

Supplementary material

Kinetics and mechanism for OH-initiated gas-phase chemistry of α -terpineol

Yan Zhao^a, Haitao Sun^b, Mei Qin^b, Renjun Wang^a, Laixiang Xu^{*,a}

Keywords: α -Terpineol; OH radicals; Reaction mechanism; Oxidation products;
Kinetic parameters

^a School of Life Sciences, Qufu Normal University, Qufu, 273165, P. R. China

^b School of Chemistry and Chemical Engineering, Qufu Normal University,
Qufu, 273165, P. R. China

*Corresponding author. E-mail: xlx150723@163.com

Fax: 86-537-4456887

Computational methods

The reliability of tunneling corrections in RRKM method

Scheme S The structure of α -terpineol.

Fig. S1 The primary reaction pathways of α -terpineol with OH radical embedded with the potential barriers ΔE (kcal mol⁻¹) and reaction heats ΔH (kcal mol⁻¹) at the BB1K/6-31+G(d,p)// BB1K/6-311+G(3df,2p) level.

Fig. S2 MPWB1K/6-31+G(d,p) optimized geometries with the bond lengths (Å) for the transition states involved in the reaction of OH with α -terpineol.

Fig. S3 MPWB1K/6-31+G(d,p) optimized geometries with the bond lengths (Å) for the intermediate states and products involved in the reaction of OH with α -terpineol.

Fig. S4 Potential energy surfaces of self-decomposition of IM2.

Table S1 The rate constants (k) at 298 K after considering the errors

Table S2 The rate constants (cm³ molecule⁻¹ s⁻¹) of the title reactions for the gas-phase oxidation of α -terpineol with OH radicals at 298 K and 1 atm

Table S3 Arrhenius formulas of rate constants (cm³ molecule⁻¹ s⁻¹) for the H-abstraction reactions at 180-380 K

Table S4 Cartesian coordinates for the optimized stationary points

Computational methods

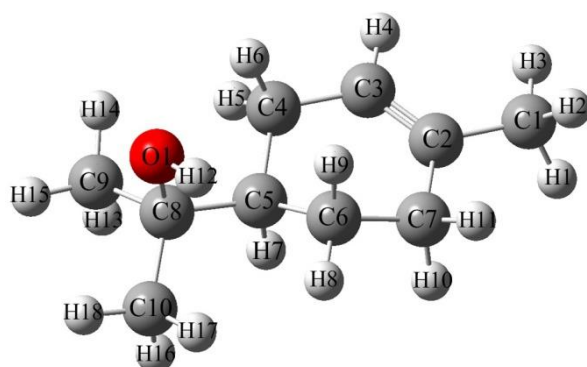
It is generally recognized that MPWB1K and BB1K methods give good results for barrier height calculations thermochemistry and thermochemical kinetics.^{1,2} In addition, these energy barriers involved in the title reactions are calculated to be about 1-5 kcal/mol at the MPWB1K/6-31+G(d,p) level. Therefore, the geometric parameters of the stationary points are optimized at the BB1K/6-31+G(d,p) level. The potential barriers ΔE (kcal mol⁻¹) and reaction heats ΔH (kcal mol⁻¹) are presented in **Fig. S1**. In addition, the rate constants of the initial steps are calculated at 298 K and 1 atm and are listed in **Table S2**. The computational results indicate that the total rate constant based on the MPWB1K method matches well with the experimental value whereas that based on the BB1K method are nearly over 1 order of magnitude lower than that

of the literature. Obviously, the MPWB1K method is suitable for thermochemistry and thermochemical kinetics of this work.

- 1 Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A*, 2004, **108**, 6908-6918.
- 2 Y. Zhao, B. J. Lynch and D. G. Truhlar, *J. Phys. Chem. A*, 2004, **108**, 2715-2719.

The reliability of the tunneling corrections in RRKM method

The CVT with SCT correction is a reliable method to calculate the rate constants including tunneling effect. In order to verify the reliability of the tunneling corrections in the RRKM method, the rate constants of the initial H-abstraction steps are also calculated employing the CVT/SCT method over a suitable range of 180-380 K. The computed data are fitted in the Arrhenius formula $k=A \exp(-E_a/RT)$. **Table S3** lists the reaction rates at 298 K and the corresponding Arrhenius equation. Comparison shows that the rates in **Table 1** and **Table S3** have the good consistence. Therefore, the RRKM method for tunneling correction in this work is effective.



Scheme S The structure of α -terpineol.

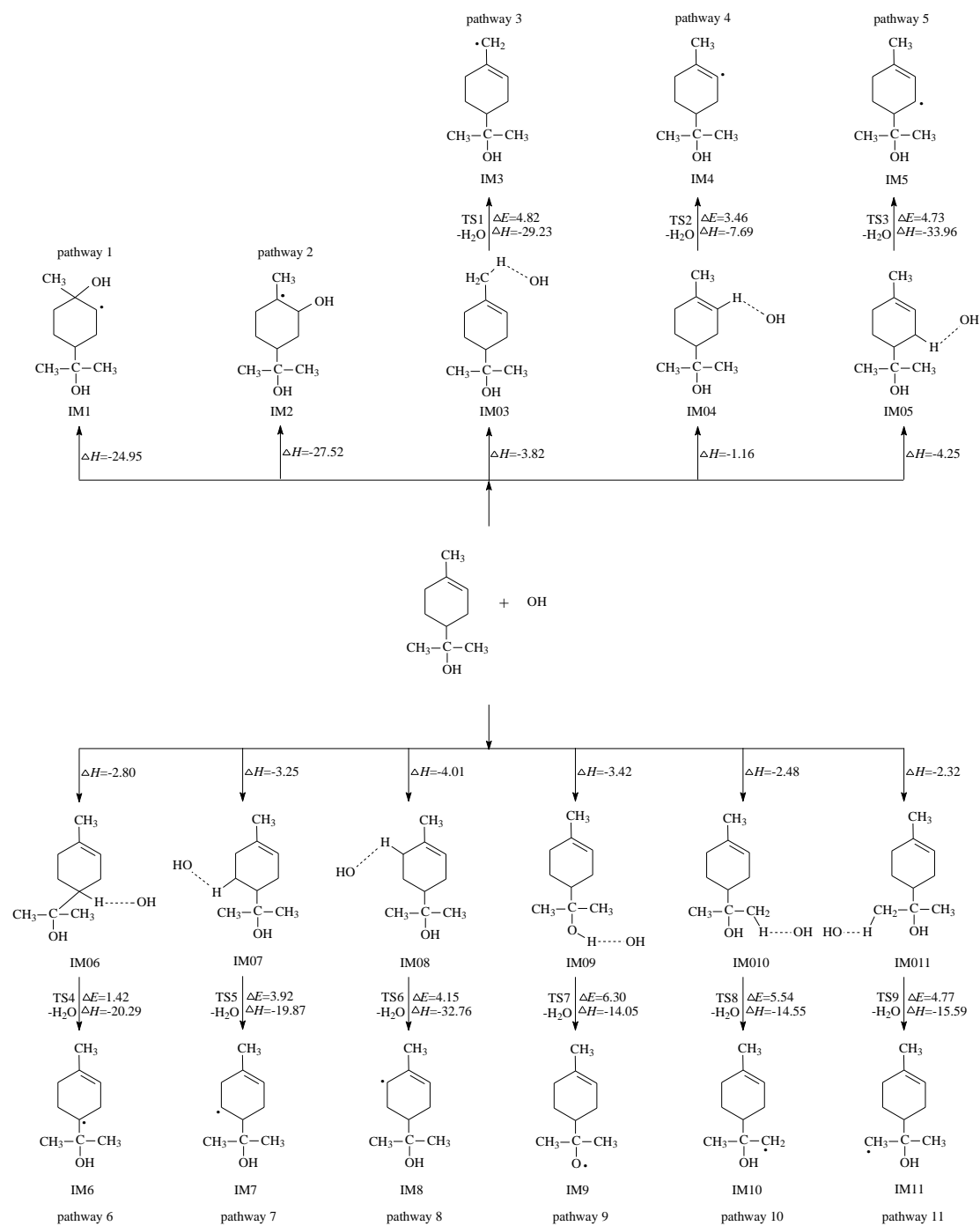


Fig. S1 The primary reaction pathways of α -terpineol with OH radical embedded with the potential barriers ΔE (kcal mol⁻¹) and reaction heats ΔH (kcal mol⁻¹) at the BB1K/6-31+G(d,p)//BB1K/6-311+G(3df,2p) level.

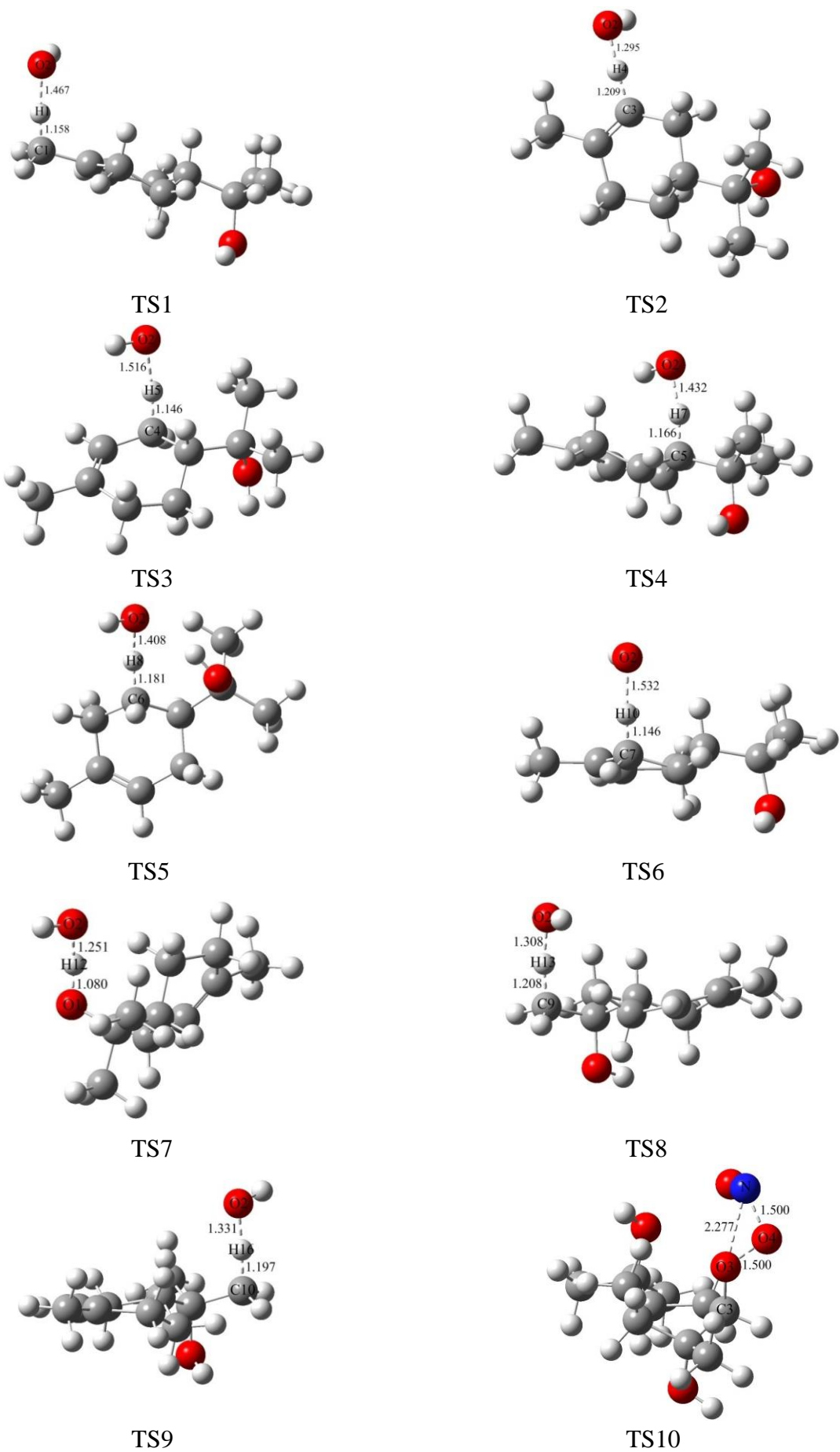
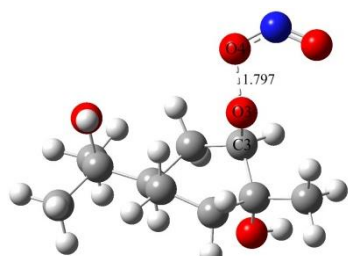
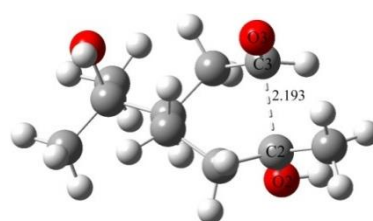


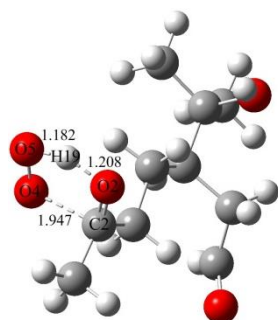
Fig. S2 MPWB1K/6-31+G(d,p) optimized geometries with the bond lengths (Å) for the transition states involved in the reaction of α -terpineol with OH radical.



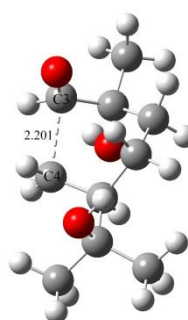
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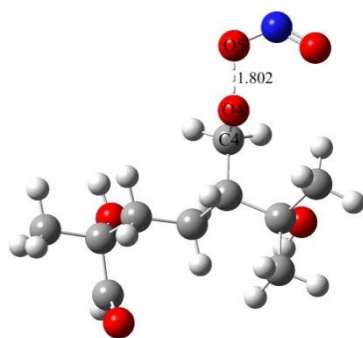
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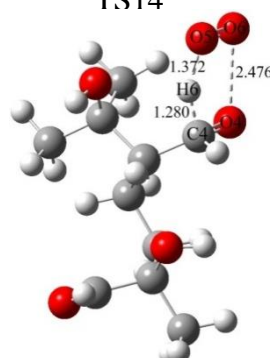
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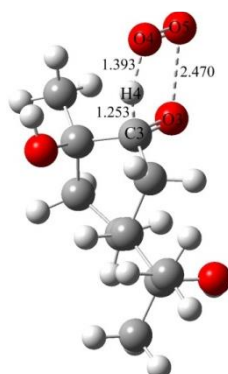
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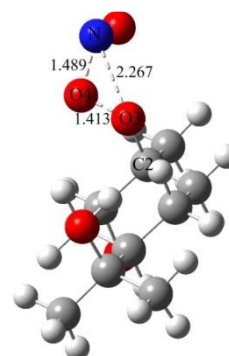
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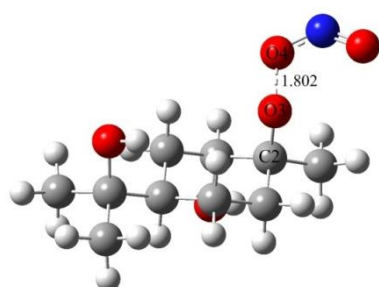
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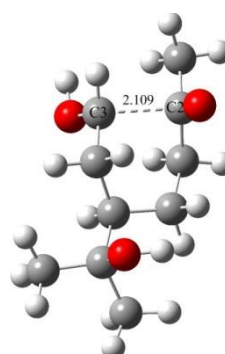
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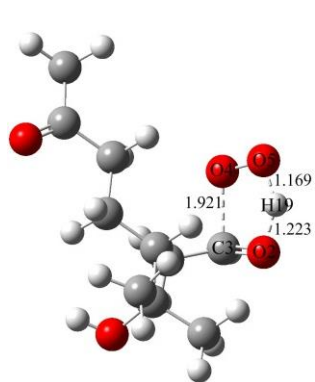


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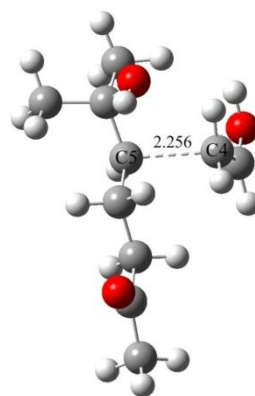


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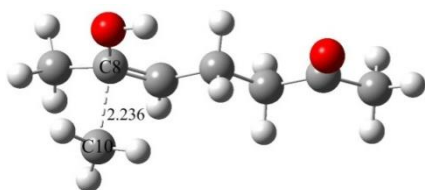
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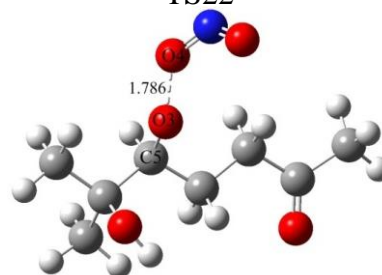
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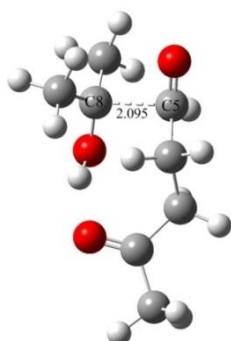
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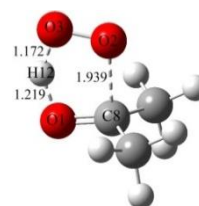
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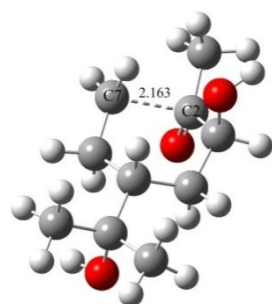
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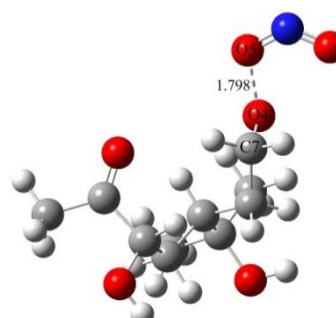
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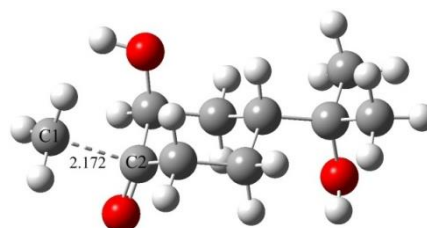
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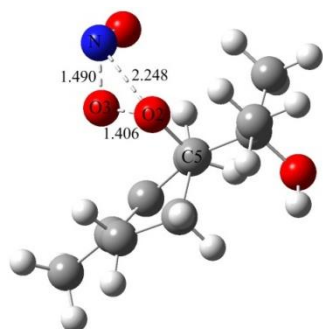


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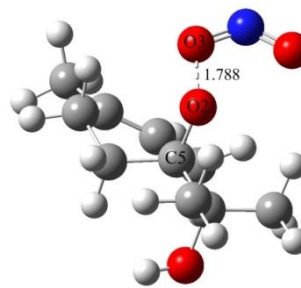


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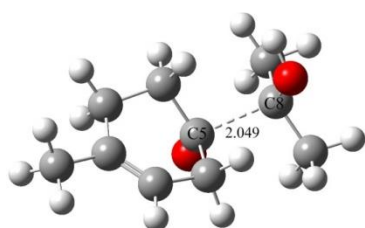
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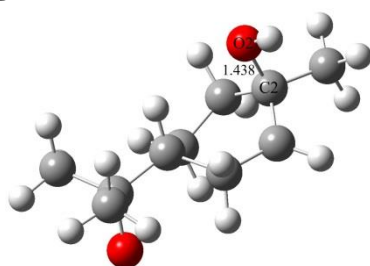


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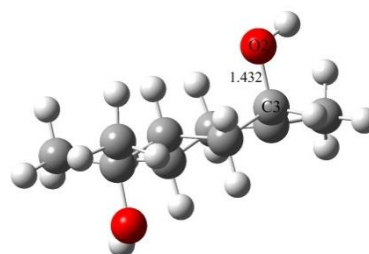


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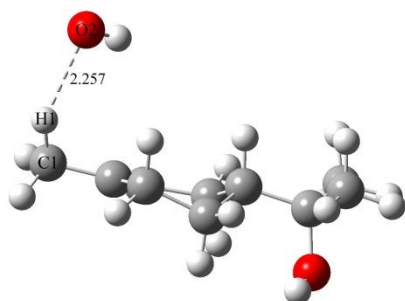
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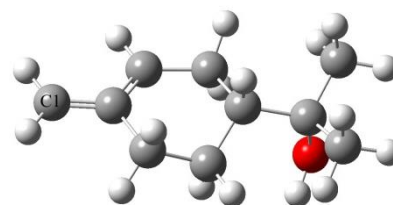
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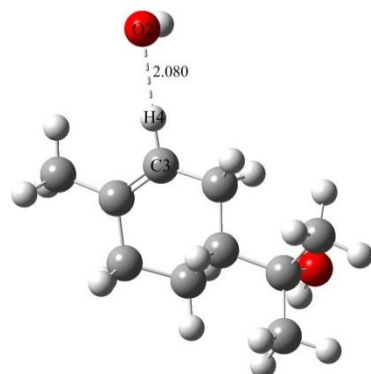
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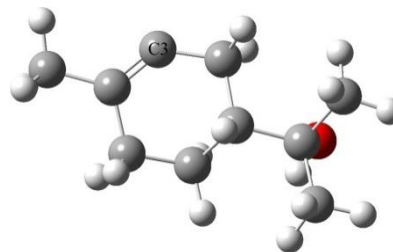
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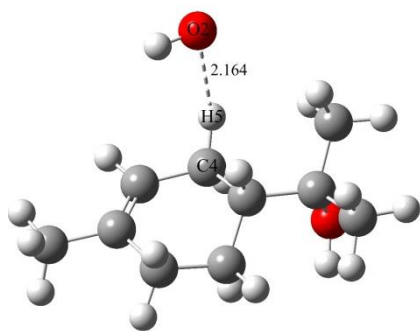


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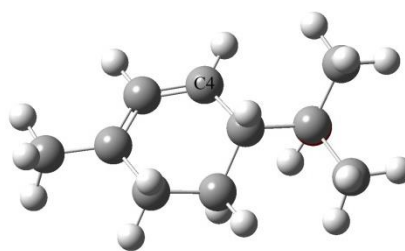


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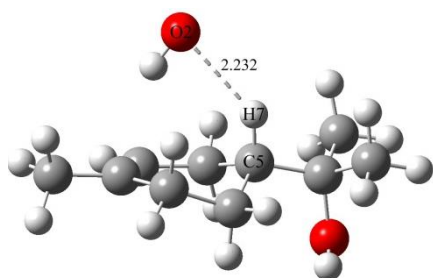
Fig. S3 MPWB1K/6-31+G(d,p) optimized geometries with the bond lengths (Å) for the intermediate states and products involved in the reaction of α -terpineol with OH radical.



