

Multiscale time-resolved fluorescence study of a glycogen phosphorylase inhibitor combined with quantum chemistry calculations.

Valentin Maffei,^{a,‡} Konstantinos Mavreas,^{b,‡} Filippo Monti,^c Michael Mamais,^{a,b,d} Thomas Gustavsson,^a Evangelia D. Chrysina,^d Dimitra Markovitsi,^{*,a} Thanasis Gimisis^{*,b} and Alessandro Venturini^{*,c}

^a LIDYL, CEA, CNRS. Université Paris-Saclay, Gif-sur-Yvette (France). e-mail: dimitra.markovitsi@cea.fr.

^b Department of Chemistry, National and Kapodistrian University of Athens, Athens (Greece). e-mail: gimisis@chem.uoa.gr.

^c Istituto ISOF, Consiglio Nazionale delle Ricerche. Bologna (Italy). e-mail: alessandro.venturini@isof.cnr.it.

^d Institute of Biology, Medicinal Chemistry & Biotechnology, National Hellenic Research Foundation, Athens (Greece). e-mail: echrysina@eie.gr.

‡ These authors contributed equally.

ELECTRONIC SUPPLEMENTARY INFORMATION

Contents

Section 1. Synthesis:

Fig. S0. ¹H NMR spectrum of 2-((4-acetamidophenyl)amino)benzoic acid in dms0-d6.....2

Section 2. Spectroscopy:

Fig. S1. GLAC uncorrected normalised fluorescence spectra, in neutral aq. solution and acetonitrile....3

Fig. S2. Normalised fluorescence decays obtained by TCSPC at 465 nm for GLAC.....3

Section 3. Theoretical Calculations:

Table S1. Ground state minima and Transition States.....4

Table S2. Bond Distances for the conformers in the Ground and Excited States.....4

Table S3. Excited State minima and Transition States.....5

Table S4. Computed M062X/6-311+gd** D_{CT} values in Å.6

Table S5. Comparison of M062X and CAM-B3LYP functionals.....6

Figure S3. Graphical representation of D_{CT} 7

Figure S4. HOMO and LUMO orbitals calculated using CAM-B3LYP Density Functional.....7

Table S6. Optimised X,Y,Z coordinates, (DFT PCM M062X 6-311g(d,p)).....8

and PCM CAM-b3lyp 6-311g(d,p)).....27

Section 1. Synthesis

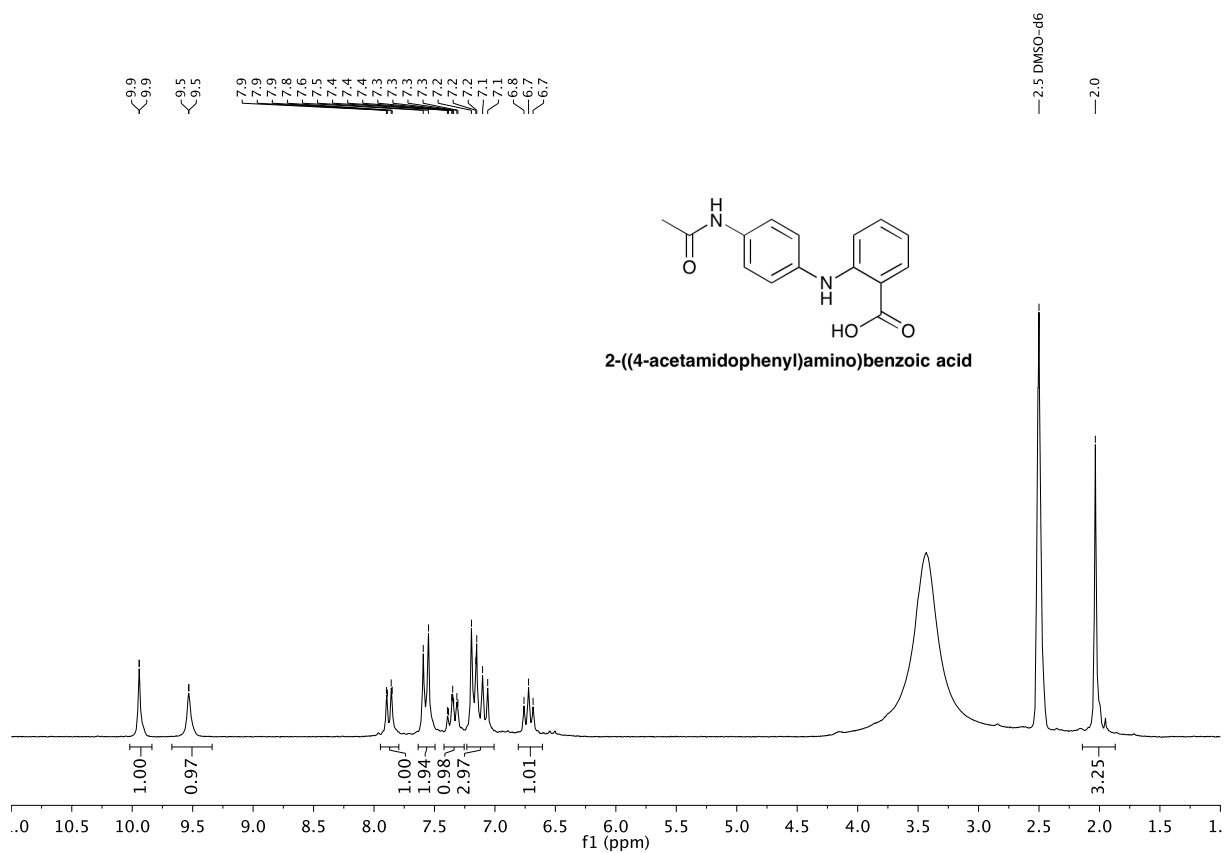


Fig. S0. ^1H NMR spectrum of 2-((4-acetamidophenyl)amino)benzoic acid in dms0-d6 .

Section 2. Spectroscopy

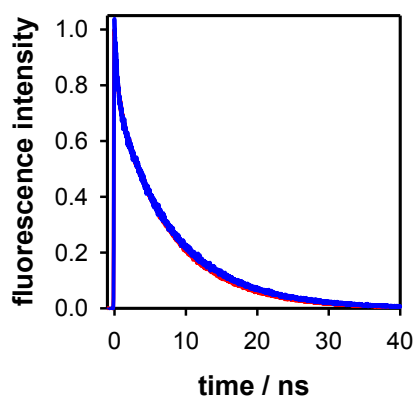


Fig. S1. Normalised fluorescence decays obtained by TCSPC at 465 nm for GLAC in water (blue) and phosphate buffer (pH 7; red). In both solutions a few drops of DMSO were added to facilitate dissolution.

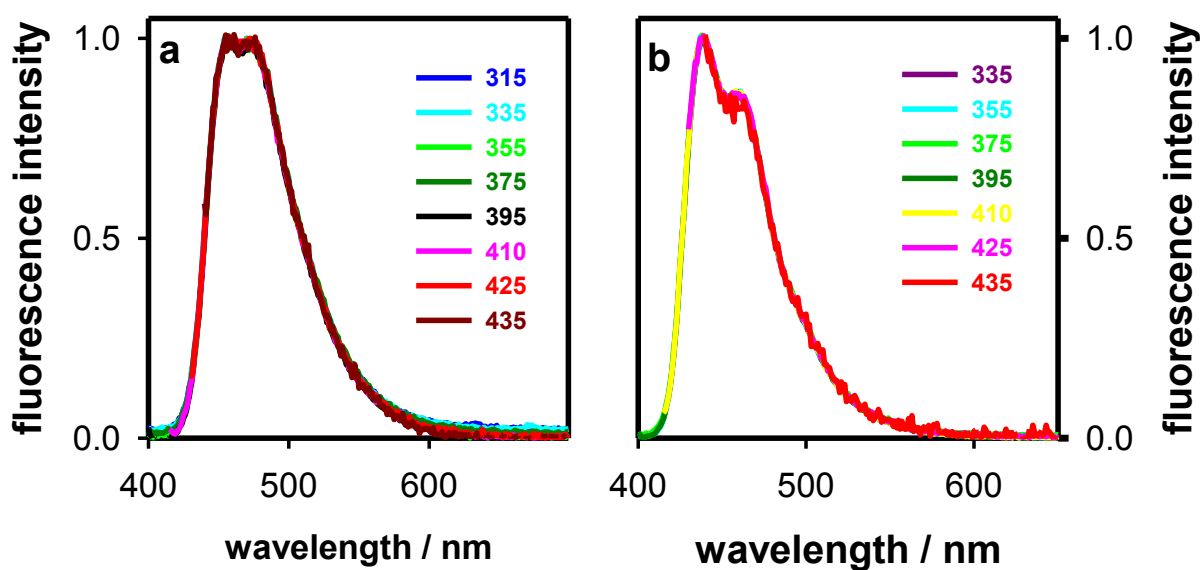


Fig. S2. Uncorrected normalized fluorescence spectra recorded for GLAC in (a) neutral aqueous solution (pH 7) and (b) acetonitrile. Different colours correspond to different excitation wavelengths.

Section 3. Theoretical Calculations

Table S1. Ground state minima and Transition States: Energies and free energies E (a.u), ΔG (a.u.) and differences, ΔE (kcal·mol⁻¹) and $\Delta\Delta G$ (kcal·mol⁻¹). Population calculated with kBT at 300 °K (pop%). Dihedral angles in degrees, α_1 and α_2 . Lower transitions in kcal·mol⁻¹, oscillator strength (f).

Isomer	Energy	ΔG	ΔE	$\Delta\Delta G$	Pop %	α_1	α_2	¹ kcal·mol ⁻¹	¹ f	² kcal·mol ⁻¹
GS-A'	-1634.66805	-1634.29824	0.4	1.0	6.0	173.9	-32.1	75.4	0.1625	76.9
GS-A''	-1634.66813	-1634.29882	0.3	0.7	9.9	-173.2	32.1	75.3	0.1648	76.9
GS-B	-1634.66823	-1634.29750	0.3	1.5	2.5	-179.1	-176.7	74.0	0.0849	75.3
GS-C'	-1634.66858	-1634.29986	0.1	0.0	31.5	4.2	56.2	75.7	0.1325	77.3
GS-C''	-1634.66864	-1634.29949	0.0	0.2	22.3	-3.8	-57.4	75.7	0.131	77.3
GS-D'	-1634.66858	-1634.29922	0.1	0.4	16.3	4.5	-128.0	75.5	0.0986	77.2
GS-D''	-1634.66867	-1634.29898	0.0	0.6	11.5	-4.3	127.5	75.5	0.0995	77.3
TS GS-A'A''	-1634.66757	-1634.29535	0.7	2.8		-179.1	1.9			
TS GS-A'B	-1634.66593	-1634.29490	1.7	3.1		177.6	100.8			
TS GS-A''B	-1634.66592	-1634.29416	1.7	3.6		-177.0	-100.8			
TS GS-A'C'	-1634.64799	-1634.27793	13.0	13.8		113.9	-23.5			
TS GS-A''C''	-1634.64800	-1634.27752	13.0	14.0		-112.7	22.5			
TS GS-BD'	-1634.64744	-1634.27768	13.3	13.9		116.6	166.7			
TS GS-BD''	-1634.64744	-1634.27778	13.3	13.9		-117.7	-167.6			
TS GS-C'D''	-1634.66742	-1634.29626	0.8	2.3		2.4	84.9			
TS GS-C''D'	-1634.66744	-1634.29623	0.8	2.3		1.4	-87.3			

¹ Single point PCM/M062X/6-311+g(d,p)//PCM/M062X/6-311g(d,p). ² PCM/M062X/6-311g(d,p)

Table S2. Bond Distances in Angstrom for the conformers in the Ground State (GS) and in the Excited State (ES).

Isomer	C ₄ -N ₄	C ₂ -N ₄
GS-A'	1.349	1.421
GS-A''	1.349	1.421
GS-B	1.349	1.415
GS-C'	1.346	1.425
GS-C''	1.346	1.425
GS-D'	1.347	1.422
GS-D''	1.347	1.423
ES-A	1.358	1.397
ES-B	1.359	1.395
ES-C'	1.355	1.405
ES-C''	1.355	1.405
ES-D'	1.359	1.397
ES-D''	1.359	1.396
ES-E'	1.411	1.351
ES-E''	1.415	1.348
ES-F'	1.412	1.351
ES-F''	1.415	1.348

Table S3. Excited State minima and Transition States: Energies and free energies E (a.u.), ΔG (a.u.), ΔE (kcal·mol⁻¹) and $\Delta\Delta G$ (kcal·mol⁻¹). Dihedral angles, α_1 and α_2 , in degrees. Lower transitions in kcal·mol⁻¹, oscillator strength (*f*).

Isomer	Energy (a.u.)	ΔG (a.u.)	ΔE	$\Delta\Delta G$	α_1	α_2	kcal·mol ⁻¹	<i>f</i>
ES-A	-1634.55827	-1634.19232	0.3	0.1	-179.7	0.1	67.4	0.153
ES-B	-1634.55772	-1634.19150	0.7	0.7	-178.4	-177.4	69.3	0.088
ES-C'	-1634.55653	-1634.19037	1.4	1.4	10.2	33.7	69.0	0.114
ES-C''	-1634.55663	-1634.19105	1.3	0.9	-10.2	-34.2	69.1	0.118
ES-D'	-1634.55701	-1634.19121	1.1	0.8	9.6	-151.6	68.9	0.087
ES-D''	-1634.55717	-1634.19137	1.0	0.7	-9.5	151.9	68.8	0.096
ES-E'	-1634.55526	-1634.18952	2.2	1.9	-86.7	-5.7	5.6	0.000
ES-E''	-1634.55854	-1634.19222	0.1	0.2	-92.1	174.4	9.1	0.001
ES-F'	-1634.55547	-1634.18906	2.1	2.2	93.7	5.4	9.2	0.001
ES-F''	-1634.55876	-1634.19254	0.0	0.0	97.5	-175.8	8.7	0.001
TS ES-AB	-1634.55084	-1634.18414	5.0	5.3	178.5	-87.7		
TS ES-AB*	-1634.55086	-1634.18424	5.0	5.2	-178.0	88.2		
TS ES-AE'	-1634.55084	-1634.18389	5.0	5.4	-137.0	8.5		
TS ES-AF'	-1634.55078	-1634.18378	5.0	5.5	141.2	-8.8		
TS ES-BE''	-1634.55481	-1634.18763	2.5	3.1	-145.8	-166.1		
TS ES-BF''	-1634.55483	-1634.18770	2.5	3.0	146.5	167.1		
TS ES-C'D''	-1634.55345	-1634.18662	3.3	3.7	1.8	91.0		

TS ES-C'D'	-1634.55343	-1634.18665	3.3	3.7	-1.8	-90.5
TS ES-C'E'	-1634.55197	-1634.18486	4.3	4.8	-46.3	-12.3
TS ES-C'F'	-1634.55119	-1634.18402	4.8	5.3	48.2	13.5
TS ES-D'E''	-1634.55507	-1634.18696	2.3	3.5	-41.6	172.1
TS ES-D'F''	-1634.55432	-1634.18605	2.8	4.1	45.5	-172.2

Table S4. Computed M062X/6-311+gd** D_{CT} values in Å.

Excited State	D_{CT}
ES-A	0.803
ES-B	0.835
ES-C'	0.731
ES-C''	0.743
ES-D'	0.993
ES-D''	1.028
ES-E'	5.053
ES-E''	4.461
ES-F'	4.454
ES-F''	4.418

Table S5. Comparison of three points of the excited surface calculated with both M062X and CAM-B3LYP functionals. Energy (a.u.), ΔG (a.u.), ΔE (kcal/mol.), $\Delta\Delta G$ (kcal/mol.), dihedral angles α_1 and α_2 (degrees), emission energy (kcal/mol.) and oscillator strength (f) computed using the linear response formalism.

