

Supporting Information

Organocatalytic Asymmetric Addition of Aldehyde to Nitroolefin by H-D-Pro-Pro-Glu-NH₂: A Mechanistic Study

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The Procedure to Construct the 12 Initial 1-Nit Structures and the Corresponding Transition States. The 12 initial 1-Nit structures (only four enantiomers) were constructed from the most preferred conformer En-01 of 1-En and β -nitrostyrene and optimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The transition state $ts(re \rightarrow re/g^-)$ corresponding to the $re \rightarrow re$ prochiral approach in the g^- orientation of the double bonds was obtained by the relaxed scan of the (2*S*,3*R*)-1-Nit along the two prochiral centers (the number of steps = 10, step size = 0.1 Å) at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The maximum energy was found at the seventh step and was reoptimized at the same level of theory. The distance between the two prochiral centers was found at 2.26 Å. The other 11 transition states were constructed by setting the distance of the two prochiral centers at 2.26 Å and then the structures were reoptimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform. For all transition states and products, the vibrational frequencies and single-point energies were calculated at the SMD M06-2X/6-31+G(d) level of theory in chloroform and at the ω B97X-D/6-311++G(d,p)//SMD M06-2X/6-31+G(d) level of theory, respectively. The torsion angles and relative thermodynamic properties of enantiomeric transition states and products for the 12 stereoselective C–C bond formation calculated at the ω B97X-D/6-311++G(d,p)//SMD M06-2X/6-31+G(d) level of theory in chloroform are listed in Table S2 of the Supporting Information.

The initial 1-Nit structures were constructed from the next most preferred conformers (En-02, En-03, and En-04) and β -nitrostyrene and optimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform. For each transition state $ts(re \rightarrow re/g^-)$, the distance of the two prochiral centers was initially assigned as 2.26 Å as found for $ts(re \rightarrow re/g^-)$ of En-01 and β -nitrostyrene and optimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The torsion angles and relative thermodynamic properties of enantiomeric transition states and products for the

additional stereoselective C–C bond formation of the next most preferred conformers calculated at the ω B97X-D/6-311++G(d,p)//SMD M06-2X/6-31+G(d) level of theory in chloroform are listed in Table S3 of the Supporting Information.

Table S1. Torsion Angles ($^{\circ}$) and Relative Thermodynamic Properties (kcal mol $^{-1}$) of 30 Local Minima for the Enamine Intermediate (**1-En**) with $\Delta G < 5$ kcal mol $^{-1}$ Calculated at the ω B97X-D/6-311++G(d,p)//SMD M06-2X/6-31+G(d) Level of Theory in Chloroform

conformer	ψ_1	ψ_2	ϕ_3	ψ_3	χ_3^1	χ_3^2	χ_3^3	ΔE^a	ΔH^a	ΔG^a	w^b
En-01	-167.4	-18.5	-78.2	-13.7	84.7	-66.0	174.8	0.0	0.0	0.0	44
En-02	40.1	-16.6	-82.6	70.2	-58.7	86.7	-178.9	3.3	2.7	0.6	17
En-03	-101.4	-11.8	-80.6	-9.1	-55.0	-169.3	-168.9	1.4	1.6	0.6	16
En-04	-150.4	150.2	-89.6	67.4	-74.9	55.6	-106.0	2.9	2.8	1.0	9
En-05	-153.9	66.3	-145.5	17.6	70.1	-65.9	125.7	1.9	1.7	1.2	6
En-06	34.7	146.1	-147.6	159.4	-57.8	-65.4	169.9	4.3	4.1	1.9	2
En-07	-162.4	70.5	-90.0	64.9	-48.5	-46.2	-56.2	3.3	3.1	2.0	2
En-08	-94.2	-10.2	79.4	-51.2	-54.5	-71.0	-172.7	3.5	3.6	2.2	1
En-09	-168.6	67.0	-86.0	71.3	-59.4	71.8	49.1	2.8	2.7	2.3	1
En-10	-123.1	153.1	-88.8	64.3	-76.4	53.4	-101.6	3.1	3.1	2.6	1
En-11	-106.3	142.5	-158.5	166.7	-99.7	-67.7	179.3	5.8	5.5	2.6	1
En-12	42.9	59.1	-93.3	63.1	-51.6	-48.0	-58.2	4.5	4.3	2.8	0
En-13	-103.3	69.9	-130.3	14.6	59.5	173.3	166.9	3.9	3.8	3.0	0
En-14	42.0	64.7	-87.7	71.2	-169.4	70.7	-170.5	5.5	5.5	3.3	0
En-15	44.8	67.8	-88.5	63.7	-62.7	179.7	29.0	5.6	5.6	3.4	0
En-16	-161.1	80.3	-90.0	67.7	-54.1	-53.1	94.0	4.1	4.2	3.4	0
En-17	-110.4	68.1	-88.2	68.2	-170.5	163.3	-171.1	4.6	4.4	3.7	0
En-18	-115.0	69.1	-114.8	9.4	-44.0	-47.8	-49.0	5.5	5.6	3.8	0
En-19	-99.5	72.0	-130.0	14.7	59.5	179.0	-20.7	4.7	4.7	3.8	0
En-20	-100.9	79.0	-85.2	66.2	-63.5	-177.3	177.3	5.6	5.3	3.8	0
En-21	-112.4	141.4	-165.0	152.6	-179.2	57.5	98.4	6.4	6.2	4.0	0
En-22	-148.9	147.1	-167.2	-36.5	65.0	-57.0	-70.2	4.6	4.6	4.0	0
En-23	-112.0	120.3	-90.4	65.6	-58.1	90.4	167.7	5.6	5.6	4.1	0
En-24	-96.4	6.0	-73.3	-13.8	90.7	-75.0	55.1	4.5	4.9	4.2	0
En-25	-164.4	-13.0	76.9	-43.8	-35.4	-49.3	-167.2	4.5	4.5	4.3	0
En-26	-91.6	89.9	-84.3	66.9	-71.4	-87.5	23.9	6.8	6.6	4.5	0
En-27	-125.7	60.3	58.7	-176.5	-96.6	-70.1	175.3	7.3	7.0	4.5	0
En-28	-94.3	80.9	-62.6	145.2	-72.2	-78.4	-174.2	5.3	5.3	4.6	0

En-29	-112.3	55.1	-87.2	52.5	56.3	-179.9	-17.0	5.8	5.0	4.7	0
En-30	-164.8	-16.2	-104.4	18.5	42.6	40.0	67.0	5.0	5.0	4.9	0

^a ΔE , ΔH , and ΔG stand for relative electronic energy, enthalpy, and Gibbs free energy. ^b The population calculated by the ΔG values at 25°C.

Table S2. Torsion Angles ($^{\circ}$) and Relative Thermodynamic Properties (kcal mol $^{-1}$) of Transition States and Products for the Stereoselective C–C Bond Formation between En-01 and β -Nitrostyrene^a

prochiral approach ^b	product configuration		ψ_1	ψ_2	ϕ_3	ψ_3	χ_3^1	χ_3^2	χ_3^3	ΔE^c	ΔH^c	ΔG^c
<i>re</i> → <i>re/g</i> ⁻	(2 <i>S</i> ,3 <i>R</i>)	ts	-170.9	-25.9	-75.9	-9.2	67.8	-84.7	-157.4	13.5	11.9	20.5
		1-Nit	-172.2	-20.4	-77.4	-13.3	75.5	-74.5	-167.2	-8.3	-8.6	1.2
<i>re</i> → <i>re/g</i> ⁺	(2 <i>S</i> ,3 <i>R</i>)	ts	-165.0	-21.9	-82.9	-13.5	86.1	-65.0	175.6	15.6	14.6	21.9
		1-D^d	-158.7	-18.2	-82.5	-5.5	78.8	-76.1	-162.1	-6.6	-6.0	-0.2
<i>re</i> → <i>re/t</i>	(2 <i>S</i> ,3 <i>R</i>)	ts	-166.6	-19.7	-77.2	-11.3	77.1	-77.7	-166.2	14.3	13.0	18.9
		1-Nit	-167.6	-18.4	-81.2	-11.2	83.2	-71.5	-172.2	5.6	6.3	13.6
<i>re</i> → <i>si/g</i> ⁻	(2 <i>S</i> ,3 <i>S</i>)	ts	-175.9	-28.6	-70.8	-11.5	54.8	-87.2	-179.8	12.6	11.2	18.2
		1-Nit	178.0	-30.3	-75.6	-12.9	71.6	-69.4	161.2	-2.8	-3.0	6.1
<i>re</i> → <i>si/g</i> ⁺	(2 <i>S</i> ,3 <i>S</i>)	ts	-170.1	-19.0	-76.9	-16.2	86.2	-65.5	173.5	18.3	17.2	23.6
		1-D^d	-165.9	-19.4	-76.5	-8.3	74.9	-78.3	-163.9	-7.7	-6.9	1.2
<i>re</i> → <i>si/t</i>	(2 <i>S</i> ,3 <i>S</i>)	ts	-168.2	-24.4	-73.7	-11.2	69.3	-80.1	-173.1	13.5	12.2	19.5
		1-Nit	-159.5	-16.6	-74.6	-14.4	75.5	-74.8	-167.2	-2.0	-1.7	5.0
<i>si</i> → <i>re/g</i> ⁻	(2 <i>R</i> ,3 <i>R</i>)	ts	-175.2	-8.8	-72.2	-7.9	82.6	-68.4	179.2	18.4	17.6	25.7
		1-Nit	-174.1	-11.5	-75.6	-7.1	83.2	-68.3	-179.1	5.3	6.3	14.3
<i>si</i> → <i>re/g</i> ⁺	(2 <i>R</i> ,3 <i>R</i>)	ts	-170.6	-17.0	-74.9	-11.3	73.9	-78.6	-170.1	14.2	13.3	20.8
		1-Nit	177.1	-21.9	-79.5	-16.3	82.4	-58.8	155.8	-5.9	-5.5	3.1
<i>si</i> → <i>re/t</i>	(2 <i>R</i> ,3 <i>R</i>)	ts	-165.7	-18.1	-69.8	-16.7	72.1	-78.7	-172.9	12.9	11.7	18.3
		1-Nit	-169.0	-15.8	-76.1	-19.4	82.9	-63.6	167.4	-4.5	-4.4	3.0
<i>si</i> → <i>si/g</i> ⁻	(2 <i>R</i> ,3 <i>S</i>)	ts	-168.6	-8.4	-68.8	-18.4	71.3	-83.5	-159.0	21.2	19.8	26.4
		1-D^d	-157.4	-18.3	-78.9	-12.0	80.0	-75.1	-170.0	-4.8	-3.9	5.3
<i>si</i> → <i>si/g</i> ⁺	(2 <i>R</i> ,3 <i>S</i>)	ts	-167.1	-16.8	-73.8	-14.4	75.6	-76.1	-169.4	14.9	13.4	21.9
		1-Nit	-174.6	-21.2	-79.0	-14.8	79.7	-66.5	176.7	-9.5	-9.4	-0.6
<i>si</i> → <i>si/t</i>	(2 <i>R</i> ,3 <i>S</i>)	ts	-166.4	-22.8	-79.6	-14.2	84.9	-65.7	175.2	19.3	18.4	25.2
		1-Nit	-177.9	-23.7	-79.8	-15.3	87.3	-63.2	170.3	6.7	7.2	14.6

^a Torsion angles are for the backbone of dPPE-NH₂. Calculated at the ω B97X-D/6-311++G(d,p)//SMD M06-2X/6-31+G(d) level of theory in chloroform. Each thermodynamic properties of ts and product were calculated relative to the reactant complex (RC) + β -styrene. ^b Represented by the enamine→nitrostyrene prochiral faces and the orientation of the double bonds of enamine and nitrostyrene around the prochiral centers. ^c ΔE , ΔH , and ΔG stand for relative electronic energy, enthalpy, and Gibbs free energy at 25 °C and 1 atm. ^d The cyclic intermediate of dihydrooxazine (*i.e.*, **1-D** in Scheme 1) was represented by product-D.

Table S3. Torsion Angles ($^{\circ}$) and Relative Thermodynamic Properties (kcal mol $^{-1}$) of Transition States and Products for the C–C Bond Formation of the Next Preferred En-02, En-03, and En-04 Conformations with β -Nitrostyrene via the *re* \rightarrow *re/g* Prochiral Approach^a

enamine	product configuration		ψ_1	ψ_2	ϕ_3	ψ_3	χ_3^1	χ_3^2	χ_3^3	ΔE^b	ΔH^b	ΔG^b
En-02	(2 <i>S</i> ,3 <i>R</i>)	ts	43.7	-19.8	-82.1	69.7	-57.4	87.7	-179.7	26.7	25.0	30.4
		1-Nit	44.1	-19.7	-81.5	70.8	-57.3	86.8	-179.9	15.0	15.3	20.6
En-03	(2 <i>S</i> ,3 <i>R</i>)	ts	-110.3	-11.6	-130.1	26.1	-57.6	-65.1	167.1	24.8	24.0	29.6
		1-D^d	-139.9	-9.9	-126.7	26.9	-57.0	-63.6	164.8	14.9	15.1	19.6
En-04	(2 <i>S</i> ,3 <i>R</i>)	ts	-106.1	163.3	-92.1	64.6	-75.9	50.6	-99.9	21.8	20.5	26.6
		1-Nit	-162.9	162.9	-91.7	65.7	-75.7	50.8	-100.5	11.0	11.7	16.8

^a Torsion angles are for the backbone of dPPE-NH₂. Calculated at the ω B97X-D/6-311++G(d,p)//SMD M06-2X/6-31+G(d) level of theory in chloroform. Each thermodynamic properties of ts and product were calculated relative to the reactant complex (RC) + β -styrene. ^b ΔE , ΔH , and ΔG stand for relative electronic energy, enthalpy, and Gibbs free energy at 25 $^{\circ}$ C and 1 atm.

Table S4. Absolute Electronic Energies, Enthalpies, Gibbs Free Energies, Single-point Energies (Hartrees) for the Transitions States and Products for the 12 Stereoselective C–C Bond Formation

prochiral approach		E_e^a	H^a	G^a	$E_{e,sp1}^b$	$E_{e,sp2}^c$
$re \rightarrow re/g^-$	ts	-1850.762193	-1850.117042	-1850.225707	-1850.711360	-1851.380597
	1-Nit	-1850.797173	-1850.150067	-1850.256885	-1850.735833	-1851.404751
$re \rightarrow re/g^+$	ts	-1850.762267	-1850.116199	-1850.226911	-1850.706618	-1851.372510
	1-Nit	-1850.797612	-1850.148979	-1850.262167	-1850.742500	-1851.408280
$re \rightarrow re/t$	ts	-1850.761912	-1850.116266	-1850.229373	-1850.706421	-1851.374648
	1-Nit	-1850.773832	-1850.125044	-1850.235794	-1850.698630	-1851.368771
$re \rightarrow si/g^-$	ts	-1850.764198	-1850.118722	-1850.229927	-1850.714675	-1851.383395
	1-Nit	-1850.789467	-1850.142132	-1850.249965	-1850.728110	-1851.396010
$re \rightarrow si/g^+$	ts	-1850.755966	-1850.109971	-1850.222170	-1850.697950	-1851.365825
	1-Nit	-1850.799502	-1850.150618	-1850.260044	-1850.748132	-1851.413822
$re \rightarrow si/t$	ts	-1850.762939	-1850.117236	-1850.228061	-1850.711889	-1851.380423
	1-Nit	-1850.786480	-1850.138439	-1850.250159	-1850.721774	-1851.391359
$si \rightarrow re/g^-$	ts	-1850.756024	-1850.109572	-1850.219146	-1850.700344	-1851.367940
	1-Nit	-1850.774999	-1850.125707	-1850.235299	-1850.700734	-1851.370299
$si \rightarrow re/g^+$	ts	-1850.764781	-1850.118634	-1850.228936	-1850.714838	-1851.380340
	1-Nit	-1850.794588	-1850.146285	-1850.254838	-1850.728490	-1851.396295
$si \rightarrow re/t$	ts	-1850.762654	-1850.116941	-1850.228718	-1850.712315	-1851.382059
	1-Nit	-1850.790616	-1850.142853	-1850.253473	-1850.726674	-1851.396125
$si \rightarrow si/g^-$	ts	-1850.755218	-1850.109662	-1850.221619	-1850.700719	-1851.364729
	1-Nit	-1850.798688	-1850.149565	-1850.257331	-1850.745476	-1851.407381
$si \rightarrow si/g^+$	ts	-1850.761146	-1850.115803	-1850.224749	-1850.711839	-1851.379897
	1-Nit	-1850.799295	-1850.151363	-1850.259659	-1850.737734	-1851.406592
$si \rightarrow si/t$	ts	-1850.754872	-1850.108616	-1850.220178	-1850.697068	-1851.364341
	1-Nit	-1850.772867	-1850.124474	-1850.235066	-1850.693404	-1851.362791

^a E_e , H , and G stand for electronic energies, enthalpies, and Gibbs free energies calculated at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The H and G values were obtained by scaling the vibrational frequencies with a factor of 0.9440. ^b Single-point energies calculated at the M06-2X/6-31+G(d) level of theory. The solvation free energy (ΔG_s) was calculated from the difference between E_e and $E_{e,sp1}$. ^c Single-point energies calculated at the ω B97X-D/6-311++G(d,p) level of theory.

Table S5. Absolute Electronic Energies, Enthalpies, Gibbs Free Energies, Single-point Energies (Hartrees) for the Protonation of the Dihydrooxazine Oxide Species (**1-D**) and Its Transition to the Cyclobutane Adduct (**1-C**)

	E_e^a	H^a	G^a	$E_{e,sp1}^b$	$E_{e,sp2}^c$
protonation of 1-D					
(2 <i>S</i> ,3 <i>R</i>)- 1-D (boat)	-1927.214471	-1926.538838	-1926.653505	-1927.162817	-1927.875717
ts	-1927.183719	-1926.515184	-1926.629922	-1927.129574	-1927.843351
protonated product	-1927.218891	-1926.542871	-1926.661164	-1927.162873	-1927.87518
transition of 1-D to 1-C					
(2 <i>S</i> ,3 <i>R</i>)- 1-D (boat)	-1927.214471	-1926.538838	-1926.653505	-1927.162817	-1927.875717
ts	-1927.188007	-1926.51406	-1926.628816	-1927.134641	-1927.854236
(2 <i>S</i> ,3 <i>R</i>)- 1-C	-1927.211131	-1926.535536	-1926.65326	-1927.163955	-1927.88579
(2 <i>S</i> ,3 <i>R</i>)- 1-D (half-chair)	-1927.215989	-1926.539464	-1926.651252	-1927.167415	-1927.877671

^a E_e , H , and G stand for electronic energies, enthalpies, and Gibbs free energies calculated at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The H and G values were obtained by scaling the vibrational frequencies with a factor of 0.9440. ^b Single-point energies calculated at the M06-2X/6-31+G(d) level of theory. The solvation free energy (ΔG_s) was calculated from the difference between E_e and $E_{e,sp1}$. ^c Single-point energies calculated at the ω B97X-D/6-311++G(d,p) level of theory.

Table S6. Absolute Electronic Energies, Enthalpies, Gibbs Free Energies, Single-point Energies (Hartrees) for the Transitions States and Products for the C–C Bond Formation of the Next Preferred En-02, En-03, and En-04 Conformations with β -Nitrostyrene via the $re \rightarrow re/g^-$ Prochiral Approach

enamine		E_e^a	H^a	G^a	$E_{e,sp1}^b$	$E_{e,sp2}^c$
En-02	ts	-1850.741676	-1850.096816	-1850.210602	-1850.679931	-1851.348580
	1-Nit	-1850.758204	-1850.110056	-1850.223915	-1850.673300	-1851.344192
En-03	ts	-1850.744511	-1850.098151	-1850.211663	-1850.679720	-1851.348571
	1-Nit	-1850.759101	-1850.111046	-1850.226246	-1850.670047	-1851.340186
En-04	ts	-1850.750025	-1850.104517	-1850.217141	-1850.693703	-1851.361879
	1-Nit	-1850.766293	-1850.117512	-1850.231829	-1850.679456	-1851.348554

^a E_e , H , and G stand for electronic energies, enthalpies, and Gibbs free energies calculated at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The H and G values were obtained by scaling the vibrational frequencies with a factor of 0.9440. ^b Single-point energies calculated at the M06-2X/6-31+G(d) level of theory. The solvation free energy (ΔG_s) was calculated from the difference between E_e and $E_{e,sp1}$. ^c Single-point energies calculated at the ω B97X-D/6-311++G(d,p) level of theory.

Table S7. Torsion Angles ($^{\circ}$) and Relative Thermodynamic Properties (kcal mol $^{-1}$) of Intermediate I7 and Transition State ts5 for the Protonation of the Four Prochiral Approach with Low Barriers of the C–C Bond Formation^a

prochiral approach		ψ_1	ψ_2	ϕ_3	ψ_3	χ_3^1	χ_3^2	χ_3^3	ΔE^b	ΔH^b	ΔG^b
<i>re</i> → <i>si/g</i> ⁻	I7	-169.9	-20.5	-83.7	-8.9	79.8	-70.9	-163.1	-10.0	-8.3	10.3
	ts5	-178.2	-29.0	-68.2	-16.5	62.6	-81.4	-179.7	6.4	4.2	23.6
<i>re</i> → <i>si/t</i>	I7	-167.6	-21.2	-76.3	-15.0	80.7	-70.3	-179.8	-12.9	-11.3	6.3
	ts5	-165.7	-19.1	-72.9	-16.2	77.8	-73.0	-173.1	3.3	0.6	22.0
<i>si</i> → <i>re/g</i> ⁺	I7	-176.3	-20.1	-76.8	-19.6	79.6	-73.2	-173.0	-12.8	-11.3	6.7
	ts5	-174.7	-19.0	-74.6	-17.3	83.5	-61.6	159.2	5.2	2.6	22.2
<i>si</i> → <i>re/t</i>	I7	-171.3	-13.0	-86.7	-7.4	77.9	-73.0	-141.0	-2.4	-0.4	16.7
	ts5	-165.0	-11.7	-97.6	1.4	83.0	-62.8	-147.4	6.7	5.7	24.3

^a Torsion angles are for the backbone and side chain of dPPE-NH₂. Calculated at the ω B97X-D/6-311++G(d,p)//SMD M06-2X/6-31+G(d) level of theory in chloroform. Each thermodynamic properties of intermediate I7 and ts5 were calculated relative to the reactant complex (RC) + β -styrene. ^b ΔE , ΔH , and ΔG stand for relative electronic energy, enthalpy, and Gibbs free energy at 25 $^{\circ}$ C and 1 atm.

Table S8. Absolute Electronic Energies, Enthalpies, Gibbs Free Energies, Single-point Energies (Hartrees) of Intermediate I7 and Transition State ts5 for the Protonation of the Four Prochiral Approaches with Low Barriers of the C–C Bond Formation

prochiral approach		E_e^a	H^a	G^a	$E_{e,sp1}^b$	$E_{e,sp2}^c$
<i>re</i> → <i>si/g</i> ⁻	I7	-1927.194851	-1926.520596	-1926.635422	-1927.125124	-1927.839378
	ts5	-1927.168137	-1926.500117	-1926.613612	-1927.101146	-1927.816059
<i>re</i> → <i>si/t</i>	I7	-1927.195893	-1926.521940	-1926.638267	-1927.119078	-1927.836863
	ts5	-1927.172469	-1926.505254	-1926.615538	-1927.102048	-1927.817547
<i>si</i> → <i>re/g</i> ⁺	I7	-1927.199185	-1926.525332	-1926.641081	-1927.125299	-1927.839700
	ts5	-1927.171715	-1926.504263	-1926.617619	-1927.107943	-1927.821141
<i>si</i> → <i>re/t</i>	I7	-1927.183776	-1926.509160	-1926.626312	-1927.111450	-1927.824607
	ts5	-1927.166781	-1926.496895	-1926.611673	-1927.102042	-1927.817778

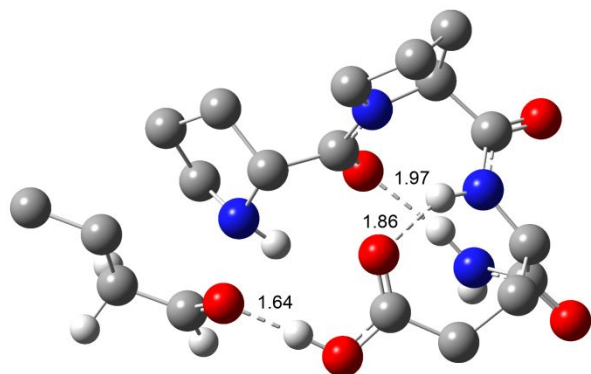
^a E_e , H , and G stand for electronic energies, enthalpies, and Gibbs free energies calculated at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The H and G values were obtained by scaling the vibrational frequencies with a factor of 0.9440. ^b Single-point energies calculated at the M06-2X/6-31+G(d) level of theory. The solvation free energy (ΔG_s) was calculated from the difference between E_e and $E_{e,sp1}$. ^c Single-point energies calculated at the ω B97X-D/6-311++G(d,p) level of theory.

Table S9. Torsion Angles (°) of dPPE-NH₂ for Reactant, Transition States, Intermediates, and Product for the Organocatalytic Addition of Butanal to β -Nitrostyrene by dPPE-NH₂^a

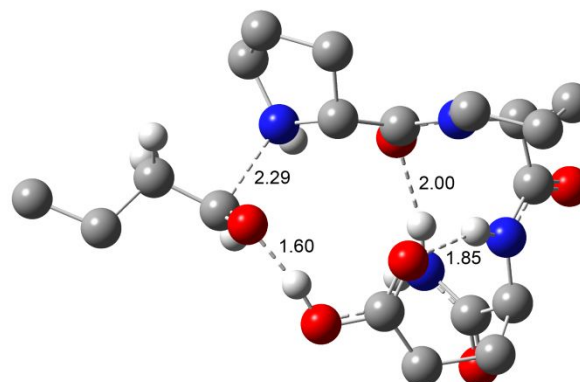
chemical species	Ψ_1	Ψ_2	ϕ_3	Ψ_3	χ_3^1	χ_3^2	χ_3^3
RC	-176.0	-21.1	-72.0	-14.7	77.4	-71.8	178.8
ts1	176.9	-24.6	-74.6	-13.4	78.7	-69.6	175.6
I1	-173.5	-21.4	-82.2	-10.4	79.1	-67.9	-179.0
I2	-172.8	-21.8	-78.6	-14.1	85.4	-63.9	173.3
ts2	-171.3	-17.7	-79.3	-14.4	83.3	-65.0	179.2
I3	-159.8	-18.7	-76.0	-11.4	77.2	-70.1	178.7
ts3	-161.5	-15.3	-83.0	-10.7	83.6	-69.3	-170.7
I4	-167.2	-21.0	-79.8	-9.7	81.1	-71.2	-174.5
I5	-170.6	-26.0	-75.3	-9.1	67.4	-82.3	-174.7
ts4	-170.9	-25.9	-75.9	-9.2	67.8	-84.7	-157.4
I6	-172.2	-20.4	-77.4	-13.3	75.5	-74.5	-167.2
I7	-170.0	-19.8	-79.7	-10.3	73.2	-81.1	-146.9
ts5	177.2	-28.2	-70.4	-13.6	68.8	-75.4	173.4
I8	-179.3	-27.0	-73.1	-14.9	73.6	-69.9	172.1
I9	-177.2	-26.6	-72.0	-17.5	71.6	-71.0	167.1
ts6	-170.8	-19.9	-80.6	-10.8	80.7	-68.5	-175.7
I10	-164.9	-23.6	-97.7	-0.7	85.0	-65.9	178.9
I11	-162.2	-10.2	-60.9	-23.4	73.8	-67.6	166.0
ts7	-168.6	-11.7	-71.1	-19.5	84.6	-64.7	169.1
PC	-170.0	-20.2	-72.3	-13.6	74.9	-75.2	-175.6

^a Optimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform.