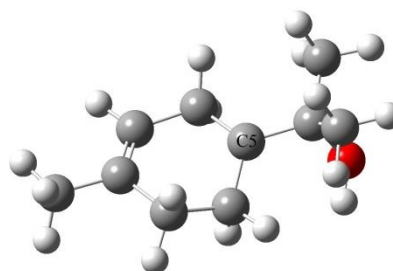
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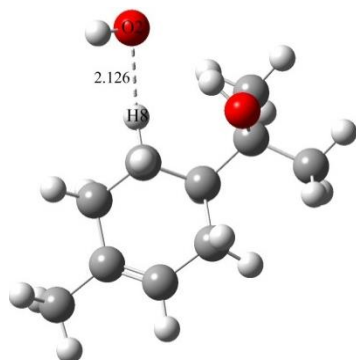
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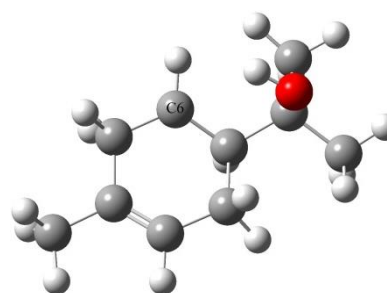
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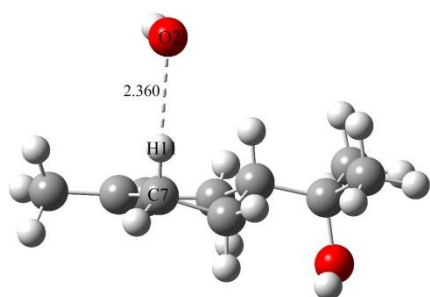
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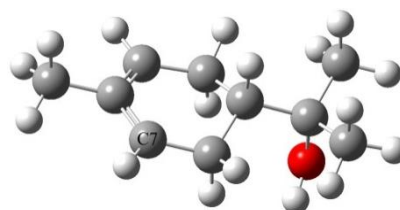
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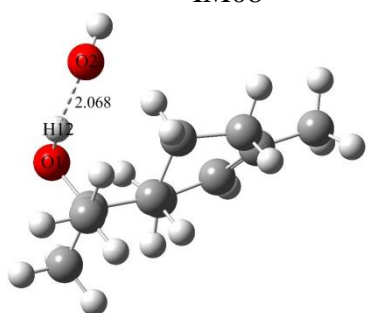
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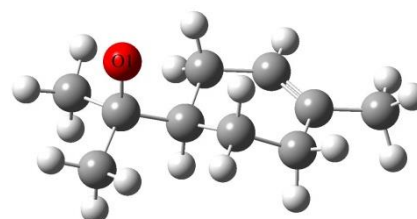
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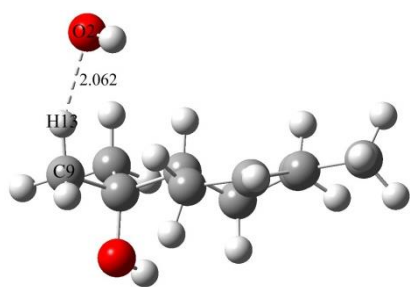


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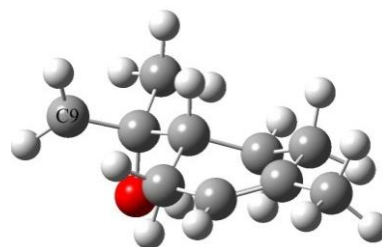


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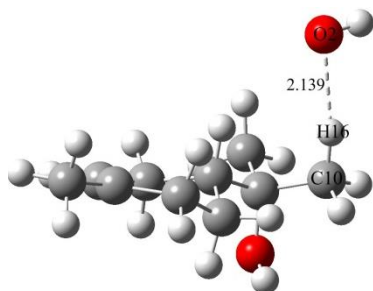
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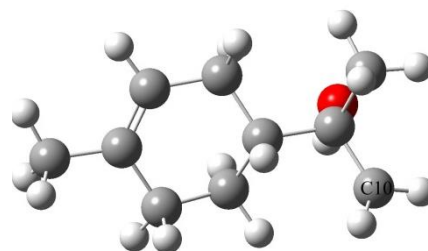
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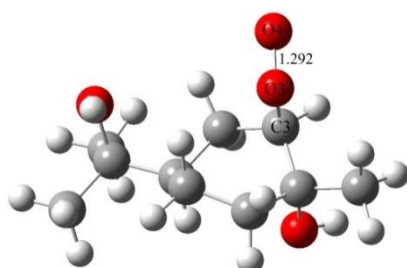
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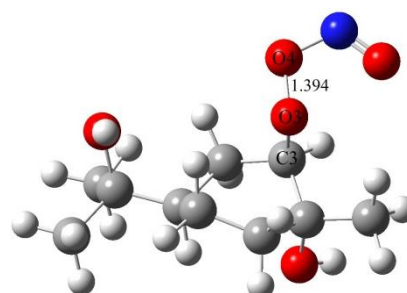
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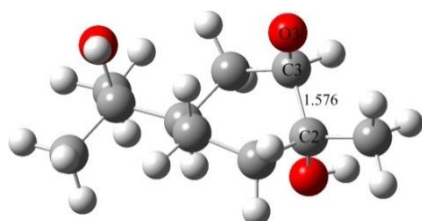
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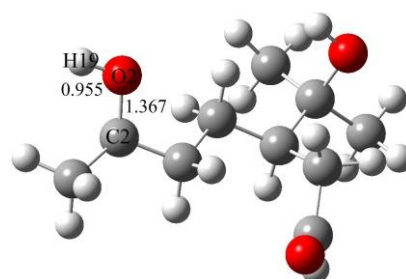
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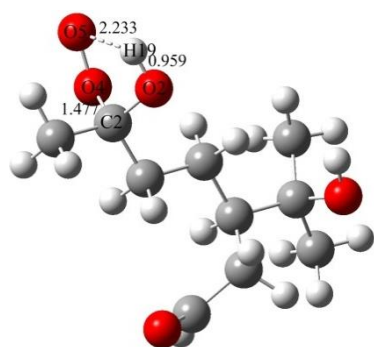
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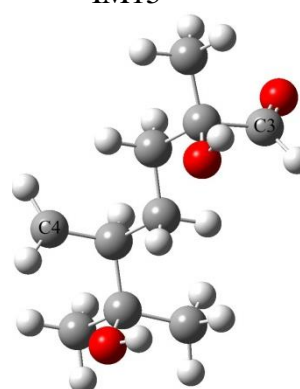
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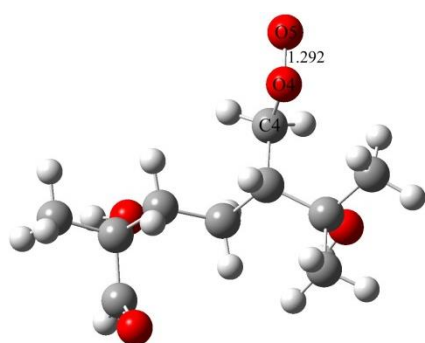


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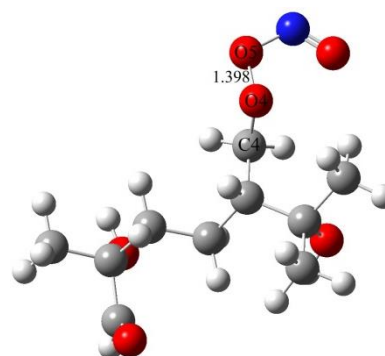


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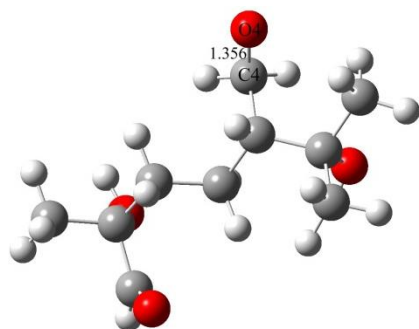
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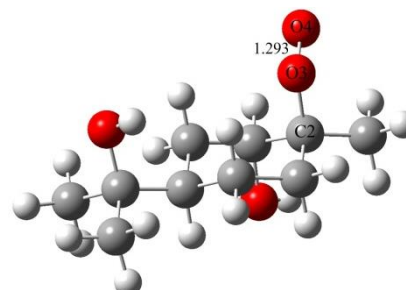
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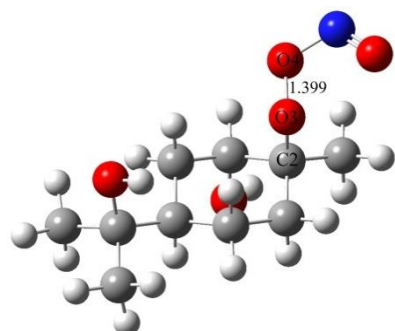
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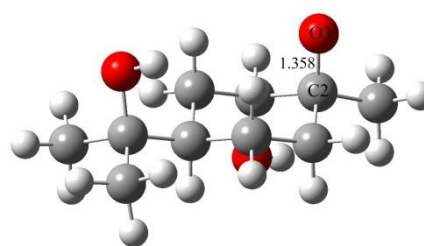
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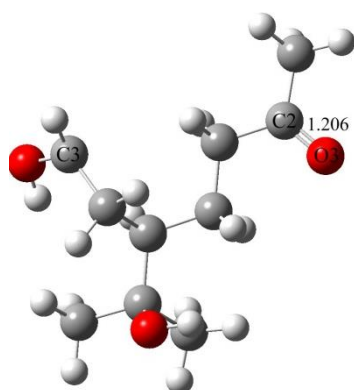
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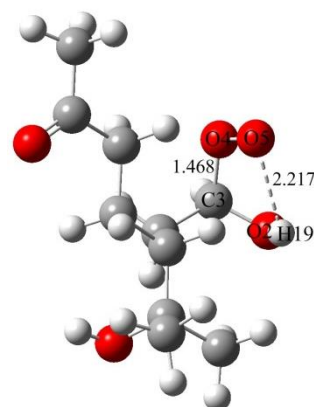
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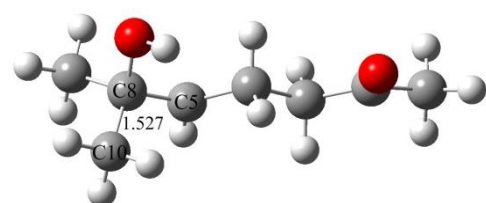
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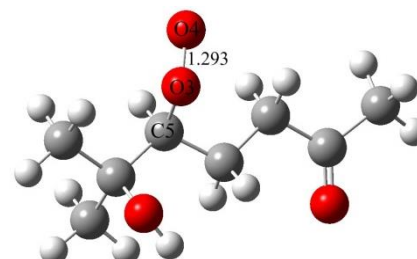
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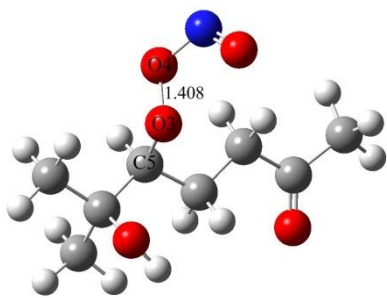


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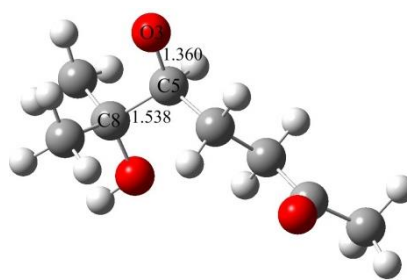


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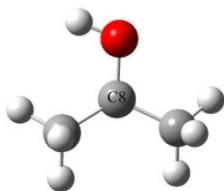
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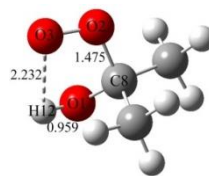
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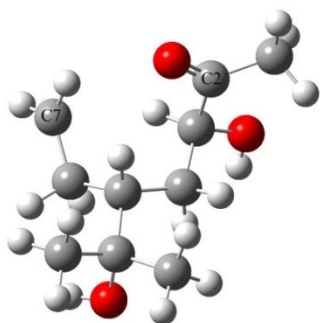
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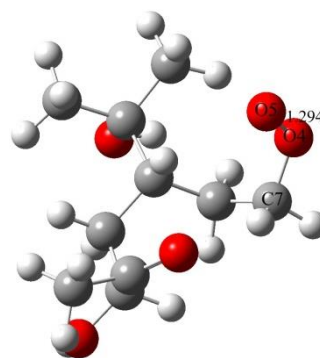
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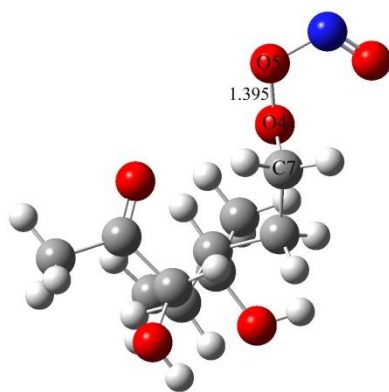
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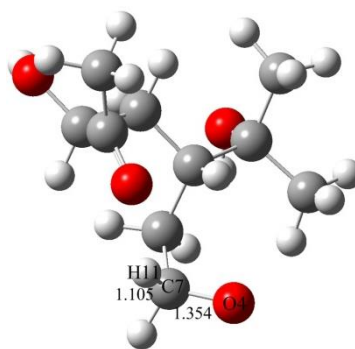
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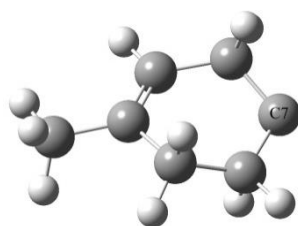
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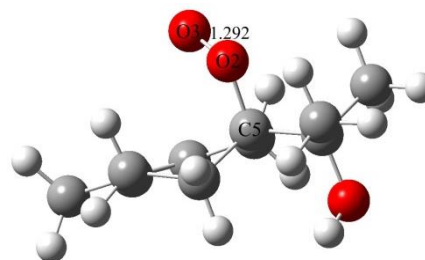
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IM36



IM37

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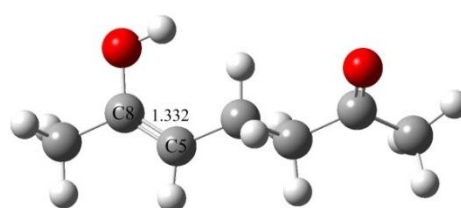
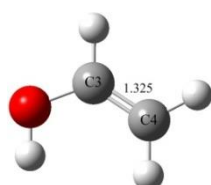
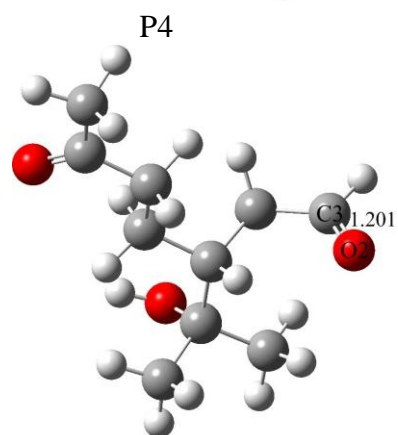
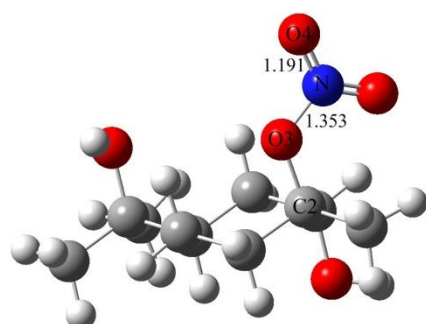
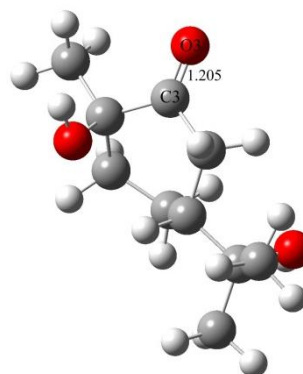
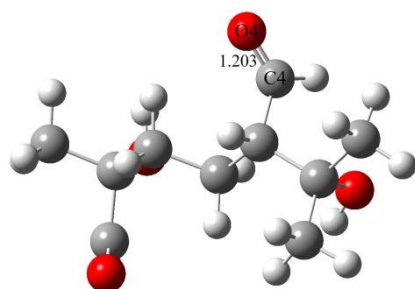
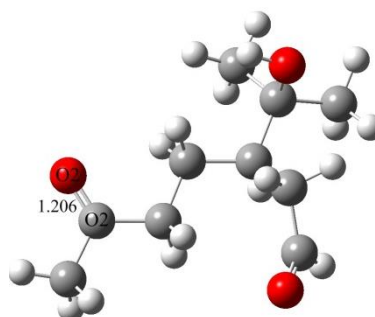
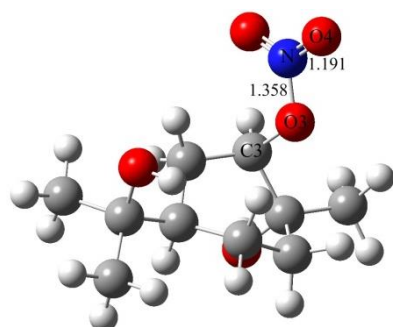
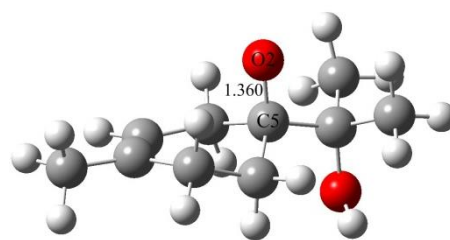
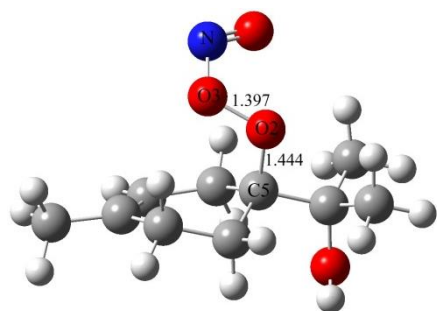


Fig. S3 (continued)

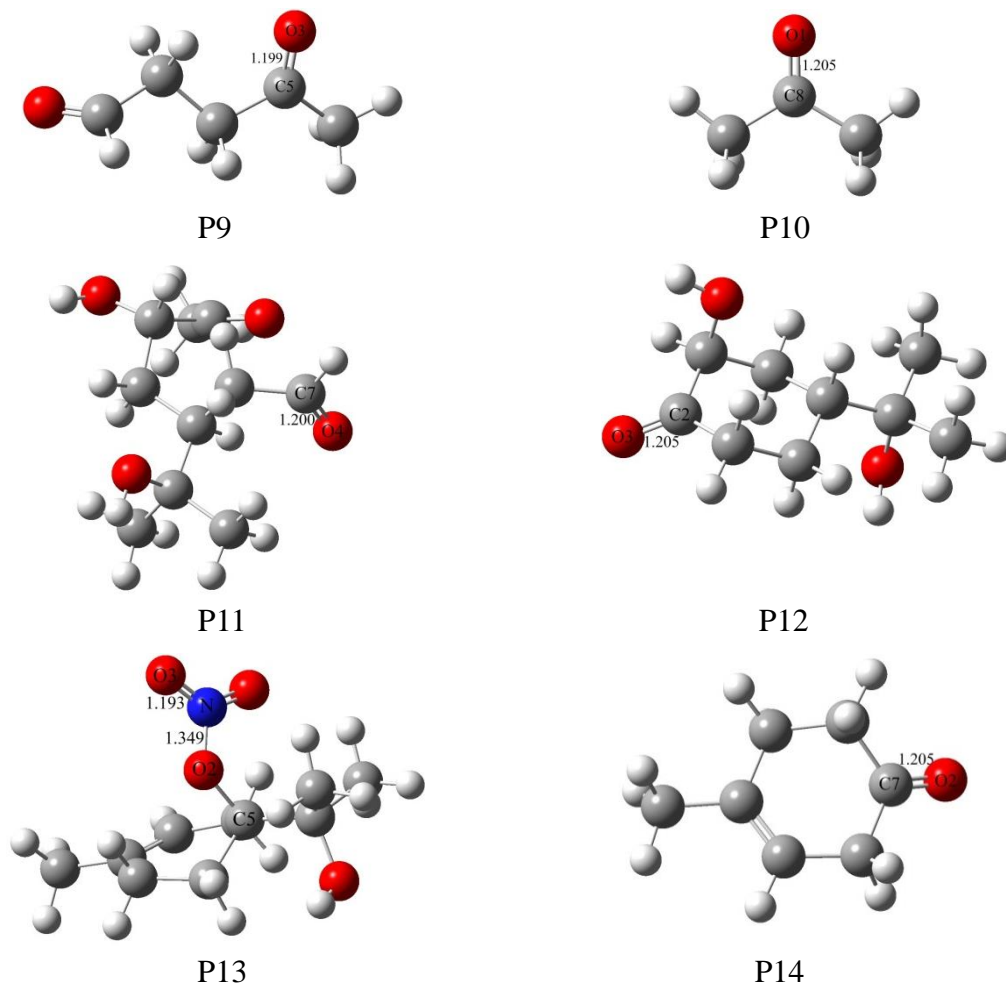


Fig. S3 (continued)

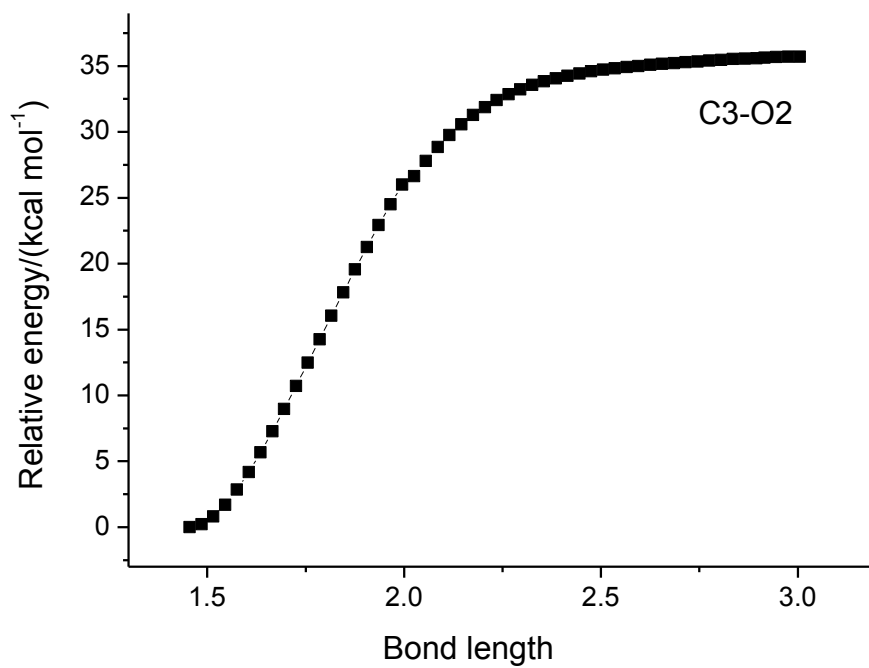


Fig. S4 Potential energy surfaces of self-decomposition of IM2.

Table S1 The rate constants (k) at 298 K after considering the errors

Reactions	Rate constants	Reactions	Rate constants
R+OH→IM1	$5.95^{+0.35}_{-0.31} \times 10^{-11}$	IM21+NO→IM22	$4.36^{+0.88}_{-0.31} \times 10^{-12}$
R+OH→IM2	$6.37^{+2.35}_{-0.66} \times 10^{-11}$	IM22→P5	$4.78^{+21.26}_{-3.89} \times 10$
R+OH→IM3+H ₂ O	$2.10^{+5.74}_{-1.64} \times 10^{-13}$	IM22→IM23+NO ₂	$5.17^{+20.13}_{-4.17} \times 10^4$
R+OH→IM4+H ₂ O	$1.31^{+31.06}_{-1.08} \times 10^{-14}$	IM23→IM24	$2.66^{+0.37}_{-1.19} \times 10^7$
R+OH→IM5+H ₂ O	$7.04^{+0.63}_{-3.43} \times 10^{-13}$	IM24+O ₂ →IM25	$5.40^{+0.09}_{-0.23} \times 10^{-12}$
R+OH→IM6+H ₂ O	$3.64^{+58.57}_{-2.81} \times 10^{-12}$	IM25→P6+HO ₂	$1.41^{+5.84}_{-1.15} \times 10^4$
R+OH→IM7+H ₂ O	$1.96^{+14.33}_{-1.28} \times 10^{-14}$	IM24→IM26	$2.85^{+10.75}_{-1.99} \times 10^{-8}$
R+OH→IM8+H ₂ O	$7.19^{+55.41}_{-3.57} \times 10^{-13}$	IM26→P8+CH ₃	$4.52^{+19.98}_{-3.72} \times 10^{-10}$
R+OH→IM9+H ₂ O	$1.73^{+36.43}_{-0.71} \times 10^{-15}$	IM26+O ₂ →IM27	$5.90^{+1.73}_{-1.20} \times 10^{-12}$
R+OH→IM10+H ₂ O	$1.27^{+8.11}_{-1.50} \times 10^{-15}$	IM27+NO→IM28	$6.21^{+0.77}_{-0.49} \times 10^{-12}$
R+OH→IM11+H ₂ O	$1.37^{+6.82}_{-1.26} \times 10^{-13}$	IM28→IM29+NO ₂	$2.96^{+5.33}_{-2.01} \times 10^7$
R+OH	$(k)1.29^{+19.98}_{-0.66} \times 10^{-10}$	IM29→IM30+P9	$2.43^{+11.28}_{-0.98} \times 10^9$
IM1+O ₂ →IM12	$5.78^{+1.20}_{-0.36} \times 10^{-12}$	IM30+O ₂ →IM31	$6.01^{+1.72}_{-1.07} \times 10^{-12}$
IM12+NO→IM13	$7.11^{+0.28}_{-0.44} \times 10^{-12}$	IM31→P10+HO ₂	$2.31^{+8.49}_{-1.84} \times 10^3$
IM13→P1	$1.06^{+4.65}_{-0.87}$	IM23→IM32	$4.32^{+7.09}_{-1.31} \times 10$
IM13→IM14+NO ₂	$2.22^{+9.54}_{-1.81} \times 10^3$	IM32+O ₂ →IM33	$5.35^{+7.80}_{-2.12} \times 10^{-12}$
IM14→IM15	$3.46^{+7.74}_{-2.54} \times 10^6$	IM33+NO→IM34	$6.45^{+0.65}_{-0.47} \times 10^{-12}$
IM15+O ₂ →IM16	$5.43^{+1.46}_{-0.76} \times 10^{-12}$	IM34→IM35+NO ₂	$0.12^{+0.61}_{-0.10}$
IM16→P2+HO ₂	$9.80^{+42.17}_{-7.96} \times 10^3$	IM35+O ₂ →P11+HO ₂	$5.71^{+48.82}_{-3.24} \times 10^{-53}$
IM14→IM17	$1.52^{+5.56}_{-1.22} \times 10^3$	IM23→P12+CH ₃	$1.09^{+8.03}_{-0.88} \times 10^{-2}$
IM17+O ₂ →IM18	$5.28^{+1.08}_{-0.82} \times 10^{-12}$	IM6+O ₂ →IM37	$5.96^{+3.42}_{-0.78} \times 10^{-12}$
IM18+NO→IM19	$5.83^{+0.32}_{-0.37} \times 10^{-12}$	IM37+NO→IM38	$6.10^{+0.65}_{-0.43} \times 10^{-12}$
IM19→IM20+NO ₂	$0.10^{+0.45}_{-0.08}$	IM38→P13	$1.08^{+5.74}_{-0.87}$
IM20+O ₂ →P3+HO ₂	$7.20^{+58.91}_{-0.96} \times 10^{-53}$	IM38→IM39+NO ₂	$7.18^{+28.22}_{-5.81} \times 10^4$
IM14+O ₂ →P4+HO ₂	$4.50^{+10.80}_{-3.66} \times 10^{-27}$	IM39→IM30+P14	$1.68^{+2.58}_{-1.02} \times 10^8$
IM2+O ₂ →IM21	$5.78^{+1.44}_{-0.79} \times 10^{-12}$		

Note: Units are s⁻¹ and cm³ molecule⁻¹ s⁻¹ for unimolecular and bimolecular reactions, respectively.

