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## ESIPT Emission Behavior of Methoxy-Substituted 2-Hydroxyphenylbenzimidazole Isomers

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#### Table of contents

S1. NMR spectra	2
S2. Optical properties	4
S3. Computational results	6

# S1. NMR spectra







Figure S2. NMR spectra of 2 in DMSO-d<sub>6</sub>.



Figure S3. NMR spectra of 3 in DMSO-d<sub>6</sub>.

## S2. Optical properties



Figure S4. UV-vis absorption spectrum of 1, 2, 3, and A in THF (10  $\mu$ M).



Table S1. Absorption characteristics in THF (10  $\mu$ M).

Figure S5. UV-vis absorption spectrum of 1, 2, and 3 in MeCN (black line), MeOH (green line), and THF/water mixed solvent in the volume ratio of 1/9 (blue line) (10  $\mu$ M).

	$\lambda_{em}/nm$	$\Phi^{a}$	LE/ESIPT <sup>b</sup>	Stokes shift <sup>c</sup> /cm <sup>-1</sup>
THF	458	0.31	0/1	10400
MeCN	456	0.27	0/1	10400
MeOH	446	0.30	0/1	10000
T1W9 <sup>d</sup>	446	0.28	0/1	9900

Table S2. Emission characteristics of 1 in various solvents (10 µM).

[a] Calculated based on quinine sulfate as a standard (0.55).

[b] Relative peak intensity of LE and ESIPT emission.

[c] Calculated for ESIPT emission.

[d] THF/water mixed solvent in the volume ratio of 1/9.

Table S3. Emission characteristics of 2 in various solvents (10  $\mu$ M).

	$\lambda_{em}/nm$	$\Phi^{\mathrm{a}}$	LE/ESIPT <sup>b</sup>	Stokes shift <sup>c</sup> /cm <sup>-1</sup>
THF	450	0.17	0/1	9300
MeCN	444	0.21	0/1	8900
MeOH	351, 433	0.21	0.29/1	8200
T1W9 <sup>d</sup>	353, 419	0.37	1.89/1	7700

[a] Calculated based on quinine sulfate as a standard (0.55).

[b] Relative peak intensity of LE and ESIPT emission.

[c] Calculated for ESIPT emission.

[d] THF/water mixed solvent in the volume ratio of 1/9.

**Table S4.** Emission characteristics of **3** in various solvents (10  $\mu$ M).

	$\lambda_{em}/nm$	$\Phi^{a}$	LE/ESIPT <sup>b</sup>	Stokes shift <sup>c</sup> /cm <sup>-1</sup>
THF	345, 486	0.04	0.91/1	12300
MeCN	345, 433	0.06	0.34/1	9900
МеОН	359, 462	0.10	3.23/1	11500
T1W9 <sup>d</sup>	354, 431	0.08	0.08/1	9800

[a] Calculated based on quinine sulfate as a standard (0.55).

[b] Relative peak intensity of LE and ESIPT emission.

[c] Calculated for ESIPT emission.

[d] THF/water mixed solvent in the volume ratio of 1/9.

# **S3.** Computational results

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		THF			MeCN			MeOH			H <sub>2</sub> O	
State	EE/eV	Abs/nm	f	EE/eV	Abs/nm	f	EE/eV	Abs/nm	f	EE/eV	Abs/nm	f
1												
$1^{1}A'$	4.068	305	0.688	4.088	303	0.677	4.091	303	0.665	4.092	303	0.672
$2^{1}A'$	4.236	293	0.265	4.227	293	0.252	4.229	293	0.256	4.226	293	0.251
3 <sup>1</sup> A'	4.698	264	0.028	4.700	264	0.027	4.701	264	0.027	4.701	264	0.027
4 <sup>1</sup> A'	5.270	235	0.032	5.277	235	0.032	5.277	235	0.032	5.278	235	0.032
5 <sup>1</sup> A'	5.488	226	0.021	5.492	226	0.019	5.492	226	0.019	5.492	226	0.019
1 <sup>1</sup> A"	5.506	225	0.001	5.543	224	0.001	5.542	224	0.001	5.547	224	0.001
2												
$1^{1}A'$	3.973	312	0.949	3.992	311	0.932	3.994	310	0.926	3.995	310	0.929
$2^{1}A'$	4.607	269	0.077	4.613	269	0.074	4.613	269	0.074	4.613	269	0.074
3 <sup>1</sup> A'	4.784	259	0.065	4.785	259	0.061	4.786	259	0.061	4.786	259	0.060
$4^{1}A'$	5.077	244	0.052	5.091	244	0.053	5.092	243	0.052	5.094	243	0.053
5 <sup>1</sup> A'	5.275	235	0.105	5.278	235	0.100	5.279	235	0.099	5.279	235	0.099
1 <sup>1</sup> A"	5.275	235	0.001	5.329	233	0.002	5.328	233	0.002	5.335	232	0.002
3												
$1^{1}$ A'	3.890	319	0.346	3.912	317	0.327	3.913	317	0.323	3.916	317	0.324
$2^{1}A'$	4.289	289	0.601	4.296	289	0.597	4.298	288	0.594	4.297	289	0.595
3 <sup>1</sup> A'	4.703	264	0.052	4.700	264	0.050	4.701	264	0.050	4.700	264	0.050
4 <sup>1</sup> A'	5.196	239	0.023	5.218	238	0.021	5.218	238	0.020	5.221	237	0.020
5 <sup>1</sup> A'	5.365	231	0.070	5.381	230	0.052	5.381	230	0.052	5.384	230	0.050
1 <sup>1</sup> A"	5.365	231	0.001	5.407	229	0.001	5.407	229	0.001	5.411	229	0.001

**Table S5**. TDDFT calculations for the excitation energies (EE in eV), absorption wavelengths (Abs in nm), and oscillator strengths (f) of **1**, **2**, and **3** in several solvents.

-								
Solvent	1 (keto)		<b>2</b> (enol)		<b>2</b> (keto)		<b>3</b> (keto)	
	EmE/eV	Flu/nm	EmE/eV	Flu/nm	EmE/eV	Flu/nm	EmE/eV	Flu/nm
THF	2.851	435	3.413	363	2.995	414	2.572	482
MeCN	2.821	439	3.360	369	2.978	426	2.530	490
MeOH	2.820	440	3.362	369	2.978	416	2.529	490
H <sub>2</sub> O	2.817	440	3.353	370	2.977	416	2.525	491

**Table S6**. DFT/TDDFT calculations for emission energy (EmE in eV) and fluorescence wavelength (Flu in nm) of **1**, **2**, and **3** in several solvents.

**Table S7**. Activation energy ( $\Delta E_a$ ) and heat of reaction ( $\Delta H$ ) for ESIPT reaction of **2** in kcal·mol<sup>-1</sup>.

Solvent	$\Delta E_{\mathrm{a}}$	$\Delta H$
THF	2.27	4.25
MeCN	2.36	4.14
МеОН	2.36	4.14
H <sub>2</sub> O	2.37	4.13



Figure S6. A typical solvation structure of **3** with six MeOH molecules in ground state optimized by  $\omega B97XD/6-31G(d,p)$  in PCM (methanol).

### Cartesian Coordinates

#### 2.17660 0.70654 -0.00003 С 2.26057 -0.70360 0.00001 С С 3.51018 -1.33361 0.00004 С 4.64142 -0.52514 0.00002 С 4.54221 0.88017 -0.00002 С 3.30768 1.52284 -0.00005 -0.00005 Ν 0.82961 0.98493 -0.20058 С 0.15369 -0.00003 -1.23635 0.00002 Ν 0.99069 Η 3.58819 -2.42127 0.00007 Н 5.63001 -0.98667 0.00005 1.47881 5.45426 -0.00003 Η Н 3.23338 2.61051 -0.00008 Н 0.36947 1.88505 -0.00008 С -0.35938 -0.00002 -1.29165 С -1.82910 -1.67371 -0.00003 С -2.19469 0.73364 0.00002 С -3.21569 -1.87301 0.00002 С -3.57146 0.52921 0.00006 С -4.06463 -0.77913 0.00006 -3.59615 Н -2.89396 0.00001 Н -4.26390 1.36688 0.00009 -0.93631 0.00010 Η -5.14445 -2.75766 -0.00011 0 -1.04359 Η -0.08924 -2.44119 -0.00020 0 -1.63345 1.97254 0.00002 -2.49495 3.10330 0.00007 С Н -3.12564 3.11791 -0.90013 Н -3.12559 3.11787 0.90031 Н -1.83726 3.97818 0.00007

Optimized geometries of 1 in the ground state in THF (angstrom)

### 8

Optimized C C C C C C C N C N H H H H H C C C C C	<pre>geometries of 1     2.17583     2.26014     3.50998     4.64103     4.54125     3.30643     0.82921     0.15316     0.98994     3.58946     5.62978     5.45308     3.23009     0.37158     -1.29208     -1.83019     -2.19458     -3.21624     -3.57185     -4.06512     -3.59852     -4.26391     -5.14491     -1.04267     -0.08808     -1.63235     -2.49114     -3.12120 </pre>	<pre>in the ground 0.70565 -0.70449 -1.33451 -0.52525 0.88041 1.52282 0.98459 -0.20009 -1.23711 -2.42209 -0.98637 1.47929 2.61020 1.88624 -0.35958 -1.67334 0.73431 -1.87306 0.52990 -0.77816 -2.89341 1.36783 -0.93515 -2.75807 -2.43990 1.97090 3.10530 3 12099</pre>	<pre>state in MeCN    -0.00001    -0.00003    -0.00005    -0.00001    0.00001    0.00001    0.00002    -0.00003    0.00001    0.00003    0.00001    0.00002    0.00002    0.00002    0.00001    0.00002    0.00001    0.00002    0.00001    0.00003    0.00001    0.00003    0.00001    0.00003    0.00001    0.00003    0.00001    0.00003    0.00001    0.00003    0.00001    0.00003    0.00004    -0.90018 </pre>	(angstrom)
H	-3.12120	3.12099	-0.90018	
Н	-1.82985	3.97705	0.00005	
		in the ground	state in MeOH	(angstrom)
Optimized	geometries of I	. In the ground	beace in neon	(anyscrom)
Optimized C	2.17585	0.70577	-0.00002	(angscrom)
Optimized C C	2.17585 2.26027	0.70577 -0.70445	-0.00002 -0.00001	(angserom)
C C C	2.17585 2.26027 3.51027	0.70577 -0.70445 -1.33424	-0.00002 -0.00001 -0.00001	(angserom)
C C C C	2.17585 2.26027 3.51027 4.64125	0.70577 -0.70445 -1.33424 -0.52501	-0.00002 -0.00001 -0.00001 -0.00001	(angserom)
C C C C C C C	2.17585 2.26027 3.51027 4.64125 4.54138	0.70577 -0.70445 -1.33424 -0.52501 0.88057	-0.00002 -0.00001 -0.00001 -0.00001 -0.00001 -0.00002	(angserom)
Optimized C C C C C C	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003	(angserom)
Optimized C C C C C C N	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003 -0.00002	(angserom)
Optimized C C C C C C C N C	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003 -0.00002 -0.00001	(angserom)
Optimized C C C C C C N C N U	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003 -0.00002 -0.00001 -0.00001	(angserom)
Optimized C C C C C C N C N H H	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003 -0.00001 -0.00001 0.00000 -0.00001	(angserom)
Optimized C C C C C C N C N H H H	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003 -0.00001 -0.00001 0.00000 -0.00001 -0.00001 -0.00001 -0.00001	(angserom)
Optimized C C C C C N C N H H H H	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00003 -0.00003	
Optimized C C C C C C N C N H H H H H	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996 0.37080	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586	-0.00002 -0.00001 -0.00001 -0.00002 -0.00002 -0.00002 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00003 -0.00003 -0.00003 -0.00002	
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Optimized C C C C C C N C N H H H H H C C	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996 0.37080 -1.29218 -1.82981	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334	-0.00002 -0.00001 -0.00001 -0.00002 -0.00002 -0.00002 -0.00001 -0.00001 -0.00001 -0.00001 -0.00003 -0.00003 -0.00003 -0.00002 -0.00001 -0.00001	
Optimized C C C C C C N C N H H H H H H C C C C	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996 0.37080 -1.29218 -1.82981 -2.19480	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440	-0.00002 -0.00001 -0.00001 -0.00002 -0.00002 -0.00002 -0.00001 -0.00001 -0.00001 -0.00001 -0.00003 -0.00003 -0.00003 -0.00002 -0.00001 -0.00001 -0.00001 0.00002	
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Optimized C C C C C C C N C N H H H H H H C C C C	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996 0.37080 -1.29218 -1.82981 -2.19480 -3.21601 -3.57202	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00003 -0.00002 -0.00001 -0.00001 -0.00001 -0.00003 -0.00003 -0.00003 -0.00003 -0.00002 -0.00001 0.00002 0.00001 0.00004	
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Optimized C C C C C C C C N N H H H H H H H C C C C	Geometries of 1 2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996 0.37080 -1.29218 -1.82981 -2.19480 -3.21601 -3.57202 -4.06521 -3.59763 4.26402	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375	-0.00002 -0.00001 -0.00001 -0.00001 -0.00002 -0.00002 -0.00001 -0.00001 -0.00001 -0.00003 -0.00003 -0.00003 -0.00003 -0.00001 0.00002 0.00001 0.00004 0.00004 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00004 0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.000001 -0.000001 -0.0000000000 -0.00000000000000000000	
Optimized C C C C C C C N C C C C C C C C C C C	geometries of 1         2.17585         2.26027         3.51027         4.64125         4.54138         3.30655         0.82918         0.15325         0.99004         3.58945         5.63006         5.45319         3.22996         0.37080         -1.29218         -1.82981         -2.19480         -3.21601         -3.57202         -4.06521         -3.59763         -4.26402         -5.14501	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375 1.36756 -0.93573	-0.00002 -0.00001 -0.00001 -0.00002 -0.00003 -0.00001 -0.00001 -0.00001 -0.00001 -0.00003 -0.00003 -0.00003 -0.00001 -0.00001 0.00002 0.00001 0.00002 0.00001 0.00004 0.00004 0.00004 0.00006 0.00006	
Optimized C C C C C C C C C C C C C C C C C C C	geometries of 1         2.17585         2.26027         3.51027         4.64125         4.54138         3.30655         0.82918         0.15325         0.99004         3.58945         5.63006         5.45319         3.22996         0.37080         -1.29218         -2.19480         -3.21601         -3.57202         -4.06521         -3.59763         -4.26402         -5.14501         -1.04230	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375 1.36756 -0.93573 -2.75774	$\begin{array}{c} -0.00002\\ -0.0001\\ -0.0001\\ -0.0001\\ -0.0002\\ -0.0002\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00003\\ -0.00003\\ -0.00003\\ -0.00002\\ -0.00001\\ -0.00001\\ 0.00002\\ 0.00001\\ 0.00004\\ 0.00004\\ 0.00004\\ 0.00006\\ -0.00006\\ -0.00006\\ -0.00006\end{array}$	
Optimized C C C C C C C C N H H H H H H C C C C C	2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996 0.37080 -1.29218 -1.82981 -2.19480 -3.21601 -3.57202 -4.06521 -3.59763 -4.26402 -5.14501 -1.04230 -0.08806	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375 1.36756 -0.93573 -2.75774 -2.43953	$\begin{array}{c} -0.00002\\ -0.0001\\ -0.0001\\ -0.00001\\ -0.00002\\ -0.00002\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00003\\ -0.00003\\ -0.00003\\ -0.00002\\ -0.00001\\ -0.00001\\ 0.00002\\ 0.00001\\ 0.00004\\ 0.00004\\ 0.00004\\ 0.00004\\ 0.00006\\ -0.00006\\ -0.00010\\ \end{array}$	
Optimized C C C C C C C C N H H H H H H H C C C C	geometries of 1         2.17585         2.26027         3.51027         4.64125         4.54138         3.30655         0.82918         0.15325         0.99004         3.58945         5.63006         5.45319         3.22996         0.37080         -1.29218         -1.82981         -2.19480         -3.57202         -4.06521         -3.59763         -4.26402         -5.14501         -1.04230         -0.08806         -1.63289	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375 1.36756 -0.93573 -2.75774 -2.43953 1.97090	$\begin{array}{c} -0.00002\\ -0.0001\\ -0.0001\\ -0.0001\\ -0.0002\\ -0.0002\\ -0.0002\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00003\\ -0.00003\\ -0.00003\\ -0.00002\\ -0.00001\\ -0.00001\\ 0.00002\\ 0.00001\\ 0.00004\\ 0.00004\\ 0.00004\\ 0.00004\\ 0.00006\\ -0.00006\\ -0.00006\\ -0.00010\\ 0.00003\\ \end{array}$	
Optimized C C C C C C C C N H H H H H H H C C C C	geometries of 1         2.17585         2.26027         3.51027         4.64125         4.54138         3.30655         0.82918         0.15325         0.99004         3.58945         5.63006         5.45319         3.22996         0.37080         -1.29218         -1.82981         -2.19480         -3.21601         -3.57202         -4.06521         -3.59763         -4.26402         -5.14501         -1.04230         -0.08806         -1.63289         -2.49165	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375 1.36756 -0.93573 -2.75774 -2.43953 1.97090 3.10505	$\begin{array}{c} -0.00002\\ -0.0001\\ -0.0001\\ -0.0001\\ -0.0002\\ -0.0002\\ -0.0002\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00003\\ -0.00003\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ 0.00002\\ 0.00001\\ 0.00004\\ 0.00001\\ 0.00004\\ 0.00004\\ 0.00006\\ -0.00000\\ -0.00000\\ -0.0000\\ -0.0000\\ -0.0000\\ -0.0000\\ -0.000$	
Optimized C C C C C C C C N H H H H H H C C C C C	geometries of 1 2.17585 2.26027 3.51027 4.64125 4.54138 3.30655 0.82918 0.15325 0.99004 3.58945 5.63006 5.45319 3.22996 0.37080 -1.29218 -1.82981 -2.19480 -3.21601 -3.57202 -4.06521 -3.59763 -4.26402 -5.14501 -1.04230 -0.08806 -1.63289 -2.49165 -3.12199	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375 1.36756 -0.93573 -2.75774 -2.43953 1.97090 3.10505 3.12075	$\begin{array}{c} -0.00002\\ -0.0001\\ -0.0001\\ -0.0001\\ -0.0002\\ -0.0002\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00003\\ -0.00003\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ 0.00002\\ 0.00001\\ 0.00004\\ 0.00001\\ 0.00004\\ 0.00004\\ 0.00004\\ 0.00001\\ 0.00006\\ -0.00006\\ -0.00010\\ 0.00006\\ -0.00015\\ \end{array}$	
Optimized C C C C C C C C N H H H H H H C C C C C	geometries of 1         2.17585         2.26027         3.51027         4.64125         4.54138         3.30655         0.82918         0.15325         0.99004         3.58945         5.63006         5.45319         3.22996         0.37080         -1.29218         -1.29218         -2.19480         -3.21601         -3.57202         -4.06521         -3.59763         -4.26402         -5.14501         -1.04230         -0.08806         -1.63289         -2.49165         -3.12199         -3.12197	0.70577 -0.70445 -1.33424 -0.52501 0.88057 1.52285 0.98444 -0.20025 -1.23707 -2.42191 -0.98612 1.47958 2.61028 1.88586 -0.35944 -1.67334 0.73440 -1.87310 0.52947 -0.77857 -2.89375 1.36756 -0.93573 -2.75774 -2.43953 1.97090 3.10505 3.12075 3.12072	$\begin{array}{c} -0.00002\\ -0.0001\\ -0.0001\\ -0.0001\\ -0.0002\\ -0.0002\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00003\\ -0.00003\\ -0.00002\\ -0.00001\\ -0.00001\\ -0.00001\\ -0.00001\\ 0.00002\\ -0.00001\\ 0.00004\\ 0.00001\\ 0.00004\\ 0.00001\\ 0.00006\\ -0.00006\\ -0.00006\\ -0.00010\\ 0.00006\\ -0.00015\\ 0.90028\\ \end{array}$	

