390
C	6.65450	-4.36420	1.74740	C	-4.19050	-0.07450	-3.08300
H	7.33940	-4.77440	3.75280	C	-3.64000	1.07730	-2.63930

C	-3.59570	2.25880	-3.53920	C	6.54620	-1.81800	-1.89820
C	-4.11680	2.18700	-4.76970	C	2.96810	-4.99900	-1.11520
C	-4.73510	0.93190	-5.24200	H	0.69120	-7.24610	-1.50050
C	-4.77150	-0.14120	-4.44340	H	2.41230	-7.48780	-1.05370
H	-3.13660	3.18270	-3.21110	H	8.85450	-0.14110	-3.42470
H	-4.08290	3.04830	-5.42430	H	8.62390	-0.18770	-1.64540
H	-5.15880	0.88290	-6.23680	O	1.77850	-5.53410	-1.44540
H	-5.22830	-1.05770	-4.79550	O	3.80400	-5.59080	-0.45880
C	-2.11710	4.90680	0.52730	O	7.13210	-2.24540	-0.92030
C	-2.71910	2.40230	-0.61850	O	7.14680	-1.05740	-2.83860
C	-1.45020	2.67300	-0.23590	Si	-4.31310	-2.42910	0.31620
C	-1.12420	4.04320	0.26160	Si	0.64200	4.60870	0.45970
H	-1.91090	5.89170	0.92000	C	-2.23970	-6.56710	-0.44150
C	-3.82020	3.35600	-0.28930	C	-1.89320	-5.50350	-1.17540
C	-3.52090	4.54750	0.26810	C	-2.52820	-4.19260	-0.92960
C	-4.59990	5.50230	0.61360	C	-3.46560	-4.06350	0.02530
C	-5.87900	5.17760	0.39910	C	-3.84630	-5.24870	0.83450
C	-6.22040	3.86340	-0.17620	C	-3.26390	-6.43330	0.61290
C	-5.25220	2.99850	-0.49900	H	-1.77530	-7.52770	-0.62190
H	-4.35690	6.46640	1.04310	H	-1.15370	-5.60250	-1.95740
H	-6.66690	5.87460	0.65370	H	-2.22320	-3.34990	-1.53520
H	-7.25860	3.59710	-0.32740	H	-4.59950	-5.16080	1.60750
H	-5.53210	2.03220	-0.89620	H	-3.54300	-7.29540	1.20460
O	-2.15520	-0.02610	0.57630	C	-8.94910	-2.76770	-0.36480
P	-0.54380	0.27780	0.29470	C	-8.18770	-3.86390	-0.44860
O	-0.43830	1.76660	-0.46900	C	-6.72770	-3.77110	-0.23850
O	-0.04440	-0.72080	-0.75080	C	-6.15700	-2.59060	0.06150
N	2.08730	-1.98550	0.59420	C	-7.00720	-1.37500	0.12240
C	3.37260	-1.46930	0.69180	C	-8.32820	-1.46100	-0.07470
C	3.23320	-3.64240	-1.67570	H	-10.01810	-2.83410	-0.52060
C	2.44740	-2.95070	-2.58110	H	-8.63870	-4.82190	-0.67250
C	4.35070	-1.50830	-3.14530	H	-6.14170	-4.67020	-0.34650
C	5.11490	-2.10210	-2.16490	H	-6.56640	-0.40450	0.29380
C	0.99740	-3.14060	-2.91280	H	-8.94220	-0.57040	-0.03710
H	0.80950	-2.93600	-3.97240	C	-3.56730	-0.73210	4.63650
H	0.66700	-4.14540	-2.67490	C	-3.19260	-1.98100	4.34000
C	4.78480	-0.48100	-4.15200	C	-3.43300	-2.52620	2.98790
H	5.50630	-0.91030	-4.85210	C	-4.02500	-1.77490	2.04460
H	3.92700	-0.10920	-4.71940	C	-4.44320	-0.39020	2.38660
H	5.26760	0.36090	-3.65710	C	-4.22130	0.10270	3.61080