Table S2 The rate constants ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) of the title reactions for the gas-phase oxidation of α -terpineol with OH radicals at 298 K and 1 atm

Reactions	Rate constants/MPWB1K	Rate constants/BB1K
R+OH→IM1	5.95×10^{-11}	6.10×10^{-12}
R+OH→IM2	6.37×10^{-11}	5.24×10^{-12}
R+OH→IM3+H ₂ O	2.10×10^{-13}	2.01×10^{-13}
R+OH→IM4+H ₂ O	1.31×10^{-14}	6.99×10^{-14}
R+OH→IM5+H ₂ O	7.04×10^{-13}	3.83×10^{-13}
R+OH→IM6+H ₂ O	3.64×10^{-12}	6.53×10^{-13}
R+OH→IM7+H ₂ O	1.96×10^{-14}	1.59×10^{-14}
R+OH→IM8+H ₂ O	7.19×10^{-13}	3.99×10^{-13}
R+OH→IM9+H ₂ O	1.73×10^{-15}	8.27×10^{-15}
R+OH→IM10+H ₂ O	1.27×10^{-15}	1.84×10^{-15}
R+OH→IM11+H ₂ O	1.37×10^{-13}	1.55×10^{-15}
R+OH	$(k)1.29 \times 10^{-10}$	$(k)1.33 \times 10^{-11}$

Table S3 Arrhenius formulas of rate constants ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for the H-abstraction reactions at 180-380 K

Reactions	$k_{298 \text{ K}}$	Arrhenius formulas	R^2
R+OH→IM3+H ₂ O	2.17×10^{-13}	$k(T)=2.00 \times 10^{-15} \exp(-295.60/T)$	0.9932
R+OH→IM4+H ₂ O	1.41×10^{-14}	$k(T)=1.32 \times 10^{-13} \exp(-656.38/T)$	0.9994
R+OH→IM5+H ₂ O	4.68×10^{-13}	$k(T)=1.12 \times 10^{-12} \exp(-249.30/T)$	0.9961
R+OH→IM6+H ₂ O	1.02×10^{-12}	$k(T)=2.05 \times 10^{-12} \exp(-198.62/T)$	0.9952
R+OH→IM7+H ₂ O	6.30×10^{-14}	$k(T)=5.60 \times 10^{-14} \exp(-387.70/T)$	0.9975
R+OH→IM8+H ₂ O	2.17×10^{-13}	$k(T)=1.40 \times 10^{-13} \exp(-134.42/T)$	0.9990
R+OH→IM9+H ₂ O	2.98×10^{-15}	$k(T)=3.09 \times 10^{-13} \exp(-1377.3/T)$	0.9997
R+OH→IM10+H ₂ O	5.31×10^{-14}	$k(T)=1.13 \times 10^{-12} \exp(-900.06/T)$	0.9993
R+OH→IM11+H ₂ O	3.68×10^{-13}	$k(T)=4.08 \times 10^{-12} \exp(-706.25/T)$	0.9991

Table S4 Cartesian coordinates for the optimized stationary points

Optimized stationary points	Cartesian coordinates			
TS1	C	-1.32310000	-0.99700800	-0.68124400
	H	-1.58290800	-1.62348800	0.17560100
	H	-1.77834500	-1.48039900	-1.54640800
	C	-1.93237900	0.35705500	-0.49587900
	C	-1.17788700	1.41090300	-0.17450200
	H	-1.65419800	2.37820700	-0.07054100
	C	0.29172300	1.35820400	0.07121800
	H	0.50831700	1.93937600	0.96737700
	H	0.82825900	1.85343100	-0.74314300
	C	0.18103700	-0.92666400	-0.85601400
	H	0.39715500	-0.48912300	-1.83361300
	H	0.58943900	-1.93510900	-0.85216800
	C	0.82024300	-0.06093800	0.21937000
	H	0.50176100	-0.44688400	1.19223800
	C	2.35887100	-0.10919100	0.19923700
	C	2.95275500	0.88378400	1.17686000
	H	4.03113400	0.75718500	1.22074500
	H	2.75079000	1.90220500	0.85990000
	H	2.54350000	0.73757000	2.17432000
	C	2.87217800	-1.50193100	0.52461300
	H	2.54466000	-2.23886300	-0.20582800
	H	3.95908900	-1.49759400	0.52716400
	H	2.52618500	-1.82723200	1.50356000
	O	2.84553900	0.29362700	-1.07012700
	H	2.63247000	-0.37918800	-1.71438800
	C	-3.39202600	0.46424900	-0.65631700
H	-3.91058900	-0.13993800	0.18423200	
H	-3.76541200	1.48132400	-0.59155600	
H	-3.76931900	-0.02500300	-1.55236200	
O	-4.47611200	-0.80646500	1.36227900	
H	-4.21590300	-0.13454400	2.00360800	
TS2	C	1.05813400	-1.87333900	-0.04894100
	H	0.99373900	-2.32944200	-1.04015500
	H	1.43923800	-2.65167000	0.61377600
	C	2.04857900	-0.74350300	-0.09399500
	C	1.59795200	0.49871500	-0.05435200
	H	2.42306500	1.37949000	-0.11792200
	C	0.19078900	0.96659000	-0.01270000
	H	0.06599300	1.77885900	-0.72656800
	H	-0.05353600	1.37522500	0.97066400
	C	-0.31107500	-1.41780400	0.41543800
	H	-0.25540100	-1.18258300	1.48074900

	H	-1.01770600	-2.23758600	0.29940900
	C	-0.77176200	-0.17504600	-0.33332600
	H	-0.70661500	-0.38192000	-1.40512000
	C	-2.23293100	0.20481700	-0.03026700
	C	-2.58719900	1.55137300	-0.62554300
	H	-3.64524500	1.75072700	-0.47899400
	H	-2.02798900	2.34468700	-0.13929800
	H	-2.37220300	1.57278600	-1.69181600
	C	-3.19396700	-0.84698800	-0.55982500
	H	-3.03203500	-1.81923200	-0.09876400
	H	-4.21609700	-0.54465400	-0.34721600
	H	-3.08659300	-0.96645000	-1.63581000
	O	-2.41665200	0.36211900	1.36599400
	H	-2.35402300	-0.49347900	1.78688600
	C	3.49262900	-1.10232500	-0.19117300
	H	4.11567700	-0.21667400	-0.26319600
	H	3.80495700	-1.68180700	0.67745500
	H	3.67171500	-1.72574900	-1.06708200
	O	3.32136300	2.29625100	0.05623000
	H	3.26848600	2.38757000	1.01330900
TS3	C	1.76535000	-1.36758800	-0.61762600
	H	1.80772600	-1.23113400	-1.70188700
	H	2.32439500	-2.28202200	-0.41420300
	C	2.44333700	-0.21743800	0.05804900
	C	1.72540900	0.74457500	0.63774000
	H	2.24107500	1.53663700	1.16727200
	C	0.24944900	0.82460500	0.59975000
	H	-0.03070800	1.85836600	0.19171800
	H	-0.18158700	0.84127600	1.60324000
	C	0.32674200	-1.52692400	-0.16619200
	H	0.32585700	-1.85830500	0.87478200
	H	-0.15220700	-2.30419300	-0.75798700
	C	-0.43186100	-0.21160900	-0.27463700
	H	-0.36664000	0.12294400	-1.31368700
	C	-1.92931900	-0.33300500	0.06365000
	C	-2.60383200	1.02200700	0.02279000
	H	-3.67006800	0.90299200	0.19608300
	H	-2.20970600	1.67628300	0.79404100
	H	-2.44815800	1.50518700	-0.93827600
	C	-2.63947600	-1.27988100	-0.88853800
	H	-2.26952600	-2.29999100	-0.80435200
	H	-3.70210000	-1.29391100	-0.66066700
	H	-2.51333700	-0.96196100	-1.92139800
	O	-2.09042200	-0.78839700	1.39722000
	H	-1.83834900	-1.70862500	1.44722300
	C	3.93359600	-0.22928500	0.07243500

	H	4.33998000	0.65295900	0.55866100
	H	4.31106100	-1.11114700	0.59009900
	H	4.32852200	-0.27094900	-0.94311400
	O	-0.16952200	3.10904600	-0.65413000
	H	0.74695600	3.10765600	-0.95677700
TS4	C	1.70767000	-0.58089900	-1.13380000
	H	1.75295200	0.26149400	-1.82834400
	H	2.25451200	-1.39362300	-1.61415100
	C	2.39995300	-0.21246300	0.14209800
	C	1.71295000	0.00972400	1.26088900
	H	2.25605200	0.24304100	2.16829900
	C	0.22191400	-0.01301200	1.36043500
	H	-0.10383600	0.85201500	1.93675700
	H	-0.11488500	-0.89105800	1.92061700
	C	0.26399800	-0.98951400	-0.91203300
	H	0.24561600	-1.97486800	-0.43796000
	H	-0.23942100	-1.07855700	-1.87185400
	C	-0.44651000	-0.01720200	0.00490500
	H	-0.27524200	1.04508800	-0.44544900
	C	-1.97448400	-0.16558300	0.05082200
	C	-2.58364700	0.74894000	1.09103900
	H	-3.66739300	0.70091200	1.03047500
	H	-2.29284800	0.44091500	2.09064300
	H	-2.26540400	1.77610000	0.92748700
	C	-2.59520600	0.12363000	-1.30390600
	H	-2.25355900	-0.57228300	-2.06752100
	H	-3.67615600	0.03521700	-1.23331700
	H	-2.34618000	1.12968800	-1.63357900
	O	-2.29868400	-1.48252200	0.46750700
	H	-2.10553600	-2.09012600	-0.24453800
	C	3.88849000	-0.12627800	0.08417700
	H	4.31170200	0.18531700	1.03490600
	H	4.32236100	-1.08957800	-0.18374000
	H	4.20739900	0.58284800	-0.68003400
	O	0.22016600	2.34741400	-0.77423800
	H	1.04723700	2.25426000	-0.28260200
TS5	C	1.71733800	1.10661900	0.27333600
	H	1.70053400	1.36461300	1.33480300
	H	2.18269400	1.95008300	-0.23875900
	C	2.56036100	-0.12206300	0.06335800
	C	2.00457800	-1.29013000	-0.24733500
	H	2.65239900	-2.14108800	-0.41709200
	C	0.53292700	-1.53208700	-0.35720300
	H	0.29100400	-2.48518400	0.11197300
	H	0.23881200	-1.62489100	-1.40607500
	C	0.32668700	0.86602500	-0.24420000

	H	0.30646700	0.84385700	-1.33301500
	H	-0.37079900	1.78252100	0.01565200
	C	-0.27031100	-0.41153300	0.29644200
	H	-0.07623300	-0.45520600	1.37121700
	C	-1.79938200	-0.50052200	0.09293400
	C	-2.28420500	-1.93342100	0.04128800
	H	-3.36966400	-1.94380800	-0.00812900
	H	-1.90345900	-2.43867500	-0.84160500
	H	-1.97158000	-2.48594900	0.92510400
	C	-2.50297000	0.22572500	1.22929000
	H	-2.15513900	1.25027400	1.33187300
	H	-3.57317500	0.24751100	1.03744400
	H	-2.33343000	-0.28884200	2.17292600
	O	-2.16121600	0.06792400	-1.14848600
	H	-2.12318100	1.02460300	-1.06436100
	C	4.03363200	0.06315300	0.20654700
	H	4.28133600	0.45706000	1.19243500
	H	4.56947600	-0.87194100	0.07091900
	H	4.40998600	0.78109700	-0.52228100
	O	-1.32204900	2.79123500	-0.22945300
	H	-0.80185400	3.33009900	-0.83625200
TS6	C	-1.63226800	0.57729900	0.82810500
	H	-1.81457600	1.49960500	0.17342100
	H	-2.18580600	0.82056400	1.73557700
	C	-2.21385000	-0.60345600	0.14522300
	C	-1.41900900	-1.48090500	-0.46861800
	H	-1.86735800	-2.35026300	-0.93401800
	C	0.06427400	-1.36037700	-0.56989000
	H	0.35797200	-1.58882800	-1.59407600
	H	0.54263900	-2.12086600	0.05381600
	C	-0.14778600	0.46965100	1.08187800
	H	0.01110800	-0.25857900	1.88265700
	H	0.22294700	1.42969100	1.43292300
	C	0.58798000	0.00975100	-0.16708200
	H	0.35364000	0.72235400	-0.96304800
	C	2.11843700	0.01289500	-0.00121900
	C	2.79901500	-0.54417600	-1.23437400
	H	3.87688300	-0.45024800	-1.13379700
	H	2.56690800	-1.59752500	-1.35806100
	H	2.48341200	-0.00697100	-2.12630300
	C	2.64232100	1.41130000	0.27651200
	H	2.27414300	1.80395700	1.22228700
	H	3.72791800	1.39097800	0.32676500
	H	2.34351800	2.10388800	-0.50725300
	O	2.50004300	-0.85764400	1.05140600
	H	2.26266100	-0.46049400	1.88724200

	C	-3.69893900	-0.74427300	0.18339400
	H	-4.18295900	0.14319400	-0.22468700
	H	-4.03437700	-1.60739300	-0.38460600
	H	-4.05424100	-0.85084200	1.20802400
	O	-1.93193700	2.49354000	-0.98694300
	H	-2.03033400	1.80435500	-1.65614300
TS7	C	1.84390500	1.05606300	0.71236600
	H	1.95315000	0.91255800	1.79134000
	H	2.24797500	2.04842100	0.50602000
	C	2.66223900	0.03165300	-0.01021400
	C	2.08195200	-0.98674100	-0.63827500
	H	2.70525400	-1.69199000	-1.17429900
	C	0.61286800	-1.25806800	-0.64080500
	H	0.45833800	-2.32030000	-0.45257600
	H	0.19363400	-1.06362700	-1.63285300
	C	0.38218500	1.00335800	0.31825000
	H	0.28112500	1.36901300	-0.70458700
	H	-0.19776900	1.67450400	0.94686600
	C	-0.13847100	-0.42473300	0.38657900
	H	0.09516700	-0.81894300	1.38031300
	C	-1.66208100	-0.53281100	0.22489400
	C	-2.11175400	-1.98629200	0.13505600
	H	-3.19667700	-2.03766500	0.13068500
	H	-1.74569400	-2.45252700	-0.77383900
	H	-1.73526000	-2.54273400	0.99087200
	C	-2.39982300	0.13440400	1.37646500
	H	-2.16579300	1.19266100	1.43162900
	H	-3.47199600	0.03135300	1.23083800
	H	-2.12997000	-0.34103600	2.31675100
	O	-2.08496900	0.02019900	-1.00080000
	H	-1.87574900	1.07437900	-1.10815700
	C	4.14126700	0.22534000	0.00981200
	H	4.51346600	0.26301000	1.03409100
	H	4.65950800	-0.57627100	-0.50925300
	H	4.41725700	1.17054000	-0.45802400
	O	-2.20729600	2.26011600	-0.88417400
	H	-3.14158100	2.29309900	-1.11080000
TS8	C	2.02160100	-0.88594800	-0.87519600
	H	1.96110600	-0.51776800	-1.90300300
	H	2.69781400	-1.74176000	-0.90847400
	C	2.61393500	0.17504600	-0.00043500
	C	1.85978200	0.84701500	0.86398300
	H	2.33038400	1.58588800	1.50091300
	C	0.38288500	0.67868700	1.01325300
	H	-0.07012500	1.66993700	1.06950900
	H	0.14900800	0.19132100	1.96418800

	C	0.65360900	-1.32557200	-0.39348000
	H	0.77502900	-1.89100900	0.53313600
	H	0.21009600	-1.99476500	-1.12889500
	C	-0.23780500	-0.12404000	-0.12012100
	H	-0.25420900	0.49718300	-1.01930600
	C	-1.69613500	-0.51919900	0.17138200
	C	-2.50171600	0.65333700	0.67732600
	H	-3.56553900	0.44289400	0.72802700
	H	-2.13931800	1.06277800	1.61320800
	H	-2.42877400	1.53210800	-0.14788300
	C	-2.37352000	-1.08189000	-1.06483700
	H	-1.86422100	-1.96657100	-1.44045600
	H	-3.39702000	-1.36049200	-0.82685200
	H	-2.39071700	-0.33651200	-1.85686100
	O	-1.75046200	-1.45486400	1.23689700
	H	-1.42371200	-2.29749400	0.92523500
	C	4.07796200	0.41897500	-0.14962800
	H	4.32411800	0.68345400	-1.17840400
	H	4.41986000	1.22225100	0.49703900
	H	4.64954600	-0.47829900	0.08824100
	O	-2.17458500	2.43616600	-1.05904200
	H	-1.38653200	2.82798400	-0.66568700
TS9	C	-1.86811900	0.96694100	0.82837800
	H	-1.71694800	1.95939200	0.39567800
	H	-2.45338300	1.12575800	1.73562200
	C	-2.65339100	0.11979900	-0.12394200
	C	-2.06654300	-0.85254700	-0.81454900
	H	-2.67300400	-1.46127200	-1.47401600
	C	-0.60608300	-1.16200400	-0.77951500
	H	-0.25679400	-1.28501600	-1.80419400
	H	-0.43467800	-2.12335900	-0.28683800
	C	-0.53098800	0.34380400	1.17833900
	H	-0.71638700	-0.53305900	1.80508600
	H	0.05007900	1.05117300	1.76718400
	C	0.21135200	-0.08733000	-0.07822100
	H	0.28588600	0.78078700	-0.73798600
	C	1.65181200	-0.54785200	0.19506300
	C	2.30611300	-1.09524300	-1.05427100
	H	3.34608400	-1.33739600	-0.85010200
	H	1.81034800	-2.00499800	-1.37656200
	H	2.26487900	-0.35963100	-1.85409500
	C	2.49610100	0.58483900	0.74351200
	H	2.13633900	1.01669700	1.67276900
	H	3.54394400	0.31324600	0.82667800
	H	2.41903500	1.48107400	-0.04611700
	O	1.68301200	-1.61196600	1.13265600

	H	1.26083500	-1.32838600	1.94235100
	C	-4.10809600	0.42808000	-0.24236300
	H	-4.26110100	1.46443300	-0.54511400
	H	-4.59663800	-0.21229700	-0.97142000
	H	-4.61398000	0.30406100	0.71544000
	O	2.35644500	2.40677500	-1.00062000
	H	3.29687300	2.59938600	-1.08524900
TS10	C	-1.02672500	-1.43680700	-1.30434900
	H	-0.91175600	-2.50224800	-1.49627400
	H	-1.65295200	-1.02972500	-2.09516500
	C	-1.76859800	-1.32192500	0.02416600
	C	-1.35991200	-0.02490600	0.72227400
	H	-1.95180300	0.10325900	1.63052600
	C	0.12350900	-0.00142600	1.04244700
	H	0.25962500	-0.38913300	2.04895100
	H	0.44307800	1.03942100	1.05529600
	C	0.33163000	-0.74119900	-1.31268400
	H	0.19621700	0.30320800	-1.59852900
	H	0.95616200	-1.20500600	-2.07278700
	C	0.98400600	-0.79569300	0.05935600
	H	0.99325600	-1.83898100	0.37828300
	C	2.44233700	-0.30838100	0.06410400
	C	2.99108100	-0.25786000	1.47516700
	H	4.03990300	0.02603300	1.45208100
	H	2.45948700	0.47850800	2.07003600
	H	2.90214300	-1.22906600	1.95722100
	C	3.32907900	-1.20298300	-0.78594300
	H	3.03579100	-1.19007400	-1.83370800
	H	4.35824300	-0.85813300	-0.72603000
	H	3.28868400	-2.23406500	-0.44128000
	O	2.52243100	1.02621600	-0.40818100
	H	2.31882000	1.03913100	-1.34175300
	C	-3.26466900	-1.42189000	-0.16903200
	H	-3.77910900	-1.42060700	0.79248700
	H	-3.63600600	-0.58099300	-0.74660200
	H	-3.50760700	-2.34658700	-0.68719300
	O	-1.31281300	-2.38848400	0.83849200
	O	-1.75459700	2.22187900	0.50305800
	O	-1.76738000	0.99227900	-0.18667600
	H	-1.88299500	-2.46207900	1.60223800
	N	-1.00773600	3.12394000	-0.43485800
	O	0.11667800	3.08660700	-0.22129600
TS11	C	0.09152800	1.92971700	-1.04532000
	H	-0.34749700	2.91552800	-0.90127700
	H	0.69186500	1.97023600	-1.95173300
	C	1.01326800	1.69849500	0.14488000

	C	1.08073600	0.18036100	0.45538900
	H	1.79302700	0.04620500	1.27567200
	C	-0.29083400	-0.35442100	0.83834100
	H	-0.39741600	-0.27872000	1.91764200
	H	-0.31133300	-1.41300500	0.58074700
	C	-0.99876200	0.87363000	-1.20132300
	H	-0.60557800	0.04510400	-1.79178500
	H	-1.82359600	1.30936500	-1.75991100
	C	-1.46032100	0.34852500	0.14881300
	H	-1.75461300	1.20613400	0.75463100
	C	-2.68703200	-0.57674200	0.06308100
	C	-3.05630000	-1.10139100	1.43548800
	H	-3.94809800	-1.71850700	1.36556300
	H	-2.25730500	-1.71430000	1.84142200
	H	-3.25205400	-0.27992200	2.12136100
	C	-3.88409400	0.13890200	-0.54044500
	H	-3.71621500	0.40236100	-1.58242000
	H	-4.75448400	-0.51101700	-0.50232300
	H	-4.11002800	1.05330500	0.00457900
	O	-2.38879500	-1.73201100	-0.70085500
	H	-2.19669700	-1.47044500	-1.59980500
	C	2.38865300	2.27933800	-0.08744900
	H	3.01151300	2.16767100	0.80019400
	H	2.88630600	1.76832000	-0.90626900
	H	2.30679100	3.33826800	-0.32097600
	O	0.40275700	2.31014000	1.26138500
	O	1.90046200	-2.10448300	-0.36181300
	O	1.59957200	-0.36713700	-0.70775200
	H	1.03049600	2.34506200	1.98178300
	N	3.04718900	-2.33014700	0.00497600
	O	3.89144700	-1.52764700	0.18020300
TS12	C	-1.33408600	-1.24066100	-0.85742100
	H	-1.21735000	-2.28054000	-0.54285500
	H	-1.90633300	-1.24452600	-1.78227400
	C	-2.14940900	-0.56974900	0.19962300
	C	-1.28864200	1.44730300	0.19794600
	H	-2.00354200	1.65874400	1.01215000
	C	0.11961700	1.12425900	0.64407900
	H	0.16569000	1.18940400	1.72894200
	H	0.73003500	1.92787400	0.22930800
	C	0.04807000	-0.64294300	-1.11961900
	H	-0.05808100	0.21350600	-1.78307700
	H	0.63457900	-1.39687000	-1.63917700
	C	0.72533100	-0.20343900	0.16956500
	H	0.53335800	-0.96562500	0.92599900
	C	2.25611200	-0.08457200	0.04950200

	C	2.86181400	0.42748200	1.34055700
	H	3.94443900	0.45550000	1.25030400
	H	2.52154300	1.43475500	1.55918900
	H	2.59815800	-0.22199200	2.17249300
	C	2.89316100	-1.42170400	-0.29601100
	H	2.59165400	-1.77859400	-1.27789200
	H	3.97469400	-1.31473700	-0.30432100
	H	2.62641400	-2.18288700	0.43458600
	O	2.60430100	0.87862300	-0.92731100
	H	2.24985100	0.61180000	-1.77427100
	C	-3.57095800	-0.24116500	-0.07609400
	H	-4.02181600	0.30809600	0.75060000
	H	-3.63413700	0.38258200	-0.96262300
	H	-4.15622300	-1.14986500	-0.23822000
	O	-1.86348000	-1.03276800	1.44560800
	O	-1.54630100	1.83843300	-0.93682600
	H	-2.49515600	-0.68979500	2.07661400
TS13	C	1.12588800	0.71327600	-0.02769900
	H	0.93075800	1.60351200	0.57399100
	H	1.13984800	1.05327800	-1.06353700
	C	2.50093300	0.24953200	0.34614400
	C	-1.36505900	2.58600300	-0.47966000
	H	-1.79756900	2.56357100	-1.49679600
	C	-1.71517000	1.41748300	0.37909500
	H	-2.79375000	1.44808000	0.53405000
	H	-1.25652900	1.53958000	1.35744200
	C	0.06580200	-0.34492600	0.19280900
	H	0.05249300	-0.60275200	1.25344600
	H	0.36979700	-1.24317500	-0.34021800
	C	-1.32579900	0.07971800	-0.26185100
	H	-1.29494300	0.20377000	-1.34957700
	C	-2.40587600	-0.98812100	0.02157700
	C	-3.66703900	-0.69062300	-0.76360700
	H	-4.43780700	-1.40699300	-0.49401900
	H	-4.05291400	0.30216500	-0.55045400
	H	-3.47811200	-0.76669900	-1.83167800
	C	-1.93109600	-2.38981700	-0.31801600
	H	-1.13298600	-2.71536100	0.34585000
	H	-2.75747000	-3.08759400	-0.21236700
	H	-1.55986600	-2.44653300	-1.33951600
	O	-2.79132900	-0.93206600	1.38249700
	H	-2.08008000	-1.26425400	1.92794900
	C	3.63723000	1.17822600	0.07533600
	H	4.58107200	0.65513000	0.18221800
	H	3.56462300	1.62387100	-0.91143600
	H	3.60251400	1.97719300	0.81473800

	O	2.62922200	-0.62838000	1.25671800
	O	-0.67518400	3.51038100	-0.14451600
	H	2.89557600	-1.60514100	0.59750800
	O	2.80462800	-0.98353500	-1.13000600
	O	3.03097000	-2.05342000	-0.48748700
TS14	C	-1.30189400	-1.13466800	-0.79381600
	H	-1.27474900	-2.15290100	-0.40756500
	H	-1.84346000	-1.15881800	-1.73643600
	C	-2.11412900	-0.32772400	0.20917000
	C	-1.86174900	1.16308400	0.05379500
	H	-2.04931000	1.75810100	0.96413300
	C	0.25086000	1.11555700	0.66874800
	H	0.07241800	1.27815700	1.72116700
	H	0.52307600	1.98681400	0.08846200
	C	0.10800800	-0.62711700	-1.05254200
	H	0.05719700	0.22138400	-1.73456000
	H	0.66103500	-1.41919800	-1.55413500
	C	0.82012600	-0.18555100	0.22418300
	H	0.64589200	-0.93283600	0.99777100
	C	2.35496100	-0.05915500	0.03468500
	C	2.99328000	0.55529800	1.26274400
	H	4.07230800	0.59252100	1.13839600
	H	2.63657700	1.57096700	1.41075200
	H	2.76271400	-0.02998600	2.15004200
	C	2.98590400	-1.41367300	-0.23887600
	H	2.62319100	-1.85584700	-1.16396800
	H	4.06296100	-1.29616100	-0.32835500
	H	2.77935800	-2.11107100	0.56998500
	O	2.64617300	0.83398300	-1.02068500
	H	2.32671300	0.46501500	-1.84262300
	C	-3.60073300	-0.56335600	0.00192000
	H	-4.18893200	-0.03695100	0.75450400
	H	-3.90842800	-0.20258400	-0.97513000
	H	-3.81677000	-1.62685100	0.07778700
	O	-1.73901500	-0.74545600	1.50753700
	O	-1.85000800	1.69687700	-1.04718400
	H	-2.40679700	-0.46915300	2.13235100
TS15	C	-1.81356800	-0.58918800	-0.55815700
	H	-1.26567600	-1.52039600	-0.71771800
	H	-2.02693500	-0.17697900	-1.54330100
	C	-3.13586800	-0.93659600	0.10547500
	C	-4.00563600	0.29046100	0.27306400
	H	-4.66188400	0.26459900	1.15765100
	C	1.28024900	-0.62841400	0.14831600
	H	0.63976000	-1.49380100	0.32267000
	H	1.76958200	-0.34611400	1.08325800