Optimized C	geometries of 2.17574	1	in the grour 0.70551	nd state in H2O (angstrom) -0.00002
С	2.26033		-0.70470	-0.00002
С	3.51046		-1.33439	-0.00002
С	4.64135		-0.52489	-0.00002
С	4.54123		0.88076	-0.00002
С	3.30627		1.52287	-0.00002
N	0.82917		0.98422	-0.00001
С	0.15319		-0.20024	-0.00001
N	0.99000		-1.23/29	-0.00001
H	3.59001		-2.42205	-0.00002
н u	5.63024		-0.98585	-0.00003
п u	3 22003		2 61023	-0.00003
н	0 37129		1 88601	-0.00001
C	-1.29229		-0.35949	0.00000
C	-1.83010		-1.67328	-0.00001
C	-2.19482		0.73455	0.00002
C	-3.21623		-1.87303	0.00001
С	-3.57215		0.52968	0.00004
С	-4.06541		-0.77827	0.00003
Н	-3.59825		-2.89357	0.00000
Н	-4.26400		1.36791	0.00005
Н	-5.14522		-0.93534	0.00005
0	-1.04224		-2.75787	-0.00004
Н	-0.08799		-2.43924	-0.00006
0	-1.63276		1.97053	0.00003
С	-2.49097		3.10537	0.00005
H	-3.12124		3.12128	-0.90015
H	-3.12122		3.12126	0.90027
H	-1.82914		3.9/6//	0.00006
Optimized	geometries of	1	in the S1 st	tate in THF (angstrom)
Optimized C	geometries of 2.19328	1	in the S1 st 0.68679	tate in THF (angstrom) -0.00041
Optimized C C	geometries of 2.19328 2.31388 3.56464	1	in the S1 st 0.68679 -0.72454 -1 34589	tate in THF (angstrom) -0.00041 0.00024 0.00051
Optimized C C C	geometries of 2.19328 2.31388 3.56464 4 69089	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760	tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010
Optimized C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501	tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054
Optimized C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497	tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082
Optimized C C C C C C N	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987	tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054
Optimized C C C C C C N C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789</pre>	tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001
Optimized C C C C C C N C N	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326</pre>	tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056
Optimized C C C C C N C N H	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117</pre>	tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100
Optimized C C C C C C N C N H H	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030</pre>
Optimized C C C C C C N C N H H H H	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085</pre>
Optimized C C C C C C N C N H H H H H	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136</pre>
Optimized C C C C C C N C N H H H H H	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00064</pre>
Optimized C C C C C C N C N H H H H C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.30113	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00064 -0.00003</pre>
Optimized C C C C C C N C N H H H H C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 2.0001	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00064 -0.00003 -0.00001</pre>
Optimized C C C C C C N C N H H H H C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 2.20057	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 1.55202	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00003 -0.00001 -0.00005 0.00005</pre>
Optimized C C C C C C N C N H H H H C C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.6063	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00001 -0.00005 -0.00010 -0.00010 -0.00028</pre>
Optimized C C C C C C N C N H H H H C C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00064 -0.00003 -0.00001 -0.00005 -0.00010 -0.00028 -0.00029</pre>
Optimized C C C C C C N C N H H H H C C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00001 -0.00005 -0.00001 -0.00028 -0.00029 -0.00013</pre>
Optimized C C C C C C N C N H H H C C C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485	1	in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00001 -0.00005 -0.00010 -0.00028 -0.00029 -0.00013 -0.00050</pre>
Optimized C C C C C C N C N H H H H C C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485 -5.23600	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231 -0.87885</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00001 -0.00005 -0.00001 -0.00005 -0.00010 -0.00028 -0.00029 -0.00013 -0.00050 -0.00050 -0.00044</pre>
Optimized C C C C C C N C N H H H H C C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485 -5.23600 -1.12227	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231 -0.87885 -2.73475</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00082 -0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00003 -0.00001 -0.00005 -0.00011 -0.00005 -0.00010 -0.00028 -0.00029 -0.00013 -0.00050 -0.00044 0.00006</pre>
Optimized C C C C C C N C N H H H H C C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485 -5.23600 -1.12227 0.70013	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231 -0.87885 -2.73475 -2.18391</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00003 -0.00001 -0.00005 -0.00010 -0.00028 -0.00028 -0.00029 -0.00013 -0.00050 -0.00050 -0.00050 -0.00058</pre>
Optimized C C C C C C N C N H H H H H C C C C C C	<pre>geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485 -5.23600 -1.12227 0.70013 -1.64426</pre>	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231 -0.87885 -2.73475 -2.18391 1.96273</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00064 -0.00003 -0.00001 -0.00005 -0.00010 -0.00028 -0.00028 -0.00029 -0.00013 -0.00050 -0.00050 -0.00050 -0.00058 -0.00058 -0.00058 -0.00006</pre>
Optimized C C C C C C N C N H H H H H C C C C C C	<pre>geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485 -5.23600 -1.12227 0.70013 -1.64426 -2.49583</pre>	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231 -0.87885 -2.73475 -2.18391 1.96273 3.10269</pre>	<pre>tate in THF (angstrom) -0.00041 0.00024 0.00051 0.00010 -0.00054 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00001 -0.00005 -0.00010 -0.00005 -0.00010 -0.00028 -0.00028 -0.00029 -0.00013 -0.00050 -0.00050 -0.00050 -0.00050 -0.00058 -0.00058 -0.00006 0.00058 -0.00006</pre>
Optimized C C C C C C C N C N H H H H C C C C C C	geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485 -5.23600 -1.12227 0.70013 -1.64426 -2.49583 -3.12462	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231 -0.87885 -2.73475 -2.18391 1.96273 3.10269 3.12928</pre>	<pre>tate in THF (angstrom) -0.00041 0.00051 0.00051 0.00054 -0.00054 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00001 -0.00005 -0.00010 -0.00005 -0.00010 -0.00028 -0.00028 -0.00029 -0.00013 -0.00050 -0.00050 -0.00050 -0.00050 -0.00058 -0.00058 -0.00006 0.00058 -0.00006 0.00122 -0.89984</pre>
Optimized C C C C C C C N C N H H H H C C C C C C	<pre>geometries of 2.19328 2.31388 3.56464 4.69089 4.57096 3.31460 0.84733 0.11690 1.04053 3.65949 5.68506 5.47232 3.22191 0.40541 -1.30113 -1.87662 -2.19201 -3.29957 -3.60663 -4.15401 -3.68622 -4.26485 -5.23600 -1.12227 0.70013 -1.64426 -2.49583 -3.12462 -3.12421</pre>	1	<pre>in the S1 st 0.68679 -0.72454 -1.34589 -0.50760 0.88501 1.51497 0.95987 -0.20789 -1.22326 -2.43117 -0.95712 1.49953 2.60059 1.86756 -0.36254 -1.71365 0.71741 -1.85903 0.52642 -0.75155 -2.87877 1.39231 -0.87885 -2.73475 -2.18391 1.96273 3.10269 3.12928 3.12754</pre>	<pre>tate in THF (angstrom) -0.00041 0.00051 0.00051 0.00054 -0.00082 -0.00054 0.00001 0.00056 0.00100 0.00030 -0.00085 -0.00136 -0.00003 -0.00001 -0.00005 -0.00010 -0.00005 -0.00010 -0.00028 -0.00028 -0.00029 -0.00013 -0.00050 -0.00050 -0.00050 -0.00058 -0.00058 -0.00058 -0.00006 0.00058 -0.00006 0.00122 -0.89984 0.90262</pre>

Optimized C C C C C C C N C C N H H H H H C C C C	<pre>geometries of 1         2.19073         2.31319         3.56446         4.68969         4.56787         3.31140         0.84607         0.11487         1.04075         3.66042         5.68437         5.46851         3.21558         0.40448         -1.29979         -1.88222         -2.19011         -3.30581         -3.60081         -4.15500         -3.69664         -4.25738         -5.23758         -1.12954         0.70653         -1.63620         -2.48394         -3.11285         -3.11242         -1.81216</pre>	<pre>in the S1 st 0.68416 -0.72776 -1.34720 -0.50805 0.88545 1.51342 0.95673 -0.21211 -1.22808 -2.43243 -0.95649 1.50108 2.59874 1.86512 -0.36374 -1.71489 0.72128 -1.85607 0.53244 -0.74644 -2.87442 1.39978 -0.86805 -2.73745 -2.18997 1.96383 3.10716 3.13492 3.13331 3.97100</pre>	<pre>tate in MeCN -0.00035 0.00018 0.00041 0.00008 -0.00044 -0.00068 -0.00049 -0.00003 0.00045 0.00024 -0.000081 0.00024 -0.00008 -0.00110 -0.00004 -0.00004 -0.00004 -0.00004 -0.00004 -0.00003 -0.00004 -0.00003 0.00041 -0.00028 0.00003 0.00044 -0.00012 0.00109 -0.89980 0.90232 0.00168</pre>	(angstrom)
Optimized C C C	geometries of <b>1</b> 2.19089 2.31329 3.56449	in the S1 st 0.68413 -0.72774 -1.34729	tate in MeOH -0.00029 0.00011 0.00027	(angstrom)
Optimized C C C	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822	tate in MeOH -0.00029 0.00011 0.00027 0.00001	(angstrom)
Optimized C C C C C C C	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054	(angstrom)
Optimized C C C C C C N	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11405	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037	(angstrom)
Optimized C C C C C C N C N N	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031	(angstrom)
Optimized C C C C C N C N H H	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.60451	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056	(angstrom)
Optimized C C C C C C N C N H H H	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076</pre>	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056 0.00013 -0.00056	(angstrom)
Optimized C C C C C N C N H H H H H	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00031 0.00056 0.00013 -0.00056 -0.00086	(angstrom)
Optimized C C C C C C N C N H H H H C	geometries of 1 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1 29996	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056 0.00013 -0.00056 -0.00086 -0.00041 -0.0002	(angstrom)
Optimized C C C C C C N C N H H H H H C C	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489</pre>	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056 0.00013 -0.00056 -0.00086 -0.00041 -0.00002 -0.00001	(angstrom)
Optimized C C C C C C N C N H H H H H C C C C	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 2.2060	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131</pre>	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056 -0.00013 -0.00056 -0.00041 -0.00001 -0.00001 -0.00001	(angstrom)
Optimized C C C C C C N C N H H H H H C C C C C C	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230</pre>	<pre>tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00037 -0.00003 0.00056 0.00013 -0.00056 -0.00056 -0.00056 -0.00041 -0.00002 -0.00001 -0.00003 -0.00013 -0.00013</pre>	(angstrom)
Optimized C C C C C C C N C N H H H H H H C C C C	geometries of <b>1</b> 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102 -4.15513	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230 -0.74667</pre>	<pre>tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00034 -0.00037 -0.00002 0.00031 0.00056 -0.00056 -0.00056 -0.00086 -0.00041 -0.00002 -0.00001 -0.00001 -0.00003 -0.00013 -0.00013 -0.00012</pre>	(angstrom)
Optimized C C C C C C N C N C N H H H H H C C C C	geometries of 1 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102 -4.15513 -3.69687 4.2520	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230 -0.74667 -2.87457 -2.87457	<pre>tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056 -0.00041 -0.00001 -0.00001 -0.00001 -0.00013 -0.00013 -0.00013 -0.00013 -0.00012 -0.00014 -0.00013 -0.00012 -0.0004</pre>	(angstrom)
Optimized C C C C C C C N C N H H H H C C C C C C	geometries of 1 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102 -4.15513 -3.69687 -4.25792 -5.23773	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230 -0.74667 -2.87457 1.39934 -0.86827</pre>	<pre>tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00013 -0.00056 -0.00056 -0.00056 -0.00056 -0.00041 -0.00001 -0.00001 -0.00001 -0.00013 -0.00013 -0.00012 -0.00014 -0.00025 -0.00018</pre>	(angstrom)
Optimized C C C C C C C N C N H H H H H C C C C C	geometries of 1 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102 -4.15513 -3.69687 -4.25792 -5.23773 -1.12961	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230 -0.74667 -2.87457 1.39934 -0.86827 -2.73738	tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056 0.00013 -0.000056 -0.000041 -0.00000 -0.00000 -0.000	(angstrom)
Optimized C C C C C C C N C N H H H H H C C C C C	geometries of 1 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102 -4.15513 -3.69687 -4.25792 -5.23773 -1.12961 0.70641 1.62020	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230 -0.74667 -2.87457 1.39934 -0.86827 -2.73738 -2.18987 1.06406</pre>	<pre>tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00031 0.00056 -0.00041 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00025 -0.00018 0.00000 0.00032</pre>	(angstrom)
Optimized C C C C C C C N C N H H H H H C C C C C	geometries of 1 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102 -4.15513 -3.69687 -4.25792 -5.23773 -1.12961 0.70641 -1.63628 -2.48367	<pre>in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230 -0.74667 -2.87457 1.39934 -0.86827 -2.73738 -2.18987 1.96406 3.10765</pre>	<pre>tate in MeOH -0.00029 0.00011 0.00027 0.00001 -0.00038 -0.00054 -0.00037 -0.00002 0.00013 -0.00056 -0.00041 -0.00001 -0.00001 -0.00001 -0.00001 -0.00013 -0.00013 -0.00013 -0.00013 -0.00012 -0.00014 -0.00025 -0.00018 0.00000 0.00032 -0.00005 0.00091</pre>	(angstrom)
Optimized C C C C C C C N C N H H H H H H C C C C	geometries of 1 2.19089 2.31329 3.56449 4.68979 4.56805 3.31163 0.84617 0.11485 1.04077 3.66021 5.68451 5.46880 3.21585 0.40431 -1.29996 -1.88237 -2.19029 -3.30601 -3.60102 -4.15513 -3.69687 -4.25792 -5.23773 -1.12961 0.70641 -1.63628 -2.48367 -3.11251	in the S1 st 0.68413 -0.72774 -1.34729 -0.50822 0.88528 1.51331 0.95668 -0.21215 -1.22801 -2.43253 -0.95659 1.50076 2.59863 1.86497 -0.36364 -1.71489 0.72131 -1.85625 0.53230 -0.74667 -2.87457 1.39934 -0.86827 -2.73738 -2.18987 1.96406 3.10765 3.13560	in MeOH           -0.00029           0.00011           0.00027           0.00001           -0.00038           -0.00034           -0.00037           -0.00031           0.00056           0.00013           -0.00056           -0.00002           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00002           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00001           -0.00002           -0.00001           -0.00001           -0.00002           -0.00001           -0.00002           -0.00001           -0.00002           -0.00001           -0.00005           -0.00005           -0.00005           -0.00005           -0.00005	(angstrom)

