Synthesis and Electrogenenerated Chemiluminescence of Donor-substituted Phenylethynylcoumarins

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Scheme 1 **Scheme 2**

Structures (Scheme 1) and synthetic scheme (Scheme 2) of preparation of donor-substituted phenylethynylcoumarins 1-10.

Corrections to be incorporated in the paper jo0493424:

Structures of compounds **6-10** in Scheme 1 to appear as 6-isomers and not as 7-isomers and all terms reading 7-coumarin derivative(s) to read as 6-coumarin derivative(s). Any reference to compounds **6-10** in the text, figures and tables implies reference to the 6-isomer and not to the 7-isomer as incorrectly reported in the paper. 4-iodosalicylaldehyde to read as 5-iodosalicylaldehyde in the text.

The correct schemes are provided in this corrected Supporting Information that also carries the corrected structures in the spectra for compounds **6-10** and corrected results of the PM3 Calculations. PM3 calculations for the 6-isomers (compounds **6** and **10**) revealed that the concept discussed in the result and discussion holds good. All the data including those given in the SI are maintainable for the corrected structures. All the results, discussion and conclusions still hold good and hence remain unaltered.

The error is regretted.

Characterization Data for 1 - 5

3-Phenylethynylcoumarin (1)

From phenylacetylene and 3-iodocoumarin in 89% yield. M.p.: 176-177 °C; ¹H-NMR (400 MHz, CDCl₃; δ, ppm) 7.93 (s, 1H), 7.57-7.46 (m, 4H), 7.35-7.26 (m, 5H); ¹³C-NMR (100 MHz, CDCl₃; δ, ppm) 159.1, 153.1, 144.5, 132.0, 131.8, 128.9, 128.2, 127.6, 124.7, 122.0, 118.8, 116.7, 113.0, 95.7, 83.3; HR-FAB M.S. m/z (M⁺): 246.0681, calculated for C₁₇H₁₀O₂: 246.0681.

3-*p*-Tolylethynylcoumarin (2)

From *p*-tolylethyne and 3-iodocoumarin in 88% yield. M.p.: 127 – 128 °C; ¹H NMR (δ, ppm): 7.91 (s, 1H), 7.53-7.46 (m, 4H), 7.33-7.26 (m, 2H), 7.15 (d, *J* = 8 Hz, 2H), 2.36 (s, 3H); ¹³C NMR (δ, ppm) : 159.17, 153.01, 144.2, 139.3, 131.8, 131.7, 129.0, 127.5, 124.6, 118.9, 118.8, 116.6, 113.1, 96.1, 82.7, 21.7; MS (M⁺) m/z: 260.0838, calculated for C₁₈H₁₂O₂: 260.0837.

3-*p*-Anisylethynylcoumarin (3)

From *p*-anisylethyne and 3-iodocoumarin in 85% yield. M.p.: 162-165 °C; ¹H-NMR (δ, ppm) 7.89 (s, 1H), 7.52-7.44 (m, 4H), 7.33-7.25 (m, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H); ¹³C-NMR (δ, ppm): 160.0, 129.2, 152.9, 143.8, 133.4, 131.7, 127.4, 124.6, 118.9, 116.6, 114.1, 113.9, 113.2, 96.1, 82.2, 55.4; HR-FAB M.S. m/z (M⁺): 276.0790, calculated for C₁₈H₁₂O₃: 276.0786.

3-(*p*-*O*-Isopropyl)phenylethynylcoumarin (4)

From 4-*O*-isopropylphenylethyne and 3-iodocoumarin in 73% yield. M.p.: 147-148 °C; ¹H-NMR (δ, ppm) 7.88 (s, 1H), 7.52-7.45 (m, 4H), 7.33-7.25 (m, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 4.57 (septet, *J* = 6.4 Hz, 1H), 1.33 (d, *J* = 6.4 Hz, 6H); ¹³C-NMR (δ ppm) 159.3, 158.5, 152.9, 143.7, 133.5, 131.7, 127.4, 124.6, 118.9, 116.7, 115.6, 113.7, 113.4, 96.3, 82.1, 69.9, 22.1; HR-FAB M.S. m/z (M⁺): 304.1095, calculated for C₂₀H₁₆O₃: 304.1099.