	C	-0.97322600	0.39634100	0.23084800
	H	-0.91159400	0.07322100	1.27073300
	H	-1.48949300	1.35467800	0.22545900
	C	0.43547200	0.55756300	-0.33740400
	H	0.38501200	0.50933000	-1.42747900
	C	1.08164500	1.90359200	0.04286100
	C	2.54927300	1.94521500	-0.32269200
	H	2.95313100	2.92254200	-0.07236400
	H	3.11411600	1.19371700	0.22028700
	H	2.68726200	1.76506500	-1.38562800
	C	0.36617200	3.06087400	-0.63416000
	H	-0.68546400	3.11962400	-0.36190300
	H	0.83905200	3.99462800	-0.34161300
	H	0.42461600	2.97139400	-1.71650500
	O	1.04050300	2.06180200	1.45031300
	H	0.13751300	2.21935300	1.72202600
	C	-3.92918500	-1.92859400	-0.73131800
	H	-4.88017200	-2.16027000	-0.25765400
	H	-4.11694400	-1.53193600	-1.72506900
	H	-3.36373300	-2.85406600	-0.83608000
	O	-2.95953900	-1.42131000	1.41680100
	O	-4.01822600	1.20533200	-0.50078200
	H	-2.63186700	-2.31802500	1.38518200
	O	2.19009600	-0.89615800	-0.86237700
	O	3.12980700	-2.31202500	-0.26264800
	N	4.22449600	-2.01373800	0.19474000
	O	4.66489400	-0.92738000	0.30042800
TS16	C	-1.71729800	-0.34074900	-0.69596500
	H	-1.36176400	-1.28995400	-1.10217800
	H	-1.95804200	0.29480600	-1.54715100
	C	-3.00052200	-0.61728400	0.06924000
	C	-3.61915100	0.66339900	0.58682400
	H	-4.16700200	0.55197700	1.53620400
	C	1.28584100	-1.07631800	-0.51471200
	H	0.58038800	-1.82554300	-0.11107900
	H	2.04122600	-1.08219300	0.51857000
	C	-0.63633300	0.32196200	0.13863100
	H	-0.53945200	-0.20958300	1.08762000
	H	-0.96469700	1.33151300	0.37165700
	C	0.71128700	0.34313000	-0.57429800
	H	0.55697300	0.56428900	-1.63252600
	C	1.67944300	1.40782300	-0.02634500
	C	3.02403500	1.33737700	-0.71907600
	H	3.68220600	2.09107100	-0.29522900
	H	3.49158900	0.36695400	-0.60491600
	H	2.91254500	1.52358400	-1.78404700

	C	1.11989800	2.81104900	-0.18303900
	H	0.21609500	2.96784200	0.40104100
	H	1.86079500	3.53202300	0.15227200
	H	0.88351400	3.02062700	-1.22375400
	O	1.93489200	1.13738900	1.34365200
	H	1.16215700	1.36784700	1.85745200
	C	-4.04097200	-1.28233300	-0.81863300
	H	-4.95988600	-1.46563200	-0.26685600
	H	-4.26556400	-0.66148300	-1.68130500
	H	-3.65940300	-2.23765300	-1.17788400
	O	-2.76790200	-1.38754200	1.22634200
	O	-3.55863100	1.71063100	0.00751700
	H	-2.63816700	-2.30169400	0.98152600
	O	2.10639300	-1.50009400	-1.38402900
	O	3.18189400	-1.50831200	1.14976300
	O	3.88949400	-1.94546300	0.27485600
TS17	C	0.32609800	2.01623100	-0.51961500
	H	0.06397100	2.84873800	0.13127800
	H	0.78254700	2.42670100	-1.41758800
	C	1.37144000	1.19225500	0.23886000
	C	1.13541000	-0.26806600	-0.18097400
	H	1.99123300	-0.88561700	0.49415000
	C	-0.19567900	-0.82580700	0.31021300
	H	-0.11569900	-1.18970300	1.33108200
	H	-0.44887200	-1.65905200	-0.34242100
	C	-0.91653100	1.21480400	-0.89138900
	H	-0.71031700	0.64345600	-1.80046500
	H	-1.72424300	1.90564300	-1.12179500
	C	-1.29063400	0.24866600	0.22316400
	H	-1.29902800	0.80702100	1.15979500
	C	-2.67889700	-0.39324700	0.06067600
	C	-2.92712700	-1.41000300	1.15558400
	H	-3.92803400	-1.82108600	1.05542300
	H	-2.22047200	-2.23135700	1.08505400
	H	-2.83441900	-0.94930200	2.13663700
	C	-3.77964000	0.65425000	0.08815200
	H	-3.71537200	1.33569000	-0.75750900
	H	-4.74851000	0.16371100	0.04224000
	H	-3.73406300	1.24640000	0.99978700
	O	-2.74916900	-1.12991400	-1.14619000
	H	-2.68441500	-0.52960000	-1.88697600
	C	2.77653800	1.65346600	-0.05531200
	H	3.50000800	1.11961300	0.56214800
	H	3.02393200	1.46234800	-1.09475500
	H	2.86980500	2.71736600	0.14836000
	O	1.06731100	1.32343500	1.61461900

	O	1.56069800	-0.61047900	-1.33507400
	H	1.81747000	1.03730500	2.13312900
	O	3.10178400	-1.70978900	0.65985200
	O	3.41795400	-1.99119800	-0.47242400
TS18	C	-0.40420200	0.73097900	1.57169500
	H	-0.16832900	1.78729200	1.69563200
	H	-0.94299200	0.40588800	2.46068900
	C	-1.32541500	0.63686300	0.37131900
	C	-0.55948200	1.04196100	-0.88979500
	H	-1.20755200	0.88757100	-1.75380900
	C	0.70516200	0.23289500	-1.06166600
	H	1.19210300	0.58994300	-1.96490300
	H	0.44567000	-0.81317400	-1.21660800
	C	0.87990700	-0.06076100	1.39661600
	H	0.63060800	-1.12277000	1.34663900
	H	1.49421000	0.08889300	2.28171100
	C	1.63300500	0.35081500	0.13825600
	H	1.91755400	1.40081000	0.24424500
	C	2.93430900	-0.45033900	-0.06292300
	C	3.67900600	0.01021000	-1.29974200
	H	4.64400800	-0.48693800	-1.35162300
	H	3.13020200	-0.24454900	-2.20034600
	H	3.84056800	1.08560300	-1.27729400
	C	3.84860300	-0.32839700	1.14545100
	H	3.41943200	-0.80064900	2.02661800
	H	4.79497900	-0.82057700	0.93707100
	H	4.04591700	0.71467300	1.38589000
	O	2.64702900	-1.81775100	-0.30065000
	H	2.27044300	-2.20116400	0.48937900
	C	-2.58194000	1.45069300	0.56556500
	H	-3.23343100	1.38074300	-0.30209200
	H	-3.12990100	1.09850000	1.43593000
	H	-2.32404100	2.49320200	0.73337600
	O	-0.19115300	2.40335600	-0.79539200
	O	-1.61999700	-0.76238700	0.30446000
	O	-2.39853500	-1.02399600	-0.84542000
	O	-4.40802100	-1.02423900	-0.00384400
	N	-3.57000000	-1.75512200	-0.28804000
	H	-0.91775100	2.95317600	-1.07611100
TS19	C	-0.33943400	0.82254700	1.55382700
	H	-0.11163900	1.88833800	1.57437000
	H	-0.85993800	0.57220600	2.47587100
	C	-1.30109800	0.63325400	0.37295300
	C	-0.54827200	0.94509900	-0.92456600
	H	-1.21165200	0.72151500	-1.76324900
	C	0.71209600	0.12353900	-1.05437500

	H	1.17889300	0.39618900	-1.99679400
	H	0.44796100	-0.93129500	-1.10613800
	C	0.94392300	0.02641900	1.41187500
	H	0.70547400	-1.03831200	1.45150900
	H	1.57489300	0.25212800	2.26891800
	C	1.66640500	0.34349500	0.10968100
	H	1.94396300	1.40050300	0.12701900
	C	2.96959900	-0.46228300	-0.05780100
	C	3.67924500	-0.09914900	-1.34641800
	H	4.65038800	-0.58575700	-1.37848400
	H	3.11451900	-0.43814900	-2.20856500
	H	3.82410800	0.97626600	-1.42014600
	C	3.91143400	-0.23469300	1.11359200
	H	3.50594600	-0.63165200	2.04205900
	H	4.85595600	-0.73846600	0.92544800
	H	4.10784800	0.82584400	1.25974000
	O	2.68829300	-1.84659300	-0.17550700
	H	2.36425700	-2.17420900	0.66141100
	C	-2.53816900	1.49007800	0.54635200
	H	-3.17685100	1.42559700	-0.33523000
	H	-3.10616200	1.14369200	1.40499500
	H	-2.27582200	2.53329800	0.70325200
	O	-0.18035200	2.30796600	-0.95122600
	O	-1.60966900	-0.71995600	0.44905900
	O	-2.68118100	-1.09311000	-0.95061400
	O	-4.29581500	-1.23955100	0.45168000
	N	-3.84370300	-1.31945600	-0.63114200
	H	-0.93081000	2.83857300	-1.20584800
TS20	C	1.35314800	-1.08861100	-0.93460700
	H	1.46776800	-0.41451700	-1.78332400
	H	1.74770000	-2.05890500	-1.24637800
	C	2.22977300	-0.63029600	0.21377500
	C	1.32988900	1.27200100	0.35247100
	H	1.98243400	1.62504400	1.14277900
	C	-0.06486600	0.92964800	0.71358100
	H	-0.59297100	1.86609600	0.90234000
	H	-0.04245400	0.37817000	1.64943500
	C	-0.10614800	-1.22656100	-0.55453200
	H	-0.16042900	-1.82431900	0.35802900
	H	-0.61052300	-1.78121900	-1.34160900
	C	-0.79977000	0.11489300	-0.34639800
	H	-0.75891500	0.66178200	-1.29215700
	C	-2.29125500	-0.03374900	0.02297300
	C	-3.00605100	1.30233600	-0.01785500
	H	-4.05640000	1.15714300	0.21990100
	H	-2.59968500	1.99506300	0.71175700

	H	-2.93134900	1.74895000	-1.00656800
	C	-3.00566100	-0.99981700	-0.90892200
	H	-2.65840200	-2.02101100	-0.76971900
	H	-4.07209700	-0.98244100	-0.70059700
	H	-2.85132700	-0.73030800	-1.95246000
	O	-2.42763500	-0.48141500	1.35930800
	H	-2.03460700	-1.34900500	1.44273100
	C	3.62460300	-0.18959300	-0.16237000
	H	4.09482000	0.32271400	0.67195100
	H	4.21642500	-1.07799400	-0.38127700
	H	3.63746800	0.43460100	-1.05336900
	O	2.01281200	-1.04528000	1.36015100
	O	1.45404700	1.90932800	-0.83419300
	H	2.32677200	2.28758500	-0.92228800
TS21	C	1.86924400	0.04876400	-0.05918400
	H	1.81653900	0.82816500	0.70219000
	H	1.77035800	0.58471800	-1.00639200
	C	3.24968800	-0.55097700	-0.01364200
	C	-1.45714600	1.85843000	0.79282000
	H	-1.55889400	2.55834700	1.62572500
	C	-0.93016900	0.51190500	1.14975300
	H	-1.66752300	0.04477500	1.80747100
	H	-0.05452300	0.66184300	1.78068200
	C	0.77689600	-0.98722600	0.08568400
	H	0.90070700	-1.49631900	1.04361200
	H	0.94788300	-1.74072500	-0.67768300
	C	-0.63206000	-0.41670500	-0.02794800
	H	-0.69316200	0.16123300	-0.95373600
	C	-1.70822700	-1.52042000	-0.13356100
	C	-3.08722000	-0.92453000	-0.32241200
	H	-3.81677200	-1.72710300	-0.38785600
	H	-3.36797400	-0.28820200	0.51111100
	H	-3.12829300	-0.32404700	-1.22658300
	C	-1.42597500	-2.48098900	-1.27679100
	H	-0.54559700	-3.09202200	-1.09169000
	H	-2.27116200	-3.15210200	-1.40325800
	H	-1.27139700	-1.94358700	-2.21037300
	O	-1.77609800	-2.23668500	1.08861200
	H	-0.99511500	-2.78063200	1.17726200
	C	4.40378200	0.40544100	-0.06084000
	H	4.44642400	0.96585600	0.87197300
	H	5.33071100	-0.14050200	-0.19072000
	H	4.27846400	1.13060100	-0.86160500
	O	3.41747400	-1.74254300	0.06771300
	O	-2.14907000	2.05926800	-0.24575200
	H	-1.36043500	2.71673500	-0.91060500

	O	-0.26837100	3.12692300	-0.98222600
	O	0.13692500	2.71438900	0.14630300
TS22	C	1.85631000	0.24961500	-0.43921600
	H	1.65164600	1.27323300	-0.11841400
	H	1.86370400	0.29427300	-1.53036900
	C	3.23983800	-0.11118700	0.02971500
	C	-1.10782800	2.64289900	0.19707300
	H	-0.28922200	3.26974400	-0.11783400
	C	-0.93388400	1.50813000	0.91584200
	H	-1.76513000	0.98752600	1.36840700
	H	0.01675600	1.37291800	1.40560000
	C	0.78656800	-0.69893600	0.05263200
	H	0.84642800	-0.76165100	1.14181600
	H	1.04455100	-1.70227300	-0.30027300
	C	-0.58496000	-0.30139100	-0.38584400
	H	-0.63907600	0.15920300	-1.36654800
	C	-1.73468400	-1.23367200	-0.09506300
	C	-3.04841400	-0.65053300	-0.57103100
	H	-3.85592900	-1.35298200	-0.38323700
	H	-3.27642000	0.26583400	-0.03545600
	H	-3.01028700	-0.43164700	-1.63480600
	C	-1.52154100	-2.59069300	-0.76093700
	H	-0.63263200	-3.08500800	-0.37433800
	H	-2.37686400	-3.23311300	-0.56402200
	H	-1.40429200	-2.48419100	-1.83716400
	O	-1.89779500	-1.42637200	1.30314100
	H	-1.13235600	-1.88275400	1.64868300
	C	4.37367900	0.70435500	-0.51813800
	H	5.28758700	0.47243200	0.01582400
	H	4.50832300	0.47220000	-1.57364300
	H	4.15909700	1.76847300	-0.45037400
	O	3.42824700	-1.01787900	0.80199100
	O	-2.27444100	3.06458000	-0.33394100
	H	-2.99447600	2.52363200	-0.01357200
TS23	C	1.58534300	-0.67997700	0.08606100
	H	1.66335200	-1.52432300	-0.60153500
	H	1.53918800	-1.12316900	1.08327000
	C	2.85448800	0.12407100	-0.00180100
	C	0.34279000	0.13344800	-0.19534400
	H	0.44705500	0.58300600	-1.18673100
	H	0.32423700	0.97790900	0.50249600
	C	-0.90654000	-0.66992200	-0.09686000
	H	-0.86473500	-1.66299500	0.32424900
	C	-2.14361300	-0.14209500	-0.33265200
	C	-3.36813200	-0.97847600	-0.48920300
	H	-4.25571500	-0.42910200	-0.19258900

	H	-3.48094400	-1.25950600	-1.53497200
	H	-3.29321500	-1.88104900	0.10798700
	C	-2.57838300	0.55881100	1.74571600
	H	-1.70137800	1.14174200	1.98642700
	H	-3.46060500	1.12074700	1.47972900
	H	-2.73026600	-0.33118300	2.33770800
	O	-2.29174400	1.05821600	-0.95667100
	H	-1.47906800	1.55922600	-0.90716700
	C	4.14301200	-0.62363400	0.17249600
	H	4.29991700	-1.27980900	-0.68232000
	H	4.96839000	0.07491300	0.24165800
	H	4.11115000	-1.25478300	1.05781100
	O	2.83410000	1.31116300	-0.21164200
TS24	C	1.58147100	-0.33240600	-0.23001500
	H	1.69253600	0.51206900	0.45129700
	H	1.67164300	0.08227200	-1.23762000
	C	2.74245600	-1.26866000	-0.02187800
	C	0.24465300	-1.00830700	-0.03491800
	H	0.18821000	-1.36801600	0.99246600
	H	0.19781300	-1.88641800	-0.67401300
	C	-0.92962600	-0.09180100	-0.32144100
	H	-0.97385200	0.13685000	-1.38992000
	C	-2.30975300	-0.69522300	0.04234300
	C	-3.40550900	0.29078900	-0.29384500
	H	-4.36840300	-0.14245500	-0.03867800
	H	-3.27193800	1.20590100	0.27208000
	H	-3.39922700	0.52847500	-1.35518500
	C	-2.51722000	-2.00298500	-0.69943400
	H	-1.81162700	-2.76587100	-0.37653500
	H	-3.52103800	-2.36816300	-0.49919900
	H	-2.40548900	-1.87397300	-1.77399500
	O	-2.39861000	-0.90320100	1.43302200
	H	-1.86004700	-1.65165700	1.68333400
	C	4.11265100	-0.66111800	-0.05643600
	H	4.23644700	-0.02753600	-0.93193100
	H	4.24838600	-0.02660500	0.81810200
	H	4.86374900	-1.44202600	-0.05161100
	O	2.57489300	-2.44703000	0.17121700
	O	-0.82036000	1.11025700	0.38045700
	O	-0.09209700	2.23599100	-0.79886000
	N	0.70489400	3.02643400	-0.31278500
	O	1.04415200	3.06903000	0.81349500
TS25	C	1.47591800	0.90131800	-0.52750200
	H	2.09899400	1.74213200	-0.82134000
	H	1.05579700	0.49544100	-1.45328700
	C	2.33703900	-0.19882600	0.02815000

	C	0.34722400	1.33055100	0.40478900
	H	0.50379400	2.35721300	0.72945500
	H	0.34895200	0.73044800	1.31220000
	C	-1.04108800	1.30822000	-0.21253900
	H	-1.04962400	1.21018900	-1.31232400
	C	-1.57910600	-0.71398300	-0.11864800
	C	-1.78024600	-0.92533800	1.34239400
	H	-2.28157000	-1.88110300	1.50624300
	H	-0.83418400	-0.95387100	1.87828500
	H	-2.39618600	-0.12854300	1.74827500
	C	-2.78889300	-0.68825500	-0.98107100
	H	-2.51868200	-0.47722500	-2.01198600
	H	-3.28307000	-1.66076200	-0.95431200
	H	-3.47780600	0.07162400	-0.62668200
	O	-0.55710000	-1.37647300	-0.68805000
	H	0.17834300	-1.46888800	-0.06293000
	C	3.80840400	-0.11725700	-0.20462000
	H	4.20801800	0.74540400	0.32678000
	H	4.29836700	-1.01998600	0.13912200
	H	4.01067500	0.04384400	-1.26185700
	O	1.84746500	-1.13188800	0.63010800
	O	-1.98253000	1.86029900	0.36777300
TS26	C	-0.56289900	-0.00036200	0.21450600
	O	0.06077000	-0.00197500	1.32043700
	H	1.21444900	-0.00268700	0.92512600
	O	1.92459900	-0.00039000	-0.00725600
	O	1.02374700	0.00269200	-0.89920400
	C	-1.16301500	1.27869100	-0.27048900
	H	-0.53087900	2.11543300	0.00503400
	H	-2.12931300	1.40500000	0.21644400
	C	-1.16215100	-1.27847200	-0.27396100
	H	-2.12596100	-1.40880700	0.21689100
	H	-1.32498000	-1.26131200	-1.34685100
	H	-0.52722000	-2.11511600	-0.00476300
	H	-1.32063500	1.26573500	-1.34402900
TS27	C	1.17541500	-1.31902100	-0.98856800
	H	1.36499900	-0.67415800	-1.83643500
	H	1.77205500	-2.21678500	-0.91797900
	C	2.28147600	-0.16732200	0.47142100
	C	-0.01502000	0.92302200	0.63027700
	H	-0.44526000	1.91945700	0.67245700
	H	-0.07096900	0.48947200	1.62719400
	C	-0.18728200	-1.33168200	-0.41347300
	H	-0.13994100	-1.77410300	0.58350200
	H	-0.80106800	-1.99321200	-1.03290900
	C	-0.80730500	0.05924800	-0.34049600

	H	-0.74153900	0.51163000	-1.33324400
	C	3.61798300	-0.21335400	-0.22650200
	H	4.28448300	0.49586000	0.26735800
	H	4.04675900	-1.20335800	-0.11617200
	H	3.55334300	0.05191800	-1.27672500
	O	2.08096000	-0.84435900	1.47813100
	C	1.44191000	1.09576300	0.26486600
	H	1.87368400	1.81846000	0.96623000
	C	-2.30389100	0.00870600	0.03224000
	C	-2.88388400	1.39847800	0.20480800
	H	-2.49823700	1.86737300	1.10395900
	H	-2.64895800	2.02719500	-0.65144100
	H	-3.96403600	1.33436800	0.30457400
	C	-3.10998400	-0.73023800	-1.02505400
	H	-2.81722200	-1.77433700	-1.11218500
	H	-4.16320600	-0.70690000	-0.75804600
	H	-2.99079000	-0.26639400	-2.00222800
	O	-2.48059300	-0.61704900	1.29081000
	H	-2.25296500	-1.54227700	1.21944500
	O	1.53520300	1.60213800	-1.04866100
	H	2.29781100	2.16833500	-1.12670600
TS28	C	-1.51983300	-0.54190900	0.80921000
	H	-1.01342100	-1.42452200	0.41857300
	H	-2.13245100	-0.80244600	1.67396500
	C	1.93630000	-1.97156700	-0.48928300
	C	1.92106500	0.30945600	0.50274000
	H	2.66561600	0.54742100	-0.25418600
	H	2.21099800	0.85736400	1.40344200
	C	-0.48513300	0.50815000	1.19181100
	H	0.01006400	0.15188700	2.09521300
	H	-1.01829900	1.40790900	1.49489900
	C	0.53899000	0.79696900	0.08592100
	H	0.22677000	0.25998000	-0.81127000
	C	3.20663100	-2.34819900	-1.17506500
	H	3.74079400	-3.06970800	-0.56100000
	H	2.98431000	-2.76782800	-2.14858300
	H	3.86244500	-1.48493800	-1.26273900
	O	0.84612300	-2.24178200	-0.93047900
	C	2.04604200	-1.18210700	0.79775000
	H	1.23560000	-1.52130800	1.44586900
	C	0.56959800	2.29329400	-0.29234700
	C	1.64237500	2.59501600	-1.32095600
	H	2.63193400	2.54512500	-0.87779100
	H	1.58992200	1.89859400	-2.15516800
	H	1.50745800	3.60307800	-1.70286300
	C	-0.77508100	2.73750900	-0.83907700

	H	-0.73400900	3.79578200	-1.08576200
	H	-1.02878900	2.17772500	-1.73577700
	H	-1.58616600	2.58182100	-0.13100200
	O	0.91760800	3.06868600	0.84541400
	H	0.13780000	3.21964600	1.37558700
	O	3.29503600	-1.47569800	1.36914800
	H	3.46973800	-0.86212800	2.07955900
	O	-2.28805400	0.05953800	-0.18238600
	O	-3.31230000	-1.26129200	-0.84618100
	O	-4.77088000	-0.73854900	0.63411600
	N	-4.39232900	-1.36862300	-0.28603300
TS29	C	0.50723400	-2.08008600	-0.36390900
	H	0.29326400	-1.97096900	-1.44082700
	H	1.57404500	-1.39433900	-0.39560700
	C	1.43481200	1.70244300	-0.65180900
	C	-0.58491900	1.18878000	0.70044900
	H	-1.03737400	2.08175500	0.27358100
	H	-0.94600300	1.11914800	1.72956600
	C	-0.43630900	-1.32574500	0.56177100
	H	0.07719300	-1.12019500	1.49994800
	H	-1.21097000	-2.04616400	0.82405400
	C	-1.04265400	-0.05689900	-0.04651300
	H	-0.70450200	0.02217500	-1.08172900
	C	1.76946300	3.10773200	-1.01501100
	H	2.60254700	3.44752500	-0.40386200
	H	2.02006400	3.16207300	-2.06732400
	H	0.93641300	3.76566300	-0.77747400
	O	1.52616600	0.78181300	-1.42971200
	C	0.92128800	1.42754200	0.74285500
	H	1.44333000	0.53527700	1.09519100
	O	1.23403500	2.53266600	1.54883900
	C	-2.58365200	-0.13710900	-0.10237300
	C	-3.20130700	1.14562100	-0.62276400
	H	-3.12719200	1.93814200	0.11504300
	H	-2.71694000	1.46825300	-1.54209400
	H	-4.25681600	0.98669400	-0.82550600
	C	-3.02367700	-1.28936400	-0.98993400
	H	-2.61994600	-2.24570500	-0.66348400
	H	-4.10815000	-1.36232800	-0.97951000
	H	-2.70101500	-1.12807900	-2.01630700
	O	-3.11170000	-0.29187500	1.20340900
	H	-2.96612400	-1.18733100	1.50318800
	O	0.98906800	-3.18920000	0.02210500
	O	3.20775000	-2.36816800	0.39619300
	O	2.91191800	-1.28935300	-0.05706200
	H	0.82860200	2.42384000	2.40639900