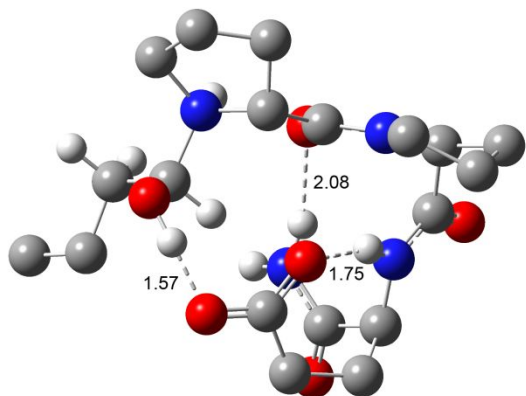
RC



ts1



I1



I2

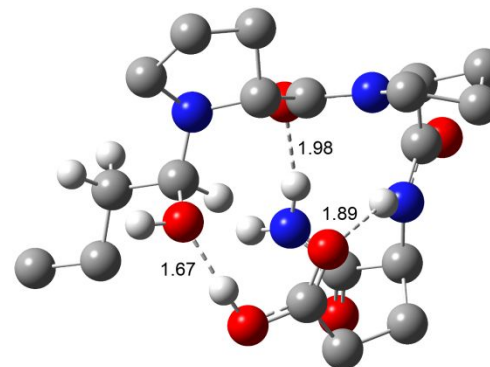
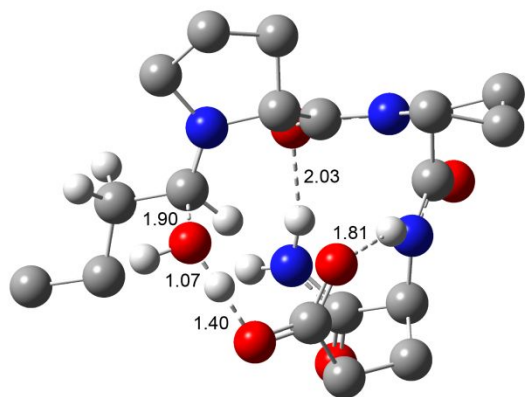
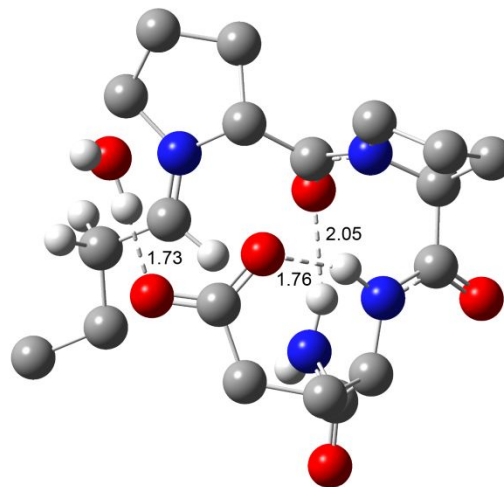


Figure S1. Optimized structures of reactant complex (RC), transition states (ts), intermediates (I), and product complex (PC) for the organocatalytic reaction of butanal and β-nitrostyrene by dPPE-NH₂ at the SMD M06-2X/6-31+G(d) level of theory in chloroform. All H-bond distances are in Å.

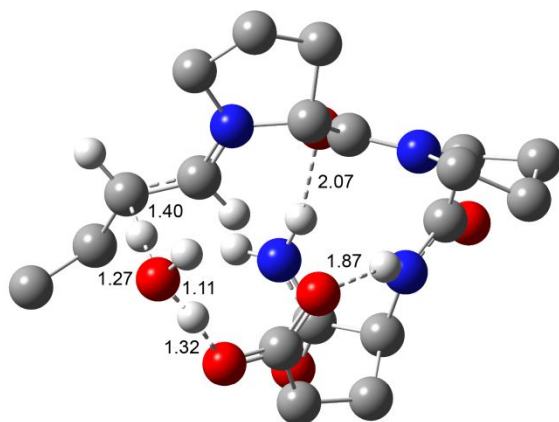
ts2



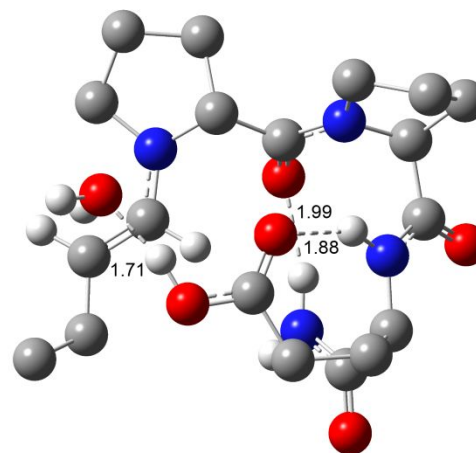
I3



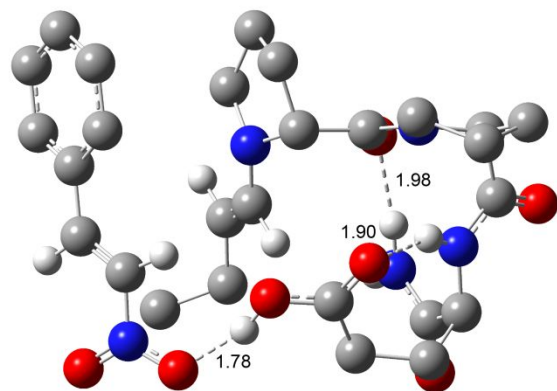
ts3



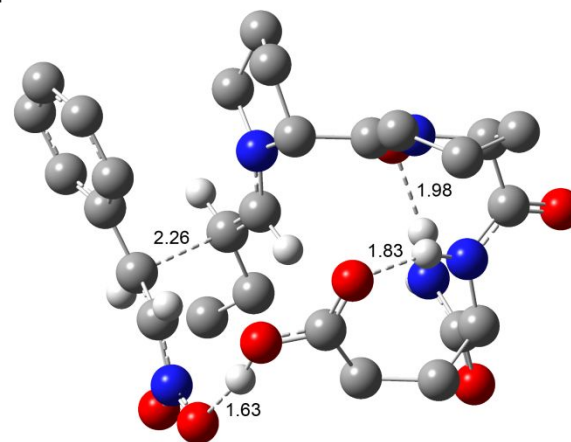
I4

**Figure S1.** (Continued.)

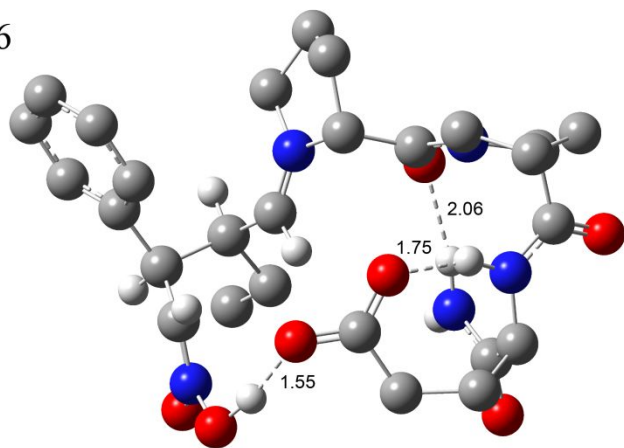
I5



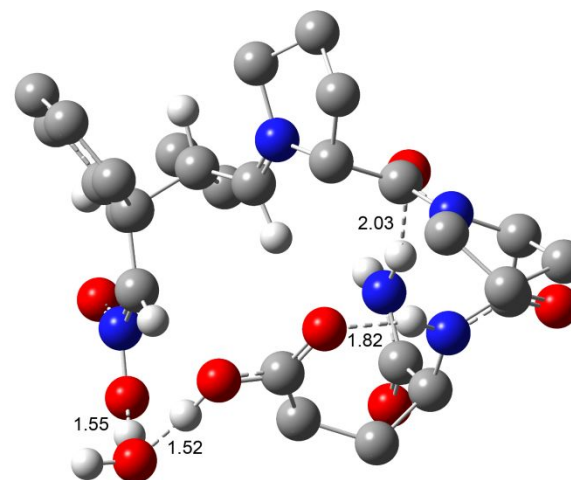
ts4

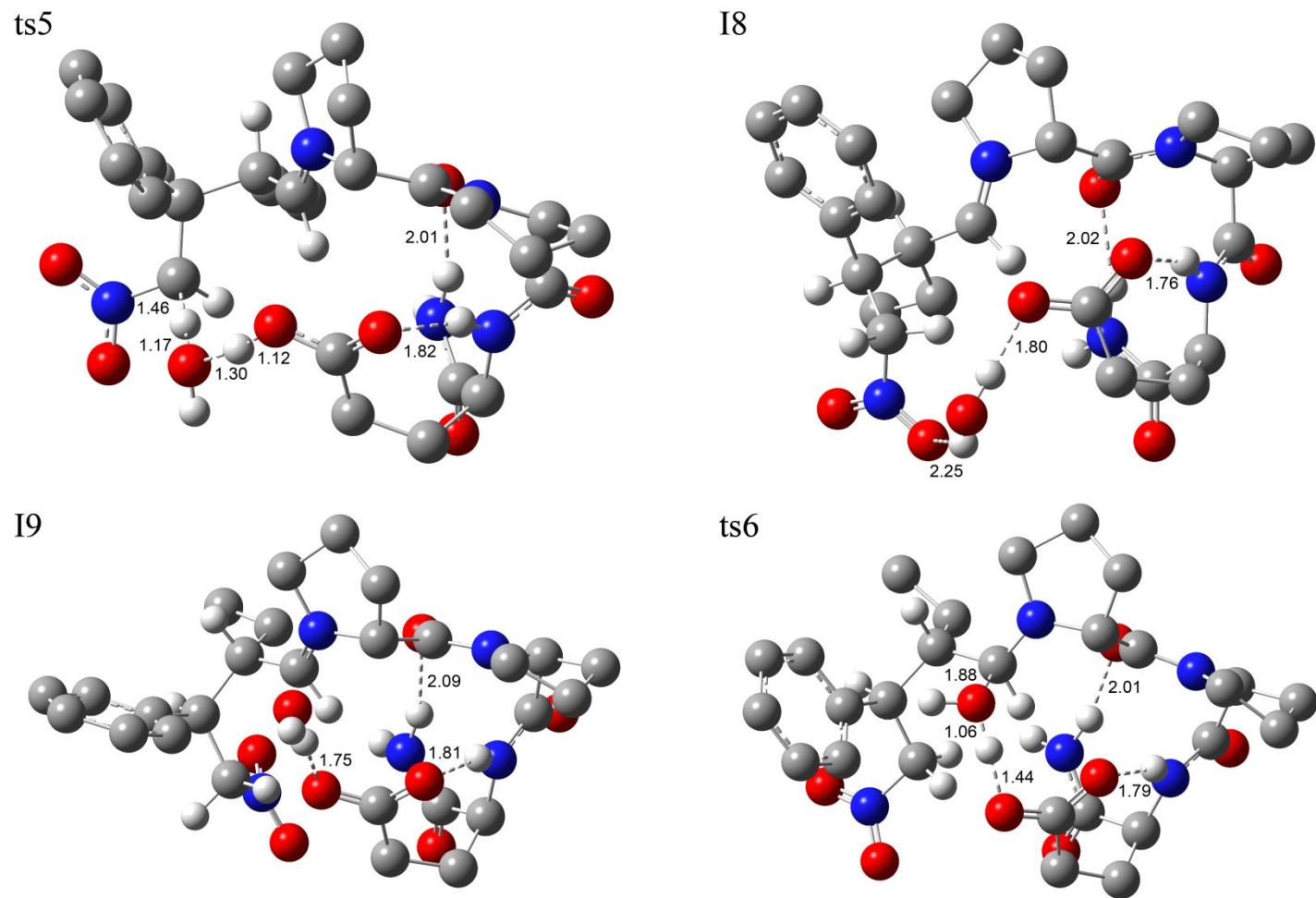


I6

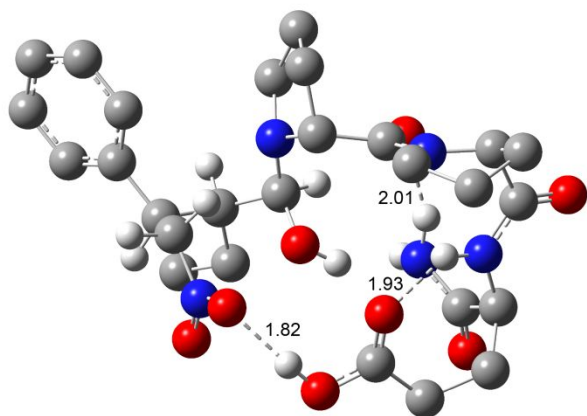


I7

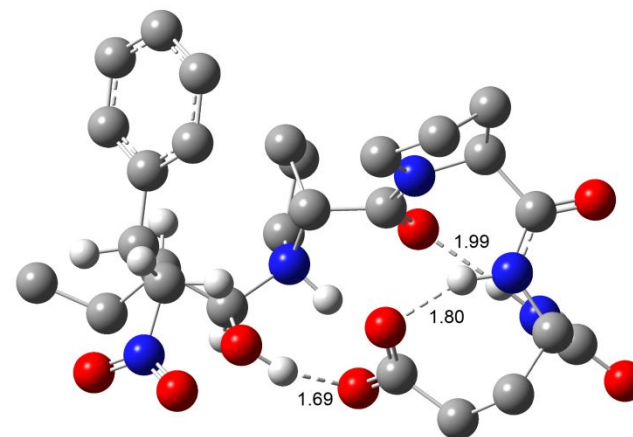
**Figure S1.** (Continued.)



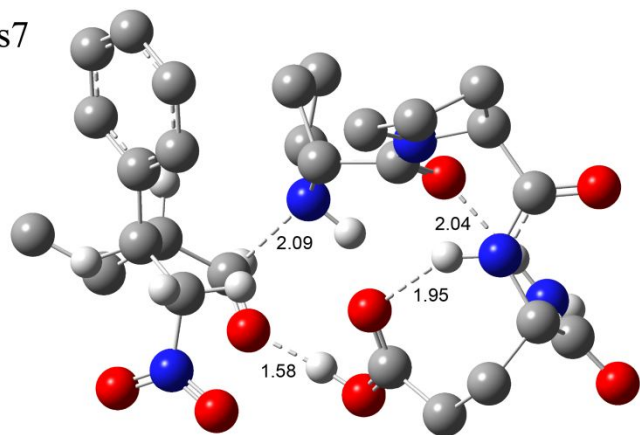
I10



I11



ts7



PC

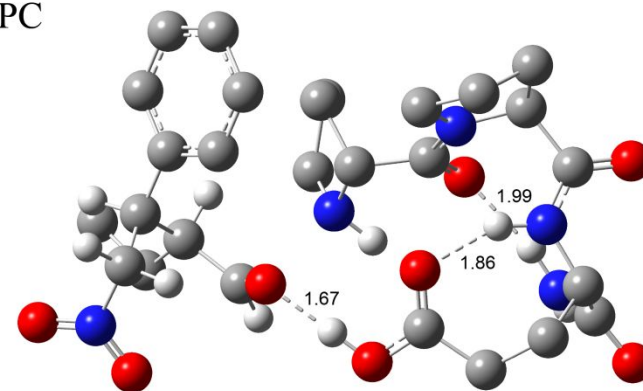
**Figure S1.** (Continued.)

Table S10. Absolute Electronic Energies, Enthalpies, Gibbs Free Energies, Single-Point Energies (Hartrees) for the Organocatalytic Addition of Butanal to β -Nitrostyrene by dPPE-NH₂

conformer	E_e^a	H^a	G^a	$E_{e,sp1}^b$	$E_{e,sp2}^c$
dPPE-NH ₂	-1180.859814	-1180.447211	-1180.524425	-1180.825163	-1181.2647754
butanal	-232.356403	-232.241316	-232.278628	-232.347763	-232.4506636
β -nitrostyrene	-513.962542	-513.821540	-513.868477	-513.945888	-514.109360
water	-76.391864	-76.368017	-76.390115	-76.383721	-76.432089
RC	-1413.220900	-1412.690387	-1412.787908	-1413.184272	-1413.730533
ts1	-1413.217694	-1412.687271	-1412.779292	-1413.180136	-1413.725189
I1	-1413.240248	-1412.707122	-1412.797406	-1413.191004	-1413.732811
I2	-1413.232720	-1412.700786	-1412.793087	-1413.193194	-1413.735710
ts2	-1413.211781	-1412.682969	-1412.774774	-1413.165843	-1413.711699
I3	-1413.224155	-1412.693995	-1412.789211	-1413.180034	-1413.726473
ts3	-1413.186216	-1412.663305	-1412.756168	-1413.141495	-1413.691625
I4	-1413.215729	-1412.685378	-1412.781100	-1413.176160	-1413.725393
I5	-1850.778595	-1850.132975	-1850.248123	-1850.730692	-1851.401941
ts4	-1850.762193	-1850.117042	-1850.225707	-1850.711360	-1851.380597
I6	-1850.797173	-1850.150067	-1850.256885	-1850.735833	-1851.404751
I7	-1927.197349	-1926.522946	-1926.638336	-1927.130296	-1927.846616
ts5	-1927.173723	-1926.505935	-1926.619143	-1927.110119	-1927.825818
I8	-1927.215032	-1926.538469	-1926.654276	-1927.152801	-1927.870175
I9	-1927.214905	-1926.538222	-1926.654588	-1927.160255	-1927.873282
ts6	-1927.206492	-1926.531625	-1926.644133	-1927.153556	-1927.866371
I10	-1927.223854	-1926.546352	-1926.659242	-1927.180971	-1927.886899
I11	-1927.217878	-1926.538131	-1926.648713	-1927.158735	-1927.864575
ts7	-1927.205976	-1926.529822	-1926.641042	-1927.156263	-1927.866148
PC	-1927.215641	-1926.539255	-1926.656582	-1927.169501	-1927.880960

^a E_e , H , and G stand for electronic energies, enthalpies, and Gibbs free energies calculated at the SMD M06-2X/6-31+G(d) level of theory in chloroform. The H and G values were obtained by scaling the vibrational frequencies with a factor of 0.9440.

^b Single-point energies calculated at the M06-2X/6-31+G(d) level of theory. The solvation free energy (ΔG_s) was calculated from the difference between E_e and $E_{e,sp1}$.

^c Single-point energies calculated at the ω B97X-D/6-311++G(d,p) level of theory.

Cartesian coordinates of transition states and products for the stereoselective C–C bond formation optimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform:

(1) <i>re</i> → <i>re/g</i> ⁻ : ts				O	-2.900446	3.595197	-1.70188
				N	-1.917109	1.585848	-2.074075
N	1.090658	-1.335208	-0.681809	H	-1.283854	3.38633	1.997386
C	0.048808	-1.982397	0.114484	H	-0.933319	2.578787	0.49124
C	0.500034	-3.450588	0.127768	C	-1.094229	1.278231	2.160773
C	1.112629	-3.626135	-1.26771	H	-1.480437	1.940383	-2.917247
C	1.815747	-2.291631	-1.533461	H	-1.886202	0.581588	-1.912752
H	0.00498	-1.535279	1.113939	O	-1.689621	0.210116	2.163466
H	-0.320786	-4.14452	0.322261	O	0.025913	1.386342	2.852599
H	1.259301	-3.582166	0.9054	C	2.851231	2.91065	-2.611967
H	1.80621	-4.468692	-1.315997	H	3.628118	3.129452	-1.874224
H	0.322073	-3.788124	-2.007273	H	3.307131	2.362308	-3.445254
H	2.870169	-2.321451	-1.240685	H	2.495003	3.870524	-2.998978
H	1.746591	-1.970021	-2.578168	H	3.910848	1.748516	-0.421956
C	1.127899	-0.016825	-0.845137	C	3.953546	-0.293353	0.318011
C	2.045669	0.715745	-1.57964	C	5.011685	-0.634362	-0.54034
C	3.372663	1.054902	0.217409	C	3.485917	-1.251832	1.22971
H	2.763911	0.173884	-2.19492	C	5.589033	-1.897618	-0.491975
C	1.689285	2.121021	-2.01534	H	5.37847	0.105919	-1.248779
H	1.246264	2.667569	-1.170838	C	4.063083	-2.519628	1.275246
H	0.900724	2.056047	-2.77789	H	2.672628	-1.014216	1.910543
H	0.388441	0.531426	-0.254376	C	5.109058	-2.848665	0.41343
C	-1.311554	-1.804166	-0.583749	H	6.412232	-2.143898	-1.156576
O	-1.381926	-1.322298	-1.719897	H	3.694994	-3.252134	1.988354
N	-2.415793	-2.170359	0.091717	H	5.556446	-3.837984	0.453265
C	-3.732709	-1.968489	-0.527643	C	2.645152	1.617967	1.266727
C	-2.507246	-2.72874	1.451317	N	2.388757	2.960831	1.31391
C	-4.015931	-0.492343	-0.834758	H	2.181164	1.048101	2.056153
C	-4.706634	-2.543525	0.518616	O	1.59023	3.388364	2.212601
H	-3.790352	-2.490608	-1.486304	O	2.913887	3.761442	0.52717
C	-3.948197	-2.40368	1.843372	H	0.529515	2.242305	2.68201
H	-1.77251	-2.267736	2.114098	(2) <i>re</i> → <i>re/g</i> ⁻ : 1-Nit			
H	-2.343322	-3.812985	1.422148	N	-0.989705	-1.473249	0.602117
O	-4.806754	-0.179277	-1.720146	C	0.092869	-2.145337	-0.150318
N	-3.363831	0.400439	-0.062468	C	-0.277275	-3.627039	-0.006822
H	-5.667377	-2.022649	0.508237	C	-0.850916	-3.698938	1.41261
H	-4.88965	-3.599843	0.296632	C	-1.653288	-2.405657	1.551235
H	-4.006614	-1.374778	2.216497	H	0.097669	-1.767238	-1.175481
H	-4.323224	-3.074167	2.620001	H	0.580951	-4.28621	-0.150704
C	-3.507294	1.832376	-0.206672	H	-1.040504	-3.878811	-0.750836
H	-2.778784	0.070422	0.704464	H	-1.480346	-4.577106	1.567622
C	-3.051689	2.561573	1.067714	H	-0.041587	-3.718384	2.149005
C	-2.7558	2.408935	-1.415725	H	-2.692747	-2.518299	1.224534
H	-4.563243	2.069503	-0.378956	H	-1.624574	-1.976005	2.554107
H	-3.63476	2.180517	1.913563	C	-1.270944	-0.235849	0.438027
H	-3.321094	3.612388	0.935566				
C	-1.551614	2.508468	1.400735				

C	-2.295448	0.523581	1.205816	H	-5.753036	0.152956	1.303719
C	-3.426156	1.001917	0.227102	C	-4.561659	-2.222056	-1.510394
H	-2.767524	-0.121643	1.954181	H	-2.930261	-0.861479	-1.78511
C	-1.548106	1.664621	1.932522	C	-5.722678	-2.521776	-0.798069
H	-1.112563	2.351498	1.196996	H	-7.056323	-1.883688	0.770762
H	-0.712021	1.212988	2.48246	H	-4.226231	-2.878271	-2.309078
H	-0.688716	0.291346	-0.324676	H	-6.295058	-3.413633	-1.036853
C	1.419895	-1.793374	0.537704	C	-2.85007	1.734241	-0.942844
O	1.430853	-1.204849	1.624511	N	-2.561476	2.997933	-0.87575
N	2.540565	-2.176842	-0.090411	H	-2.554592	1.235967	-1.854498
C	3.849267	-1.942512	0.534636	O	-1.857982	3.539568	-1.925409
C	2.648079	-2.739293	-1.450152	O	-2.852903	3.798399	0.044475
C	4.193673	-0.456922	0.692306	H	-1.148677	2.833728	-2.156508
C	4.818266	-2.64405	-0.431985				
H	3.869742	-2.371282	1.539934				
C	4.121931	-2.512104	-1.790299	(3) $re \rightarrow re/g^+$: ts			
H	1.971005	-2.218834	-2.131996	N	0.739511	-1.384763	-0.669439
H	2.407625	-3.808821	-1.436966	C	-0.444571	-2.063039	-0.155429
O	5.068511	-0.113712	1.486601	C	-0.252648	-3.505512	-0.658455
N	3.517901	0.390731	-0.100617	C	0.429207	-3.302193	-2.016803
H	5.81353	-2.194321	-0.402798	C	1.370789	-2.11702	-1.781504
H	4.907697	-3.698835	-0.151008	H	-0.448149	-1.986701	0.937726
H	4.257556	-1.502572	-2.193419	H	-1.195699	-4.05375	-0.729658
H	4.486152	-3.230433	-2.528097	H	0.409519	-4.025731	0.040119
C	3.710761	1.823682	-0.071056	H	0.968748	-4.191608	-2.350028
H	2.774571	0.06065	-0.727737	H	-0.311875	-3.041911	-2.778895
C	3.223419	2.466267	-1.384443	H	2.374917	-2.441214	-1.492715
C	3.023304	2.505097	1.117103	H	1.448364	-1.456	-2.651454
H	4.779915	2.030955	0.044628	C	1.021299	-0.134873	-0.326999
H	3.666641	1.906472	-2.216465	C	2.201955	0.515274	-0.678084
H	3.648252	3.474124	-1.413312	C	3.408415	-0.323258	0.83914
C	1.709693	2.60485	-1.584917	H	2.770085	0.080194	-1.4995
O	3.256344	3.686477	1.360542	C	2.344299	2.015709	-0.500495
N	2.1233	1.770769	1.803477	H	2.820834	2.245977	0.463899
H	1.5294	3.319661	-2.395632	H	1.350857	2.480825	-0.46757
H	1.242098	3.057885	-0.697928	H	0.330397	0.319107	0.380162
C	0.893264	1.355407	-1.919585	C	-1.709771	-1.448455	-0.759235
H	1.707359	2.186465	2.628919	O	-1.658792	-0.748917	-1.778361
H	2.032186	0.7662	1.674904	N	-2.883864	-1.741614	-0.167411
O	1.374481	0.204641	-1.768355	C	-4.143313	-1.37677	-0.825641
O	-0.295082	1.552652	-2.319722	C	-3.087624	-2.490132	1.085482
C	-2.441246	2.423952	2.90822	C	-4.376323	0.134268	-0.911944
H	-3.24367	2.95355	2.388724	C	-5.206871	-2.082752	0.036516
H	-2.881871	1.74516	3.647986	H	-4.143273	-1.732178	-1.859829
H	-1.85119	3.171933	3.447091	C	-4.548007	-2.182729	1.416447
H	-4.061626	1.684409	0.800755	H	-2.395594	-2.148299	1.858463
C	-4.248946	-0.206069	-0.192159	H	-2.932991	-3.563021	0.91712
C	-5.415641	-0.515586	0.514017	O	-5.163011	0.591767	-1.736655
C	-3.829481	-1.073494	-1.208622	N	-3.699041	0.887316	-0.021893
C	-6.148748	-1.663705	0.215355				