Optimized C C C C C C C C N C C N C C C C C C C	<pre>geometries of : 2.19038 2.31319 3.56453 4.68956 4.56737 3.31089 0.84594 0.11450 1.04085 3.66053 5.68441 5.46794 3.21421 0.40425 -1.29963 -1.88332 -2.18990 -3.30709 -3.59984 -4.15520 -3.69881 -4.25636 -5.23791 -1.13080 0.70771 -1.63484 -2.48179 -3.11066 -3.11033 -1.80928</pre>	<pre>I in the S1 stat 0.68362 -0.72836 -1.34748 -0.50812 0.88556 1.51313 0.95607 -0.21298 -1.22898 -2.43270 -0.95621 1.50131 2.59837 1.86454 -0.36389 -1.71517 0.72203 -1.85573 0.53348 -0.74572 -2.87376 1.40085 -0.86628 -2.73787 -2.19109 1.96425 3.10824 3.13505 3.97147</pre>	<pre>te in H2O (angstrom) -0.00024 0.00005 0.00016 -0.00004 -0.00032 -0.00029 -0.00029 -0.00023 0.00038 0.00033 -0.00047 -0.00066 -0.00031 -0.00001 0.00000 0.00000 0.00000 -0.00008 -0.00001 -0.00001 -0.00018 -0.00011 0.00000 0.000022 -0.00004 0.00079 -0.90011 0.90195 0.00117</pre>	
Optimized C	geometries of 2.81295	2 in the ground -0.77820	state in THF (angst 0.00005	rom)
С	2.66267	0.62602	-0.00003	
С	3.79112	1.45199	-0.00008	
С	5.04110	0.84080	-0.00004	
С	5.17436	-0.56052	0.00004	
С	4.06126	-1.39768	0.00008	
Ν	1.52675	-1.27545	0.00006	
С	0.66627	-0.21329	0.00002	
N	1.32036	0.94333	-0.00005	
Н	3.68870	2.53762	-0.00014	
Н	5.93992	1.45919	-0.00008	
Н	6.17209	-1.00164	0.00006	
Н	4.16615	-2.48298	0.00014	
Н	1.26870	-2.25096	0.00017	
С	0 77064		0 0000	
С	-0.77964	-0.30648	0.00002	
С	-1.54925	-0.30648 0.88178	0.00002	
	-1.54925 -1.46348	-0.30648 0.88178 -1.53585	0.00002 0.00001 0.00001	
С	-1.54925 -1.46348 -2.94884	-0.30648 0.88178 -1.53585 0.82186	0.00002 0.00001 0.00001 -0.00001	
C C	-1.54925 -1.46348 -2.94884 -2.84179	-0.30648 0.88178 -1.53585 0.82186 -1.60581	0.00002 0.00001 0.00001 -0.00001 -0.00001	
C C H	-0.77964 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075	0.00002 0.00001 0.00001 -0.00001 0.00000	
C C H C	-0.77984 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401	0.00002 0.00001 0.00001 -0.00001 -0.00001 0.00000 -0.00002	
C C H C H	-0.77984 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080 -3.49545	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401 1.76250	0.00002 0.00001 -0.00001 -0.00001 0.00000 -0.00002 -0.00001	
C C H C H H	-0.77964 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080 -3.49545 -3.36193	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401 1.76250 -2.56288	0.00002 0.00001 -0.00001 -0.00001 0.00000 -0.00002 -0.00001 -0.00003	
С С Н Н Н Н О	-0.77964 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080 -3.49545 -3.36193 -0.98156	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401 1.76250 -2.56288 2.09586	0.00002 0.00001 -0.00001 -0.00001 0.00000 -0.00002 -0.00001 -0.00003 0.00004	
С С Н С Н Н Н О Н	-0.77964 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080 -3.49545 -3.36193 -0.98156 0.01076 -4.92287	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401 1.76250 -2.56288 2.09586 1.96117 -0.56707	0.00002 0.00001 -0.00001 -0.00001 0.00000 -0.00002 -0.00001 -0.00003 0.00004 0.00010 -0.00004	
С С Н Н Н Н О Н	-0.77964 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080 -3.49545 -3.36193 -0.98156 0.01076 -4.93387 -5.72769	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401 1.76250 -2.56288 2.09586 1.96117 -0.56797 0.60250	0.00002 0.00001 -0.00001 -0.00001 0.00000 -0.00002 -0.00001 -0.00003 0.00004 0.00010 -0.00004 -0.00004	
С С Н Н Н О Н О С С	-0.77964 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080 -3.49545 -3.36193 -0.98156 0.01076 -4.93387 -5.73768 -6.77400	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401 1.76250 -2.56288 2.09586 1.96117 -0.56797 0.60259 0.25242	0.00002 0.00001 -0.00001 -0.00001 -0.00000 -0.00002 -0.00001 -0.00003 0.00004 0.00010 -0.00004 -0.00004 -0.00004 -0.00004	
С С Н Н Н О Н О С Н Н Н	-0.77964 -1.54925 -1.46348 -2.94884 -2.84179 -0.90062 -3.59080 -3.49545 -3.36193 -0.98156 0.01076 -4.93387 -5.73768 -6.77499 -5.55460	-0.30648 0.88178 -1.53585 0.82186 -1.60581 -2.47075 -0.41401 1.76250 -2.56288 2.09586 1.96117 -0.56797 0.60259 0.25343 1.20887	0.00002 0.00001 -0.00001 -0.00001 0.00000 -0.00002 -0.00003 0.00004 0.00010 -0.00004 -0.00004 -0.00004 -0.00004 -0.00006 0.89946	

Optimized C C C C C C C N C N N H H H H H C C C C	<pre>geometries of 2     2.81257     2.66275     3.79119     5.04143     5.17431     4.06117     1.52709     0.66661     1.32007     3.68932     5.94030     6.17196     4.16520     1.27022     0.77990     -1.54940     -1.46378     -2.94904     -2.84231     -0.90131     -3.59114     -3.49618     -3.36199     -0.97966     0.01288     -4.93417     -5.73837     -6.77560     -5.55538 </pre>	<pre>in the ground -0.77806 0.62639 1.45281 0.84134 -0.56041 -1.39780 -1.27548 -0.21444 0.94337 2.53862 1.45969 -1.00179 -2.48301 -2.25189 -0.30749 0.88083 -1.53704 0.82233 -1.60583 -2.47187 -0.41380 1.76279 -2.56325 2.09532 1.95849 -0.56718 0.60395 0.25490 1.21018 1.21018</pre>	<pre>state in MeCN         0.00005         -0.00002         -0.00003         0.00002         0.00002         -0.00002         -0.00002         -0.00008         0.00001         0.00012         0.00014         0.00003         -0.00003         -0.00003         -0.00003         -0.00002         -0.00004         -0.00003         -0.00002         -0.00004         -0.00003         -0.00004         -0.00003         -0.00002         -0.00004         -0.00003         -0.00003         -0.00003         -0.00002         -0.00004         -0.00003         -0.00004         -0.00003         -0.00004         -0.00003         -0.00004         -0.00003         -0.00003         -0.00003         -0.00002         -0.00002         -0.00002         -0.00003         -0.00003         -0.00003         -0.00003         -0.00002         -0.00004         -0.00003         -0.00003         -0.00003         -0.00003         -0.00004         -0.00003         -0.00003         -0.00003         -0.00004         -0.00003         -0.00002         -0.00003         -0.00003         -0.00003         -0.00003         -0.00004         -0.0003         -0.00003         -0.00003         -0.00003         -0.00003         -0.00003         -0.00003         -0.00003         -0.00003         -0.00003         -0.00002         -0.00004         -0.00003         -0.00004         -0.0003</pre>	(angstrom)
Ontimized	geometries of 2	in the ground	state in MeOH	(angstrom)
C	2.81262	-0.77801	0.00005	
C C	2.81262	-0.77801 0.62640	0.00005 -0.00003	
C C	2.81262 2.66274 3.79121	-0.77801 0.62640 1.45276	0.00005 -0.00003 -0.00008	
	2.81262 2.66274 3.79121 5.04130	-0.77801 0.62640 1.45276 0.84130	0.00005 -0.00003 -0.00008 -0.00003	
	2.81262 2.66274 3.79121 5.04130 5.17423	-0.77801 0.62640 1.45276 0.84130 -0.56038	0.00005 -0.00003 -0.00008 -0.00003 0.00005	
	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774	0.00005 -0.00003 -0.00008 -0.00003 0.00005	
C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554	0.00005 -0.00003 -0.00008 -0.00003 0.00005 0.00009	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454	0.00005 -0.00003 -0.00008 -0.00003 0.00005 0.00009 0.00006 0.00001	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328	0.00005 -0.00003 -0.00008 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855	0.00005 -0.00003 -0.00008 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961	0.00005 -0.00003 -0.00008 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161	0.00005 -0.00003 -0.00008 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007 0.00008	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298	0.00005 -0.00003 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007 0.00008 0.00016	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183	0.00005 -0.00003 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007 0.00007 0.00008 0.00016 0.00022	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739	0.00005 -0.00003 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007 0.00007 0.00008 0.00016 0.00022 0.00000	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 0.00000	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 0.00000 -0.00002	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 0.00001 -0.00006 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 0.00000 -0.00002 -0.00001	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 -0.00001 -0.00006 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 0.00000 -0.00001 -0.00001 -0.00003	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 -0.00001 -0.00006 -0.00015 -0.00007 0.00008 0.00016 0.000022 0.00000 0.00000 -0.00002 -0.00001 -0.00003 -0.00003	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123 -3.59118	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 -0.00001 -0.00006 -0.00015 -0.00007 0.00008 0.00016 0.00002 0.00000 -0.00002 -0.00001 -0.00003 -0.00003 -0.00003 -0.00002	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123 -3.59118 -3.49576	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 -0.00001 -0.00001 -0.00007 0.00008 0.00016 0.00002 0.00000 -0.00000 -0.00001 -0.00003 -0.00003 -0.00003 -0.00002 -0.00001	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123 -3.59118 -3.49576 -3.36186	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284 -2.56307	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00009 0.00006 -0.00001 -0.000015 -0.00007 0.00008 0.00016 0.00002 0.00000 -0.00000 -0.00001 -0.00003 -0.00003 -0.00003 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123 -3.59118 -3.49576 -3.36186 -0.97951	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284 -2.56307 2.09519	0.00005 -0.00003 -0.00003 -0.00005 0.00005 0.00006 0.00001 -0.000015 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 -0.00002 -0.00002 -0.00003 -0.00003 -0.00002 -0.00003 -0.00002 -0.00003 -0.00002 -0.00003 -0.00003 -0.00003 -0.00004 0.00003	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123 -3.59118 -3.49576 -3.36186 -0.97951 0.01298	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284 -2.56307 2.09519 1.95746	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00006 0.00001 -0.00015 -0.00015 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 -0.00002 -0.00001 -0.00003 -0.00003 -0.00001 -0.00003 -0.00004 0.00003 0.00003 0.00004 0.00003 0.00003 0.00004	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123 -3.59118 -3.49576 -3.36186 -0.97951 0.01298 -4.93416	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284 -2.56307 2.09519 1.95746 -0.56711	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00006 0.00001 -0.00015 -0.00015 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 -0.00002 -0.00001 -0.00003 -0.00003 -0.00003 -0.00004 0.00006 -0.00003	
C C C C C C C C C C C C C C C C C C C	2.81262 2.66274 3.79121 5.04130 5.17423 4.06114 1.52697 0.66656 1.32011 3.68948 5.94019 6.17193 4.16511 1.27018 -0.77976 -1.54925 -1.46370 -2.94875 -2.84226 -0.90123 -3.59118 -3.49576 -3.36186 -0.97951 0.01298 -4.93416 -5.73885	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284 -2.56307 2.09519 1.95746 -0.56711 0.60389	0.00005 -0.00003 -0.00003 -0.00005 0.00005 0.00006 0.00001 -0.00015 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 -0.00002 -0.00002 -0.00003 -0.000003 -0.000003 -0.000003 -0.000003 -0.000003 -0.000003 -0.00003 -0.00003 -0.00003 -0.00003 -0.00003 -0.00003 -0.000003 -0.00003 -0.00003 -0.00003 -0.00003 -0.00003 -0.00003 -0.00000000000000000000000000000000000	
C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 2.81262\\ 2.66274\\ 3.79121\\ 5.04130\\ 5.17423\\ 4.06114\\ 1.52697\\ 0.66656\\ 1.32011\\ 3.68948\\ 5.94019\\ 6.17193\\ 4.16511\\ 1.27018\\ -0.77976\\ -1.54925\\ -1.46370\\ -2.94875\\ -2.84226\\ -0.90123\\ -3.59118\\ -3.49576\\ -3.36186\\ -0.97951\\ 0.01298\\ -4.93416\\ -5.73885\\ -6.77597\end{array}$	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284 -2.56307 2.09519 1.95746 -0.56711 0.60389 0.25443	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00006 0.00001 -0.00015 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 -0.00002 -0.00002 -0.00003 -0.000003 -0.0000003 -0.000003 -0.000003 -0.000003 -0.00000	
C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 2.81262\\ 2.66274\\ 3.79121\\ 5.04130\\ 5.17423\\ 4.06114\\ 1.52697\\ 0.66656\\ 1.32011\\ 3.68948\\ 5.94019\\ 6.17193\\ 4.16511\\ 1.27018\\ -0.77976\\ -1.54925\\ -1.46370\\ -2.94875\\ -2.84226\\ -0.90123\\ -3.59118\\ -3.49576\\ -3.36186\\ -0.97951\\ 0.01298\\ -4.93416\\ -5.73885\\ -6.77597\\ -5.55574\end{array}$	-0.77801 0.62640 1.45276 0.84130 -0.56038 -1.39774 -1.27554 -0.21454 0.94328 2.53855 1.45961 -1.00161 -2.48298 -2.25183 -0.30739 0.88078 -1.53684 0.82237 -1.60564 -2.47175 -0.41369 1.76284 -2.56307 2.09519 1.95746 -0.56711 0.60389 0.25443 1.20989	0.00005 -0.00003 -0.00003 -0.00003 0.00005 0.00006 0.00001 -0.00015 -0.00015 -0.00007 0.00008 0.00016 0.00022 0.00000 -0.00002 -0.00001 -0.00003 -0.000003 -0.000003 -0.000003 -0.000003 -0.000003 -0.0000	