3-(*p*-*N,N*-Dimethylamino)phenylethynylcoumarin (5)

From *N,N*-dimethylaminophenylethyne and 3-iodocoumarin in 88% yield. M.p.: 205-206 °C; ¹H-NMR (δ, ppm) 7.84 (s, 1H), 7.50-7.43 (m, 4H), 7.32-7.26 (m, 2H), 6.62 (d, *J* = 8.8 Hz, 2H), 2.99 (s, 6H); ¹³C-NMR (δ, ppm) 159.4, 152.8, 150.4, 142.6, 133.1, 131.3, 127.2, 124.5, 119.2, 116.6, 113.8, 111.5, 108.6, 97.9, 81.9, 40.2; HR-FAB M.S. m/z (M⁺): 289.1098, calculated for C₁₉H₁₅NO₂: 289.1103.

Characterization Data for 6 - 10

6-Phenylethynylcoumarin (6)

From phenylacetylene and 6-iodocoumarin in 86% yield. M.p.: 74-76 °C; ¹H-NMR (δ, ppm) 7.65-7.67 (m, 2H), 7.62 (s, 1H), 7.51-7.49 (m, 2H), 7.36 (d, *J* = 4.4 Hz, 2H), 7.34-7.20 (m, 2H), 6.3 (d, *J* = 9.6 Hz, 1H); ¹³C-NMR (δ, ppm) 160.0, 153.2, 142.6, 134.6, 131.4, 130.6, 128.5, 128.2, 122.4, 119.6, 118.7, 117.1, 116.9, 89.9, 87.4; HR-FAB M.S. *m/z* (M⁺): 246.0682, calculated for C₁₇H₁₀O₂: 246.0714.

6-*p*-Tolylethynylcoumarin (7)

From *p*-tolylacetylene and 6-iodocoumarin in 90% yield. M.p.: 183-186 °C; ¹H-NMR (δ, ppm) 7.67 (s, 1H), 7.65-7.63 (m, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 9.2 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 2H), 6.44 (d, *J* = 9.2 Hz, 1H), 2.36 (s, 3H); ¹³C-NMR (δ, ppm) 160.0, 153.1, 142.6, 138.7, 134.6, 131.3, 130.5, 129.0, 119.6, 119.3, 118.6, 117.1, 116.9, 90.1, 86.8, 21.6; HR-FAB M.S. *m/z* (M⁺): 260.0839, calculated for C₁₈H₁₂O₂: 260.0837.

6-*p*-Anisylethynylcoumarin (8)

From *p*-anisylethyne and 6-iodocoumarin in 85% yield. M.p.: 102-107 °C; ¹H-NMR (δ, ppm) 7.63-7.67 (m, 2H), 7.61 (s, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.43 (d, *J* = 8.2 Hz, 1H), 3.82 (s, 3H); ¹³C-NMR (δ, ppm) 160.1, 159.6, 153.1, 142.7, 134.6, 132.9, 130.4, 120.1, 118.7, 117.2, 117.0, 114.5, 113.9, 90.1, 86.2, 55.4; HR-FAB M.S. *m/z* (M⁺): 276.0789, calculated for C₁₈H₁₂O₃: 277.0786.

6-(4-*O*-Isopropyl)phenylethynylcoumarin (9)

From 4-*O*-isopropylphenylethyne and 6-iodocoumarin in 85% yield. M.p.: 112-116 °C; ¹H-NMR (δ ppm) 7.66 (d, *J* = 6.8 Hz, 1H), 7.60 (s, 1H), 7.42 (d, *J* = 8.8 Hz), 7.27 (d, *J* = 8.4 Hz, H), 6.84 (d, *J* = 8.2 Hz, 2H), 6.42 (d, *J* = 8.8 Hz, 1H), 4.55 (q, *J* = 5.2 Hz, 1H), 1.33 (d, *J* = 6.0 Hz, 6H); ¹³C-NMR (δ ppm) 160.0, 158.0, 153.0, 142.7, 134.5, 132.9, 130.4, 120.1, 118.7, 117.1, 116.9, 115.6, 114.1, 90.2, 86.1, 69.9, 22.0; HR-FAB M.S. *m/z* (M⁺): 304.1103, calculated for C₂₀H₁₆O₃: 304.1099.