Excited State surface	CAM-b3lyp/6-311g**						Emission 6-311+g**	
Conformer	Energy (a.u.)	ΔG (a.u.)	ΔE	$\Delta\Delta G$	α_1	α_2	kcal/mol.	f
ES-A	-1634.42255	-1634.05620	0.0	0.0	-179.7	0.2	66.2	0.1903
ES-F'	-1634.41716	-1634.05122	3.4	3.1	90.5	5.7	44.6	0.0003
TS ES-AF'	1634.41283	-1634.046026	6.1	6.4	134.4	-6.8		

Excited State surface	M062x/6-311g**						Emission 6-311+g**	
Conformer	Energy (a.u.)	ΔG (a.u.)	ΔE	$\Delta\Delta G$	α_1	α_2	kcal/mol.	f
ES-A	-1634.55827	-1634.19232	0.0	0.0	0.3	-179.9	65.8	0.1991
ES-F'	-1634.55547	-1634.18906	1.8	2.0	-78.9	178.3	41.1	0.0009
TS ES-AF'	1634.55078	-1634.18378	4.7	5.4	141.2	-8.8		

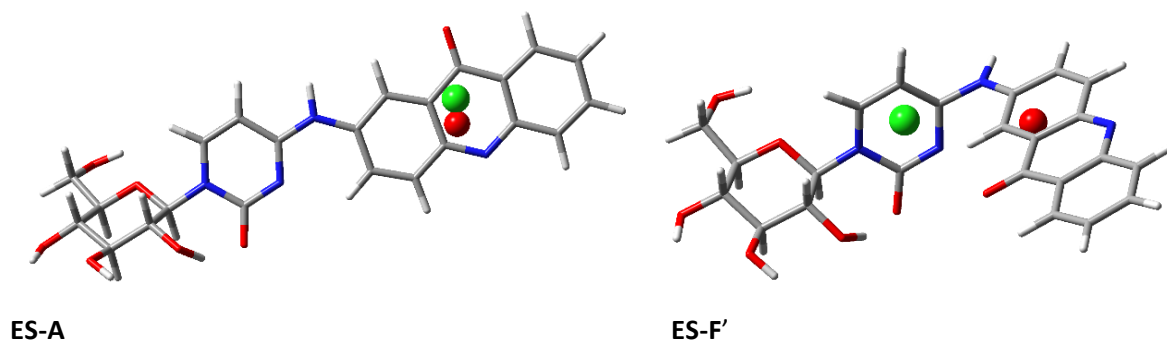
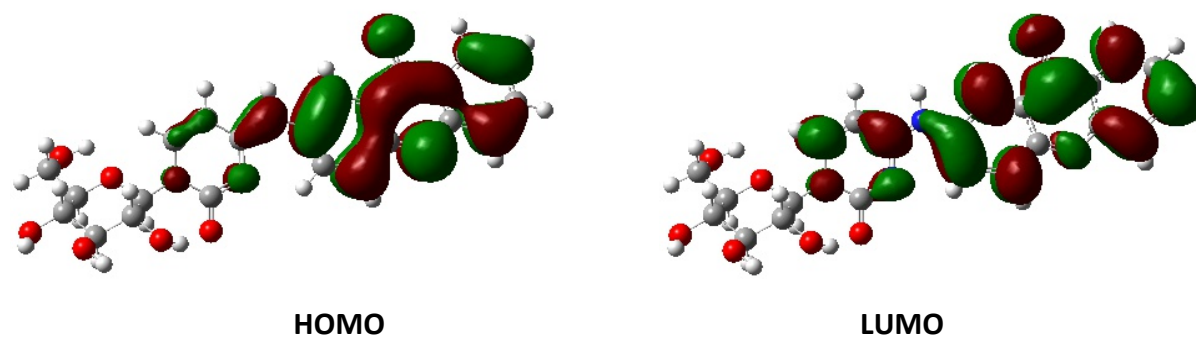


Fig. S3. Graphical representation of D_{CT} with the barycentre of charge R_+ and R_- . Green circle is R_+ and red circle is R_- , where R_- accounts for the density depletion zone.

a)



b)

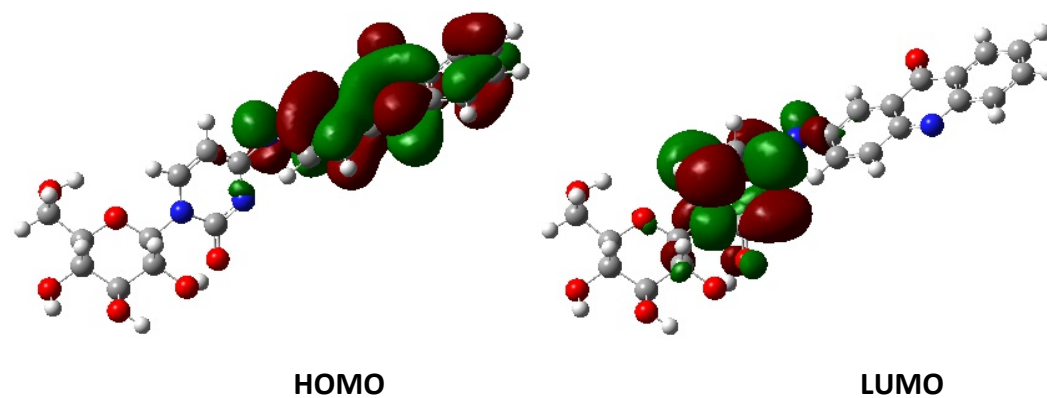


Fig. S4. HOMO and LUMO orbitals calculated using CAM-B3LYP Density Functional: **a)** In the planar excited state conformer **ES-A**. **b)** In the twisted non-emissive conformer **ES-F**. Compare with Fig. 11 in the manuscript.

Table S6. Optimized Molecular Structures
(X,Y,Z coordinates, DFT M062X 6-311g(d,p)).

Ground State

M062x 6-311g(d,p) solvent=water

GS-A'

E=-1634.66805

O	-0.02669900	0.20590100	0.04287800
C	1.35747600	0.43036400	0.12111100
C	1.66266000	1.87894300	-0.27062200
C	0.90117500	2.79369700	0.67956500
C	-0.58161900	2.47558600	0.65415900
C	-0.77794800	0.99792600	0.96831300
N	2.00814900	-0.52961200	-0.77051200
C	3.33233900	-0.90328300	-0.47553200
N	3.91682700	-1.85430800	-1.23472500
C	3.27901200	-2.35633800	-2.28017100
C	1.96027000	-1.93536600	-2.65870000
C	1.36216800	-1.02548600	-1.86228200
N	3.87724600	-3.30220900	-3.03345500
O	3.89902400	-0.34344800	0.46705000
O	3.03767700	2.19349000	-0.24052300
O	1.05177200	4.15066000	0.31815300
O	-1.28319900	3.22187000	1.62552100
C	-2.21559600	0.54421100	0.83193600
O	-2.34955000	-0.82335300	1.15908800
H	3.50794700	1.48678300	0.23203400
H	1.99692700	4.33967100	0.31640300
H	-1.73037800	-1.30285700	0.59854400
H	-1.01778800	4.14181300	1.51480900
H	1.45887100	-2.33819800	-3.52585200
H	0.35941600	-0.65707000	-2.02703000
H	-2.55383900	0.74629900	-0.19227200
H	-2.83496600	1.11452200	1.52354300
H	1.72963500	0.22438100	1.13080000
H	1.29506700	2.03912700	-1.29184500
H	1.27553100	2.62893400	1.70100400
H	-0.96743600	2.68341400	-0.35416700
H	-0.42395700	0.79026500	1.98712200
H	3.30920500	-3.71616000	-3.75884100
C	5.15635400	-3.89116000	-2.84010300
C	5.31044800	-5.23633800	-3.06848600
C	6.29133700	-3.10911700	-2.49945700
C	6.57128000	-5.85731000	-2.96227100
H	4.46160800	-5.85491500	-3.34132300
C	7.51924600	-3.69771300	-2.37842100
H	6.17107500	-2.04822100	-2.33070800
C	7.71895900	-5.09607800	-2.60055100

C	6.69199300	-7.28596100	-3.21666600
H	8.38977100	-3.10685000	-2.11706700
N	8.96269700	-5.59679300	-2.46351300
C	8.04521100	-7.79975900	-3.06108800
O	5.72424200	-7.99874900	-3.53629500
C	9.10514200	-6.92024100	-2.69188600
C	8.30550000	-9.17116900	-3.27717900
C	10.40777000	-7.49199900	-2.55733200
C	9.56900600	-9.68928800	-3.13978100
H	7.46764000	-9.80042600	-3.55629000
C	10.63077200	-8.82607400	-2.77322100
H	11.21506900	-6.82464900	-2.27673200
H	9.75837600	-10.74250900	-3.30782300
H	11.63231200	-9.22749900	-2.66233400

GS-A''

E=-1634.66813

O	0.02195000	0.14579700	0.03499100
C	1.40629600	0.37513400	0.09707900
C	1.69688800	1.84300000	-0.22814200
C	0.94609100	2.70645500	0.77691300
C	-0.53492900	2.38026900	0.76158200
C	-0.71686800	0.88838400	1.00996000
N	2.04260500	-0.53624200	-0.85380900
C	3.37228100	-0.92223300	-0.60292200
N	3.93977700	-1.83953500	-1.41381900
C	3.27862300	-2.29876400	-2.46473400
C	1.95716500	-1.85292600	-2.80402000
C	1.37759300	-0.97635600	-1.95808900
N	3.85636500	-3.22077600	-3.26184000
O	3.96027100	-0.40005200	0.34844500
O	3.07044400	2.16420000	-0.20169100
O	1.08241300	4.08002200	0.47762900
O	-1.22418900	3.07616900	1.77810500
C	-2.15402900	0.43179300	0.87797900
O	-2.27369200	-0.95067100	1.14206100
H	3.55416200	1.42903200	0.21053600
H	2.02611000	4.27597300	0.47086200
H	-1.66152600	-1.39862400	0.54868700
H	-0.96738400	4.00225600	1.70456400
H	1.43836900	-2.21589200	-3.67868900
H	0.37473200	-0.59525400	-2.09019300
H	-2.51221700	0.67986600	-0.12921200
H	-2.76406000	0.96436600	1.60697500
H	1.80024300	0.12165600	1.08747500
H	1.31221100	2.05014600	-1.23469800
H	1.33880600	2.49640400	1.78303700
H	-0.93908700	2.63186900	-0.22944100
H	-0.34334900	0.63541200	2.01149300
H	3.35296200	-3.45712000	-4.10498000
C	5.14879600	-3.79717000	-3.13216800
C	5.89237000	-4.02492800	-4.26380300
C	5.65203700	-4.21871300	-1.87329300

C 7.14780500 -4.66199700 -4.19922300
 H 5.52694200 -3.72287500 -5.23976800
 C 6.87425000 -4.82571900 -1.79069600
 H 5.06074600 -4.05022200 -0.98418800
 C 7.68015700 -5.07569800 -2.94501200
 C 7.90196100 -4.88779900 -5.42419600
 H 7.26502300 -5.14950200 -0.83273900
 N 8.87084700 -5.68458900 -2.77738000
 C 9.18236300 -5.54788000 -5.21390200
 O 7.48676100 -4.54597000 -6.54559600
 C 9.59261700 -5.90860100 -3.89671400
 C 10.01595400 -5.83164400 -6.31824600
 C 10.86021400 -6.55480300 -3.76474300
 C 11.22838300 -6.45447300 -6.15748100
 H 9.66000000 -5.53914200 -7.29980200
 C 11.64783300 -6.81764200 -4.85408000
 H 11.17433900 -6.83027200 -2.76419200
 H 11.86040300 -6.66802300 -7.01089500
 H 12.60458900 -7.31024400 -4.71804300

GS-B

E=-1634.66823

O -0.11833700 0.17350600 -0.03900500
 C 1.25866600 0.39345500 0.12880500
 C 1.55402000 1.89203700 0.02092600
 C 0.74646700 2.61003900 1.09399700
 C -0.72925400 2.28763000 0.95623300
 C -0.91255800 0.77555200 0.98826100
 N 1.95469600 -0.37979900 -0.89908000
 C 3.26967500 -0.79409700 -0.62715400
 N 3.89323800 -1.58924800 -1.52463700
 C 3.30130100 -1.89733200 -2.66720100
 C 1.99395100 -1.41293800 -3.01491000
 C 1.35701800 -0.66593400 -2.09050400
 N 3.92439200 -2.69280100 -3.56108300
 O 3.79824800 -0.41341400 0.42033600
 O 2.92244200 2.20710600 0.15707300
 O 0.88749900 4.01153900 0.99194200
 O -1.47618200 2.83730100 2.02038500
 C -2.33766200 0.34130600 0.72054600
 O -2.46180700 -1.06406000 0.78884700
 H 3.38647500 1.43156000 0.51305100
 H 1.82886900 4.20682000 1.06063400
 H -1.81653900 -1.42847600 0.17374100
 H -1.22265700 3.76471900 2.08839400
 H 1.52783200 -1.65065000 -3.95960200
 H 0.35850300 -0.27469000 -2.22526000
 H -2.64472200 0.72365200 -0.26120000
 H -2.98825200 0.77060100 1.48195500
 H 1.60026600 0.00858500 1.09598800
 H 1.21909200 2.23413300 -0.96614300
 H 1.08804800 2.26497800 2.08138100
 H -1.08315200 2.67229700 -0.01101900
 H -0.58966500 0.38805400 1.96402900
 H 3.40528500 -2.86380500 -4.41076300
 C 5.18788900 -3.32735400 -3.51725500

C 6.06192900 -3.31086400 -2.45373100
 C 5.54972400 -4.04568400 -4.69186300
 C 7.29602300 -3.99467600 -2.52792000
 H 5.82842400 -2.77792500 -1.54669800
 C 6.73805200 -4.71068300 -4.77559700
 H 4.86382900 -4.06161700 -5.53362000
 C 7.67164600 -4.71805900 -3.69347900
 C 8.19326000 -3.95460400 -1.38025800
 H 7.00558800 -5.25559100 -5.67348700
 N 8.82519500 -5.39883700 -3.84779000
 C 9.43017900 -4.69911000 -1.57019200
 O 7.92581500 -3.33967500 -0.33258400
 C 9.67496400 -5.37978100 -2.79907000
 C 10.38762400 -4.74614800 -0.53259900
 C 10.91063900 -6.08805700 -2.91626800
 C 11.56509700 -5.43646400 -0.67632100
 H 10.15632300 -4.21427900 0.38348300
 C 11.82089300 -6.11543300 -1.89325000
 H 11.09887700 -6.60536000 -3.85047100
 H 12.29274800 -5.46603000 0.12560900
 H 12.74919100 -6.66311800 -2.01514900

GS-C'

E=-1634.66858

O 0.11281500 0.12849600 0.14593900
 C 1.50972500 0.17974600 0.01090600
 C 1.95044200 1.63371000 -0.18016300
 C 1.48602800 2.42867800 1.03279600
 C -0.01202700 2.28747100 1.22198600
 C -0.36429100 0.80795300 1.31189900
 N 1.87214300 -0.65843100 -1.13254700
 C 3.16493800 -1.22115300 -1.14668400
 N 3.48521200 -2.05830600 -2.15070600
 C 2.62412100 -2.28614500 -3.13763600
 C 1.32807400 -1.67873900 -3.18812800
 C 0.99855100 -0.87832300 -2.14957200
 N 3.02846700 -3.14103900 -4.09590800
 O 3.94184200 -0.91319100 -0.23731300
 O 3.34301500 1.78438400 -0.34744200
 O 1.76902100 3.80433100 0.88456400
 O -0.43959500 2.90743700 2.41591300
 C -1.85534200 0.55207300 1.36154500
 O -2.13058700 -0.82898900 1.47051700
 H 3.77762700 0.95219500 -0.09617600
 H 2.71888500 3.88333000 0.74102300
 H -1.68337000 -1.25854700 0.73366900
 H -0.06946700 3.79734800 2.41554800
 H 0.62978800 -1.87216100 -3.98645600
 H 0.03595800 -0.39475100 -2.05799100
 H -2.31749600 0.98339300 0.46454700
 H -2.27059600 1.04493500 2.24016400
 H 2.00248900 -0.25480100 0.88756500
 H 1.45100200 2.02357800 -1.07583900
 H 1.98970400 2.03139600 1.92681800
 H -0.51800600 2.72534000 0.34958700
 H 0.11164800 0.37157600 2.20045600

H 3.92711900 -3.57443700 -3.92786500
 C 2.32096000 -3.46967100 -5.28863300
 C 2.01720800 -4.77521600 -5.58032000
 C 1.97017000 -2.44872600 -6.20953000
 C 1.35830000 -5.11820700 -6.77791800
 H 2.28134400 -5.57161300 -4.89333200
 C 1.31039000 -2.75631800 -7.36624900
 H 2.23611400 -1.42140800 -5.98392700
 C 0.97421800 -4.10523300 -7.70505400
 C 1.05741000 -6.51625100 -7.05695700
 H 1.03551200 -1.98179700 -8.07278800
 N 0.33145000 -4.32988100 -8.86593400
 C 0.36068700 -6.72852900 -8.31826300
 O 1.36681200 -7.44047000 -6.28618800
 C 0.03777800 -5.61841200 -9.15128300
 C 0.00640900 -8.03730900 -8.71243500
 C -0.64565800 -5.89917700 -10.37340600
 C -0.65093600 -8.27410100 -9.89397500
 H 0.27363300 -8.84858800 -8.04460700
 C -0.97750800 -7.17944000 -10.73089600
 H -0.89181700 -5.05580400 -11.00877800
 H -0.91891600 -9.28163800 -10.18784000
 H -1.49662500 -7.35767400 -11.66641100

GS-C''

E=-1634.66864

O 0.09228100 0.15481600 0.01757800
 C 1.49631700 0.14096200 -0.01209800
 C 2.01879200 1.57930500 -0.07287200
 C 1.50142100 2.31781300 1.15438800
 C -0.01172400 2.24507200 1.22369300
 C -0.44026400 0.78351800 1.18795900
 N 1.90167200 -0.64373700 -1.17916900
 C 3.16495300 -1.26821400 -1.14083600
 N 3.51216800 -2.06912500 -2.16511200
 C 2.70723800 -2.20583900 -3.21404900
 C 1.45757400 -1.51504600 -3.32492000
 C 1.09896400 -0.74838100 -2.27066900
 N 3.13824000 -3.02121600 -4.19458200
 O 3.89123200 -1.04918600 -0.16589400
 O 3.42542500 1.66925900 -0.12604000
 O 1.86145200 3.68302900 1.12226700
 O -0.49837400 2.81008800 2.42236400
 C -1.94106700 0.60324800 1.10949600
 O -2.28880700 -0.76581600 1.10741600
 H 3.80050400 0.79774700 0.08587700
 H 2.82218000 3.72014500 1.05314300
 H -1.80348100 -1.17252300 0.38178600
 H -0.08384500 3.67582700 2.50995700
 H 0.82996800 -1.59393500 -4.19811300
 H 0.17071600 -0.19565100 -2.22952700
 H -2.31087100 1.11215300 0.21030600
 H -2.39985700 1.06218000 1.98479400
 H 1.90037400 -0.37244200 0.86725700
 H 1.60736600 2.05109700 -0.97392200
 H 1.91549700 1.83685300 2.05331800