Optimized	geometries of ${\bf 2}$	in the ground s	tate in H2O	(angstrom)
С	2.81263	-0.77791	0.00005	
С	2.66249	0.62649	-0.00003	
С	3.79093	1.45304	-0.00008	
С	5.04109	0.84165	-0.00004	
С	5.17419	-0.56010	0.00004	
С	4.06121	-1.39761	0.00009	
N	1.52705	-1.27575	0.00007	
С	0.66657	-0.21518	0.00002	
N	1.31980	0.94307	-0.00005	
H	3.68932	2.53886	-0.00015	
H	5.93994	1.46004	-0.00008	
H	6.17199	-1.00112	0.00007	
H	4.16501	-2.48284	0.00015	
Н	1.27077	-2.25225	0.00018	
С	-0.77975	-0.30780	0.00001	
С	-1.54917	0.88041	0.00001	
С	-1.46382	-1.53722	0.00000	
С	-2.94861	0.82230	-0.00001	
С	-2.84243	-1.60575	-0.00002	
Н	-0.90152	-2.47221	-0.00001	
С	-3.59133	-0.41376	-0.00002	
Н	-3.49575	1.76273	-0.00001	
Н	-3.36184	-2.56330	-0.00003	
0	-0.97899	2.09497	0.00004	
Н	0.01374	1.95710	0.00008	
0	-4.93418	-0.56681	-0.00004	
С	-5.73868	0.60478	-0.00004	
Н	-6.77580	0.25545	-0.00004	
Н	-5.55520	1.21047	0.89951	
H	-5.55519	1.21048	-0.89957	
Optimized	geometries of <b>2</b>	in the S1 state	keto form -	in THF (angstrom)
Optimized	geometries of <b>2</b>	in the S1 state	e keto form : 0.00006	in THF (angstrom)
Optimized C	geometries of 2 2.82127 2.72063	in the S1 state -0.76990 0.64509	e keto form : 0.00006 -0.00004	in THF (angstrom)
Optimized c c c	geometries of 2 2.82127 2.72063 3.86235	in the S1 state -0.76990 0.64509 1.45372	<pre>keto form : 0.00006 -0.00004 -0.00009</pre>	in THF (angstrom)
Optimized C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043	in the S1 state -0.76990 0.64509 1.45372 0.79819	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004</pre>	in THF (angstrom)
Optimized c c c c c	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799	in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006</pre>	in THF (angstrom)
Optimized C C C C C C	geometries of <b>2</b> 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012</pre>	in THF (angstrom)
Optimized C C C C C C N	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008</pre>	in THF (angstrom)
Optimized C C C C C C N C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003</pre>	in THF (angstrom)
Optimized C C C C C C N C N	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006</pre>	in THF (angstrom)
Optimized C C C C C C N C N H	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016</pre>	in THF (angstrom)
Optimized C C C C C C N C N H H	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008</pre>	in THF (angstrom)
Optimized C C C C C C N C N H H H	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00016 -0.00008 0.00010</pre>	in THF (angstrom)
Optimized C C C C C C N C N H H H H	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00016 -0.00008 0.00010 0.00020</pre>	in THF (angstrom)
Optimized C C C C C C N C N H H H H H H	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00016 -0.00010 0.00020 0.00021</pre>	in THF (angstrom)
Optimized C C C C C C N C N H H H H H C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00016 -0.00010 0.00020 0.00021 -0.00001</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00016 -0.00016 0.00020 0.00021 -0.00001 0.00001</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00016 -0.00016 0.00020 0.00021 -0.00001 0.00000 -0.00005</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00006 -0.00016 0.00020 0.00021 -0.00001 0.00001 0.00000 -0.00005 -0.00002</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00006 -0.00016 0.00020 0.00021 -0.00001 0.000021 -0.00001 0.00005 -0.00005 -0.00002 -0.00004</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H H H H	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00006 -0.00016 0.00020 0.00021 -0.00001 0.000021 -0.00001 0.00005 -0.00005 -0.00002 -0.00004 -0.00008</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00005 -0.00002 -0.00004 -0.00008 -0.00008 -0.00008</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00001 0.00005 -0.00002 -0.00004 -0.00008 -0.00003 -0.00003 -0.00001</pre>	in THF (angstrom)
Optimized C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144 -3.38042	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835 -2.54351</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00005 -0.00003 -0.00003 -0.00001 -0.00005</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144 -3.38042 -1.01012	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835 -2.54351 2.07476</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00005 -0.00003 -0.00003 -0.00001 -0.00005 0.00005 0.00002</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144 -3.38042 -1.01012 0.89982	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835 -2.54351 2.07476 1.83463</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00005 -0.00003 -0.00003 -0.00001 -0.00005 0.00002 -0.00005</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144 -3.38042 -1.01012 0.89982 -4.99549	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835 -2.54351 2.07476 1.83463 -0.58368</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00002 -0.00003 -0.00003 -0.00003 -0.00003 -0.00003 -0.00005 0.00002 -0.00008 -0.00008 -0.00008 -0.00008 -0.00008 -0.00008 -0.00008</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144 -3.38042 -1.01012 0.89982 -4.99549 -5.80639	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835 -2.54351 2.07476 1.83463 -0.58368 0.57881</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00002 -0.00004 -0.00003 -0.00003 -0.00003 -0.00003 -0.00002 0.00002 -0.00008 -0.00002 0.00002 -0.00008 -0.00002</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144 -3.38042 -1.01012 0.89982 -4.99549 -5.80639 -6.84213	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835 -2.54351 2.07476 1.83463 -0.58368 0.57881 0.22387</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00002 -0.00004 -0.00003 -0.00003 -0.00003 -0.00001 -0.00002 0.00002 0.00001 0.00001</pre>	in THF (angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of 2 2.82127 2.72063 3.86235 5.10043 5.19799 4.05639 1.53229 0.63385 1.38827 3.78887 6.01429 6.18413 4.13184 1.27539 -0.78728 -1.58947 -1.46632 -3.00952 -2.87616 -0.91912 -3.64643 -3.56144 -3.38042 -1.01012 0.89982 -4.99549 -5.80639 -6.84213 -5.62912	<pre>in the S1 state -0.76990 0.64509 1.45372 0.79819 -0.59900 -1.41594 -1.24772 -0.20400 0.93903 2.54038 1.39425 -1.06514 -2.50290 -2.22340 -0.29328 0.94577 -1.51534 0.84012 -1.57673 -2.45887 -0.40818 1.77835 -2.54351 2.07476 1.83463 -0.58368 0.57881 0.22387 1.18921</pre>	<pre>keto form : 0.00006 -0.00004 -0.00009 -0.00004 0.00006 0.00012 0.00008 0.00003 -0.00006 -0.00016 -0.00008 0.00010 0.00020 0.00021 -0.00001 0.00002 -0.00005 -0.00002 -0.00004 -0.00003 -0.00003 -0.00003 -0.00003 -0.00003 -0.00001 0.00002 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001 0.00001</pre>	in THF (angstrom)

Optimized C C C C C C C N C C N H H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363     -3.56709     -3.37318     -1.01314     0.90911     -4.99213     -5.80866     -6.84283     -5.63350</pre>	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00007 -0.00011 0.00021 0.00023 -0.00001 0.00000 -0.00001 -0.00001 -0.00005 -0.00001 -0.00005 -0.00001 -0.00002 -0.00007 0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.89865 -0.89860	in MeCN	(angstrom)
Optimized	geometries of 2	in the S1 st	ate keto form	in MeOH	(angstrom)
Optimized C	geometries of 2 2.81810 2.72094	in the S1 st -0.77028	ate keto form 0.00006 -0.00004	in MeOH	(angstrom)
Optimized C C	geometries of 2 2.81810 2.72094 3.86449	in the S1 st -0.77028 0.64648 1 45217	ate keto form 0.00006 -0.00004 -0.00009	in MeOH	(angstrom)
Optimized C C C	geometries of 2 2.81810 2.72094 3.86449 5.10084	in the S1 st -0.77028 0.64648 1.45217 0 79424	ate keto form 0.00006 -0.00004 -0.00009 -0.00004	in MeOH	(angstrom)
Optimized C C C C	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506	<pre>! in the S1 st -0.77028 0.64648 1.45217 0.79424 -0 60448</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007	in MeOH	(angstrom)
Optimized C C C C C	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256	<pre>! in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1 41864</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012	in MeOH	(angstrom)
Optimized C C C C C C C N	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256 1 53037	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1 24552</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00008	in MeOH	(angstrom)
Optimized C C C C C C C N C	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256 1.53037 0.63203	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00008 0.00003	in MeOH	(angstrom)
Optimized C C C C C C C N C N N	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256 1.53037 0.63203 1.39056	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00008 0.00003 -0.00007	in MeOH	(angstrom)
Optimized C C C C C C C N C N H	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256 1.53037 0.63203 1.39056 3.79277	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00008 0.00003 -0.00007 -0.00017	in MeOH	(angstrom)
Optimized C C C C C C C N C N H H	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256 1.53037 0.63203 1.39056 3.79277 6.01612	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00008 0.00003 -0.00007 -0.00017 -0.00018	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00008 0.00003 -0.00007 -0.00017 -0.00011	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00008 0.00003 -0.00007 -0.00017 -0.00017 -0.00008 0.00011 0.00021	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H H	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00007 -0.00017 -0.00011 0.00021 0.00023	in MeOH	(angstrom)
Optimized C C C C C C C N C N H H H H C	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256 1.53037 0.63203 1.39056 3.79277 6.01612 6.18029 4.12488 1.27314 -0.78495	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00007 -0.00017 -0.00001 0.00021 0.00023 -0.00001	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H H C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179</pre>	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.000017 -0.00001 0.00021 0.00023 -0.00001 0.00001 0.00001	in MeOH	(angstrom)
Optimized C C C C C C C N C N H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328</pre>	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00017 -0.00011 0.00021 0.00023 -0.00001 0.00000 -0.00006	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154 -0.28888 0.95107 -1.51588 0.84221</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00007 0.00012 0.00003 -0.00007 -0.00007 -0.00017 -0.00001 0.00021 0.00023 -0.00001 0.00000 -0.00006 -0.00001	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154 -0.28888 0.95107 -1.51588 0.84221 -1.57661</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00007 0.00012 0.00003 -0.00007 -0.00007 -0.00017 -0.00001 0.00021 0.00023 -0.00001 0.00000 -0.00000 -0.00006 -0.00001 -0.00005	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154 -0.28888 0.95107 -1.51588 0.84221 -1.57661 -2.45804</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00007 -0.00011 0.00021 0.00023 -0.00001 0.00000 -0.00000 -0.00006 -0.00001 -0.00005 -0.00010	in MeOH	(angstrom)
Optimized C C C C C C C N C N H H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154 -0.28888 0.95107 -1.51588 0.84221 -1.57661 -2.45804 -0.40664</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00007 -0.00011 0.00021 0.00023 -0.00001 0.00000 -0.00001 -0.00005 -0.00010 -0.00003	in MeOH	(angstrom)
Optimized C C C C C C C N C N H H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363     -3.56709</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154 -0.28888 0.95107 -1.51588 0.84221 -1.57661 -2.45804 -0.40664 1.77844</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00017 -0.00011 0.00021 0.00023 -0.00001 0.00000 -0.00001 -0.00005 -0.00010 -0.00003 0.00000	in MeOH	(angstrom)
Optimized C C C C C C C N C N H H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363     -3.56709     -3.37318</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154 -0.28888 0.95107 -1.51588 0.84221 -1.57661 -2.45804 -0.40664 1.77844 -2.54390</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00001 0.00021 0.00023 -0.00001 0.00001 -0.00001 -0.00005 -0.00010 -0.00003 0.00000 -0.00007	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363     -3.56709     -3.37318     -1.01314</pre>	<pre>2 in the S1 st -0.77028 0.64648 1.45217 0.79424 -0.60448 -1.41864 -1.24552 -0.19937 0.94399 2.53896 1.38814 -1.07264 -2.50572 -2.22154 -0.28888 0.95107 -1.51588 0.84221 -1.57661 -2.45804 -0.40664 1.77844 -2.54390 2.08007</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00001 0.00021 0.00023 -0.00001 0.00001 -0.00005 -0.00010 -0.00005 -0.00010 -0.00005 -0.00000 -0.00007 0.00007 0.00007 0.00007	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363     -3.56709     -3.37318     -1.01314     0.90911 </pre>	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00007 -0.00011 0.00021 0.00023 -0.00001 0.00001 -0.00005 -0.00001 -0.00005 -0.00001 -0.00005 -0.00000 -0.00007 0.00002 -0.00007 0.00002 -0.00009	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H H C C C C	geometries of 2 2.81810 2.72094 3.86449 5.10084 5.19506 4.05256 1.53037 0.63203 1.39056 3.79277 6.01612 6.18029 4.12488 1.27314 -0.78495 -1.59179 -1.46328 -3.01159 -2.86951 -0.91434 -3.64363 -3.56709 -3.37318 -1.01314 0.90911 -4.99213	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00007 -0.00011 0.00021 0.00023 -0.00001 0.00001 -0.00005 -0.00001 -0.00005 -0.00001 -0.00005 -0.00000 -0.00007 0.00002 -0.00009 -0.00002	in MeOH	(angstrom)
Optimized C C C C C C C N C C N C N H H H H H H C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.10084     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363     -3.56709     -3.37318     -1.01314     0.90911     -4.99213     -5.80866     6     2022 </pre>	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00001 0.00021 0.00023 -0.00001 0.00001 -0.00005 -0.00001 -0.00005 -0.00001 -0.00005 -0.00000 -0.00007 0.00002 -0.00002	in MeOH	(angstrom)
Optimized C C C C C C C C N C C C C C C C C C C	<pre>geometries of 2     2.81810     2.72094     3.86449     5.19506     4.05256     1.53037     0.63203     1.39056     3.79277     6.01612     6.18029     4.12488     1.27314     -0.78495     -1.59179     -1.46328     -3.01159     -2.86951     -0.91434     -3.64363     -3.56709     -3.37318     -1.01314     0.90911     -4.99213     -5.80866     -6.84283     _5.2320 </pre>	<pre>2 in the S1 st</pre>	ate keto form 0.00006 -0.00004 -0.00009 -0.00004 0.00007 0.00012 0.00003 -0.00007 -0.00017 -0.00001 0.00021 0.00023 -0.00001 0.00000 -0.00001 -0.00005 -0.00001 -0.00005 -0.00001 -0.00005 -0.00000 -0.00007 0.00002 -0.00002 -0.00002 0.00001 0.00002 -	in MeOH	(angstrom)