6-(4-*N,N*-Dimethylamino)phenylethynylcoumarin (10)

From *N,N*-dimethylaminophenylethyne and 6-iodocoumarin in 92% yield. M.p.: 125-129 °C; ¹H-NMR (δ, ppm) 7.65 (d, *J* = 9.6 Hz, 2H), 7.56 (s, 1H), 7.38 (d, *J* = 8.8 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 1H), 6.66 (d, *J* = 9.2 Hz, 2H), 6.42 (d, *J* = 9.6 Hz, 1H), 2.98 (s, 6H); ¹³C-NMR (δ, ppm): 160.2, 152.8, 150.6, 142.8, 134.4, 132.6, 130.1, 120.7, 118.7, 117.1, 116.9, 111.7, 109.0, 91.4, 85.6, 40.2; HR-FAB M.S. *m/z* (M⁺): 289.1096, calculated for C₂₀H₁₆O₃: 289.1103.

RHL-5-3

Pulse Sequence: s2pu1

RHL-5-3

Pulse Sequence: s2pu1

RHL-5-1

Pulse Sequence: s2pu1

RHL-5-1

Pulse Sequence: s2pul

RHL-5-2

Pulse Sequence: s2pu1

RHL-5-2

Pulse Sequence: s2pu1

RHL-5-5

Pulse Sequence: s2pu1

RHL-5-5

Pulse Sequence: s2pul

RHL-5-4

Pulse Sequence: s2pu1

RHL-5-4

Pulse Sequence: s2pu1

benzene

Pulse Sequence: s2pu1

benzene

Pulse Sequence; s2pu1

p2071

Pulse Sequence: s2pu1

p2071

Pulse Sequence: s2pu1

ome

Pulse Sequence: s2pu1

ome

Pulse Sequence: s2pu1

i-pr

Pulse Sequence: s2pu1

i-pr

Pulse Sequence: s2pul

p2075-c13

Pulse Sequence: s2pu1

X-ray crystal structure (ORTEP) of compound **4**

Table 1. Crystal data and structure refinement for IC10547. (Compound 4)

Identification code	ic10547
Diffractionmeter used	Nonius KappaCCD
Empirical formula	$C_{20}H_{16}O_3$
Formula weight	304.33
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	$a = 34.0680(4)$ Å $\alpha = 90^\circ$ $b = 5.9080(2)$ Å $\beta = 115.704(2)^\circ$ $c = 17.5600(7)$ Å $\gamma = 90^\circ$
Volume, Z	$3184.6(2)$ Å ³ , 8
Density (calculated)	1.269 Mg/m ³
Absorption coefficient	0.085 mm ⁻¹
F(000)	1280
Crystal size	0.30 x 0.20 x 0.15 mm
θ range for data collection	2.57 to 27.48°
Limiting indices	$-44 \leq h \leq 44$, $-6 \leq k \leq 7$, $-19 \leq l \leq 22$
Reflections collected	8600
Independent reflections	3576 ($R_{int} = 0.0434$)
Absorption correction	Multi-scan
Max. and min. transmission	0.988 and 0.914
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3523 / 0 / 209
Goodness-of-fit on F^2	1.008
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0582$, $wR2 = 0.1354$
R indices (all data)	$R1 = 0.1377$, $wR2 = 0.1734$
Extinction coefficient	$0.0045(12)$
Largest diff. peak and hole	0.258 and -0.165 eÅ ⁻³

Table 2. Bond lengths [Å] and angles [°] for 10547. (Compound 4)