H	-6.153627	-1.537119	0.040912	C	0.308608	3.630288	-1.946023
H	-5.389947	-3.082981	-0.369273	C	-0.872891	2.749767	-1.537415
H	-4.613791	-1.222721	1.941444	H	1.083122	2.241261	0.97629
H	-4.996402	-2.952137	2.049017	H	2.173095	4.014464	-0.824483
C	-3.75124	2.333495	-0.010406	H	0.671857	4.391195	0.053321
H	-3.042321	0.442142	0.613603	H	-0.014919	4.612704	-2.298968
C	-3.47101	2.895074	1.400635	H	0.883022	3.145469	-2.741829
C	-2.790957	2.990675	-1.011002	H	-1.654611	3.366695	-1.070473
H	-4.758234	2.63484	-0.314276	H	-1.307019	2.217577	-2.389418
H	-3.956765	2.239918	2.131532	C	-1.158267	1.267065	0.421586
H	-3.954623	3.872864	1.47017	C	-2.237349	0.355677	-0.170764
C	-2.001435	3.106173	1.769906	C	-3.49883	0.42717	0.721136
O	-2.856176	4.202938	-1.202511	H	-2.519048	0.742575	-1.158745
N	-1.843138	2.200613	-1.555563	C	-1.653082	-1.059625	-0.335204
H	-1.945421	3.594705	2.751635	H	-1.87911	-1.643868	0.567965
H	-1.522416	3.796694	1.062722	H	-0.558878	-0.974744	-0.392648
C	-1.151183	1.860707	1.86063	H	-0.563626	0.710076	1.148605
H	-1.253302	2.609628	-2.272393	C	2.114061	1.392965	-0.724924
H	-1.910297	1.183728	-1.538112	O	1.938133	0.758542	-1.771307
O	-1.551845	0.719664	1.75215	N	3.316142	1.377164	-0.105669
O	0.153325	2.057323	2.094072	C	4.447245	0.695749	-0.740511
C	3.170255	2.640987	-1.62403	C	3.678821	2.022779	1.16702
H	4.166296	2.184293	-1.677266	C	4.274212	-0.824582	-0.809091
H	2.682596	2.497089	-2.595084	C	5.644273	1.107517	0.134298
H	3.301625	3.71657	-1.466349	H	4.555395	1.027147	-1.777067
H	2.967935	0.333179	1.586146	C	5.014557	1.35944	1.507856
C	4.723468	0.121401	0.313458	H	2.91581	1.839174	1.926681
C	5.351967	1.228221	0.895479	H	3.791279	3.105275	1.027066
C	5.348484	-0.522268	-0.763765	O	4.965234	-1.493874	-1.573116
C	6.579588	1.683846	0.414614	N	3.352839	-1.349411	0.024509
H	4.877774	1.730154	1.735527	H	6.425561	0.343692	0.1421
C	6.57299	-0.068415	-1.24457	H	6.073891	2.033765	-0.260941
H	4.86147	-1.370674	-1.241357	H	4.83252	0.409081	2.022971
C	7.1915	1.039296	-0.658466	H	5.633212	1.987315	2.153144
H	7.054563	2.54372	0.878867	C	3.009312	-2.752611	0.040039
H	7.044217	-0.572999	-2.08353	H	2.810527	-0.730686	0.62214
H	8.144322	1.396421	-1.038886	C	2.491347	-3.195747	1.419924
C	3.162272	-1.688389	1.021138	C	1.991741	-3.151952	-1.038961
N	2.079417	-2.086367	1.765132	H	3.917207	-3.322771	-0.182705
H	3.735525	-2.494601	0.585337	H	3.168402	-2.802707	2.186028
O	1.845398	-3.312339	1.90738	H	2.565119	-4.285478	1.449771
O	1.337083	-1.225055	2.291031	C	1.038573	-2.850153	1.76956
H	0.367414	3.006335	2.149442	O	1.669172	-4.335114	-1.15082
				N	1.462332	-2.164402	-1.778482
				H	0.72001	-3.485306	2.604108
				H	0.364326	-3.093961	0.933793
				C	0.753224	-1.415945	2.149828
				H	0.812196	-2.414642	-2.515151
				H	1.757649	-1.190998	-1.711026
				O	1.457762	-0.45833	1.901065
(4) $re \rightarrow re/g^+$: 1-D							
N	-0.300329	1.806518	-0.55889				
C	1.014242	2.265314	-0.114608				
C	1.136928	3.702685	-0.660471				

O	-0.398735	-1.195265	2.800126	C	3.963083	1.798759	0.137307
C	-2.134746	-1.809083	-1.575358	C	2.645707	1.936562	2.197633
H	-3.219435	-1.958193	-1.573144	C	4.286363	0.469989	-0.548462
H	-1.870771	-1.253261	-2.483138	C	4.883193	2.07345	1.340018
H	-1.66151	-2.796058	-1.634404	H	4.054169	2.562769	-0.639909
H	-3.214924	0.08429	1.728763	C	4.084321	1.541066	2.533533
C	-4.614614	-0.452428	0.20443	H	1.911152	1.262122	2.644484
C	-4.92155	-1.653552	0.84697	H	2.428934	2.964725	2.51201
C	-5.3098	-0.113123	-0.962207	O	5.201355	0.403545	-1.364367
C	-5.894688	-2.509851	0.329744	N	3.532286	-0.589032	-0.187778
H	-4.392907	-1.921025	1.759631	H	5.860677	1.600083	1.220542
C	-6.285164	-0.962926	-1.479161	H	5.034667	3.153522	1.436007
H	-5.078576	0.816736	-1.479013	H	4.16424	0.449448	2.589855
C	-6.577127	-2.167469	-0.836572	H	4.412803	1.959293	3.487709
H	-6.120371	-3.442038	0.840315	C	3.696567	-1.891249	-0.79589
H	-6.815041	-0.687404	-2.386805	H	2.784065	-0.472933	0.491061
H	-7.335119	-2.832189	-1.241064	C	3.139746	-3.010394	0.099598
C	-3.908036	1.86753	0.78414	C	3.071047	-1.998507	-2.193201
N	-3.011943	2.770604	1.018397	H	4.767746	-2.067219	-0.938887
H	-4.908067	2.236939	0.592298	H	3.526817	-2.867961	1.114894
O	-3.150664	4.015373	1.087434	H	3.557526	-3.947673	-0.276032
O	-1.729971	2.321264	1.311358	C	1.619213	-3.186506	0.128571
H	-0.887016	-2.023563	2.957492	O	3.27321	-3.008345	-2.864376

(5) $re \rightarrow re/t: ts$

N	-0.901754	1.668875	-0.31811	H	1.373836	-4.183396	0.509576
C	0.174623	2.036093	0.593136	H	1.188904	-3.150493	-0.882998
C	-0.083019	3.536583	0.819669	C	0.838965	-2.205123	0.960974
C	-0.598934	4.001215	-0.549487	H	1.896094	-1.02496	-3.528909
C	-1.445573	2.825572	-1.050014	H	2.17997	-0.118792	-2.072764
H	0.100089	1.445842	1.511187	O	1.244205	-1.145453	1.41239
H	0.811724	4.073353	1.14523	O	-0.415053	-2.61456	1.156158
H	-0.856911	3.651685	1.586047	C	-1.794661	-1.714614	-3.064206
H	-1.179539	4.923687	-0.484389	H	-2.225756	-1.079112	-3.845958
H	0.241083	4.171695	-1.229612	H	-0.719107	-1.508895	-3.018007
H	-2.511342	2.938204	-0.82278	H	-1.928409	-2.759387	-3.365824
H	-1.342158	2.653666	-2.126584	H	-3.465591	1.30958	0.353835
C	-1.237187	0.409383	-0.560567	C	-3.37115	-0.63397	1.315769
C	-2.35001	-0.004736	-1.287484	C	-2.562559	-0.12949	2.345424
C	-3.769525	0.274726	0.210348	C	-3.784441	-1.971236	1.381027
H	-2.814103	0.733234	-1.943165	C	-2.193889	-0.931653	3.425471
C	-2.460792	-1.445177	-1.711846	H	-2.23651	0.908691	2.302647
H	-3.52537	-1.710624	-1.775165	C	-3.415868	-2.775345	2.45917
H	-2.01307	-2.091865	-0.944762	H	-4.395667	-2.39173	0.586845
H	-0.643086	-0.329806	-0.023071	C	-2.625716	-2.259505	3.487151
C	1.536588	1.808584	-0.07253	H	-1.576091	-0.520118	4.218992
O	1.629691	1.641084	-1.292449	H	-3.744829	-3.809887	2.493668
N	2.620766	1.835575	0.72737	H	-2.342171	-2.886708	4.327251
				C	-5.008214	0.089467	-0.412839
				N	-5.491823	1.064825	-1.256234
				H	-5.610016	-0.806179	-0.374668

O	-6.581952	0.878028	-1.835708
O	-4.835689	2.117102	-1.431127
H	-0.887096	-1.969799	1.725936

(6) *re*→*re/t*: 1-Nit

N	-0.727836	1.821502	-0.008378
C	0.448541	2.087672	0.844192
C	0.285209	3.577258	1.188345
C	-0.346004	4.158119	-0.081987
C	-1.32384	3.077402	-0.539386
H	0.405522	1.430622	1.716337
H	1.235963	4.048718	1.446763
H	-0.395791	3.672984	2.039909
H	-0.856322	5.104915	0.102967
H	0.419206	4.320544	-0.846879
H	-2.328445	3.184934	-0.120497
H	-1.409835	2.989977	-1.624068
C	-1.139725	0.632572	-0.261038
C	-2.385373	0.30834	-0.986041
C	-3.539374	0.330127	0.119216
H	-2.646174	1.129457	-1.663179
C	-2.198892	-1.0022	-1.762521
H	-2.015382	-1.826059	-1.059452
H	-1.282599	-0.901023	-2.359494
H	-0.541959	-0.172389	0.171174
C	1.714894	1.812163	0.028146
O	1.660788	1.674124	-1.19708
N	2.869456	1.752749	0.712238
C	4.140231	1.648319	-0.014613
C	3.048473	1.786818	2.17661
C	4.319294	0.312328	-0.740081
C	5.189409	1.849514	1.09234
H	4.194603	2.418586	-0.788811
C	4.492906	1.312576	2.346217
H	2.329052	1.12774	2.669669
H	2.915933	2.808502	2.550717
O	5.161793	0.20643	-1.626088
N	3.531748	-0.705033	-0.332039
H	6.126892	1.339569	0.859477
H	5.396764	2.918987	1.200448
H	4.524499	0.217371	2.360481
H	4.936404	1.682732	3.272993
C	3.558646	-2.004086	-0.970049
H	2.835499	-0.554488	0.392917
C	3.105595	-3.120328	-0.00923
C	2.730035	-2.070557	-2.259447
H	4.591725	-2.205823	-1.269643
H	3.564812	-2.939126	0.969102

H	3.520993	-4.056697	-0.390072
C	1.600489	-3.345527	0.138639
O	2.783524	-3.079413	-2.95746
N	1.908954	-1.031217	-2.517267
H	1.42409	-4.291383	0.663308
H	1.118454	-3.4663	-0.84105
C	0.819726	-2.297229	0.883085
H	1.429747	-1.027907	-3.411316
H	1.983432	-0.144594	-2.024006
O	1.231967	-1.21161	1.266488
O	-0.437238	-2.683727	1.089525
C	-3.351567	-1.349108	-2.702322
H	-4.259315	-1.627963	-2.162644
H	-3.602818	-0.49971	-3.347801
H	-3.069429	-2.191211	-3.343097
H	-3.390069	1.279452	0.652239
C	-3.379243	-0.787158	1.128927
C	-2.695255	-0.529675	2.32527
C	-3.872213	-2.079319	0.915147
C	-2.5186	-1.526272	3.288887
H	-2.324032	0.475798	2.519642
C	-3.696161	-3.079515	1.872616
H	-4.405565	-2.311773	-0.002996
C	-3.021353	-2.808372	3.062536
H	-1.997856	-1.297058	4.214828
H	-4.090094	-4.074758	1.686685
H	-2.889465	-3.587175	3.807955
C	-4.889518	0.394238	-0.50717
N	-5.261875	1.510852	-1.107869
H	-5.595881	-0.422733	-0.526828
O	-6.410262	1.611949	-1.663452
O	-4.45923	2.518612	-1.139128
H	-0.924386	-2.014204	1.617257

(7) *re*→*si/g*⁻: ts

N	-0.708358	1.737408	0.027892
C	0.634256	2.036918	0.516168
C	0.557554	3.540122	0.835431
C	-0.43077	4.061709	-0.212747
C	-1.469312	2.944762	-0.310506
H	0.852696	1.438363	1.41125
H	1.52757	4.037493	0.783981
H	0.156667	3.668843	1.845977
H	-0.874846	5.019999	0.065642
H	0.074584	4.182365	-1.177024
H	-2.286302	3.0852	0.408092
H	-1.897592	2.851514	-1.313756
C	-1.064269	0.503854	-0.353461

C	-2.263026	0.127984	-0.932512	H	-5.346805	-2.012815	-0.182989
C	-3.558444	-0.22249	0.937998	C	-7.370846	0.643999	-0.796789
C	-2.361634	-1.214759	-1.605107	H	-6.923987	2.693473	-0.292256
H	-3.353017	-1.656481	-1.434873	H	-7.532857	-1.472498	-1.169646
H	-1.631975	-1.899422	-1.150864	H	-8.338289	0.875602	-1.233502
H	-0.320033	-0.265088	-0.152211	C	-3.214512	-1.478822	1.411821
C	1.683876	1.68931	-0.556732	N	-2.01062	-1.641838	2.05013
O	1.345878	1.243856	-1.658773	H	-3.760912	-2.398141	1.260255
N	2.986964	1.825661	-0.236943	O	-1.653322	-2.756601	2.462267
C	3.996062	1.378167	-1.206749	O	-1.261082	-0.633201	2.17805
C	3.581168	2.300773	1.026303	H	0.249288	-0.767604	2.824912
C	3.869497	-0.122212	-1.506205	H	-3.060275	0.631156	1.387325
C	5.328336	1.745539	-0.528456	H	-2.933272	0.908066	-1.289475
H	3.860653	1.883882	-2.165968				
C	5.000458	1.733235	0.9692				
H	3.014157	1.938343	1.888412	(8) $re \rightarrow si/g^-$: 1-Nit			
H	3.600678	3.39664	1.041817	N	0.33208	1.987532	-0.687074
O	4.207981	-0.58411	-2.589771	C	-1.122117	2.023848	-0.973665
N	3.361282	-0.876119	-0.502756	C	-1.336123	3.473803	-1.421765
H	6.129964	1.055134	-0.803361	C	-0.356324	4.254414	-0.543247
H	5.621961	2.751375	-0.845868	C	0.87824	3.358357	-0.492975
H	5.011582	0.712586	1.364013	H	-1.354331	1.274475	-1.740479
H	5.698449	2.332292	1.558705	H	-2.366479	3.80651	-1.297855
C	3.167988	-2.309205	-0.600237	H	-1.070791	3.560207	-2.480176
H	3.288941	-0.455398	0.417617	H	-0.119099	5.240959	-0.945579
C	2.899459	-2.907778	0.79055	H	-0.769103	4.380873	0.463053
C	2.025198	-2.706749	-1.547012	H	1.574404	3.561271	-1.311961
H	4.065738	-2.777741	-1.019722	H	1.408125	3.401876	0.460215
H	3.811691	-2.831506	1.389948	C	0.980676	0.898348	-0.482871
H	2.690693	-3.96977	0.64162	C	2.379563	0.859531	0.031225
C	1.732891	-2.269215	1.555341	C	3.264822	-0.207201	-0.694526
O	1.870124	-3.893552	-1.824585	C	2.271588	0.628565	1.572498
N	1.196984	-1.735917	-1.980931	H	2.483389	-0.425957	1.785916
H	1.304197	-2.990571	2.261579	H	1.24337	0.811387	1.907217
H	0.902575	-1.994556	0.887025	H	0.41977	-0.02896	-0.613904
C	2.124788	-1.051879	2.375638	C	-1.845796	1.634324	0.331144
H	0.506879	-1.999471	-2.675439	O	-1.194453	1.281394	1.322956
H	1.407202	-0.744993	-1.882957	N	-3.185827	1.635334	0.337777
O	3.263457	-0.619954	2.434925	C	-3.88223	1.108197	1.524112
O	1.165971	-0.45346	3.065946	C	-4.111609	1.952997	-0.766998
C	-2.12874	-1.119284	-3.116914	C	-3.48597	-0.343967	1.830569
H	-2.914151	-0.516407	-3.58736	C	-5.368961	1.22739	1.138682
H	-1.170826	-0.637468	-3.344481	H	-3.625562	1.690045	2.412403
H	-2.142374	-2.110638	-3.584259	C	-5.36023	1.157234	-0.392762
C	-4.872877	0.038926	0.328412	H	-3.684603	1.651659	-1.724922
C	-5.337288	1.362446	0.282472	H	-4.325942	3.028095	-0.768275
C	-5.67951	-0.978932	-0.202158	O	-3.514801	-0.771913	2.981753
C	-6.576913	1.664434	-0.270502	N	-3.149125	-1.086103	0.758585
H	-4.715234	2.156156	0.691045	H	-5.970817	0.445042	1.608216
C	-6.918262	-0.675207	-0.761485				

H	-5.750296	2.197811	1.472838	C	-0.740155	3.761765	-1.101855
H	-5.258045	0.123144	-0.739032	C	-1.434959	2.521827	-1.678041
H	-6.262084	1.581953	-0.839884	H	-0.308797	1.358875	1.210532
C	-2.778117	-2.485477	0.825492	H	0.329651	3.990325	0.810268
H	-3.218644	-0.684808	-0.179427	H	-1.381303	3.514747	0.959179
C	-2.900131	-3.122263	-0.572556	H	-1.365304	4.652466	-1.193249
C	-1.361118	-2.721341	1.36487	H	0.203553	3.944987	-1.624893
H	-3.450215	-3.003106	1.519033	H	-2.520044	2.640032	-1.723674
H	-3.904337	-2.909012	-0.955422	H	-1.076639	2.260103	-2.679258
H	-2.821191	-4.205177	-0.440525	C	-1.41508	0.169124	-0.884226
C	-1.833463	-2.688332	-1.581554	C	-2.531721	-0.259463	-1.598276
O	-0.993519	-3.862377	1.622286	C	-3.856384	0.042357	0.032436
N	-0.542796	-1.643533	1.453722	C	-2.670636	-1.710941	-2.00501
H	-1.9253	-3.312293	-2.481236	H	-2.554911	-2.357354	-1.126163
H	-0.826627	-2.887656	-1.200026	H	-1.847514	-1.970561	-2.684808
C	-1.898117	-1.246355	-2.080415	H	-0.874729	-0.538817	-0.256377
H	0.344419	-1.789207	1.922959	C	1.322265	1.704573	-0.178487
H	-0.921341	-0.699675	1.470274	O	1.60181	1.445989	-1.352908
O	-2.959052	-0.592177	-1.977017	N	2.280011	1.896391	0.753426
O	-0.846492	-0.756163	-2.614873	C	3.684056	2.018438	0.346424
C	3.215159	1.533988	2.364337	C	2.088544	2.076716	2.204339
H	4.259929	1.392114	2.0708	C	4.290753	0.714219	-0.170963
H	2.959411	2.588642	2.209968	C	4.376828	2.506899	1.630849
H	3.131058	1.322369	3.435161	H	3.773946	2.734991	-0.475122
C	4.679251	-0.129582	-0.135563	C	3.5091	1.922468	2.749309
C	5.523649	0.876939	-0.618741	H	1.399567	1.325081	2.598171
C	5.150823	-0.963395	0.882581	H	1.687176	3.07438	2.419316
C	6.800538	1.058259	-0.092052	O	5.324092	0.732231	-0.833835
H	5.174366	1.526416	-1.419493	N	3.643946	-0.418909	0.17121
C	6.430248	-0.786154	1.411247	H	5.422125	2.191945	1.674766
H	4.529274	-1.755954	1.288819	H	4.345572	3.601005	1.659445
C	7.257318	0.226693	0.931268	H	3.739333	0.86103	2.895951
H	7.440663	1.844199	-0.48348	H	3.639288	2.437313	3.703883
H	6.77674	-1.444542	2.203086	C	4.062131	-1.717503	-0.311148
H	8.252303	0.362639	1.345493	H	2.757699	-0.359709	0.664295
C	2.692706	-1.590902	-0.628081	C	3.520346	-2.849737	0.585938
N	1.87905	-2.049074	-1.531848	C	3.656305	-1.988649	-1.765266
H	2.935322	-2.313672	0.139099	H	5.155516	-1.748096	-0.292839
O	1.369044	-3.198063	-1.561523	H	3.574139	-2.519023	1.628755
O	1.562715	-1.211156	-2.559565	H	4.195032	-3.703222	0.482334
H	0.501814	-1.202775	-2.613438	C	2.116447	-3.35782	0.257489
H	3.310006	0.087586	-1.746734	O	4.125796	-2.962314	-2.350108
H	2.853591	1.830542	-0.144513	N	2.709308	-1.187835	-2.292202
				H	1.888229	-4.222423	0.895444
				H	2.073234	-3.727773	-0.775156
				C	0.985112	-2.377534	0.45593
				H	2.469577	-1.323773	-3.268209
				H	2.432485	-0.306222	-1.862585
				O	1.075698	-1.282101	0.976323
				O	-0.219901	-2.78421	0.039492
(9) $re \rightarrow si/g^+$: ts							
N	-1.062458	1.437845	-0.748182				
C	-0.128156	1.896283	0.27503				
C	-0.470398	3.395508	0.362739				

C	-3.992143	-2.001401	-2.714234	C	-2.878229	1.881023	-2.063655
H	-4.85795	-1.788051	-2.079343	C	-4.188002	-0.385536	0.296639
H	-4.087581	-1.391111	-3.619612	C	-5.103604	1.318691	-1.362181
H	-4.049808	-3.053668	-3.011062	H	-4.485494	1.657031	0.724282
C	-3.591726	-1.09906	0.944274	C	-4.15846	1.210612	-2.563336
C	-4.399712	-2.241685	0.887961	H	-1.982863	1.494832	-2.555998
C	-2.546846	-1.063202	1.878456	H	-2.91994	2.969415	-2.19645
C	-4.175204	-3.316713	1.747656	O	-5.083508	-0.810973	1.022526
H	-5.216721	-2.283681	0.171234	N	-3.177353	-1.14616	-0.167924
C	-2.319108	-2.13498	2.735026	H	-5.93236	0.606794	-1.390415
H	-1.895256	-0.193026	1.929912	H	-5.521879	2.328582	-1.298842
C	-3.133544	-3.267116	2.673091	H	-3.956548	0.158875	-2.79691
H	-4.816692	-4.192184	1.695183	H	-4.55246	1.692272	-3.461361
H	-1.499881	-2.088999	3.447843	C	-2.986949	-2.527002	0.212866
H	-2.955889	-4.104273	3.342634	H	-2.46725	-0.722647	-0.761116
C	-3.738477	1.33909	0.559225	C	-2.109724	-3.272699	-0.807479
N	-4.203169	2.421478	-0.134972	C	-2.389784	-2.701088	1.617667
H	-3.250397	1.584845	1.4914	H	-3.966831	-3.01594	0.245018
O	-4.050347	3.569456	0.346844	H	-2.511448	-3.091079	-1.810364
O	-4.738273	2.263619	-1.257969	H	-2.225396	-4.33938	-0.600105
H	-0.182166	-3.667642	-0.371114	C	-0.604395	-2.975038	-0.781916
H	-4.666957	-0.102652	-0.676968	O	-2.27746	-3.833319	2.087502
H	-3.007875	0.465228	-2.25977	N	-1.96198	-1.591928	2.242762

(10) $re \rightarrow si/g^+$: 1-D

N	0.552219	2.066847	0.621859	H	-1.604441	-1.683796	3.1867
C	-0.558002	2.318577	-0.287173	H	-2.093682	-0.652917	1.868813
C	-0.727989	3.851661	-0.273773	O	-0.88791	-0.750323	-1.72225
C	-0.290772	4.213568	1.148514	O	1.136385	-1.570854	-1.716334
C	0.888791	3.271817	1.39523	C	1.748005	-1.184272	3.213339
H	-0.332786	1.944129	-1.290508	H	2.773305	-1.570109	3.243316
H	-1.74478	4.178453	-0.510475	H	1.662855	-0.412958	3.987554
H	-0.040131	4.287645	-1.006162	H	1.080976	-2.009352	3.486622
H	-0.007735	5.264187	1.25218	C	3.869847	-0.961654	-0.056656
H	-1.097429	4.000932	1.858557	C	3.701874	-2.299234	0.328491
H	1.822285	3.718685	1.021022	C	4.158431	-0.688771	-1.397454
H	1.013319	3.040269	2.458255	C	3.791683	-3.33399	-0.60312
C	1.599272	1.222035	0.206109	H	3.509556	-2.536836	1.372298
C	2.286452	0.517798	1.37475	C	4.259817	-1.72062	-2.331406
C	3.739703	0.135331	0.99752	H	4.306084	0.335418	-1.727797
C	1.377112	-0.618074	1.845712	C	4.069578	-3.04566	-1.942415
H	1.366425	-1.414792	1.089918	H	3.661973	-4.36354	-0.279786
H	0.358057	-0.213994	1.885903	H	4.482626	-1.483651	-3.367952
H	1.208003	0.481653	-0.496982	H	4.149122	-3.847796	-2.670977
C	-1.837529	1.645716	0.230874	C	4.416999	1.420233	0.629016
O	-1.946029	1.254196	1.398424	N	3.807334	2.295272	-0.106076
N	-2.873531	1.537224	-0.632267	H	5.387409	1.728544	0.997077
C	-4.181191	1.078891	-0.152851	O	4.216454	3.423886	-0.466701
				O	2.577115	1.951304	-0.654935

H	1.659388	-2.348807	-1.438415
H	4.231079	-0.226643	1.907564
H	2.380901	1.236449	2.199498

(11) *re*→*si/t*: ts

N	-0.820805	-1.453799	0.634414
C	0.290722	-2.064659	-0.092778
C	-0.032606	-3.565358	-0.014677
C	-0.703435	-3.695856	1.357868
C	-1.547574	-2.424345	1.473209
H	0.312322	-1.687284	-1.120566
H	0.856262	-4.192621	-0.117495
H	-0.733345	-3.821575	-0.816285
H	-1.311011	-4.599659	1.443409
H	0.055997	-3.713249	2.146284
H	-2.562959	-2.571857	1.091409
H	-1.60755	-2.040009	2.496654
C	-0.929591	-0.134316	0.759055
C	-1.988025	0.54872	1.344348
C	-3.100841	0.642252	-0.546148
C	-1.837202	1.989081	1.784622
H	-1.742784	2.648446	0.913831
H	-0.906726	2.106049	2.354063
H	-0.135513	0.439943	0.277886
C	1.620299	-1.718341	0.595856
O	1.642634	-1.182474	1.709356
N	2.754406	-1.993762	-0.074725
C	4.046914	-1.626997	0.518524
C	2.893798	-2.605875	-1.407474
C	4.183939	-0.114228	0.732418
C	5.068541	-2.16933	-0.498546
H	4.159394	-2.079951	1.506946
C	4.299283	-2.172545	-1.824084
H	2.119953	-2.243218	-2.086988
H	2.824218	-3.697529	-1.326882
O	4.958722	0.329674	1.57429
N	3.42025	0.662931	-0.064182
H	5.978829	-1.565226	-0.521524
H	5.343919	-3.191337	-0.218741
H	4.262946	-1.16422	-2.25249
H	4.733011	-2.846708	-2.566058
C	3.409686	2.108496	0.010685
H	2.866488	0.230154	-0.799606
C	2.803879	2.721225	-1.26368
C	2.670074	2.653454	1.241395
H	4.440055	2.468303	0.108522
H	3.360329	2.344592	-2.12907
H	2.982332	3.797948	-1.207056

C	1.29922	2.517305	-1.480296
O	2.722298	3.855831	1.487473
N	1.935682	1.781738	1.961025
H	0.931286	3.273535	-2.18483
H	0.727758	2.691903	-0.555831
C	0.88561	1.17192	-2.040188
H	1.519393	2.122477	2.82028
H	1.998557	0.773796	1.836488
O	1.639275	0.226831	-2.208159
O	-0.393195	1.032821	-2.3656
C	-3.009353	2.439877	2.653607
H	-3.964214	2.322321	2.130088
H	-3.056475	1.85045	3.576859
H	-2.907981	3.49398	2.929338
C	-3.848097	-0.627442	-0.432473
C	-3.470768	-1.699856	-1.250007
C	-4.908257	-0.79461	0.469581
C	-4.139259	-2.921646	-1.167109
H	-2.655608	-1.568428	-1.958408
C	-5.567506	-2.015116	0.559159
H	-5.199483	0.029487	1.118062
C	-5.181607	-3.084106	-0.256388
H	-3.84157	-3.746561	-1.808739
H	-6.38038	-2.138475	1.269154
H	-5.6973	-4.037422	-0.181382
C	-3.761677	1.873326	-0.546669
N	-3.165249	3.0033	-1.036039
H	-4.751547	2.041309	-0.146974
O	-3.788842	4.077279	-1.01089
O	-1.987669	2.978013	-1.51618
H	-0.958716	1.811452	-2.105526
H	-2.235772	0.571732	-1.193558
H	-2.716879	-0.045376	1.894127