Optimized	geometries of ${\bf 2}$	in the S1 stat	e keto form	in H2O	(angstrom)
С	2.81742	-0.77050	0.00006		
С	2.72048	0.64660	-0.00004		
С	3.86416	1.45224	-0.00008		
С	5.10030	0.79420	-0.00003		
С	5.19436	-0.60485	0.00006		
С	4.05204	-1.41895	0.00011		
N	1.53015	-1.24567	0.00008		
С	0.63160	-0.19924	0.00002		
N	1.39045	0.94436	-0.00006		
Н	3.79218	2.53901	-0.00015		
Н	6.01579	1.38779	-0.00007		
Н	6.17966	-1.07286	0.00010		
Н	4.12403	-2.50602	0.00019		
H	1.27296	-2.22179	0.00020		
С	-0.78466	-0.28869	-0.00001		
С	-1.59163	0.95182	0.0000		
С	-1.46315	-1.51654	-0.00004		
С	-3.01146	0.84281	-0.00002		
С	-2.86854	-1.57676	-0.00004		
Н	-0.91370	-2.45832	-0.00007		
С	-3.64283	-0.40598	-0.00002		
Н	-3.56748	1.77876	-0.00001		
Н	-3.37324	-2.54356	-0.00005		
0	-1.01243	2.08048	0.00000		
Н	0.90931	1.84293	-0.00008		
0	-4.99127	-0.58878	-0.00002		
С	-5.80871	0.57006	0.00001		
Н	-6.84262	0.21011	0.00001		
Н	-5.63386	1.18109	0.89863		
Н	-5.63388	1.18112	-0.89860		
Optimized	geometries of 2	in the S1 stat	e encl form	in THF	(angstrom)
Optimized	geometries of 2	in the S1 stat	e enol form	in THF	(angstrom)
Optimized C	geometries of 2 2.80553 2.64136	in the S1 stat -0.79289	e enol form 0.00003 -0.00002	in THF	(angstrom)
Optimized C C	geometries of 2 2.80553 2.64136 3.78928	in the S1 stat -0.79289 0.64062 1 47329	e enol form 0.00003 -0.00002 -0.00004	in THF	(angstrom)
Optimized C C C	geometries of <b>2</b> 2.80553 2.64136 3.78928 5.03263	in the S1 stat -0.79289 0.64062 1.47329 0.85400	e enol form 0.00003 -0.00002 -0.00004 0.00001	in THF	(angstrom)
Optimized C C C C	geometries of <b>2</b> 2.80553 2.64136 3.78928 5.03263 5.17180	in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00006	in THF	(angstrom)
Optimized C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751	<pre>in the S1 stat    -0.79289    0.64062    1.47329    0.85400    -0.55329    -1 40405</pre>	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00006 0.00007	in THF	(angstrom)
Optimized C C C C C C N	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1 29868</pre>	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00006 0.00007 0.00001	in THF	(angstrom)
Optimized C C C C C C C N C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187</pre>	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00006 0.00007 0.00001 -0.00001	in THF	(angstrom)
Optimized C C C C C C N C N	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481</pre>	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00006 0.00007 0.00001 -0.00001 -0.00005	in THF	(angstrom)
Optimized C C C C C C N C N H	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818</pre>	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00006 0.00007 0.00001 -0.00001 -0.00005 -0.00007	in THF	(angstrom)
Optimized C C C C C N C N H H	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752</pre>	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00007 0.00001 -0.00001 -0.00005 -0.00007 0.00007	in THF	(angstrom)
Optimized C C C C C N C N H H H	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641</pre>	e enol form 0.00003 -0.00002 -0.00004 0.00001 0.00007 0.00001 -0.00001 -0.00005 -0.00007 0.00007 0.00000 0.00009	in THF	(angstrom)
Optimized C C C C C N C N H H H H	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834</pre>	<pre>e enol form     0.00003     -0.00002     -0.00004     0.00001     0.00007     0.00001     -0.00001     -0.00001     -0.00005     -0.00007     0.00000     0.00009     0.00011</pre>	in THF	(angstrom)
Optimized C C C C C N C N H H H H H	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796</pre>	<pre>e enol form     0.00003     -0.00002     -0.00004     0.00001     0.00007     0.00001     -0.00001     -0.00005     -0.00007     0.00000     0.00009     0.00011     0.00018</pre>	in THF	(angstrom)
Optimized C C C C C N C N H H H H H C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749</pre>	<pre>e enol form     0.00003     -0.00002     -0.00004     0.00001     0.00001     0.00001     -0.00001     -0.00001     -0.00005     -0.00007     0.00000     0.00009     0.00011     0.00018     -0.00001</pre>	in THF	(angstrom)
Optimized C C C C C C N C N H H H H C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490</pre>	<pre>e enol form     0.00003     -0.00002     -0.00004     0.00001     0.00007     0.00001     -0.00001     -0.00005     -0.00007     0.00000     0.00009     0.00011     0.00018     -0.00001     -0.00003</pre>	in THF	(angstrom)
Optimized C C C C C C N C C N H H H H C C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386</pre>	<pre>e enol form     0.00003     -0.00002     -0.00004     0.00001     0.00001     0.00001     -0.00001     -0.00001     -0.00007     0.00000     0.00009     0.00011     0.00001     -0.00001     -0.00001     -0.00003     0.00000</pre>	in THF	(angstrom)
Optimized C C C C C C N C C N H H H H C C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00001 -0.00003 0.00000 -0.00002	in THF	(angstrom)
Optimized C C C C C C C N C C N H H H H C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00001 -0.00003 0.00000 -0.00002 0.00001	in THF	(angstrom)
Optimized C C C C C C C N C C N H H H H C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00001 -0.00002 0.00001 -0.00001 -0.00001 -0.00001	in THF	(angstrom)
Optimized C C C C C C C N H H H H H C C C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00001 -0.00002 0.00001 -0.00001 -0.00001 0.00001 -0.00001 0.00001 -0.00001 0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00002 -0.00001 -0.00001 -0.000000 -0.000000 -0.00000 -0.000000 -0.000000 -0.00000 -0.00000	in THF	(angstrom)
Optimized C C C C C C C N H H H H H C C C C C C H C H	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 0.00001 -0.00000 -0.000000 -0.000000 -0.00000 -0.00000 -0.00000 -0.00000	in THF	(angstrom)
Optimized C C C C C C N C N H H H H H C C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572 -3.38407	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699 -2.55037</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 0.00001 -0.00001 -0.00001 0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00002 -0.00001 -0.00001 -0.00002 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.000000 -0.000000 -0.00000 -0.00000 -0.00000 -0.00000	in THF	(angstrom)
Optimized C C C C C C C N H H H H H C C C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572 -3.38407 -0.96039	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699 -2.55037 2.08291</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00001 0.00001 -0.00000 -0.000000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.0000	in THF	(angstrom)
Optimized C C C C C C C N H H H H H H C C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572 -3.38407 -0.96039 0.04061	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699 -2.55037 2.08291 1.93031</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00000 -0.000000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000	in THF	(angstrom)
Optimized C C C C C C C N H H H H H H C C C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572 -3.38407 -0.96039 0.04061 -4.93585	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699 -2.55037 2.08291 1.93031 -0.55603</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00001 0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00001 -0.00002 -0.00002 -0.00005 -0.00007 0.00007 0.00007 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00007 -0.0007 -0.00007 -0.0007 -0.0007 -0.0007 -0.0007 -0.0007 -0.0007 -0.0007	in THF	(angstrom)
Optimized C C C C C C C N C C N H H H H H C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572 -3.38407 -0.96039 0.04061 -4.93585 -5.74480	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699 -2.55037 2.08291 1.93031 -0.55603 0.61027</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00009 0.00011 0.00001 -0.00001 -0.00001 -0.00001 0.00001 -0.00002 -0.00002 -0.00005 -0.00005 -0.00007 0.00001 0.000000 0.00000 0.000000 0.00000 0.000000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000000	in THF	(angstrom)
Optimized C C C C C C C N C C N H H H H H C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572 -3.38407 -0.96039 0.04061 -4.93585 -5.74480 -6.78061	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699 -2.55037 2.08291 1.93031 -0.55603 0.61027 0.25702</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00001 0.00001 -0.00001 -0.00001 -0.00001 0.00001 -0.00002 -0.00005 -0.00005 -0.00007 0.00001 0.00002 -0.00001 0.00001 0.00002 -0.00001 0.000000 -0.000000 -0.000000 -0.00000 -0.00000 -0.00000 -0.00000	in THF	(angstrom)
Optimized C C C C C C C N C C N H H H H H H C C C C	geometries of 2 2.80553 2.64136 3.78928 5.03263 5.17180 4.05751 1.53954 0.63917 1.33780 3.68688 5.93538 6.17319 4.16719 1.29740 -0.75326 -1.55706 -1.46529 -2.94292 -2.84381 -0.91555 -3.59383 -3.48572 -3.38407 -0.96039 0.04061 -4.93585 -5.74480 -6.78061 -5.56194	<pre>in the S1 stat -0.79289 0.64062 1.47329 0.85400 -0.55329 -1.40405 -1.29868 -0.23187 0.95481 2.55818 1.46752 -0.98641 -2.48834 -2.27796 -0.32749 0.89490 -1.57386 0.84406 -1.60308 -2.51477 -0.40138 1.78699 -2.55037 2.08291 1.93031 -0.55603 0.61027 0.25702 1.21730</pre>	e encl form 0.00003 -0.00002 -0.00004 0.00001 0.00001 -0.00001 -0.00001 -0.00005 -0.00007 0.00000 0.00001 0.00001 -0.00001 -0.00001 -0.00001 0.00001 0.00002 -0.00005 -0.00005 -0.00005 -0.00005 -0.00005 -0.00007 0.00001 0.00002 -0.00005 -0.00007 0.00001 0.00002 -0.00005 -0.00007 0.00001 0.00002 -0.00001 0.00002 -0.00002 -0.00005 -0.00005 -0.00007 0.00001 0.00002 -0.00002 -0.00002 0.89952	in THF	(angstrom)

Optimized	geometries of ${\bf 2}$	in the S1 state	e enol form	in MeCN	(angstrom)
С	2.80485	-0.79339	0.00004		
С	2.64109	0.64119	-0.00002		
С	3.78974	1.47383	-0.00005		
С	5.03306	0.85397	-0.00001		
С	5.17154	-0.55385	0.00005		
С	4.05717	-1.40470	0.00008		
N	1.54005	-1.29898	0.00002		
С	0.63855	-0.23262	0.00001		
N	1.33858	0.95568	-0.00004		
Н	3.68824	2.55891	-0.00010		
Н	5.93614	1.46707	-0.00003		
Н	6.17289	-0.98715	0.00008		
Н	4.16597	-2.48892	0.00013		
Н	1.29936	-2.27904	0.00020		
С	-0.75262	-0.32709	0.00000		
С	-1.55746	0.89509	-0.00002		
С	-1.46573	-1.57409	0.00000		
С	-2.94247	0.84408	-0.00002		
С	-2.84328	-1.60375	0.00000		
Н	-0.91563	-2.51468	-0.00001		
С	-3.59408	-0.40173	-0.00001		
Н	-3.48657	1.78639	-0.00003		
Н	-3.38234	-2.55177	0.00000		
0	-0.96015	2.08467	-0.00003		
Н	0.04003	1.93109	-0.00003		
0	-4.93528	-0.55605	0.00000		
С	-5.74635	0.61025	0.00000		
Н	-6.78148	0.25547	0.00001		
Н	-5.56375	1.21681	0.89960		
Н	-5.56376	1.21680	-0.89961		
Optimized	commetries of 2	in the S1 state	encl form	in MoOH	(angstrom)
Optimized	geometries of 2	in the S1 state	e enol form	in MeOH	(angstrom)
Optimized C	geometries of <b>2</b> 2.80496 2.64128	in the S1 state -0.79334	e enol form 0.00003 -0.00002	in MeOH	(angstrom)
Optimized C C	geometries of <b>2</b> 2.80496 2.64128 3.79001	in the S1 state -0.79334 0.64109 1 47360	e enol form 0.00003 -0.00002 -0.00005	in MeOH	(angstrom)
Optimized C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324	in the S1 state -0.79334 0.64109 1.47360 0.85357	e enol form 0.00003 -0.00002 -0.00005 -0.00001	in MeOH	(angstrom)
Optimized C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162	in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005	in MeOH	(angstrom)
Optimized C C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711	in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1 40490	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007	in MeOH	(angstrom)
Optimized C C C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53003	in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1 29857	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003	in MeOH	(angstrom)
Optimized C C C C C C N C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001	in MeOH	(angstrom)
Optimized C C C C C C N C N	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0 95586</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004	in MeOH	(angstrom)
Optimized C C C C C C N C N H	<pre>geometries of 2     2.80496     2.64128     3.79001     5.03324     5.17162     4.05711     1.53993     0.63856     1.33873     3.68855</pre>	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2 55866</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009	in MeOH	(angstrom)
Optimized C C C C C C N C N H H	<pre>geometries of 2     2.80496     2.64128     3.79001     5.03324     5.17162     4.05711     1.53993     0.63856     1.33873     3.68855     5.93640</pre>	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1 46654</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H	<pre>geometries of 2     2.80496     2.64128     3.79001     5.03324     5.17162     4.05711     1.53993     0.63856     1.33873     3.68855     5.93640     6.17292</pre>	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2 48913</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00007	in MeOH	(angstrom)
Optimized C C C C C N C N H H H H H	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00012 0.00017	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H H C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00012 0.00017 0.00000	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H H C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00012 0.00017 0.00000 -0.00002	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H H C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00012 0.00017 0.00000 -0.00002 0.00000	in MeOH	(angstrom)
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00012 0.00017 0.00002 0.00000 -0.00002 0.00000	in MeOH	(angstrom)
Optimized C C C C C C C N C N H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00012 0.00017 0.00002 0.00000 -0.00002 0.00000	in MeOH	(angstrom)
Optimized C C C C C C C N N H H H H H H C C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00004 -0.00009 -0.00003 0.00007 0.00012 0.00007 0.00002 0.00000 -0.00002 0.00000 0.00000 0.00000 0.00000	in MeOH	(angstrom)
Optimized C C C C C C C N N H H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00009 -0.00003 0.00007 0.00012 0.00017 0.00002 0.00000 -0.00002 0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000	in MeOH	(angstrom)
Optimized C C C C C C C N N H H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00009 -0.00003 0.00007 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00001 -0.00001 -0.00003	in MeOH	(angstrom)
Optimized C C C C C C N C C N H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682 -3.38206	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642 -2.55173</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00003 0.00007 0.00003 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00002 0.00000 -0.00001 -0.00003 0.00001	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682 -3.38206 -0.96057	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642 -2.55173 2.08506</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00005 0.00007 0.00003 0.00001 -0.00003 0.00007 0.00002 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00001 -0.00003 0.00001 -0.00003 0.00001 -0.00003	in MeOH	(angstrom)
Optimized C C C C C C C N C C C C C C C C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682 -3.38206 -0.96057 0.03955	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642 -2.55173 2.08506 1.93237</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00007 0.00003 0.00001 -0.00003 0.00007 0.00003 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00002 0.00001 -0.00003 0.00001 -0.00003 -0.00003 -0.00003 -0.00003 -0.00002	in MeOH	(angstrom)
Optimized C C C C C C C N C C C C C C C C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682 -3.38206 -0.96057 0.03955 -4.93528	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642 -2.55173 2.08506 1.93237 -0.55649</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00007 0.00003 0.00001 -0.00003 0.00007 0.00003 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00002 0.00000 -0.00003 0.00001 -0.00003 0.00001 -0.00003 -0.00002 0.00002 0.00000 -0.00003 -0.00002 0.00000 -0.00003 -0.00002 0.00000	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682 -3.38206 -0.96057 0.03955 -4.93528 -5.74632	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642 -2.55173 2.08506 1.93237 -0.55649 0.60964</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00007 0.00003 0.00001 -0.00003 0.00007 0.00003 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00002 0.00000 -0.00001 -0.00003 -0.00003 -0.00002 0.00000 -0.00003 -0.00002 0.00000 -0.00003 -0.00002 0.00000 -0.00000 -0.00002 0.00000 -0.00002 0.00000 -0.00002 0.00000 -0.00000 -0.00002 0.00000 -0.00002 0.00000 -0.000000 -0.00000 -0.000000 -0.000000 -0.00000 -0.00000	in MeOH	(angstrom)
Optimized C C C C C C C N C C N H H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682 -3.38206 -0.96057 0.03955 -4.93528 -5.74632 -6.78133	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642 -2.55173 2.08506 1.93237 -0.55649 0.60964 0.25452</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00007 0.00003 0.00001 -0.00003 0.00007 0.00003 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00000 0.00000 -0.00001 -0.00003 -0.00001 -0.00000 -0.00000 -0.000000 -0.000000 -0.000000 -0.00000 -0.000000 -0.000000 -0.000000 -0.00000	in MeOH	(angstrom)
Optimized C C C C C C N C C N H H H H H H H H C C C C	geometries of 2 2.80496 2.64128 3.79001 5.03324 5.17162 4.05711 1.53993 0.63856 1.33873 3.68855 5.93640 6.17292 4.16581 1.29905 -0.75267 -1.55768 -1.46558 -2.94275 -2.84313 -0.91558 -3.59407 -3.48682 -3.38206 -0.96057 0.03955 -4.93528 -5.74632 -6.78133 -5.56388	<pre>in the S1 state -0.79334 0.64109 1.47360 0.85357 -0.55421 -1.40490 -1.29857 -0.23213 0.95586 2.55866 1.46654 -0.98764 -2.48913 -2.27854 -0.32670 0.89531 -1.57380 0.84414 -1.60365 -2.51444 -0.40180 1.78642 -2.55173 2.08506 1.93237 -0.55649 0.60964 0.25452 1.21626</pre>	e enol form 0.00003 -0.00002 -0.00005 -0.00001 0.00007 0.00003 0.00001 -0.00003 0.00007 0.00003 0.00007 0.00002 0.00000 -0.00002 0.00000 -0.00000 -0.00000 0.00000 -0.00001 -0.00003 -0.00001 -0.00000 -0.000000 -0.000000 -0.000000 -0.00000 -0.00000 -0.000000 -0.00000 -0.00000	in MeOH	(angstrom)