O(1)-C(9)	1.371(2)	O(1)-C(1)	1.382(2)
O(2)-C(9)	1.201(3)	O(3)-C(15)	1.357(2)
O(3)-C(18)	1.445(3)	C(1)-C(2)	1.378(3)
C(1)-C(6)	1.389(3)	C(2)-C(3)	1.381(3)
C(3)-C(4)	1.384(3)	C(4)-C(5)	1.369(3)
C(5)-C(6)	1.393(3)	C(6)-C(7)	1.428(3)
C(7)-C(8)	1.354(3)	C(8)-C(10)	1.463(3)
C(8)-C(9)	1.466(3)	C(10)-C(11)	1.125(3)
C(11)-C(12)	1.473(3)	C(12)-C(13)	1.391(3)
C(12)-C(17)	1.400(3)	C(13)-C(14)	1.371(3)
C(14)-C(15)	1.383(3)	C(15)-C(16)	1.386(3)
C(16)-C(17)	1.362(3)	C(18)-C(19)	1.492(3)
C(18)-C(20)	1.503(3)		
C(9)-O(1)-C(1)	122.7(2)	C(15)-O(3)-C(18)	120.1(2)
C(2)-C(1)-O(1)	116.8(2)	C(2)-C(1)-C(6)	122.5(2)
O(1)-C(1)-C(6)	120.6(2)	C(1)-C(2)-C(3)	117.9(2)
C(2)-C(3)-C(4)	121.2(2)	C(5)-C(4)-C(3)	119.6(2)
C(4)-C(5)-C(6)	121.0(2)	C(1)-C(6)-C(5)	117.6(2)
C(1)-C(6)-C(7)	118.2(2)	C(5)-C(6)-C(7)	124.1(2)
C(8)-C(7)-C(6)	121.2(2)	C(7)-C(8)-C(10)	124.3(2)
C(7)-C(8)-C(9)	120.3(2)	C(10)-C(8)-C(9)	115.5(2)
O(2)-C(9)-O(1)	117.5(2)	O(2)-C(9)-C(8)	125.6(2)
O(1)-C(9)-C(8)	116.9(2)	C(11)-C(10)-C(8)	174.9(2)
C(10)-C(11)-C(12)	178.3(2)	C(13)-C(12)-C(17)	117.8(2)
C(13)-C(12)-C(11)	119.5(2)	C(17)-C(12)-C(11)	122.6(2)
C(14)-C(13)-C(12)	121.1(2)	C(13)-C(14)-C(15)	120.5(2)
O(3)-C(15)-C(14)	125.8(2)	O(3)-C(15)-C(16)	115.6(2)
C(14)-C(15)-C(16)	118.6(2)	C(17)-C(16)-C(15)	121.2(2)
C(16)-C(17)-C(12)	120.7(2)	O(3)-C(18)-C(19)	110.8(2)
O(3)-C(18)-C(20)	104.8(2)	C(19)-C(18)-C(20)	112.4(2)

Crystal packing diagram showing π -interaction in **4**

Current / 1e-5A

Mar. 18, 2004 14:14:02

Tech: CV

File: 3-H-2.bin

Init E (V) = 0

High E (V) = 2.5

Low E (V) = -2

Init P/N = N

Scan Rate (V/s) = 0.05

Segment = 3

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-5

CV curve of 1

Current / 1e-5A

Feb. 20, 2004 12:55:30

Tech: CV

File: 3-CH3.bin

Init E (V) = 0

High E (V) = 2

Low E (V) = -2

Init P/N = N

Scan Rate (V/s) = 0.05

Segment = 3

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-5

2nd E (V) = 0

Sens 2 (A/V) = 1e-6

Current / 1e-5A

Mar. 18, 2004 15:58:56
Tech: CV
File: 3-OCH3.bin

Init E (V) = 0
High E (V) = 2
Low E (V) = -3
Init P/N = N
Scan Rate (V/s) = 0.05
Segment = 3
Smpl Interval (V) = 0.001
Quiet Time (s) = 2
Sensitivity (A/V) = 1e-5

Current / 1e-5A

Mar. 18, 2004 17:09:10
Tech: CV
File: 3-oisopropyl-2
Init E (V) = 0
High E (V) = 2
Low E (V) = -2.5
Init P/N = N
Scan Rate (V/s) = 0.05
Segment = 3
Smpl Interval (V) = 0.001
Quiet Time (s) = 2
Sensitivity (A/V) = 1e-5
2nd E (V) = 0
Sens 2 (A/V) = 1e-6