TS30	C	1.30839300	-1.21874400	-0.72241500
	H	1.44120800	-0.74264000	-1.69098100
	H	1.76691300	-2.20337400	-0.73122300
	C	1.92238300	-0.38372100	0.36948900
	C	1.39133000	1.04134900	0.38460300
	H	1.90161100	1.59401700	1.17338500
	C	-0.09178000	0.92936300	0.70046000
	H	-0.49243600	1.93919700	0.72282000
	H	-0.21378400	0.49731900	1.69306500
	C	-0.18519400	-1.30661300	-0.40972900
	H	-0.30262600	-1.83059900	0.54189300
	H	-0.66210900	-1.91066100	-1.17794200
	C	-0.83160300	0.07271400	-0.32149400
	H	-0.73141700	0.55293600	-1.29784900
	C	-2.34002000	-0.00298500	-0.00797000
	C	-2.95584900	1.37977600	0.06869500
	H	-4.03615800	1.29565300	0.15024500
	H	-2.60139100	1.91161500	0.94536800
	H	-2.71597700	1.96175000	-0.81840400
	C	-3.08064000	-0.82175600	-1.05284200
	H	-2.77340700	-1.86554800	-1.04467600
	H	-4.14792500	-0.79076200	-0.85001300
	H	-2.90728800	-0.42948500	-2.05305900
	O	-2.55122300	-0.56762300	1.27468800
	H	-2.35248900	-1.50166600	1.24576100
	C	3.89221300	-0.06802200	-0.49034000
	H	4.26573500	0.69456100	0.17540000
	H	4.28443100	-1.06068400	-0.34533500
	H	3.62357100	0.21584800	-1.49634900
	O	2.31837400	-0.88772300	1.42270800
	O	1.49511700	1.69419200	-0.85842600
	H	2.37998900	2.03358200	-0.96461300
TS31	C	1.79909400	-1.10060100	-1.02822400
	H	1.84134500	-0.32553700	-1.79643700
	H	2.34884500	-1.95210000	-1.43094600
	C	2.46941600	-0.61256800	0.21612100
	C	1.74377000	-0.16967400	1.23594300
	H	2.24618600	0.17204400	2.13219100
	C	0.25440200	-0.07274700	1.24826000
	H	-0.03873300	0.92885800	1.55588900
	H	-0.15479100	-0.75992900	1.99089600
	C	0.36182600	-1.50778100	-0.77261900
	H	0.35746300	-2.38922400	-0.13065600
	H	-0.12225400	-1.76528500	-1.71184500
	C	-0.41594100	-0.40922900	-0.07022100
	C	-1.91218100	-0.77529400	0.15106800

	C	-2.60584600	0.27451100	0.99349500
	H	-3.66447600	0.04043700	1.06074400
	H	-2.20223400	0.28761700	2.00102800
	H	-2.49158500	1.26031800	0.55159600
	C	-2.65218500	-0.95275600	-1.16250700
	H	-2.23385500	-1.76174200	-1.75837200
	H	-3.69110600	-1.19310500	-0.95191500
	H	-2.61396100	-0.04541000	-1.75795300
	O	-1.97273300	-1.96868400	0.90517600
	H	-1.81398200	-2.71423100	0.32926500
	C	3.95996600	-0.63309900	0.23050500
	H	4.35861400	-0.23230300	1.15830000
	H	4.34014000	-1.64688100	0.10353000
	H	4.36020500	-0.04206800	-0.59379200
	O	-0.50148200	0.71315800	-0.97606000
	O	0.56792400	1.60941100	-0.80301400
	N	-0.14657400	2.90083000	-0.59743100
	O	-0.32042600	3.09463500	0.52134300
TS32	C	1.58317700	-1.32255300	-1.02027300
	H	1.74165400	-0.55714500	-1.78318200
	H	2.02558100	-2.23652600	-1.41774200
	C	2.28867300	-0.92926100	0.23835500
	C	1.61151700	-0.40086700	1.25171100
	H	2.14292900	-0.13022500	2.15575900
	C	0.14396800	-0.11928300	1.25015900
	H	-0.04287600	0.90777500	1.56400100
	H	-0.35375500	-0.75946500	1.98028700
	C	0.09963000	-1.53339200	-0.79448400
	H	-0.03219100	-2.41093000	-0.16105200
	H	-0.39666100	-1.71679600	-1.74477900
	C	-0.53160800	-0.33990300	-0.09745200
	C	-2.08619500	-0.52896800	0.12621900
	C	-2.63590600	0.58894400	0.98513300
	H	-3.71918700	0.51264500	1.02324300
	H	-2.26209900	0.50954900	2.00108000
	H	-2.35548900	1.55624300	0.57827500
	C	-2.83044500	-0.59141300	-1.19307900
	H	-2.48995400	-1.41744400	-1.81461500
	H	-3.89016000	-0.73126000	-0.99490700
	H	-2.69450200	0.32783500	-1.75578700
	O	-2.28369700	-1.71735900	0.85405100
	H	-2.22289400	-2.46550800	0.26267200
	C	3.76474000	-1.13582100	0.27480900
	H	4.19605800	-0.79345000	1.21128200
	H	4.01683100	-2.18837500	0.14562200
	H	4.24843200	-0.59498100	-0.53917900

	O	-0.51109300	0.79040500	-0.91530000
	O	1.06337000	1.63434800	-0.83280300
	N	1.00216100	2.71788000	-0.26877500
	O	0.05990200	3.17235700	0.27453500
TS33	C	-1.86357000	-1.24219000	0.03478600
	H	-1.98777400	-1.60565700	1.05716400
	H	-2.36713000	-1.96443900	-0.60933600
	C	-2.52098300	0.09714900	-0.09797400
	C	-1.80965600	1.22046700	-0.09916900
	H	-2.32646000	2.16706400	-0.19881600
	C	-0.32052600	1.29180800	0.05324600
	H	-0.06000100	2.02621300	0.81321900
	H	0.12916300	1.60879200	-0.88920500
	C	-0.37961500	-1.19060700	-0.30096800
	H	-0.26812500	-1.01035900	-1.37137200
	H	0.09744900	-2.12982300	-0.03519200
	C	0.22583800	-0.05302900	0.49259300
	C	2.12697600	0.04055700	-0.26818200
	C	2.68035500	1.25123600	0.39764700
	H	3.74660200	1.32760400	0.18006500
	H	2.19867500	2.15054200	0.02790500
	H	2.53619900	1.17861600	1.47034300
	C	2.72178300	-1.26916100	0.12746000
	H	2.27622900	-2.09890100	-0.41783100
	H	3.79161700	-1.26171200	-0.08725300
	H	2.56956800	-1.43589800	1.18838500
	O	1.98840700	0.23978200	-1.60407900
	H	1.82284900	-0.59323100	-2.04465500
	C	-4.00959200	0.09419900	-0.20006500
	H	-4.41070500	1.10235600	-0.25292200
	H	-4.34094200	-0.45288000	-1.08285400
	H	-4.45432000	-0.40258500	0.66259200
	O	0.50422300	-0.24581600	1.69826900
IM1	C	1.51519200	1.33421400	-0.08968100
	H	1.62615800	1.85092900	0.86234500
	H	2.04088600	1.92198400	-0.83974400
	C	2.20987800	-0.02183200	0.06775100
	C	1.47656400	-1.06928900	-0.68895300
	H	2.02158500	-1.79306600	-1.27933100
	C	0.01923800	-1.23276700	-0.46946400
	H	-0.17059300	-2.12035100	0.14248000
	H	-0.48378200	-1.41847800	-1.42352900
	C	0.04467300	1.21788000	-0.46960000
	H	-0.03670700	1.10973000	-1.55399800
	H	-0.46203000	2.14334700	-0.20232500
	C	-0.60673900	0.00195700	0.17485800

	H	-0.35778300	0.00618800	1.23705300
	C	-2.13969300	-0.00150500	0.05690600
	C	-2.72130000	-1.32455200	0.50933900
	H	-3.80681500	-1.27129200	0.50560600
	H	-2.42449100	-2.12299600	-0.16377900
	H	-2.38621100	-1.56903200	1.51505400
	C	-2.75655500	1.12213900	0.87297100
	H	-2.41988200	2.10178800	0.53970200
	H	-3.83889200	1.09114200	0.77599000
	H	-2.50001100	1.02335500	1.92550100
	O	-2.53157800	0.12361400	-1.30093700
	H	-2.30634800	0.99971800	-1.60919200
	C	3.66953500	0.05910000	-0.32445400
	H	4.17498900	-0.88670400	-0.13309900
	H	3.77338700	0.28791400	-1.38274400
	H	4.16714200	0.83445400	0.25266100
	O	2.11625900	-0.31155500	1.47286400
	H	2.44717600	-1.19717700	1.61789800
IM2	C	1.48649600	-1.40442900	-0.47004600
	H	1.57864300	-1.23992100	-1.55250100
	H	1.92076700	-2.38568100	-0.27746000
	C	2.24943300	-0.35343700	0.24821900
	C	1.63226500	0.99920400	0.29499900
	H	2.14829400	1.61660000	1.03495700
	C	0.15593900	0.95982600	0.62383500
	H	-0.22329400	1.97155000	0.50800800
	H	0.02223000	0.67310400	1.66710100
	C	0.00863500	-1.39836700	-0.10803400
	H	-0.09336900	-1.71963200	0.93173800
	H	-0.50625500	-2.13003800	-0.72740100
	C	-0.60689100	-0.01389400	-0.26129900
	H	-0.47961300	0.30428500	-1.29915100
	C	-2.11968600	-0.00445800	0.03208800
	C	-2.68895800	1.39854200	-0.02648800
	H	-3.77340700	1.35776400	0.03202800
	H	-2.33548900	1.99165700	0.81051600
	H	-2.40610000	1.89391400	-0.95266800
	C	-2.87505800	-0.88816000	-0.94745400
	H	-2.58250200	-1.93291100	-0.86578400
	H	-3.94137900	-0.82616200	-0.74567100
	H	-2.69844100	-0.57168300	-1.97344100
	O	-2.37052900	-0.44416000	1.35786700
	H	-2.19199600	-1.38091600	1.41408500
	C	3.71439900	-0.50334500	0.42069300
	H	4.12172400	0.25064000	1.09191100
	H	3.96969400	-1.48522200	0.81783200

	H	4.25310600	-0.41603400	-0.53171900
	O	1.72470600	1.63972600	-0.98218100
	H	2.64452700	1.71526400	-1.22694000
IM013	C	1.40487000	0.27978700	-1.18638900
	H	1.71024900	1.28305500	-0.87069000
	H	1.84702700	0.14074600	-2.17446100
	C	1.98692700	-0.72679100	-0.24489600
	C	1.21745300	-1.38574300	0.61677100
	H	1.67452100	-2.12683100	1.26147400
	C	-0.24996300	-1.16030200	0.78951100
	H	-0.46504000	-1.12123300	1.85683400
	H	-0.82063700	-2.00764700	0.39938100
	C	-0.10531700	0.17694100	-1.27564700
	H	-0.35749900	-0.73985700	-1.81418600
	H	-0.48843800	1.01212500	-1.85804800
	C	-0.73243900	0.11297500	0.11001400
	H	-0.36102600	0.96709100	0.68536000
	C	-2.26943100	0.21551800	0.09476800
	C	-2.84801200	-0.02260000	1.47421600
	H	-3.92074500	0.15032500	1.45799600
	H	-2.68136000	-1.04828800	1.78786400
	H	-2.39772700	0.64717200	2.20387000
	C	-2.73592900	1.57060500	-0.41254300
	H	-2.40969700	1.76468400	-1.43128900
	H	-3.82225000	1.60687600	-0.40024000
	H	-2.35717300	2.37304700	0.21722000
	O	-2.82146100	-0.81191200	-0.71084500
	H	-2.59739900	-0.64563400	-1.62473000
	C	3.46715300	-0.90179300	-0.32095200
	H	3.92371000	0.06297700	-0.11491000
	H	3.82935500	-1.62289400	0.40700600
	H	3.78919100	-1.21391100	-1.31336100
	O	3.82729100	2.04302300	0.96330900
	H	3.04642400	1.71772900	1.43607700
IM3	C	1.78709900	-1.25735400	-0.18683500
	H	1.76739500	-1.55992400	-1.23552600
	H	2.33578500	-2.03207900	0.34597400
	C	2.52126000	0.05087200	-0.06271600
	C	1.78711300	1.21410200	0.05322900
	H	2.32644500	2.14539700	0.16683700
	C	0.30208900	1.28886200	0.05546700
	H	-0.01023200	2.09522900	-0.60918200
	H	-0.05145200	1.57642800	1.05202200
	C	0.36698400	-1.16122200	0.33431300
	H	0.39811800	-0.98344800	1.41210600
	H	-0.13696600	-2.11265800	0.17416800

	C	-0.37620900	-0.01566300	-0.33603400
	H	-0.28057700	-0.14535400	-1.41820100
	C	3.90263800	0.06234300	-0.06238900
	H	4.45000100	0.98956100	0.00823100
	H	4.47182300	-0.85114900	-0.13486400
	C	-1.88313400	-0.00299200	-0.02051400
	C	-2.57752500	-1.22293300	-0.60295500
	H	-2.19018200	-2.15108200	-0.18771200
	H	-3.64042700	-1.17752200	-0.38029000
	H	-2.45232300	-1.26366100	-1.68299800
	C	-2.54605800	1.25063900	-0.55188300
	H	-3.62030900	1.19180700	-0.39862500
	H	-2.18200600	2.12818500	-0.02670600
	H	-2.35101500	1.37087600	-1.61549900
	O	-2.09114600	0.04099100	1.38104600
	H	-1.81045100	-0.78845800	1.76380600
IMO4	C	0.86490126	-2.01066052	-0.04081404
	H	0.77020526	-2.47615452	-1.02520704
	H	1.20650826	-2.79949752	0.63095596
	C	1.91539126	-0.93748552	-0.10642804
	C	1.53360026	0.32797348	-0.08210104
	H	2.32698626	1.08643048	-0.15477504
	C	0.15438226	0.87273248	-0.04035504
	H	0.07027026	1.68071348	-0.76496204
	H	-0.06181474	1.30763248	0.93831996
	C	-0.47476974	-1.47448052	0.42360696
	H	-0.40045474	-1.22801952	1.48523296
	H	-1.22580474	-2.25585652	0.32245496
	C	-0.87091374	-0.21878452	-0.34034704
	H	-0.82307674	-0.44365052	-1.40942604
	C	-2.30743174	0.24465948	-0.03573004
	C	-2.59079674	1.60027248	-0.64817504
	H	-3.63553374	1.85926548	-0.49942704
	H	-1.98636974	2.36839148	-0.17577804
	H	-2.38082074	1.59520048	-1.71565104
	C	-3.32745174	-0.76012952	-0.54590104
	H	-3.21639974	-1.73334352	-0.07200204
	H	-4.33033174	-0.39937852	-0.33271604
	H	-3.23269374	-0.90009252	-1.62059904
	O	-2.47458974	0.43099148	1.35903896
	H	-2.45653174	-0.42087752	1.79160496
	C	3.33709926	-1.37615052	-0.20540004
	H	4.00724526	-0.52702352	-0.29280904
	H	3.62204326	-1.95985452	0.66979096
	H	3.47700026	-2.02044452	-1.07330604
	O	3.84960174	2.48594352	0.06749804

	H	3. 80706474	2. 59318652	1. 02344004
IM4	C	1. 80054000	-1. 20714500	-0. 12083000
	H	1. 86407100	-1. 58025600	-1. 14651700
	H	2. 34744200	-1. 92228500	0. 49588400
	C	2. 47936800	0. 13967600	-0. 04028100
	C	1. 70783100	1. 19152600	0. 10171300
	C	0. 24684600	1. 33340800	0. 13561000
	H	-0. 06404000	2. 14827200	-0. 51657500
	H	-0. 10186800	1. 57907900	1. 14046100
	C	0. 35202800	-1. 13935600	0. 33047400
	H	0. 33641900	-0. 99800400	1. 41359700
	H	-0. 13169400	-2. 09132700	0. 11906600
	C	-0. 39897700	0. 01623000	-0. 31968900
	H	-0. 27155900	-0. 06277600	-1. 40267400
	C	3. 96918500	0. 17051400	-0. 12907100
	H	4. 30902100	-0. 29146800	-1. 05616700
	H	4. 34583800	1. 18747200	-0. 09522400
	H	4. 41802300	-0. 39127900	0. 69001200
	C	-1. 91209900	-0. 00565200	-0. 03593300
	C	-2. 57289000	-1. 21761300	-0. 67245800
	H	-2. 18036700	-2. 15198300	-0. 27662500
H	-3. 64125600	-1. 19472100	-0. 47346900	
H	-2. 42225100	-1. 22260400	-1. 74990100	
C	-2. 58335000	1. 25374400	-0. 54251100	
H	-3. 65976300	1. 17201600	-0. 41800300	
H	-2. 24801000	2. 11945300	0. 02013400	
H	-2. 36494400	1. 41252400	-1. 59646400	
O	-2. 14946200	-0. 00945000	1. 36089700	
H	-1. 87025400	-0. 84850400	1. 72314300	
IM05	C	1. 76951600	-1. 34770300	-0. 68992900
	H	1. 82305100	-1. 14308900	-1. 76292100
	H	2. 32534200	-2. 27480800	-0. 54116400
	C	2. 44554200	-0. 24270500	0. 06096300
	C	1. 73012000	0. 66794100	0. 71610900
	H	2. 25040900	1. 43035500	1. 28427400
	C	0. 24191600	0. 70532700	0. 75542900
	H	-0. 09918200	1. 73520100	0. 60130700
	H	-0. 11563800	0. 45418500	1. 75823100
	C	0. 32598500	-1. 53758800	-0. 26442300
	H	0. 31579600	-1. 96090700	0. 74314700
	H	-0. 14916600	-2. 25936000	-0. 92545800
	C	-0. 42689600	-0. 21545700	-0. 25056100
	H	-0. 34484700	0. 23140400	-1. 24580500
	C	-1. 92900100	-0. 36427100	0. 05612400
	C	-2. 60745000	0. 98910800	0. 11007800
	H	-3. 67918000	0. 85619700	0. 23251800

	H	-2.24662700	1.57000600	0.95278900
	H	-2.41961300	1.55563900	-0.79861500
	C	-2.63030700	-1.23810100	-0.96933100
	H	-2.26045700	-2.26152300	-0.95699400
	H	-3.69492300	-1.26871300	-0.75237200
	H	-2.49494400	-0.84570400	-1.97521000
	O	-2.10450600	-0.91851300	1.35036300
	H	-1.85455000	-1.84052500	1.33226800
	C	3.93695600	-0.24591700	0.05773600
	H	4.34277300	0.60620300	0.59586800
	H	4.32188100	-1.15537100	0.51946600
	H	4.32674700	-0.22370100	-0.96032300
	O	-0.17399500	3.47616900	-0.68180500
	H	0.74285500	3.30946100	-0.94263000
IM5	C	-1.77239600	1.21682500	-0.29039300
	H	-1.83368700	1.44799600	-1.35995600
	H	-2.31903500	2.01564000	0.21309900
	C	-2.43187000	-0.09433300	-0.02721100
	C	-1.64457300	-1.22533900	0.06541100
	H	-2.12558900	-2.17020500	0.28314800
	C	-0.27897500	-1.21219400	-0.12196100
	H	0.27799800	-2.12906100	-0.01624100
	C	-0.31632400	1.23252100	0.14554800
	H	-0.28198100	1.19050800	1.23781000
	H	0.14180900	2.17228700	-0.15302100
	C	0.45523900	0.05051500	-0.43235800
	H	0.48483200	0.18898400	-1.52097600
	C	-3.91080200	-0.12841700	0.09313100
	H	-4.38920400	0.26060100	-0.80845900
	H	-4.27914000	-1.13746100	0.25737900
	H	-4.25728500	0.49790500	0.91766500
	C	1.92681500	-0.02792200	0.02524300
	C	2.69731800	-1.00772500	-0.83557500
	H	3.70532700	-1.11751600	-0.44434600
	H	2.23116600	-1.98837000	-0.83855400
	H	2.75821300	-0.64943100	-1.86045700
	C	2.60540900	1.32989000	-0.02777100
	H	2.18841100	2.01006000	0.71163900
	H	3.66446400	1.21449700	0.18742500
	H	2.49833400	1.78892400	-1.00942100
	O	2.01323200	-0.54551700	1.33998100
	H	1.45046200	-0.03414400	1.91903000
IM06	C	-1.58157100	-0.97593900	0.94375900
	H	-1.70529000	-0.32570300	1.81464100
	H	-2.06756800	-1.91715600	1.20415600
	C	-2.28860200	-0.36925300	-0.22932600

	C	-1.60189000	0.20835800	-1.21549800
	H	-2.14579800	0.60634100	-2.06396000
	C	-0.11487800	0.36014400	-1.24079500
	H	0.12580900	1.37845900	-1.54505800
	H	0.31426200	-0.29295700	-2.00563600
	C	-0.10898200	-1.20531100	0.66767600
	H	-0.01118200	-2.01481500	-0.05938700
	H	0.38080500	-1.52772900	1.58429700
	C	0.53925100	0.04595300	0.09692600
	H	0.33786600	0.87357200	0.78736500
	C	2.07095100	-0.06047100	-0.02438200
	C	2.64497100	1.12874500	-0.76631000
	H	3.73061600	1.08693800	-0.74340600
	H	2.33491000	1.11824000	-1.80655600
	H	2.32049500	2.06194200	-0.31103500
	C	2.72809700	-0.16278600	1.34154400
	H	2.41081600	-1.05071500	1.88465200
	H	3.80721600	-0.21483400	1.22199700
	H	2.48974400	0.70463600	1.95317400
	O	2.41970100	-1.18760500	-0.81082600
	H	2.23980900	-1.98313100	-0.31306600
	C	-3.77784800	-0.46100300	-0.22905100
	H	-4.21448700	0.04185200	-1.08736600
	H	-4.09943000	-1.50226000	-0.24276400
	H	-4.19399400	-0.01810200	0.67616300
	O	-1.34032000	2.44338700	1.12806700
	H	-1.74665300	1.87854400	0.44660100
IM6	C	-1.68688200	-1.23416800	0.11322500
	H	-1.59510100	-1.56602600	1.15010500
	H	-2.27664100	-1.99750000	-0.39651900
	C	-2.42029700	0.07126600	0.07250000
	C	-1.76911000	1.21967000	-0.08190300
	H	-2.33523500	2.14181000	-0.12144200
	C	-0.28330800	1.35251000	-0.17004200
	H	0.05453400	2.05968800	0.59008000
	H	-0.02090800	1.83144700	-1.12572700
	C	-0.31115900	-1.13103500	-0.52649000
	H	-0.45289400	-1.04527800	-1.61215200
	H	0.24424000	-2.05389600	-0.36003100
	C	0.43472900	0.05894200	-0.03923200
	C	1.93358400	-0.00871100	0.06311400
	C	2.56590900	1.33186800	0.36511200
	H	3.64615900	1.21851900	0.38657700
	H	2.31831300	2.05801300	-0.40387500
	H	2.23687300	1.71122500	1.32912900
	C	2.37220500	-1.02454000	1.10861400

	H	1. 97598500	-2. 01591800	0. 89803400
	H	3. 45777600	-1. 09135000	1. 11662500
	H	2. 02985700	-0. 73286600	2. 09861800
	O	2. 48171900	-0. 38151000	-1. 20480900
	H	2. 15199800	-1. 24756400	-1. 43962600
	C	-3. 90348000	0. 00577400	0. 21959000
	H	-4. 35162800	0. 99548500	0. 21678400
	H	-4. 35134000	-0. 57500400	-0. 58692100
	H	-4. 17888800	-0. 48816100	1. 15188600
IM07	C	1. 78942451	1. 05434100	0. 33053872
	H	1. 80081351	1. 29476800	1. 39686672
	H	2. 20939351	1. 92606300	-0. 17511228
	C	2. 66906851	-0. 13111500	0. 07900572
	C	2. 15330751	-1. 31100600	-0. 25526128
	H	2. 83012751	-2. 13361500	-0. 45078628
	C	0. 68949251	-1. 60403100	-0. 36338528
	H	0. 49044451	-2. 58272900	0. 07215672
	H	0. 39351851	-1. 67401100	-1. 41394628
	C	0. 37892151	0. 80004800	-0. 13882928
	H	0. 32546751	0. 83393000	-1. 22660628
	H	-0. 27354949	1. 60886400	0. 24891372
	C	-0. 14772749	-0. 54059500	0. 33007072
	H	0. 04475051	-0. 62328800	1. 40354472
	C	-1. 67472349	-0. 67080300	0. 12892872
	C	-2. 11597649	-2. 11617200	0. 05250372
	H	-3. 20081549	-2. 16166500	0. 00641872
	H	-1. 72162149	-2. 59156900	-0. 84097428
	H	-1. 78072049	-2. 67468200	0. 92415372
	C	-2. 40038449	0. 01717400	1. 27490072
	H	-2. 08567849	1. 05176100	1. 38965272
	H	-3. 47109249	0. 00816300	1. 08472372
	H	-2. 21286349	-0. 50083500	2. 21305172
	O	-2. 06481649	-0. 09270300	-1. 10184928
	H	-2. 06056949	0. 86165100	-1. 00224628
	C	4. 13439251	0. 10775900	0. 22066572
	H	4. 36955751	0. 49113000	1. 21396572
	H	4. 70854051	-0. 80099100	0. 06378072
	H	4. 47820651	0. 85644900	-0. 49340728
	O	-1. 73970551	3. 04790600	-0. 29827972
	H	-1. 16060151	3. 54632900	-0. 89062572
IM7	C	1. 75641200	-1. 26489500	0. 01220300
	H	2. 03041300	-1. 82669300	-0. 89357100
	H	2. 17154000	-1. 85824900	0. 83180600
	C	2. 43675200	0. 06747300	-0. 02534100
	C	1. 74073700	1. 19762200	0. 02573700
	H	2. 27961800	2. 13698000	0. 02636000

	C	0.25203000	1.28329400	0.08520100
	H	-0.07580200	2.11908600	-0.53110300
	H	-0.07208400	1.51112700	1.10358400
	C	0.28387400	-1.18293600	0.13778000
	H	-0.24868700	-2.10206300	0.33938400
	C	-0.44312700	0.00538000	-0.37858900
	H	-0.38788800	-0.01071200	-1.47773700
	C	3.92635100	0.04013200	-0.10010000
	H	4.26358400	-0.48936800	-0.99162500
	H	4.34295400	1.04300600	-0.12475300
	H	4.35190100	-0.48386300	0.75610600
	C	-1.93762200	-0.01774000	-0.00805500
	C	-2.64123500	-1.20264900	-0.65052100
	H	-2.22054100	-2.15213100	-0.32897300
	H	-3.69100000	-1.19406100	-0.36938700
	H	-2.57166400	-1.15532800	-1.73569300
	C	-2.63222200	1.26132000	-0.42420800
	H	-3.69372300	1.18856100	-0.20260500
	H	-2.23437500	2.10988000	0.12332100
	H	-2.51197000	1.43916200	-1.49085000
	O	-2.08305700	-0.07772500	1.39854200
	H	-1.51952800	-0.77554200	1.73275500
IM08	C	1.61733900	0.25325100	-1.01218600
	H	1.83625100	1.22167700	-0.61327600
	H	2.15175300	0.26468900	-1.96263800
	C	2.17687700	-0.76815200	-0.09436300
	C	1.37015800	-1.45282400	0.71737400
	H	1.80113600	-2.21403600	1.35628900
	C	-0.10422700	-1.25165700	0.82048700
	H	-0.37506400	-1.23332200	1.87581500
	H	-0.62769100	-2.11182700	0.39354600
	C	0.12304700	0.15297000	-1.20378500
	H	-0.08544400	-0.72850100	-1.81726300
	H	-0.22376400	1.02482900	-1.75327200
	C	-0.59086000	0.01432700	0.13183300
	H	-0.30770200	0.87639200	0.74252500
	C	-2.12452100	0.04347000	0.00200900
	C	-2.78721600	-0.19561100	1.34285300
	H	-3.86360400	-0.08214300	1.24666900
	H	-2.58899200	-1.20339500	1.69469800
	H	-2.42622800	0.51371600	2.08465800
	C	-2.60658800	1.36493000	-0.57112300
	H	-2.25318500	1.52094900	-1.58846700
	H	-3.69324000	1.37868900	-0.59248700
	H	-2.26011000	2.20212000	0.03080300
	O	-2.56806300	-1.02364500	-0.82019300