Optimized C C C C C C C N C N H H H H H C C C C C	<pre>geometries of 2     2.80484     2.64108     3.78979     5.03315     5.17158     4.05718     1.54015     0.63836     1.33862     3.68840     5.93627     6.17293     4.16586     1.29974     -0.75264     -1.55759     -1.46589     -2.94255     -2.84330     -0.91598     -3.59414     -3.48676     -3.38219     -0.95994     0.04023     -4.93524     -5.74640     -6.78136     -5.56390     -5.56392</pre>	<pre>e in the S1 -0.79343 0.64119 1.47385 0.85387 -0.55398 -1.40484 -1.29883 -0.23262 0.95574 2.55894 1.46691 -0.98731 -2.48904 -2.27900 -0.32704 0.89522 -1.57412 0.84420 -1.60378 -2.51478 -0.40171 1.78644 -2.55190 2.08487 1.93127 -0.55613 0.61016 0.25499 1.21668 1.21667</pre>	state	enol form 0.00004 -0.00002 -0.00004 0.00006 0.00008 0.00002 0.00009 -0.00002 0.00009 0.00013 0.00019 -0.00001 -0.00001 -0.00001 -0.00002 0.00000 -0.00002 -0.00001 -0.00002 0.00000 -0.00003 0.00000 -0.00005 0.00000 0.00000 0.00000 0.00002 0.89963 -0.89963	in H2O (angstrom)
Ontimized	geometries of 2	in the Cl	state	TS in THF	(angstrom)
C	2.82251	0.79016		0.00003	(ango er om)
C C	2.82251 2.61398	0.79016 -0.62997		0.00003	(angoerom)
C C C	2.82251 2.61398 3.71902	0.79016 -0.62997 -1.50635		0.00003 -0.00005 0.00003	(ango or om)
C C C C	2.82251 2.61398 3.71902 4.98930	0.79016 -0.62997 -1.50635 -0.93156		0.00003 -0.00005 0.00003 0.00021	(4119002000)
C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061	0.79016 -0.62997 -1.50635 -0.93156 0.46396		0.00003 -0.00005 0.00003 0.00021 0.00030	(4119002011)
C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484		0.00003 -0.00005 0.00003 0.00021 0.00030 0.00020	(4119002011)
C C C C C C C N	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191		0.00003 -0.00005 0.00003 0.00021 0.00030 0.00020 -0.00008	(4119002011)
C C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769		0.00003 -0.00005 0.00003 0.00021 0.00030 0.00020 -0.00008 -0.00022	(4119002011)
C C C C C C C C C N C N	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602		0.00003 -0.00005 0.00003 0.00021 0.00030 0.00020 -0.00008 -0.00022 -0.00026	(4119002011)
C C C C C C C C C C N N H	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.26620	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644		0.00003 -0.00005 0.00021 0.00030 0.00020 -0.00008 -0.00022 -0.00026 -0.00026 -0.00006	(4119002011)
C C C C C C C C C N C N H H	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.10676	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128		0.00003 -0.00005 0.00021 0.00020 -0.00020 -0.00020 -0.00022 -0.00022 -0.00026 -0.00026 0.00028	(4119002011)
C C C C C C C C C C N C C N H H H	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473		0.00003 -0.00005 0.00021 0.00020 -0.00020 -0.00022 -0.00022 -0.00026 0.00028 0.00043 0.00026	(4119) 22 011)
C C C C C C C C C C N C N H H H H	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00008 -0.00022 -0.00026 -0.00028 0.00028 0.00026 -0.00009	(4119) 22 011)
C C C C C C C C C C N C N H H H H C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00028 -0.00026 -0.00028 0.00028 0.00028 0.00026 -0.00009 -0.00028	(4119) 22 011)
C C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00022 -0.00022 -0.00026 -0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00028	
C C C C C C C C C C C N C C N C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00022 -0.00022 -0.00026 -0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00013 -0.00025	
C C C C C C C C C C C N C C N H H H H H	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00028 -0.00026 -0.00028 0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00028 -0.00025 0.00005	
C C C C C C C C C C C N C N H H H H H C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569 -2.90644	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00028 -0.00026 -0.00028 0.00043 0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00013 -0.00025 0.00005 -0.00013	
C C C C C C C C C C C N C N H H H H H H	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569 -2.90644 -1.00845	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00028 -0.00026 -0.00026 -0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00013 -0.00025 0.00005 -0.00013 -0.00030	
C C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569 -2.90644 -1.00845 -3.60917	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00008 -0.00022 -0.00026 -0.00006 0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00013 -0.00025 0.00005 -0.00013 -0.00030 0.00003	
C C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569 -2.90644 -1.00845 -3.60917 -3.42098	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119 -1.81758		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00028 -0.00026 -0.00026 -0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00013 -0.00025 0.00005 -0.00013 -0.00013 -0.00030 0.00003 0.00003	
C C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569 -2.90644 -1.00845 -3.60917 -3.42098 -3.48435 -0.84046	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119 -1.81758 2.51600 -1.27811		0.00003 -0.00005 0.0003 0.00021 0.00030 0.00020 -0.00022 -0.00026 -0.00026 -0.00028 0.00043 0.00026 -0.00028 -0.00028 -0.00013 -0.00013 -0.00013 -0.00011 -0.00014	
C C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569 -2.90644 -1.00845 -3.60917 -3.42098 -3.48435 -0.84946 0.32929	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119 -1.81758 2.51600 -1.97811 -1.69164		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00028 -0.00026 -0.00028 0.00028 0.00028 0.00028 -0.00028 -0.00028 -0.00028 -0.00028 -0.00025 0.00003 -0.00013 -0.00013 -0.00014 -0.00014 -0.00015	
C C C C C C C C C C C C C C C C C C C	2.82251 2.61398 3.71902 4.98930 5.18061 4.09723 1.57491 0.63014 1.28572 3.57710 5.86629 6.19676 4.24433 1.37579 -0.77000 -1.51359 -1.51806 -2.91569 -2.90644 -1.00845 -3.60917 -3.42098 -3.48435 -0.84946 0.32929 -4.95935	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119 -1.81758 2.51600 -1.97811 -1.69164 0.47358		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00028 -0.00028 -0.00028 0.00043 0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00013 -0.00013 -0.00013 -0.00018 -0.00011 -0.00014 -0.00018	
C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 2.82251\\ 2.61398\\ 3.71902\\ 4.98930\\ 5.18061\\ 4.09723\\ 1.57491\\ 0.63014\\ 1.28572\\ 3.57710\\ 5.86629\\ 6.19676\\ 4.24433\\ 1.37579\\ -0.77000\\ -1.51359\\ -1.51806\\ -2.91569\\ -2.90644\\ -1.00845\\ -3.60917\\ -3.42098\\ -3.48435\\ -0.84946\\ 0.32929\\ -4.95935\\ -5.72331\end{array}$	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119 -1.81758 2.51600 -1.97811 -1.69164 0.47358 -0.72126		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00022 -0.00026 -0.00026 -0.00028 0.00028 0.00043 0.00026 -0.00009 -0.00028 -0.00013 -0.00025 0.00005 -0.00013 -0.00013 -0.00013 -0.00014 -0.00014 -0.00014 -0.00057 0.00018 0.00018	
C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 2.82251\\ 2.61398\\ 3.71902\\ 4.98930\\ 5.18061\\ 4.09723\\ 1.57491\\ 0.63014\\ 1.28572\\ 3.57710\\ 5.86629\\ 6.19676\\ 4.24433\\ 1.37579\\ -0.77000\\ -1.51359\\ -1.51806\\ -2.91569\\ -2.90644\\ -1.00845\\ -3.60917\\ -3.42098\\ -3.48435\\ -0.84946\\ 0.32929\\ -4.95935\\ -5.72331\\ -6.77206\end{array}$	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119 -1.81758 2.51600 -1.97811 -1.69164 0.47358 -0.72126 -0.40788		0.00003 -0.00005 0.00021 0.00020 -0.00022 -0.00022 -0.00026 -0.00026 -0.00028 0.00028 0.00028 0.00028 -0.00029 -0.00028 -0.00029 -0.00025 0.00025 0.00013 -0.00025 0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00013 -0.00018 -0.00014 -0.00014 -0.00018 0.00037 0.00047	
C C C C C C C C C C C C C C C C C C C	$\begin{array}{c} 2.82251\\ 2.61398\\ 3.71902\\ 4.98930\\ 5.18061\\ 4.09723\\ 1.57491\\ 0.63014\\ 1.28572\\ 3.57710\\ 5.86629\\ 6.19676\\ 4.24433\\ 1.37579\\ -0.77000\\ -1.51359\\ -1.51806\\ -2.91569\\ -2.90644\\ -1.00845\\ -3.60917\\ -3.42098\\ -3.48435\\ -0.84946\\ 0.32929\\ -4.95935\\ -5.72331\\ -6.77206\\ -5.51857\end{array}$	0.79016 -0.62997 -1.50635 -0.93156 0.46396 1.35484 1.35191 0.33769 -0.86602 -2.58644 -1.58128 0.86088 2.43473 2.34091 0.41800 -0.86014 1.62380 -0.85404 1.59110 2.58729 0.36119 -1.81758 2.51600 -1.97811 -1.69164 0.47358 -0.72126 -0.40788 -1.32221		0.00003 -0.00005 0.00003 0.00021 0.00020 -0.00022 -0.00026 -0.00026 -0.00028 0.00028 0.00028 0.00028 -0.00028 -0.00028 -0.00029 -0.00028 -0.00013 -0.00025 0.00005 -0.00013 -0.00013 -0.00013 -0.00013 -0.00014 -0.00011 -0.00014 -0.00057 0.00018 0.00037 0.00047 -0.89876	

Optimized C C C C C C C N N H H H H H H C C C C C	<pre>geometries of     2.82085     2.61212     3.71731     4.98760     5.17899     4.09641     1.57532     0.62835     1.28525     3.57512     5.86472     6.19535     4.24337     1.37818     -0.76928     -1.51273     -1.51273     -1.51273     -1.51925     -2.91381     -2.90545     -1.00875     -3.60775     -3.42083     -3.48389     -0.84779     0.33265     -4.95725     -5.72235     -6.77076     -5.51731     -5.51738</pre>	2	in the S1 0.79119 -0.63051 -1.50738 -0.93290 0.46358 1.35489 1.35349 0.33982 -0.86598 -2.58748 -1.58245 0.86004 2.43456 2.34336 0.41830 -0.86088 1.62608 -0.85431 1.59283 2.58895 0.36127 -1.81710 2.51748 -1.97999 -1.69108 0.47259 -0.72275 -0.40867 -1.32314 -1.32315	state	TS in MeCN -0.00004 0.00005 0.00004 -0.00017 -0.00016 0.00010 0.00016 0.00012 -0.00023 -0.00023 -0.00008 0.00010 0.00006 0.00001 0.00006 0.00001 0.00002 0.00006 -0.00001 0.00001 0.00003 -0.00001 0.00007 0.00002 -0.00001 0.00002 -0.00001 0.00007 0.00029 -0.00006 -0.00001 0.00007 0.00029 -0.00006 -0.00001 0.00007 0.00029 -0.00001 0.00007 0.00029 -0.00001 0.00002 -0.00001 0.00002 -0.00001 0.00002 -0.00001 0.00002 -0.00001 0.00002 -0.00001 0.00002 -0.00002 -0.00001 0.00002 -0.00001 0.00002 -0.00001 0.00001 0.00001 0.00000 -0.00000 -0.00000 -0.0000000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.000000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000000	(angstrom)
Optimized	geometries of	2	in the S1	state	TS in MeOH	(angstrom)
C C	2.82093 2.61233		0.79113 -0.63055		0.00004 -0.00006	
C C	2.82093 2.61233 3.71748		0.79113 -0.63055 -1.50737		0.00004 -0.00006 0.00002	
C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909		0.79113 -0.63055 -1.50737 -0.93277		0.00004 -0.00006 0.00002 0.00021 0.00032	
C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493		0.00004 -0.00006 0.00002 0.00021 0.00032 0.00022	
C C C C C C C N	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338		0.00004 -0.00006 0.00002 0.00021 0.00032 0.00022 -0.00008	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969		0.00004 -0.00006 0.00002 0.00021 0.00032 0.00022 -0.00008 -0.00023	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 2.57552		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58740		0.00004 -0.00006 0.00002 0.00021 0.00032 0.00022 -0.00008 -0.00023 -0.00027	
C C C C C C C C C C C N C N H H	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237		0.00004 -0.00006 0.00022 0.00021 0.00032 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028	
C C C C C C C C C C N C N H H H	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540		$\begin{array}{c} 0.79113 \\ -0.63055 \\ -1.50737 \\ -0.93277 \\ 0.46364 \\ 1.35493 \\ 1.35338 \\ 0.33969 \\ -0.86597 \\ -2.58749 \\ -1.58237 \\ 0.86025 \end{array}$		0.00004 -0.00006 0.00022 0.00021 0.00022 -0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460		0.00004 -0.00006 0.00022 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00046 0.00029	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 0.76226		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327		0.00004 -0.00006 0.00022 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00046 0.00029 -0.00008	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327 0.41834 -0.86099		0.00004 -0.00006 0.00022 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00028 0.00046 0.00029 -0.00008 -0.00030 -0.00014	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327 0.41834 -0.86099 1.62603		0.00004 -0.00006 0.0002 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00046 0.00029 -0.00008 -0.00030 -0.00014 -0.00027	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327 0.41834 -0.86099 1.62603 -0.85437		0.00004 -0.00006 0.00022 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00046 0.00029 -0.00008 -0.00030 -0.00014 -0.00027 0.00005	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327 0.41834 -0.86099 1.62603 -0.85437 1.59269 2.58905		0.00004 -0.00006 0.00021 0.00022 -0.00023 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00029 -0.00008 -0.00008 -0.00008 -0.000030 -0.00014 -0.00027 0.00005 -0.00015 -0.00032	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898 -3.60786		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327 0.41834 -0.86099 1.62603 -0.85437 1.59269 2.58905 0.36119		0.00004 -0.00006 0.0002 0.00021 0.00022 -0.00023 -0.00023 -0.00027 -0.00008 0.00028 0.00029 -0.00008 -0.00030 -0.00014 -0.00027 0.00027 0.00005 -0.00015 -0.00032 0.0003	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898 -3.60786 -3.42091		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327 0.41834 -0.86099 1.62603 -0.85437 1.59269 2.58905 0.36119 -1.81719		0.00004 -0.00006 0.0002 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00029 -0.00008 -0.00008 -0.00014 -0.00027 0.00005 -0.00015 -0.00032 0.0003 0.00019	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898 -3.60786 -3.42091 -3.48378		0.79113 - $0.63055$ - $1.50737$ - $0.93277$ 0.46364 1.35493 1.35338 0.33969 - $0.86597$ - $2.58749$ - $1.58237$ 0.86025 2.43460 2.34327 0.41834 - $0.86099$ 1.62603 - $0.85437$ 1.59269 2.58905 0.36119 - $1.81719$ 2.51745		0.00004 -0.00006 0.00021 0.00022 -0.00023 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00029 -0.00008 -0.00030 -0.00015 -0.00013 0.00015 -0.00013 0.00015	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898 -3.60786 -3.42091 -3.48378 -0.84781 0.33322		0.79113 -0.63055 -1.50737 -0.93277 0.46364 1.35493 1.35338 0.33969 -0.86597 -2.58749 -1.58237 0.86025 2.43460 2.34327 0.41834 -0.86099 1.62603 -0.85437 1.59269 2.58905 0.36119 -1.81719 2.51745 -1.97985 -1.69087		0.00004 -0.00006 0.00021 0.00022 -0.00023 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00029 -0.00008 -0.00030 -0.00014 -0.00027 0.00005 -0.00015 -0.00015 -0.00013 -0.00015 -0.000015 -0.000015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898 -3.60786 -3.42091 -3.48378 -0.84781 0.33322 -4.95745		0.79113 - $0.63055$ - $1.50737$ - $0.93277$ 0.46364 1.35493 1.35338 0.33969 - $0.86597$ - $2.58749$ - $1.58237$ 0.86025 2.43460 2.34327 0.41834 - $0.86099$ 1.62603 - $0.85437$ 1.59269 2.58905 0.36119 - $1.81719$ 2.51745 - $1.97985$ - $1.69087$ 0.47263		0.00004 -0.00006 0.0002 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00029 -0.00008 -0.00008 -0.00014 -0.00027 0.00005 -0.00015 -0.00015 -0.00013 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00019	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898 -3.60786 -3.42091 -3.48378 -0.84781 0.33322 -4.95745 -5.72269		0.79113 - $0.63055$ - $1.50737$ - $0.93277$ 0.46364 1.35493 1.35338 0.33969 - $0.86597$ - $2.58749$ - $1.58237$ 0.86025 2.43460 2.34327 0.41834 - $0.86099$ 1.62603 - $0.85437$ 1.59269 2.58905 0.36119 - $1.81719$ 2.51745 - $1.97985$ - $1.69087$ 0.47263 - $0.72261$		0.00004 -0.00006 0.0002 0.00021 0.00022 -0.00008 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00029 -0.00008 -0.00008 -0.00003 -0.00015 -0.0	
C C C C C C C C C C C C C C C C C C C	2.82093 2.61233 3.71748 4.98780 5.17909 4.09643 1.57532 0.62844 1.28535 3.57552 5.86487 6.19540 4.24335 1.37828 -0.76926 -1.51282 -1.51921 -2.91398 -2.90553 -1.00898 -3.60786 -3.42091 -3.48378 -0.84781 0.3322 -4.95745 -5.72269 -6.77108 -5.51785		0.79113 - $0.63055$ - $1.50737$ - $0.93277$ 0.46364 1.35493 1.35338 0.33969 - $0.86597$ - $2.58749$ - $1.58237$ 0.86025 2.43460 2.34327 0.41834 - $0.86099$ 1.62603 - $0.85437$ 1.59269 2.58905 0.36119 - $1.81719$ 2.51745 - $1.97985$ - $1.69087$ 0.47263 - $0.72261$ - $0.40847$ - $1.32314$		0.00004 -0.00006 0.00021 0.00022 -0.00023 -0.00023 -0.00027 -0.00008 0.00028 0.00028 0.00029 -0.00008 -0.00030 -0.00014 -0.00027 0.00005 -0.00015 -0.00015 -0.00013 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00015 -0.00019 0.00039 0.00050 -0.89876	