(12) *re*→*si/t*: 1-Nit

N	-0.580518	-1.808955	0.636116
C	0.551631	-2.493165	-0.021292
C	0.471259	-3.902761	0.581251
C	0.038401	-3.639148	2.03204
C	-0.908539	-2.435563	1.941015
H	0.414915	-2.456354	-1.102099
H	1.422608	-4.435438	0.508411
H	-0.291736	-4.473177	0.042415
H	-0.460464	-4.503501	2.474057
H	0.90366	-3.385976	2.648582
H	-1.962508	-2.726628	1.908327
H	-0.754725	-1.700689	2.734296
C	-1.141882	-0.779883	0.12168

C	-2.126266	0.090685	0.817776	H	-4.961953	-0.468794	1.636845
C	-3.20537	0.53956	-0.222115	C	-6.147478	-2.593596	-0.738622
C	-1.286155	1.239576	1.452772	H	-5.441876	-2.689173	-2.77247
H	-1.115112	2.02352	0.708053	H	-6.639934	-2.254163	1.334386
H	-0.294103	0.849674	1.715208	H	-6.887357	-3.377916	-0.87055
H	-0.784283	-0.470646	-0.861756	C	-3.858514	1.835983	0.141517
C	1.834931	-1.78507	0.429147	N	-3.550047	3.004486	-0.340155
O	1.853103	-1.170285	1.502158	H	-4.657154	1.881338	0.872004
N	2.922193	-1.942415	-0.337897	O	-4.116909	4.080248	-0.020488
C	4.242246	-1.528686	0.153882	O	-2.588203	3.18573	-1.298154
C	2.964652	-2.501529	-1.701908	H	-1.882174	2.452552	-1.350253
C	4.411268	-0.01315	0.293924	H	-2.698436	0.662046	-1.182355
C	5.196984	-2.122392	-0.895043	H	-2.6103	-0.459391	1.632993
H	4.408909	-1.941403	1.152901				
C	4.363881	-2.107381	-2.18027				
H	2.175537	-2.060106	-2.315695	(13) <i>si</i> → <i>re/g</i> ⁻ : <i>ts</i>			
H	2.839788	-3.590782	-1.668309	N	1.249374	-2.053969	0.781294
O	5.345401	0.431176	0.960934	C	-0.174336	-2.385229	0.936181
N	3.514767	0.752084	-0.349153	C	-0.227385	-3.91695	0.688084
H	6.125193	-1.55075	-0.966209	C	1.048543	-4.204425	-0.104302
H	5.445966	-3.151232	-0.614533	C	2.052708	-3.265466	0.53847
H	4.334894	-1.09674	-2.602286	H	-0.488591	-2.134624	1.955311
H	4.742772	-2.790277	-2.943796	H	-1.128274	-4.214544	0.147519
C	3.506599	2.195087	-0.237698	H	-0.210627	-4.442512	1.648212
H	2.726569	0.341908	-0.86389	H	1.357839	-5.250128	-0.043323
C	2.703605	2.832365	-1.387285	H	0.922529	-3.934696	-1.158927
C	2.959059	2.694252	1.105158	H	2.405022	-3.649908	1.507426
H	4.538947	2.556022	-0.289709	H	2.922255	-3.056429	-0.083161
H	3.058896	2.396996	-2.328569	C	1.770594	-0.905869	1.199279
H	2.972523	3.892666	-1.402323	C	3.128574	-0.595742	1.154652
C	1.174985	2.751448	-1.309645	C	3.313858	0.036835	-0.846715
O	3.083035	3.877837	1.412188	C	3.651567	0.545321	1.994334
N	2.294967	1.798487	1.861731	H	2.945967	1.383866	1.958617
H	0.749526	3.475189	-2.01365	H	4.593783	0.908847	1.564527
H	0.817926	3.074026	-0.320135	H	1.048604	-0.1483	1.508016
C	0.498132	1.4157	-1.608466	C	-1.099232	-1.64737	-0.03594
H	1.966023	2.096782	2.772685	O	-0.691176	-0.948177	-0.964073
H	2.268277	0.80636	1.638456	N	-2.421132	-1.872428	0.172737
O	1.155374	0.345206	-1.660029	C	-3.410901	-1.587161	-0.871026
O	-0.76053	1.447479	-1.780237	C	-3.027674	-2.509119	1.359492
C	-1.931445	1.819914	2.709221	C	-3.756296	-0.106582	-1.017848
H	-2.910499	2.263074	2.504319	C	-4.63127	-2.40202	-0.417459
H	-2.058448	1.047814	3.47679	H	-3.027778	-1.906397	-1.845045
H	-1.293208	2.606738	3.124132	C	-4.527838	-2.34258	1.108724
C	-4.247024	-0.5562	-0.399496	H	-2.692609	-2.010959	2.27407
C	-4.393008	-1.19239	-1.634682	H	-2.757822	-3.569441	1.415605
C	-5.062336	-0.954418	0.66716	O	-4.443417	0.278831	-1.959702
C	-5.337138	-2.207222	-1.804274	N	-3.262305	0.712451	-0.067581
H	-3.770206	-0.885489	-2.472467	H	-5.562458	-1.993046	-0.815295
C	-6.008835	-1.96252	0.499374				

H	-4.525957	-3.433984	-0.768191	C	0.706856	-4.145579	-0.488813
H	-4.865002	-1.365616	1.473317	C	1.817892	-3.12494	-0.272762
H	-5.111817	-3.117576	1.610047	H	-0.442103	-2.035354	1.848632
C	-3.34487	2.151196	-0.185085	H	-1.216867	-4.344189	0.546768
H	-2.648961	0.332403	0.64843	H	0.200753	-4.352181	1.61679
C	-3.106595	2.84068	1.170043	H	1.102911	-5.161653	-0.530548
C	-2.390754	2.717815	-1.24588	H	0.184211	-3.93981	-1.428284
H	-4.351902	2.406039	-0.530927	H	2.614534	-3.513279	0.368931
H	-3.65127	2.284573	1.94058	H	2.243362	-2.736624	-1.198367
H	-3.555844	3.835491	1.112958	C	1.704806	-0.938715	0.874672
C	-1.651138	3.046777	1.590681	C	3.158623	-0.653026	0.769104
O	-2.433231	3.917581	-1.518242	C	3.530823	0.301011	-0.425965
N	-1.508888	1.865321	-1.794997	C	3.631089	-0.130213	2.135738
H	-1.628362	3.675631	2.490643	H	3.076747	0.778406	2.401394
H	-1.105516	3.611528	0.824156	H	4.685509	0.152095	2.033043
C	-0.850758	1.811294	1.928551	H	1.060454	-0.234331	1.406486
H	-0.902911	2.209654	-2.531399	C	-1.258	-1.767122	-0.13743
H	-1.455759	0.876785	-1.55705	O	-0.902609	-1.195395	-1.168453
O	-1.269348	0.670404	1.949019	N	-2.554607	-1.947229	0.192168
O	0.425555	2.019891	2.27794	C	-3.615635	-1.668785	-0.78193
C	3.889165	0.132861	3.449777	C	-3.086788	-2.423809	1.486219
H	2.949256	-0.165995	3.928049	C	-3.86188	-0.177298	-1.012496
H	4.58146	-0.714791	3.510338	C	-4.83884	-2.351273	-0.153101
H	4.317626	0.959658	4.027703	H	-3.347942	-2.088979	-1.755523
H	4.382066	-0.147993	-0.756331	C	-4.59228	-2.178029	1.347796
C	2.932041	1.468603	-0.780898	H	-2.640682	-1.863245	2.313004
C	3.939881	2.438864	-0.711128	H	-2.874619	-3.489695	1.624801
C	1.594574	1.881718	-0.811799	O	-4.572248	0.195584	-1.941281
C	3.623522	3.796361	-0.681556	N	-3.265391	0.661319	-0.141313
H	4.981081	2.124996	-0.691442	H	-5.774277	-1.908084	-0.501479
C	1.279316	3.239069	-0.801877	H	-4.83553	-3.412859	-0.421591
H	0.803224	1.132817	-0.841999	H	-4.836777	-1.155434	1.656103
C	2.290629	4.200349	-0.731094	H	-5.173878	-2.869492	1.961238
H	4.418218	4.535819	-0.631175	C	-3.300464	2.097581	-0.302658
H	0.242015	3.556787	-0.86693	H	-2.653006	0.289369	0.578776
H	2.037294	5.257037	-0.726521	C	-3.013839	2.814775	1.028861
C	2.639642	-0.807104	-1.737686	C	-2.352105	2.602168	-1.398286
N	3.2081	-1.994932	-2.122844	H	-4.306078	2.374731	-0.636056
H	1.649501	-0.635371	-2.134872	H	-3.559303	2.295009	1.82393
O	2.593215	-2.734255	-2.923151	H	-3.435561	3.820323	0.954339
O	4.320066	-2.342821	-1.6552	C	-1.544496	2.993005	1.413453
H	0.691429	2.949432	2.148286	O	-2.35376	3.796717	-1.694535
H	3.819521	-1.428533	1.027929	N	-1.52164	1.702376	-1.952448
				H	-1.485008	3.647434	2.293393
				H	-1.002853	3.519547	0.617613
				C	-0.762128	1.751272	1.765464
				H	-0.941957	1.997866	-2.730221
				H	-1.522576	0.715233	-1.70706
				O	-1.195514	0.613637	1.794287
				O	0.515457	1.942226	2.116408
(14) <i>si</i> → <i>re/g</i> ˚: 1-Nit							
N	1.140152	-2.01898	0.468341				
C	-0.249887	-2.386756	0.832169				
C	-0.223241	-3.92184	0.703617				

C	3.484171	-1.176929	3.239284	C	3.37493	2.416792	1.219806
H	2.432954	-1.445771	3.407455	C	3.938393	0.204055	-1.417675
H	4.02901	-2.09304	2.983973	C	5.025926	2.311791	-0.51686
H	3.879512	-0.803682	4.189197	H	3.416894	2.159091	-2.015011
H	4.617598	0.411362	-0.307386	C	4.861576	2.134332	0.995491
C	2.912499	1.681269	-0.3079	H	2.972346	1.883448	2.08462
C	3.600425	2.686765	0.38263	H	3.18908	3.49122	1.341665
C	1.675224	1.99752	-0.881174	O	4.497904	-0.12838	-2.460128
C	3.077916	3.975311	0.492911	N	3.489572	-0.672368	-0.49897
H	4.567534	2.460174	0.826495	H	5.924775	1.840924	-0.921856
C	1.166508	3.294985	-0.808652	H	5.048261	3.376266	-0.773914
H	1.105133	1.23183	-1.403084	H	5.091136	1.102276	1.284737
C	1.862006	4.287897	-0.11691	H	5.498482	2.803891	1.578101
H	3.633576	4.740419	1.028557	C	3.574751	-2.101748	-0.698038
H	0.226146	3.53814	-1.297038	H	3.051599	-0.336223	0.35689
H	1.465398	5.298654	-0.067142	C	3.43545	-2.851593	0.635299
C	3.260919	-0.347823	-1.746818	C	2.539876	-2.633223	-1.69963
N	3.948053	-1.416923	-2.10893	H	4.553244	-2.335064	-1.13117
H	2.513711	-0.011323	-2.450313	H	4.145685	-2.422538	1.350951
O	3.690171	-2.021196	-3.211078	H	3.745607	-3.88354	0.449845
O	4.860611	-1.894354	-1.340313	C	2.031235	-2.906743	1.241716
H	0.811234	2.858239	1.946552	O	2.624627	-3.796841	-2.092845
H	3.694853	-1.580026	0.539476	N	1.565522	-1.788905	-2.070577

(15) $si \rightarrow re/g^+$: ts

N	-0.890714	1.924637	0.568795	H	1.27572	-3.163395	0.488205
C	0.490365	2.342591	0.773146	C	1.544865	-1.667884	1.963817
C	0.404314	3.868434	0.559463	H	0.816773	-2.144231	-2.652907
C	-0.637737	3.984133	-0.559063	H	1.455921	-0.863019	-1.664363
C	-1.663221	2.907501	-0.199258	O	2.132763	-0.600515	2.008285
H	0.813521	2.070218	1.781354	O	0.412513	-1.815314	2.653587
H	1.364634	4.317699	0.295119	C	-3.658113	0.447404	3.609928
H	0.0399	4.33631	1.48012	H	-2.749766	0.890381	4.033497
H	-1.089596	4.976915	-0.613926	H	-4.377284	1.255737	3.435145
H	-0.177949	3.760612	-1.5266	H	-4.085856	-0.230175	4.357443
H	-2.46543	3.306503	0.436878	H	-2.184857	-0.160622	-1.059516
H	-2.118078	2.436995	-1.076031	C	-4.360431	-0.342771	-1.03642
C	-1.456772	0.924425	1.248516	C	-4.509349	0.680459	-1.98418
C	-2.808934	0.602686	1.228151	C	-5.510308	-0.971862	-0.536384
C	-3.000958	-0.705502	-0.592739	C	-5.771699	1.062715	-2.428302
C	-3.347496	-0.299221	2.308705	H	-3.622174	1.168748	-2.38153
H	-2.618459	-1.09526	2.512644	C	-6.773862	-0.583279	-0.974715
H	-4.260694	-0.793466	1.953114	H	-5.424195	-1.767301	0.198692
H	-0.770522	0.333387	1.856122	C	-6.909265	0.434802	-1.919337
C	1.441725	1.741223	-0.267069	H	-5.86878	1.84955	-3.171002
O	1.034083	1.208141	-1.300389	H	-7.655793	-1.077554	-0.577032
N	2.760912	1.92188	-0.025816	H	-7.896343	0.734916	-2.25958
C	3.743037	1.682377	-1.085966	C	-2.716609	-1.972641	-0.098939
				N	-1.431989	-2.228296	0.300391
				H	-3.435181	-2.72294	0.197033
				O	-1.185172	-3.279972	0.965423

O	-0.534488	-1.398672	0.069057
H	-0.101544	-2.576313	2.288069
H	-3.497747	1.333504	0.80759

(16) *si*→*re/g*⁺: 1-Nit

N	-0.498736	2.271352	0.249145
C	0.94159	2.427868	0.559129
C	1.122753	3.945217	0.414896
C	0.244494	4.273515	-0.795625
C	-0.991838	3.402538	-0.586799
H	1.137073	2.022574	1.555624
H	2.161324	4.239282	0.26893
H	0.745488	4.43784	1.317421
H	-0.017655	5.331508	-0.852164
H	0.755095	3.994613	-1.722919
H	-1.77071	3.922242	-0.022356
H	-1.412481	3.000452	-1.510287
C	-1.21113	1.291112	0.664675
C	-2.682207	1.176545	0.427723
C	-2.995729	-0.201374	-0.237209
C	-3.396207	1.394279	1.780629
H	-3.01177	0.690473	2.527947
H	-4.455481	1.15889	1.630891
H	-0.699345	0.521164	1.261135
C	1.744264	1.628536	-0.480598
O	1.173283	0.988394	-1.365934
N	3.085199	1.705626	-0.390663
C	3.922685	1.095238	-1.432004
C	3.87686	2.229141	0.741316
C	3.833777	-0.432502	-1.477175
C	5.337937	1.543637	-1.03071
H	3.62133	1.457334	-2.418166
C	5.261096	1.623653	0.49747
H	3.432783	1.918443	1.691012
H	3.929746	3.322193	0.703004
O	4.19351	-1.042192	-2.482229
N	3.413766	-1.020588	-0.34495
H	6.099714	0.851724	-1.397153
H	5.536939	2.533642	-1.454617
H	5.319545	0.622919	0.938444
H	6.052903	2.237719	0.932611
C	3.30976	-2.455575	-0.182448
H	3.074961	-0.456484	0.436523
C	3.320901	-2.801231	1.32192
C	2.04789	-3.053975	-0.815483
H	4.164763	-2.926558	-0.676684
H	4.079694	-2.175514	1.805427
H	3.643618	-3.841301	1.424602

C	1.972016	-2.665407	2.032826
O	1.956484	-4.274923	-0.933039
N	1.06146	-2.193847	-1.122991
H	2.109917	-2.914025	3.093965
H	1.27087	-3.40961	1.639919
C	1.285734	-1.297016	2.017893
H	0.155124	-2.554842	-1.420448
H	1.194902	-1.187341	-1.086891
O	1.963432	-0.247861	1.911787
O	0.020142	-1.30572	2.169676
C	-3.255245	2.82257	2.302068
H	-2.207444	3.09083	2.486311
H	-3.675685	3.543919	1.592688
H	-3.790769	2.935692	3.249483
H	-2.421536	-0.25534	-1.171819
C	-4.471349	-0.292559	-0.601862
C	-4.938972	0.41755	-1.712434
C	-5.378149	-1.041459	0.151348
C	-6.287327	0.38649	-2.061052
H	-4.236734	0.988785	-2.317483
C	-6.729437	-1.075874	-0.196387
H	-5.030889	-1.6096	1.011364
C	-7.188439	-0.360223	-1.300427
H	-6.632134	0.936696	-2.932392
H	-7.420994	-1.667699	0.39702
H	-8.239671	-0.390067	-1.57301
C	-2.497388	-1.296618	0.645747
N	-1.91088	-2.335735	0.141989
H	-2.497534	-1.237073	1.725636
O	-1.266158	-3.169631	1.015699
O	-1.852703	-2.655895	-1.07434
H	-0.697539	-2.518016	1.586041
H	-3.017034	1.95504	-0.264823

(17) *si*→*re/t*: ts

N	-0.844295	-1.955673	-0.953331
C	0.566155	-2.195641	-1.262809
C	0.663384	-3.734902	-1.23046
C	-0.342602	-4.11141	-0.137082
C	-1.499602	-3.141044	-0.371545
H	0.795807	-1.779013	-2.247371
H	1.677331	-4.088138	-1.024854
H	0.34561	-4.131727	-2.200332
H	-0.664373	-5.153219	-0.200489
H	0.091322	-3.941786	0.85375
H	-2.219108	-3.529752	-1.105036
H	-2.035547	-2.883915	0.544527
C	-1.501668	-0.919577	-1.464841

C	-2.852213	-0.62194	-1.305925
C	-2.687638	0.639987	0.478185
C	-3.527033	0.251391	-2.331832
H	-2.818887	0.997823	-2.711856
H	-4.345579	0.805057	-1.853557
H	-0.883238	-0.225107	-2.031442
C	1.504714	-1.599228	-0.20928
O	1.108147	-1.293409	0.918955
N	2.806223	-1.506681	-0.553591
C	3.820067	-1.256901	0.476362
C	3.390344	-1.728391	-1.888567
C	3.774521	0.15774	1.053861
C	5.141133	-1.547553	-0.255903
H	3.659154	-1.926707	1.326337
C	4.820847	-1.214126	-1.715737
H	2.834996	-1.170862	-2.646637
H	3.374285	-2.796216	-2.140659
O	4.320865	0.405743	2.125938
N	3.114657	1.07902	0.325304
H	5.970294	-0.967596	0.156426
H	5.380703	-2.611065	-0.153544
H	4.84493	-0.129943	-1.874274
H	5.51224	-1.678726	-2.422267
C	2.92961	2.436432	0.791415
H	2.695799	0.816501	-0.564687
C	2.440668	3.350464	-0.343105
C	1.959767	2.540717	1.975821
H	3.887253	2.819366	1.159428
H	3.124938	3.246554	-1.192539
H	2.529747	4.377063	0.021673
C	0.992653	3.153994	-0.801425
O	1.890964	3.590119	2.608764
N	1.158522	1.47944	2.203928
H	0.667677	4.044658	-1.353728
H	0.302221	3.079486	0.050478
C	0.733277	1.979194	-1.717812
H	0.561482	1.509069	3.022886
H	1.322757	0.576567	1.764602
O	1.55747	1.139023	-2.041365
O	-0.49136	1.898648	-2.228536
C	-4.094536	-0.559139	-3.502158
H	-3.298188	-1.074395	-4.050363
H	-4.802786	-1.316154	-3.145517
H	-4.624792	0.092515	-4.205186
H	-1.662396	0.966781	0.317306
C	-2.855028	-0.42423	1.495538
C	-1.740504	-0.840944	2.228998
C	-4.095815	-1.033367	1.739586
C	-1.855304	-1.847049	3.188732
H	-0.773282	-0.395441	2.025563

C	-4.209455	-2.04241	2.689241
H	-4.970448	-0.734692	1.165494
C	-3.08804	-2.453721	3.418077
H	-0.976589	-2.159038	3.746976
H	-5.173131	-2.513564	2.861962
H	-3.180997	-3.242289	4.159624
C	-3.674053	1.619127	0.341445
N	-3.424391	2.820183	-0.268365
H	-4.701331	1.501584	0.656369
O	-4.346164	3.6437	-0.387519
O	-2.260656	3.11506	-0.674924
H	-1.156405	2.451338	-1.739384
H	-3.482509	-1.384952	-0.850485

(18) *si*→*rel*: 1-Nit

N	-0.670701	-2.108311	-1.010382
C	0.778219	-2.35128	-1.182983
C	0.881845	-3.877741	-1.02524
C	-0.194514	-4.185822	0.02197
C	-1.348348	-3.261615	-0.360362
H	1.08231	-1.98142	-2.164016
H	1.880431	-4.192984	-0.714598
H	0.646001	-4.356632	-1.981065
H	-0.501168	-5.233315	0.013336
H	0.165667	-3.936926	1.024698
H	-2.013136	-3.714589	-1.102483
H	-1.931409	-2.904562	0.490667
C	-1.215945	-1.015258	-1.39603
C	-2.649762	-0.65511	-1.251243
C	-2.716339	0.346303	-0.02253
C	-3.146071	-0.08054	-2.588821
H	-2.594745	0.838077	-2.814088
H	-4.200526	0.188721	-2.471784
H	-0.552981	-0.269766	-1.842947
C	1.540173	-1.629127	-0.066604
O	0.956297	-1.210524	0.936448
N	2.873835	-1.563107	-0.216236
C	3.723706	-1.168809	0.911862
C	3.642771	-1.853838	-1.4418
C	3.61661	0.311061	1.281097
C	5.13268	-1.534924	0.418597
H	3.433588	-1.726546	1.806568
C	5.039047	-1.329155	-1.096354
H	3.201391	-1.338008	-2.299362
H	3.657044	-2.93299	-1.637496
O	4.06359	0.703694	2.357575
N	3.048711	1.116268	0.366541
H	5.901201	-0.924246	0.897829

H	5.332634	-2.586617	0.649675	C	-0.768102	3.605875	-1.317339
H	5.105378	-0.263129	-1.339626	C	-1.788654	2.641953	-0.719901
H	5.820441	-1.856497	-1.647943	H	0.620483	2.292357	1.420132
C	2.83783	2.52825	0.612098	H	1.211573	4.157522	-0.530188
H	2.624594	0.737911	-0.48373	H	-0.136411	4.409875	0.600192
C	2.614535	3.278626	-0.716607	H	-1.22274	4.555683	-1.607738
C	1.654302	2.805136	1.545018	H	-0.297604	3.159985	-2.199518
H	3.724101	2.92805	1.113362	H	-2.534119	3.177425	-0.114122
H	3.328184	2.885794	-1.449586	H	-2.307396	2.036328	-1.465419
H	2.869474	4.328706	-0.545911	C	-1.527546	0.959759	1.05771
C	1.190537	3.237156	-1.27142	C	-2.882595	0.658355	1.134175
O	1.520465	3.915591	2.050165	C	-3.140268	-0.848347	-0.345378
N	0.749414	1.811272	1.67912	C	-3.392924	-0.017721	2.384419
H	1.147545	3.858839	-2.175192	H	-2.636104	-0.729237	2.739425
H	0.49324	3.704301	-0.56526	H	-4.293103	-0.598776	2.147753
C	0.614083	1.883356	-1.678293	H	-0.82069	0.473425	1.728303
H	-0.039008	1.969498	2.296571	C	1.439827	1.56061	-0.437977
H	0.947292	0.860903	1.37534	O	1.163445	0.805214	-1.364101
O	1.353665	0.880756	-1.829772	N	2.721766	1.861015	-0.103634
O	-0.642868	1.855961	-1.895544	C	3.825473	1.488073	-0.989347
C	-2.998489	-1.087287	-3.728451	C	3.168771	2.65571	1.054206
H	-1.946136	-1.320848	-3.933525	C	4.211434	0.011385	-0.908976
H	-3.515071	-2.02692	-3.497534	C	4.970215	2.394026	-0.511382
H	-3.426627	-0.688058	-4.652749	H	3.548057	1.671211	-2.031785
H	-1.730549	0.804629	0.106894	C	4.693473	2.531745	0.988221
C	-3.037365	-0.435359	1.24371	H	2.756617	2.249732	1.982359
C	-2.056982	-0.634275	2.217652	H	2.851083	3.701025	0.952236
C	-4.299241	-1.016156	1.424701	O	5.025516	-0.459086	-1.700244
C	-2.328499	-1.397435	3.355289	N	3.624817	-0.705525	0.069004
H	-1.065874	-0.212565	2.075832	H	5.949281	1.968504	-0.742587
C	-4.573999	-1.77531	2.559104	H	4.889071	3.368435	-1.005135
H	-5.074268	-0.878599	0.672814	H	5.016176	1.627494	1.516521
C	-3.586908	-1.969553	3.528756	H	5.193415	3.390783	1.441658
H	-1.553062	-1.542185	4.10252	C	3.830847	-2.130742	0.188441
H	-5.558937	-2.215609	2.688325	H	2.942553	-0.265086	0.68255
H	-3.802739	-2.560709	4.414319	C	3.302508	-2.653201	1.532372
C	-3.709563	1.440474	-0.255103	C	3.184568	-2.929851	-0.950806
N	-3.413058	2.700786	-0.373421	H	4.903938	-2.341173	0.132153
H	-4.771379	1.238392	-0.33176	H	3.75927	-2.070122	2.340266
O	-4.246886	3.628422	-0.530952	H	3.665769	-3.679412	1.631617
O	-2.109729	3.113039	-0.266741	C	1.77732	-2.692777	1.703676
H	-1.538336	2.637117	-0.990363	O	3.520636	-4.102548	-1.129011
H	-3.244106	-1.5417	-1.004592	N	2.233006	-2.307036	-1.656389
				H	1.53028	-3.450334	2.456416
				H	1.271187	-2.999369	0.777103
				C	1.121095	-1.400823	2.133115
				H	1.680968	-2.838495	-2.318558
				H	1.866715	-1.386242	-1.422958
				O	1.602177	-0.288105	2.037329
				O	-0.089012	-1.517259	2.696416
(19) $si \rightarrow si/g^-$: ts							
N	-0.981306	1.784357	0.164394				
C	0.373084	2.316257	0.355933				
C	0.254344	3.757081	-0.187862				