H -0.42807500 2.76382700 0.34835700
 H -0.05557600 0.26767100 2.07809200
 H 4.06521800 -3.40190400 -4.05542900
 C 2.41374100 -3.38769900 -5.36619000
 C 2.93932700 -3.15476700 -6.61163500
 C 1.16156400 -4.04471100 -5.24788800
 C 2.25471700 -3.55698200 -7.77596700
 H 3.89620100 -2.65694000 -6.72436600
 C 0.47062300 -4.42425700 -6.36424600
 H 0.76321500 -4.24457500 -4.25873400
 C 0.98571000 -4.20038300 -7.68043900
 C 2.84666400 -3.29962000 -9.08209600
 H -0.48718200 -4.92471700 -6.28217000
 N 0.25229300 -4.61234900 -8.73089000
 C 2.03117000 -3.75598000 -10.19930400
 O 3.94676100 -2.74042600 -9.22623800
 C 0.77777900 -4.38859100 -9.95648200
 C 2.48717700 -3.56995300 -11.52259900
 C 0.03103900 -4.81228800 -11.09765900
 C 1.74496900 -3.98816000 -12.59898300
 H 3.44757400 -3.08443600 -11.65563200
 C 0.49767500 -4.61866400 -12.37125600
 H -0.92279900 -5.29449500 -10.91548100
 H 2.10286200 -3.84121400 -13.61072700
 H -0.09485600 -4.95261500 -13.21614100

GS-D'

E=-1634.66858

O 0.09183800 0.09256400 0.04833400
 C 1.49395500 0.14804000 -0.00252100
 C 1.94396000 1.61100600 -0.05393700
 C 1.41099200 2.30805500 1.19101300
 C -0.09554500 2.15954300 1.28368900
 C -0.45226300 0.67932200 1.23487600
 N 1.92051600 -0.60384900 -1.18360400
 C 3.21321100 -1.16529100 -1.16863500
 N 3.58749300 -1.93292200 -2.20852500
 C 2.77968400 -2.09666000 -3.25233500
 C 1.48618000 -1.48733900 -3.32795300
 C 1.10057200 -0.75928800 -2.25595700
 N 3.24475800 -2.89297900 -4.23463500
 O 3.94101600 -0.92154900 -0.20063000
 O 3.34343600 1.77084400 -0.12822700
 O 1.70322200 3.68950400 1.17111800
 O -0.58931700 2.68383900 2.49782400
 C -1.94354400 0.42622000 1.17670600
 O -2.22357100 -0.95816200 1.16072600
 H 3.76399100 0.91795900 0.07361100
 H 2.65957500 3.77415500 1.08504100
 H -1.73119400 -1.33068200 0.42161200
 H -0.22265000 3.57066100 2.58758600
 H 0.82981800 -1.62560400 -4.17127800
 H 0.13174600 -0.28540100 -2.18237200
 H -2.35213800 0.92802900 0.29040600
 H -2.41058700 0.85030700 2.06511400
 H 1.93599900 -0.35376800 0.86525600

H 1.49531900 2.07234900 -0.94249800
 H 1.86306800 1.83682000 2.07680600
 H -0.55151700 2.66838800 0.42240900
 H -0.02870800 0.17176300 2.11199400
 H 4.13237300 -3.33327500 -4.02684200
 C 2.62969500 -3.17913400 -5.48490700
 C 2.20884400 -2.18451400 -6.33265400
 C 2.48448100 -4.53488000 -5.87507100
 C 1.60203400 -2.49191100 -7.56671000
 H 2.33212900 -1.13856100 -6.07295900
 C 1.92527500 -4.85414700 -7.08072000
 H 2.82378000 -5.31376900 -5.20077700
 C 1.45039700 -3.84791300 -7.97953200
 C 1.14721600 -1.41015900 -8.43051900
 H 1.81570700 -5.88800100 -7.38702900
 N 0.89962200 -4.23974500 -9.14368600
 C 0.55666300 -1.86365500 -9.68186800
 O 1.25519100 -0.21098000 -8.12301900
 C 0.46752500 -3.25751100 -9.96535000
 C 0.07244800 -0.91854000 -10.61288200
 C -0.12205500 -3.63186500 -11.21127600
 C -0.48926200 -1.31095300 -11.80223000
 H 0.16165700 0.13015200 -10.35205600
 C -0.58275600 -2.69318300 -12.09639300
 H -0.18996000 -4.69187100 -11.42918400
 H -0.85757400 -0.57871900 -12.51039700
 H -1.02501000 -3.01153300 -13.03422000

GS-D"

E=-1634.66867

O 0.08473300 0.12310000 -0.04516800
 C 1.48862500 0.12401200 -0.00647500
 C 1.99649100 1.56770200 0.04929300
 C 1.41024400 2.22351900 1.29265700
 C -0.10359300 2.13201900 1.28204900
 C -0.51114000 0.67155400 1.13474900
 N 1.95910400 -0.58209100 -1.19864000
 C 3.22210200 -1.20371600 -1.13610300
 N 3.62013500 -1.94567400 -2.18608600
 C 2.86740100 -2.02586500 -3.27926400
 C 1.62472800 -1.32657400 -3.41186400
 C 1.21347900 -0.62147200 -2.33433400
 N 3.35760100 -2.78914400 -4.27545200
 O 3.90156300 -1.03776500 -0.11785900
 O 3.40307400 1.67126200 0.07317300
 O 1.75440300 3.59142500 1.36270600
 O -0.65572900 2.61610500 2.48768100
 C -2.00414800 0.48201500 0.97306400
 O -2.33369300 -0.88733200 0.86666800
 H 3.77648500 0.79014800 0.24460500
 H 2.71691000 3.64158800 1.34827300
 H -1.81025100 -1.24127200 0.13985300
 H -0.25962000 3.48006200 2.64793600
 H 1.03961200 -1.35422000 -4.31639300
 H 0.28328700 -0.07105900 -2.30836600
 H -2.33792100 1.04424900 0.09172300

H -2.50935700 0.87908100 1.85305400
 H 1.85590500 -0.44027000 0.85773000
 H 1.62531300 2.09214300 -0.84012600
 H 1.78536200 1.69164300 2.17996000
 H -0.48315500 2.70035200 0.42084300
 H -0.16284100 0.10445500 2.00851800
 H 4.28267000 -3.16031600 -4.09875100
 C 2.72929900 -3.10784500 -5.51132300
 C 1.46556100 -3.64154300 -5.56611000
 C 3.44970700 -2.89779900 -6.71455700
 C 0.86096700 -3.94911800 -6.80088400
 H 0.90110900 -3.83746800 -4.66081900
 C 2.89237400 -3.21537700 -7.92161300
 H 4.44938200 -2.48030900 -6.66120400
 C 1.56852600 -3.74781500 -8.02216000
 C -0.48996500 -4.49469500 -6.82010600
 H 3.43935900 -3.06128400 -8.84455300
 N 1.08135300 -4.02351900 -9.24644900
 C -0.99025300 -4.78221800 -8.15695000
 O -1.15124800 -4.69412800 -5.78699700
 C -0.17173500 -4.52799400 -9.29556700
 C -2.28945000 -5.31076100 -8.32181100
 C -0.72600700 -4.83193300 -10.57635100
 C -2.79342000 -5.59179300 -9.56715400
 H -2.87481100 -5.48586100 -7.42608200
 C -1.98975000 -5.34453000 -10.70671000
 H -0.10457000 -4.63980100 -11.44383700
 H -3.79125800 -5.99684000 -9.68366100
 H -2.38054000 -5.56385600 -11.69444600

TS GS-A'A"

E=-1634.66757

C -5.98618400 1.11416400 -0.63774400
 O -5.96266700 2.14895700 -1.32720400
 C -8.46308400 1.06326100 -0.50379700
 C -9.64229500 0.50270000 -0.08202200
 C -9.60167200 -0.67721600 0.70194100
 C -8.40688200 -1.25546100 1.03822300
 C -3.63598200 -1.37905800 0.93717700
 C -2.41719800 -0.87992000 0.56069400
 C -2.34724800 0.29795400 -0.23190100
 C -3.52040500 0.91829800 -0.60416400
 N 2.75587200 -0.05904300 -0.18278300
 C 1.75919900 -0.93037600 0.28960600
 O 2.11078400 -1.98462200 0.82595100
 N 0.46575100 -0.57429300 0.13511000
 C 0.15004200 0.53520000 -0.51483000
 C -4.86897800 -0.76291200 0.57077600
 N -1.13985000 0.89763900 -0.66560600
 C 1.14423700 1.40019800 -1.08808300
 C -7.15990600 -0.69765400 0.61662800
 C 2.43417900 1.06428100 -0.88450800
 C -7.21493600 0.48986400 -0.17270200
 C -4.77644000 0.41644700 -0.22062700
 N -6.02338700 -1.32243100 0.98878000
 H -3.50689000 1.82059900 -1.20824300

H -3.69078500 -2.27790900 1.54102400
 H -1.50598100 -1.37382200 0.85724100
 H -8.36795100 -2.15837800 1.63740900
 H-10.52926300 -1.12717900 1.03911600
 H-10.59401100 0.95037900 -0.34122000
 H -8.45350500 1.96530600 -1.10556600
 H 0.87900900 2.29128300 -1.63736100
 H 3.26616500 1.65597600 -1.23927100
 H -1.27924500 1.75139300 -1.18817100
 C 4.15008200 -0.40766300 0.08993500
 O 4.88710600 0.78780600 0.10531700
 C 4.72957200 -1.34979100 -0.96898700
 H 4.16632200 -0.88858900 1.07417500
 C 6.25205200 0.60235100 0.49362300
 C 6.18896800 -1.60847100 -0.61839900
 O 4.03727800 -2.57439200 -1.07454200
 H 4.68004300 -0.84128400 -1.93984400
 C 6.95240400 -0.30221200 -0.51246800
 C 6.85434400 1.98899700 0.56938000
 H 6.28138700 0.13572700 1.48750200
 O 6.82333200 -2.39403100 -1.60574100
 H 6.23150100 -2.11688500 0.35656200
 H 3.45534100 -2.66979100 -0.30242300
 O 8.27220900 -0.51418700 -0.05851300
 H 6.95034100 0.18564500 -1.49768400
 O 6.18959100 2.77976600 1.53265500
 H 6.80923200 2.44806400 -0.42637800
 H 7.89860100 1.90631400 0.86930700
 H 6.31909700 -3.21187800 -1.68305500
 H 8.64745300 -1.21053600 -0.60922800
 H 5.25463100 2.76735700 1.30200900

TS GS-A'B

E=-1634.66593

C -5.11446700 0.96508000 0.62181200
 O -4.73478600 1.94960000 1.27792000
 C -7.24637900 2.04115900 -0.05530600
 C -8.44949900 2.03650500 -0.71626800
 C -8.82771200 0.88454200 -1.44796200
 C -8.01006800 -0.21346900 -1.50060100
 C -3.99498400 -2.51480400 -0.34766800
 C -2.78529800 -2.57857200 0.28816700
 C -2.31819700 -1.48247200 1.05310300
 C -3.08200500 -0.34828300 1.14904000
 N 2.45675300 -0.18680100 0.33648200
 C 1.26473100 0.06249400 -0.36989400
 O 1.33290700 0.73263400 -1.40468100
 N 0.11067200 -0.44070900 0.11489100
 C 0.10185900 -1.08661800 1.27075300
 C -4.82186700 -1.35048800 -0.27130300
 N -1.06238500 -1.58215900 1.73217900
 C 1.28483700 -1.28059400 2.06044700
 C -6.75224100 -0.24149500 -0.82443200
 C 2.44183500 -0.81994600 1.54186400
 C -6.38366700 0.92388100 -0.09166300
 C -4.32786400 -0.25529700 0.49796600

N -6.00080900 -1.36070300 -0.92213400
 H -2.73853300 0.50169200 1.72778200
 H -4.36280400 -3.34975400 -0.93280200
 H -2.16866400 -3.46790400 0.21710100
 H -8.29252700 -1.09923200 -2.05852300
 H -9.77679300 0.87225800 -1.97294200
 H -9.10479000 2.89834300 -0.68260900
 H -6.92148900 2.90388800 0.51571800
 H 1.25803900 -1.78742200 3.01350400
 H 3.40038900 -0.93555800 2.02798300
 H -1.03102000 -2.10133600 2.59790800
 C 3.71033500 0.27412300 -0.26013500
 O 4.73674500 -0.55257800 0.22581700
 C 4.01839500 1.73127400 0.09538200
 H 3.60169200 0.16367400 -1.34460200
 C 6.00472000 -0.29141200 -0.38398200
 C 5.35967800 2.09385500 -0.52830800
 O 3.02900300 2.63882900 -0.33769300
 H 4.10029600 1.80381600 1.18713600
 C 6.44027200 1.13400900 -0.06878400
 C 6.95169700 -1.33898100 0.16102800
 H 5.91069700 -0.41340900 -1.47151700
 O 5.76218600 3.39671200 -0.16059700
 H 5.26932200 2.01888800 -1.62240200
 H 2.43835300 2.18072000 -0.95894400
 O 7.65876000 1.37321400 -0.74035600
 H 6.56445800 1.24039200 1.01839700
 O 6.52022000 -2.64016300 -0.17957300
 H 7.02803200 -1.21391900 1.24862600
 H 7.93749200 -1.18913500 -0.27828000
 H 5.06108300 3.99751900 -0.43732100
 H 7.83692600 2.31746200 -0.66532900
 H 5.61471900 -2.72230100 0.13794500

TS GS-A"B

E=-1634.66592

C 4.96709500 1.22615100 0.45997500
 O 4.49662100 2.29041000 0.89577100
 C 7.02632100 2.30936000 -0.40365400
 C 8.24330300 2.26688200 -1.03752800
 C 8.72948900 1.02354700 -1.51007300
 C 8.00174500 -0.12492100 -1.34121000
 C 4.14583200 -2.45764600 0.21779400
 C 2.92487600 -2.48694900 0.83392100
 C 2.35103600 -1.29776700 1.34551300
 C 3.02293700 -0.11022300 1.21657900
 N -2.45107200 -0.44210200 0.27386400
 C -1.26351400 -0.41533800 -0.48171400
 O -1.34508800 -0.13093000 -1.68054700
 N -0.09928100 -0.70254300 0.13618900
 C -0.09669500 -1.07697300 1.40644200
 C 4.87777900 -1.23901600 0.06165600
 N 1.07976800 -1.35548200 2.00001600
 C -1.29862000 -1.20130700 2.18122100
 C 6.73204200 -0.11523800 -0.68723000
 C -2.45179400 -0.86074200 1.56962300

C 6.25451200 1.14204200 -0.21633800
 C 4.27895200 -0.05262700 0.58054100
 N 6.07208800 -1.28773300 -0.55834700
 H 2.59660100 0.80970600 1.60052500
 H 4.59537900 -3.36195800 -0.17586400
 H 2.37976900 -3.41859700 0.93912800
 H 8.36717700 -1.08069000 -1.69988700
 H 9.69027600 0.98090400 -2.01165300
 H 8.82842600 3.16771000 -1.17702300
 H 6.61994100 3.24158600 -0.02739900
 H -1.28353400 -1.53037900 3.20940200
 H -3.41516200 -0.88277800 2.05954900
 H 1.04953000 -1.68299700 2.95507100
 C -3.68875800 -0.02773700 -0.38720300
 O -4.55919700 0.44342200 0.60948100
 C -4.35444100 -1.18206000 -1.14209500
 H -3.42071700 0.77514700 -1.08274800
 C -5.76875300 0.99970900 0.08493800
 C -5.65533200 -0.66501900 -1.74172300
 O -3.54611200 -1.73204000 -2.15907800
 H -4.58486400 -1.97284800 -0.41724700
 C -6.54444200 -0.07690000 -0.66302400
 C -6.51952700 1.55810000 1.27470600
 H -5.51786800 1.81654700 -0.60514300
 O -6.37796300 -1.70163100 -2.37250900
 H -5.41670500 0.12739000 -2.46690300
 H -2.79129400 -1.13874100 -2.31087500
 O -7.69530200 0.52400300 -1.21719200
 H -6.81926600 -0.87624000 0.04004800
 O -5.77285700 2.57077900 1.91676000
 H -6.75303500 0.73531900 1.96231300
 H -7.45325800 2.00076100 0.92903500
 H -5.79779400 -2.08422500 -3.04046900
 H -8.08482900 -0.12190700 -1.81722300
 H -4.91643900 2.18686500 2.13280800

TS GS-A'C'

E=-1634.64799

N -2.34462800 -0.87601200 0.45164100
 C -1.80442900 -1.39261900 1.63945400
 N -0.64843800 -2.12113500 1.54541700
 C -0.04938800 -2.23739800 0.39314900
 C -0.52000200 -1.64934500 -0.80812500
 C -1.70111300 -0.98270800 -0.73597900
 N 1.14667000 -3.01283400 0.36966700
 C 2.35192100 -2.34058300 0.08730700
 C 3.42471300 -3.09697200 -0.46208600
 C 4.62171800 -2.47894900 -0.70404300
 C 4.82519800 -1.11043300 -0.42521600
 C 3.76019800 -0.34074900 0.13050700
 C 2.52134000 -1.00580900 0.37562000
 N 3.84492800 0.96895600 0.43799300
 C 5.02996000 1.57162300 0.19134900
 C 6.17190200 0.92398800 -0.36257800
 C 6.10978400 -0.49353700 -0.70339600
 C 7.36179900 1.64912400 -0.58212500

C 7.45434700 2.98441900 -0.27180800
 C 6.32809300 3.63954100 0.28027800
 C 5.15922900 2.95886600 0.50408600
 O -2.37946700 -1.18423200 2.70172600
 H 1.72014000 -0.41728500 0.80820200
 H 5.45323600 -3.03295200 -1.12503900
 H 3.27953700 -4.14907200 -0.67995400
 H 8.20225000 1.11071300 -1.00613600
 H 8.37259900 3.53260500 -0.44424200
 H 6.39084600 4.69343600 0.52950500
 H 4.29219900 3.45455100 0.92664100
 H 0.02102600 -1.74900700 -1.73663800
 H -2.19394400 -0.52977900 -1.58505500
 H 1.03321300 -3.85729200 -0.18041700
 O 7.07302300 -1.11393400 -1.18893800
 C -3.63880100 -0.19145200 0.54920500
 O -4.27071100 -0.30579000 -0.69629600
 C -3.47646000 1.28929200 0.90499400
 H -4.20648700 -0.71420700 1.32674100
 C -5.61036000 0.20290800 -0.68999900
 C -4.86851500 1.90747600 0.95171200
 O -2.79493600 1.51338200 2.11835700
 H -2.89955100 1.76947500 0.10610500
 C -5.59011800 1.69157000 -0.36597900
 C -6.17712900 -0.10197100 -2.05994700
 H -6.19071800 -0.33142700 0.07394400
 O -4.80302400 3.29912300 1.17615700
 H -5.44614100 1.41884700 1.75083300
 H -2.86054400 0.71702800 2.66631800
 O -6.92798800 2.13484800 -0.29689500
 H -5.04007800 2.22426800 -1.15489000
 O -6.20652300 -1.49322600 -2.30035000
 H -5.57817300 0.42329700 -2.81455400
 H -7.20152700 0.26603700 -2.10825100
 H -4.31801800 3.43197900 1.99853300
 H -6.90713300 3.03373400 0.05027000
 H -5.30708600 -1.81507800 -2.17890100