H	-3.38960	-0.33070	5.62570	H	0.41540	-2.42500	-2.31130
H	-2.71140	-2.59590	5.08950	C	8.52860	-0.74610	-2.57910
H	-3.13130	-3.53900	2.78830	H	9.12010	-1.66120	-2.50750
H	-4.88950	0.24960	1.63940	C	1.53100	-6.85810	-0.92570
H	-4.51040	1.11850	3.84800	H	1.27580	-6.79100	0.13370
C	2.73410	4.90630	-3.72040	O	0.14450	0.31130	1.62510
C	3.37990	5.29610	-2.61570	C	5.22120	-1.72420	4.59520
C	2.73400	5.16210	-1.29350	C	3.91440	-1.27950	4.47190
C	1.50020	4.63930	-1.19100	C	3.27550	-1.18460	3.21870
C	0.78000	4.23190	-2.42400	C	4.00810	-1.57240	2.06490
C	1.36840	4.35510	-3.62020	C	5.33130	-2.02000	2.21510
H	3.20720	5.00130	-4.68920	C	5.94660	-2.09730	3.45910
H	4.37810	5.70800	-2.68700	H	5.67650	-1.78180	5.57990
H	3.26160	5.51590	-0.41640	H	3.33330	-0.98350	5.33900
H	-0.22790	3.84630	-2.37500	H	5.88510	-2.32250	1.33020
H	0.84140	4.05800	-4.51770	H	6.96920	-2.45110	3.54060
C	2.74350	2.14640	3.82600	H	1.35880	-1.48400	0.05180
C	3.38970	2.36760	2.67570	C	0.54250	-5.38680	2.57550
C	2.71910	3.09420	1.57770	C	1.91910	-5.17270	2.55010
C	1.45690	3.52520	1.72650	C	2.45490	-4.06360	1.89980
C	0.73170	3.23880	2.98750	C	1.61070	-3.12840	1.27380
C	1.34370	2.58740	3.98330	C	0.22130	-3.35540	1.28190
H	3.24050	1.63400	4.63890	C	-0.29190	-4.47470	1.92720
H	4.41340	2.03760	2.55760	H	0.12340	-6.24660	3.08960
H	3.28110	3.31530	0.68490	H	2.59450	-5.87420	3.03070
H	-0.29160	3.56960	3.11460	H	3.52680	-3.94350	1.88050
H	0.81640	2.38600	4.90660	H	-0.43630	-2.65430	0.78060
C	0.84420	9.05940	1.92040	H	-1.35920	-4.64180	1.93170
C	0.34000	8.76810	0.71590	C	4.47970	2.09000	-1.53440
C	0.27440	7.36400	0.26100	C	5.34280	1.52490	-0.59670
C	0.70900	6.37190	1.05730	C	4.94460	0.41370	0.14400
C	1.27780	6.70300	2.38740	C	3.67540	-0.16740	-0.03690
C	1.33830	7.97700	2.79500	C	2.80900	0.42280	-0.96880
H	0.89390	10.08750	2.25500	C	3.20810	1.54100	-1.70020
H	-0.02000	9.55960	0.07150	H	4.79390	2.95190	-2.11400
H	-0.13150	7.14930	-0.72010	H	6.32680	1.95310	-0.42870
H	1.65150	5.92460	3.03770	H	5.62760	-0.00090	0.87370
H	1.75300	8.21750	3.76540	H	1.80930	0.03430	-1.13070
N	3.03880	-1.90460	-3.24670	H	2.50660	1.97870	-2.40170
H	2.44500	-1.37300	-3.86920	O	2.00420	-0.75970	3.27360