C	-3.728718	0.975425	3.500382	C	-3.336564	-2.212952	1.544577
H	-2.837588	1.532847	3.810703	C	-4.311003	0.378496	-0.623213
H	-4.478532	1.70019	3.162448	C	-5.41058	-1.631732	0.485788
H	-4.130972	0.460102	4.379894	H	-4.360607	-1.559289	-1.448183
C	-4.594896	-0.677245	-0.594811	C	-4.740059	-1.694766	1.861521
C	-5.084212	0.345156	-1.419464	H	-2.593574	-1.873485	2.270244
C	-5.505193	-1.569803	-0.016282	H	-3.314375	-3.309441	1.495072
C	-6.448188	0.465158	-1.666362	O	-5.09677	0.892511	-1.415476
H	-4.390247	1.056217	-1.862949	N	-3.460329	1.081927	0.150697
C	-6.872854	-1.451575	-0.264433	H	-6.283509	-0.975446	0.451969
H	-5.137339	-2.371373	0.62008	H	-5.722174	-2.633185	0.170695
C	-7.348185	-0.434071	-1.089036	H	-4.671264	-0.691287	2.297199
H	-6.811464	1.262849	-2.308491	H	-5.268835	-2.340641	2.566543
H	-7.565368	-2.157371	0.185813	C	-3.313132	2.515897	0.037012
H	-8.41304	-0.33922	-1.28227	H	-2.81757	0.586894	0.763593
C	-2.275736	-0.761039	-1.434005	C	-2.741385	3.126483	1.329533
N	-0.996144	-1.258384	-1.328301	C	-2.437842	2.953669	-1.145394
H	-2.542402	-0.409678	-2.420729	H	-4.303906	2.945712	-0.138892
O	-0.325533	-1.41886	-2.365346	H	-3.270291	2.691881	2.185078
O	-0.549673	-1.564482	-0.197601	H	-2.97838	4.193159	1.309479
H	-0.419655	-2.431694	2.640596	C	-1.227536	3.019271	1.53601
H	-3.570228	1.347775	0.646261	O	-2.373047	4.15401	-1.425056
H	-2.876212	-1.588392	0.407182	N	-1.730869	2.000775	-1.760449

(20) $si \rightarrow si/g^-$: 1-D

N	0.590453	-1.936915	-0.260119	H	-1.045494	2.252651	-2.464711
C	-0.723779	-2.388929	0.150336	H	-1.754685	1.017098	-1.496686
C	-0.752761	-3.806885	-0.451379	O	-1.318836	0.62547	1.963079
C	-0.062269	-3.6105	-1.81287	O	0.595577	1.638028	2.314492
C	0.916129	-2.434722	-1.602649	C	2.455132	-2.419191	2.347572
H	-0.780037	-2.396863	1.243643	H	1.361851	-2.394754	2.413847
H	-1.763608	-4.215961	-0.541873	H	2.728813	-3.246358	1.682187
H	-0.16521	-4.466575	0.195177	H	2.841792	-2.645922	3.346643
H	0.44965	-4.518195	-2.142122	C	4.773834	0.560204	-0.057311
H	-0.800095	-3.345028	-2.574027	C	5.476798	-0.28081	-0.927581
H	1.962317	-2.761101	-1.638193	C	5.492054	1.355278	0.838468
H	0.761038	-1.664112	-2.366965	C	6.869093	-0.325574	-0.900726
C	1.116535	-0.73043	0.236978	H	4.93025	-0.905662	-1.632621
C	2.647848	-0.759684	0.398971	C	6.886405	1.312237	0.869214
C	3.260479	0.580834	-0.065406	H	4.954817	2.012173	1.519811
C	3.0296	-1.095863	1.844623	C	7.57832	0.471132	-0.000328
H	2.697341	-0.275187	2.495878	H	7.401549	-0.982167	-1.583574
H	4.123486	-1.132977	1.911168	H	7.430777	1.9372	1.571983
H	0.644208	-0.522912	1.199823	H	8.663993	0.436813	0.020665
C	-1.889504	-1.595364	-0.443454	C	2.722161	0.871863	-1.432701
O	-1.785265	-1.016195	-1.527201	N	1.447686	0.780285	-1.63476
N	-3.071546	-1.629902	0.218867	H	3.322158	1.126794	-2.298045
C	-4.284201	-1.140076	-0.440552	O	0.809664	0.989455	-2.695406
				O	0.672112	0.477748	-0.520109

H	1.002814	2.520816	2.248639
H	3.049436	-1.541842	-0.257279
H	2.914692	1.363228	0.627674

(21) $si \rightarrow si/g^+$: ts

N	-1.111694	-1.847841	-0.818908
C	0.265406	-2.112216	-1.254688
C	0.309157	-3.654718	-1.310837
C	-0.603722	-4.053272	-0.147145
C	-1.74897	-3.049639	-0.250997
H	0.428628	-1.65151	-2.231539
H	1.323963	-4.050198	-1.219555
H	-0.112501	-3.990195	-2.264207
H	-0.956163	-5.084542	-0.21858
H	-0.082012	-3.92798	0.807696
H	-2.525812	-3.391792	-0.949051
H	-2.214735	-2.826406	0.711563
C	-1.816651	-0.830305	-1.31844
C	-3.180588	-0.609019	-1.180949
C	-3.259967	0.676217	0.615819
C	-3.856239	0.293604	-2.190314
H	-3.224792	1.173491	-2.371538
H	-4.802686	0.665618	-1.784479
H	-1.222083	-0.087293	-1.854401
C	1.326517	-1.624319	-0.265767
O	1.060423	-1.363659	0.910019
N	2.594694	-1.593733	-0.729723
C	3.715922	-1.459877	0.206355
C	3.033519	-1.753082	-2.127915
C	3.820271	-0.074019	0.84471
C	4.938455	-1.787751	-0.667368
H	3.595479	-2.162736	1.035875
C	4.504587	-1.338214	-2.065701
H	2.44517	-1.112136	-2.78927
H	2.924866	-2.797158	-2.447679
O	4.505189	0.096446	1.850823
N	3.134268	0.908897	0.231375
H	5.841379	-1.29015	-0.305803
H	5.111637	-2.868887	-0.651691
H	4.585527	-0.249225	-2.157218
H	5.093137	-1.795493	-2.864313
C	3.06367	2.253901	0.75683
H	2.570059	0.697285	-0.589681
C	2.599488	3.243603	-0.325088
C	2.151899	2.377104	1.984573
H	4.061955	2.550801	1.095122
H	3.207564	3.082792	-1.222459
H	2.827859	4.246203	0.046005

C	1.110731	3.232156	-0.684742
O	2.152067	3.416992	2.636997
N	1.321143	1.342787	2.232865
H	0.871735	4.156686	-1.224587
H	0.479936	3.25807	0.215156
C	0.6199	2.09164	-1.552701
H	0.764321	1.380786	3.079897
H	1.424754	0.441128	1.771457
O	1.266673	1.099032	-1.851853
O	-0.611134	2.22128	-2.027306
C	-4.122898	-0.422445	-3.518237
H	-3.184122	-0.739546	-3.987246
H	-4.739597	-1.315606	-3.363783
H	-4.649006	0.234569	-4.219765
C	-2.931114	-0.339001	1.629324
C	-1.618209	-0.557765	2.058122
C	-3.96384	-1.128644	2.159995
C	-1.337911	-1.545772	2.999201
H	-0.805761	0.016307	1.627599
C	-3.687055	-2.107778	3.107407
H	-4.985968	-0.965047	1.82431
C	-2.369977	-2.321557	3.526501
H	-0.308702	-1.719791	3.301139
H	-4.494294	-2.707352	3.51888
H	-2.152599	-3.092628	4.260675
C	-2.481645	1.818009	0.420855
N	-2.990097	2.900411	-0.246039
H	-1.429597	1.896795	0.6599
O	-2.172028	3.810438	-0.607149
O	-4.19811	3.017802	-0.496987
H	-1.106256	2.973768	-1.590217
H	-3.787994	-1.403123	-0.747737
H	-4.320523	0.793165	0.403353

(22) $si \rightarrow si/g^+$: 1-Nit

N	0.619177	2.289085	-0.334677
C	-0.822795	2.403108	-0.657843
C	-1.07936	3.90163	-0.442177
C	-0.207199	4.219172	0.776855
C	1.068417	3.416913	0.526327
H	-0.983548	2.047301	-1.677584
H	-2.134907	4.122138	-0.274875
H	-0.741197	4.456073	-1.323653
H	0.00468	5.285149	0.876806
H	-0.695152	3.874876	1.693696
H	1.811889	3.988395	-0.036723
H	1.524887	3.008163	1.430732
C	1.368318	1.345854	-0.774483

C	2.849315	1.29267	-0.602211	H	5.252813	-0.698671	1.809725
C	3.346241	-0.063221	-0.003717	C	2.962418	-0.33041	4.298649
C	3.427176	1.515112	-2.023982	H	0.897338	0.222641	3.994242
H	3.047709	0.737047	-2.697152	H	5.050244	-0.865619	4.271231
H	4.510401	1.371356	-1.954903	H	2.870836	-0.407358	5.378486
H	0.889299	0.586941	-1.407874	C	2.666741	-1.21863	-0.672038
C	-1.615672	1.549632	0.337523	N	3.176197	-1.771802	-1.730589
O	-1.056759	1.032556	1.311695	H	1.698071	-1.585818	-0.349836
N	-2.935447	1.44728	0.122553	O	2.390172	-2.687505	-2.386076
C	-3.789115	0.771447	1.108961	O	4.304699	-1.555305	-2.237202
C	-3.672403	1.860142	-1.08786	H	1.538691	-2.137283	-2.61427
C	-3.494566	-0.726079	1.242684	H	3.193695	2.099213	0.052982
C	-5.204228	1.021691	0.560348	H	4.412512	-0.115645	-0.245792
H	-3.636511	1.207235	2.099601				
C	-4.991354	1.095629	-0.954976				
H	-3.112808	1.584555	-1.985154	(23) <i>si</i> → <i>si/t</i> : <i>ts</i>			
H	-3.842888	2.943007	-1.079755	N	-0.927668	2.059427	0.318696
O	-3.86045	-1.339117	2.244363	C	0.42355	2.543273	0.021885
N	-2.868658	-1.290915	0.197266	C	0.153512	3.860637	-0.722448
H	-5.901411	0.238487	0.8676	C	-1.087121	4.397447	-0.00635
H	-5.573356	1.979972	0.940668	C	-1.923583	3.14501	0.261782
H	-4.88129	0.090072	-1.374979	H	0.948674	2.735608	0.965346
H	-5.808062	1.599735	-1.476229	H	-0.072086	3.641582	-1.77293
C	-2.509497	-2.690829	0.147356	H	1.00594	4.541732	-0.679246
H	-2.542411	-0.727155	-0.594211	H	-0.796332	4.866081	0.939794
C	-2.329706	-3.13634	-1.317435	H	-1.632662	5.133587	-0.600595
C	-1.243314	-3.024307	0.94351	H	-2.468886	3.192313	1.209841
H	-3.315207	-3.274129	0.604552	H	-2.648378	2.940037	-0.53259
H	-3.171026	-2.733918	-1.893594	C	-1.21581	0.834271	0.745486
H	-2.417157	-4.226649	-1.338178	C	-2.499647	0.36043	1.01611
C	-1.000941	-2.77564	-1.985525	C	-3.256261	-0.182683	-0.883897
O	-0.939369	-4.196419	1.143477	C	-2.655643	-0.854552	1.894468
N	-0.466641	-1.981429	1.31692	H	-1.749347	-1.474051	1.835349
H	-0.962496	-3.264451	-2.967788	H	-3.489672	-1.470382	1.530842
H	-0.163465	-3.209464	-1.42183	H	-0.371612	0.151105	0.814561
C	-0.669336	-1.303201	-2.244121	C	1.233293	1.561938	-0.816808
H	0.327481	-2.179196	1.916932	O	0.699719	0.620571	-1.410955
H	-0.817092	-1.026467	1.299392	N	2.561221	1.777184	-0.905853
O	-1.490945	-0.390299	-1.990109	C	3.367701	0.912866	-1.777087
O	0.479893	-1.080211	-2.743392	C	3.36442	2.807206	-0.224069
C	3.117934	2.901828	-2.581776	C	3.415117	-0.543166	-1.298176
H	2.040848	3.068527	-2.705571	C	4.756031	1.576245	-1.741008
H	3.514004	3.687114	-1.927439	H	2.942721	0.884134	-2.783894
H	3.578555	3.025497	-3.566439	C	4.789464	2.274099	-0.377666
C	3.19756	-0.13794	1.505731	H	3.060925	2.908985	0.820943
C	1.976485	0.120378	2.137584	H	3.246637	3.773741	-0.727798
C	4.299166	-0.49199	2.290442	O	3.703788	-1.44688	-2.076999
C	1.857438	0.024353	3.523924	N	3.161652	-0.733572	0.013092
H	1.096474	0.396329	1.560465	H	5.557895	0.847203	-1.880274
C	4.183816	-0.588162	3.677306				

H	4.820796	2.315173	-2.546115	C	-1.240484	4.31064	0.129578
H	5.003533	1.551253	0.417862	C	-1.975123	3.017377	-0.186901
H	5.533092	3.07269	-0.325416	H	0.787152	2.413889	1.263231
C	3.115551	-2.037995	0.63808	H	0.395791	4.043872	-1.271584
H	2.881029	0.058242	0.584384	H	0.929677	4.608379	0.323166
C	3.355382	-1.919598	2.159125	H	-1.354737	4.55622	1.190613
C	1.797986	-2.78879	0.410063	H	-1.613972	5.145998	-0.465496
H	3.904797	-2.657344	0.20129	H	-2.959157	2.891859	0.265175
H	4.140036	-1.17369	2.325397	H	-2.065049	2.866132	-1.269051
H	3.740985	-2.879972	2.509628	C	-1.33088	0.819497	0.750363
C	2.128095	-1.603479	3.01745	C	-2.708497	0.272013	0.830419
O	1.704196	-3.960418	0.76823	C	-3.223664	-0.164575	-0.603645
N	0.759542	-2.068621	-0.062983	C	-2.788592	-0.804334	1.914928
H	2.41369	-1.650751	4.076933	H	-1.964689	-1.52177	1.795747
H	1.354208	-2.370977	2.882692	H	-3.723383	-1.35876	1.778276
C	1.485173	-0.251853	2.814677	H	-0.486667	0.205563	1.07161
H	-0.089559	-2.581398	-0.285673	C	1.174136	1.615478	-0.699805
H	0.902333	-1.193747	-0.565719	O	0.647811	0.680698	-1.308459
O	1.910473	0.642743	2.109995	N	2.47728	1.908771	-0.836182
O	0.35747	-0.033465	3.501118	C	3.294619	1.144991	-1.789719
C	-2.949666	-0.47712	3.350326	C	3.249275	2.942486	-0.124108
H	-2.178906	0.187077	3.754861	C	3.426794	-0.335617	-1.417775
H	-3.908412	0.049483	3.420095	C	4.651065	1.872396	-1.743531
H	-3.013238	-1.368618	3.985436	H	2.839058	1.167747	-2.783062
C	-2.484124	-1.350621	-1.376883	C	4.689922	2.478977	-0.337127
C	-2.74853	-2.662642	-0.954144	H	2.961762	2.984603	0.930001
C	-1.509932	-1.146441	-2.363873	H	3.080249	3.922519	-0.584621
C	-2.059117	-3.738852	-1.510795	O	3.719027	-1.166419	-2.271855
H	-3.50374	-2.848975	-0.195898	N	3.2447	-0.631485	-0.114164
C	-0.828995	-2.222938	-2.928791	H	5.482866	1.195314	-1.952225
H	-1.285928	-0.134552	-2.687213	H	4.657801	2.666058	-2.497855
C	-1.101861	-3.523633	-2.505299	H	4.949776	1.714701	0.404284
H	-2.273959	-4.748499	-1.171692	H	5.40222	3.302115	-0.248045
H	-0.075702	-2.04406	-3.691105	C	3.303763	-1.980134	0.408968
H	-0.566849	-4.36391	-2.938766	H	2.962609	0.101079	0.529413
C	-4.624806	-0.353538	-0.645332	C	3.624755	-1.964532	1.919967
N	-5.427349	0.740712	-0.421367	C	2.021673	-2.791021	0.184408
H	-5.125002	-1.304013	-0.531802	H	4.099608	-2.514231	-0.118083
O	-6.638497	0.562934	-0.167675	H	4.344104	-1.160435	2.10874
O	-4.937162	1.892467	-0.468486	H	4.121384	-2.906639	2.165501
H	0.092933	-0.815797	4.020035	C	2.426137	-1.842402	2.862706
H	-3.279106	1.116253	1.115199	O	2.021489	-3.993079	0.434427
H	-2.953622	0.771818	-1.307628	N	0.911673	-2.101686	-0.161319
				H	2.777118	-1.899329	3.902072
				H	1.742636	-2.690978	2.729134
				C	1.624445	-0.567639	2.759176
				H	0.094408	-2.655209	-0.406266
				H	0.975415	-1.182761	-0.596691
				O	1.949963	0.428733	2.141854
				O	0.467479	-0.537469	3.430486
(24) <i>si</i> → <i>si/t</i> : 1-Nit							
N	-1.03211	1.993329	0.318864				
C	0.361303	2.493842	0.257941				
C	0.217303	3.963304	-0.193383				

C	-2.768524	-0.191545	3.314457	H	-0.304678	-2.126146	-3.682613
H	-1.889268	0.445464	3.466187	H	-0.746244	-4.430857	-2.852319
H	-3.661131	0.423962	3.47287	C	-4.70456	-0.367113	-0.564527
H	-2.755807	-0.968113	4.087151	N	-5.506216	0.669888	-0.393602
C	-2.510133	-1.369187	-1.189619	H	-5.181205	-1.330195	-0.679827
C	-2.748029	-2.672452	-0.730214	O	-6.777849	0.527035	-0.365392
C	-1.62388	-1.196416	-2.259138	O	-5.006691	1.849567	-0.251425
C	-2.116325	-3.76671	-1.322231	H	0.283112	-1.384012	3.878404
H	-3.448214	-2.841351	0.08376	H	-3.386199	1.095638	1.092969
C	-0.993159	-2.287775	-2.857474	H	-3.014838	0.693587	-1.256077
H	-1.425082	-0.194079	-2.629323				
C	-1.23772	-3.578768	-2.391183				
H	-2.317274	-4.768788	-0.952618				

Cartesian coordinates of reactants, transition states, and products for the protonation of (2*S*,3*R*)-**1-D** and its transition to (2*S*,3*R*)-**1-C** optimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform:

(A) Protonation of **1-D/W** (boat)

(1) **1-D/W**

				H	-3.034753	2.809555	2.244609
N	0.244078	-1.794732	-0.8695	H	-2.41804	4.287762	1.512919
C	-1.06351	-2.288273	-0.435259	C	-0.922751	2.798035	1.734955
C	-1.218444	-3.656246	-1.133951	O	-1.690175	4.421086	-1.114528
C	-0.365551	-3.486936	-2.394263	N	-1.575836	2.281268	-1.859641
C	0.830433	-2.685803	-1.884746	H	-0.522276	3.420938	2.540277
H	-1.094371	-2.394894	0.652932	H	-0.288126	3.004288	0.859752
H	-2.261837	-3.911399	-1.343317	C	-0.669624	1.360817	2.11658
H	-0.791639	-4.432001	-0.489032	H	-0.980924	2.556562	-2.632654
H	-0.065046	-4.441408	-2.833735	H	-1.87964	1.310035	-1.81108
H	-0.909641	-2.909565	-3.148376	O	-1.369994	0.406173	1.805226
H	1.572687	-3.360294	-1.430513	O	0.441036	1.21102	2.824697
H	1.315333	-2.110726	-2.678964	C	2.068044	1.918595	-1.713703
C	1.0809	-1.261528	0.119371	H	3.139681	2.124583	-1.627478
C	2.159052	-0.319071	-0.415927	H	1.897218	1.401945	-2.665915
C	3.385748	-0.380402	0.523281	H	1.546451	2.881738	-1.756038
H	2.483541	-0.671812	-1.403407	H	3.04999	-0.072701	1.527192
C	1.538715	1.083998	-0.549805	C	4.497008	0.542986	0.078357
H	1.680589	1.621872	0.398662	C	4.76745	1.718368	0.781434
H	0.454571	0.965185	-0.684129	C	5.227624	0.262746	-1.081918
H	0.465557	-0.735897	0.855414	C	5.746785	2.604977	0.330673
C	-2.172007	-1.343607	-0.904666	H	4.203536	1.945033	1.684112
O	-2.051111	-0.660885	-1.928221	C	6.207858	1.143526	-1.532255
N	-3.322332	-1.328182	-0.195222	H	5.020774	-0.644905	-1.646994
C	-4.484451	-0.605049	-0.719279	C	6.468106	2.320229	-0.827653
C	-3.599378	-2.002236	1.085872	H	5.945364	3.517829	0.885574
C	-4.295821	0.913986	-0.74484	H	6.765842	0.913919	-2.435878
C	-5.620635	-1.031294	0.226417	H	7.229924	3.009695	-1.180489
H	-4.673761	-0.895886	-1.756563	C	3.842556	-1.807698	0.568094
C	-4.89528	-1.330589	1.541685	N	2.975945	-2.750397	0.747395
H	-2.780408	-1.84371	1.791377	H	4.86168	-2.137405	0.40356
H	-3.737912	-3.079381	0.928537	O	3.147025	-3.989492	0.793653
O	-5.025394	1.615068	-1.442499	O	1.661157	-2.347093	0.99767
N	-3.32053	1.401035	0.047718	H	0.577489	0.247608	3.059543
H	-6.389875	-0.260219	0.314399	O	0.881319	-1.343239	3.482598
H	-6.088981	-1.940811	-0.163878	H	1.266036	-1.877895	2.759824
H	-4.660341	-0.397494	2.067117	H	1.435043	-1.493079	4.265567
H	-5.474649	-1.967512	2.214208				
C	-2.973403	2.803293	0.095619				
H	-2.746294	0.760822	0.593539	(2) ts for protonation			
C	-2.377695	3.197086	1.457902	N	0.364992	-1.625913	-0.648882
C	-2.025212	3.239228	-1.031995	C	-0.916194	-2.106558	-0.091052
H	-3.892085	3.380769	-0.054586	C	-0.885021	-3.595966	-0.457542

C	-0.231776	-3.587424	-1.843871	O	-0.103168	1.075356	2.752141
C	0.860397	-2.523262	-1.726814	C	2.805423	1.999881	-2.373159
H	-0.920405	-1.898223	0.983668	H	3.575897	2.4466	-1.74019
H	-1.877125	-4.050741	-0.458818	H	3.294214	1.292616	-3.052493
H	-0.257246	-4.123946	0.267592	H	2.363634	2.79808	-2.97892
H	0.187532	-4.557855	-2.115569	H	2.675977	1.250553	0.905228
H	-0.962198	-3.299967	-2.606622	C	4.520342	0.744175	-0.012549
H	1.81514	-2.935789	-1.395795	C	5.135675	1.850592	0.584506
H	1.002706	-1.934947	-2.635893	C	5.247152	0.001404	-0.950534
C	0.919519	-0.547027	-0.244293	C	6.436247	2.220048	0.246141
C	2.16844	0.052854	-0.783227	H	4.582722	2.436014	1.317206
C	3.108816	0.367108	0.413181	C	6.548293	0.370181	-1.292414
H	2.645075	-0.646587	-1.473495	H	4.800444	-0.871008	-1.41919
C	1.709147	1.314567	-1.558476	C	7.146862	1.481678	-0.699931
H	1.270283	2.024901	-0.844704	H	6.891542	3.087195	0.717213
H	0.90118	1.015415	-2.239989	H	7.095918	-0.214699	-2.026865
H	0.381007	-0.000026	0.530555	H	8.158983	1.76839	-0.971773
C	-2.044468	-1.350418	-0.805179	C	3.127143	-0.681195	1.531183
O	-1.798445	-0.595383	-1.753263	N	3.605584	-1.976382	1.200717
N	-3.296078	-1.565064	-0.370063	H	3.682216	-0.338647	2.405312
C	-4.429723	-0.94595	-1.072166	O	4.07044	-2.686251	2.097543
C	-3.71086	-2.326466	0.823403	O	3.45264	-2.41046	0.047178
C	-4.424661	0.585956	-1.007954	H	0.235853	0.043854	2.753116
C	-5.648757	-1.538317	-0.342653	O	0.776459	-1.218698	2.567341
H	-4.404316	-1.206504	-2.133408	H	1.868692	-0.990687	2.086806
C	-5.125374	-1.8037	1.072959	H	0.925408	-1.664845	3.41722
H	-3.028682	-2.137113	1.655436				
H	-3.726271	-3.399331	0.600346				
O	-5.056328	1.242072	-1.832775	(3) protonated 1-D/W			
N	-3.730567	1.122831	0.011503	N	0.205133	2.099905	-0.711846
H	-6.507411	-0.863496	-0.374532	C	1.62967	2.113869	-0.300944
H	-5.933095	-2.479615	-0.824495	C	2.093828	3.547352	-0.614959
H	-5.083391	-0.872187	1.648632	C	1.111007	4.028442	-1.687181
H	-5.734653	-2.522936	1.624856	C	-0.21256	3.413659	-1.250313
C	-3.593616	2.545793	0.22898	H	1.665749	1.886203	0.768032
H	-3.211122	0.520638	0.650578	H	3.130648	3.579326	-0.956341
C	-3.238052	2.837447	1.700697	H	2.002616	4.150702	0.292222
C	-2.554706	3.207528	-0.684787	H	1.049712	5.116883	-1.745771
H	-4.54874	3.027873	-0.003573	H	1.394661	3.639212	-2.670997
H	-3.91721	2.255901	2.33468	H	-0.671519	3.968569	-0.425754
H	-3.457527	3.894085	1.876779	H	-0.926438	3.272191	-2.061505
C	-1.784757	2.606663	2.125124	C	-0.51115	1.042968	-0.626174
O	-2.451364	4.43179	-0.697648	C	-1.929027	0.877565	-1.059081
N	-1.739637	2.387269	-1.379074	C	-2.709549	0.249731	0.133805
H	-1.619945	3.070525	3.104244	H	-2.377039	1.841961	-1.325307
H	-1.090414	3.119178	1.445154	C	-1.868303	-0.041722	-2.313709
C	-1.303517	1.175772	2.246793	H	-1.904542	-1.085323	-1.980699
H	-1.101934	2.812685	-2.042343	H	-0.896388	0.09514	-2.805048
H	-1.919112	1.389547	-1.468495	H	-0.017752	0.153508	-0.239964
O	-1.957177	0.18954	1.897599				

C	2.388081	1.005113	-1.039929
O	1.858527	0.340177	-1.938933
N	3.635709	0.760152	-0.612023
C	4.37872	-0.377011	-1.170335
C	4.362017	1.432739	0.483148
C	3.696497	-1.722535	-0.88675
C	5.748773	-0.271731	-0.478176
H	4.448813	-0.295619	-2.257687
C	5.425352	0.401597	0.859787
H	3.686818	1.666181	1.309267
H	4.821844	2.355194	0.109565
O	3.931206	-2.693614	-1.604008
N	2.870044	-1.756622	0.175344
H	6.22519	-1.2495	-0.372811
H	6.405244	0.36797	-1.077134
H	5.003334	-0.323253	1.564661
H	6.297855	0.866376	1.324617
C	2.142068	-2.945194	0.570839
H	2.748926	-0.93563	0.778921
C	1.626826	-2.806487	2.01684
C	0.968282	-3.274279	-0.359894
H	2.811999	-3.810761	0.514648
H	2.476756	-2.535103	2.653119
H	1.292098	-3.800597	2.327396
C	0.470761	-1.825518	2.233397
O	0.369332	-4.337859	-0.230069
N	0.591796	-2.322334	-1.246074
H	0.049531	-1.989198	3.23341
H	-0.356793	-2.035276	1.541834
C	0.777767	-0.325463	2.154902
H	-0.092267	-2.594429	-1.943543
H	1.197595	-1.5384	-1.476179
O	1.969522	0.065211	2.0443
O	-0.225568	0.443403	2.200419
C	-2.969456	0.227634	-3.337613
H	-3.963111	-0.00711	-2.947803
H	-2.963573	1.278162	-3.650862
H	-2.802861	-0.386584	-4.228421
H	-2.097746	-0.579499	0.510227
C	-4.054347	-0.309648	-0.286577
C	-4.220326	-1.691314	-0.410294
C	-5.131085	0.528202	-0.597618
C	-5.430073	-2.228069	-0.850176
H	-3.395102	-2.352477	-0.151917
C	-6.343672	-0.004087	-1.032431
H	-5.027348	1.608606	-0.518169
C	-6.495059	-1.384873	-1.16486
H	-5.541124	-3.30525	-0.939362
H	-7.169554	0.660048	-1.272453
H	-7.439355	-1.799877	-1.505935