TS GS-A"C"

E=-1634.64800

N -2.29974800 -0.94477200 0.45423900
 C -1.81705500 -1.52766300 1.63615000
 N -0.67666600 -2.28154700 1.55121600
 C -0.03735900 -2.36218400 0.41763200
 C -0.46074800 -1.72866000 -0.77803400
 C -1.62030200 -1.02420100 -0.71534700
 N 1.15266200 -3.14685400 0.41003900
 C 1.15795000 -4.32077200 -0.36702200
 C 2.41151800 -4.81074800 -0.82892800
 C 2.45008100 -5.98008600 -1.53919500
 C 1.28138000 -6.71597100 -1.83006800
 C 0.01756700 -6.23760100 -1.37200600
 C 0.00095700 -5.01670600 -0.63309300
 N -1.15815700 -6.86040000 -1.58883600
 C -1.10931500 -8.01476900 -2.29130100
 C 0.08146800 -8.60312100 -2.80729800

C 1.36845300 -7.95144800 -2.58769500
 C 0.01967800 -9.81442900 -3.52756800
 C -1.17520400 -10.45513600 -3.75030400
 C -2.36538900 -9.88190900 -3.24309100
 C -2.33419000 -8.70533000 -2.54006200
 O -2.42320600 -1.34801100 2.68629200
 H -0.96097000 -4.66608400 -0.27616800
 H 3.39274600 -6.37287900 -1.90330600
 H 3.31590800 -4.25403600 -0.61042100
 H 0.95352600 -10.22155500 -3.89930400
 H -1.21222800 -11.38515700 -4.30447800
 H -3.31403600 -10.37986000 -3.41290000
 H -3.24210000 -8.26048700 -2.14802000
 H 0.09908600 -1.82115500 -1.69609200
 H -2.06700800 -0.51684100 -1.55913100
 H 1.97846200 -2.57592800 0.26729900
 O 2.44162900 -8.41622700 -3.01302200
 C -3.57120300 -0.21727800 0.54051200
 O -4.16451300 -0.25288600 -0.72863200
 C -3.36701500 1.23951000 0.96744700
 H -4.18293800 -0.75219300 1.27497600
 C -5.48316600 0.30846800 -0.74399200
 C -4.73604900 1.90781600 0.99752300
 O -2.71706100 1.38554000 2.20977600
 H -2.74714100 1.73189900 0.20924900
 C -5.41736900 1.77932300 -0.35235300
 C -6.01251900 0.08723100 -2.14461400
 H -6.11068800 -0.23488400 -0.02505900
 O -4.62657200 3.28439100 1.28802300
 H -5.35917600 1.40644500 1.75355800
 H -2.83272900 0.57144700 2.72219900
 O -6.73875600 2.27248000 -0.30933200
 H -4.81911500 2.32363300 -1.09699500
 O -6.08875500 -1.28969000 -2.44853000
 H -5.36672300 0.61990400 -2.85405700
 H -7.01911200 0.49905300 -2.21064200
 H -4.16257100 3.36144600 2.12942700
 H -6.69565800 3.15388700 0.07825600
 H -5.20801100 -1.65400100 -2.31092700

TS GS-BD'

E=-1634.64744

N 2.63570000 -0.68059300 -0.53458700
 C 2.14565500 -1.09625300 -1.78342300
 N 0.87989600 -1.61784900 -1.82461000
 C 0.14975200 -1.63003600 -0.74402000
 C 0.58355700 -1.13574200 0.51169000
 C 1.86134900 -0.67868100 0.57639300
 N -1.16297800 -2.17970500 -0.86389000
 C -2.24058300 -1.28262900 -0.68598400
 C -2.12896100 0.04251800 -1.19019900
 C -3.19642800 0.89275300 -1.06224000
 C -4.40314700 0.49214100 -0.45326900
 C -4.53133500 -0.83781400 0.04932200
 C -3.40318400 -1.69961700 -0.08098400
 N -5.63754100 -1.32563700 0.64600700

C -6.68421100 -0.47777500 0.76198800
 C -6.69313600 0.87145200 0.30333600
 C -5.51010100 1.42713000 -0.34465500
 C -7.84207900 1.67179400 0.47450400
 C -8.97305900 1.18094600 1.08059600
 C -8.97790700 -0.15724300 1.54092000
 C -7.87518900 -0.95716300 1.38762400
 O 2.85669700 -0.98410600 -2.77496500
 H -3.49228200 -2.70778600 0.31038700
 H -3.13920400 1.90829500 -1.43781700
 H -1.21810500 0.35968600 -1.68356700
 H -7.79794900 2.69122000 0.10743300
 H -9.85052800 1.80337500 1.20717300
 H -9.86573600 -0.55484700 2.02095400
 H -7.87297600 -1.98323900 1.73838300
 H -0.06208400 -1.14327600 1.37675100
 H 2.32971600 -0.31514300 1.48069600
 H -1.26315600 -3.00825300 -0.28637000
 O -5.45685300 2.59664600 -0.76504800
 C 4.02422100 -0.21033400 -0.48566300
 O 4.50246000 -0.43845600 0.81148200
 C 4.12886200 1.28162200 -0.81452500
 H 4.57832800 -0.80621200 -1.21895100
 C 5.89850300 -0.14538000 0.94802500
 C 5.59621900 1.67841200 -0.70586300
 O 3.61376100 1.62210100 -2.08183400
 H 3.55349900 1.83661100 -0.06460800
 C 6.13902500 1.33322600 0.66922300
 C 6.27456900 -0.55643600 2.35525700
 H 6.46237400 -0.75172100 0.22658100
 O 5.76609200 3.06683300 -0.89229200
 H 6.17144800 1.11885600 -1.45871500
 H 3.63231800 0.83750500 -2.64951800
 O 7.52878700 1.56495700 0.74499900
 H 5.59942800 1.93230900 1.41667200
 O 6.06625600 -1.93893200 2.55406900
 H 5.69252600 0.04366600 3.06592800
 H 7.33363900 -0.35344200 2.51126400
 H 5.39620900 3.28583900 -1.75505000
 H 7.68071500 2.46124200 0.42477500
 H 5.14455300 -2.11473000 2.33760500

TS GS-BD''

E=-1634.64744

N 2.65552200 -0.65806000 -0.50601800
 C 2.14325800 -1.11172500 -1.73252200
 N 0.87633100 -1.63271400 -1.73517600
 C 0.16232800 -1.60198200 -0.64432700
 C 0.62099200 -1.07477600 0.58913500
 C 1.89936300 -0.61604700 0.61665100
 N -1.15332900 -2.15312300 -0.72249300
 C -1.38705000 -3.32448800 0.03488500
 C -0.37052300 -4.31651500 0.10428900
 C -0.61876300 -5.47246400 0.79764500
 C -1.85206300 -5.71061900 1.43810400
 C -2.88406400 -4.72669100 1.36880600

C -2.59795300 -3.52623100 0.65440800
 N -4.09810400 -4.85096200 1.94180400
 C -4.32930400 -5.99608100 2.62245700
 C -3.39168900 -7.05923200 2.76852300
 C -2.07068000 -6.95343800 2.15848400
 C -3.73641300 -8.21366800 3.50241900
 C -4.97050700 -8.34614200 4.09130000
 C -5.91128400 -7.29804800 3.95398600
 C -5.60286700 -6.16509900 3.24624700
 O 2.83675600 -1.03117300 -2.73931300
 H -3.37420700 -2.76944000 0.61065300
 H 0.13778500 -6.24593600 0.86732200
 H 0.57414000 -4.15997800 -0.40251800
 H -2.98765600 -8.99368700 3.58472300
 H -5.22555800 -9.23645000 4.65314500
 H -6.88861000 -7.39241500 4.41513900
 H -6.31948200 -5.35851400 3.13775600
 H -0.00449700 -1.06724500 1.46889900
 H 2.38311100 -0.22308300 1.50031400
 H -1.85243200 -1.44132700 -0.53566400
 O -1.21081300 -7.84782300 2.24945400
 C 4.04777200 -0.19664200 -0.49282700
 O 4.54415500 -0.39140300 0.80316100
 C 4.15856100 1.28386700 -0.86728800
 H 4.58589200 -0.81786300 -1.21686800
 C 5.94372400 -0.10333200 0.91186600
 C 5.62977400 1.67309000 -0.78989200
 O 3.62959400 1.58925800 -2.13787300
 H 3.59695200 1.86559400 -0.12722500
 C 6.18880300 1.36503000 0.58728400
 C 6.33703100 -0.47588600 2.32507900
 H 6.49405500 -0.73355100 0.20047400
 O 5.80643000 3.05412000 -1.01991100
 H 6.19087500 1.08719000 -1.53327100
 H 3.63205300 0.78681100 -2.68036500
 O 7.58074800 1.59029900 0.63783100
 H 5.66277900 1.98873400 1.32422400
 O 6.12378400 -1.85067700 2.56692900
 H 5.76830000 0.14818100 3.02585500
 H 7.39929400 -0.27467200 2.46045300
 H 5.42700700 3.24994800 -1.88408000
 H 7.73354800 2.47617100 0.29022400
 H 5.19831200 -2.02747000 2.36799100

TS GS-C'D"

E=-1634.64742

N 2.59843600 -0.90295500 0.51496300
 C 2.39473300 -1.95227100 1.43381600
 N 1.13374400 -2.36484200 1.66271900
 C 0.12337700 -1.84140400 0.97711400
 C 0.30393700 -0.83280300 -0.02371100
 C 1.56768000 -0.38981400 -0.20733900
 N -1.10590100 -2.30624400 1.26229700
 C -2.31608700 -1.84130300 0.65152000
 C -3.02388500 -0.77658800 1.25893900
 C -4.17902500 -0.33455400 0.66367600

C -4.66370300 -0.91319400 -0.52717600
 C -3.95453800 -1.98484400 -1.14698500
 C -2.75573000 -2.42520300 -0.50555800
 N -4.33073100 -2.60449400 -2.28081100
 C -5.47036300 -2.16110300 -2.85785100
 C -6.27834500 -1.10251100 -2.35199400
 C -5.89455400 -0.41280000 -1.12738900
 C -7.45316200 -0.71866700 -3.03464900
 C -7.84452700 -1.34665600 -4.19097200
 C -7.04966400 -2.40004500 -4.70445800
 C -5.90503100 -2.79322400 -4.06221400
 O 3.38593500 -2.44233100 1.98426700
 H -2.19798600 -3.23706800 -0.95799600
 H -4.75306300 0.47804900 1.09417900
 H -2.64324500 -0.33622400 2.17209800
 H -8.03459800 0.09193100 -2.60967500
 H -8.74750300 -1.04556100 -4.70793500
 H -7.35158100 -2.90148600 -5.61760300
 H -5.29139700 -3.59912800 -4.44885200
 H -0.52173100 -0.42987200 -0.58845600
 H 1.82543500 0.39133900 -0.90887800
 H -1.15542900 -2.99167100 2.00476500
 O -6.55487000 0.51769700 -0.63675000
 C 3.96148500 -0.39397100 0.35676600
 O 3.86506100 0.93906100 -0.07429400
 C 4.76522300 -1.20399800 -0.66442300
 H 4.43455600 -0.45180700 1.34307200
 C 5.13222500 1.60036900 -0.14551400
 C 6.14147800 -0.56471600 -0.79343700
 O 4.90115300 -2.56603600 -0.32343500
 H 4.24911800 -1.13849100 -1.63042600
 C 6.01762200 0.89972500 -1.16820900
 C 4.83038600 3.03967300 -0.50397900
 H 5.61220200 1.56211300 0.84174800
 O 6.90965700 -1.19778700 -1.79529400
 H 6.65325600 -0.63383300 0.17823700
 H 4.62283300 -2.68399500 0.60041800
 O 7.27591300 1.53957300 -1.16209500
 H 5.54680800 0.96932600 -2.15930200
 O 4.03130800 3.65305900 0.48614400
 H 4.34064200 3.06348300 -1.48571000
 H 5.76668000 3.59345300 -0.56683700
 H 6.96509900 -2.13120000 -1.56128200
 H 7.86860500 0.99342400 -1.69065200
 H 3.24797500 3.10229000 0.58887600

TS GS-C'D"

E=-1634.64744

N 2.60453800 -0.89718100 0.50965200
 C 2.39453600 -1.96711600 1.40288500
 N 1.13073000 -2.37293400 1.62787000
 C 0.12149600 -1.81693100 0.96656900
 C 0.30709500 -0.78451900 -0.00874600
 C 1.57507200 -0.35375200 -0.19217700
 N -1.11161600 -2.27146500 1.25099300
 C -2.31604700 -1.80382700 0.63079900

C -2.78252700	-2.45305900	-0.53720600	O -0.04202800	0.32624400	0.17909400
C -3.93393300	-1.99290000	-1.12614000	C 1.33046100	0.61658600	0.11334500
C -4.64773800	-0.89835500	-0.59660300	C 1.53520300	1.95343600	-0.60519200
C -4.18158400	-0.23617700	0.57821700	C 0.78321000	3.02477700	0.17332400
C -2.98146300	-0.73683100	1.17093400	C -0.67985100	2.65172500	0.31816900
N -4.78453000	0.81633200	1.16109500	C -0.77982300	1.27306100	0.95857000
C -5.91546300	1.26346500	0.56990300	N 1.98019100	-0.49085800	-0.58672300
C -6.49597300	0.70066600	-0.60285000	C 3.33461900	-0.73749700	-0.30222000
C -5.86611500	-0.44053600	-1.25388200	N 3.92538000	-1.81337400	-0.86813800
C -7.68240700	1.24691100	-1.13876200	C 3.25458500	-2.56276400	-1.72822600
C -8.30174900	2.32275000	-0.55247300	C 1.90179400	-2.28763500	-2.10762700
C -7.73453400	2.89152700	0.61353800	C 1.30046100	-1.24152900	-1.50050100
C -6.58408800	2.38113100	1.15518800	N 3.84975300	-3.64463600	-2.29382700
O 3.38350600	-2.48105300	1.93555000	O 3.92571600	0.03899400	0.45212800
H -2.60577800	-0.24929900	2.06308400	O 2.89093300	2.31976700	-0.73966300
H -4.32711700	-2.46047900	-2.02155100	O 0.84165200	4.27353200	-0.48348500
H -2.22709700	-3.29146300	-0.93876300	O -1.36284900	3.56523300	1.14981700
H -8.08520200	0.78361800	-2.03245000	C -2.19715700	0.74520000	1.02083000
H -9.21155500	2.73543800	-0.97104600	O -2.24032400	-0.52175200	1.64373200
H -8.21721500	3.74187200	1.08295900	H 3.42401800	1.76100500	-0.15058500
H -6.14333700	2.81105000	2.04758600	H 1.77406500	4.49295900	-0.59081100
H -0.51786800	-0.35613800	-0.55557400	H -1.62821700	-1.08740400	1.16113900
H 1.83772900	0.43982300	-0.87775100	H -1.15785000	4.44796900	0.82160800
H -1.15983500	-3.01749800	1.93256400	H 1.37380300	-2.89442600	-2.82829600
O -6.32377000	-0.97595600	-2.27687300	H 0.27411500	-0.95545100	-1.68098400
C 3.97242200	-0.39935300	0.35576400	H -2.60380700	0.70513800	0.00233600
O 3.88767300	0.94338000	-0.04663500	H -2.80470200	1.42872000	1.61321600
C 4.76328000	-1.19517000	-0.68654300	H 1.76957200	0.65469100	1.11635400
H 4.44959100	-0.48284800	1.33826100	H 1.10077000	1.86961900	-1.60902100
C 5.16078700	1.59391500	-0.10993900	H 1.22404800	3.10292800	1.17848500
C 6.14543300	-0.56699400	-0.80742600	H -1.13340500	2.61768700	-0.68277800
O 4.88767000	-2.56566300	-0.37665100	H -0.35760600	1.30905200	1.97200100
H 4.24363500	-1.10296000	-1.64847100	H 3.26360800	-4.14954100	-2.94516900
C 6.03502800	0.90611600	-1.15080800	C 5.12855700	-4.18746000	-2.14867300
C 4.87116800	3.04306100	-0.43757500	C 5.39319300	-5.34091700	-2.94195500
H 5.64459100	1.53086800	0.87414800	C 6.12112300	-3.68546700	-1.30201600
O 6.90349800	-1.18649900	-1.82531200	C 6.62447400	-5.97737100	-2.89184200
H 6.66003300	-0.66195200	0.16061500	H 4.63046000	-5.74066300	-3.60093000
H 4.60912200	-2.70195700	0.54471600	C 7.36176900	-4.32268500	-1.25171900
O 7.29977800	1.53295600	-1.13668200	H 5.92394700	-2.81500300	-0.69927300
H 5.56105600	1.00118300	-2.13825400	C 7.65498000	-5.46976900	-2.03055100
O 4.08228300	3.64370200	0.56838000	C 6.88906500	-7.16297900	-3.70498600
H 4.37741200	3.09161900	-1.41638300	H 8.14244400	-3.94530100	-0.60229600
H 5.81246600	3.58907600	-0.49331200	N 8.87289600	-6.02511500	-1.92897900
H 6.95021700	-2.12514500	-1.61111800	C 8.22186900	-7.73400300	-3.57076200
H 7.88499100	0.99123500	-1.67799300	O 6.02044500	-7.64710000	-4.46428800
H 3.29354900	3.09916100	0.66256800	C 9.16473600	-7.13344000	-2.67900400
			C 8.60012800	-8.86698600	-4.30112100
			C 10.44270700	-7.69540100	-2.56091800
			C 9.88373000	-9.41082400	-4.16586100
			H 7.87452100	-9.30940900	-4.97277200
			C 10.80485000	-8.83121200	-3.30053700
			H 11.14023600	-7.22273200	-1.87920000
			H 10.15706600	-10.28865400	-4.74055700
			H 11.79769800	-9.25161200	-3.19568300