H	1.53510	-0.47310	2.45210	H	4.09650	-2.26660	-0.08920
C	4.49160	-3.05450	-1.26620	H	5.16430	-3.71040	-0.72320

**OOH-Type II Z**

C	3.44520	1.40210	0.98420	C	-3.22440	-1.10550	0.94400
C	3.92940	3.99180	-0.06040	C	-5.90250	0.91640	0.54360
C	2.67730	3.51970	-0.01900	C	-5.53690	1.99130	-0.23820
C	2.40830	2.15060	0.50950	C	-5.22800	0.51510	-2.17110
H	4.14100	4.97110	-0.46450	C	-5.62370	-0.56990	-1.41930
C	5.06040	3.16790	0.39020	C	-5.52480	3.44470	0.14370
C	4.84750	1.91900	0.85810	H	-5.15910	4.06030	-0.68360
C	6.03130	1.06860	1.18210	H	-6.52590	3.78340	0.41750
C	7.27160	1.55670	1.06890	C	-4.88380	0.53940	-3.63340
C	7.48470	2.93900	0.60570	H	-4.00090	-0.07980	-3.81820
C	6.43830	3.70150	0.27590	H	-5.69500	0.12540	-4.23220
H	5.91380	0.03880	1.48780	H	-4.68020	1.55820	-3.97410
H	8.12420	0.93190	1.30220	C	-6.00970	-1.90210	-1.96600
H	8.49070	3.32880	0.51940	C	-6.41910	0.99670	1.93500
H	6.60340	4.71140	-0.07870	H	-7.03820	3.41540	3.99040
C	3.40420	-2.71990	2.14870	H	-7.95840	1.87640	3.89050
C	3.24380	0.02560	1.50220	H	-5.60260	-4.09540	-3.45370
C	2.75200	-0.90330	0.66310	H	-7.26930	-3.48440	-3.63850
C	3.01160	-2.33900	0.92360	O	-6.52770	2.25320	2.41320
H	3.60250	-3.76430	2.35960	O	-6.73180	0.01080	2.57510
C	3.68810	-0.38870	2.86280	O	-6.50640	-2.76970	-1.27540
C	3.71900	-1.70480	3.17890	O	-5.80920	-2.03020	-3.29100
C	4.13940	-2.13020	4.53340	Si	1.28310	4.54450	-0.72040
C	4.46840	-1.21520	5.45260	Si	3.05210	-3.57860	-0.46840
C	4.41280	0.22260	5.12090	C	-0.83260	1.77850	-3.85040
C	4.04050	0.61730	3.89750	C	-1.57040	2.45160	-2.95990
H	4.18300	-3.18280	4.78390	C	-0.92030	3.32530	-1.96180
H	4.77490	-1.52650	6.44280	C	0.41520	3.46440	-1.95810
H	4.67000	0.95720	5.87290	C	1.22960	2.71790	-2.94890
H	3.99390	1.67520	3.67340	C	0.63750	1.91540	-3.84180
O	1.08880	1.76010	0.61270	H	-1.31040	1.13010	-4.57350
P	0.60270	0.24870	0.13010	H	-2.64370	2.35150	-2.96070
O	1.97320	-0.51900	-0.39830	H	-1.54110	3.83710	-1.24160
O	-0.33030	0.37000	-1.05040	H	2.30840	2.81290	-2.94870
N	-2.51590	-1.21790	-0.25160	H	1.23380	1.36570	-4.55850

C	2.83630	8.43170	-2.82520	H	4.07790	-0.27300	-4.08010
C	2.95050	8.29350	-1.49920	H	4.36820	-1.37500	-1.81270
C	2.46290	7.06530	-0.83840	H	1.21540	-4.16080	-2.85120
C	1.91420	6.07690	-1.56520	H	1.02430	-3.15610	-5.03780
C	1.77900	6.24150	-3.03350	C	-0.17790	-6.81370	0.53650
C	2.21940	7.35710	-3.62870	C	-0.55240	-5.59130	0.14470
H	3.19230	9.33100	-3.31090	C	0.46620	-4.57290	-0.18750
H	3.39920	9.08080	-0.90750	C	1.77190	-4.87280	-0.10380
H	2.55750	6.97530	0.23700	C	2.18180	-6.22730	0.34230
H	1.32300	5.46810	-3.63570	C	1.25610	-7.14680	0.64140
H	2.12120	7.47610	-4.70000	H	-0.92390	-7.55690	0.78650
C	-1.49630	6.17380	2.67410	H	-1.60220	-5.34480	0.08560
C	-0.46380	5.38180	2.98710	H	0.14480	-3.58600	-0.49590
C	0.40540	4.84070	1.92170	H	3.22810	-6.47950	0.44780
C	0.15990	5.13810	0.63420	H	1.55630	-8.13280	0.97170
C	-0.97390	6.03160	0.29530	N	-5.15310	1.73190	-1.53190
C	-1.76260	6.51580	1.26240	H	-4.86230	2.52450	-2.08680
H	-2.13640	6.56610	3.45350	H	-4.87850	3.60090	1.00900
H	-0.26590	5.13120	4.02120	C	-6.21740	-3.29090	-3.85850
H	1.24200	4.21660	2.20410	H	-6.05670	-3.18960	-4.93130
H	-1.16720	6.29820	-0.73630	C	-6.98040	2.34850	3.77740
H	-2.59250	7.16420	1.01310	H	-6.26640	1.86070	4.44380
C	7.31250	-5.49120	-0.85880	O	0.06670	-0.41770	1.38080
C	6.29180	-5.96100	-1.58510	C	-3.48440	-4.67380	3.39580
C	4.95040	-5.35560	-1.45520	C	-2.25160	-4.22230	2.95310
C	4.74220	-4.34710	-0.59170	C	-2.11960	-3.04750	2.18110
C	5.88490	-3.81270	0.19090	C	-3.30630	-2.35010	1.81750
C	7.10040	-4.35990	0.06630	C	-4.53770	-2.80490	2.31640
H	8.29630	-5.93230	-0.95390	C	-4.64380	-3.95150	3.09570
H	6.44620	-6.78480	-2.26990	H	-3.54220	-5.58230	3.98930
H	4.13990	-5.74250	-2.06090	H	-1.33420	-4.74980	3.19370
H	5.75730	-2.96460	0.84860	H	-5.43620	-2.24010	2.09570
H	7.93400	-3.96610	0.63340	H	-5.61440	-4.27710	3.45550
C	2.55580	-1.59100	-4.68040	H	-1.79760	-0.50460	-0.47880
C	3.45740	-1.11870	-3.81320	C	-2.51450	-4.24120	-3.19570
C	3.61200	-1.75450	-2.48940	C	-1.76580	-3.07020	-3.33840
C	2.81390	-2.77490	-2.12810	C	-1.76050	-2.09820	-2.34570
C	1.82730	-3.30450	-3.09950	C	-2.54300	-2.26860	-1.18100
C	1.71760	-2.74980	-4.31400	C	-3.31630	-3.43560	-1.04720
H	2.44380	-1.13070	-5.65350	C	-3.28240	-4.41090	-2.04440