C	-2.818531	1.286723	1.245733
N	-2.984746	0.666953	2.60274
H	-1.932239	1.915974	1.345786
O	-2.930482	1.432584	3.549695
O	-3.192551	-0.526276	2.691888
H	-0.02456	2.147929	2.172912
O	-0.050825	3.116974	1.952987
H	-3.689541	1.939615	1.140693
H	-0.238432	3.566958	2.790506

(B) Transition of 1-D (boat) to 1-C

(1) 1-D/W

N	0.244078	-1.794732	-0.8695
C	-1.06351	-2.288273	-0.435259
C	-1.218444	-3.656246	-1.133951
C	-0.365551	-3.486936	-2.394263
C	0.830433	-2.685803	-1.884746
H	-1.094371	-2.394894	0.652932
H	-2.261837	-3.911399	-1.343317
H	-0.791639	-4.432001	-0.489032
H	-0.065046	-4.441408	-2.833735
H	-0.909641	-2.909565	-3.148376
H	1.572687	-3.360294	-1.430513
H	1.315333	-2.110726	-2.678964
C	1.0809	-1.261528	0.119371
C	2.159052	-0.319071	-0.415927
C	3.385748	-0.380402	0.523281
H	2.483541	-0.671812	-1.403407
C	1.538715	1.083998	-0.549805
H	1.680589	1.621872	0.398662
H	0.454571	0.965185	-0.684129
H	0.465557	-0.735897	0.855414
C	-2.172007	-1.343607	-0.904666
O	-2.051111	-0.660885	-1.928221
N	-3.322332	-1.328182	-0.195222
C	-4.484451	-0.605049	-0.719279
C	-3.599378	-2.002236	1.085872
C	-4.295821	0.913986	-0.74484
C	-5.620635	-1.031294	0.226417
H	-4.673761	-0.895886	-1.756563
C	-4.89528	-1.330589	1.541685
H	-2.780408	-1.84371	1.791377
H	-3.737912	-3.079381	0.928537
O	-5.025394	1.615068	-1.442499
N	-3.32053	1.401035	0.047718
H	-6.389875	-0.260219	0.314399
H	-6.088981	-1.940811	-0.163878

H	-4.660341	-0.397494	2.067117	C	1.553848	4.053484	-1.134079
H	-5.474649	-1.967512	2.214208	C	1.079929	3.702995	-2.550285
C	-2.973403	2.803293	0.095619	C	-0.149446	2.833469	-2.305008
H	-2.746294	0.760822	0.593539	H	0.923708	3.008577	0.687505
C	-2.377695	3.197086	1.457902	H	2.605685	4.344295	-1.098569
C	-2.025212	3.239228	-1.031995	H	0.951972	4.868152	-0.719929
H	-3.892085	3.380769	-0.054586	H	0.835224	4.588687	-3.140266
H	-3.034753	2.809555	2.244609	H	1.847542	3.127382	-3.07333
H	-2.41804	4.287762	1.512919	H	-1.045525	3.438575	-2.115295
C	-0.922751	2.798035	1.734955	H	-0.356775	2.118687	-3.10402
O	-1.690175	4.421086	-1.114528	C	-0.49715	1.1506	-0.525183
N	-1.575836	2.281268	-1.859641	C	-1.654692	0.418743	-1.152631
H	-0.522276	3.420938	2.540277	C	-2.536192	0.345552	0.12314
H	-0.288126	3.004288	0.859752	H	-2.149315	1.073773	-1.881055
C	-0.669624	1.360817	2.11658	C	-1.212872	-0.88003	-1.834498
H	-0.980924	2.556562	-2.632654	H	-0.47041	-1.373758	-1.19766
H	-1.87964	1.310035	-1.81108	H	-0.687106	-0.621373	-2.761813
O	-1.369994	0.406173	1.805226	H	-0.052921	0.67078	0.354123
O	0.441036	1.21102	2.824697	C	2.500286	1.851984	-0.280076
C	2.068044	1.918595	-1.713703	O	3.112647	1.600308	-1.325187
H	3.139681	2.124583	-1.627478	N	2.863115	1.325911	0.901267
H	1.897218	1.401945	-2.665915	C	4.110862	0.55504	0.976137
H	1.546451	2.881738	-1.756038	C	2.208169	1.475295	2.219855
H	3.04999	-0.072701	1.527192	C	4.095804	-0.716379	0.126384
C	4.497008	0.542986	0.078357	C	4.266891	0.26526	2.481854
C	4.76745	1.718368	0.781434	H	4.93743	1.152307	0.580999
C	5.227624	0.262746	-1.081918	C	2.835663	0.337677	3.023472
C	5.746785	2.604977	0.330673	H	1.121381	1.376308	2.148387
H	4.203536	1.945033	1.684112	H	2.455194	2.453408	2.650125
C	6.207858	1.143526	-1.532255	O	5.150415	-1.15889	-0.321494
H	5.020774	-0.644905	-1.646994	N	2.89221	-1.300292	-0.061026
C	6.468106	2.320229	-0.827653	H	4.754097	-0.696724	2.660531
H	5.945364	3.517829	0.885574	H	4.884141	1.048361	2.933658
H	6.765842	0.913919	-2.435878	H	2.294644	-0.594098	2.820265
H	7.229924	3.009695	-1.180489	H	2.796141	0.530113	4.097968
C	3.842556	-1.807698	0.568094	C	2.719673	-2.49167	-0.866079
N	2.975945	-2.750397	0.747395	H	2.067154	-0.951843	0.423072
H	4.86168	-2.137405	0.40356	C	2.05944	-3.664702	-0.122844
O	3.147025	-3.989492	0.793653	C	2.046211	-2.184714	-2.211847
O	1.661157	-2.347093	0.99767	H	3.734135	-2.814475	-1.130622
H	0.577489	0.247608	3.059543	H	2.546556	-3.745514	0.855503
O	0.881319	-1.343239	3.482598	H	2.31601	-4.570895	-0.678683
H	1.266036	-1.877895	2.759824	C	0.537085	-3.68806	0.043983
H	1.435043	-1.493079	4.265567	O	1.50693	-3.078688	-2.861918
				N	2.12491	-0.909383	-2.640708
				H	0.232396	-4.679492	0.391217
				H	0.048508	-3.547779	-0.929998
(2) ts for transition				C	-0.0653	-2.673902	0.981935
N	0.1946	2.113111	-1.065382	H	1.812359	-0.706797	-3.582895
C	1.287301	2.780469	-0.315294	H	2.622889	-0.181985	-2.132624

O	0.385282	-1.553293	1.19002	H	-0.107644	0.34723	0.103041
O	-1.183078	-3.101622	1.542238	C	2.263615	2.053629	-0.215759
C	-2.359034	-1.840603	-2.138101	O	2.973658	1.964819	-1.22482
H	-2.819129	-2.220844	-1.220239	N	2.66917	1.535066	0.963148
H	-3.144807	-1.355257	-2.728747	C	4.026312	0.993315	1.071419
H	-1.987241	-2.698003	-2.708711	C	1.92078	1.453862	2.232067
H	-2.115083	-0.426355	0.77735	C	4.248988	-0.256572	0.2171
C	-4.013897	0.082593	-0.081651	C	4.180755	0.720082	2.578056
C	-4.655298	-0.92264	0.64805	H	4.75093	1.724612	0.703389
C	-4.766499	0.847657	-0.979773	C	2.74614	0.454518	3.044352
C	-6.017785	-1.166748	0.47549	H	0.902623	1.097892	2.059229
H	-4.08078	-1.51214	1.35986	H	1.882254	2.435767	2.718988
C	-6.127828	0.605603	-1.154838	O	5.38428	-0.551752	-0.147733
H	-4.291217	1.643358	-1.550699	N	3.14853	-0.983563	-0.07293
C	-6.757649	-0.405944	-0.429073	H	4.866571	-0.107558	2.775891
H	-6.500779	-1.954182	1.047911	H	4.578343	1.617649	3.063263
H	-6.697515	1.207928	-1.857537	H	2.441856	-0.567052	2.788382
H	-7.818316	-0.597469	-0.566366	H	2.612493	0.59402	4.119593
C	-2.239625	1.712267	0.705491	C	3.178561	-2.153609	-0.92276
N	-1.640691	1.945658	1.883154	H	2.257417	-0.75008	0.3579
H	-2.664491	2.598437	0.247644	C	2.720547	-3.445596	-0.224464
O	-1.468369	3.129393	2.283126	C	2.448835	-1.915679	-2.252334
O	-1.146797	0.98337	2.568734	H	4.232148	-2.290349	-1.194788
H	-1.574061	-2.397352	2.151857	H	3.185314	-3.462061	0.768015
O	-2.324791	-1.341178	3.11547	H	3.146481	-4.280679	-0.787978
H	-1.929547	-0.447585	2.934837	C	1.221596	-3.730962	-0.112552
H	-2.186433	-1.515215	4.059994	O	2.118952	-2.86872	-2.958491
				N	2.231515	-0.633511	-2.595826
				H	1.076153	-4.768277	0.204131
				H	0.745464	-3.652822	-1.099934
				C	0.415983	-2.86357	0.818392
				H	1.834628	-0.44507	-3.508751
				H	2.565504	0.157397	-2.048359
				O	0.690803	-1.717103	1.146972
				O	-0.687964	-3.471683	1.230166
				C	-2.356069	-2.13833	-2.278629
				H	-2.900227	-2.468974	-1.386336
				H	-3.080398	-1.67084	-2.956507
				H	-1.954621	-3.028053	-2.774959
				H	-2.193001	-0.773054	0.655473
				C	-4.111342	-0.102426	-0.047665
				C	-4.771633	-1.09937	0.677352
				C	-4.867861	0.773063	-0.836022
				C	-6.159613	-1.223797	0.612172
				H	-4.189635	-1.779487	1.296466
				C	-6.254122	0.651532	-0.901592
				H	-4.372787	1.556966	-1.407094
				C	-6.904347	-0.349423	-0.177942
				H	-6.658029	-2.006131	1.178107
				H	-6.82812	1.336857	-1.51943
(3) 1-C/W							
N	0.008027	1.98583	-1.157021				
C	0.909607	2.757295	-0.284602				
C	1.030531	4.142845	-0.960387				
C	0.427735	3.93752	-2.355244				
C	-0.652004	2.894365	-2.095444				
H	0.487741	2.868146	0.720919				
H	2.062175	4.500863	-0.990182				
H	0.432864	4.864832	-0.394731				
H	0.02697	4.861045	-2.781062				
H	1.177859	3.528337	-3.038805				
H	-1.548183	3.37077	-1.658187				
H	-0.952725	2.354696	-2.998143				
C	-0.767817	0.998235	-0.488101				
C	-1.752364	0.106083	-1.271421				
C	-2.614419	0.016987	0.022576				
H	-2.297423	0.712685	-2.007303				
C	-1.235524	-1.168279	-1.913393				
H	-0.53344	-1.648113	-1.220876				
H	-0.654556	-0.907297	-2.806616				

H	-7.985228	-0.446165	-0.231158
C	-1.999696	1.364715	0.420898
N	-1.725388	1.650212	1.848976
H	-2.551504	2.227921	0.046452
O	-1.678414	2.817009	2.195395
O	-1.495414	0.717374	2.611514
H	-1.21592	-2.873956	1.832512
O	-2.211803	-2.011163	2.865562
H	-1.950214	-1.07179	2.838518
H	-2.126925	-2.290966	3.791531

(C) (2*S*,3*R*)-1-D/W (half-chair)

N	1.084982	-1.231474	0.175786
C	-0.123593	-2.02679	0.274931
C	0.379636	-3.447179	-0.029426
C	1.444324	-3.187555	-1.101728
C	2.109366	-1.881359	-0.649481
H	-0.559946	-1.940746	1.275204
H	-0.413781	-4.120499	-0.366037
H	0.830476	-3.863595	0.877548
H	2.164342	-4.004934	-1.189964
H	0.965837	-3.046431	-2.075965
H	3.005319	-2.088107	-0.053274
H	2.407219	-1.265181	-1.505641
C	0.981779	0.139792	0.46087
C	1.995402	1.095336	-0.169315
C	3.405051	0.926629	0.478914
H	2.053746	0.867077	-1.24005
C	1.480473	2.537026	-0.00567
H	1.509475	2.809001	1.057987
H	0.427147	2.5628	-0.308262
H	-0.035134	0.503831	0.272305
C	-1.160315	-1.60628	-0.776263
O	-0.839296	-0.917956	-1.755003
N	-2.425816	-2.042136	-0.614365
C	-3.429715	-1.793123	-1.652488
C	-2.96419	-2.791031	0.534897
C	-3.791921	-0.312141	-1.804053
C	-4.629193	-2.637339	-1.188185
H	-3.050688	-2.108414	-2.628894
C	-4.475593	-2.666207	0.335802
H	-2.62545	-2.34992	1.475231
H	-2.639663	-3.838117	0.491722
O	-4.377613	0.080626	-2.81089
N	-3.445722	0.485663	-0.774977
H	-5.578263	-2.215992	-1.528025

H	-4.535854	-3.648224	-1.59859
H	-4.829019	-1.724263	0.771211
H	-5.020882	-3.487788	0.806016
C	-3.635622	1.917813	-0.786821
H	-2.941473	0.095338	0.021458
C	-3.753768	2.484463	0.638168
C	-2.537966	2.672622	-1.552645
H	-4.568141	2.13412	-1.319725
H	-4.518081	1.909762	1.173592
H	-4.13174	3.504848	0.536036
C	-2.466982	2.568388	1.475049
O	-2.622003	3.89284	-1.685588
N	-1.498533	1.950304	-2.009112
H	-2.591549	3.323271	2.255393
H	-1.62317	2.911891	0.857581
C	-2.008417	1.292983	2.143994
H	-0.799947	2.42741	-2.567597
H	-1.447376	0.934584	-1.944868
O	-2.099989	0.175363	1.646385
O	-1.460234	1.496792	3.322699
C	2.242554	3.569093	-0.832421
H	3.299533	3.638039	-0.550211
H	2.194683	3.327932	-1.901204
H	1.803636	4.56262	-0.696037
H	3.751321	1.942678	0.725306
C	4.485585	0.359212	-0.442798
C	5.27016	-0.752027	-0.121938
C	4.72965	1.013065	-1.657605
C	6.263759	-1.202367	-0.993366
H	5.108461	-1.29611	0.804174
C	5.719691	0.567093	-2.529353
H	4.137249	1.883955	-1.928529
C	6.493266	-0.546706	-2.199937
H	6.855377	-2.072976	-0.723798
H	5.88774	1.091509	-3.46612
H	7.265274	-0.898896	-2.87825
C	3.345175	0.220343	1.799828
N	2.257939	0.00078	2.456092
H	4.239951	-0.078385	2.332281
O	2.168617	-0.523246	3.612655
O	1.037801	0.359737	1.933096
H	-1.089402	0.630672	3.692415
O	-0.436316	-0.682452	4.374852
H	0.505739	-0.67186	4.069692
H	-0.402253	-0.61902	5.34254

Cartesian coordinates of reactants, reactant complex, intermediates, transition states, and product complex for the organocatalytic addition optimized at the SMD M06-2X/6-31+G(d) level of theory in chloroform:

(A) Reactans

(1) dPPE-NH₂

N	-2.510789	-1.612625	-0.378955
C	-2.492798	-0.199699	0.025877
C	-3.840593	0.407815	-0.45454
C	-4.748763	-0.823892	-0.692565
C	-3.914917	-2.018895	-0.199171
H	-2.436162	-0.173855	1.116871
H	-3.700225	0.976981	-1.379336
H	-4.247768	1.088393	0.297621
H	-5.704361	-0.746514	-0.167261
H	-4.962756	-0.935711	-1.759805
H	-4.079471	-2.19853	0.8689
H	-4.110104	-2.947787	-0.739377
C	-1.276474	0.481934	-0.574387
O	-0.727351	0.00908	-1.580081
N	-0.838472	1.618727	-0.002518
C	0.246691	2.388274	-0.619321
C	-1.350258	2.240533	1.23155
C	1.605261	1.681105	-0.560337
C	0.23622	3.704127	0.175235
H	0.042112	2.540857	-1.682826
C	-0.276345	3.281429	1.555531
H	-1.460724	1.49249	2.020644
H	-2.322467	2.710897	1.04222
O	2.527426	2.053319	-1.280906
N	1.708619	0.652968	0.305763
H	1.222801	4.173014	0.197462
H	-0.466137	4.400835	-0.29405
H	0.529623	2.814457	2.132904
H	-0.676178	4.115488	2.136725
C	2.877214	-0.20465	0.359411
H	0.906949	0.399544	0.876736
C	2.773734	-1.189629	1.54153
C	3.101403	-0.998143	-0.934982
H	3.772272	0.412428	0.489978
H	2.496298	-0.622141	2.436678
H	3.773603	-1.597791	1.711954
C	1.817589	-2.372254	1.34369
O	4.198198	-1.515271	-1.139033
N	2.039004	-1.163918	-1.742968
H	1.877339	-3.023496	2.225807
H	2.109292	-2.985927	0.486544
C	0.359708	-1.994273	1.198963

H	2.169306	-1.688464	-2.600082
H	1.1516	-0.68282	-1.60854
O	-0.123462	-0.988501	1.716102
O	-0.352942	-2.838253	0.490567
H	-1.280891	-2.411008	0.263951
H	-2.273475	-1.643092	-1.375051

(2) butanal

C	1.557133	0.410975	0.000011
C	0.093571	0.743635	0
C	-0.828221	-0.469112	0.00002
H	-0.607694	-1.087991	0.877509
H	-0.60766	-1.088049	-0.87742
C	-2.299629	-0.064287	-0.000022
H	-2.54491	0.533824	0.885323
H	-2.544879	0.53375	-0.885426
H	-2.952409	-0.943208	0.000004
H	-0.0889	1.387529	0.874185
H	-0.088891	1.387498	-0.874211
O	2.006163	-0.71586	0.000001
H	2.248915	1.276263	-0.000022

(3) nitrostyrene

C	0.616869	0.460168	0.023608
H	0.910218	1.507319	0.069091
C	-0.819533	0.180329	0.014831
C	-1.703685	1.268484	-0.014266
C	-1.342101	-1.123427	0.03428
C	-3.080934	1.062435	-0.029674
H	-1.303673	2.279455	-0.026244
C	-2.716077	-1.326971	0.019874
H	-0.674278	-1.979454	0.066584
C	-3.588757	-0.235301	-0.013531
H	-3.755139	1.913447	-0.053263
H	-3.111046	-2.338502	0.036779
H	-4.662366	-0.400469	-0.02419
C	1.591143	-0.454709	-0.026777
N	2.975821	-0.035276	-0.00674
H	1.494976	-1.530397	-0.084502

O	3.813147	-0.928891	-0.038001
O	3.252979	1.155075	0.039608
(4) water			
H	0.769888	-0.471270	0.000000
O	0.000000	0.117720	0.000000
H	-0.769888	-0.470492	0.000000

(B) Local minima and transition states

(1) RC

N	2.084362	-0.121469	1.40191
C	1.553821	0.767678	0.369483
C	2.483426	2.01849	0.389832
C	3.51599	1.719373	1.490324
C	2.790088	0.716351	2.380762
H	1.577642	0.252199	-0.600674
H	1.907722	2.915201	0.645183
H	2.948465	2.192275	-0.584176
H	4.411156	1.257639	1.060647
H	3.822345	2.618499	2.031261
H	3.465281	0.104505	2.988554
H	2.092335	1.236813	3.055254
C	3.245641	-2.073289	0.072161
C	4.637296	-1.534608	0.176944
C	5.017683	-0.586849	-0.95344
H	4.280854	0.226165	-0.998651
H	4.947666	-1.116964	-1.90984
C	0.104255	1.16677	0.65967
O	-0.459343	0.829015	1.710148
N	-0.531416	1.920352	-0.260617
C	-1.843973	2.507463	0.029284
C	-0.022929	2.288436	-1.591469
C	-2.960778	1.474198	0.191405
C	-2.087528	3.429935	-1.180236
H	-1.8111	3.059841	0.973035
C	-1.28691	2.766352	-2.305769
H	0.444613	1.42667	-2.074649
H	0.713614	3.097455	-1.510692
O	-3.999433	1.76965	0.778271
N	-2.733789	0.269003	-0.364319
H	-3.152279	3.537277	-1.401544
H	-1.681054	4.42296	-0.961957
H	-1.833689	1.906183	-2.708994
H	-1.062377	3.448258	-3.129196
C	-3.658143	-0.836877	-0.237974

H	-1.837809	0.082834	-0.809852
C	-3.338515	-1.939322	-1.264458
C	-3.689242	-1.451017	1.16793
H	-4.672128	-0.46744	-0.423866
H	-3.203115	-1.467674	-2.244196
H	-4.223179	-2.578109	-1.331618
C	-2.150296	-2.847918	-0.942442
O	-4.572155	-2.258687	1.452102
N	-2.683155	-1.125872	2.000258
H	-2.155974	-3.703647	-1.629091
H	-2.236265	-3.282756	0.060975
C	-0.774624	-2.236686	-1.060755
H	-2.71046	-1.495474	2.943571
H	-2.006204	-0.39262	1.794732
O	-0.534151	-1.095883	-1.432765
O	0.183387	-3.089789	-0.738607
C	6.422351	-0.018966	-0.771748
H	6.509839	0.531944	0.172503
H	7.171179	-0.819858	-0.758606
H	6.681366	0.666707	-1.584998
H	1.081314	-2.651824	-0.857165
H	4.744608	-1.062871	1.162001
H	5.303206	-2.412826	0.191971
O	2.582057	-2.008836	-0.956495
H	1.314893	-0.622617	1.846336
H	2.866957	-2.643672	0.934843

(2) ts1

N	-2.156058	0.887609	-0.98016
C	-1.203535	1.466734	-0.021538
C	-1.709033	2.904639	0.264517
C	-3.130462	2.906271	-0.304718
C	-2.995246	1.980593	-1.505309
H	-1.212219	0.860678	0.896993
H	-1.09187	3.637329	-0.26987
H	-1.677129	3.145122	1.329196
H	-3.829709	2.476751	0.42143
H	-3.479148	3.906326	-0.575314
H	-3.949183	1.592723	-1.871809
H	-2.492027	2.499974	-2.334024
C	-3.162383	-0.865632	0.097967
C	-4.57079	-0.549626	-0.312726
C	-5.492801	-1.689834	0.150003
H	-5.451343	-1.759244	1.243105
H	-5.118114	-2.644169	-0.243147
C	0.214238	1.426586	-0.591679
O	0.443258	0.904804	-1.69375
N	1.205693	1.97784	0.132251

C	2.558757	2.090095	-0.427162	H	0.744888	-1.755187	1.069874
C	1.108873	2.517348	1.499158	H	0.735707	-3.997642	-1.038738
C	3.227355	0.73809	-0.688481	H	0.353567	-4.154728	0.691197
C	3.313241	2.893379	0.64995	H	2.65844	-3.653874	1.329032
H	2.528916	2.605049	-1.391465	H	2.876893	-4.739723	-0.060155
C	2.570066	2.546991	1.944803	H	3.983847	-2.203957	-0.019508
H	0.476988	1.874816	2.117857	H	3.357069	-2.892154	-1.541324
H	0.68895	3.529745	1.479091	C	2.437516	-0.213188	0.032608
O	4.141224	0.638845	-1.503689	C	3.479943	0.454653	-0.849297
N	2.772695	-0.286282	0.0572	C	3.776095	1.867683	-0.347751
H	4.376788	2.64321	0.672719	H	4.139387	1.810408	0.684459
H	3.217206	3.962658	0.434167	H	2.841051	2.443646	-0.319875
H	2.870923	1.557939	2.308706	C	-0.396496	-1.56039	-0.752242
H	2.740861	3.274926	2.741315	O	-0.191509	-0.903442	-1.78711
C	3.261689	-1.64167	-0.070686	N	-1.624834	-1.820763	-0.298845
H	1.993487	-0.134381	0.694068	C	-2.799781	-1.326781	-1.029772
C	2.895374	-2.468816	1.177305	C	-1.979278	-2.500858	0.961843
C	2.751382	-2.361807	-1.325221	C	-2.895606	0.203687	-1.05039
H	4.352014	-1.611155	-0.166745	C	-3.971271	-1.955488	-0.255744
H	3.137334	-1.873186	2.064761	H	-2.759757	-1.648259	-2.073404
H	3.549105	-3.344783	1.187477	C	-3.431449	-2.073013	1.173795
C	1.456123	-2.982492	1.253923	H	-1.314467	-2.178841	1.767527
O	3.234057	-3.44937	-1.634677	H	-1.906362	-3.586179	0.830109
N	1.727844	-1.787923	-1.985926	O	-3.591549	0.760777	-1.898469
H	1.370561	-3.692417	2.0865	N	-2.218695	0.843517	-0.083181
H	1.18994	-3.554493	0.356747	H	-4.878249	-1.351468	-0.333993
C	0.37353	-1.952254	1.475058	H	-4.182116	-2.948841	-0.665963
H	1.415282	-2.227332	-2.844373	H	-3.463221	-1.100755	1.677853
H	1.409848	-0.83958	-1.794884	H	-3.983873	-2.794455	1.780064
O	0.564328	-0.760961	1.689077	C	-2.194113	2.283034	0.05787
O	-0.83657	-2.475674	1.435071	H	-1.634019	0.335768	0.593705
C	-6.931126	-1.472097	-0.309924	C	-1.912007	2.670194	1.524577
H	-7.330892	-0.53097	0.084813	C	-1.174317	2.963849	-0.862664
H	-6.99222	-1.430509	-1.403529	H	-3.172594	2.677965	-0.235127
H	-7.582207	-2.283466	0.031679	H	-2.553288	2.047768	2.15964
H	-1.538254	-1.745586	1.50068	H	-2.242043	3.705761	1.650242
H	-4.888916	0.395908	0.142116	C	-0.456282	2.5978	1.993758
H	-4.624818	-0.45527	-1.402684	O	-1.142398	4.189489	-0.938329
O	-2.783824	-0.760225	1.274436	N	-0.300288	2.159878	-1.50586
H	-1.634493	0.434314	-1.731583	H	-0.385457	3.060448	2.985498
H	-2.58816	-1.507998	-0.590751	H	0.181821	3.214639	1.347092
				C	0.232548	1.235077	2.111017
				H	0.324254	2.58737	-2.18014
				H	-0.431765	1.153062	-1.552055
				O	-0.369026	0.172924	1.79268
(3) II				O	1.426398	1.275426	2.525222
N	2.033482	-1.554099	-0.58042	C	4.799724	2.582498	-1.22473
C	0.783796	-2.114876	0.036066	H	5.746133	2.029914	-1.254926
C	0.979176	-3.631251	-0.033752	H	4.437072	2.683026	-2.254585
C	2.473033	-3.775964	0.257407	H	5.010565	3.587318	-0.845072
C	3.10811	-2.621184	-0.513995				

H	2.313465	0.116744	1.934381
H	4.402333	-0.140342	-0.852285
H	3.102909	0.499061	-1.881607
O	2.869581	-0.463038	1.312737
H	1.511076	0.378183	0.022449
H	1.791067	-1.354388	-1.561712