S₁ Excited State

M062x 6-311g(d,p) solvent=water

S1 excited state

ES-A

E=-1634.55827

ES-B

E=-1634.55772

O	-0.12671600	0.17279900	-0.03743100
C	1.24908200	0.40011200	0.13468900
C	1.53733300	1.90019700	0.02136800
C	0.72078900	2.62006700	1.08608700
C	-0.75246500	2.28920100	0.94327500
C	-0.92770400	0.77640400	0.98325900
N	1.95281900	-0.37321200	-0.88577100
C	3.27310300	-0.77862900	-0.60728700
N	3.90586300	-1.56500500	-1.49979600
C	3.31925200	-1.88110700	-2.64646500
C	2.01343500	-1.40951200	-3.00064600
C	1.36375300	-0.66293900	-2.08162800
N	3.95248300	-2.67469500	-3.55033300
O	3.79059000	-0.39031500	0.44494400
O	2.90352600	2.22169900	0.16524000
O	0.85505400	4.02192100	0.97709800
O	-1.50724800	2.84122300	2.00081300
C	-2.34951400	0.33295200	0.71303000
O	-2.46582900	-1.07281000	0.78794800
H	3.36999300	1.44528300	0.51741800
H	1.79515100	4.22220300	1.04861500
H	-1.81508800	-1.43628200	0.17804600
H	-1.25908800	3.77041400	2.06417800
H	1.55297400	-1.65113200	-3.94735300
H	0.36386800	-0.27838500	-2.22413700
H	-2.65528100	0.70846700	-0.27175700
H	-3.00526500	0.76236400	1.46993400
H	1.58845500	0.02242700	1.10548600
H	1.20643200	2.23555500	-0.96948600
H	1.05942700	2.28236400	2.07700700
H	-1.10394800	2.66635900	-0.02780900
H	-0.60636600	0.39638300	1.96252500
H	3.42805900	-2.83302300	-4.40041500
C	5.19123900	-3.31506500	-3.52839000
C	6.08796600	-3.29053300	-2.42765400
C	5.53081500	-4.03107000	-4.68605200
C	7.29705900	-3.97655000	-2.50446600
H	5.84701400	-2.74541900	-1.53169500
C	6.73509700	-4.71301500	-4.76863000
H	4.84075100	-4.04779800	-5.52328600
C	7.65583000	-4.70993900	-3.68440600
C	8.22412900	-3.95886500	-1.37104400
H	7.00308500	-5.26616200	-5.66013200
N	8.80286900	-5.38788200	-3.81989400
C	9.45936200	-4.70776200	-1.55265400
O	7.96345500	-3.33632700	-0.31864100
C	9.69857900	-5.39582600	-2.78178300
C	10.42458000	-4.76931600	-0.53878800
C	10.89236600	-6.11050100	-2.94247700
C	11.60969200	-5.48998700	-0.72211200
H	10.22967200	-4.24403700	0.38813000
C	11.84807000	-6.16036000	-1.91768400
H	11.05040200	-6.62377800	-3.88387300
H	12.34442600	-5.52458500	0.07448000
H	12.76571900	-6.71829600	-2.05914100

ES-C'

E=-1634.55653

O	0.09483600	0.31331400	0.27179400
C	1.48478000	0.23595400	0.09040100
C	2.05006200	1.64322400	-0.12279100
C	1.70069000	2.47956300	1.10142200
C	0.20310000	2.47522700	1.34243200
C	-0.27894700	1.03420400	1.45038400
N	1.73058000	-0.63600700	-1.05921300
C	2.96594000	-1.31352600	-1.11205200
N	3.17373100	-2.17846100	-2.12268600
C	2.26346200	-2.33103800	-3.07949800
C	1.02133900	-1.62510900	-3.08140900
C	0.79949600	-0.79538500	-2.03524200
N	2.57989000	-3.23869900	-4.03447600
O	3.79886800	-1.07541600	-0.23257300
O	3.44401300	1.66640500	-0.33752100
O	2.10172900	3.82351100	0.93644800
O	-0.12477600	3.13247400	2.54794600
C	-1.78457700	0.91508300	1.55073900
O	-2.18033400	-0.43491700	1.67672200
H	3.81074700	0.80089100	-0.09154200
H	3.04968100	3.81616600	0.76204800
H	-1.79931600	-0.90549900	0.92783800
H	0.32287700	3.98585400	2.53047700
H	0.26850900	-1.77764500	-3.83677700
H	-0.12074200	-0.24338800	-1.90542000
H	-2.23541900	1.38423100	0.66706300
H	-2.12344500	1.44607800	2.43981700
H	1.96499900	-0.23958500	0.95256800
H	1.55856500	2.07537300	-1.00318300
H	2.19643800	2.04030300	1.98013300
H	-0.29070500	2.95666200	0.48621700
H	0.18474400	0.55688200	2.32421600
H	3.39290000	-3.79901200	-3.80567800
C	1.92873200	-3.53139800	-5.24491700
C	1.91352300	-4.88348200	-5.66463000
C	1.37043000	-2.53732100	-6.04413200
C	1.31542100	-5.24083700	-6.87151900
H	2.34457900	-5.65587500	-5.03945600
C	0.75486300	-2.88777300	-7.25165800
H	1.44715300	-1.49737000	-5.75366900
C	0.70819400	-4.23069700	-7.69128300
C	1.28265600	-6.63292800	-7.30389200
H	0.32066100	-2.13044500	-7.89233200
N	0.10476100	-4.50149900	-8.86501700
C	0.61828400	-6.88500600	-8.57942000
O	1.79508000	-7.54865400	-6.62393800
C	0.05508000	-5.79260400	-9.30916300
C	0.52251700	-8.17718400	-9.10043700
C	-0.58045900	-6.04903300	-10.53356200
C	-0.11697800	-8.40949500	-10.32746700
H	0.95451800	-8.99257900	-8.53332300
C	-0.66652000	-7.35282600	-11.04249000
H	-1.00136300	-5.20653900	-11.06963900

H -0.17984000 -9.41945900 -10.71635500
 H -1.16024000 -7.53181400 -11.99001300

ES-C''

E=-1634.55663

O 0.10362900 0.15141400 0.17335400
 C 1.50266900 0.18823200 0.05782700
 C 1.97858800 1.64385900 0.07694400
 C 1.51486600 2.27216200 1.38462900
 C 0.01160400 2.14182400 1.53757300
 C -0.37352500 0.67283700 1.41779600
 N 1.85436700 -0.49233600 -1.18886900
 C 3.13191900 -1.08098500 -1.27695600
 N 3.42398000 -1.80423000 -2.37447500
 C 2.55189100 -1.89361400 -3.37379700
 C 1.29534200 -1.21348500 -3.36442700
 C 0.99183500 -0.52623100 -2.23874300
 N 2.95842000 -2.63980300 -4.42922800
 O 3.91786400 -0.90876700 -0.34031900
 O 3.37644200 1.78313800 -0.04983600
 O 1.83044200 3.64784800 1.43341500
 O -0.41730700 2.60064400 2.80174900
 C -1.87022100 0.44613300 1.41642000
 O -2.17536100 -0.93013600 1.32771000
 H 3.78795400 0.91046400 0.06847300
 H 2.78412100 3.72340900 1.31557900
 H -1.72764600 -1.26183600 0.54218300
 H -0.02769300 3.47316300 2.92802300
 H 0.62535600 -1.22421400 -4.20824300
 H 0.06525500 0.01532700 -2.10879200
 H -2.31158200 1.00907200 0.58420900
 H -2.28655600 0.82000600 2.35134500
 H 1.97737800 -0.37604200 0.86804000
 H 1.50073300 2.16805200 -0.76013000
 H 1.99742600 1.74196300 2.21938400
 H -0.47347700 2.70792800 0.72957000
 H 0.08155200 0.10656900 2.24161600
 H 3.93784000 -2.89765000 -4.39057800
 C 2.23379500 -3.06243500 -5.55651200
 C 2.92208500 -3.11563300 -6.79283600
 C 0.90718500 -3.47671100 -5.46804600
 C 2.27248200 -3.56033500 -7.94246500
 H 3.95160500 -2.78650100 -6.86160400
 C 0.24220200 -3.91268100 -6.61920500
 H 0.40664500 -3.49704200 -4.50833700
 C 0.89670800 -3.96373900 -7.87217800
 C 2.96866100 -3.60170700 -9.22334300
 H -0.78639300 -4.24775700 -6.57244100
 N 0.20226700 -4.39845200 -8.94100200
 C 2.18256200 -4.07953100 -10.35680200
 O 4.16391200 -3.25289300 -9.33680900
 C 0.81951800 -4.46183800 -10.15861000
 C 2.73903200 -4.16993200 -11.63489800
 C 0.07533000 -4.91937400 -11.25636600
 C 1.97543500 -4.63067400 -12.71761800
 H 3.77339100 -3.87672500 -11.76628900

C 0.65004700 -5.00445600 -12.53240200
 H -0.95620300 -5.20302500 -11.08365100
 H 2.42515300 -4.69492100 -13.70191900
 H 0.06031000 -5.36058200 -13.36842200

ES-D'

E=-1634.55701

O 0.05556200 0.17935900 0.08889900
 C 1.45820500 0.14199500 0.03063600
 C 2.00420100 1.57160400 -0.03547500
 C 1.52418500 2.31459300 1.20410100
 C 0.01167500 2.26595900 1.30438100
 C -0.44136700 0.81176500 1.27276300
 N 1.82935300 -0.64369000 -1.14605700
 C 3.08135500 -1.29495700 -1.12890100
 N 3.39772200 -2.09058300 -2.16470100
 C 2.57833600 -2.20055300 -3.21069200
 C 1.33098400 -1.51087100 -3.28553800
 C 0.99740400 -0.74973300 -2.21579400
 N 2.99873800 -3.06890300 -4.16744600
 O 3.82551900 -1.09563200 -0.16264900
 O 3.41098600 1.63575900 -0.11689300
 O 1.90529500 3.67405700 1.16860800
 O -0.44085600 2.83453000 2.51470000
 C -1.94626100 0.65599600 1.22664500
 O -2.31601100 -0.70731300 1.22786700
 H 3.77422900 0.75845100 0.09150400
 H 2.86479900 3.69615900 1.07921300
 H -1.85600100 -1.11867700 0.48851400
 H -0.01122800 3.69348300 2.59606000
 H 0.64611000 -1.62961900 -4.10821700
 H 0.05934100 -0.21817300 -2.14057900
 H -2.32758600 1.17393000 0.33751000
 H -2.37829000 1.11905200 2.11332300
 H 1.87089600 -0.38087200 0.90045600
 H 1.58372900 2.05338900 -0.92690700
 H 1.94876600 1.82429400 2.09302000
 H -0.41413500 2.79449300 0.43950900
 H -0.04602100 0.28623700 2.15251500
 H 3.79675000 -3.61947800 -3.87269800
 C 2.53789000 -3.28820400 -5.46747100
 C 1.88431800 -2.28023700 -6.22312900
 C 2.79982500 -4.53389300 -6.04379500
 C 1.45948600 -2.54849500 -7.52254900
 H 1.75593900 -1.27776300 -5.84161400
 C 2.38801900 -4.80749000 -7.34421500
 H 3.30987300 -5.29140800 -5.45909500
 C 1.69927100 -3.83344100 -8.11522100
 C 0.78333600 -1.51577600 -8.30331300
 H 2.57548300 -5.77262000 -7.79782500
 N 1.32097600 -4.15416400 -9.36119200
 C 0.38567700 -1.90145100 -9.65205500
 O 0.56109800 -0.37885100 -7.83471100
 C 0.67049000 -3.21944900 -10.12238300
 C -0.27401600 -1.00239800 -10.49671200
 C 0.27730300 -3.57920500 -11.41887200

C -0.65835500 -1.38439600 -11.78719200
 H -0.47986600 -0.00580800 -10.12555600
 C -0.38608600 -2.66771100 -12.25000000
 H 0.50479700 -4.58422200 -11.75458700
 H -1.17052700 -0.67450900 -12.42668800
 H -0.68357900 -2.96335800 -13.24876700

ES-D''

E=-1634.55717

O 0.09566300 0.08756000 0.02803000
 C 1.49873400 0.15124800 0.00551600
 C 1.94383500 1.61473600 0.08901300
 C 1.38516100 2.20258600 1.37805000
 C -0.12200800 2.04241500 1.42927100
 C -0.47083000 0.57047500 1.25012600
 N 1.94472600 -0.49273600 -1.22930200
 C 3.24098300 -1.05051600 -1.24782300
 N 3.62460900 -1.72841700 -2.34271900
 C 2.82294400 -1.80768000 -3.40517800
 C 1.55078400 -1.16290500 -3.45816100
 C 1.15360200 -0.51838000 -2.33506600
 N 3.34604600 -2.49070200 -4.45733500
 O 3.95599200 -0.88838100 -0.25261400
 O 3.34397700 1.78246400 0.05626300
 O 1.67150300 3.58185000 1.47974800
 O -0.64121800 2.46224000 2.67302600
 C -1.95992600 0.31943200 1.14577500
 O -2.23422900 -1.05903400 1.00563200
 H 3.76359900 0.91369700 0.17771900
 H 2.62907100 3.67619800 1.42212400
 H -1.72941400 -1.36473400 0.24453900
 H -0.27866000 3.33869100 2.84438500
 H 0.94034900 -1.15014600 -4.34553300
 H 0.20574100 -0.00532000 -2.25251400
 H -2.35616400 0.89502400 0.29963200
 H -2.44275600 0.66412500 2.05975700
 H 1.92951400 -0.42301700 0.83311500
 H 1.51015600 2.14969100 -0.76521700
 H 1.82257800 1.66004800 2.22961700
 H -0.56401500 2.61979300 0.60464400
 H -0.05996700 -0.00805200 2.08852100
 H 4.32804400 -2.70796800 -4.33351400
 C 2.74522400 -2.97066600 -5.62207600
 C 1.36051000 -3.27479800 -5.69620400
 C 3.57324100 -3.21588000 -6.72124300
 C 0.81999100 -3.77816700 -6.87702600
 H 0.71159800 -3.18411200 -4.83738300
 C 3.04301700 -3.72195400 -7.90276500
 H 4.63140800 -2.99031100 -6.64764200
 C 1.65569900 -4.00715400 -8.02114900
 C -0.60303400 -4.09993000 -6.95557600
 H 3.67318100 -3.90545200 -8.76394400
 N 1.19886900 -4.48882000 -9.18559500
 C -1.06377200 -4.61757000 -8.23785300
 O -1.36771800 -3.93509700 -5.98123300
 C -0.13329800 -4.78517300 -9.30815700

C -2.40674900 -4.95338400 -8.44107300
 C -0.59163200 -5.27933900 -10.53714500
 C -2.84169800 -5.44358700 -9.67719900
 H -3.09880800 -4.82157300 -7.61819000
 C -1.94035800 -5.60665700 -10.72465300
 H 0.13221200 -5.39934000 -11.33476500
 H -3.88669700 -5.69609300 -9.81660800
 H -2.27720100 -5.98605300 -11.68174000

ES-E'

E=-1634.55526

C 6.00922900 1.04137600 -0.20646900
 O 6.29104700 2.23123800 -0.32504300
 C 8.38359500 0.30331300 -0.22579100
 C 9.34660200 -0.68318400 -0.17032500
 C 8.95351900 -2.02570900 -0.03364700
 C 7.61907600 -2.36195500 0.04483300
 C 2.98989800 -1.26355700 0.11939700
 C 1.96892900 -0.37208900 0.07234200
 C 2.24087100 1.02810500 -0.07306100
 C 3.58148100 1.45939200 -0.15601800
 N -2.65971000 0.74787700 0.25807700
 C -1.89900300 1.13840000 1.39224000
 O -2.49398000 1.11968000 2.49640700
 N -0.63142400 1.49987300 1.23956400
 C -0.12789900 1.57917700 -0.03861500
 C 4.36979000 -0.85381200 0.02668600
 N 1.23586800 1.92836500 -0.14009300
 C -0.90394600 1.39289200 -1.19825200
 C 6.61602600 -1.36901500 -0.00966600
 C -2.19197400 0.99295200 -1.04093400
 C 7.02113800 -0.02050100 -0.14742300
 C 4.62371700 0.56004100 -0.11124800
 N 5.30576900 -1.78113300 0.07642400
 H 3.80688700 2.51534400 -0.26335500
 H 2.80034300 -2.32386500 0.23372200
 H 0.93906200 -0.69454100 0.15229400
 H 7.30247300 -3.39258200 0.15075800
 H 9.70645400 -2.80388700 0.01079500
 H 10.39730100 -0.42862000 -0.23100400
 H 8.65329400 1.34765900 -0.33035300
 H -0.48758800 1.55750900 -2.18212300
 H -2.88404600 0.80449900 -1.84509600
 H 1.50650900 2.90896200 -0.16011400
 C -4.02761600 0.33193100 0.46466900
 O -4.38048600 -0.53316000 -0.59781800
 C -5.00341700 1.51455200 0.50490200
 H -4.06772300 -0.20224700 1.41991700
 C -5.67952300 -1.10291600 -0.45601600
 C -6.41930800 0.97991500 0.64372000
 O -4.73121800 2.39752800 1.57379200
 H -4.91740100 2.06208300 -0.44364900
 C -6.73129600 -0.00103300 -0.46804400
 C -5.83044500 -2.08188500 -1.60131700
 H -5.73547600 -1.64637900 0.49791500
 O -7.37958600 2.01751000 0.58362700
 H -6.49785300 0.45009700 1.60505300