Optimized C C C C C C C N C C N C N H H H H H C C C C	<pre>geometries of 2 2.82065 2.61184 3.71700 4.98734 5.17878 4.09637 1.57545 0.62811 1.28517 3.57474 5.86444 6.19519 4.24340 1.37868 -0.76915 -1.51259 -1.51259 -1.51949 -2.91351 -2.90538 -1.00892 -3.60759 -3.42073 -3.48388 -0.84752 0.33315 -4.95701 -5.72224 -6.77061 -5.51722</pre>	2 i	n the S1 0.79137 -0.63057 -1.50758 -0.93320 0.46341 1.35483 1.35381 0.34025 -0.86589 -2.58766 -1.58278 0.85978 2.43443 2.34385 0.41844 -0.86092 1.62647 -0.85433 1.59308 2.58928 0.36127 -1.81704 2.51771 -1.98022 -1.69092 0.47236 -0.72310 -0.40896 -1.32341 -1.32341	state	TS in H2O -0.00004 0.00005 0.00003 -0.00016 -0.00014 0.00010 0.00010 -0.00010 -0.00024 -0.00020 -0.00007 0.00009 0.00006 0.00004 0.00001 0.00001 0.00001 0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00002 -0.00006 0.00008 -0.00008 -0.00011 -0.89927 0.89912	(angstrom)
Optimized C C C C C C C N C N H H H H H C C C C C	<pre>geometries of : -2.78551 -2.46935 -3.49010 -4.80326 -5.10303 -4.09976 -1.56853 -0.58832 -1.09930 -3.25763 -5.62202 -6.14654 -4.33497 -1.42925 0.84090 1.72883 1.35326 3.12493 2.71761 0.67723 3.60763 3.11010 4.67971 1.31518 0.31465 3.89478 5.30028 5.73094 5.63411 5.63412</pre>	3 i	n the grc 0.68959 -0.68658 -1.64301 -1.18610 0.19020 1.15498 1.33622 0.38418 -0.84102 -2.70831 -1.90700 0.50833 2.21936 2.33574 0.65314 -0.44228 1.96535 -0.20421 2.18371 2.82070 1.09951 3.20061 1.28876 -1.71615 -1.69870 -1.31980 -1.14035 -2.14681 -0.60021 -0.60013	ound st	<pre>cate in THF -0.00002 -0.00003 -0.00005 -0.00005 -0.00004 -0.00001 -0.00001 -0.00001 -0.00006 -0.00008 -0.00008 -0.00008 -0.00003 0.00000 0.00000 0.00001 0.00001 0.00007 -0.00007 -0.00007 -0.00007 -0.00007 -0.00007 -0.00007 -0.00005 0.00015 0.00015 0.00015 0.00015 0.00015 0.00010 -0.89922 0.89926</pre>	(angstrom)

Optimized	geometries of	3	in the ground	state in MeCN	(angstrom)
c	-2.78531		0.68930	-0.00003	
С	-2.46882		-0.68685	-0.00002	
С	-3.48932		-1.64395	-0.00004	
С	-4.80267		-1.18703	-0.00005	
С	-5.10273		0.18961	-0.00005	
С	-4.09976		1.15479	-0.00004	
N	-1.56930		1.33691	-0.00001	
С	-0.58878		0.38680	0.00001	
N	-1.09844		-0.83991	-0.00001	
Н	-3.25747		-2.70947	-0.00004	
Н	-5.62133		-1.90810	-0.00006	
Н	-6.14636		0.50735	-0.00007	
Н	-4.33367		2.21941	-0.00004	
Н	-1.43295		2.33714	-0.00002	
С	0.84101		0.65525	0.00001	
С	1.72838		-0.44066	0.00005	
С	1.35463		1.96693	-0.00004	
С	3.12432		-0.20498	0.00002	
С	2.71971		2.18311	-0.00006	
Н	0.68001		2.82319	-0.00007	
С	3.60885		1.09833	-0.00003	
Н	3.11335		3.19954	-0.00010	
Н	4.68107		1.28658	-0.00005	
0	1.31156		-1.71531	0.00014	
Н	0.30997		-1.69394	0.00020	
0	3.89366		-1.32178	0.00006	
С	5.30066		-1.14242	0.00005	
Н	5.73108		-2.14890	0.00009	
Н	5.63387		-0.60225	-0.89906	
Н	5.63388		-0.60217	0.89912	
Ontimized	acometries of	2	in the ground	atata in MaOH	(anget rom)
Optimized	geometries of	3	in the ground	state in MeOH	(angstrom)
Optimized 6	geometries of -2.78531	3	in the ground 0.68930	state in MeOH -0.00003	(angstrom)
Optimized 6 6	geometries of -2.78531 -2.46882 -3.48932	3	in the ground 0.68930 -0.68685 -1.64395	<pre>state in MeOH    -0.00003    -0.00002    -0.00004</pre>	(angstrom)
Optimized 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267	3	in the ground 0.68930 -0.68685 -1.64395 -1 18703	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005</pre>	(angstrom)
Optimized 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273	3	in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00005</pre>	(angstrom)
Optimized 6 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976	3	<pre>in the ground     0.68930     -0.68685     -1.64395     -1.18703     0.18961     1 15479</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00005    -0.00005</pre>	(angstrom)
Optimized 6 6 6 6 6 6 7	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56030	3	<pre>in the ground     0.68930     -0.68685     -1.64395     -1.18703     0.18961     1.15479     1.32691</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00005    -0.00004    -0.00004</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878	3	<pre>in the ground     0.68930     -0.68685     -1.64395     -1.18703     0.18961     1.15479     1.33691     0 38680</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00005    -0.00004    -0.00001    0.00001</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0 83991</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00005    -0.00004    -0.00001    0.00001    -0.00001</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 1	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2 70947</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00004    -0.00001    0.00001    -0.00001    -0.00001    -0.00001    -0.00001</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 7 1 1	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1 90810</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00004    -0.00001    0.00001    -0.00001    -0.00001    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00006</pre>	(angstrom)
Optimized 6 6 6 6 6 6 7 6 7 1 1 1	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00004    -0.00001    0.00001    -0.00001    -0.00001    -0.00004    -0.00004    -0.00004    -0.00006    -0.00007</pre>	(angstrom)
Optimized 6 6 6 6 6 6 7 6 7 1 1 1 1	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00004    -0.00001    -0.00001    -0.00001    -0.00004    -0.0004</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 1 1 1 1 1	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2 33714</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00001    -0.00001    -0.00001    -0.00001    -0.00004    -0.00004    -0.00004    -0.00007    -0.00004    -0.00004    -0.00002</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 1 1 1 1 1 1 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00001    -0.00001    -0.00001    -0.00001    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00002    0.00001</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 1 1 1 1 1 1 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00001    -0.00001    -0.00001    -0.00001    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00002    0.00001    0.00005</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 1 1 1 1 1 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00004 -0.00002 0.00001 0.00005 -0.00004</pre>	(angstrom)
Optimized 6 6 6 6 6 6 7 6 7 1 1 1 1 1 1 6 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498</pre>	<pre>state in MeOH    -0.00003    -0.00002    -0.00004    -0.00005    -0.00001    -0.00001    -0.00001    -0.00004    -0.00004    -0.00004    -0.00004    -0.00004    -0.00002    0.00001    0.00005    -0.00004    0.00002</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 7 1 1 1 1 1 1 6 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00004 -0.00002 0.00001 0.00005 -0.00004 0.00002 -0.00004</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 7 1 1 1 1 1 1 6 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00004 -0.00002 0.00001 0.00005 -0.00004 0.00002 -0.00006 -0.00006 -0.00007</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 1 1 1 1 1 1 6 6 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00004 -0.00002 0.00001 0.00002 -0.00004 0.00002 -0.00004 -0.00002 -0.00004 -0.00007 -0.00003</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 1 1 1 1 1 1 1 6 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00007 -0.00004 -0.00002 0.00005 -0.00004 0.00002 -0.00004 0.00002 -0.00004 0.00007 -0.00003 -0.00003 -0.00010</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 7 1 1 1 1 1 1 1 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335 4.68107	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954 1.28658</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00007 -0.00004 -0.00002 0.00001 0.00005 -0.00004 -0.00004 -0.00005 -0.00006 -0.00007 -0.00003 -0.00003 -0.00010 -0.00005</pre>	(angstrom)
Optimized 6 6 6 6 6 7 6 7 7 1 1 1 1 1 1 1 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335 4.68107 1.31156	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954 1.28658 -1.71531</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00007 -0.00004 -0.00002 0.00001 0.00002 -0.00004 -0.00005 -0.00007 -0.00003 -0.00003 -0.00010 -0.00005 0.00014</pre>	(angstrom)
Optimized 6 6 6 6 6 7 7 6 7 1 1 1 1 1 1 1 1 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335 4.68107 1.31156 0.30997	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954 1.28658 -1.71531 -1.69394</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00007 -0.00004 -0.00002 0.00001 0.00005 -0.00004 -0.00007 -0.00004 -0.00005 -0.00007 -0.00003 -0.00003 -0.00010 -0.00005 0.00014 0.00020</pre>	(angstrom)
Optimized 6 6 6 6 6 7 7 6 7 1 1 1 1 1 1 1 1 6 6 6 6	geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335 4.68107 1.31156 0.30997 3.89366	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954 1.28658 -1.71531 -1.69394 -1.32178</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00007 -0.00004 -0.00002 0.00001 0.00005 -0.00004 -0.00005 -0.00007 -0.00003 -0.00003 -0.00010 -0.00010 -0.00014 0.00020 0.00014 0.00020 0.00006</pre>	(angstrom)
Optimized 6 6 6 6 6 7 7 6 7 1 1 1 1 1 1 1 1 6 6 6 6	<pre>geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335 4.68107 1.31156 0.30997 3.89366 5.30066</pre>	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954 1.28658 -1.71531 -1.69394 -1.32178 -1.14242</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00007 -0.00004 -0.00002 0.00001 0.00002 -0.00004 -0.00005 -0.00004 -0.00005 -0.00007 -0.00003 -0.00003 -0.00010 -0.00005 0.00014 0.00020 0.0006 0.00005</pre>	(angstrom)
Optimized 6 6 6 6 6 7 7 6 7 1 1 1 1 1 1 1 1 1 6 6 6 6	<pre>geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335 4.68107 1.31156 0.30997 3.89366 5.30066 5.73108</pre>	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954 1.28658 -1.71531 -1.69394 -1.32178 -1.14242 -2.14890</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00004 -0.00002 0.00001 0.00002 -0.00004 -0.00002 -0.00004 -0.00005 -0.00007 -0.00003 -0.00007 -0.00003 -0.00005 -0.00010 -0.00005 0.00014 0.00020 0.00005 0.00005 0.00009</pre>	(angstrom)
Optimized 6 6 6 6 6 7 7 6 7 1 1 1 1 1 1 1 1 1 6 6 6 6	<pre>geometries of -2.78531 -2.46882 -3.48932 -4.80267 -5.10273 -4.09976 -1.56930 -0.58878 -1.09844 -3.25747 -5.62133 -6.14636 -4.33367 -1.43295 0.84101 1.72838 1.35463 3.12432 2.71971 0.68001 3.60885 3.11335 4.68107 1.31156 0.30997 3.89366 5.30066 5.73108 5.63387</pre>	3	<pre>in the ground 0.68930 -0.68685 -1.64395 -1.18703 0.18961 1.15479 1.33691 0.38680 -0.83991 -2.70947 -1.90810 0.50735 2.21941 2.33714 0.65525 -0.44066 1.96693 -0.20498 2.18311 2.82319 1.09833 3.19954 1.28658 -1.71531 -1.69394 -1.32178 -1.14242 -2.14890 -0.60225</pre>	<pre>state in MeOH -0.00003 -0.00002 -0.00004 -0.00005 -0.00001 -0.00001 -0.00001 -0.00004 -0.00004 -0.00007 -0.00004 -0.00002 0.00001 0.00005 -0.00004 -0.00005 -0.00007 -0.00003 -0.00003 -0.00010 -0.00005 0.00014 0.00020 0.00014 0.00005 0.00005 0.00005 0.00009 -0.89906</pre>	(angstrom)

Optimized	geometries of :	3 in the ground	state in H2O (angstrom)
6 0	-2.78529	0.68920	-0.00002
6 0	-2.46886	-0.68/00	-0.00005
6 0	-3.48942	-1.64414	-0.00009
6 0	-4.80280	-1.18/09	-0.00009
6 0	-5.10275	0.18969	-0.00007
6 U	-4.09972	1.15487	-0.00003
7 0	-1.56947	1.33688	0.00001
6 0	-0.58893	0.38709	0.00002
/ 0	-1.09842	-0.83988	-0.00003
1 0	-3.25//6	-2.70974	-0.00011
1 0	-5.62149	-1.90813	-0.00012
1 0	-6.14637	0.50749	-0.00007
1 0	-4.33323	2.21958	-0.00001
1 0	-1.43353	2.33/25	0.00002
6 0	0.84102	0.65556	0.00003
6 0	1.72839	-0.44044	0.00008
6 0	1.35478	1.96721	-0.00004
6 0	3.12432	-0.20501	0.00002
6 0	2.71997	2.18308	-0.00009
1 0	0.68035	2.82357	-0.00008
6 0	3.60905	1.09823	-0.00006
1 0	3.11378	3.19943	-0.00015
1 0	4.68128	1.28634	-0.00010
8 0	1.31121	-1.71531	0.00022
1 0	0.30942	-1.69379	0.00034
8 0	3.89366	-1.32198	0.00007
6 0	5.30095	-1.14267	0.00004
1 0	5.73140	-2.14913	0.00009
1 0	5.63415	-0.60250	-0.89901
1 0	5.63418	-0.60239	0.89900
Optimized	geometries of :	<b>3</b> in the S1 stat	e in THF (angstrom)
Optimized C	geometries of : -2.80185	<b>3</b> in the S1 stat 0.68579	e in THF (angstrom) 0.00019
Optimized C C	geometries of : -2.80185 -2.52951	<b>3</b> in the S1 stat 0.68579 -0.70363	e in THF (angstrom) 0.00019 -0.00069
Optimized C C C	geometries of : -2.80185 -2.52951 -3.56248	3 in the S1 stat 0.68579 -0.70363 -1.64489	e in THF (angstrom) 0.00019 -0.00069 -0.00125
Optimized C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090
Optimized C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004
Optimized C C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055
Optimized C C C C C C N	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053
Optimized C C C C C C N C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012	<pre>3 in the S1 stat     0.68579     -0.70363     -1.64489     -1.14726     0.22448     1.17523     1.31975     0.39375</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010
Optimized C C C C C C N C N	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096
Optimized C C C C C N C N H	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00055 0.00053 0.00010 -0.00096 -0.00188
Optimized C C C C C N C N H H	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131
Optimized C C C C C N C N H H H	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666	<pre>3 in the S1 stat     0.68579     -0.70363     -1.64489     -1.14726     0.22448     1.17523     1.31975     0.39375     -0.83229     -2.71440     -1.85211     0.56863</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021
Optimized C C C C C N C N H H H H	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356	<pre>3 in the S1 stat     0.68579     -0.70363     -1.64489     -1.14726     0.22448     1.17523     1.31975     0.39375     -0.83229     -2.71440     -1.85211     0.56863     2.24456</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127
Optimized C C C C C N C N H H H H H	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741	<pre>3 in the S1 stat     0.68579     -0.70363     -1.64489     -1.14726     0.22448     1.17523     1.31975     0.39375     -0.83229     -2.71440     -1.85211     0.56863     2.24456     2.31957</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157
Optimized C C C C C N C N H H H H C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.00001
Optimized C C C C C N C N H H H H H C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.00001 0.00041
Optimized C C C C C C N C N H H H H H C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.00001 0.00041 -0.00043
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.0001 0.00041 -0.00043 0.00027
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940	3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036
Optimized C C C C C C N C N H H H H H H H C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00127 0.00157 0.000157 0.0001 0.00041 -0.00043 0.00027 -0.00036 -0.00093
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00005
Optimized C C C C C C N C N H H H H H H H C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00127 0.00157 0.000157 0.0001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00005 -0.00058
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139 4.75022	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495 1.30828</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00005 -0.00058 -0.00006
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139 4.75022 1.33811	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495 1.30828 -1.69590</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00127 0.00157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00058 -0.00058 -0.00006 0.00092
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139 4.75022 1.33811 -0.56967	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495 1.30828 -1.69590 -1.65942</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00055 -0.00058 -0.00057
Optimized C C C C C C N C N H H H H H H H C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139 4.75022 1.33811 -0.56967 3.96079	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495 1.30828 -1.69590 -1.65942 -1.30470</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00005 -0.00058 -0.00058 -0.00057 0.00057 0.00057 0.00057 0.00057
Optimized C C C C C C N C N H H H H H H H C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139 4.75022 1.33811 -0.56967 3.96079 5.37166	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495 1.30828 -1.69590 -1.65942 -1.30470 -1.13660</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.00011 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00005 -0.00058 -0.00058 -0.00057 0.00062 0.00067
Optimized C C C C C C N C N H H H H H H H H C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139 4.75022 1.33811 -0.56967 3.96079 5.37166 5.78999	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495 1.30828 -1.69590 -1.65942 -1.30470 -1.13660 -2.14769</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00005 -0.00058 -0.00058 -0.00057 0.000057 0.00062 0.00067 0.00100
Optimized C C C C C C N C N H H H H H H H C C C C	geometries of : -2.80185 -2.52951 -3.56248 -4.87457 -5.14155 -4.10533 -1.57844 -0.56012 -1.16821 -3.35567 -5.70741 -6.17666 -4.31356 -1.44741 0.85028 1.76574 1.37788 3.18216 2.77940 0.71989 3.68066 3.14139 4.75022 1.33811 -0.56967 3.96079 5.37166 5.78999 5.70506	<pre>3 in the S1 stat 0.68579 -0.70363 -1.64489 -1.14726 0.22448 1.17523 1.31975 0.39375 -0.83229 -2.71440 -1.85211 0.56863 2.24456 2.31957 0.63872 -0.50349 1.92305 -0.21351 2.15662 2.79365 1.10942 3.18495 1.30828 -1.69590 -1.65942 -1.30470 -1.13660 -2.14769 -0.60006</pre>	e in THF (angstrom) 0.00019 -0.00069 -0.00125 -0.00090 -0.00004 0.00055 0.00053 0.00010 -0.00096 -0.00188 -0.00131 0.00021 0.00127 0.00157 0.000157 0.000157 0.00001 0.00041 -0.00043 0.00027 -0.00036 -0.00093 -0.00005 -0.00058 -0.00005 -0.00057 0.00005 -0.00057 0.00062 0.00067 0.00100 -0.89952