(4) I2

N	-2.271554	1.475959	-0.404772
C	-1.054551	2.099017	0.097421
C	-1.302326	3.593308	-0.15628
C	-2.784675	3.731441	0.197909
C	-3.403283	2.413896	-0.291494
H	-0.918666	1.91719	1.176099
H	-1.133264	3.814074	-1.217182
H	-0.66061	4.241246	0.443928
H	-2.892523	3.814308	1.285099
H	-3.250851	4.609095	-0.257283
H	-4.160924	2.052753	0.41599
H	-3.889837	2.53053	-1.267148
C	-2.486809	0.127698	0.011692
C	-3.570177	-0.574804	-0.793777
C	-3.690079	-2.063253	-0.468844
H	-3.948679	-2.196958	0.589453
H	-2.710871	-2.540974	-0.609089
C	0.180108	1.585658	-0.640746
O	0.101865	0.866277	-1.64245
N	1.389985	1.972566	-0.170635
C	2.597393	1.667185	-0.945357
C	1.682545	2.740679	1.050936
C	2.919634	0.173193	-1.020913
C	3.698765	2.444783	-0.201477
H	2.476972	1.998909	-1.980527
C	3.18176	2.506684	1.238906
H	1.082606	2.379899	1.890298
H	1.474881	3.80592	0.894741
O	3.659523	-0.257618	-1.902473
N	2.384299	-0.594153	-0.050933
H	4.67439	1.962388	-0.299557
H	3.771741	3.453869	-0.620324
H	3.350894	1.550933	1.748204
H	3.650668	3.299028	1.827166
C	2.544495	-2.031891	-0.011492
H	1.724688	-0.184898	0.606771
C	2.33618	-2.574288	1.419358
C	1.617084	-2.777977	-0.979275
H	3.564229	-2.266343	-0.331681
H	2.802939	-1.870849	2.117701

H	2.884334	-3.517032	1.496176
C	0.893845	-2.868218	1.834623
O	1.781683	-3.98175	-1.165154
N	0.596692	-2.074634	-1.510837
H	0.888656	-3.322774	2.833484
H	0.439329	-3.613711	1.171399
C	-0.044836	-1.690361	1.898453
H	0.0179	-2.540787	-2.200957
H	0.563721	-1.056153	-1.486873
O	0.275785	-0.516672	1.77087
O	-1.297186	-2.058632	2.126458
C	-4.733026	-2.757546	-1.340634
H	-5.723604	-2.307596	-1.204124
H	-4.474358	-2.677291	-2.402924
H	-4.811886	-3.821678	-1.09496
H	-1.895194	-1.261338	2.040654
H	-4.536331	-0.074354	-0.625958
H	-3.324472	-0.442463	-1.85453
O	-2.766905	0.030412	1.437891
H	-1.537116	-0.405953	-0.110285
H	-3.725118	0.085499	1.591282

(5) ts2

N	-2.245113	1.466043	-0.261819
C	-1.002422	2.105601	0.176479
C	-1.258132	3.597369	-0.104113
C	-2.770252	3.729273	0.091976
C	-3.315482	2.441183	-0.522365
H	-0.859884	1.916529	1.246961
H	-0.988634	3.828832	-1.141873
H	-0.682394	4.245643	0.558557
H	-3.007413	3.758024	1.161027
H	-3.18407	4.622165	-0.38194
H	-4.248635	2.111098	-0.058765
H	-3.470474	2.538622	-1.60357
C	-2.438125	0.168653	-0.120927
C	-3.585506	-0.512804	-0.810969
C	-3.581774	-2.02984	-0.627038
H	-3.654653	-2.28134	0.437329
H	-2.61797	-2.427588	-0.968816
C	0.198017	1.571366	-0.602621
O	0.060288	0.866674	-1.608625
N	1.414791	1.950177	-0.166961
C	2.608465	1.629847	-0.95619
C	1.732967	2.662243	1.083998
C	2.937105	0.13496	-0.993856
C	3.713538	2.431376	-0.248587
H	2.465098	1.936082	-1.996181
C	3.244829	2.463251	1.209108

H	1.179479	2.231285	1.922514	H	3.502706	-2.135483	-1.777895
H	1.483713	3.725791	0.991455	C	2.110059	-0.024031	-0.555655
O	3.718125	-0.298616	-1.840305	C	3.379021	0.725299	-0.753733
N	2.358357	-0.620086	-0.04446	C	3.145907	2.22555	-0.92168
H	4.696592	1.974774	-0.385465	H	2.539324	2.579339	-0.07939
H	3.743201	3.445585	-0.660932	H	2.567496	2.403405	-1.836764
H	3.454303	1.505477	1.698188	C	-0.413633	-1.484844	-0.876866
H	3.714698	3.258578	1.79226	O	-0.329643	-0.746423	-1.866033
C	2.519412	-2.056095	0.019707	N	-1.594912	-1.832509	-0.342845
H	1.655342	-0.228874	0.588952	C	-2.839191	-1.323965	-0.931883
C	2.254488	-2.569766	1.450748	C	-1.823077	-2.621891	0.882828
C	1.625499	-2.8099	-0.97129	C	-2.988919	0.196588	-0.788361
H	3.549289	-2.297805	-0.260884	C	-3.925015	-2.080696	-0.150047
H	2.728831	-1.86857	2.147165	H	-2.86624	-1.534505	-2.004165
H	2.776049	-3.526327	1.552763	C	-3.281267	-2.305389	1.22169
C	0.794599	-2.810921	1.839424	H	-1.135338	-2.309818	1.671823
O	1.800458	-4.01211	-1.156916	H	-1.681108	-3.688335	0.671246
N	0.620086	-2.110461	-1.538918	O	-3.789978	0.80375	-1.498549
H	0.768258	-3.280814	2.830142	N	-2.220958	0.778152	0.148636
H	0.336203	-3.543444	1.162954	H	-4.860736	-1.518033	-0.109869
C	-0.157415	-1.620964	1.907874	H	-4.120483	-3.039569	-0.641679
H	0.068944	-2.576547	-2.250653	H	-3.328616	-1.388386	1.819362
H	0.575176	-1.094251	-1.497431	H	-3.753362	-3.111154	1.7882
O	0.222983	-0.450765	1.667652	C	-2.195844	2.206417	0.379322
O	-1.355219	-1.923919	2.22384	H	-1.551785	0.235276	0.708119
C	-4.720857	-2.693734	-1.394898	C	-1.625123	2.517983	1.778608
H	-5.695302	-2.328353	-1.050061	C	-1.402204	2.978063	-0.681552
H	-4.6471	-2.487904	-2.469007	H	-3.219781	2.590679	0.320939
H	-4.704351	-3.779585	-1.259427	H	-2.129698	1.861939	2.497443
H	-2.238548	-0.85329	2.021218	H	-1.919078	3.544593	2.017466
H	-4.538933	-0.077456	-0.485005	C	-0.105271	2.42329	1.946577
H	-3.484837	-0.272718	-1.879736	O	-1.422751	4.206322	-0.683441
O	-2.905185	-0.073232	1.708901	N	-0.64528	2.251106	-1.532588
H	-1.523227	-0.408743	0.004278	H	0.166428	2.86035	2.915262
H	-3.810911	-0.415451	1.80394	H	0.403732	3.049366	1.200853
				C	0.558644	1.042361	1.903061
				H	-0.190852	2.74707	-2.29116
				H	-0.758095	1.244979	-1.630584
				O	-0.141794	0.006385	1.731218
				O	1.815447	1.032664	2.022441
				C	4.461526	2.994313	-0.978625
				H	5.031801	2.8567	-0.05287
				H	5.085119	2.654831	-1.814134
				H	4.284057	4.066427	-1.107299
				H	2.453667	-0.567639	2.149609
				H	4.000787	0.529647	0.134264
				H	3.922846	0.306503	-1.61217
				O	2.88458	-1.463201	2.143557
				H	1.177687	0.517774	-0.427319
				H	3.18153	-1.609343	3.053818
(6) I3							
N	2.046235	-1.303142	-0.531036				
C	0.825607	-2.077012	-0.217579				
C	1.179963	-3.487459	-0.699882				
C	2.669923	-3.582277	-0.358972				
C	3.209342	-2.201867	-0.724509				
H	0.734566	-2.043639	0.871668				
H	1.019389	-3.56445	-1.781915				
H	0.573781	-4.24447	-0.19779				
H	2.798814	-3.749404	0.71392				
H	3.181225	-4.374135	-0.909948				
H	4.025032	-1.864336	-0.08421				

(7) ts3

N	-1.960751	1.75692	-0.466897
C	-0.694991	2.309256	0.02115
C	-0.813664	3.795841	-0.35031
C	-2.304344	4.071378	-0.138219
C	-2.984678	2.797683	-0.646396
H	-0.64826	2.185369	1.109029
H	-0.544559	3.926326	-1.405407
H	-0.163811	4.42594	0.260544
H	-2.510385	4.207253	0.928741
H	-2.650363	4.959873	-0.670437
H	-3.88446	2.542058	-0.077398
H	-3.249666	2.857838	-1.708328
C	-2.190491	0.467276	-0.622878
C	-3.44311	-0.131969	-0.790211
C	-3.507487	-1.590152	-1.216257
H	-2.616107	-2.111364	-0.841049
H	-3.47529	-1.663493	-2.311702
C	0.518676	1.660034	-0.628784
O	0.44191	1.075332	-1.713874
N	1.689045	1.818172	0.016877
C	2.935089	1.388422	-0.621835
C	1.899497	2.363937	1.371876
C	3.066327	-0.132928	-0.726409
C	4.014678	1.997559	0.285867
H	2.98276	1.768368	-1.645928
C	3.354541	1.991037	1.66761
H	1.20299	1.908294	2.080503
H	1.753092	3.450525	1.368985
O	3.922353	-0.622221	-1.461868
N	2.226089	-0.857264	0.035217
H	4.948633	1.432734	0.24231
H	4.215893	3.024718	-0.036527
H	3.397378	0.986458	2.102809
H	3.819276	2.688525	2.36811
C	2.199894	-2.302795	0.001525
H	1.492916	-0.415393	0.594843
C	1.704053	-2.874938	1.344771
C	1.356486	-2.864557	-1.149074
H	3.221123	-2.653137	-0.177171
H	2.172829	-2.292687	2.146808
H	2.093089	-3.894371	1.422101
C	0.192261	-2.960572	1.554423
O	1.359341	-4.073081	-1.372009
N	0.58587	-1.988155	-1.825907
H	-0.006158	-3.562866	2.447806
H	-0.274363	-3.515481	0.72903

C	-0.61609	-1.677664	1.719261
H	0.070181	-2.332597	-2.627908
H	0.69237	-0.981035	-1.728049
O	-0.128159	-0.544865	1.510035
O	-1.826145	-1.891744	2.073618
C	-4.763812	-2.289838	-0.699854
H	-4.78069	-2.311066	0.395494
H	-5.668593	-1.77219	-1.04051
H	-4.813489	-3.32311	-1.058442
H	-2.744387	-0.940264	2.031502
H	-3.575461	-0.146188	0.60459
H	-4.270956	0.499165	-1.119797
O	-3.613571	-0.265403	1.865757
H	-1.32884	-0.176035	-0.449634
H	-3.421291	0.59392	2.279223

(8) I4

N	2.06235	-1.498476	-0.734809
C	0.910395	-2.098812	-0.087623
C	1.135406	-3.601123	-0.3298
C	2.659241	-3.723417	-0.243348
C	3.166515	-2.434356	-0.899878
H	0.904384	-1.878973	0.990061
H	0.785784	-3.862274	-1.336072
H	0.611675	-4.225094	0.397801
H	2.965764	-3.74621	0.808151
H	3.041485	-4.622564	-0.732638
H	4.072428	-2.054244	-0.404883
H	3.401155	-2.56722	-1.965116
C	2.241816	-0.143551	-0.79543
C	3.371711	0.511824	-1.144468
C	3.455914	2.014601	-1.173846
H	2.474465	2.43756	-0.918746
H	3.688984	2.359412	-2.19125
C	-0.403745	-1.622882	-0.699394
O	-0.446775	-1.02671	-1.780708
N	-1.536292	-1.900478	-0.016512
C	-2.834417	-1.564502	-0.609634
C	-1.662462	-2.543272	1.302005
C	-3.057752	-0.055424	-0.747959
C	-3.841353	-2.208265	0.360004
H	-2.908123	-1.971792	-1.621653
C	-3.100157	-2.205486	1.700602
H	-0.924455	-2.142931	2.001118
H	-1.521484	-3.627189	1.211591
O	-3.902933	0.379797	-1.526103
N	-2.300112	0.722517	0.050359
H	-4.790093	-1.666427	0.380664

H	-4.040399	-3.236385	0.039742	C	1.288795	2.406605	-2.148041
H	-3.134652	-1.208031	2.154339	H	0.671645	2.840352	-1.348719
H	-3.507594	-2.923287	2.416243	H	0.742396	2.580422	-3.087253
C	-2.339827	2.167844	0.019462	H	0.238078	0.828257	-0.195648
H	-1.599735	0.293943	0.651666	C	-1.379255	-1.737152	-0.532006
C	-1.861335	2.762818	1.358999	O	-1.48585	-1.303651	-1.685035
C	-1.527552	2.781803	-1.129067	N	-2.466158	-2.165029	0.146149
H	-3.376795	2.476424	-0.148588	C	-3.788886	-2.041392	-0.477206
H	-2.327294	2.19265	2.170613	C	-2.527877	-2.728693	1.503323
H	-2.253051	3.781657	1.415457	C	-4.141107	-0.582019	-0.795916
C	-0.349826	2.86164	1.574106	C	-4.734881	-2.658205	0.57129
O	-1.579699	3.995551	-1.321228	H	-3.81995	-2.571883	-1.432592
N	-0.730546	1.952347	-1.827771	C	-3.984272	-2.482698	1.896962
H	-0.147654	3.490777	2.448764	H	-1.816553	-2.233039	2.167072
H	0.135335	3.375516	0.733459	H	-2.306383	-3.802767	1.473289
C	0.404538	1.573931	1.79457	O	-4.939127	-0.30509	-1.685609
H	-0.221466	2.33443	-2.617164	N	-3.532813	0.342498	-0.021437
H	-0.775688	0.938466	-1.74252	H	-5.719572	-2.183699	0.560451
O	-0.063993	0.44602	1.722435	H	-4.868097	-3.722234	0.350624
O	1.678575	1.79089	2.082949	H	-4.098304	-1.4604	2.275074
C	4.515299	2.567365	-0.215706	H	-4.324488	-3.174851	2.670834
H	4.270967	2.31334	0.822707	C	-3.730656	1.76823	-0.165125
H	5.503949	2.150245	-0.442675	H	-2.968727	0.024493	0.761241
H	4.587817	3.658491	-0.287216	C	-3.2857	2.507467	1.107953
H	2.178788	0.928742	2.149821	C	-3.004675	2.374522	-1.376602
H	4.096284	-0.218034	2.544286	H	-4.795541	1.968605	-0.328961
H	4.255252	-0.044216	-1.459019	H	-3.841765	2.103729	1.961083
O	3.298297	-0.353562	2.007124	H	-3.584811	3.551293	0.986073
H	1.357377	0.432462	-0.522895	C	-1.781164	2.483735	1.408479
H	3.566561	-0.200919	1.077758	O	-3.199963	3.557328	-1.65594
				N	-2.140559	1.589413	-2.039554
				H	-1.525305	3.3305	2.057901
(9) I5				H	-1.1855	2.625548	0.493936
				C	-1.271612	1.23765	2.102109
N	1.000092	-1.064889	-0.583987	H	-1.666558	1.977099	-2.847277
C	-0.020456	-1.749997	0.186418	H	-2.012823	0.597568	-1.847993
C	0.556968	-3.168632	0.299123	O	-1.940934	0.251107	2.345103
C	1.213575	-3.379604	-1.074893	O	0.009823	1.242979	2.468645
C	1.639036	-1.972507	-1.533404	C	2.624588	3.150645	-2.232229
H	-0.140203	-1.270531	1.166338	H	3.186112	3.065523	-1.295709
H	-0.198173	-3.925092	0.528305	H	3.249209	2.737608	-3.033424
H	1.305379	-3.175339	1.097601	H	2.474208	4.216111	-2.437851
H	2.057696	-4.07329	-1.025351	H	4.848926	1.728017	0.178298
H	0.482115	-3.7928	-1.776534	C	4.498832	-0.414713	0.374467
H	2.726693	-1.82398	-1.509035	C	5.39431	-0.716508	-0.662653
H	1.292965	-1.765024	-2.55619	C	3.933586	-1.461365	1.121647
C	0.867678	0.274887	-0.896275	C	5.70357	-2.039875	-0.96555
C	1.451369	0.928725	-1.916363	H	5.837877	0.094271	-1.235821
C	4.187463	0.989166	0.627668	C	4.255436	-2.780435	0.826509
H	2.07994	0.384741	-2.621679	H	3.256697	-1.239798	1.942899

C	5.134691	-3.07235	-0.220608
H	6.390007	-2.264053	-1.776682
H	3.82531	-3.586451	1.414582
H	5.380361	-4.105879	-0.4489
C	3.132327	1.431111	1.325157
N	2.910212	2.848559	1.436535
H	2.339744	0.838077	1.764357
O	1.790444	3.216596	1.817966
O	3.792437	3.635587	1.151096
H	0.487237	2.066576	2.216501

(10) ts4

N	1.090658	-1.335208	-0.681809
C	0.048808	-1.982397	0.114484
C	0.500034	-3.450588	0.127768
C	1.112629	-3.626135	-1.26771
C	1.815747	-2.291631	-1.533461
H	0.00498	-1.535279	1.113939
H	-0.320786	-4.14452	0.322261
H	1.259301	-3.582166	0.9054
H	1.80621	-4.468692	-1.315997
H	0.322073	-3.788124	-2.007273
H	2.870169	-2.321451	-1.240685
H	1.746591	-1.970021	-2.578168
C	1.127899	-0.016825	-0.845137
C	2.045669	0.715745	-1.57964
C	3.372663	1.054902	0.217409
H	2.763911	0.173884	-2.19492
C	1.689285	2.121021	-2.01534
H	1.246264	2.667569	-1.170838
H	0.900724	2.056047	-2.77789
H	0.388441	0.531426	-0.254376
C	-1.311554	-1.804166	-0.583749
O	-1.381926	-1.322298	-1.719897
N	-2.415793	-2.170359	0.091717
C	-3.732709	-1.968489	-0.527643
C	-2.507246	-2.72874	1.451317
C	-4.015931	-0.492343	-0.834758
C	-4.706634	-2.543525	0.518616
H	-3.790352	-2.490608	-1.486304
C	-3.948197	-2.40368	1.843372
H	-1.77251	-2.267736	2.114098
H	-2.343322	-3.812985	1.422148
O	-4.806754	-0.179277	-1.720146
N	-3.363831	0.400439	-0.062468
H	-5.667377	-2.022649	0.508237
H	-4.88965	-3.599843	0.296632
H	-4.006614	-1.374778	2.216497

H	-4.323224	-3.074167	2.620001
C	-3.507294	1.832376	-0.206672
H	-2.778784	0.070422	0.704464
C	-3.051689	2.561573	1.067714
C	-2.7558	2.408935	-1.415725
H	-4.563243	2.069503	-0.378956
H	-3.63476	2.180517	1.913563
H	-3.321094	3.612388	0.935566
C	-1.551614	2.508468	1.400735
O	-2.900446	3.595197	-1.70188
N	-1.917109	1.585848	-2.074075
H	-1.283854	3.38633	1.997386
H	-0.933319	2.578787	0.49124
C	-1.094229	1.278231	2.160773
H	-1.480437	1.940383	-2.917247
H	-1.886202	0.581588	-1.912752
O	-1.689621	0.210116	2.163466
O	0.025913	1.386342	2.852599
C	2.851231	2.91065	-2.611967
H	3.628118	3.129452	-1.874224
H	3.307131	2.362308	-3.445254
H	2.495003	3.870524	-2.998978
H	3.910848	1.748516	-0.421956
C	3.953546	-0.293353	0.318011
C	5.011685	-0.634362	-0.54034
C	3.485917	-1.251832	1.22971
C	5.589033	-1.897618	-0.491975
H	5.37847	0.105919	-1.248779
C	4.063083	-2.519628	1.275246
H	2.672628	-1.014216	1.910543
C	5.109058	-2.848665	0.41343
H	6.412232	-2.143898	-1.156576
H	3.694994	-3.252134	1.988354
H	5.556446	-3.837984	0.453265
C	2.645152	1.617967	1.266727
N	2.388757	2.960831	1.31391
H	2.181164	1.048101	2.056153
O	1.59023	3.388364	2.212601
O	2.913887	3.761442	0.52717
H	0.529515	2.242305	2.68201

(11) I6

N	-0.989705	-1.473249	0.602117
C	0.092869	-2.145337	-0.150318
C	-0.277275	-3.627039	-0.006822
C	-0.850916	-3.698938	1.41261
C	-1.653288	-2.405657	1.551235
H	0.097669	-1.767238	-1.175481

H	0.580951	-4.28621	-0.150704	H	-2.881871	1.74516	3.647986
H	-1.040504	-3.878811	-0.750836	H	-1.85119	3.171933	3.447091
H	-1.480346	-4.577106	1.567622	H	-4.061626	1.684409	0.800755
H	-0.041587	-3.718384	2.149005	C	-4.248946	-0.206069	-0.192159
H	-2.692747	-2.518299	1.224534	C	-5.415641	-0.515586	0.514017
H	-1.624574	-1.976005	2.554107	C	-3.829481	-1.073494	-1.208622
C	-1.270944	-0.235849	0.438027	C	-6.148748	-1.663705	0.215355
C	-2.295448	0.523581	1.205816	H	-5.753036	0.152956	1.303719
C	-3.426156	1.001917	0.227102	C	-4.561659	-2.222056	-1.510394
H	-2.767524	-0.121643	1.954181	H	-2.930261	-0.861479	-1.78511
C	-1.548106	1.664621	1.932522	C	-5.722678	-2.521776	-0.798069
H	-1.112563	2.351498	1.196996	H	-7.056323	-1.883688	0.770762
H	-0.712021	1.212988	2.48246	H	-4.226231	-2.878271	-2.309078
H	-0.688716	0.291346	-0.324676	H	-6.295058	-3.413633	-1.036853
C	1.419895	-1.793374	0.537704	C	-2.85007	1.734241	-0.942844
O	1.430853	-1.204849	1.624511	N	-2.561476	2.997933	-0.87575
N	2.540565	-2.176842	-0.090411	H	-2.554592	1.235967	-1.854498
C	3.849267	-1.942512	0.534636	O	-1.857982	3.539568	-1.925409
C	2.648079	-2.739293	-1.450152	O	-2.852903	3.798399	0.044475
C	4.193673	-0.456922	0.692306	H	-1.148677	2.833728	-2.156508
C	4.818266	-2.64405	-0.431985				
H	3.869742	-2.371282	1.539934				
C	4.121931	-2.512104	-1.790299	(12) I7			
H	1.971005	-2.218834	-2.131996				
H	2.407625	-3.808821	-1.436966	N	-0.690226	-1.873992	0.838094
O	5.068511	-0.113712	1.486601	C	0.481918	-2.322381	0.051428
N	3.517901	0.390731	-0.100617	C	0.390474	-3.857908	0.096782
H	5.81353	-2.194321	-0.402798	C	-0.364872	-4.13571	1.39873
H	4.907697	-3.698835	-0.151008	C	-1.403344	-3.02318	1.448993
H	4.257556	-1.502572	-2.193419	H	0.38168	-1.919603	-0.959647
H	4.486152	-3.230433	-2.528097	H	1.375842	-4.327993	0.075471
C	3.710761	1.823682	-0.071056	H	-0.182394	-4.209954	-0.766768
H	2.774571	0.06065	-0.727737	H	-0.831224	-5.122508	1.413222
C	3.223419	2.466267	-1.384443	H	0.309467	-4.05431	2.257365
C	3.023304	2.505097	1.117103	H	-2.277408	-3.240539	0.823198
H	4.779915	2.030955	0.044628	H	-1.724932	-2.763098	2.457287
H	3.666641	1.906472	-2.216465	C	-1.001516	-0.635655	0.957443
H	3.648252	3.474124	-1.413312	C	-2.193345	-0.107937	1.663287
C	1.709693	2.60485	-1.584917	C	-3.199151	0.421138	0.563383
O	3.256344	3.686477	1.360542	H	-2.703522	-0.918744	2.193462
N	2.1233	1.770769	1.803477	C	-1.754899	0.97163	2.671393
H	1.5294	3.319661	-2.395632	H	-1.455011	1.872856	2.123646
H	1.242098	3.057885	-0.697928	H	-0.869229	0.609487	3.210862
C	0.893264	1.355407	-1.919585	H	-0.346492	0.079012	0.451413
H	1.707359	2.186465	2.628919	C	1.756143	-1.75302	0.688212
H	2.032186	0.7662	1.674904	O	1.726261	-1.177722	1.780586
O	1.374481	0.204641	-1.768355	N	2.887053	-1.893085	-0.020326
O	-0.295082	1.552652	-2.319722	C	4.146305	-1.3569	0.514417
C	-2.441246	2.423952	2.90822	C	3.042188	-2.474052	-1.368955
H	-3.24367	2.95355	2.388724	C	4.138915	0.171707	0.648877

C	5.1883	-1.835363	-0.510986	O	-1.78918	3.270243	-3.060625
H	4.329756	-1.749849	1.51768	H	-2.090102	3.484013	-2.107041
C	4.393326	-1.916735	-1.817828	H	-0.995634	1.97082	-3.012428
H	2.220191	-2.168422	-2.020578				
H	3.067778	-3.568169	-1.306068				
O	4.956868	0.725869	1.378208	(13) ts5			
N	3.220981	0.827613	-0.08768	N	0.623937	1.60545	0.702844
H	6.046676	-1.161395	-0.560182	C	-0.590339	2.00663	-0.049101
H	5.546944	-2.828705	-0.221764	C	-0.465839	3.535667	-0.113616
H	4.259027	-0.918601	-2.249274	C	0.240588	3.884101	1.195864
H	4.867721	-2.554679	-2.566854	C	1.281777	2.782351	1.331496
C	3.063013	2.26504	-0.058212	H	-0.571919	1.528873	-1.035802
H	2.567271	0.312466	-0.676596	H	-1.429501	4.032693	-0.217037
C	2.413453	2.787352	-1.351523	H	0.156109	3.803533	-0.973713
C	2.267608	2.770196	1.153263	H	0.702679	4.872828	1.178842
H	4.055901	2.718244	0.030601	H	-0.464182	3.841086	2.033291
H	2.986076	2.401503	-2.202791	H	2.188476	2.9948	0.753461
H	2.543898	3.87233	-1.342792	H	1.549448	2.551753	2.362356
C	0.911583	2.527129	-1.564231	C	0.99282	0.383552	0.831689
O	2.180035	3.977105	1.356077	C	2.130361	-0.079821	1.67954
N	1.639673	1.84262	1.906466	C	3.361655	-0.50355	0.813506
H	0.524434	3.276793	-2.259973	H	2.480172	0.755612	2.293493
H	0.343669	2.679199	-0.6315	C	1.595144	-1.176448	2.625286
C	0.5347	1.154485	-2.085805	H	1.121232	-1.974854	2.043395
H	1.169245	2.163679	2.745314	H	0.805223	-0.730827	3.242866
H	1.837506	0.848912	1.822976	H	0.405798	-0.360877	0.288828
O	1.134357	0.124105	-1.7865	C	-1.815664	1.476874	0.726598
O	-0.512339	1.073828	-2.876759	O	-1.664773	0.756194	1.720107
C	-2.857376	1.299703	3.67311	N	-3.035551	1.775943	0.254348
H	-3.746103	1.683355	3.165721	C	-4.212914	1.188837	0.917493
H	-3.132019	0.415423	4.26049	C	-3.397118	2.546906	-0.952599
H	-2.516236	2.073257	4.368473	C	-4.194927	-0.345876	0.895076
H	-4.066995	0.778977	1.128391	C	-5.391149	1.758789	0.107164
C	-3.619234	-0.760202	-0.298262	H	-4.242664	1.477368	1.970824
C	-4.73622	-1.522303	0.060832	C	-4.790219	2.014247	-1.27944
C	-2.85714	-1.171911	-1.399934	H	-2.670455	2.380503	-1.7501
C	-5.085597	-2.66646	-0.657724	H	-3.445433	3.614464	-0.708398
H	-5.339807	-1.21338	0.912152	O	-4.767149	-0.992521	1.767237
C	-3.199799	-2.317711	-2.117467	N	-3.538286	-0.902925	-0.142105
H	-1.985438	-0.600324	-1.716953	H	-6.243409	1.074904	0.09654
C	-4.31452	-3.071253	-1.747193	H	-5.715134	2.70228	0.558641
H	-5.962762	-3.238825	-0.368333	H	-4.712189	1.082307	-1.850187
H	-2.598655	-2.614165	-2.973237	H	-5.370319	2.728857	-1.867706
H	-4.585098	-3.960083	-2.310287	C	-3.415037	-2.331517	-0.344768
C	-2.667536	1.563661	-0.241468	H	-3.152143	-0.305809	-0.872369
N	-2.893048	2.813517	0.111688	C	-2.905579	-2.622279	-1.768498
H	-2.148356	1.427984	-1.177619	C	-2.49533	-3.018698	0.672756
H	-2.592413	3.204355	-3.600967	H	-4.395382	-2.805054	-0.22058
O	-2.45404	3.793365	-0.632037	H	-3.580174	-2.137276	-2.482465
O	-3.52628	3.116182	1.167657				