H	-2.49380	-5.00720	-3.96510	H	-2.57410	3.52220	3.68570
H	-1.17710	-2.91090	-4.23500	H	-2.07100	3.43320	1.24130
H	-1.14090	-1.21060	-2.43160	H	-2.32050	1.35610	-0.00370
H	-3.93010	-3.59630	-0.17360	H	-3.58520	-0.64560	3.59260
H	-3.86340	-5.31830	-1.90320	H	-3.31730	1.45420	4.84880
C	-2.69740	2.59840	3.12930	O	-0.87220	-2.72120	1.84760
C	-2.42290	2.55060	1.76180	H	-0.64830	-1.76690	1.58710
C	-2.58210	1.36560	1.04790	C	-5.77150	-0.42310	0.01140
C	-2.99210	0.18900	1.69630	H	-4.46700	-0.90820	0.57910
C	-3.26790	0.24930	3.07220	H	-6.35070	-1.19580	0.50370
C	-3.11930	1.44000	3.78080				

### Re-optimization with the delocalised bonding model

#### **TS6-E**

(B3LYP/6-31G\*\*:UFF) Energy = -1868.143404

(B3LYP/6-31G\*\*:UFF) Free Energy = -1866.967209

M06-2X/6-31G\*\* Derived free energy = -4601.512062

M06-2X/6-31G\*\* Derived free energy in solution = -4601.528501

Number of Imaginary Frequencies = 1 (-770.87)

#### ONIOM (B3LYP/6-31G\*\*:UFF) Geometry

O		2.17720	0.23500		-0.78660		
P	0.67380	0.11320	-0.14120	H	-4.40700	-4.15070	-4.49610
O	0.32010	1.58300	0.54990	C	-6.65000	-2.40260	-0.45740
O	-0.22800	-0.16650	-1.32000	H	-7.28770	-1.99570	-1.24940
O	0.66910	-0.85240	1.02710	H	-6.61500	-3.48980	-0.54030
H	-4.28750	-0.05730	-0.19520	H	-7.08970	-2.14970	0.51030
C	-5.25630	-1.79840	-0.54720	H	-5.70160	-0.29100	0.73930
C	-2.74120	-2.92020	-3.86810	N	-5.20920	-0.47540	-0.12580
C	-2.26650	-2.01880	-2.92510	C	-2.99210	-3.93010	0.74430
C	-3.08400	-1.62100	-1.84980	C	-1.70450	-3.42510	0.73670
C	-4.39610	-2.15150	-1.71780	N	-1.43180	-2.32680	1.49640
C	-4.83260	-3.07620	-2.68390	H	-0.50790	-1.81690	1.33800
C	-4.03060	-3.45280	-3.75500	C	-2.30480	-1.72770	2.35700
H	-2.10150	-3.20820	-4.69790	C	-1.67320	-0.63970	3.17800
H	-1.27020	-1.59510	-2.99450	H	-0.76340	-1.02170	3.65000
H	-5.82680	-3.49890	-2.59920	H	-1.35160	0.17670	2.52350