	H	-2.34186800	-0.83330700	-1.72865700
	C	3.65423500	-0.97506200	-0.13148500
	H	4.18139700	-0.03961500	0.05677500
	H	3.97571500	-1.70263100	0.60838900
	H	3.97472200	-1.32230500	-1.11340800
	O	2.13411800	3.11879400	0.75852000
	H	2.22800500	2.59299000	1.56300900
IM8	C	1.77376200	-1.19592300	0.04285800
	H	2.31829200	-2.12874800	0.00231600
	C	2.46089700	-0.00064700	-0.02335300
	C	1.76948200	1.18994400	0.08821500
	H	2.31720400	2.12211700	0.09332900
	C	0.28886500	1.24550200	0.22068600
	H	-0.07769300	2.13147900	-0.29496600
	H	0.00188100	1.37163700	1.26989300
	C	0.29596500	-1.24745700	0.21451700
	H	0.06441100	-1.36073500	1.28175400
	H	-0.08925400	-2.14037400	-0.27470300
	C	-0.39654300	-0.00058800	-0.32377900
	H	-0.26922200	-0.00520200	-1.40950500
	C	3.94858300	0.00603500	-0.21680900
	H	4.40598000	0.85928700	0.27731200
	H	4.40321100	-0.89699900	0.18195300
	H	4.20326200	0.06372600	-1.27369900
	C	-1.91219700	0.00552700	-0.04872900
	C	-2.58372800	-1.22319900	-0.63838600
	H	-2.24340600	-2.13827700	-0.15726100
	H	-3.65962200	-1.15551200	-0.49910900
	H	-2.37716600	-1.31010500	-1.70327600
	C	-2.56241000	1.25431200	-0.60871000
	H	-3.64184200	1.18541400	-0.50353400
	H	-2.23330600	2.13447700	-0.06560600
	H	-2.32105700	1.37926400	-1.66207500
	O	-2.16656300	0.05952400	1.34531000
	H	-1.96522000	-0.78868000	1.73563100
IM09	C	1.76482600	1.00370200	0.69891100
	H	1.84950800	0.89748100	1.78408400
	H	2.16661200	1.99267800	0.46988700
	C	2.60635400	-0.03685500	0.02757000
	C	2.04558600	-1.08027400	-0.57642200
	H	2.68651200	-1.79758900	-1.07473300
	C	0.57926600	-1.36455300	-0.60196000
	H	0.42958600	-2.42035400	-0.37813500
	H	0.18006900	-1.20971100	-1.60825100
	C	0.31129500	0.92023900	0.27795800
	H	0.22766100	1.23873900	-0.76447100

	H	-0.28231200	1.60269900	0.88565100
	C	-0.20944100	-0.50522700	0.37432000
	H	-0.01028500	-0.86558000	1.38831400
	C	-1.72968300	-0.61013300	0.14679200
	C	-2.16905500	-2.05903200	0.08050200
	H	-3.25360300	-2.11198400	0.03380100
	H	-1.77503600	-2.53718900	-0.81102000
	H	-1.82931000	-2.61096500	0.95477900
	C	-2.49856100	0.09692300	1.25112400
	H	-2.28301300	1.16271000	1.28021700
	H	-3.56625500	-0.01927900	1.08182300
	H	-2.25666300	-0.32522700	2.22449100
	O	-2.07413300	-0.05674400	-1.10880600
	H	-2.09008900	0.89915600	-1.03854600
	C	4.08314100	0.17076500	0.07307800
	H	4.43429400	0.24059100	1.10318200
	H	4.61787700	-0.64154800	-0.41141900
	H	4.36337400	1.10390400	-0.41645400
	O	-1.81596300	2.90941000	-0.64036500
	H	-1.19053100	3.36681900	-1.22107100
IM9	C	1.73068800	-1.25275600	-0.08579700
	H	1.79103900	-1.65976100	-1.09949600
	H	2.27717700	-1.95675200	0.54399800
	C	2.41633800	0.07686200	-0.04823300
	C	1.71725000	1.20301200	0.04935900
	H	2.25000700	2.14477200	0.09875500
	C	0.22538100	1.27958200	0.07732300
	H	-0.09134900	2.08184000	-0.58912500
	H	-0.11588800	1.56229100	1.07751300
	C	0.28533800	-1.17452300	0.36321700
	H	0.24367200	-1.00941900	1.44113300
	H	-0.20512200	-2.12551100	0.16740900
	C	-0.44354300	-0.02692300	-0.31749500
	H	-0.35289300	-0.15256200	-1.40064500
	C	3.90632700	0.06025700	-0.12177500
	H	4.24474400	-0.44576200	-1.02650900
	H	4.32021700	1.06479400	-0.12135900
	H	4.33269100	-0.48551900	0.72011300
	C	-1.94638300	-0.03395200	0.01762400
	C	-2.66730700	-1.24636400	-0.56075000
	H	-2.29449600	-2.17091100	-0.13126200
	H	-3.72911600	-1.18059300	-0.34183200
	H	-2.53144100	-1.28955300	-1.63933900
	C	-2.64000400	1.23790200	-0.50079300
	H	-3.71016800	1.17158700	-0.33336000
	H	-2.26200200	2.12433800	-0.00338500

	H	-2.44826900	1.32118000	-1.56851400
	O	-2.15291400	0.03336900	1.37122800
IM010	C	2.00723827	-0.73901637	-1.00629700
	H	1.93452727	-0.20270237	-1.95649400
	H	2.68869227	-1.57135337	-1.19006600
	C	2.60148427	0.16328563	0.03025000
	C	1.85118027	0.67261663	1.00261800
	H	2.32363127	1.29622063	1.75175300
	C	0.37729127	0.46712763	1.13570900
	H	-0.08457573	1.42814663	1.36927100
	H	0.15829027	-0.17809537	1.99137800
	C	0.64712527	-1.26503737	-0.59357800
	H	0.78279527	-1.97839837	0.22238600
	H	0.20036427	-1.80409237	-1.42736100
	C	-0.25332073	-0.13754537	-0.10921400
	H	-0.28536873	0.62522463	-0.89181800
	C	-1.70429473	-0.59715837	0.12959900
	C	-2.52895973	0.43329863	0.86482100
	H	-3.55351273	0.08593063	0.96782700
	H	-2.12937673	0.64288763	1.85165900
	H	-2.59068173	1.37335563	0.29457300
	C	-2.38776273	-0.93874237	-1.18296500
	H	-1.87512773	-1.73769937	-1.71461300
	H	-3.40685473	-1.26515237	-0.99142800
	H	-2.41892073	-0.06445637	-1.82965200
	O	-1.72897273	-1.71020337	1.00763400
	H	-1.38235873	-2.47644637	0.55393400
	C	4.06234827	0.44104463	-0.08811200
	H	4.29656227	0.87801763	-1.05930700
	H	4.40542827	1.12587063	0.68240800
	H	4.64234227	-0.47876437	-0.01087800
	O	-2.07979927	2.96409237	-0.91389700
	H	-1.28873427	3.21176537	-0.41534000
IM10	C	1.70520700	-1.25184700	-0.10923600
	H	1.75705100	-1.63862900	-1.13102300
	H	2.24563600	-1.97437500	0.50476900
	C	2.40391300	0.07118700	-0.04373400
	C	1.71697900	1.20223900	0.08521700
	H	2.26136700	2.13595900	0.15663100
	C	0.22658700	1.29044200	0.12106700
	H	-0.10082900	2.11505400	-0.51233100
	H	-0.11587600	1.53942500	1.12822700
	C	0.25977500	-1.16719200	0.34364500
	H	0.24225500	-1.01876400	1.42606300
	H	-0.23782300	-2.11248000	0.13494000
	C	-0.44693900	0.00211500	-0.32172500

	H	-0.32130300	-0.10031100	-1.40384200
	C	3.89338800	0.03906500	-0.12538400
	H	4.22217300	-0.44626400	-1.04496600
	H	4.31798900	1.03881100	-0.10107000
	H	4.31883900	-0.53279900	0.69962700
	C	-1.96499300	0.04405800	-0.05148500
	C	-2.66701800	-1.19463700	-0.60749900
	H	-2.32829200	-2.10259700	-0.11012000
	H	-3.73832400	-1.10459500	-0.45266300
	H	-2.47745100	-1.30337700	-1.67276300
	C	-2.56605200	1.25241900	-0.66774900
	H	-2.38070300	1.47650100	-1.70611600
	H	-3.28003400	1.83568200	-0.11109200
	O	-2.22012600	0.14379400	1.33792200
	H	-1.98875900	-0.68469500	1.75365000
IM011	C	-1.86413200	0.75208000	1.03262600
	H	-1.68281200	1.81516800	0.85255400
	H	-2.46656400	0.70538000	1.94147500
	C	-2.64601000	0.17838700	-0.10770400
	C	-2.06398300	-0.61563100	-1.00080100
	H	-2.66806700	-1.03332600	-1.79713000
	C	-0.61157300	-0.96319500	-1.01528800
	H	-0.24175700	-0.84667700	-2.03363200
	H	-0.47313400	-2.01889300	-0.76531100
	C	-0.54877300	0.02909700	1.24673000
	H	-0.76507300	-0.96634800	1.64429500
	H	0.03437400	0.56186500	1.99559500
	C	0.21567000	-0.11355300	-0.06073100
	H	0.33094200	0.88416700	-0.49227100
	C	1.63639200	-0.67605900	0.12563500
	C	2.30657400	-0.90957300	-1.21184400
	H	3.33591300	-1.22478100	-1.06005000
	H	1.79735300	-1.69437800	-1.76189100
	H	2.29967000	0.00394000	-1.80252500
	C	2.49400800	0.24037200	0.97627100
	H	2.13733400	0.31729600	2.00091600
	H	3.52424100	-0.10430800	0.99143800
	H	2.46060700	1.26405800	0.57040000
	O	1.60583400	-1.94420100	0.75746100
	H	1.21596100	-1.84763200	1.62473200
	C	-4.09074200	0.54420800	-0.17334500
	H	-4.21473000	1.62658200	-0.22160100
	H	-4.57631000	0.10976700	-1.04279000
	H	-4.62101200	0.20814600	0.71806900
	O	2.42257900	2.98560400	-0.69851800
	H	3.38117700	3.11195400	-0.70311600

IM11	C	1. 71980300	-1. 24658200	-0. 13014200
	H	1. 77796500	-1. 61544500	-1. 15819400
	H	2. 26903300	-1. 97143700	0. 47304000
	C	2. 39973300	0. 08504000	-0. 04087000
	C	1. 69779200	1. 20579400	0. 09793000
	H	2. 23091600	2. 14450600	0. 18629300
	C	0. 20527900	1. 28152800	0. 11727400
	H	-0. 10923900	2. 10379300	-0. 52515500
	H	-0. 14924800	1. 53026000	1. 12121200
	C	0. 27546300	-1. 17974000	0. 32342800
	H	0. 25786600	-1. 03915700	1. 40659200
	H	-0. 23176200	-2. 12073400	0. 10887600
	C	-0. 44791300	-0. 01417300	-0. 33049700
	H	-0. 32372000	-0. 10636900	-1. 41389000
	C	3. 89024000	0. 07463700	-0. 10898100
	H	4. 23350100	-0. 39463700	-1. 03153500
	H	4. 30132400	1. 07945500	-0. 06786200
	H	4. 31537000	-0. 50244800	0. 71249200
	C	-1. 96004400	-0. 04464900	-0. 05352700
	C	-2. 57427900	-1. 26240000	-0. 64604100
	H	-3. 55429700	-1. 56820500	-0. 31220100
	H	-2. 16555100	-1. 71569900	-1. 53599400
	C	-2. 65342600	1. 19469600	-0. 60156200
	H	-3. 72823400	1. 10061600	-0. 47672400
	H	-2. 32496300	2. 07472500	-0. 05446900
	H	-2. 43105700	1. 32756600	-1. 65740100
	O	-2. 21443500	-0. 00543100	1. 34279500
	H	-1. 96831300	-0. 84825100	1. 72049100
IM12	C	-1. 16940300	-1. 18589100	-1. 12691700
	H	-1. 14014100	-2. 27346000	-1. 09387300
	H	-1. 75614000	-0. 90361100	-1. 99818400
	C	-1. 90676400	-0. 74618700	0. 13557500
	C	-1. 37604000	0. 60708200	0. 58687600
	H	-1. 95648600	0. 99974100	1. 42055200
	C	0. 10060800	0. 56918200	0. 92378100
	H	0. 19745100	0. 35857500	1. 98533500
	H	0. 50032200	1. 56922200	0. 75510600
	C	0. 24128500	-0. 61696700	-1. 25266800
	H	0. 19372500	0. 35465200	-1. 74718500
	H	0. 82295900	-1. 27431300	-1. 89418000
	C	0. 89601800	-0. 45146600	0. 11049800
	H	0. 84389600	-1. 41468500	0. 61982900
	C	2. 38155100	-0. 05678200	0. 04039500
	C	2. 94583800	0. 14071400	1. 43238400
	H	4. 00579200	0. 37192300	1. 37023800
	H	2. 45361100	0. 96863500	1. 93359100

	H	2.81780900	-0.75890100	2.03039400
	C	3.20227900	-1.10349600	-0.69358600
	H	2.92155300	-1.17574600	-1.74228900
	H	4.25509200	-0.83666400	-0.65180400
	H	3.07562200	-2.08655900	-0.24448400
	O	2.53202300	1.19969600	-0.59600800
	H	2.27931100	1.11966700	-1.51413900
	C	-3.40310100	-0.72403400	-0.08086100
	H	-3.92657100	-0.49004600	0.84661900
	H	-3.67342500	0.02888100	-0.81607600
	H	-3.74104500	-1.69614500	-0.43138200
	O	-1.57025500	-1.67873600	1.14793900
	O	-1.51355500	2.74152600	-0.17869300
	O	-1.63435800	1.50076100	-0.51993400
	H	-2.15780200	-1.56006100	1.89264900
IM13	C	0.24972800	1.77662500	-1.08850900
	H	-0.11161100	2.79963500	-1.00026500
	H	0.87286500	1.72753400	-1.97878100
	C	1.11950800	1.52947700	0.14136800
	C	1.05538400	0.05104200	0.51654000
	H	1.74788800	-0.14870800	1.33581300
	C	-0.35161200	-0.38769200	0.87621600
	H	-0.48021200	-0.27371000	1.94939600
	H	-0.43894500	-1.45052100	0.65072900
	C	-0.91777400	0.80418600	-1.22575100
	H	-0.57905900	-0.07946400	-1.76843700
	H	-1.69266900	1.27653200	-1.82452500
	C	-1.44822200	0.37660400	0.13441100
	H	-1.68062300	1.28136900	0.69798100
	C	-2.74162400	-0.45281600	0.05677400
	C	-3.17475100	-0.89941900	1.43808900
	H	-4.11160100	-1.44593800	1.37026000
	H	-2.43492300	-1.56019600	1.87960100
	H	-3.31600000	-0.04229000	2.09281300
	C	-3.86809000	0.33175100	-0.59483300
	H	-3.65955500	0.54792700	-1.64049600
	H	-4.78664900	-0.24803600	-0.55553800
	H	-4.03344800	1.27828400	-0.08403800
	O	-2.51980900	-1.65374400	-0.66134300
	H	-2.32157800	-1.44199300	-1.57187200
	C	2.54027400	1.99614200	-0.07854200
	H	3.12981100	1.88198800	0.83169500
	H	3.02076100	1.41005900	-0.85592600
	H	2.54419200	3.04504700	-0.36515600
	O	0.52571500	2.24548900	1.20966300
	O	1.77922200	-1.96257600	-0.32652600

	O	1. 55387300	-0. 62379700	-0. 64435100
	H	1. 14627200	2. 29574000	1. 93506300
	N	3. 07876900	-2. 20959400	0. 04859200
	O	3. 76809600	-1. 27306000	0. 11092700
IM14	C	1. 35758800	1. 28724900	-0. 63726700
	H	1. 42320900	2. 24249700	-0. 11874700
	H	1. 91604600	1. 38019700	-1. 56635000
	C	2. 06295200	0. 27476000	0. 25229200
	C	1. 42021800	-1. 14453900	0. 01651800
	H	1. 99501100	-1. 83602100	0. 64888300
	C	-0. 04880900	-1. 11683600	0. 43337100
	H	-0. 10272400	-1. 40594600	1. 48067500
	H	-0. 56368800	-1. 88216700	-0. 14659800
	C	-0. 09550900	0. 94420900	-0. 94682400
	H	-0. 12588200	0. 30477500	-1. 82949000
	H	-0. 62323400	1. 86336700	-1. 18973300
	C	-0. 75037100	0. 22328700	0. 22085500
	H	-0. 60248800	0. 83805400	1. 10980500
	C	-2. 26853300	0. 03098900	0. 05837600
	C	-2. 83723900	-0. 71760200	1. 24628300
	H	-3. 91388400	-0. 81794000	1. 13734700
	H	-2. 41320600	-1. 71518000	1. 30982000
	H	-2. 62667500	-0. 18652900	2. 17200100
	C	-2. 98744500	1. 36125500	-0. 09168400
	H	-2. 72229300	1. 86211300	-1. 02026400
	H	-4. 06166500	1. 19598000	-0. 10287700
	H	-2. 74818100	2. 03212300	0. 73116600
	O	-2. 55361100	-0. 79137100	-1. 05957100
	H	-2. 26630500	-0. 34918100	-1. 85658100
	C	3. 55195000	0. 23978400	0. 00416600
	H	4. 04309400	-0. 45317800	0. 68736000
	H	3. 76196400	-0. 08816900	-1. 00934000
	H	3. 97273000	1. 23102100	0. 15690000
	O	1. 79012300	0. 62529700	1. 58494700
	O	1. 62229300	-1. 41319800	-1. 28753400
	H	2. 35893100	0. 12302100	2. 16676600
IM15	C	1. 63617100	0. 08920000	-0. 27696500
	H	1. 69185600	0. 88778300	0. 47272400
	H	1. 63610900	0. 58869500	-1. 24714600
	C	2. 85159100	-0. 75831700	-0. 18641500
	C	-0. 31522800	2. 55689400	-0. 16987100
	H	-0. 73192300	2. 75178500	-1. 17594900
	C	-0. 90283000	1. 38114200	0. 53673500
	H	-1. 92537400	1. 65714500	0. 79799500
	H	-0. 37533900	1. 22818000	1. 47500000
	C	0. 35156800	-0. 70428100	-0. 09965800

	H	0.35098500	-1.13421700	0.90457700
	H	0.37665200	-1.54223600	-0.79302600
	C	-0.91673700	0.11228800	-0.32081000
	H	-0.93949000	0.40411200	-1.37662900
	C	-2.20852400	-0.69642800	-0.06819700
	C	-3.41093200	0.01509600	-0.65403000
	H	-4.31472300	-0.52990000	-0.39614900
	H	-3.51394300	1.02435400	-0.26592700
	H	-3.33209800	0.06715400	-1.73727700
	C	-2.13167700	-2.09647400	-0.65153800
	H	-1.39038600	-2.70383300	-0.13705400
	H	-3.09646400	-2.58577000	-0.54683800
	H	-1.86909000	-2.07113500	-1.70755400
	O	-2.46404500	-0.77516500	1.32223400
	H	-1.78523900	-1.30525500	1.73721200
	C	4.17272200	-0.23186700	-0.60570100
	H	4.91106200	-1.02855400	-0.70155900
	H	4.10003600	0.26443100	-1.56911300
	H	4.56705400	0.49678300	0.11276600
	O	2.83457400	-1.56051200	0.92005700
	O	0.53247100	3.28107500	0.27546800
	H	3.65957400	-2.03622200	0.99058800
IM16	C	1.10054100	0.59023000	-0.12094600
	H	0.96116500	1.46197500	0.51444600
	H	1.08961500	0.94920300	-1.15056500
	C	2.47836200	0.04848400	0.15896200
	C	-1.32478100	2.57306500	-0.42911600
	H	-1.78506500	2.59230500	-1.43423700
	C	-1.68803000	1.39134400	0.40602400
	H	-2.75735500	1.46256100	0.60560900
	H	-1.18652700	1.46279400	1.36810300
	C	0.00677400	-0.43772800	0.09916800
	H	0.01598500	-0.72813200	1.15134600
	H	0.25416700	-1.32847800	-0.47325700
	C	-1.38055300	0.06038100	-0.29087700
	H	-1.38371700	0.21911200	-1.37466500
	C	-2.49367500	-0.97102900	-0.00142000
	C	-3.77179100	-0.59512300	-0.72279800
	H	-4.55931900	-1.29113700	-0.44819500
	H	-4.10959600	0.40277700	-0.45825100
	H	-3.62848500	-0.63800200	-1.79977900
	C	-2.09060000	-2.37678800	-0.40941500
	H	-1.27607000	-2.75395200	0.20531100
	H	-2.93840800	-3.04575600	-0.28887400
	H	-1.76817600	-2.41063000	-1.44833500
	O	-2.82176500	-0.95043000	1.37546800

	H	-2.09832400	-1.32145900	1.87825700
	C	3.58402700	1.06039300	0.00751800
	H	4.54673200	0.57288700	0.14238100
	H	3.55939200	1.51468200	-0.97824800
	H	3.46687500	1.83405000	0.75955300
	O	2.48741300	-0.57211900	1.37949200
	O	-0.59963200	3.46740700	-0.08733000
	H	3.34137800	-0.99442900	1.49151200
	O	2.69715100	-0.97418400	-0.88460100
	O	3.70359400	-1.72314200	-0.58861800
IM17	C	-1.15449000	-0.64085600	-0.47515000
	H	-1.07955700	-1.72643600	-0.43857300
	H	-1.23180500	-0.34847300	-1.52259000
	C	-2.45628800	-0.24782100	0.20948500
	C	-2.65577300	1.25087900	0.06301500
	H	-2.57448600	1.82648600	1.00190300
	C	1.54129400	-1.83939000	-0.70204100
	H	1.15971100	-2.38708600	-1.54839900
	H	1.98796200	-2.38723200	0.11312400
	C	0.07535800	-0.01475500	0.15503200
	H	0.13574700	-0.34563400	1.19218800
	H	-0.04119500	1.06934000	0.16601200
	C	1.37268100	-0.36916100	-0.58676600
	H	1.29365400	0.06022000	-1.58938600
	C	2.61622500	0.26753000	0.07642600
	C	3.84968900	-0.02813900	-0.74976000
	H	4.72574600	0.39765000	-0.26783700
	H	3.99581200	-1.10032700	-0.84439900
	H	3.75471200	0.39807700	-1.74586700
	C	2.46370400	1.76852300	0.25065300
	H	1.70373800	2.01455400	0.98976300
	H	3.40433600	2.19365800	0.59126100
	H	2.18677600	2.24789300	-0.68641100
	O	2.85971400	-0.33527200	1.33422800
	H	2.17486400	-0.07165200	1.94627400
	C	-3.63413700	-0.96926600	-0.41420000
	H	-4.56387600	-0.72087400	0.09729300
	H	-3.74065200	-0.67475300	-1.45387400
	H	-3.48078700	-2.04356700	-0.35575200
	O	-2.31908300	-0.55630500	1.57743000
	O	-2.88290900	1.78714200	-0.98471100
	H	-3.18205500	-0.63162000	1.97954000
IM18	C	1.38739300	0.49417700	-0.52017300
	H	1.09551000	1.54219200	-0.58705900
	H	1.45252600	0.10734800	-1.53567600
	C	2.77512000	0.45245500	0.08880400

	C	3.32440400	-0.96213800	0.10221700
	H	4.03217600	-1.16801000	0.92562400
	C	-1.56206300	1.24000700	0.33681700
	H	-0.75956600	1.95820900	0.48027100
	H	-2.06782600	1.07704200	1.28631600
	C	0.35369900	-0.30015500	0.25701300
	H	0.40864000	-0.03207200	1.31258600
	H	0.61158500	-1.35464200	0.18156200
	C	-1.06683400	-0.06146500	-0.25407200
	H	-1.03754100	0.05422500	-1.34023700
	C	-2.01133600	-1.23731200	0.06594800
	C	-3.45624200	-0.89208000	-0.22585000
	H	-4.07842200	-1.76452700	-0.04636900
	H	-3.80514200	-0.09337100	0.42157700
	H	-3.57958100	-0.57192600	-1.25702100
	C	-1.62808400	-2.48007000	-0.71873500
	H	-0.61098200	-2.80749800	-0.51490600
	H	-2.29986400	-3.29238700	-0.45407700
	H	-1.71103000	-2.30167900	-1.78847500
	O	-1.96899000	-1.50239900	1.45718600
	H	-1.12065300	-1.88356000	1.67887400
	C	3.74929400	1.31173800	-0.69776600
	H	4.75324400	1.26012800	-0.27580200
	H	3.80350300	0.98376400	-1.73194900
	H	3.41716400	2.34710500	-0.67355600
	O	2.67606600	0.89379800	1.42462900
	O	3.05045400	-1.80297200	-0.70582700
	H	3.50632600	1.26920700	1.71034100
	O	-2.49355900	1.83884200	-0.57757100
	O	-2.91424200	2.98267000	-0.14807300
IM19	C	-1.76753300	-0.56317100	-0.54961800
	H	-1.23551400	-1.50500100	-0.70141400
	H	-1.97423500	-0.15498800	-1.53785500
	C	-3.09533400	-0.88509400	0.11568400
	C	-3.94556500	0.35722500	0.27390600
	H	-4.60253400	0.34812400	1.15827400
	C	1.31296500	-0.64147400	0.17564100
	H	0.67944200	-1.51258200	0.32828600
	H	1.81266700	-0.39107200	1.11192000
	C	-0.91181600	0.41574900	0.23214900
	H	-0.86508400	0.10272800	1.27625500
	H	-1.40923600	1.38334400	0.21412100
	C	0.50467700	0.53881800	-0.32857000
	H	0.46184400	0.46746800	-1.41788800
	C	1.16244200	1.88632900	0.02774900
	C	2.63157000	1.90009700	-0.33451800