H -4.01233100 2.00769000 2.11091300
 O -7.99829200 -0.59952900 -0.28497900
 H -6.68475400 0.52869400 -1.43048300
 O -4.83194500 -3.08081000 -1.54445400
 H -5.78533400 -1.52712500 -2.54746400
 H -6.80013700 -2.57387100 -1.53029900
 H -7.15319700 2.64761900 1.27681500
 H -8.61784400 0.11666000 -0.10554100
 H -3.99058100 -2.61629900 -1.47657200

ES-E''

E=-1634.55854

C -5.12126600 2.99513700 0.11419700
 C -4.98047900 1.60390300 0.00216800
 C -6.12559400 0.78234900 -0.11869000
 C -7.39491300 1.40188700 -0.12374400
 C -7.51422500 2.77029000 -0.01310500
 C -6.37104500 3.57956100 0.10748300
 N -6.08492000 -0.58842600 -0.23100700
 C -4.89985100 -1.16440100 -0.22575100
 C -3.64569700 -0.46530200 -0.11257800
 C -3.64381200 0.99551500 0.01038300
 C -4.84233900 -2.60519800 -0.33678600
 C -3.66682800 -3.27405500 -0.33458000
 C -2.42393800 -2.56037800 -0.22814000
 C -2.44766500 -1.15456300 -0.11496000
 N -1.25671500 -3.23443400 -0.24251700
 C -0.00840900 -2.58367300 -0.10174000
 N 0.35085800 -2.25655000 1.18512600
 C 1.47519200 -1.57460300 1.36736400
 N 2.20990800 -1.11919200 0.24147900
 C 1.92606000 -1.59780900 -1.04584200
 C 0.79007300 -2.32020300 -1.22876800
 O 1.95185800 -1.29849600 2.49427600
 O -2.60993800 1.65532900 0.11080300
 H -1.52241300 -0.60283100 -0.01583000
 H -5.78655700 -3.12907900 -0.42161700
 H -3.64076300 -4.35471100 -0.41791900
 H -8.26628300 0.76487500 -0.21677700
 H -8.49727400 3.22624700 -0.01870600
 H -6.47421200 4.65401000 0.19429300
 H -4.22153200 3.59196300 0.20563900
 H 0.50723300 -2.67449100 -2.21007000
 H 2.61886300 -1.32490300 -1.82452500
 H -1.30784300 -4.24926200 -0.23828900
 C 3.40819800 -0.34696500 0.47611200
 O 3.62518000 0.46808400 -0.65986700
 C 4.64097800 -1.22769500 0.71360200
 H 3.23120600 0.27307600 1.36150300
 C 4.72273900 1.36579400 -0.51136100
 C 5.85950000 -0.33336700 0.87249200
 O 4.50662800 -2.04069800 1.86123200
 H 4.77808900 -1.86979100 -0.16717000
 C 6.01384900 0.57808800 -0.32779500
 C 4.72331200 2.22877400 -1.75569200

H 4.55643300 1.99915600 0.37159600
 O 7.05018400 -1.08787000 0.99645500
 H 5.71638000 0.29273800 1.76610700
 H 3.66927800 -1.79789600 2.30548700
 O 7.06889800 1.49957300 -0.14121600
 H 6.18771600 -0.03930400 -1.22091900
 O 3.50414700 2.93303300 -1.87990900
 H 4.90413200 1.58817800 -2.62859900
 H 5.52706800 2.96134900 -1.68705200
 H 6.92528800 -1.68404600 1.74336600
 H 7.82991000 0.99025900 0.15945800
 H 2.80457600 2.27474300 -1.80531300

ES-F'

E=-1634.55547

C 6.01662400 -1.21962100 -0.26714700
 O 6.21264800 -2.41980000 -0.44171800
 C 8.43850100 -0.65577300 -0.24520100
 C 9.47018100 0.25451800 -0.14092300
 C 9.17461400 1.61393400 0.05911800
 C 7.86763400 2.04203800 0.15095100
 C 3.17110300 1.28180400 0.15731800
 C 2.08774100 0.47092300 0.06697200
 C 2.25813600 -0.93770400 -0.14157900
 C 3.56405800 -1.46191600 -0.24232400
 N -2.67368400 -0.48771900 0.22094600
 C -1.82128700 -0.66102300 1.34351400
 O -2.30324400 -0.36437400 2.46270800
 N -0.58374200 -1.10637300 1.16486200
 C -0.14328100 -1.30560500 -0.12370900
 C 4.51771300 0.77665700 0.05081000
 N 1.18883800 -1.75656500 -0.25008000
 C -0.88213900 -0.93986300 -1.26469400
 C 6.79563400 1.12820900 0.04675300
 C -2.15454000 -0.50181000 -1.08171400
 C 7.10264400 -0.23809200 -0.15433800
 C 4.66899800 -0.64403900 -0.15310800
 N 5.51833100 1.62990400 0.14827300
 H 3.71218800 -2.52573400 -0.39757600
 H 3.05861300 2.34678500 0.31959800
 H 1.08470800 0.86438000 0.16327600
 H 7.62594000 3.08676400 0.30518100
 H 9.98158900 2.33254500 0.14185300
 H 10.49998800 -0.07243000 -0.21202400
 H 8.63236600 -1.71071000 -0.39923700
 H -0.45085700 -1.00329800 -2.25389900
 H -2.82881400 -0.21242900 -1.87094500
 H 1.38262100 -2.75188300 -0.31824200
 C -4.01611600 -0.00908200 0.45344000
 O -4.82628200 -0.45751300 -0.61657000
 C -4.08818400 1.52043600 0.54133100
 H -4.35927100 -0.44228100 1.39891500
 C -6.20636800 -0.13957100 -0.45233100
 C -5.54047900 1.93537800 0.70826000
 O -3.32840000 2.03095600 1.61768700
 H -3.70107300 1.93655800 -0.39870800

C -6.38834100 1.37251000 -0.41409300
 C -6.92468200 -0.79590700 -1.61250200
 H -6.56828900 -0.57137300 0.49161500
 O -5.68845300 3.34258100 0.69518300
 H -5.91125400 1.52717500 1.66053000
 H -2.99030100 1.27231800 2.13434900
 O -7.75968800 1.64527400 -0.20938400
 H -6.04303400 1.79964800 -1.36667400
 O -6.72336000 -2.19493300 -1.60258500
 H -6.56547600 -0.34834100 -2.54823800
 H -7.99503600 -0.61138700 -1.52486300
 H -5.12559000 3.68870900 1.39675200
 H -7.82578300 2.58360300 0.00071600
 H -5.77077700 -2.32923500 -1.54949700

ES-F"

E=-1634.55876

C 5.30847700 2.74349100 1.02277600
 C 5.10710200 1.43539500 0.55775800
 C 6.21564400 0.61918500 0.23253100
 C 7.51146800 1.15900000 0.38988800
 C 7.69043500 2.44636400 0.84783700
 C 6.58310800 3.25091000 1.16866300
 N 6.11485900 -0.67319500 -0.22878400
 C 4.90496500 -1.17484400 -0.37402900
 C 3.68217700 -0.46999200 -0.08647800
 C 3.74451000 0.90868500 0.40775200
 C 4.78379900 -2.53336400 -0.85465300
 C 3.57901800 -3.12293200 -1.02862800
 C 2.36848000 -2.40326800 -0.74199000
 C 2.45393000 -1.07718300 -0.26844500
 N 1.17198500 -2.99416800 -0.93401400
 C -0.04783900 -2.34882700 -0.62122300
 N -0.35436300 -2.27796600 0.71799600
 C -1.47009500 -1.65323600 1.07525900
 N -2.34555600 -1.15502400 0.07503300
 C -1.92834500 -1.05959600 -1.26056900
 C -0.77895000 -1.68632200 -1.62369900
 O -1.81136300 -1.45762400 2.26597700
 O 2.74017800 1.56829100 0.67331700
 H 1.55407000 -0.52597600 -0.03080100
 H 5.70416700 -3.06204800 -1.07059500
 H 3.50535000 -4.14260600 -1.38943100
 H 8.35476400 0.52677100 0.13904500
 H 8.69294400 2.84172300 0.96175900
 H 6.73308900 4.26137800 1.52794500
 H 4.43512500 3.33852600 1.26221600
 H -0.43511800 -1.67080100 -2.64842400
 H -2.58769500 -0.53698800 -1.93380300
 H 1.17552600 -3.97042200 -1.21344900
 C -3.55252600 -0.48574400 0.50004600
 O -4.50329600 -0.60480200 -0.54095400
 C -3.32364400 0.99818200 0.81262400
 H -3.90952000 -0.99458000 1.40171500
 C -5.78315000 -0.07810800 -0.19896500
 C -4.65486400 1.63283900 1.17994600

O -2.40585000 1.18801700 1.86997000
 H -2.93154900 1.48279100 -0.09178800
 C -5.67153800 1.41608300 0.07747300
 C -6.69032400 -0.40089900 -1.36756100
 H -6.15505000 -0.58608300 0.70222900
 O -4.53232500 3.02772000 1.38370300
 H -5.02867700 1.15050400 2.09577900
 H -2.18862300 0.30990600 2.24178200
 O -6.94841200 1.88962800 0.45501600
 H -5.31987700 1.92401200 -0.83217100
 O -6.76010500 -1.79672400 -1.57947900
 H -6.31553200 0.11903500 -2.25870200
 H -7.69729900 -0.04446100 -1.15231700
 H -3.86107000 3.15204600 2.06403000
 H -6.82084200 2.77971300 0.80202500
 H -5.84932700 -2.10571000 -1.63678800

TS ES-AB

E=-1634.55084

C 4.21543300 -3.41497700 0.04252700
 O 3.57959200 -4.31721100 -0.54572300
 C 5.90315400 -4.99524300 0.96171000
 C 7.06020500 -5.25253300 1.71946200
 C 7.73424500 -4.21398900 2.34720900
 C 7.25695100 -2.89993600 2.22505800
 C 4.16578400 0.32003400 0.61300000
 C 3.02369700 0.69482200 -0.11642700
 C 2.29204700 -0.27559700 -0.77821200
 C 2.67037600 -1.63115600 -0.73179400
 N -2.64083800 0.13273500 -0.15701800
 C -1.56650800 -0.14539100 0.70950700
 O -1.81993400 -0.35174500 1.90045600
 N -0.31798600 -0.17189000 0.20061900
 C -0.11277200 0.13224000 -1.07217100
 C 4.57317800 -1.02516200 0.67654400
 N 1.14525000 0.10200800 -1.54918800
 C -1.17599800 0.50044500 -1.96339900
 C 6.10186700 -2.61762000 1.47384800
 C -2.42640400 0.47545900 -1.45725900
 C 5.41422200 -3.69566400 0.82852000
 C 3.80407900 -2.01785500 -0.01308100
 N 5.68642200 -1.32605900 1.39365600
 H 2.08837600 -2.38098100 -1.25224600
 H 4.75927700 1.05623100 1.14077900
 H 2.70966500 1.73001300 -0.16859400
 H 7.76244600 -2.06975400 2.70398600
 H 8.62518300 -4.41384500 2.93014900
 H 7.42417100 -6.26962400 1.81075300
 H 5.37075800 -5.79827500 0.46752200
 H -0.99129000 0.76456900 -2.99384900
 H -3.30903400 0.70248000 -2.03862500
 H 1.27884800 0.31402800 -2.52788400
 C -3.99477600 0.05486400 0.39212300
 O -4.86487300 -0.23235600 -0.67246900
 C -4.42444100 1.36359500 1.06141700
 H -3.99136000 -0.76110800 1.12294500

C -6.21193800 -0.46715500 -0.25014500
 C -5.85620500 1.19210500 1.55140000
 O -3.59532400 1.74862500 2.13573700
 H -4.39847300 2.15602500 0.30305400
 C -6.76759700 0.78940100 0.40802800
 C -6.97178400 -0.87589300 -1.49378500
 H -6.22147000 -1.29418000 0.47264000
 O -6.36025400 2.39370000 2.09611700
 H -5.87412200 0.39456300 2.30931700
 H -3.02377100 0.99819700 2.37051300
 O -8.07030000 0.49829500 0.86743200
 H -6.78487100 1.60429900 -0.32978000
 O -6.43534300 -2.05803700 -2.05053300
 H -6.94541100 -0.04662100 -2.21207100
 H -8.00931500 -1.07447100 -1.22674000
 H -5.76093800 2.65562400 2.80420300
 H -8.34377900 1.24091700 1.41761400
 H -5.49715000 -1.89427600 -2.19366600

TS ES-AB*

E=-1634.55086

C 4.81761500 1.35448300 1.51078500
 O 4.46904000 2.55556100 1.50029500
 C 6.75355300 1.77659300 3.01411300
 C 7.87070000 1.31880800 3.73609000
 C 8.22024500 -0.02448400 3.71205300
 C 7.45406000 -0.93028200 2.96240800
 C 3.83023700 -2.00570900 0.09229400
 C 2.69430800 -1.66311700 -0.66249400
 C 2.27012300 -0.34621200 -0.69107900
 C 2.95533800 0.65547900 0.02321200
 N -2.66665600 0.11346500 -0.13668200
 C -1.61017200 -0.20340900 0.73844800
 O -1.88429800 -0.42888200 1.92131400
 N -0.35554500 -0.24520100 0.24576600
 C -0.12697000 0.08197300 -1.01732500
 C 4.53946600 -1.02835700 0.81445700
 N 1.13381100 0.01805200 -1.48354300
 C -1.16915800 0.49811400 -1.91232200
 C 6.33273100 -0.49674800 2.23234000
 C -2.42696200 0.48521800 -1.42449800
 C 5.97971800 0.89085700 2.26433100
 C 4.08787400 0.33076600 0.77348000
 N 5.62915300 -1.41920600 1.52417200
 H 2.61060100 1.68121200 -0.00503600
 H 4.18717000 -3.02729800 0.13512100
 H 2.14848800 -2.41332500 -1.22126700
 H 7.70404600 -1.98396700 2.92519800
 H 9.08076500 -0.37537600 4.26873700
 H 8.45945900 2.02269900 4.31332000
 H 6.47170600 2.82212300 3.02536100
 H -0.96423900 0.78489900 -2.93286800
 H -3.29653500 0.74462100 -2.01197100
 H 1.29287200 0.30119600 -2.44019100
 C -4.03009100 0.04361300 0.38937300
 O -4.88666200 -0.20774400 -0.69509800

C -4.45199800 1.34310900 1.08097100
 H -4.04986400 -0.78807400 1.10200800
 C -6.24361000 -0.43227200 -0.29994400
 C -5.89407300 1.18162700 1.54348600
 O -3.63554000 1.69085700 2.17743300
 H -4.40211500 2.15202100 0.34140000
 C -6.79215000 0.81747700 0.37678500
 C -6.98829800 -0.80262400 -1.56465100
 H -6.27674400 -1.27471100 0.40416000
 O -6.39032800 2.37796300 2.10666200
 H -5.93581900 0.36787000 2.28301300
 H -3.07521900 0.92859100 2.40100200
 O -8.10622100 0.53546500 0.80867000
 H -6.78571400 1.64852500 -0.34297000
 O -6.45835000 -1.97915500 -2.13931900
 H -6.93905100 0.04206200 -2.26349900
 H -8.03263800 -0.99301200 -1.31911400
 H -5.80231500 2.61285500 2.83344200
 H -8.37726700 1.26901700 1.37209400
 H -5.51593200 -1.82462000 -2.26378500

TS ES-AE'

E=-1634.55084

C -6.04533000 -1.04778500 -0.53332400
 O -6.18028500 -2.18784000 -0.98051200
 C -8.48697800 -0.67188000 -0.25745100
 C -9.55651700 0.11794800 0.11155000
 C -9.32597200 1.41321700 0.61342700
 C -8.03950300 1.89393800 0.73799200
 C -3.31763200 1.46894800 0.32638500
 C -2.19512000 0.77590600 0.00389900
 C -2.29101300 -0.55916500 -0.51013200
 C -3.58035600 -1.12818900 -0.68342700
 N 2.69384200 -0.42054300 0.05797000
 C 1.66714300 -0.24305200 1.02335300
 O 2.02572100 0.13272200 2.16058700
 N 0.40597900 -0.49280600 0.68571000
 C 0.14333300 -0.97747900 -0.56396700
 C -4.63653900 0.90920700 0.17455400
 N -1.19798100 -1.27349000 -0.86263000
 C 1.14298200 -1.31752000 -1.49051200
 C -6.92863400 1.10482900 0.36744700
 C 2.43735800 -1.05288100 -1.15467400
 C -7.16920100 -0.20072100 -0.13965800
 C -4.71870000 -0.42909500 -0.35504400
 N -5.67904700 1.64745400 0.52172300
 H -3.68053900 -2.13745800 -1.06867000
 H -3.25436100 2.48213200 0.70521100
 H -1.21705000 1.21547200 0.13261600
 H -7.84399600 2.88781000 1.12321600
 H -10.16432500 2.03533400 0.90381300
 H -10.56938500 -0.25373600 0.01643900
 H -8.63680000 -1.67235400 -0.64648000
 H 0.90041800 -1.76983000 -2.44237500
 H 3.28946500 -1.25615300 -1.78327300
 H -1.37236300 -2.13901900 -1.36102700