H	-2.34550	-0.27320	3.94440	C	5.70610	1.32660	3.38330
C	-0.52380	-3.95400	-0.02500	H	3.26800	4.10710	2.20460
H	-0.28930	-4.97460	0.28410	H	4.75380	4.50700	4.10720
H	-0.74140	-3.98380	-1.09480	H	6.31420	2.74940	4.87770
H	0.33530	-3.30750	0.15060	H	6.38990	0.56630	3.74200
C	-3.62010	-2.15550	2.36920	C	2.91290	4.00610	-0.55120
C	-3.46520	-5.12370	0.01340	C	2.08340	5.02750	-1.07380
C	-4.70970	-1.61320	3.21180	C	2.65500	6.16930	-1.65910
H	-3.50140	-7.66950	-0.71990	C	4.04120	6.29610	-1.74810
H	-3.57980	-6.63240	-2.16330	C	4.86770	5.28410	-1.26300
C	-2.94040	-6.97130	-1.34510	C	4.31400	4.14520	-0.67450
H	-2.03730	-7.44180	-1.73320	H	2.02920	6.96120	-2.05370
C	-5.37580	-0.58320	5.22760	H	4.47550	7.17690	-2.20320
H	-5.93600	0.19330	4.70270	H	5.94260	5.37990	-1.34700
H	-6.06350	-1.38240	5.51290	H	4.99180	3.37490	-0.33290
H	-4.87890	-0.17250	6.10570	Si	-1.76930	3.65710	-0.43740
O	-4.64400	-5.43440	-0.05400	Si	4.13960	-2.13530	-0.22640
O	-5.88510	-1.65340	2.87640	C	-3.23280	1.07760	-4.05490
O	-4.31980	-1.10320	4.39930	C	-4.16300	1.63800	-3.17720
O	-2.48620	-5.84820	-0.57090	C	-3.72920	2.41130	-2.09650
O	-2.64100	-0.74440	-0.93150	C	-2.35700	2.60310	-1.86450
H	-1.66360	-0.46990	-1.10390	C	-1.43150	2.06690	-2.77440
C	-4.03490	-3.17040	1.40950	C	-1.86820	1.30000	-3.85870
H	-4.64680	-2.50430	0.39290	H	-3.56920	0.47830	-4.89080
H	-4.93280	-3.73040	1.66180	H	-5.22160	1.48490	-3.34220
C	3.12330	0.52660	0.15840	H	-4.46900	2.88830	-1.46970
C	3.15350	1.81900	0.70830	H	-0.37010	2.23340	-2.65150
C	4.90270	-0.17090	1.64700	H	-1.14740	0.87480	-4.54500
C	4.04250	-0.45130	0.57930	C	-3.44610	7.99360	-0.86050
H	5.59160	-0.93310	1.99370	C	-3.63880	7.07400	-1.89450
C	2.31850	2.86880	0.05630	C	-3.14350	5.77170	-1.77670
C	0.91120	2.69990	0.00240	C	-2.45680	5.37900	-0.61640
C	0.10030	3.75310	-0.47350	C	-2.25590	6.31250	0.41250
C	0.69400	4.90000	-1.01150	C	-2.75250	7.61360	0.29100
H	0.07430	5.69300	-1.41140	H	-3.82870	9.00170	-0.95430
C	4.86610	1.07470	2.28690	H	-4.16760	7.37200	-2.79060
C	3.98440	2.08460	1.82420	H	-3.28630	5.08570	-2.59940
C	3.94880	3.32080	2.50310	H	-1.71200	6.03900	1.30690
C	4.78780	3.55410	3.59500	H	-2.59670	8.32840	1.08870
C	5.66640	2.56230	4.03100	C	-3.19830	2.37120	3.82180