	H	3.04942400	2.87682100	-0.10636700
	H	3.18182300	1.15313200	0.22863300
	H	2.76918800	1.69294400	-1.39279300
	C	0.46343500	3.03995200	-0.67077300
	H	-0.58754500	3.11854400	-0.40108200
	H	0.94882700	3.97270500	-0.39617700
	H	0.52128500	2.92878000	-1.75124900
	O	1.12168800	2.06713700	1.43262300
	H	0.22023500	2.23868700	1.70098200
	C	-3.90424100	-1.86971800	-0.71454900
	H	-4.85995000	-2.08137000	-0.24096000
	H	-4.08378100	-1.47728800	-1.71144400
	H	-3.35475600	-2.80564800	-0.81164300
	O	-2.92629300	-1.36363300	1.43018400
	O	-3.94280600	1.26649000	-0.50657100
	H	-2.63679800	-2.27358800	1.40546400
	O	2.27099700	-0.97241600	-0.82398100
	O	2.81834300	-2.21773100	-0.50239000
	N	3.99039000	-2.13376900	0.20891100
	O	4.32411800	-1.05705300	0.49762900
IM20	C	1.26926800	0.49575600	-0.55185600
	H	1.12578300	1.57164800	-0.67220000
	H	1.29055500	0.06683000	-1.55255700
	C	2.63091200	0.27686600	0.08601600
	C	2.95528400	-1.19718300	0.19822100
	H	3.58378900	-1.45900200	1.06438700
	C	-1.53869300	1.73981100	0.25788700
	H	-0.59357900	2.24440700	0.47642600
	H	-2.10575100	1.59909000	1.18486500
	C	0.12138600	-0.10896100	0.23333600
	H	0.21069500	0.17059600	1.28365300
	H	0.21486400	-1.19245700	0.18197300
	C	-1.24384100	0.31954200	-0.29679500
	H	-1.19673500	0.38820200	-1.38506200
	C	-2.36714500	-0.66896300	0.06364300
	C	-3.73626200	-0.11596000	-0.26795500
	H	-4.48839100	-0.86799700	-0.04524000
	H	-3.95436200	0.76974400	0.31972400
	H	-3.80074600	0.15424000	-1.31832400
	C	-2.17575100	-1.99053800	-0.66316100
	H	-1.22858400	-2.46745500	-0.42072900
	H	-2.97460500	-2.67175800	-0.38263400
	H	-2.20960800	-1.84741200	-1.74074500
	O	-2.37742500	-0.87923800	1.46390000
	H	-1.60374300	-1.38283500	1.71258800
	C	3.73723300	0.91060700	-0.74347900

	H	4.70914500	0.73681100	-0.28787600
	H	3.74294900	0.50755200	-1.75227400
	H	3.57616900	1.98626100	-0.80811500
	O	2.67561600	0.74506000	1.41425800
	O	2.59674000	-2.01826100	-0.59760800
	H	2.71323900	1.69963200	1.41584800
	O	-2.26060900	2.40594400	-0.67665800
IM21	C	-1.05879300	-0.47490300	1.49036700
	H	-1.04025400	0.39310600	2.14844000
	H	-1.53653000	-1.28902500	2.03397300
	C	-1.91709800	-0.10237900	0.30484900
	C	-1.22991400	0.97980800	-0.53000700
	H	-1.81872900	1.12959000	-1.43659800
	C	0.18353900	0.59708800	-0.90301800
	H	0.59887100	1.43221800	-1.45966900
	H	0.16709100	-0.26592000	-1.56813900
	C	0.36002800	-0.84546000	1.09727500
	H	0.33010100	-1.75286000	0.48950100
	H	0.91276400	-1.08034500	2.00387400
	C	1.03745300	0.27057200	0.31302400
	H	1.07800100	1.15827400	0.94950400
	C	2.48719700	-0.07177000	-0.08090200
	C	3.12922300	1.06306300	-0.85345600
	H	4.18207400	0.84721800	-1.01401800
	H	2.66554000	1.17918000	-1.82753700
	H	3.04347200	2.00042700	-0.30832300
	C	3.33220900	-0.38435400	1.14334900
	H	2.99729200	-1.28916700	1.64635100
	H	4.36570900	-0.53718300	0.84392300
	H	3.29715500	0.43134200	1.86295500
	O	2.51137500	-1.17655700	-0.96839200
	H	2.25881400	-1.96667100	-0.49430000
	C	-3.32371000	0.27038600	0.69903600
	H	-3.91442200	0.52361100	-0.17727800
	H	-3.80309900	-0.55984500	1.21137600
	H	-3.30268100	1.11733900	1.37950600
	O	-1.16448800	2.17121800	0.22243100
	O	-1.96624500	-1.31091300	-0.50451500
	O	-2.69124800	-1.17338200	-1.56625100
	H	-1.99710700	2.63314500	0.16716600
IM22	C	-0.45812400	0.52418000	1.60554300
	H	-0.22013700	1.55271900	1.87398800
	H	-1.02364600	0.08931400	2.42813600
	C	-1.34728600	0.59690500	0.38181300
	C	-0.54733300	1.14715700	-0.80234800
	H	-1.17199500	1.10513200	-1.69624200

	C	0.71816000	0.35675000	-1.03979700
	H	1.22817400	0.81638000	-1.88157700
	H	0.46129000	-0.66160600	-1.32608800
	C	0.82490100	-0.24950700	1.36077700
	H	0.57369100	-1.29401100	1.16274400
	H	1.41451300	-0.22525700	2.27447600
	C	1.61412400	0.32151200	0.18903500
	H	1.88787900	1.35011100	0.43792700
	C	2.92526900	-0.44136500	-0.08056100
	C	3.72004200	0.21109500	-1.19408800
	H	4.68005000	-0.28743500	-1.29788600
	H	3.20295000	0.12670200	-2.14418800
	H	3.89366200	1.26326900	-0.98032700
	C	3.78664200	-0.51760400	1.16916200
	H	3.32581000	-1.13262900	1.93944800
	H	4.74749700	-0.96229500	0.92375600
	H	3.95942700	0.47179400	1.58864600
	O	2.65329800	-1.75206700	-0.54685500
	H	2.27600100	-2.26725000	0.16379400
	C	-2.60453300	1.38854000	0.64970500
	H	-3.24406200	1.42563900	-0.23082200
	H	-3.16207400	0.94260100	1.46828800
	H	-2.34627000	2.40639600	0.92909500
	O	-0.17806100	2.48345300	-0.52959000
	O	-1.66574100	-0.78213500	0.13194600
	O	-2.44979400	-0.87636100	-1.02362300
	O	-4.00965400	-1.43153800	0.35347600
	N	-3.74144900	-1.27835400	-0.76703600
	H	-0.88418000	3.07210400	-0.78217600
IM23	C	1.33545900	-1.13925000	-0.83039200
	H	1.45586300	-0.60761000	-1.77412000
	H	1.80432200	-2.11586400	-0.93122900
	C	2.13616500	-0.31822400	0.20379600
	C	1.42614700	1.04939400	0.35568100
	H	1.93380900	1.59698000	1.15326000
	C	-0.03269400	0.89708700	0.70579500
	H	-0.44281700	1.89860000	0.80291800
	H	-0.11986700	0.40693200	1.67302400
	C	-0.13365100	-1.26822600	-0.48809000
	H	-0.23412400	-1.83795800	0.43777900
	H	-0.61042500	-1.84261900	-1.27971900
	C	-0.79881300	0.09279600	-0.33328600
	H	-0.72421200	0.61207100	-1.29207700
	C	-2.29775400	-0.00379300	0.01099300
	C	-2.93843600	1.36879900	0.05545800
	H	-4.00973200	1.26707700	0.20686100

	H	-2.54497700	1.95621300	0.87832900
	H	-2.76624900	1.90603900	-0.87434800
	C	-3.04075200	-0.86883600	-0.99423600
	H	-2.72645600	-1.90924900	-0.94084100
	H	-4.10703700	-0.83577200	-0.78652700
	H	-2.87479300	-0.52008800	-2.01193000
	O	-2.47776300	-0.53356500	1.31292500
	H	-2.20670400	-1.44976600	1.32044800
	C	3.58182000	-0.16745400	-0.23582800
	H	4.13081500	0.45365000	0.47017500
	H	4.05666800	-1.14440800	-0.26047300
	H	3.65816700	0.27181800	-1.22780700
	O	1.51044200	1.77058900	-0.85108000
	O	2.03219500	-0.99988000	1.37313700
	H	2.38381700	2.14304500	-0.94292300
IM24	C	1.80224100	0.32648800	-0.15189700
	H	1.75751600	1.13318900	0.58196200
	H	1.75915100	0.83311600	-1.11842600
	C	3.14807800	-0.33237000	-0.01392700
	C	-0.68432100	2.50022300	0.37080500
	H	-0.34396900	3.30955800	0.99745100
	C	-0.88587000	1.13580400	0.91477900
	H	-1.87375300	1.05091700	1.37811300
	H	-0.18356900	0.98019800	1.73271500
	C	0.65215700	-0.64249800	0.00654700
	H	0.74025300	-1.13120100	0.97926800
	H	0.77565000	-1.42721900	-0.73570000
	C	-0.71489500	0.01409700	-0.12776800
	H	-0.75581500	0.45153900	-1.13201100
	C	-1.88318600	-0.99061700	-0.05763600
	C	-3.17202600	-0.32344900	-0.49583500
	H	-4.00233800	-1.01301300	-0.37183000
	H	-3.39136700	0.56154900	0.09621500
	H	-3.11573300	-0.04356600	-1.54683400
	C	-1.64482000	-2.21689900	-0.92197200
	H	-0.83830300	-2.83318900	-0.53065900
	H	-2.54515900	-2.82518900	-0.94694000
	H	-1.38771800	-1.93847100	-1.94253000
	O	-2.10557000	-1.39124900	1.28168200
	H	-1.36616700	-1.91997500	1.57747000
	C	4.34828600	0.51510100	-0.31594900
	H	5.24949900	0.01100500	0.01263400
	H	4.40659600	0.68292000	-1.39052800
	H	4.26892800	1.49189200	0.15539600
	O	3.25621200	-1.48735900	0.31646300
	O	-1.52877400	2.94262300	-0.59649900

	H	-1.92251300	2.19854300	-1.05181200
IM25	C	-1.87038400	0.09656000	0.06358800
	H	-1.79058700	0.86765200	-0.70480900
	H	-1.81287500	0.64468400	1.00583800
	C	-3.24238500	-0.51047600	-0.05468000
	C	1.22694800	2.04000000	-0.71798900
	H	1.38330400	2.64476200	-1.60542200
	C	0.92276400	0.60674900	-1.08937900
	H	1.76607200	0.24674400	-1.67486800
	H	0.07976500	0.62323400	-1.77906200
	C	-0.76855500	-0.93373100	-0.03790700
	H	-0.88149200	-1.46971000	-0.98246700
	H	-0.94008100	-1.66739800	0.74469200
	C	0.64166900	-0.36192400	0.06845600
	H	0.70287300	0.16990700	1.02343900
	C	1.71744600	-1.47283800	0.11918200
	C	3.08303000	-0.89158900	0.42056700
	H	3.82537100	-1.68408300	0.38621500
	H	3.37062000	-0.12974600	-0.29679300
	H	3.09865100	-0.45213300	1.41647800
	C	1.39548300	-2.53363200	1.15865200
	H	0.54064900	-3.14069700	0.86955900
H	2.24742500	-3.19832400	1.27342600	
H	1.17568600	-2.08483300	2.12565800	
O	1.84511100	-2.07847900	-1.15474900	
H	1.06410300	-2.59934200	-1.33500400	
C	-4.40677400	0.40750400	0.16904600	
H	-5.32732300	-0.08523900	-0.12074600	
H	-4.45907100	0.67066300	1.22451000	
H	-4.28529800	1.33606800	-0.38375100	
O	-3.39676300	-1.67959800	-0.30908300	
O	2.28818800	2.22930600	0.10799000	
H	2.09200700	1.82215900	0.95441900	
O	-0.01342800	2.48946400	1.14714600	
O	0.02123500	2.64004500	-0.13362100	
IM26	C	1.60387500	-0.67872700	0.14469100
	H	1.64578800	-1.51350900	-0.55688300
	H	1.62054300	-1.13519500	1.13752900
	C	2.86336800	0.13289700	0.00537000
	C	0.34423700	0.13347400	-0.05194200
	H	0.34985300	0.56852000	-1.05323700
	H	0.38695300	0.99693700	0.62447200
	C	-0.89407400	-0.64937900	0.15320000
	H	-0.84724600	-1.59579500	0.67639800
	C	-2.24510400	-0.03283500	-0.02485300
	C	-3.23385300	-1.05370800	-0.55066600

	H	-4.21630600	-0.59992400	-0.65326700
	H	-2.91358200	-1.41255500	-1.52444100
	H	-3.30666000	-1.90011600	0.12768500
	C	-2.73694500	0.54543600	1.30027500
	H	-2.04246500	1.29635700	1.67582300
	H	-3.70884300	1.01369600	1.15883700
	H	-2.82790700	-0.23123900	2.05576700
	O	-2.21160900	0.99435400	-0.99854300
	H	-1.68596700	1.72274400	-0.67183200
	C	4.15797800	-0.62470200	0.00067800
	H	4.25783100	-1.15553600	-0.94510500
	H	4.98912500	0.06187700	0.11015200
	H	4.17956700	-1.37180100	0.79069200
	O	2.83191200	1.33324700	-0.10309500
IM27	C	1.70286500	0.38260700	-0.23261700
	H	1.73819100	1.28434800	0.37852500
	H	1.71622300	0.74047500	-1.26490900
	C	2.96444400	-0.40780400	-0.00942900
	C	0.45778400	-0.42841200	0.04627600
	H	0.43980800	-0.70491700	1.09929100
	H	0.50959300	-1.35442800	-0.52169100
	C	-0.81774600	0.30215100	-0.29926900
	H	-0.81479400	0.63082800	-1.33714400
	C	-2.10729900	-0.47518500	-0.01274200
	C	-3.30781800	0.43260700	-0.17366900
	H	-4.21633400	-0.14357500	-0.02498900
	H	-3.27918800	1.22958000	0.56157900
	H	-3.32994300	0.87359400	-1.16749600
	C	-2.21021500	-1.66052800	-0.95705900
	H	-1.40421700	-2.37502000	-0.80046500
	H	-3.15185000	-2.17318900	-0.78113400
	H	-2.18153200	-1.34391900	-1.99727700
	O	-2.13407700	-0.91039900	1.32758800
	H	-1.54449500	-1.65451000	1.43721600
	C	4.25403600	0.35354500	-0.06479400
	H	4.34284400	0.96777300	0.83024900
	H	5.08974400	-0.33483400	-0.10643400
	H	4.27657600	1.02818800	-0.91744700
	O	2.93413500	-1.59327600	0.21051300
	O	-0.86067300	1.51217700	0.48636700
	O	-0.41525200	2.53346400	-0.17047500
IM28	C	1.65320200	-0.19785700	-0.27857200
	H	1.73636800	0.71352800	0.31313700
	H	1.69079100	0.12070600	-1.32353300
	C	2.87384100	-1.04340400	-0.02377300
	C	0.36822900	-0.93261100	0.02592900

	H	0.33633300	-1.15156400	1.09268400
	H	0.38627500	-1.88988100	-0.48921000
	C	-0.87213600	-0.16698700	-0.37382400
	H	-0.89456000	-0.01829400	-1.45304800
	C	-2.19637900	-0.82714000	0.03957300
	C	-3.35874200	0.04764200	-0.37616700
	H	-4.28949100	-0.42979500	-0.08410400
	H	-3.29480700	1.01343100	0.11291300
	H	-3.36496800	0.19692200	-1.45349400
	C	-2.31207200	-2.20330000	-0.59082400
	H	-1.55922500	-2.88798800	-0.20524300
	H	-3.29036200	-2.61753000	-0.36333200
	H	-2.20187600	-2.15716300	-1.67230100
	O	-2.27486400	-0.92139600	1.44392800
	H	-1.70662700	-1.62433600	1.75359200
	C	4.20147600	-0.35465100	-0.11739200
	H	4.26421700	0.25615700	-1.01509200
	H	4.31761500	0.31546600	0.73320600
	H	5.00002900	-1.08686500	-0.10495800
	O	2.78255800	-2.21437400	0.24887000
	O	-0.85940300	1.12995900	0.23435700
	O	-0.44003600	2.03338500	-0.76048700
	N	0.34511000	3.03011100	-0.27580400
	O	0.58049500	2.98571000	0.86579700
IM29	C	1.44847800	-0.11858900	-0.54884000
	H	1.58290800	0.05582600	-1.61882600
	H	1.12693800	-1.15591800	-0.45398100
	C	2.78792700	0.00613500	0.12186900
	C	0.40909100	0.81037300	0.03590000
	H	0.70374900	1.84388100	-0.12850500
	H	0.37379100	0.66537700	1.11204700
	C	-0.98446100	0.63144400	-0.57015500
	H	-0.85318600	0.29406100	-1.61591400
	C	-1.88515400	-0.40487300	0.12254400
	C	-2.33704200	0.10796000	1.47561500
	H	-2.99192700	-0.61946100	1.95354200
	H	-1.49043700	0.28410600	2.13304700
	H	-2.89264500	1.03530100	1.35947300
	C	-3.07928400	-0.70679700	-0.75877500
	H	-2.75284100	-1.14873100	-1.69761800
	H	-3.75361600	-1.40644000	-0.26689200
	H	-3.63161700	0.20460500	-0.97215900
	O	-1.07467100	-1.55486400	0.27013000
	H	-1.57221100	-2.23003400	0.72762800
	C	3.92553800	-0.74786200	-0.50210000
	H	4.20479500	-0.26737300	-1.43879800

	H	4.77960400	-0.74658200	0.16486900
	H	3.63500100	-1.76859000	-0.73989800
	O	2.94309900	0.67890700	1.11061100
	O	-1.64078500	1.81261100	-0.72753600
IM30	C	0.00878500	0.03028900	-0.23221200
	C	-1.21599300	-0.76292900	0.03381700
	H	-1.41025100	-0.86572800	1.10896600
	H	-2.09882400	-0.30459100	-0.41283300
	H	-1.12336800	-1.76326700	-0.37954200
	C	1.34979900	-0.53524000	0.02661700
	H	2.12128300	0.10123500	-0.39888800
	H	1.55303200	-0.62065500	1.10080300
	H	1.43980700	-1.52749900	-0.40667100
	O	-0.04968000	1.36278800	0.06041400
	H	-0.93978500	1.68548000	-0.06447800
IM31	C	0.36281300	0.02856700	0.06352400
	C	0.38772500	1.48581600	-0.32338900
	H	0.49991400	1.59911400	-1.39739100
	H	-0.54055000	1.96319100	-0.01904300
	H	1.21771600	1.97467500	0.17710100
	C	1.55150400	-0.76262700	-0.39203600
	H	1.43842400	-1.79720100	-0.08543100
	H	1.64778700	-0.71338100	-1.47190700
	H	2.44856600	-0.35591800	0.06352100
	O	0.18651000	-0.16050900	1.40783600
	H	-0.64322500	0.25069700	1.65892500
	O	-1.89407300	-0.18926900	-0.13598200
	O	-0.77754700	-0.57918500	-0.64864900
IM32	C	0.05234300	2.68072100	0.04969600
	H	-0.47370800	2.56255500	-0.88381800
	H	-0.01669100	3.62270300	0.57142300
	C	-2.35620200	0.00229400	-0.64224700
	C	-0.27554400	-0.55510600	0.61209900
	H	-0.39370500	-1.53716800	0.15808900
	H	0.08005500	-0.72831900	1.63175300
	C	0.96596800	1.62584300	0.54295400
	H	0.86808400	1.51784100	1.62879300
	H	1.99527100	1.97796600	0.39933900
	C	0.79398800	0.25205900	-0.11384900
	H	0.48121600	0.40004300	-1.14812600
	C	-3.52211500	-0.91971300	-0.77890600
	H	-4.31044800	-0.61592200	-0.09440000
	H	-3.87400000	-0.90417900	-1.80326400
	H	-3.24012100	-1.92729200	-0.48141000
	O	-1.94078300	0.66416400	-1.56269100
	C	-1.66240900	0.07430200	0.70172800

	H	-1.58384500	1.13336300	0.95878100
	C	2.13582900	-0.51378300	-0.14639100
	C	1.96777900	-1.96750500	-0.53953100
	H	1.48785300	-2.53053000	0.25466300
	H	1.37730200	-2.06019300	-1.44863800
	H	2.94388300	-2.41213200	-0.71354300
	C	3.10633000	0.13880900	-1.11785900
	H	3.28003800	1.18924800	-0.89474800
	H	4.06261900	-0.37622300	-1.07369900
	H	2.72779300	0.07689600	-2.13558100
	O	2.70056800	-0.55360900	1.15529000
	H	3.01158300	0.31989400	1.38682200
	O	-2.46535700	-0.60830700	1.63331400
	H	-2.01440000	-0.63405700	2.47411100
IM33	C	-0.90387100	2.02023700	-1.03462600
	H	0.00497600	2.33985300	-0.53314400
	H	-1.06467700	2.59208600	-1.94438500
	C	2.44673200	0.62149700	0.45260600
	C	0.82161400	-1.05155000	-0.41950000
	H	1.11884500	-1.67942000	0.41812500
	H	0.64638600	-1.72355500	-1.26428400
	C	-0.91746600	0.53426500	-1.30941700
	H	-0.26703200	0.35196500	-2.16447200
	H	-1.91563600	0.27375700	-1.65944900
	C	-0.49155800	-0.33775000	-0.11836300
	H	-0.35259400	0.31177700	0.74812700
	C	3.52225000	0.04969000	1.31380800
	H	4.45942300	0.05291700	0.76183900
	H	3.61336000	0.63682900	2.21947100
	H	3.31222000	-0.99227200	1.54492800
	O	1.89086200	1.66348800	0.69988700
	C	2.02170600	-0.17504700	-0.76143700
	H	1.76964600	0.54960500	-1.53776500
	C	-1.58459600	-1.36191300	0.26284000
	C	-1.12622000	-2.29244500	1.36898900
	H	-0.39347200	-3.00415600	1.00190400
	H	-0.69572700	-1.73203600	2.19617600
	H	-1.97410800	-2.86089600	1.74084000
	C	-2.85588500	-0.66246900	0.70591200
	H	-3.24960000	0.00923100	-0.05425900
	H	-3.61626200	-1.40609600	0.93230800
	H	-2.67693700	-0.06443000	1.59580000
	O	-1.85311200	-2.20694800	-0.84700800
	H	-2.47768000	-1.77706000	-1.42754200
	O	3.11365900	-0.96504500	-1.15707700
	H	2.82343600	-1.60438500	-1.80424000

	O	-2.01478500	2.37951100	-0.19852700
	O	-1.71922400	2.33639400	1.06086800
IM34	C	-1.44094900	-0.78059500	0.77498400
	H	-0.84665900	-1.61370700	0.40641400
	H	-2.06307100	-1.09256000	1.61242200
	C	2.07386400	-1.84045400	-0.48084100
	C	1.84645000	0.44736500	0.47892800
	H	2.56430800	0.74832300	-0.28137100
	H	2.08163200	1.02974800	1.37414200
	C	-0.57830800	0.40038300	1.14622800
	H	-0.05848700	0.15356800	2.07150900
	H	-1.24325600	1.22375900	1.40430800
	C	0.42659900	0.80623500	0.05770600
	H	0.17841500	0.26402000	-0.85562800
	C	3.37273900	-2.18024500	-1.13070500
	H	3.94232900	-2.83113000	-0.47141400
	H	3.18608900	-2.66580900	-2.08073600
	H	3.97701100	-1.28565600	-1.26394000
	O	1.00626400	-2.16664300	-0.93963600
	C	2.11517500	-1.02146200	0.79182200
	H	1.34436400	-1.42626500	1.45099100
	C	0.32052600	2.30807800	-0.28348400
	C	1.39188400	2.74192300	-1.26543600
	H	2.36738600	2.76883500	-0.79009900
	H	1.43174400	2.07155200	-2.12156800
	H	1.17505100	3.74511600	-1.62165400
	C	-1.04195000	2.63374700	-0.86747700
	H	-1.85751700	2.38715600	-0.19169400
	H	-1.09498600	3.69650700	-1.09102200
	H	-1.20891900	2.07539200	-1.78517800
	O	0.55388700	3.08198300	0.88382800
	H	-0.24933800	3.12883500	1.39845100
	O	3.38784300	-1.18484600	1.36263000
	H	3.50170200	-0.55153200	2.06803100
	O	-2.27605400	-0.31644100	-0.28103700
	O	-2.99133900	-1.40182300	-0.78627900
	O	-4.48078800	-0.78294200	0.63333700
	N	-4.23463800	-1.53575700	-0.22072200
IM35	C	0.73723900	2.41689700	0.59333000
	H	-0.29983800	2.50424100	0.22170600
	H	0.85070600	3.17955200	1.37207000
	C	-2.40238900	0.36649200	-0.50043300
	C	-0.52855000	-0.93580200	0.50357100
	H	-0.73747200	-1.69972600	-0.24299500
	H	-0.24000000	-1.46507500	1.41580500
	C	0.95361400	1.00784800	1.12088400