H	-2.990219	-3.701349	-1.921062	H	2.477001	-2.946931	-0.721415
C	-1.456586	-2.216549	-2.058816	H	1.79827	-2.488895	-2.311904
O	-2.451587	-4.244636	0.71065	C	1.092044	-0.416118	-0.68627
N	-1.704765	-2.227273	1.432208	C	2.219215	0.181425	-1.460363
H	-1.129944	-2.702298	-2.988135	C	3.37187	0.607598	-0.495564
H	-0.776238	-2.587497	-1.279999	H	2.649135	-0.579332	-2.120584
C	-1.19724	-0.72892	-2.255799	C	1.641995	1.312303	-2.336932
H	-1.190648	-2.678588	2.18066	H	1.306634	2.146167	-1.706977
H	-1.874679	-1.228687	1.523635	H	0.738448	0.927669	-2.827399
O	-2.106785	0.101842	-2.310065	H	0.437229	0.246642	-0.117489
O	0.043584	-0.357336	-2.371979	C	-1.616191	-1.703128	-0.675997
C	2.682877	-1.758572	3.523685	O	-1.503458	-1.017363	-1.699151
H	3.427016	-2.321285	2.950442	N	-2.812362	-2.042949	-0.175627
H	3.204705	-0.967984	4.075274	C	-4.033732	-1.560612	-0.840176
H	2.24153	-2.442709	4.254668	C	-3.094361	-2.732267	1.098334
H	4.164947	-0.671745	1.545306	C	-4.121096	-0.029513	-0.893356
C	3.786355	0.691715	-0.027695	C	-5.156662	-2.159579	0.025523
C	4.747609	1.578517	0.468626	H	-4.066905	-1.905939	-1.876332
C	3.167325	0.99363	-1.244955	C	-4.51845	-2.278252	1.414052
C	5.074187	2.744944	-0.22341	H	-2.369679	-2.437833	1.860507
H	5.252113	1.346226	1.405253	H	-3.061669	-3.81761	0.950414
C	3.483058	2.162668	-1.937179	O	-4.785391	0.521632	-1.769519
H	2.431316	0.315328	-1.667844	N	-3.470923	0.625937	0.083374
C	4.435113	3.045811	-1.426478	H	-6.055681	-1.538606	0.0081
H	5.830344	3.416346	0.174792	H	-5.417775	-3.151641	-0.358151
H	2.988974	2.374905	-2.881913	H	-4.497346	-1.305253	1.916984
H	4.687094	3.952434	-1.969793	H	-5.037883	-2.988897	2.06111
C	3.101365	-1.788995	0.051956	C	-3.453418	2.068553	0.202267
N	4.290549	-2.446185	-0.358049	H	-2.930901	0.117309	0.793182
H	2.497212	-2.526846	0.579038	C	-2.976856	2.475306	1.610698
H	2.407496	-1.796007	-1.228174	C	-2.577124	2.760621	-0.847122
O	4.215444	-3.632926	-0.713003	H	-4.466278	2.454113	0.042833
O	5.350553	-1.813053	-0.423397	H	-3.571182	1.915616	2.342002
O	1.871229	-1.924256	-2.260009	H	-3.221419	3.53461	1.734962
H	1.701092	-2.871489	-2.389642	C	-1.482238	2.300938	1.897356
H	0.822568	-1.161509	-2.338046	O	-2.633919	3.980186	-0.976985
				N	-1.70601	1.985245	-1.531398
				H	-1.253822	2.792993	2.852231
				H	-0.879179	2.831903	1.148421
				C	-0.923104	0.875981	2.018627
				H	-1.196665	2.425481	-2.289324
				H	-1.793121	0.972072	-1.55096
				O	-1.706849	-0.108228	2.037732
				O	0.337012	0.776993	2.099907
				C	2.62072	1.783495	-3.40943
				H	3.546049	2.179208	-2.982254
				H	2.877113	0.959348	-4.084664
				H	2.167038	2.579228	-4.007878
				H	4.162639	1.028826	-1.124673
				C	3.926663	-0.631416	0.185699
(14) I8							
N	0.821487	-1.666387	-0.61928				
C	-0.370665	-2.165581	0.10516				
C	-0.149646	-3.683663	0.1283				
C	0.589317	-3.947974	-1.185191				
C	1.555071	-2.773044	-1.287673				
H	-0.403921	-1.696707	1.095667				
H	-1.082603	-4.242682	0.205295				
H	0.479585	-3.939171	0.987026				
H	1.118467	-4.902623	-1.190958				
H	-0.112132	-3.931484	-2.026187				

C	4.961549	-1.337267	-0.435953	H	4.120401	-0.995752	2.16281
C	3.378271	-1.133375	1.372809	C	4.731953	-2.125686	-0.92379
C	5.443521	-2.525152	0.110605	H	2.642208	-2.694512	-1.313552
H	5.393279	-0.949397	-1.356801	H	3.480271	-3.686205	-0.080368
C	3.860038	-2.323751	1.920191	O	4.480201	1.405933	1.419557
H	2.567284	-0.605181	1.87495	N	3.224111	0.831388	-0.383111
C	4.889751	-3.023699	1.29024	H	6.099554	-0.836731	0.241779
H	6.253398	-3.056521	-0.381511	H	5.683536	-2.378505	1.01129
H	3.431195	-2.700967	2.844702	H	4.597459	-1.327408	-1.661953
H	5.265295	-3.947674	1.721094	H	5.366322	-2.897922	-1.365035
C	2.97209	1.66106	0.53643	C	3.035834	2.181294	-0.871812
N	2.922401	3.053461	-0.030148	H	2.818202	0.083064	-0.95267
H	3.727002	1.736313	1.326677	C	2.523247	2.154571	-2.3239
H	1.996555	1.498649	0.998366	C	2.084869	3.017437	-0.007324
O	3.7489	3.373593	-0.863284	H	3.995277	2.709662	-0.842726
O	2.073741	3.80806	0.416108	H	3.200858	1.52402	-2.910732
O	1.674226	2.889648	3.3124	H	2.609944	3.17498	-2.709069
H	1.64363	3.55807	2.610744	C	1.075717	1.694296	-2.509731
H	1.175239	2.128469	2.940489	O	2.034584	4.229766	-0.168024
				N	1.268122	2.347333	0.851048
				H	0.773715	1.898747	-3.545667
(15) I9				H	0.398017	2.292294	-1.887845
				C	0.766288	0.210609	-2.27737
N	-0.725515	-1.7518	0.796927	H	0.766074	2.926993	1.517166
C	0.57488	-2.236884	0.277664	H	1.51601	1.41176	1.166755
C	0.539104	-3.744621	0.568796	O	1.707971	-0.619682	-2.202957
C	-0.381082	-3.858738	1.78573	O	-0.462395	-0.09239	-2.187494
C	-1.464637	-2.82753	1.502609	C	-2.761159	1.26263	3.628499
H	0.628366	-2.017029	-0.792578	H	-3.210281	2.167809	3.211839
H	1.530816	-4.1578	0.757407	H	-3.556776	0.528643	3.805745
H	0.103322	-4.250169	-0.297915	H	-2.327192	1.527641	4.59783
H	-0.800284	-4.859149	1.908226	H	-3.698505	1.64359	1.191619
H	0.15796	-3.589635	2.70086	C	-4.114213	0.15556	-0.263014
H	-2.225687	-3.204032	0.811196	C	-5.454141	0.1137	0.13271
H	-1.938632	-2.430163	2.399946	C	-3.698347	-0.630382	-1.34319
C	-1.079457	-0.5217	0.717068	C	-6.367565	-0.698558	-0.539121
C	-2.257165	0.069226	1.415002	H	-5.782765	0.721216	0.973741
C	-3.121081	1.005834	0.515802	C	-4.60965	-1.446605	-2.011835
H	-2.933816	-0.730573	1.730891	H	-2.659754	-0.610332	-1.668285
C	-1.678842	0.688926	2.719204	C	-5.946158	-1.482041	-1.613302
H	-0.930564	1.45172	2.487298	H	-7.407108	-0.71818	-0.223279
H	-1.151315	-0.115602	3.246229	H	-4.271275	-2.055409	-2.845771
H	-0.406902	0.133259	0.167036	H	-6.65554	-2.116656	-2.1374
C	1.706531	-1.456343	0.963316	C	-2.392745	1.918746	-0.470888
O	1.474768	-0.575121	1.798978	N	-1.723404	3.110925	0.151485
N	2.954925	-1.738625	0.556918	H	-3.109449	2.365978	-1.165921
C	4.07304	-0.936651	1.07272	H	-1.622059	1.426534	-1.076466
C	3.372113	-2.679891	-0.500649	O	-1.876283	3.32624	1.34296
C	3.935234	0.550488	0.724601	O	-1.080929	3.82242	-0.594852
C	5.298643	-1.565982	0.386075	O	-1.165328	-2.730091	-2.120512

H	-0.876382	-1.791219	-2.245688
H	-1.159675	-3.126313	-3.004091

(16) ts6

N	0.097191	2.287454	0.190333
C	-1.207139	2.364291	-0.471499
C	-1.501133	3.877365	-0.530718
C	-0.673348	4.449655	0.623729
C	0.599758	3.610267	0.586821
H	-1.133624	1.918093	-1.467556
H	-2.566638	4.100064	-0.437646
H	-1.149059	4.273928	-1.48817
H	-0.469152	5.516611	0.511605
H	-1.189665	4.289953	1.576898
H	1.308807	3.978634	-0.166518
H	1.101651	3.55953	1.556174
C	0.810587	1.174248	0.161513
C	1.994727	1.049467	1.094838
C	2.956468	-0.148218	0.840217
H	2.593371	1.963443	0.997495
C	1.442618	0.996419	2.544076
H	1.139923	-0.033135	2.776787
H	0.532419	1.60006	2.616901
H	0.217475	0.2773	-0.020841
C	-2.246031	1.579204	0.332658
O	-1.997291	1.13013	1.457745
N	-3.446724	1.399143	-0.249484
C	-4.508224	0.690952	0.472328
C	-3.828331	1.748412	-1.630516
C	-4.180202	-0.784209	0.729139
C	-5.721521	0.849297	-0.458474
H	-4.666879	1.14361	1.454484
C	-5.09107	0.913346	-1.853192
H	-3.024755	1.49153	-2.325608
H	-4.043091	2.821172	-1.705227
O	-4.793214	-1.409581	1.593374
N	-3.230749	-1.318581	-0.059131
H	-6.437425	0.032855	-0.336647
H	-6.231348	1.790914	-0.227757
H	-4.816001	-0.091118	-2.193335
H	-5.751091	1.360764	-2.59985
C	-2.771975	-2.683281	0.067765
H	-2.718383	-0.745438	-0.734958
C	-2.197289	-3.197929	-1.268348
C	-1.74891	-2.877814	1.19349
H	-3.629252	-3.306013	0.343603
H	-2.885248	-2.891222	-2.06475
H	-2.22283	-4.290778	-1.225168

C	-0.76166	-2.797132	-1.617209
O	-1.38871	-4.010547	1.499974
N	-1.236747	-1.761961	1.765916
H	-0.429445	-3.383592	-2.481389
H	-0.077828	-3.084532	-0.804978
C	-0.457315	-1.337669	-1.940772
H	-0.693668	-1.895992	2.611956
H	-1.657831	-0.84459	1.62767
O	-1.319671	-0.438559	-1.81704
O	0.747052	-1.113194	-2.30292
C	2.463075	1.489413	3.567512
H	3.389112	0.904338	3.552488
H	2.724198	2.537475	3.378497
H	2.051785	1.423257	4.579493
H	3.443745	-0.319708	1.806133
C	4.082836	0.171827	-0.136016
C	5.007094	1.156924	0.239195
C	4.254825	-0.465601	-1.369963
C	6.063862	1.50781	-0.594187
H	4.898508	1.646281	1.20617
C	5.316608	-0.114417	-2.209863
H	3.561987	-1.234455	-1.706786
C	6.220495	0.872051	-1.828018
H	6.769277	2.271515	-0.278363
H	5.430288	-0.620741	-3.164254
H	7.045929	1.141382	-2.480708
C	2.199601	-1.42756	0.512758
N	3.086132	-2.638548	0.63509
H	1.787752	-1.476977	-0.496703
H	1.394922	-1.616164	1.232106
O	3.94212	-2.649136	1.501669
O	2.868403	-3.561213	-0.128312
O	1.529942	1.134427	-1.571822
H	1.194755	0.223835	-1.997569
H	2.504086	1.134028	-1.607656

(17) I10

N	-1.343209	1.232493	-0.367053
C	-0.28231	1.912369	0.363496
C	-0.835697	3.344863	0.450334
C	-1.468301	3.553052	-0.935059
C	-1.890623	2.139809	-1.386195
H	-0.154591	1.460204	1.35161
H	-0.067124	4.086921	0.686433
H	-1.596054	3.376046	1.237874
H	-2.310739	4.249212	-0.901493
H	-0.726942	3.960085	-1.629014
H	-2.979797	2.028376	-1.437952

H	-1.479232	1.90749	-2.380125	C	-4.505663	1.210746	0.564467
C	-1.087656	-0.120018	-0.842528	C	-6.827171	0.129575	-0.528867
C	-2.384853	-0.926416	-1.005946	H	-5.709515	-1.702233	-0.689013
C	-3.281103	-1.024037	0.274865	C	-5.646733	2.000683	0.422876
H	-2.97638	-0.397066	-1.767323	H	-3.595846	1.64971	0.967837
C	-2.040111	-2.305824	-1.590754	C	-6.811256	1.464518	-0.125799
H	-1.524636	-2.905613	-0.832018	H	-7.729535	-0.301728	-0.953961
H	-1.325826	-2.155562	-2.412572	H	-5.622738	3.040301	0.739556
H	-0.602118	-0.080366	-1.832826	H	-7.699253	2.080852	-0.236722
C	1.065615	1.924649	-0.35581	C	-2.602406	-0.752925	1.617484
O	1.153493	1.689471	-1.569754	N	-1.643499	-1.820737	2.047664
N	2.162249	2.247718	0.365465	H	-3.343338	-0.744133	2.425322
C	3.431436	2.498121	-0.322837	H	-2.027372	0.169731	1.649182
C	2.241993	2.483444	1.817117	O	-1.748918	-2.943263	1.606967
C	4.030505	1.24627	-0.965559	O	-0.812819	-1.496574	2.892205
C	4.329546	3.073172	0.788085	O	-0.21857	-0.759683	0.073519
H	3.281425	3.205608	-1.143384	H	0.674565	-2.484152	2.536629
C	3.749606	2.471361	2.07245	H	0.542747	-1.112162	-0.421688
H	1.717462	1.697306	2.364804				
H	1.80033	3.455261	2.072149				
O	4.832709	1.349308	-1.890546	(18) I11			
N	3.6388	0.070585	-0.431936	N	0.639144	-0.61832	1.48405
H	5.38308	2.830937	0.627404	C	0.411213	0.651471	0.722188
H	4.227477	4.163232	0.800838	C	1.098127	1.729233	1.577944
H	4.093276	1.438443	2.201603	C	0.812487	1.272985	3.013483
H	4.019489	3.036864	2.967375	C	0.854736	-0.255947	2.939776
C	4.073004	-1.211299	-0.939597	H	0.806482	0.535465	-0.288031
H	3.012216	0.067644	0.369642	H	0.705415	2.726174	1.358106
C	4.46759	-2.194904	0.182294	H	2.17171	1.740057	1.378147
C	3.047332	-1.850023	-1.882859	H	1.55502	1.6549	3.717687
H	4.959742	-1.020742	-1.553787	H	-0.174825	1.606634	3.339026
H	5.009822	-1.625321	0.944685	H	1.825145	-0.656389	3.241179
H	5.171888	-2.913287	-0.245501	H	0.074686	-0.742995	3.524846
C	3.343444	-3.0086	0.821057	C	1.71957	-1.597357	0.95901
O	3.256776	-2.957077	-2.360952	C	3.158286	-1.044051	0.862676
N	1.891105	-1.157768	-2.100818	C	3.65573	-0.443883	-0.512064
H	3.773254	-3.741012	1.515447	H	3.25521	-0.233573	1.596992
H	2.807528	-3.601573	0.069996	C	4.076178	-2.183329	1.377549
C	2.316849	-2.233723	1.606055	H	3.96115	-3.063938	0.736877
H	1.319559	-1.512066	-2.862798	H	3.704839	-2.46652	2.370361
H	1.870548	-0.143573	-1.972006	H	1.692871	-2.348582	1.760551
O	2.323206	-1.028866	1.794165	C	-1.090042	0.941031	0.737743
O	1.371707	-3.027767	2.098595	O	-1.788085	0.477756	1.647477
C	-3.24614	-3.069088	-2.133994	N	-1.555693	1.808036	-0.173637
H	-3.961268	-3.329859	-1.345497	C	-2.871685	2.443126	-0.022379
H	-3.77922	-2.478318	-2.889006	C	-0.835153	2.265478	-1.373547
H	-2.929832	-4.006432	-2.603742	C	-4.064026	1.502208	-0.219213
H	-3.654923	-2.051673	0.327929	C	-2.829039	3.565391	-1.070793
C	-4.510843	-0.131344	0.165476	H	-2.975574	2.830265	0.996101
C	-5.687212	-0.659064	-0.379036				

C	-1.9272	2.987457	-2.16516	H	-0.229529	-1.18659	1.404719
H	-0.420612	1.408798	-1.913044				
H	-0.020523	2.946457	-1.093109				
O	-5.191659	1.885562	0.089271	(19) ts7			
N	-3.796918	0.280395	-0.707132				
H	-3.829711	3.830402	-1.419064	N	0.8009	-0.088025	1.887569
H	-2.369048	4.455806	-0.628793	C	0.448241	0.99098	0.953267
H	-2.483515	2.262043	-2.769144	C	1.22127	2.213358	1.482524
H	-1.517238	3.749255	-2.831893	C	1.11713	2.031539	2.999132
C	-4.792852	-0.773049	-0.725591	C	1.25717	0.516209	3.168829
H	-2.833183	-0.001932	-0.906861	H	0.736165	0.723391	-0.065446
C	-4.220453	-2.029732	-1.409506	H	0.809661	3.161931	1.127747
C	-5.289552	-1.147102	0.676901	H	2.26372	2.148386	1.150655
H	-5.676092	-0.434041	-1.276134	H	1.886803	2.582736	3.545075
H	-3.787224	-1.724288	-2.368752	H	0.137228	2.366193	3.355091
H	-5.066878	-2.686889	-1.631914	H	2.307725	0.237043	3.328183
C	-3.199542	-2.83125	-0.596437	H	0.673177	0.121348	4.003378
O	-6.357755	-1.743125	0.804588	C	2.064302	-1.673514	1.391883
N	-4.468735	-0.866439	1.705716	C	3.325464	-1.03289	0.832254
H	-2.968136	-3.753709	-1.145658	C	3.343368	-0.674466	-0.694883
H	-3.621098	-3.156233	0.360757	H	3.511557	-0.117669	1.408442
C	-1.845983	-2.177765	-0.319238	C	4.442891	-2.044145	1.203477
H	-4.759306	-1.132306	2.638912	H	4.324724	-2.936063	0.579295
H	-3.58801	-0.368087	1.594718	H	4.289104	-2.3614	2.242881
O	-1.475168	-1.180348	-0.985972	H	2.105524	-1.804244	2.486867
O	-1.126766	-2.730124	0.576104	C	-1.055984	1.263171	1.00366
C	5.552915	-1.827156	1.51889	O	-1.757722	0.814367	1.918409
H	6.05162	-1.666696	0.557814	N	-1.568935	2.055019	0.040509
H	5.687552	-0.92691	2.131091	C	-2.93453	2.572877	0.148849
H	6.081503	-2.645959	2.017771	C	-0.881929	2.510696	-1.180647
H	4.697621	-0.765357	-0.589998	C	-4.014363	1.515873	-0.085896
C	3.721832	1.082462	-0.486486	C	-2.968651	3.677143	-0.918543
C	4.640155	1.691899	0.379913	H	-3.107952	2.958636	1.157441
C	2.914089	1.907104	-1.27625	C	-2.011415	3.151678	-1.992798
C	4.726905	3.077413	0.481499	H	-0.423368	1.662561	-1.698004
H	5.294392	1.066957	0.985037	H	-0.099442	3.237505	-0.932399
C	2.998318	3.298337	-1.179118	O	-5.187768	1.767736	0.177287
H	2.203142	1.479556	-1.978307	N	-3.602475	0.336282	-0.591738
C	3.896757	3.889268	-0.294824	H	-3.982349	3.858141	-1.282425
H	5.446779	3.523889	1.162038	H	-2.584131	4.606216	-0.485275
H	2.359923	3.918489	-1.803142	H	-2.510151	2.390693	-2.602856
H	3.961609	4.971022	-0.219214	H	-1.641734	3.935615	-2.657498
C	3.012909	-0.886762	-1.826104	C	-4.506024	-0.787772	-0.723234
N	3.184038	-2.345404	-2.13	H	-2.609013	0.150839	-0.711197
H	3.530924	-0.399187	-2.659741	C	-3.899403	-1.872534	-1.63551
H	1.944447	-0.710336	-1.913091	C	-4.885029	-1.410947	0.625815
O	2.406898	-2.834477	-2.926532	H	-5.440442	-0.429318	-1.164431
O	4.119774	-2.941768	-1.626099	H	-3.405413	-1.373526	-2.476723
O	1.30976	-2.12761	-0.23272	H	-4.727629	-2.454046	-2.049099
H	0.411525	-2.535318	-0.083918	C	-2.950903	-2.865813	-0.965469

O	-5.838233	-2.183347	0.691613	C	2.170311	-1.561888	0.339719
N	-4.069326	-1.143369	1.664574	C	3.366706	-0.750689	0.77969
H	-2.651132	-3.624958	-1.699745	C	4.200098	-0.123484	-0.374093
H	-3.456694	-3.417325	-0.165024	H	2.91833	0.095791	1.321375
C	-1.659116	-2.320682	-0.403354	C	4.176512	-1.532983	1.831851
H	-4.30637	-1.536191	2.568401	H	4.659349	-2.413646	1.391722
H	-3.345073	-0.428344	1.631573	H	3.455426	-1.918023	2.564426
O	-1.20606	-1.201567	-0.624812	H	1.830549	-2.34018	1.040668
O	-1.039832	-3.211987	0.343583	C	-1.556755	1.030761	1.040474
C	5.863223	-1.500348	1.077807	O	-2.229366	0.542137	1.959242
H	6.105311	-1.195658	0.053542	N	-2.128574	1.804604	0.094392
H	6.018259	-0.638492	1.737578	C	-3.534019	2.205624	0.21181
H	6.58512	-2.272064	1.364516	C	-1.487043	2.320214	-1.127025
H	4.261388	-1.115481	-1.101842	C	-4.518373	1.038884	0.090508
C	3.479911	0.835081	-0.918431	C	-3.702472	3.218103	-0.934783
C	4.559569	1.508291	-0.32626	H	-3.718811	2.650438	1.193616
C	2.592838	1.589737	-1.692929	C	-2.685062	2.745106	-1.978149
C	4.736031	2.879842	-0.484355	H	-0.884889	1.539386	-1.598841
H	5.276199	0.950723	0.270345	H	-0.841895	3.17572	-0.89049
C	2.763	2.967618	-1.853087	O	-5.668653	1.149109	0.508365
H	1.744882	1.120612	-2.182463	N	-4.04408	-0.069395	-0.509641
C	3.831089	3.621272	-1.246202	H	-4.730432	3.247746	-1.303898
H	5.584068	3.369632	-0.01367	H	-3.437999	4.217373	-0.572949
H	2.054361	3.5254	-2.460039	H	-3.07589	1.879758	-2.525785
H	3.964207	4.692129	-1.370578	H	-2.422238	3.520756	-2.70141
C	2.212934	-1.227085	-1.565576	C	-4.818767	-1.283774	-0.644427
N	2.230818	-2.71755	-1.736848	H	-3.075894	-0.094503	-0.823345
H	2.33566	-0.873872	-2.595001	C	-4.187456	-2.223072	-1.687318
H	1.201679	-1.003998	-1.224637	C	-4.999771	-2.043242	0.676855
O	1.192272	-3.233557	-2.105191	H	-5.829041	-1.021721	-0.976591
O	3.277816	-3.318622	-1.577679	H	-3.996905	-1.646989	-2.600042
O	1.406346	-2.478965	0.708405	H	-4.941411	-2.976097	-1.931314
H	-0.112272	-2.899224	0.575288	C	-2.922274	-2.972511	-1.26049
H	-0.031274	-0.657815	2.048741	O	-5.787547	-2.986135	0.725851
				N	-4.215992	-1.675347	1.706919
				H	-2.732963	-3.790821	-1.965301
				H	-3.049624	-3.45626	-0.283374
				C	-1.643713	-2.171153	-1.203981
				H	-4.354559	-2.138029	2.597897
				H	-3.633051	-0.840707	1.687826
				O	-1.545542	-0.969042	-1.410685
				O	-0.592062	-2.921566	-0.915983
				C	5.212848	-0.680235	2.559153
				H	6.050954	-0.403142	1.911317
				H	4.762311	0.242489	2.946191
				H	5.630909	-1.230984	3.40749
				H	5.193557	0.071538	0.04324
				C	3.653892	1.227095	-0.811577
				C	4.214684	2.380781	-0.250594
				C	2.587631	1.366885	-1.70742
(20) PC							
N	0.396228	-0.225085	1.896921				
C	-0.044205	0.810417	0.961462				
C	0.698803	2.079484	1.426859				
C	0.690862	1.92237	2.950285				
C	0.897037	0.414424	3.136537				
H	0.22254	0.534915	-0.067217				
H	0.227445	3.004236	1.082416				
H	1.722432	2.057826	1.034774				
H	1.464795	2.517995	3.442571				
H	-0.282126	2.225974	3.352733				
H	1.965466	0.184244	3.262119				
H	0.37205	0.02351	4.013459				

C	3.719655	3.645801	-0.563264	H	5.158555	-0.59537	-2.266099
H	5.046693	2.284617	0.445048	H	3.507476	-1.296711	-2.11456
C	2.098237	2.633527	-2.029405	O	6.195449	-2.334197	-0.821956
H	2.121903	0.488235	-2.144369	O	4.265495	-3.281826	-0.988339
C	2.656757	3.775803	-1.456408	O	1.611663	-1.425798	-0.739416
H	4.168356	4.52756	-0.11389	H	0.228209	-2.347906	-0.896798
H	1.276477	2.725769	-2.735003	H	-0.390117	-0.833789	2.114832
H	2.270646	4.759686	-1.708964				
C	4.42356	-1.03474	-1.590782				
N	5.012681	-2.325805	-1.114738				