Current / 1e-5A

Mar. 18, 2004 17:53:06

Tech: CV

File: 3-nnMe.bin

Init E (V) = 0

High E (V) = 2

Low E (V) = -2.5

Init P/N = N

Scan Rate (V/s) = 0.05

Segment = 3

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-5

ECL spectrum of **1**

ECL spectrum of **2**

6.22
6.23
6.24

ECL spectrum of **3**

ECL spectrum of **4**

ECL spectrum of **5**

Current / 1e-5A

Feb. 9, 2004 17:54:24
Tech: CV
File: H-1.bin
Init E (V) = 0
High E (V) = 2.5
Low E (V) = -2
Init P/N = N
Scan Rate (V/s) = 0.05
Segment = 3
Smpl Interval (V) = 0.001
Quiet Time (s) = 2
Sensitivity (A/V) = 1e-5
2nd E (V) = 0
Sens 2 (A/V) = 1e-6

CV curve of 6

Current / 1e-5A

Feb. 9, 2004 18:22:59

Tech: CV

File: ch3

Init E (V) = 0

High E (V) = 2.5

Low E (V) = -2

Init P/N = N

Scan Rate (V/s) = 0.05

Segment = 3

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-5

2nd E (V) = 0

Sens 2 (A/V) = 1e-6

CV curve of 7

Current / 1e-5A

Dec. 26, 2003 14:23:47
Tech: CV
File: ome.bin
Init E (V) = 0
High E (V) = 2
Low E (V) = -2
Init P/N = N
Scan Rate (V/s) = 0.1
Segment = 3
Smpl Interval (V) = 0.001
Quiet Time (s) = 2
Sensitivity (A/V) = 1e-5

Mar. 10, 2004 13:52:59
Tech: CV
File: i-pro.bin
Init E (V) = 0
High E (V) = 3
Low E (V) = -3
Init P/N = N
Scan Rate (V/s) = 0.05
Segment = 3
Smpl Interval (V) = 0.001
Quiet Time (s) = 2
Sensitivity (A/V) = 2e-5

Current / 1e-5A

Feb. 9, 2004 17:37:36

Tech: CV

File: n-me2

Init E (V) = 0

High E (V) = 2.5

Low E (V) = -2

Init P/N = N

Scan Rate (V/s) = 0.05

Segment = 3

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-5

2nd E (V) = 0

Sens 2 (A/V) = 1e-6

CV curve of 10

ECL spectrum of **6**

Procedure used for performing theoretical calculations

The program used:	Spartan'04 (for Windows)
Level of theory:	Semi-empirical Parameterization Method 3 (also called Parameter Model 3, PM3)
Basis set:	Predefined basis sets as provided by Spartan'04 (restricted to minimal valence-only representation; incorporates restricted Hartree-Fock model)

Computational method:

Structures were drawn at the Entry-level of input and minimized. Calculations were set up to perform geometry optimization in order to obtain equilibrium geometry for the molecule at the ground state with Semi-empirical method PM3 from its initial geometry subject to symmetry. The total charge was neutral and multiplicity was Singlet.

Print was requested for atomic charges, thermodynamics, vibrational modes, orbitals and energies. The required surfaces were selected and the problem was submitted. When the calculations were completed, the orbital surfaces were mapped and other properties were outputted.

The following pages contain the minimum energy structures of **1**, **6**, **5** and **10** as appropriate and their energies and Cartesian coordinates. No imaginary frequencies were present.