	H	0.34301000	0.87288100	2.01327000
	H	1.98306400	0.94278700	1.47225100
	C	0.64904000	-0.06999900	0.07378800
	H	0.39401700	0.43806900	-0.85866300
	C	-3.41492900	-0.43830700	-1.24256300
	H	-4.33317200	-0.47580900	-0.66060000
	H	-3.59970700	0.01300400	-2.20980300
	H	-3.08312500	-1.46840600	-1.34870700
	O	-2.00118400	1.43588700	-0.89254800
	C	-1.84256100	-0.21207800	0.78033000
	H	-1.68846500	0.62849600	1.45944700
	C	1.88472600	-0.94112200	-0.23894200
	C	1.55917400	-2.05054400	-1.22049500
	H	0.95480700	-2.82085900	-0.75171300
	H	1.02961800	-1.66057500	-2.08722600
	H	2.47856500	-2.51944500	-1.55988600
	C	3.00998100	-0.09695300	-0.80880500
	H	3.31468200	0.70238900	-0.13650600
	H	3.87268600	-0.72954600	-1.00318000
	H	2.70119000	0.37799900	-1.73633300
	O	2.31619400	-1.60687100	0.93824600
	H	2.81641100	-0.99793700	1.47798400
	O	-2.79857700	-1.09985300	1.30081700
	H	-2.40362200	-1.61121500	2.00385600
	O	1.48539000	2.70966100	-0.49711000
IM36	C	-0.22387700	-1.17734000	0.36456500
	H	-0.13786700	-1.29334800	1.44837600
	H	-0.79435000	-2.03785200	0.01644600
	C	-0.94014900	0.09697200	0.04384000
	C	-0.21991900	1.20990100	-0.05333100
	H	-0.69451500	2.15191600	-0.29365200
	C	1.26155100	1.20076700	0.14992600
	H	1.51177600	1.21004200	1.23177900
	H	1.74813300	2.10010800	-0.22134100
	C	1.17204800	-1.18853200	-0.24541200
	H	1.09272900	-1.14468700	-1.35256900
	H	1.70849300	-2.11611300	-0.05766200
	C	2.03197600	-0.01274400	-0.16082900
	C	-2.41736400	0.04751800	-0.13673300
	H	-2.82786400	1.03060700	-0.34974800
	H	-2.68766100	-0.62220900	-0.95307800
	H	-2.90447200	-0.33773000	0.75928500
IM37	C	1.75416700	-0.46014000	-1.15796000
	H	1.82041000	0.46663300	-1.73304900
	H	2.27217500	-1.21705300	-1.74741500
	C	2.44113200	-0.28160600	0.15726300

	C	1.73318900	-0.01229800	1.24679600
	H	2.24563900	0.11276000	2.19217200
	C	0.25304700	0.16726500	1.28429700
	H	0.02055800	1.13674300	1.72421300
	H	-0.19459700	-0.58780600	1.93153900
	C	0.30352700	-0.86689500	-0.99103500
	H	0.26468900	-1.86761200	-0.55889700
	H	-0.18873900	-0.89565000	-1.96007200
	C	-0.44580900	0.06441600	-0.05606000
	C	-1.94283000	-0.31478900	0.11391800
	C	-2.62764700	0.63923300	1.06981500
	H	-3.68161200	0.38485800	1.13494700
	H	-2.20305600	0.55967000	2.06550700
	H	-2.53308800	1.66489200	0.72423700
	C	-2.68299500	-0.33566600	-1.21128700
	H	-2.30039700	-1.10670200	-1.87750800
	H	-3.73231000	-0.54819400	-1.02507700
	H	-2.60523000	0.61984000	-1.72171800
	O	-2.01119700	-1.58643000	0.72483000
	H	-1.85500700	-2.26236500	0.06798900
	C	3.92762400	-0.39361500	0.16423500
	H	4.33794000	-0.21802400	1.15469800
	H	4.24930800	-1.38022400	-0.16977000
	H	4.37168700	0.33069200	-0.51910700
	O	-0.50368000	1.35698800	-0.73298100
	O	0.44377800	2.17595500	-0.41717100
IM38	C	1.80238900	-1.03998800	-1.06057000
	H	1.90054200	-0.23872100	-1.79543600
	H	2.32793000	-1.89666700	-1.48438600
	C	2.46234900	-0.63117800	0.21713700
	C	1.73428400	-0.22014600	1.24877400
	H	2.23406400	0.06410200	2.16621400
	C	0.24591200	-0.09818400	1.25593900
	H	-0.04742400	0.88918700	1.61257200
	H	-0.17479100	-0.80937900	1.96874800
	C	0.34373300	-1.40496500	-0.86201200
	H	0.29981600	-2.33652400	-0.29707000
	H	-0.13172500	-1.56932700	-1.82599300
	C	-0.43031600	-0.36230100	-0.07741800
	C	-1.92143500	-0.76515800	0.13681500
	C	-2.63162800	0.24133800	1.01711100
	H	-3.67992700	-0.03254300	1.09589500
	H	-2.21235300	0.23884400	2.01862800
	H	-2.54955700	1.24061700	0.60127200
	C	-2.66420600	-0.91339300	-1.17867100
	H	-2.23916600	-1.69891200	-1.80096200

	H	-3.69845200	-1.17394400	-0.96973400
	H	-2.64434500	0.01239100	-1.74566400
	O	-1.94950100	-1.98571900	0.84744500
	H	-1.80330900	-2.70926100	0.24099500
	C	3.95162700	-0.69076400	0.25377200
	H	4.34412100	-0.34288800	1.20514800
	H	4.30760300	-1.70756400	0.08784100
	H	4.38128400	-0.07404600	-0.53603100
	O	-0.56587800	0.83444800	-0.87462300
	O	0.59146300	1.61545800	-0.81885000
	N	0.39540600	2.81984700	-0.19952800
	O	-0.66838400	3.00007800	0.23970200
IM39	C	1.77485800	-1.23587700	-0.03735700
	H	1.80058600	-1.56819100	-1.07662000
	H	2.32305500	-1.98191400	0.53901000
	C	2.46355100	0.08609300	0.07323900
	C	1.75865100	1.20724200	0.16636500
	H	2.27945400	2.15276200	0.25199900
	C	0.27161300	1.28950400	0.12802900
	H	-0.03510600	2.05579200	-0.58159800
	H	-0.14306300	1.56992800	1.09885900
	C	0.34211700	-1.17318700	0.44597900
	H	0.32876400	-0.98814200	1.51997100
	H	-0.15099000	-2.12593000	0.26318600
	C	-0.42164000	-0.04229300	-0.24749900
	C	-1.92820100	0.01337000	0.13976500
	C	-2.58120200	1.26597100	-0.39972300
	H	-3.65471600	1.21477600	-0.24029000
	H	-2.21069600	2.14582300	0.11743300
	H	-2.38496600	1.36573100	-1.46354300
	C	-2.64794700	-1.21099900	-0.39424800
	H	-2.26693400	-2.13201100	0.04343300
	H	-3.70739300	-1.14278200	-0.16142300
	H	-2.52986700	-1.27641500	-1.47336800
	O	-2.04949400	0.08525800	1.54606700
	H	-1.89963500	-0.78077900	1.92052100
	C	3.95433100	0.07156400	0.04954000
	H	4.36748300	1.07490600	0.10226500
	H	4.35358100	-0.50790400	0.88191500
	H	4.31964300	-0.39784800	-0.86415800
	O	-0.28875500	-0.12352600	-1.59883400
P1	C	0.46454300	1.75197400	-1.17871300
	H	0.10839100	2.78023700	-1.19991000
	H	1.12712900	1.62033000	-2.03106100
	C	1.27292800	1.61265900	0.10869700
	C	1.16832400	0.18349900	0.63317500

	H	1.81256200	0.05005700	1.49872500
	C	-0.26192100	-0.21125100	0.95152900
	H	-0.44101000	-0.00159000	2.00233200
	H	-0.35540800	-1.28927700	0.82465400
	C	-0.70398300	0.77769300	-1.28065200
	H	-0.35338500	-0.15743200	-1.71982800
	H	-1.44317000	1.19369600	-1.96060200
	C	-1.30703200	0.48994000	0.08464800
	H	-1.55511400	1.44608000	0.54702300
	C	-2.60416100	-0.33550300	0.02192500
	C	-3.10967200	-0.64497100	1.41657000
	H	-4.05536600	-1.17662400	1.35523600
	H	-2.40793800	-1.27804800	1.95103500
	H	-3.25928800	0.27088700	1.98426300
	C	-3.68889600	0.38811900	-0.75706800
	H	-3.42266600	0.51510100	-1.80436600
	H	-4.61026300	-0.18716300	-0.71833100
	H	-3.87927700	1.37427900	-0.33856100
	O	-2.35636400	-1.60115100	-0.56596000
	H	-2.17895400	-1.48735800	-1.49813300
	C	2.70854600	2.04245600	-0.09022700
	H	3.25761700	2.01253600	0.85144000
	H	3.21435000	1.38940400	-0.79554900
	H	2.73683200	3.05965200	-0.47267100
	O	0.64406800	2.43467200	1.07522500
	O	2.04251300	-2.18337300	1.06162100
	O	1.71286800	-0.61686500	-0.43667400
	H	1.22911200	2.54725700	1.82297800
	N	2.10198700	-1.87237400	-0.09394400
	O	2.47315100	-2.52116900	-1.02176000
P2	C	1.67209000	0.05342000	-0.17626800
	H	1.75861100	0.89091500	0.51773400
	H	1.72996100	0.50815500	-1.16875400
	C	2.88669600	-0.81620600	0.01190900
	C	-0.25259000	2.55501300	-0.23551600
	H	-0.72386400	2.76990500	-1.21232300
	C	-0.85952200	1.42051700	0.51895100
	H	-1.88224500	1.70982600	0.76136700
	H	-0.33794000	1.29784400	1.46518900
	C	0.37715500	-0.70688600	0.00442600
	H	0.34077800	-1.08779300	1.02751100
	H	0.41142900	-1.58380800	-0.63650800
	C	-0.87022200	0.11767600	-0.29039400
	H	-0.85884300	0.36515500	-1.35760100
	C	-2.18171000	-0.66059500	-0.04175900
	C	-3.35391300	0.04901600	-0.68819200

	H	-4.27401200	-0.47136400	-0.43788100
	H	-3.45092500	1.07317400	-0.33942500
	H	-3.24299900	0.06081200	-1.76980600
	C	-2.11327300	-2.08318800	-0.56785900
	H	-1.39668200	-2.68349200	-0.01153800
	H	-3.08886400	-2.55218600	-0.47132100
	H	-1.82300000	-2.10370200	-1.61661900
	O	-2.47353000	-0.67832900	1.34344700
	H	-1.85249700	-1.25137900	1.79032600
	C	4.21915800	-0.17639800	-0.23877800
	H	5.01386900	-0.84685600	0.06615000
	H	4.32256600	0.04390000	-1.30022700
	H	4.30061600	0.76983200	0.29114700
	O	2.78882000	-1.97130600	0.34497000
	O	0.67356400	3.22174200	0.13951600
P3	C	1.22164500	0.43227200	-0.56532000
	H	1.09021500	1.51080200	-0.66370600
	H	1.27001300	0.02741300	-1.57491000
	C	2.55628400	0.17921600	0.11391400
	C	2.85484600	-1.30005000	0.21861000
	H	3.46413700	-1.57951200	1.09308500
	C	-1.47807800	1.71466800	0.11639200
	H	-1.84710100	1.79430000	1.15216800
	C	0.04206500	-0.17701300	0.16911200
	H	0.11512300	0.06662000	1.23067300
	H	0.10186900	-1.26083500	0.08496500
	C	-1.30038000	0.31210300	-0.38280300
	H	-1.25411900	0.34761700	-1.47139400
	C	-2.49391100	-0.56299000	0.04180600
	C	-3.79393700	0.11233000	-0.34332900
	H	-4.63430200	-0.51812100	-0.06666000
	H	-3.90623600	1.06231300	0.17411600
	H	-3.82893500	0.29699900	-1.41415000
	C	-2.42514200	-1.94047200	-0.58905700
	H	-1.53320100	-2.48655800	-0.28930400
	H	-3.29184700	-2.52024600	-0.28195800
	H	-2.42302100	-1.87114900	-1.67427900
	O	-2.52963600	-0.66885500	1.45318800
	H	-1.82047100	-1.23977000	1.74483800
	C	3.69958500	0.80741600	-0.66855500
	H	4.65209700	0.61481000	-0.18074900
	H	3.73531500	0.41674700	-1.68165000
	H	3.55427800	1.88551400	-0.72497300
	O	2.56321300	0.62856800	1.44991300
	O	2.49691400	-2.10991600	-0.58931900
	H	2.57179800	1.58406100	1.46358000

	O	-1.19467500	2.70071800	-0.51182000
P4	C	-1.28055900	-1.46564000	-0.49797000
	H	-1.30314000	-2.30338800	0.19706100
	H	-1.81140300	-1.77294100	-1.39617400
	C	-2.05470700	-0.33873400	0.18432300
	C	-1.43223200	0.99557000	-0.20514700
	C	0.02575300	1.14455000	0.12993900
	H	0.08454100	1.68945200	1.07163200
	H	0.46902400	1.77698700	-0.63806600
	C	0.15919300	-1.10034700	-0.84496900
	H	0.17754000	-0.57747900	-1.80495600
	H	0.73017600	-2.01704600	-0.97379000
	C	0.76987500	-0.18586400	0.20793600
	H	0.60312800	-0.63258200	1.18808500
	C	2.28657400	0.01214200	0.04757500
	C	2.79792700	1.05879400	1.01562800
	H	3.87961100	1.13120900	0.94209400
	H	2.38274700	2.03423600	0.78109100
	H	2.53316500	0.80060600	2.03874400
	C	3.03823400	-1.28928500	0.26866400
	H	2.76712600	-2.04700600	-0.46398000
	H	4.10728500	-1.11254500	0.18334200
	H	2.83239700	-1.69383500	1.25725600
	O	2.58358100	0.52640000	-1.23933000
	H	2.44082200	-0.15710000	-1.89158800
	C	-3.52861800	-0.38455400	-0.12254000
H	-4.06043100	0.39903200	0.41313900	
H	-3.70295100	-0.22001800	-1.18141100	
H	-3.93263200	-1.35235200	0.16356100	
O	-1.81870100	-0.49126400	1.57925300	
O	-2.07498200	1.87489300	-0.72030400	
H	-2.40482300	0.09475500	2.05637400	
P5	C	0.47397500	-0.97529800	1.54581000
	H	0.25372800	-2.04066400	1.51283600
	H	0.96288200	-0.76680100	2.49601300
	C	1.45660800	-0.70748200	0.42090600
	C	0.75700700	-0.95719000	-0.91974500
	H	1.42978400	-0.70883600	-1.73666700
	C	-0.51773000	-0.15413000	-1.04713600
	H	-0.95137900	-0.39959300	-2.01245300
	H	-0.28481100	0.91069100	-1.05628800
	C	-0.81490200	-0.18448600	1.41416500
	H	-0.58894800	0.87885200	1.51610700
	H	-1.46512700	-0.45857800	2.24175600
	C	-1.50007300	-0.43840700	0.07904200
	H	-1.77060900	-1.49616000	0.03239900

	C	-2. 80174100	0. 37142600	-0. 08386600
	C	-3. 46980000	0. 07687100	-1. 41178600
	H	-4. 44242600	0. 56001500	-1. 44699300
	H	-2. 88129300	0. 46639600	-2. 23606400
	H	-3. 60538700	-0. 99345000	-1. 54968000
	C	-3. 77603200	0. 07795000	1. 04478000
	H	-3. 39796300	0. 42157400	2. 00557200
	H	-4. 71590600	0. 59086900	0. 85827600
	H	-3. 97424700	-0. 98917000	1. 12482100
	O	-2. 51988700	1. 75994900	-0. 11845700
	H	-2. 25559200	2. 05146600	0. 75216500
	C	2. 71818700	-1. 51957800	0. 60875000
	H	3. 38297700	-1. 46216700	-0. 24621600
	H	3. 25154200	-1. 17634000	1. 49181800
	H	2. 44298000	-2. 55780100	0. 77297600
	O	0. 41453100	-2. 32741900	-0. 97661800
	O	1. 71703000	0. 71708500	0. 60764100
	O	3. 11066200	0. 73914500	-1. 09408900
	O	2. 78583500	2. 48714700	0. 11484600
	N	2. 60772000	1. 34954400	-0. 19132700
	H	1. 13738900	-2. 82243500	-1. 35319000
P6	C	-1. 85663300	0. 43446900	0. 27026700
	H	-1. 79315300	1. 40942400	-0. 21780500
	H	-1. 78360400	0. 65091000	1. 33854600
	C	-3. 23125200	-0. 12301000	0. 00840100
	C	1. 70798900	2. 34002900	-0. 38879000
	H	2. 02292400	3. 07475000	-1. 14911200
	C	0. 95948200	1. 16019600	-0. 91710200
	H	1. 50455800	0. 74600100	-1. 76824100
	H	0. 04779800	1. 57593800	-1. 35670700
	C	-0. 74548800	-0. 49683900	-0. 16105900
	H	-0. 86663700	-0. 72419100	-1. 22099900
	H	-0. 89091300	-1. 43736100	0. 36384800
	C	0. 64624800	0. 07047000	0. 09801100
	H	0. 66802300	0. 52262500	1. 09171200
	C	1. 73785200	-1. 02029500	0. 08288100
	C	3. 11981800	-0. 41866900	0. 23302400
	H	3. 85745500	-1. 21414400	0. 29283300
	H	3. 37554700	0. 19483700	-0. 62677700
	H	3. 17855700	0. 19660600	1. 12649800
	C	1. 52611800	-2. 04065700	1. 18877700
	H	0. 59979200	-2. 59712200	1. 06829800
	H	2. 34329400	-2. 75690500	1. 17915300
	H	1. 50372200	-1. 55708200	2. 16298000
	O	1. 74898100	-1. 66765000	-1. 17844100
	H	0. 95933700	-2. 19973800	-1. 26501600

	C	-4.39620200	0.75531200	0.35692800
	H	-4.41238600	1.62168800	-0.30253700
	H	-5.32119000	0.20250300	0.24388700
	H	-4.30768000	1.13092200	1.37398600
	O	-3.38560600	-1.22203300	-0.46269400
	O	1.94999600	2.53897000	0.77081300
P7	C	0.03310600	0.43755000	-0.00005200
	H	-0.03281800	1.51425000	0.00022100
	C	1.19146100	-0.20475500	-0.00003000
	H	2.11192500	0.35222500	0.00021700
	H	1.25378300	-1.28312200	-0.00007800
	O	-1.19435300	-0.11404400	-0.00003600
	H	-1.12547100	-1.06777000	0.00041600
P8	C	-1.12981700	-0.59844500	0.06425300
	H	-0.85791100	-0.74382400	1.11216000
	H	-1.24209900	-1.60489400	-0.34255400
	C	-2.46755900	0.09040000	0.03381800
	C	-0.04274400	0.16879300	-0.66473500
	H	-0.03587200	1.18794600	-0.27846800
	H	-0.33486400	0.27726000	-1.70948200
	C	1.28841300	-0.49553100	-0.56545400
	H	1.38325200	-1.47442600	-1.01224100
	C	2.37554100	-0.00318300	0.02647000
	C	3.68186600	-0.70215600	0.11314800
	H	4.45731400	-0.10879500	-0.36680200
	H	3.96992600	-0.83054700	1.15451200
	H	3.63511900	-1.67485200	-0.36343200
	O	2.44194200	1.20669100	0.63186300
	H	1.60741000	1.66475600	0.54727800
	C	-3.64381800	-0.69174000	0.53815400
	H	-3.41026600	-1.19059700	1.47595600
	H	-4.49818700	-0.03703200	0.66347300
	H	-3.89315900	-1.46816700	-0.18387000
	O	-2.58593700	1.21760200	-0.37817000
P9	C	0.18356100	-0.52857500	0.09972800
	H	0.13368300	-1.34629800	-0.61907100
	H	0.12879600	-1.00156400	1.08456600
	C	1.54079600	0.12559800	0.01422400
	C	-0.95357400	0.45402100	-0.09194200
	H	-1.03350100	0.77933000	-1.12468200
	H	-0.74804800	1.33589400	0.51753300
	C	-2.25622200	-0.12666900	0.34574000
	H	-2.27510400	-0.51158700	1.38225100
	C	2.71878200	-0.79129600	-0.11196900
	H	2.73800800	-1.20925700	-1.11760100
	H	3.63636900	-0.24168600	0.06054300

	H	2.64271100	-1.62679500	0.58016500
	O	1.66287000	1.32284400	0.04869600
	O	-3.24074100	-0.19490700	-0.33599500
P10	C	-0.00000400	0.18021900	-0.00005200
	O	-0.00001200	1.38509400	0.00001000
	C	-1.27796300	-0.60697000	-0.00166100
	H	-2.12486700	0.06217700	-0.09566600
	H	-1.36279900	-1.17166400	0.92544300
	C	1.27797600	-0.60695900	0.00164700
	H	1.28265400	-1.32894600	0.81576900
	H	1.36244200	-1.17256200	-0.92492500
	H	2.12489400	0.06231100	0.09471500
	H	-1.28228800	-1.32980900	-0.81502500
P11	C	-0.92488900	2.36132600	-0.60965900
	H	-0.87130200	3.15338900	-1.37451100
	C	2.35498100	0.48361200	0.25709500
	C	0.50840700	-1.09920900	-0.35265600
	H	0.67578600	-1.73139200	0.51782800
	H	0.17118900	-1.75339800	-1.15915300
	C	-0.74916500	0.96965900	-1.12860800
	H	0.10503100	1.01065800	-1.80072300
	H	-1.60107700	0.73780600	-1.77300300
	C	-0.59057600	-0.08750000	-0.04039900
	H	-0.33531000	0.43840500	0.88045700
	C	3.26479200	0.03121900	1.34886600
	H	4.20688100	-0.29805800	0.91654800
	H	3.42668800	0.84293100	2.04755100
	H	2.84567500	-0.83693100	1.85374200
	O	1.96571600	1.62065600	0.15113300
	C	1.88008200	-0.55075900	-0.74006500
	H	1.83928700	-0.04738400	-1.70602600
	O	2.82645100	-1.59004000	-0.77521400
	C	-1.92244200	-0.80555000	0.23268600
	C	-1.79075400	-1.84343600	1.33594700
	H	-1.16570500	-2.67433800	1.02424300
	H	-1.37216600	-1.40475800	2.23973900
	H	-2.77102900	-2.24494500	1.58873800
	C	-3.01243600	0.18235200	0.60619500
	H	-3.21996600	0.87054400	-0.20813900
	H	-3.93415100	-0.35298400	0.83342500
	H	-2.72786300	0.76782700	1.47575200
	O	-2.26060500	-1.45189000	-0.98719100
	H	-3.12644000	-1.84602500	-0.90114400
	O	-1.12540400	2.64802100	0.53831900
	H	2.49721400	-2.29561900	-1.32811600
P12	C	1.58098900	-1.34305500	-0.65267700

	H	1.68062600	-0.99840200	-1.68272900
	H	2.03689200	-2.32449500	-0.56584400
	C	2.32115200	-0.38002200	0.22038700
	C	1.73014400	1.01441100	0.23482900
	H	2.28764100	1.61745800	0.95077100
	C	0.26395900	0.95761300	0.60417900
	H	-0.11734000	1.97402900	0.55371000
	H	0.15956100	0.61850800	1.63542500
	C	0.10129200	-1.36098900	-0.27790600
	H	0.00193500	-1.77696100	0.72789800
	H	-0.41238100	-2.03722400	-0.95662300
	C	-0.52407100	0.02832700	-0.31004000
	H	-0.44917500	0.41332800	-1.32962500
	C	-2.02113400	0.00537400	0.05963900
	C	-2.60895100	1.40224200	0.06153700
	H	-3.68781100	1.34563800	0.17748500
	H	-2.22015100	1.98278000	0.89167100
	H	-2.38349100	1.92096300	-0.86759100
	C	-2.81270500	-0.86806800	-0.89933900
	H	-2.51418500	-1.91294900	-0.84155200
	H	-3.87018800	-0.81225200	-0.65472300
	H	-2.67890700	-0.53940100	-1.92788700
	O	-2.19198300	-0.46641700	1.38594600
	H	-2.07182900	-1.41393800	1.40283700
	O	3.29681300	-0.66713500	0.86745200
	O	1.81207500	1.56082100	-1.06594900
	H	2.71951400	1.78977500	-1.25647000
P13	C	1.90824600	-0.84674900	-1.12209200
	H	1.94882500	0.00615200	-1.80060000
	H	2.48721300	-1.63952000	-1.59775200
	C	2.55509200	-0.47269600	0.17314300
	C	1.83649300	-0.32645600	1.28126700
	H	2.33685200	-0.06273400	2.20355100
	C	0.35135400	-0.47945200	1.35136800
	H	-0.07250600	0.24925000	2.03294300
	H	0.08416900	-1.45873700	1.75657000
	C	0.47711800	-1.31974000	-0.94714800
	H	0.47349800	-2.31240800	-0.50516600
	H	-0.01473200	-1.37843000	-1.91858100
	C	-0.31153500	-0.41120400	-0.00729300
	C	-1.82989600	-0.78636000	0.00424800
	C	-2.56498300	-0.44240200	1.28320400
	H	-3.58698700	-0.79738100	1.18347500
	H	-2.12080800	-0.95706600	2.12963600
	H	-2.57434300	0.62142700	1.47833600
	C	-2.54091400	-0.18005500	-1.19064000

	H	-2.01460700	-0.38213700	-2.12232300
	H	-3.53872600	-0.60596300	-1.25186200
	H	-2.63800200	0.89763900	-1.09141800
	O	-1.91383500	-2.20021600	-0.04899100
	H	-1.73374400	-2.49781900	-0.93911800
	C	4.03094700	-0.26180500	0.13979700
	H	4.41461100	0.03875100	1.11044400
	H	4.54871100	-1.17042500	-0.16676100
	H	4.29363200	0.51053800	-0.58304100
	O	-0.07709300	0.86086100	-0.69431000
	O	0.02134000	2.97730400	-0.77909500
	N	-0.35477300	2.05228200	-0.12678900
	O	-0.94055900	2.07885200	0.91915400
P14	C	0.59868600	-1.23862300	-0.14679200
	H	0.52686900	-1.53117500	-1.19681800
	H	1.18785400	-2.01764300	0.33640200
	C	1.31741200	0.07321800	-0.04462900
	C	0.65160500	1.21299700	0.11518600
	H	1.20569700	2.13990100	0.18610900
	C	-0.83730600	1.32564700	0.16153600
	H	-1.21201100	2.00329200	-0.60379400
	H	-1.15918800	1.75096900	1.11650600
	C	-0.78682000	-1.18842700	0.47918300
	H	-0.67570400	-1.09003500	1.56113300
	H	-1.36744700	-2.08200400	0.27328700
	C	-1.54871700	0.01020500	0.00341900
	C	2.80438800	0.02419400	-0.15018200
	H	3.24313600	1.01701400	-0.11326500
	H	3.23332700	-0.57053800	0.65607600
	H	3.10951700	-0.44692300	-1.08466800
	O	-2.66094100	-0.06101500	-0.45466200