C	-3.97700	2.05500	2.70680	C	3.21810	-1.03260	-4.12590
C	-3.53880	2.39870	1.42540	C	3.83530	-1.14270	-2.87620
C	-2.31200	3.05480	1.24510	C	3.37250	-2.07570	-1.93320
C	-1.53240	3.36390	2.37270	C	2.28370	-2.89750	-2.26860
C	-1.97220	3.01810	3.65390	C	1.66620	-2.78300	-3.51730
H	-3.54100	2.10730	4.81380	H	1.64990	-1.75870	-5.41000
H	-4.92660	1.55290	2.83410	H	3.57330	-0.30250	-4.84160
H	-4.17510	2.16850	0.59100	H	4.64470	-0.46960	-2.63750
H	-0.59270	3.89060	2.26740	H	1.89530	-3.61970	-1.57160
H	-1.36690	3.26140	4.51740	H	0.82090	-3.41340	-3.76210
C	1.90310	-5.24370	2.45510	C	8.69240	-3.13190	-0.59180
C	1.98760	-3.90890	2.85770	C	7.83080	-4.04520	0.01960
C	2.67120	-2.98010	2.06760	C	6.46700	-3.75730	0.13160
C	3.26430	-3.37840	0.85830	C	5.95120	-2.55570	-0.38200
C	3.18060	-4.72380	0.46500	C	6.82960	-1.63360	-0.97400
C	2.50300	-5.65170	1.26130	C	8.19260	-1.92420	-1.08320
H	1.37210	-5.96110	3.06710	H	9.74820	-3.35490	-0.67450
H	1.52200	-3.59270	3.78220	H	8.22090	-4.97500	0.41320
H	2.72480	-1.95390	2.40290	H	5.82990	-4.47290	0.62770
H	3.63300	-5.05360	-0.46200	H	6.47230	-0.67720	-1.32750
H	2.43680	-6.68570	0.94890	H	8.86290	-1.20820	-1.54090
C	2.13250	-1.85060	-4.44560				

### TS7-E

(B3LYP/6-31G\*\*):UFF) Energy = -1868.132024

(B3LYP/6-31G\*\*):UFF) Free Energy = -1866.955790

M06-2X/6-31G\*\* Derived free energy = -4601.506584

M06-2X/6-31G\*\* Derived free energy in solution = -4601.524033

Number of Imaginary Frequencies = 1 (-789.69)

### ONIOM (B3LYP/6-31G\*\*):UFF) Geometry

O	1.95960	-0.07100	-0.61290	O	-0.44830	0.14520	-1.30980
P	0.41940	0.18710	-0.07480	O	0.10160	-0.76810	1.05880
O	0.35300	1.69900	0.61260	H	-4.01050	-1.38460	-2.43260

C	-5.43950	-1.79160	-1.03930	H	-5.19210	-3.15950	5.66500
C	-4.11590	1.16680	1.79870	O	-4.47780	-5.00060	-2.35480
C	-3.26500	0.79070	0.76660	O	-6.06750	-3.80480	2.13540
C	-3.68830	-0.13130	-0.20530	O	-4.57720	-3.26500	3.74070
C	-4.99690	-0.69130	-0.12600	O	-2.25800	-5.07640	-2.75280
C	-5.82720	-0.28060	0.93170	O	-2.87450	-0.52230	-1.20170
C	-5.40750	0.64330	1.88320	H	-1.91430	-0.15060	-1.17920
H	-3.76200	1.86510	2.54820	C	-4.13340	-3.82070	0.14220
H	-2.26780	1.21070	0.69750	H	-4.85520	-2.80450	-0.41340
H	-6.82530	-0.69520	1.01060	H	-4.94290	-4.54220	0.05820
H	-6.07680	0.94580	2.68200	C	2.88990	0.00540	0.39330
C	-6.88560	-2.26830	-0.97140	C	3.13290	1.24560	1.00480
H	-7.56100	-1.46880	-1.29430	C	4.45350	-1.05720	1.91260
H	-7.01450	-3.12070	-1.64420	C	3.63750	-1.12480	0.77670
H	-7.15490	-2.59570	0.03310	H	4.99770	-1.93660	2.23710
H	-5.15200	-2.58420	-2.89160	C	2.63260	2.46530	0.31570
N	-4.94550	-1.76600	-2.33400	C	1.23780	2.65210	0.15900
C	-3.01980	-3.99310	-0.77480	C	0.75270	3.89460	-0.31120
C	-1.82920	-3.34510	-0.49440	C	1.65580	4.85770	-0.77910
N	-1.70280	-2.69230	0.69690	H	1.29290	5.78990	-1.19030
H	-0.89110	-2.02110	0.81500	C	4.57500	0.13640	2.63490
C	-2.62190	-2.72050	1.70970	C	3.92130	1.30760	2.17860
C	-2.18390	-2.03850	2.97660	C	4.07190	2.50320	2.91150
H	-2.96830	-1.37510	3.34250	C	4.86430	2.53350	4.06130
H	-1.99990	-2.78010	3.75940	C	5.51360	1.37840	4.49800
H	-1.27490	-1.46340	2.79590	C	5.37180	0.18380	3.78990
C	-0.63100	-3.25500	-1.39060	H	3.57040	3.41370	2.60970
H	-0.28910	-4.25470	-1.65880	H	4.97330	3.45590	4.61700
H	-0.88100	-2.73060	-2.31540	H	6.12770	1.40860	5.38880
H	0.16870	-2.70410	-0.90000	H	5.88530	-0.70230	4.14390
C	-3.82860	-3.35790	1.48230	C	3.53700	3.42120	-0.21600
C	-3.33490	-4.72450	-2.01600	C	3.03200	4.62570	-0.75810
C	-4.93210	-3.49290	2.45750	C	3.91290	5.59060	-1.27470
H	-3.07720	-6.70310	-3.77620	C	5.28850	5.36000	-1.27480
H	-3.16310	-5.15030	-4.63560	C	5.79620	4.16530	-0.76740
C	-2.54780	-5.76940	-3.97830	C	4.93280	3.19950	-0.24620
H	-1.57910	-5.96740	-4.43620	H	3.53690	6.52100	-1.68390
C	-5.64500	-3.37330	4.69730	H	5.96190	6.10550	-1.67750
H	-6.43500	-2.65250	4.47410	H	6.86320	3.98370	-0.78230
H	-6.07130	-4.37900	4.68490	H	5.36810	2.27710	0.11330