C 4.05181800 -0.09559400 0.43980500
 O 4.76105500 0.23802700 -0.73524100
 C 4.75635300 -1.26117300 1.14680300
 H 4.00361900 0.76471100 1.11629900
 C 6.09113000 0.68920200 -0.48328700
 C 6.19184300 -0.85523400 1.44104100
 O 4.11813300 -1.62943900 2.35149600
 H 4.75827800 -2.12241200 0.46517000
 C 6.89762800 -0.42539000 0.17083700
 C 6.64579800 1.11748700 -1.82546400
 H 6.05713300 1.55653400 0.19095800
 O 6.93119200 -1.92210300 2.00309100
 H 6.17611600 -0.00117400 2.13477500
 H 3.40436300 -0.98533300 2.52572900
 O 8.19143800 0.07147300 0.44489400
 H 6.94537900 -1.28367300 -0.51479700
 O 5.86529600 2.15360800 -2.38638800
 H 6.68250000 0.24269500 -2.48742700
 H 7.65833300 1.49714800 -1.69119200
 H 6.46302300 -2.19830800 2.79896300
 H 8.61869500 -0.57328100 1.02002600
 H 4.95517100 1.83773200 -2.38536400

TS ES-AF'

E=-1634.55078

C 6.00233700 -1.25927000 -0.38787000
 O 6.03494100 -2.42724000 -0.78021500
 C 8.45882000 -1.11696500 -0.03633200
 C 9.59033000 -0.42106400 0.33704700
 C 9.47679100 0.91381300 0.77051400
 C 8.24213900 1.52659000 0.82356900
 C 3.51728200 1.55577500 0.25390100
 C 2.34099700 0.96378300 -0.07912600
 C 2.31731800 -0.39731600 -0.52848500
 C 3.54768300 -1.10085900 -0.62414300
 N -2.70744500 -0.02581600 -0.09752600
 C -1.66714800 0.38170600 0.77868300
 O -2.00574800 1.04960500 1.77933000
 N -0.41226400 0.04221100 0.50001800
 C -0.14842500 -0.59571000 -0.67681400
 C 4.77708300 0.86068600 0.17726700
 N 1.17237000 -1.01966100 -0.89562800
 C -1.12899400 -0.88329300 -1.64115200
 C 7.06993200 0.83577900 0.44702500
 C -2.42406700 -0.58160800 -1.34095500
 C 7.19236700 -0.51104700 0.00926700
 C 4.73993000 -0.50374800 -0.28619000
 N 5.87735900 1.50762100 0.52845100
 H 3.55837300 -2.13315600 -0.95763600
 H 3.54459300 2.58728800 0.58450400
 H 1.40838000 1.50272800 -0.00360900
 H 8.13611200 2.55273400 1.15567900
 H 10.36401600 1.46215600 1.06427100
 H 10.56255400 -0.89690800 0.29789000
 H 8.51911200 -2.14528300 -0.37326100
 H -0.87170800 -1.32975000 -2.59174200

H -3.26535900 -0.77296100 -1.98748800
 H 1.28449700 -1.91808700 -1.35148900
 C -4.07133800 0.29484000 0.26853600
 O -4.91510500 -0.66097100 -0.33828200
 C -4.48377900 1.70117800 -0.18586400
 H -4.14004500 0.23089500 1.36017400
 C -6.28617000 -0.52332500 0.03261300
 C -5.94560900 1.91835900 0.17205800
 O -3.70178300 2.71444400 0.41075900
 H -4.36780700 1.75452400 -1.27673600
 C -6.81174900 0.82994200 -0.42897500
 C -7.00690400 -1.69210900 -0.60553000
 H -6.37385600 -0.59297600 1.12596500
 O -6.42103600 3.16068800 -0.30859400
 H -6.04507500 1.87490300 1.26711300
 H -3.11240100 2.29566600 1.06785400
 O -8.15375600 0.94721200 -0.00329100
 H -6.74257500 0.88748600 -1.52479600
 O -6.48333300 -2.92066200 -0.14312000
 H -6.91992600 -1.60672600 -1.69636600
 H -8.06172800 -1.65538200 -0.33473300
 H -5.84896300 3.84166000 0.06278500
 H -8.40654500 1.86768800 -0.13673100
 H -5.53109000 -2.87884600 -0.28320600

TS ES-BE''

E=-1634.55481

C -5.99196800 2.78069900 0.51006500
 C -5.62255600 1.45784700 0.21497900
 C -6.63071500 0.46836500 0.05777300
 C -7.97884800 0.84816400 0.20510300
 C -8.32264400 2.15524600 0.49788600
 C -7.32171600 3.12995000 0.65151900
 N -6.36176400 -0.84543800 -0.23701800
 C -5.09465500 -1.20641500 -0.36726900
 C -3.96866500 -0.32305700 -0.22259100
 C -4.21557600 1.09584200 0.07162900
 C -4.81190700 -2.58436500 -0.69085700
 C -3.53499600 -3.03235000 -0.82485600
 C -2.42531400 -2.15408200 -0.64842300
 C -2.67190800 -0.78105800 -0.37126500
 N -1.17385800 -2.66198500 -0.80059200
 C 0.03101900 -2.02508200 -0.50434900
 N 0.05650000 -1.22134400 0.58847000
 C 1.19122500 -0.59822100 0.90841800
 N 2.32681800 -0.76383700 0.07639000
 C 2.33523100 -1.69751200 -0.94622600
 C 1.17693200 -2.33369500 -1.26741100
 O 1.33094400 0.11618700 1.92048500
 O -3.29330500 1.91229100 0.18999400
 H -1.85279100 -0.08897700 -0.25429300
 H -5.65712300 -3.24902900 -0.82054900
 H -3.34090900 -4.07386500 -1.05973100
 H -8.73418900 0.08088400 0.08125600
 H -9.36520300 2.42847400 0.60846900
 H -7.59397600 4.15329900 0.88054500

H -5.20437100 3.51620000 0.62436000
 H 1.14037700 -3.03558700 -2.08895000
 H 3.27125200 -1.83457700 -1.46474700
 H -1.10791900 -3.58765800 -1.20545200
 C 3.53541700 -0.03780700 0.42012200
 O 4.27380800 0.14702200 -0.76754500
 C 4.39616600 -0.78698500 1.44485900
 H 3.22595500 0.92727400 0.83616000
 C 5.43980300 0.95164800 -0.58930300
 C 5.66832100 0.01177800 1.68403900
 O 3.73135600 -0.98855200 2.67407500
 H 4.65989300 -1.76399200 1.01845700
 C 6.39507100 0.26506700 0.37840700
 C 6.02647800 1.14312900 -1.97188100
 H 5.14531900 1.92777100 -0.17931000
 O 6.55786600 -0.67286800 2.54395000
 H 5.39226200 0.98277200 2.12199200
 H 2.88531200 -0.50294300 2.64647400
 O 7.51023000 1.11129400 0.56659600
 H 6.70406200 -0.70086400 -0.04648200
 O 5.10508500 1.78990000 -2.82599500
 H 6.31945200 0.16292900 -2.36947500
 H 6.91402600 1.77132000 -1.90115600
 H 6.07903300 -0.84625800 3.36224100
 H 8.00916800 0.75093000 1.30833300
 H 4.28860400 1.28069400 -2.78025700

TS ES-BF"

E=-1634.55483

C 6.34781100 -2.58917900 -0.42947900
 C 5.87192300 -1.27948300 -0.25121200
 C 6.78915700 -0.19398800 -0.26243700
 C 8.15718200 -0.46786700 -0.45512800
 C 8.60612700 -1.76388200 -0.63140500
 C 7.69498200 -2.83375500 -0.61805800
 N 6.41428100 1.11573800 -0.08963300
 C 5.12844100 1.37540400 0.08797500
 C 4.08511000 0.38555300 0.11319800
 C 4.44648700 -1.02870000 -0.05717300
 C 4.73559500 2.74988200 0.28692300
 C 3.43269700 3.09448900 0.46783800
 C 2.40365100 2.10698100 0.46673600
 C 2.76237200 0.73977800 0.31109200
 N 1.12259700 2.51801500 0.66034700
 C -0.03759000 1.75182900 0.53907900
 N -0.06469900 0.80946100 -0.43560200
 C -1.17289000 0.08923400 -0.61104500
 N -2.33499400 0.42256900 0.12876500
 C -2.29125500 1.35135600 1.15475000
 C -1.13608100 2.03362900 1.37844500
 O -1.26310400 -0.86937700 -1.40286100
 O 3.59929400 -1.93040500 -0.03838000
 H 2.00642400 -0.02941100 0.32280800
 H 5.51982500 3.49683000 0.28627800
 H 3.15472800 4.13382800 0.60915100
 H 8.84273100 0.37155000 -0.46003100

H 9.66232300 -1.95484700 -0.77911900
 H 8.04991100 -3.84812000 -0.75545000
 H 5.62812900 -3.39925200 -0.41492100
 H -1.06858800 2.76228500 2.17412900
 H -3.20261100 1.49412300 1.71386500
 H 0.99833600 3.47768200 0.95806100
 C -3.56159700 -0.29298200 -0.17147100
 O -4.64249300 0.55011300 0.15987100
 C -3.67708500 -1.60464200 0.61475600
 H -3.55597000 -0.50963100 -1.24565100
 C -5.91422900 0.00592300 -0.19468500
 C -5.01794700 -2.24493100 0.28995900
 O -2.63982600 -2.51436600 0.31577200
 H -3.64307000 -1.36353000 1.68551700
 C -6.15447100 -1.28478700 0.57805200
 C -6.92874300 1.08548100 0.11807800
 H -5.92778500 -0.20704400 -1.27268800
 O -5.23699100 -3.41136200 1.05862000
 H -5.03505700 -2.49097500 -0.78242000
 H -2.11438700 -2.14693400 -0.42007200
 O -7.39500400 -1.81833000 0.16382100
 H -6.16426000 -1.06209700 1.65474300
 O -6.66484100 2.25740100 -0.62611700
 H -6.90995700 1.28516000 1.19718300
 H -7.92303900 0.73317300 -0.15511500
 H -4.49840700 -4.00528300 0.88350100
 H -7.44331100 -2.71326900 0.51846500
 H -5.74456300 2.48569700 -0.45597400

ES-C'D"

E=-1634.55345

O -4.03646900 0.94322000 -0.69506700
 C -4.00156900 -0.35956500 -0.17089500
 C -4.47055600 -0.33588400 1.28700000
 C -5.88146400 0.23597800 1.31842200
 C -5.91782200 1.60482800 0.66755400
 C -5.35517300 1.49708000 -0.74392000
 N -2.62758000 -0.84656800 -0.30073100
 C -2.43266900 -2.23978300 -0.38058200
 N -1.18558900 -2.70036800 -0.59188400
 C -0.16111800 -1.85539800 -0.64911500
 C -0.31255500 -0.43928600 -0.49372300
 C -1.57495000 0.01485700 -0.33026700
 N 1.05584400 -2.38899800 -0.85225000
 O -3.41953700 -2.97226000 -0.25073800
 O -4.45675200 -1.60355200 1.90574300
 O -6.34710800 0.38135900 2.64391100
 O -7.23910600 2.09253800 0.57106200
 C -5.21791600 2.83652700 -1.43542300
 O -4.72068500 2.68191400 -2.74844000
 H -4.32837400 -2.28150900 1.22064300
 H -6.29935900 -0.48828400 3.05688900
 H -3.89477000 2.19208100 -2.67488800
 H -7.63502200 1.99776700 1.44471600
 H 0.53072500 0.23249100 -0.52418200
 H -1.82005500 1.06312900 -0.23268600

H -4.56440000 3.47961600 -0.83241600
 H -6.20044200 3.30257300 -1.50388800
 H -4.63153000 -1.03437000 -0.76079900
 H -3.80245800 0.33075900 1.84666500
 H -6.54553800 -0.43601600 0.75440800
 H -5.28902400 2.28923000 1.25482300
 H -5.99803700 0.83970400 -1.34472900
 H 1.08077200 -3.39344200 -0.97348500
 C 2.26123000 -1.62880300 -0.97947800
 C 2.60985400 -1.10810000 -2.24140500
 C 3.05628900 -1.40915500 0.13201600
 C 3.78750400 -0.36927500 -2.39244500
 H 1.97579100 -1.28386300 -3.10101100
 C 4.24226300 -0.66439400 -0.00448200
 H 2.75907600 -1.81587300 1.09086700
 C 4.62457900 -0.13901400 -1.25288900
 C 4.17297900 0.16624900 -3.69047700
 H 4.88793800 -0.47829100 0.84463800
 N 5.78070900 0.56955300 -1.32297200
 C 5.42542300 0.91982200 -3.72248500
 O 3.47675600 -0.00735300 -4.71381700
 C 6.17745900 1.08572100 -2.51576700
 C 5.90153300 1.47823400 -4.90755500
 C 7.38132100 1.81239900 -2.55901300
 C 7.10840500 2.19905300 -4.92610800
 H 5.31935300 1.34240200 -5.81052500
 C 7.84460300 2.36639300 -3.76030200
 H 7.93485300 1.92662100 -1.63455200
 H 7.46258400 2.62548700 -5.85763800
 H 8.77405400 2.92254300 -3.77644100

TS ES-C"D'

E=-1634.55343

O -4.05367000 0.92138400 -0.71974600
 C -4.00567300 -0.36579900 -0.15908300
 C -4.44269400 -0.30159900 1.30732000
 C -5.85226500 0.27235800 1.35504300
 C -5.90329700 1.62210100 0.66621300
 C -5.37347400 1.47359700 -0.75419600
 N -2.63417700 -0.85479700 -0.30455500
 C -2.43811600 -2.24930300 -0.35273700
 N -1.19456800 -2.71321600 -0.57779700
 C -0.17357500 -1.86820300 -0.67948800
 C -0.32426000 -0.44898100 -0.55289000
 C -1.58364400 0.00709500 -0.37325900
 N 1.03752900 -2.40279000 -0.91300200
 O -3.42056200 -2.97957600 -0.18347200
 O -4.41559600 -1.55258000 1.95886500
 O -6.28680800 0.45616900 2.68632900
 O -7.22631700 2.10807500 0.58628400
 C -5.25269000 2.79255500 -1.48698600
 O -4.78343200 2.60003900 -2.80531000
 H -4.30145700 -2.24847800 1.28950200
 H -6.22829700 -0.40095700 3.12339300
 H -3.95623500 2.11189800 -2.73497300
 H -7.60001200 2.04434800 1.47242800

H 0.51724300 0.22295200 -0.61348400
 H -1.82824100 1.05693400 -0.29233400
 H -4.58699400 3.45303500 -0.91703300
 H -6.23691000 3.25603700 -1.54787000
 H -4.64710500 -1.05800500 -0.71542700
 H -3.76212800 0.37903900 1.83416400
 H -6.52960500 -0.41492200 0.82627800
 H -5.26084700 2.32262300 1.21868300
 H -6.02967400 0.79926700 -1.32091600
 H 1.07102500 -3.41299000 -0.96313600
 C 2.24572900 -1.64436700 -1.02339500
 C 2.96398200 -1.32811700 0.14676300
 C 2.67912800 -1.22104700 -2.26797900
 C 4.14495200 -0.58361100 0.06315100
 H 2.60984600 -1.66149700 1.11388900
 C 3.86620600 -0.47269800 -2.36736500
 H 2.10217200 -1.47335900 -3.14924500
 C 4.60967200 -0.14346000 -1.21849800
 C 4.90466000 -0.24824000 1.25957100
 H 4.23438400 -0.13065200 -3.32649000
 N 5.74479500 0.58418200 -1.37744000
 C 6.11729600 0.53986600 1.04434500
 O 4.54200100 -0.60958300 2.39968300
 C 6.48190400 0.92043800 -0.28653900
 C 6.92613100 0.92590500 2.11196200
 C 7.65230500 1.67617400 -0.48174500
 C 8.09129400 1.68115500 1.89188100
 H 6.63409100 0.62918300 3.11170000
 C 8.45368600 2.05471500 0.60410000
 H 7.90971800 1.95357600 -1.49703300
 H 8.70764900 1.97171800 2.73492600
 H 9.35173400 2.63685600 0.43662500

TS ES-C"E'

E=-1634.55197

C 6.02784300 -1.03372800 0.00218900
 O 6.25797500 -2.24238200 -0.05415200
 C 8.41958600 -0.41053700 0.27133000
 C 9.41554700 0.53168500 0.42825200
 C 9.07917400 1.89692300 0.48469600
 C 7.76320000 2.29638400 0.38488600
 C 3.11498200 1.41692100 -0.12310500
 C 2.05941500 0.57401700 -0.26101300
 C 2.26385200 -0.84305000 -0.32101000
 C 3.58965800 -1.33966800 -0.24308000
 N -2.74384300 -0.79576800 -0.30967100
 C -2.22248600 -1.64488400 -1.32262500
 O -3.04287100 -2.11426500 -2.14027300
 N -0.91615300 -1.89318000 -1.35020200
 C -0.13798300 -1.40457600 -0.34200300
 C 4.47018800 0.93674300 -0.01931300
 N 1.23253500 -1.70768800 -0.45061600
 C -0.64809700 -0.75354800 0.79227400
 C 6.72669600 1.35099400 0.22438700
 C -1.97787200 -0.45119300 0.80193500
 C 7.07381600 -0.02399800 0.16694800