Optimized C C C C C C C N C N H H H H H H C C C C	<pre>geometries of : -2.80097 -2.53269 -3.56820 -4.87890 -5.14187 -4.10322 -1.57749 -0.55959 -1.17196 -3.36448 -5.71352 -6.17594 -4.30717 -1.44619 0.84682 1.76972 1.37301 3.18533 2.77292 0.71474 3.67997 3.13279 4.74854 1.34460 -0.58226 3.96723 5.37860 5.80161 5.70893 5.70885</pre>	<pre>3 in the S1 0.68464 -0.70619 -1.64368 -1.14307 0.23033 1.17724 1.31582 0.38760 -0.83918 -2.71387 -1.84583 0.57768 2.24748 2.31581 0.63468 -0.50509 1.92202 -0.21216 2.15549 2.79201 1.11124 3.18470 1.31456 -1.69905 -1.67086 -1.30245 -1.12807 -2.13715 -0.58970 -0.58918</pre>	state	in MeCN 0.00017 -0.00067 -0.00123 -0.00092 -0.00010 0.00048 0.00052 0.00015 -0.00091 -0.00133 0.0012 0.00133 0.0012 0.0016 0.00042 -0.00032 -0.00032 -0.00054 -0.00054 -0.00055 0.00055 -0.00049 0.00055 0.00055 0.0	(angstrom)
Optimized C	geometries of : -2.80101	3 in the S1 0.68481	state	in MeOH 0.00009	(angstrom)
Optimized C C	geometries of : -2.80101 -2.53272 -3.56801	3 in the S1 0.68481 -0.70590 -1.64371	state	in MeOH 0.00009 -0.00054 -0.00101	(angstrom)
Optimized C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874	3 in the S1 0.68481 -0.70590 -1.64371 -1.14333	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084	(angstrom)
Optimized C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190	3 in the S1 0.68481 -0.70590 -1.64371 -1.14333 0.23006	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022	(angstrom)
Optimized C C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350	<b>3</b> in the S1 0.68481 -0.70590 -1.64371 -1.14333 0.23006 1.17714	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027	(angstrom)
Optimized C C C C C C N	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750	3 in the S1 0.68481 -0.70590 -1.64371 -1.14333 0.23006 1.17714 1.31597	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041	(angstrom)
Optimized C C C C C C N C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 1.17105	3 in the S1 0.68481 -0.70590 -1.64371 -1.14333 0.23006 1.17714 1.31597 0.38775 0.23250	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015	(angstrom)
Optimized C C C C C N C N H	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393	3 in the S1 0.68481 -0.70590 -1.64371 -1.14333 0.23006 1.17714 1.31597 0.38775 -0.83859 -2.71381	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146	(angstrom)
Optimized C C C C C N C N H H	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118	(angstrom)
Optimized C C C C C N C N H H H	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604       0.57708</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00011	(angstrom)
Optimized C C C C C N C N H H H H H	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604       0.57708       2.24730</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00011 0.00077	(angstrom)
Optimized C C C C C N C N H H H H H H	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604       0.57708       2.24730       2.31587</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00011 0.00077 0.00124	(angstrom)
Optimized C C C C C C N C N H H H H H H C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00011 0.00077 0.00124 0.00009	(angstrom)
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         102222</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00041 0.00015 -0.00043 -0.00146 -0.00118 -0.00011 0.00077 0.00124 0.00009 0.00034	(angstrom)
Optimized C C C C C C N C N H H H H C C C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         1.92223         -0.21237</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00146 -0.00118 -0.00118 -0.00118 0.00077 0.00124 0.00009 0.00034 -0.00018 0.00025	(angstrom)
Optimized C C C C C C N C N H H H H H C C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         1.92223         -0.21237         2.15538</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00118 -0.00018 0.00034 -0.00018 0.00025 -0.00013	(angstrom)
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604       0.57708       2.24730       2.31587       0.63506       -0.50500       1.92223       -0.21237       2.15538       2.79234</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00018 0.00077 0.00124 0.00009 0.00034 -0.00018 0.00025 -0.00013 -0.00048	(angstrom)
Optimized C C C C C C N C N H H H H H H C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.68017	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604       0.57708       2.24730       2.31587       0.63506       -0.50500       1.92223       -0.21237       2.15538       2.79234       1.11076</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00118 -0.00011 0.00077 0.00124 0.00009 0.00034 -0.00018 0.00025 -0.00013 -0.00048 0.00005	(angstrom)
Optimized C C C C C C N C N C N H H H H H C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.68017 3.13390	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         1.92223         -0.21237         2.15538         2.79234         1.1076         3.18436</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00084 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00118 -0.00118 -0.00011 0.00077 0.00124 0.00009 0.00034 -0.00018 0.00025 -0.00013 -0.00048 0.00005 -0.00028	(angstrom)
Optimized C C C C C C C N C N H H H H H C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.68017 3.13390 4.74874	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         1.92223         -0.21237         2.15538         2.79234         1.11076         3.18436         1.31405 </pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00043 -0.00146 -0.00118 -0.00118 -0.00011 0.00077 0.00124 0.00009 0.00034 -0.00018 0.00025 -0.00013 -0.00048 0.00005 -0.00028 0.00004	(angstrom)
Optimized C C C C C C C N C N H H H H H C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.68017 3.13390 4.74874 1.34400 -0.58252	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         1.92223         -0.21237         2.15538         2.79234         1.11076         3.18436         1.31405         -1.69877         -1.67040</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00043 -0.00118 -0.00118 -0.00118 0.00077 0.00124 0.00009 0.00034 -0.00018 0.00025 -0.00013 -0.00048 0.00005 -0.00028 0.00004 0.00004 0.00068 -0.00040	(angstrom)
Optimized C C C C C C C N C C C C C C C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.66017 3.13390 4.74874 1.34400 -0.58252 3.96706	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         1.92223         -0.21237         2.15538         2.79234         1.11076         3.18436         1.31405         -1.69877         -1.67040         -1.30299</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00043 -0.00146 -0.00118 -0.00118 -0.00011 0.00077 0.00124 0.000034 -0.00018 0.00025 -0.00013 -0.00048 0.00004 0.00048	(angstrom)
Optimized C C C C C C C N C C C C C C C C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.68017 3.13390 4.74874 1.34400 -0.58252 3.96706 5.37827	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604       0.57708       2.24730       2.31587       0.63506       -0.50500       1.92223       -0.21237       2.15538       2.79234       1.11076       3.18436       1.31405       -1.69877       -1.67040       -1.30299       -1.12820</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00118 -0.00011 0.00077 0.00124 0.00009 0.00034 -0.00018 0.00025 -0.00013 -0.00048 0.000048 0.00048 0.00048 0.00048 0.00048	(angstrom)
Optimized C C C C C C C N C N H H H H H H H C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.68017 3.13390 4.74874 1.34400 -0.58252 3.96706 5.37827 5.80142	<pre>3 in the S1       0.68481       -0.70590       -1.64371       -1.14333       0.23006       1.17714       1.31597       0.38775       -0.83859       -2.71381       -1.84604       0.57708       2.24730       2.31587       0.63506       -0.50500       1.92223       -0.21237       2.15538       2.79234       1.11076       3.18436       1.31405       -1.69877       -1.67040       -1.30299       -1.12820       -2.13723</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00118 -0.00118 0.00077 0.00124 0.00077 0.00124 0.000034 -0.00018 0.00025 -0.00013 -0.00048 0.000048 0.00048	(angstrom)
Optimized C C C C C C C N C C N C N C N H H H H C C C C	geometries of : -2.80101 -2.53272 -3.56801 -4.87874 -5.14190 -4.10350 -1.57750 -0.55952 -1.17185 -3.36393 -5.71342 -6.17611 -4.30768 -1.44578 0.84707 1.76958 1.37338 3.18514 2.77343 0.71535 3.68017 3.13390 4.74874 1.34400 -0.58252 3.96706 5.37827 5.80142 5.70860	<pre>3 in the S1         0.68481         -0.70590         -1.64371         -1.14333         0.23006         1.17714         1.31597         0.38775         -0.83859         -2.71381         -1.84604         0.57708         2.24730         2.31587         0.63506         -0.50500         1.92223         -0.21237         2.15538         2.79234         1.11076         3.18436         1.31405         -1.69877         -1.67040         -1.30299         -1.12820         -2.13723         -0.58975</pre>	state	in MeOH 0.00009 -0.00054 -0.00101 -0.00022 0.00027 0.00041 0.00015 -0.00063 -0.00146 -0.00118 -0.00118 -0.00118 -0.00124 0.00077 0.00124 0.00034 -0.00018 0.00025 -0.00013 -0.00048 0.000048 0.00048	(angstrom)

Optimized	geometries of	3	in the S1	state	in H2O	(angstrom)
С	-2.80089		0.68456		0.00013	
С	-2.53326		-0.70644		-0.00061	L
С	-3.56908		-1.64353		-0.00113	3
С	-4.87957		-1.14245		-0.00090	)
С	-5.14197		0.23118		-0.00017	7
С	-4.10303		1.17763		0.00038	
N	-1.57733		1.31530		0.00047	
С	-0.55958		0.38669		0.00016	
Ν	-1.17252		-0.83993		-0.00076	5
Н	-3.36568		-2.71377		-0.00166	5
Н	-5.71455		-1.84482		-0.00129	9
Н	-6.17595		0.57889		-0.00001	L
Н	-4.30640		2.24799		0.00098	
Н	-1.44569		2.31524		0.00143	
С	0.84646		0.63412		0.00007	
С	1.77016		-0.50548		0.00041	
С	1.37243		1.92179		-0.00029	9
С	3.18570		-0.21220		0.00026	
С	2.77224		2.15517		-0.00024	1
Н	0.71420		2.79171		-0.00068	3
С	3.67995		1.11113		0.00000	
Н	3.13205		3.18438		-0.00044	1
Н	4.74841		1.31494		-0.00002	2
0	1.34526		-1.69960		0.00081	
H	-0.58406		-1.67224		-0.00044	1
0	3.96836		-1.30229		0.00055	
С	5.37965		-1.12636		0.00054	
Н	5.80376		-2.13497		0.00079	
Н	5.70940		-0.58759		-0.89936	5
Н	5.70937		-0.58714		0.90017	

Optimized	geometries of	<b>3</b> +(MeOH) <sub>6</sub> in	the ground state	in MeOH	(angstrom)
С	-2.66592	-1.85799	-0.10177		
C	-2.64154	-0.68222	-0.87508		
C	-3.82251	0.02/1/	-1.112//		
C	-4.99121	-0.45645	-0.54384		
C	-3 83574	-2 35235	0.24241		
N	-1.35593	-2.28183	-0.06292		
C	-0.61041	-1.38451	-0.77074		
N	-1.34505	-0.41612	-1.27646		
Н	-3.81579	0.93314	-1.70827		
Н	-5.92257	0.07678	-0.69991		
Н	-5.93002	-1.96804	0.67665		
Н	-3.83842	-3.25172	1.07938		
H	-0.99541	-3.07535	0.44427		
C	0.83828	-1.53840	-0.95144		
C	1.69245	-0.439/6	-0.81/32		
C	1.30190	-2.80030	-1.08272		
C	2 71671	-2 95837	-1 49489		
Н	0.68791	-3.64404	-1.38277		
C	3.57463	-1.85783	-1.40899		
H	3.12027	-3.93153	-1.74992		
Н	4.63354	-1.98950	-1.59493		
0	1.29721	0.79554	-0.44194		
Н	0.50107	0.74817	0.13819		
0	3.80476	0.52542	-0.96716		
С	5.21307	0.42250	-1.07983		
H	5.60238	1.41783	-0.87126		
H	5.61829	-0.2869/	-0.34928		
Н	5.5093L 2.22210	0.116//	-2.08902		
U u	2 85027	2.02955	1.45892		
	-0 74423	3 10284	-0 29699		
н	-0 54758	2 65581	-1 14308		
0	-0.53843	1.80777	-2.71912		
H	-0.75132	0.96538	-2.25349		
0	-0.30446	0.48363	1.67626		
Н	-1.27594	0.35996	1.75529		
0	-2.97913	0.54384	2.15223		
Н	-3.50026	-0.10319	1.66226		
0	1.13847	-1.47244	3.05594		
Н	0.61938	-0.89629	2.46656		
U U	0.02878	1.61409	2.48550		
п	-0 59887	2 46783	2.27010		
H	-0.09018	1.37889	3.54820		
C	-3.34655	1.84675	1.69753		
Н	-4.42255	1.91039	1.51299		
Н	-3.08334	2.55098	2.48955		
Н	-2.79828	2.12056	0.78956		
С	3.62193	0.90306	2.22080		
Н	4.32082	0.25807	1.67139		
Н	4.12906	1.26776	3.11781		
H	2.76508	0.29243	2.53720		
С	1.85799	-2.39538	2.27082		
n u	2.33143 2 /6610	-1.908/1	1.33129 2 0//01		
H	2.40019 1 20193	-3.00368	2.944U1 1 70621		
C	-1 72602	2 24591	-3 35075		
H	-1,46492	3.02923	-4.06644		
Н	-2.22047	1.43235	-3.89591		
Н	-2.44127	2.66900	-2.63113		
С	0.31517	3.98938	-0.02050		

Н	0.06814	4.53659	0.89413
Н	1.26476	3.46552	0.15099
Н	0.46576	4.72510	-0.82345