Si	-1.07840	4.29740	-0.37880	H	-4.77170	5.10390	2.87170
Si	3.63890	-2.69920	-0.22740	C	0.47670	-5.66270	1.52120
C	-3.09160	1.66420	-3.66690	C	0.67470	-4.41730	2.12110
C	-1.71800	1.91360	-3.70560	C	1.62090	-3.52990	1.60010
C	-1.11740	2.68520	-2.70610	C	2.37640	-3.88270	0.47060
C	-1.88480	3.19540	-1.64670	C	2.19770	-5.15180	-0.10340
C	-3.26860	2.96130	-1.62950	C	1.24310	-6.03260	0.41370
C	-3.86720	2.19350	-2.63320	H	-0.26210	-6.34480	1.92130
H	-3.55540	1.06390	-4.43880	H	0.09220	-4.13770	2.98870
H	-1.11810	1.51160	-4.51170	H	1.75990	-2.57390	2.08500
H	-0.05450	2.88120	-2.76400	H	2.80170	-5.46500	-0.94530
H	-3.89040	3.35840	-0.84300	H	1.10180	-7.00440	-0.04110
H	-4.93220	2.00250	-2.60460	C	2.86470	-1.54310	-4.69610
C	-1.66390	8.74200	-1.67180	C	3.74240	-0.79110	-3.91290
C	-2.08090	7.71440	-2.52210	C	3.98000	-1.15260	-2.58390
C	-1.90840	6.37870	-2.14590	C	3.33690	-2.26960	-2.02290
C	-1.31380	6.06470	-0.91350	C	2.46200	-3.02210	-2.82170
C	-0.90010	7.10160	-0.06290	C	2.22580	-2.65830	-4.15060
C	-1.07390	8.43560	-0.44280	H	2.67870	-1.26110	-5.72430
H	-1.79820	9.77520	-1.96500	H	4.23290	0.07750	-4.33280
H	-2.53790	7.95300	-3.47370	H	4.64020	-0.53720	-1.98770
H	-2.23630	5.59990	-2.82070	H	1.95830	-3.88920	-2.43220
H	-0.44090	6.87800	0.89220	H	1.54550	-3.24190	-4.75750
H	-0.75140	9.23170	0.21570	C	7.92960	-4.51800	0.12570
C	-3.04310	4.28900	3.86120	C	6.83090	-5.23540	0.60390
C	-1.73330	3.82980	3.70560	C	5.54350	-4.69990	0.49910
C	-1.14360	3.80640	2.43810	C	5.34480	-3.44290	-0.09630
C	-1.87130	4.21740	1.30880	C	6.45730	-2.72170	-0.55840
C	-3.17880	4.70170	1.47960	C	7.74290	-3.26010	-0.45160
C	-3.76330	4.73050	2.74910	H	8.92570	-4.93290	0.20970
H	-3.49570	4.31260	4.84400	H	6.97720	-6.20500	1.06210
H	-1.16840	3.50620	4.57020	H	4.71510	-5.26650	0.89790
H	-0.11380	3.49510	2.35740	H	6.33920	-1.73880	-0.99010
H	-3.73760	5.09180	0.63930	H	8.59550	-2.69910	-0.81190