C 4.66271300 -0.48923200 -0.09392800
 N 5.44108200 1.82184800 0.13315300
 H 3.77109500 -2.40844800 -0.28223100
 H 2.96926800 2.49003100 -0.09444500
 H 1.05295400 0.96259700 -0.34613400
 H 7.48713200 3.34340200 0.42681200
 H 9.85931100 2.63889100 0.60764400
 H 10.45130100 0.22514200 0.50722300
 H 8.65052400 -1.46838600 0.22437600
 H -0.00964200 -0.48844500 1.62391500
 H -2.48535800 0.07480600 1.59462300
 H 1.46422600 -2.67047000 -0.67878800
 C -4.15459800 -0.47679100 -0.34756000
 O -4.32983500 0.76865300 0.29598600
 C -5.01585400 -1.53735700 0.35103700
 H -4.44536800 -0.40944300 -1.40172700
 C -5.66935800 1.25581100 0.23080200
 C -6.46557800 -1.07980000 0.32701300
 O -4.91635700 -2.80523500 -0.26274900
 H -4.68039500 -1.61713100 1.39391500
 C -6.60405500 0.29344100 0.95239700
 C -5.64008200 2.63599100 0.85263200
 H -5.97405000 1.33658100 -0.82216200
 O -7.30423100 -1.96501000 1.04380400
 H -6.79234000 -1.01723700 -0.72193400
 H -4.37638200 -2.70899300 -1.07145600
 O -7.92244600 0.78519000 0.82586900
 H -6.30946000 0.23179000 2.00994300
 O -4.76446100 3.48980500 0.14436700
 H -5.34167000 2.54240400 1.90478900
 H -6.63835700 3.07075300 0.80965100
 H -7.18911300 -2.83804900 0.65206500
 H -8.50963900 0.08114700 1.12332800
 H -3.92063300 3.02802100 0.09132200

TS ES-C'F'

E=-1634.55119

C 6.01314300 -1.18175200 -0.26794800
 O 6.13765200 -2.40289800 -0.37670200
 C 8.42636400 -0.72189500 -0.64908800
 C 9.48857100 0.15086400 -0.77028300
 C 9.27218600 1.53460500 -0.63506900
 C 8.00626100 2.02120700 -0.38264800
 C 3.34487300 1.45681400 0.38521400
 C 2.23057900 0.68936600 0.50311700
 C 2.31108000 -0.73446200 0.37146700
 C 3.57973200 -1.32246600 0.13144200
 N -2.74013100 -0.49626400 0.45034000
 C -2.19210600 -1.29248000 1.48956300
 O -2.97230900 -1.63792800 2.40205700
 N -0.90055600 -1.61378200 1.45388800
 C -0.12700300 -1.10487300 0.45305100
 C 4.64139600 0.88682900 0.11499800
 N 1.21635000 -1.52277300 0.46943300
 C -0.60786200 -0.25173200 -0.55234900
 C 6.90434100 1.14851900 -0.25514900

C -1.93207300 0.07369300 -0.52891600
 C 7.13032000 -0.24639400 -0.39200600
 C 4.71126900 -0.54787400 0.00216400
 N 5.67433400 1.70395700 -0.00601100
 H 3.66669700 -2.39847800 0.02502300
 H 3.29438800 2.53255700 0.50282200
 H 1.27176700 1.14250500 0.71955500
 H 7.82126200 3.08365000 -0.27597600
 H 10.10458400 2.22181000 -0.73000000
 H 10.48499600 -0.22489400 -0.96786900
 H 8.56573300 -1.79207000 -0.74823300
 H 0.04462500 0.13799100 -1.32154000
 H -2.42020700 0.71431900 -1.24526400
 H 1.37653400 -2.52038800 0.57576100
 C -4.15970300 -0.20912900 0.49185500
 O -4.59321200 0.02075600 -0.83186900
 C -4.48214200 1.01793000 1.35426600
 H -4.65846900 -1.08968800 0.91192700
 C -6.00388000 0.20617600 -0.94160900
 C -5.97792400 1.28271400 1.28143600
 O -4.10200200 0.84752200 2.70370200
 H -3.94294100 1.87893100 0.93730500
 C -6.42368900 1.44326300 -0.15793600
 C -6.29346100 0.31375300 -2.42392800
 H -6.51749900 -0.67491300 -0.53209600
 O -6.33276400 2.46314800 1.97507800
 H -6.50518800 0.41876300 1.71341700
 H -3.80501100 -0.07545200 2.82069100
 O -7.82818500 1.56491400 -0.25057800
 H -5.92569600 2.32530400 -0.58575000
 O -5.88912100 -0.85761900 -3.10334300
 H -5.78239200 1.20101400 -2.81937100
 H -7.36630500 0.43280300 -2.57280500
 H -6.02365700 2.35827800 2.88191800
 H -8.09057500 2.23340800 0.39224800
 H -4.96856800 -1.00671700 -2.86158700

TS ES-D"E"

E=-1634.55507

C -5.63299000 2.94769300 -0.32764700
 C -5.36823900 1.57352700 -0.21570400
 C -6.44286500 0.65226200 -0.12963200
 C -7.76189600 1.15559400 -0.16023900
 C -8.00165700 2.50875800 -0.27153100
 C -6.93045500 3.41681900 -0.35629200
 N -6.27904100 -0.70585900 -0.01704100
 C -5.04369000 -1.17472700 0.01577100
 C -3.85494600 -0.36887500 -0.06265700
 C -3.98714000 1.08831800 -0.18620100
 C -4.85981800 -2.60275100 0.13396200
 C -3.62596900 -3.16061400 0.16532300
 C -2.44690400 -2.34520700 0.09278400
 C -2.59684200 -0.94317200 -0.03347800
 N -1.23862700 -2.94311200 0.15846500
 C 0.01233200 -2.28841600 0.14477600
 N 0.85495700 -2.65558100 1.15297600

C 2.06686000 -2.11251100 1.19959200
 N 2.40856400 -1.10203100 0.25887100
 C 1.61701500 -0.87045900 -0.86208400
 C 0.39689200 -1.47291800 -0.93282200
 O 2.94964100 -2.43327000 2.02456300
 O -3.00961900 1.83696600 -0.25742600
 H -1.73204300 -0.29791600 -0.10293000
 H -5.75278600 -3.21261700 0.19784400
 H -3.50719000 -4.23493700 0.25536400
 H -8.57468800 0.44207700 -0.09317400
 H -9.02109500 2.87542900 -0.29355500
 H -7.12627300 4.47850400 -0.44306800
 H -4.78966800 3.62542300 -0.38966400
 H -0.25397200 -1.31202700 -1.78093400
 H 2.01066800 -0.18864600 -1.59898800
 H -1.22022700 -3.93530600 0.37118800
 C 3.70993700 -0.47840400 0.37167700
 O 3.61613300 0.81154000 -0.19643400
 C 4.80702700 -1.27416000 -0.34768700
 H 3.94770500 -0.41282700 1.43906400
 C 4.80888300 1.58183700 -0.05543900
 C 6.11467600 -0.50540100 -0.24425700
 O 4.98183700 -2.56684900 0.19319100
 H 4.52533300 -1.36346200 -1.40561800
 C 5.95466600 0.89870100 -0.79097000
 C 4.48313500 2.95457400 -0.60493400
 H 5.06173900 1.66588700 1.01090100
 O 7.14906800 -1.13574600 -0.97464300
 H 6.39300300 -0.43410500 0.81802000
 H 4.41045700 -2.64542200 0.98215400
 O 7.12402900 1.66546000 -0.58882700
 H 5.70816300 0.83598000 -1.86068100
 O 3.42156300 3.54752600 0.11523800
 H 4.23761700 2.85835900 -1.67043000
 H 5.35624900 3.59864200 -0.50406600
 H 7.22350800 -2.03460200 -0.63489300
 H 7.86259100 1.13060700 -0.90088700
 H 2.70118100 2.90787800 0.11108700

TS ES-D'F"

E=-1634.55432

C 6.02334000 2.81317300 -0.07579700
 C 5.65487100 1.45931300 -0.12314200
 C 6.65352400 0.45950100 -0.24157100
 C 8.00416500 0.86526700 -0.30799500
 C 8.34649900 2.20021200 -0.26018500
 C 7.35020000 3.18664000 -0.14312800
 N 6.38637100 -0.88599800 -0.29564800
 C 5.12153200 -1.26380100 -0.23265900
 C 4.00051200 -0.37059600 -0.11437900
 C 4.24392200 1.07610000 -0.04994600
 C 4.82886000 -2.67745900 -0.29032100
 C 3.55769600 -3.14305800 -0.24339700
 C 2.44711500 -2.24194600 -0.12158700
 C 2.70399400 -0.85035500 -0.06967000
 N 1.19966000 -2.75290200 -0.05413500

C 0.00518800 -2.01191800 0.08553800
 N -0.78524000 -2.39367900 1.12997300
 C -1.96191200 -1.79550100 1.29155100
 N -2.39416900 -0.83781300 0.33494000
 C -1.55694000 -0.40930400 -0.68956100
 C -0.35138300 -1.02521800 -0.84727900
 O -2.72987800 -2.00991900 2.25405500
 O 3.32867300 1.89591700 0.05784400
 H 1.89366400 -0.13983300 0.01566600
 H 5.67104800 -3.35365800 -0.37318700
 H 3.35753700 -4.20812300 -0.28925000
 H 8.75822400 0.09231800 -0.39804600
 H 9.38890800 2.49137800 -0.31303300
 H 7.62622600 4.23331800 -0.10623500
 H 5.23560500 3.55184300 0.01514300
 H 0.30687700 -0.75164900 -1.66034400
 H -1.93677900 0.37058000 -1.32959600
 H 1.11364500 -3.76090800 0.02391400
 C -3.70320600 -0.24268800 0.51456600
 O -4.17420400 0.15935200 -0.75416100
 C -3.66596100 0.97082300 1.45241600
 H -4.35676900 -1.01216900 0.94026800
 C -5.50878300 0.66399500 -0.72796600
 C -5.06101500 1.57122600 1.52563200
 O -3.23131600 0.63857600 2.75431400
 H -2.97712300 1.71078300 1.02343100
 C -5.56946800 1.91457300 0.13996900
 C -5.88299900 0.92219600 -2.17225700
 H -6.17683400 -0.10170200 -0.30925800
 O -5.07805000 2.75753500 2.29560600
 H -5.73764500 0.82500400 1.96857800
 H -3.14287800 -0.33296900 2.80548900
 O -6.91096100 2.35602700 0.17908800
 H -4.91672000 2.68522400 -0.29466400
 O -5.81430400 -0.26775600 -2.93164200
 H -5.21489200 1.69305500 -2.57740000
 H -6.90812500 1.28881300 -2.21780300
 H -4.72930200 2.53124000 3.16515200
 H -6.96093700 3.02821400 0.86801300
 H -4.93719600 -0.63590500 -2.77927400

S₁ Excited State

CAM-b3lyp 6-311g(d,p) solvent=water

ES A

E=-1634.42254117

O -0.023725 0.340781 0.150400
 C 1.348465 0.637252 0.104376
 C 1.556054 1.997041 -0.568380
 C 0.762979 3.039498 0.206969
 C -0.696320 2.650875 0.322723
 C -0.791366 1.261286 0.935334
 N 2.000940 -0.460177 -0.615110
 C 3.357974 -0.695114 -0.355944

N 3.943452 -1.779146 -0.900604
 C 3.266783 -2.558803 -1.726243
 C 1.907361 -2.298955 -2.080088
 C 1.310550 -1.245547 -1.489107
 N 3.854740 -3.650483 -2.274220
 O 3.964350 0.107519 0.363634
 O 2.908746 2.397726 -0.627558
 O 0.818336 4.303131 -0.426628
 O -1.399897 3.547658 1.158999
 C -2.197215 0.706777 0.971492
 O -2.233093 -0.564523 1.589245
 H 3.448088 1.737356 -0.151544
 H 1.747937 4.549568 -0.488102
 H -1.608639 -1.123075 1.114309
 H -1.187515 4.437250 0.855026
 H 1.366575 -2.928082 -2.771396
 H 0.277979 -0.978060 -1.652058
 H -2.591364 0.664859 -0.051577
 H -2.826597 1.375455 1.557058
 H 1.779874 0.648748 1.110339
 H 1.159992 1.936014 -1.589014
 H 1.182908 3.110534 1.219941
 H -1.137132 2.632720 -0.682958
 H -0.386511 1.283806 1.954744
 H 3.258208 -4.172127 -2.900233
 C 5.138316 -4.189636 -2.144611
 C 5.390155 -5.353900 -2.919007
 C 6.141286 -3.671986 -1.329530
 C 6.622138 -5.987061 -2.881257
 H 4.618224 -5.767606 -3.556935
 C 7.383603 -4.305047 -1.289350
 I 5.949049 -2.790173 -0.742445
 C 7.663496 -5.461958 -2.049523
 C 6.875926 -7.181800 -3.676189
 H 8.174766 -3.914118 -0.661446
 N 8.882857 -6.015948 -1.962089
 C 8.208507 -7.749822 -3.558459
 O 5.994178 -7.681174 -4.414225
 C 9.164478 -7.135074 -2.696110
 C 8.575512 -8.891398 -4.275454
 C 10.442150 -7.692766 -2.592399
 C 9.859658 -9.430985 -4.155457
 H 7.838522 -9.344485 -4.926199
 C 10.792464 -8.838031 -3.318611
 H 11.151687 -7.208865 -1.931805
 H 10.123453 -10.317484 -4.721222
 H 11.787884 -9.255093 -3.224524

ES TS AF'

E=-1634.41283467

C 6.002952 -1.283082 -0.320890
 O 6.033128 -2.473340 -0.647814
 C 8.461332 -1.121353 -0.014507
 C 9.594494 -0.407854 0.301851
 C 9.484965 0.946070 0.660246
 C 8.253517 1.558525 0.696668

C 3.525141 1.551992 0.200209
 C 2.348983 0.942101 -0.081988
 C 2.321651 -0.438195 -0.458556
 C 3.549597 -1.140905 -0.528824
 N -2.706690 0.015548 -0.099322
 C -1.683589 0.398065 0.800505
 O -2.034549 1.081247 1.791427
 N -0.432122 0.032184 0.563254
 C -0.143575 -0.625766 -0.597372
 C 4.783625 0.858971 0.141126
 N 1.175068 -1.082189 -0.769408
 C -1.105381 -0.905950 -1.577981
 C 7.078955 0.849024 0.377439
 C -2.398400 -0.574786 -1.321424
 C 7.196209 -0.516323 0.015115
 C 4.744141 -0.527737 -0.243114
 N 5.886620 1.521717 0.437892
 H 3.559782 -2.188858 -0.805873
 H 3.553908 2.597916 0.479743
 H 1.415259 1.478097 -0.010157
 H 8.151958 2.601222 0.972136
 H 10.375353 1.510931 0.909937
 H 10.566627 -0.884679 0.275548
 H 8.516941 -2.166306 -0.293707
 H -0.834944 -1.373936 -2.514427
 H -3.222708 -0.762836 -1.987627
 H 1.284086 -2.017810 -1.141641
 C -4.078064 0.313770 0.263264
 O -4.908262 -0.618494 -0.398002
 C -4.503644 1.737189 -0.118050
 H -4.157910 0.196006 1.348931
 C -6.288894 -0.518969 -0.045214
 C -5.976328 1.915466 0.211851
 O -3.758552 2.725513 0.562910
 H -4.362208 1.858027 -1.199589
 C -6.822739 0.848127 -0.447809
 C -6.978072 -1.671011 -0.741276
 H -6.391990 -0.641843 1.040861
 O -6.459944 3.174803 -0.221536
 H -6.097754 1.826163 1.300455
 H -3.124121 2.266405 1.157978
 O -8.172978 0.936974 -0.033890
 H -6.745708 0.957708 -1.537956
 O -6.450187 -2.912309 -0.314784
 H -6.873612 -1.546628 -1.826600
 H -8.038361 -1.659530 -0.492477
 H -5.915418 3.846439 0.203897
 H -8.428740 1.862024 -0.121995
 H -5.495262 -2.856312 -0.430042

ES F'

E=-1634.41715462

C 6.038313 -1.260184 -0.240858
 O 6.159984 -2.478301 -0.374735
 C 8.487821 -0.848379 -0.233682
 C 9.571044 -0.003076 -0.159736

C 9.360357 1.375322 -0.009574
C 8.085067 1.884468 0.063894
C 3.355154 1.413990 0.093138
C 2.228094 0.667378 0.033451
C 2.311320 -0.751039 -0.121913
C 3.579548 -1.352066 -0.205442
N -2.667454 -0.240438 0.227532
C -1.821881 -0.390566 1.349907
O -2.320574 -0.102076 2.467831
N -0.574363 -0.803117 1.188835
C -0.114490 -1.009028 -0.090238
C 4.666200 0.827352 0.005290
N 1.198079 -1.514153 -0.198232
C -0.872833 -0.726020 -1.238421
C 6.960724 1.037524 -0.009327
C -2.153545 -0.319656 -1.073859
C 7.181140 -0.348618 -0.160846
C 4.731936 -0.603290 -0.147475
N 5.717168 1.617172 0.072134
H 3.665223 -2.426477 -0.322256
H 3.306604 2.488450 0.216211
H 1.251409 1.123035 0.114200
H 7.908797 2.946663 0.179989
H 10.210044 2.045372 0.049176
H 10.578600 -0.395593 -0.216594
H 8.616392 -1.917380 -0.349421
H -0.447381 -0.824665 -2.227158
H -2.832592 -0.083267 -1.873982
H 1.346342 -2.519251 -0.225023
C -4.059022 0.080962 0.460029
O -4.801371 -0.392956 -0.647387
C -4.309547 1.582803 0.636623
H -4.364777 -0.439163 1.373672
C -6.213808 -0.244892 -0.506268
C -5.803029 1.821938 0.777365
O -3.652640 2.106189 1.772843
H -3.947940 2.098929 -0.262076
C -6.567118 1.230773 -0.387387
C -6.822780 -0.919880 -1.714842
H -6.542192 -0.768192 0.401456
O -6.109235 3.204548 0.835575
H -6.144407 1.327889 1.697912
H -3.173194 1.363248 2.208428
O -7.964780 1.338971 -0.191692
H -6.266036 1.747826 -1.308447
O -6.465810 -2.288026 -1.766206
H -6.498470 -0.390880 -2.620139
H -7.908599 -0.863127 -1.651576
H -5.608962 3.570598 1.573370
H -8.136997 2.250097 0.071054
H -5.505945 -2.320519 -1.688118