### 1,3-diene-1,4-diol-phosphoric acid

(B3LYP/6-31G\*\*) Energy = -797.723048

(B3LYP/6-31G\*\*) Free Energy = -797.661026

M06-2X/6-31G\*\* Derived free energy = -797.452409

Number of Imaginary Frequencies = 0

#### B3LYP/6-31G\*\* Geometry

O	0.10530	-1.05800	-0.77540	H	-3.16460	1.11700	0.03310
P	0.96810	-0.02720	0.13420	C	-1.17800	1.58040	-0.04460
O	0.18500	1.38650	-0.02250	H	-1.38620	2.64090	-0.11960
O	1.28130	-0.45940	1.50860	C	-1.08040	-1.55660	-0.23850
C	-2.11090	-0.77530	0.10240	H	-1.08460	-2.63690	-0.15800
H	-3.00210	-1.28400	0.45790	O	2.21800	0.25870	-0.82440
C	-2.17060	0.67940	0.02600	H	3.03710	-0.01900	-0.38930

### 2-(1-iminoethyl)phenol

(B3LYP/6-31G\*\*) Energy = -440.266553

(B3LYP/6-31G\*\*) Free Energy = -440.144013

M06-2X/6-31G\*\* Derived free energy = -439.947721

Number of Imaginary Frequencies = 0

#### B3LYP/6-31G\*\* Geometry

C	1.66920	-0.12960	0.00000	O	-0.04250	2.20220	-0.00000
C	-2.61220	-0.35220	-0.00000	H	0.95590	2.07040	-0.00000
C	-1.85560	-1.53320	0.00000	N	2.22130	1.03970	0.00000
C	-0.47170	-1.45050	0.00000	H	3.23970	0.99800	0.00000
C	0.19970	-0.21040	0.00000	C	2.48230	-1.40630	0.00000
C	-0.58590	0.98110	-0.00000	H	2.25950	-2.01490	-0.88220
C	-1.98940	0.88580	-0.00000	H	3.55080	-1.17770	0.00000
H	-3.69750	-0.40430	-0.00000	H	2.25950	-2.01490	0.88230
H	-2.34560	-2.50130	0.00000				
H	0.10830	-2.36750	0.00000				
H	-2.55790	1.80960	-0.00000				

**dimethyl 2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate**

(B3LYP/6-31G\*\*) Energy = -783.887286

(B3LYP/6-31G\*\*) Free Energy = -783.681520

M06-2X/6-31G\*\* Derived free energy = -783.350852

Number of Imaginary Frequencies = 0

**B3LYP/6-31G\*\* Geometry**

C	-1.26780	0.22790	0.00010	H	4.21470	-2.34700	0.88700
C	-1.22730	1.58800	0.00010	O	-2.40130	-1.81190	0.00010
C	1.22730	1.58800	0.00010	O	-3.67520	0.05450	-0.00030
C	1.26770	0.22790	0.00010	O	3.67520	0.05450	-0.00030
C	-2.41310	2.51770	-0.00000	O	2.40130	-1.81190	0.00010
H	-2.08670	3.56310	0.00030	N	0.00000	2.23110	0.00010
H	-3.04690	2.34290	-0.87150	H	0.00000	3.23850	0.00010
C	2.41310	2.51770	0.00000	H	-3.04740	2.34240	0.87090
H	3.04690	2.34290	-0.87140	C	3.61610	-2.57060	-0.00000
H	2.08680	3.56300	0.00050	H	3.31000	-3.61700	0.00020
H	3.04750	2.34230	0.87090	C	-3.61610	-2.57060	-0.00000
C	2.56470	-0.45890	-0.00010	H	-4.21460	-2.34710	0.88710
C	-2.56470	-0.45890	-0.00010	C	-0.00000	-0.61360	0.00020
H	-4.21450	-2.34710	-0.88720	H	-0.00000	-1.28950	-0.86470
H	-3.31000	-3.61700	0.00000	H	-0.00000	-1.28920	0.86540
H	4.21440	-2.34720	-0.88730				

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