Optimized ground state structure of **1**

Energy: 38.11 kcal/mol

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
1 H H1	-2.0388082	0.0000000	-5.2892747
2 C C1	-1.0151203	0.0000000	-4.8969663
3 C C4	1.6031850	0.0000000	-3.8796035
4 C C2	-0.7866845	0.0000000	-3.5110668
5 C C6	0.0749204	0.0000000	-5.7503883
6 C C5	1.3794273	0.0000000	-5.2448048
7 C C3	0.5186479	0.0000000	-2.9898926
8 H H6	-0.0844317	0.0000000	-6.8342435
9 H H5	2.2274379	0.0000000	-5.9377119
10 H H4	2.6246014	0.0000000	-3.4822174
11 C C7	0.7045554	0.0000000	-1.5578525
12 H H7	1.7261790	0.0000000	-1.1601745
13 C C8	-0.3796842	0.0000000	-0.7455194
14 C C9	-1.7330331	0.0000000	-1.3396594
15 O O1	-1.9039649	0.0000000	-2.7101632
16 O O2	-2.8281232	0.0000000	-0.8241290
17 C C10	-0.2663860	0.0000000	0.6584845
18 C C11	-0.1747357	0.0000000	1.8503971
19 C C12	-0.0763243	0.0000000	3.2617537
20 C C13	0.1100179	0.0000000	6.0380631
21 C C14	-1.2399629	0.0000000	4.0392197
22 C C15	1.1802958	0.0000000	3.8772385
23 C C16	1.2664305	0.0000000	5.2643942
24 C C17	-1.1393608	0.0000000	5.4255061
25 H H2	-2.2227436	0.0000000	3.5547655
26 H H3	2.0899818	0.0000000	3.2677744
27 H H8	2.2483986	0.0000000	5.7488496
28 H H9	-2.0480416	0.0000000	6.0366762
29 H H10	0.1833287	0.0000000	7.1305318

Optimized ground state structure of **6**

Energy: 37.23 kcal/mol; μ = 4.63 D; Pt.gp:Cs

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
1	H	H1	-4.3396197	0.0000000	-0.2518891
2	C	C1	-3.3127239	0.0000000	-0.6363544
3	C	C4	-0.6848425	0.0000000	-1.6447841
4	C	C2	-3.0751521	0.0000000	-2.0212267
5	C	C6	-2.2334047	0.0000000	0.2284133
6	C	C5	-0.9187997	0.0000000	-0.2724624
7	C	C3	-1.7662256	0.0000000	-2.5343691
8	H	H4	0.3397985	0.0000000	-2.0347295
9	C	C7	-1.5766386	0.0000000	-3.9699514
10	H	H7	-0.5525132	0.0000000	-4.3605122
11	C	C8	-2.6497677	0.0000000	-4.7791978
12	H	H3	-2.5748397	0.0000000	-5.8716413
13	C	C9	-3.9974381	0.0000000	-4.1964392
14	O	O1	-5.0812964	0.0000000	-4.7373830
15	O	O2	-4.1879404	0.0000000	-2.8287238
16	H	H15	-2.3992553	0.0000000	1.3116858
17	C	C10	0.1719447	0.0000000	0.6295463
18	C	C11	1.0923065	0.0000000	1.3914736
19	C	C12	2.1836893	0.0000000	2.2941185
20	C	C13	4.3291996	0.0000000	4.0661150
21	C	C14	2.7216260	-1.2123727	2.7389648
22	C	C15	2.7216260	1.2123727	2.7389648
23	C	C16	3.7933080	1.2055099	3.6239548
24	C	C17	3.7933080	-1.2055099	3.6239548
25	H	H2	2.2986859	-2.1606627	2.3908596
26	H	H6	2.2986859	2.1606627	2.3908596
27	H	H5	4.2163071	2.1529858	3.9738156
28	H	H8	4.2163071	-2.1529858	3.9738156
29	H	H9	5.1736545	0.0000000	4.7630895

Minimum energy structure of **6**
after imposing dihedral constraint of 0°.

Energy: 37.01 kcal/mol; μ = 4.63 D; Pt.gp.: Cs

Cartesian Coordinates (Angstroms)

	Atom	X	Y	Z
1 H	H1	-2.9001522	0.0000000	-3.2363120
2 C	C1	-1.9006250	0.0000000	-2.7854425
3 C	C4	0.6747958	0.0000000	-1.6495459
4 C	C2	-0.7561977	0.0000000	-3.6007996
5 C	C6	-1.7441068	0.0000000	-1.4114467
6 C	C5	-0.4582283	0.0000000	-0.8400404
7 C	C3	0.5342305	0.0000000	-3.0425910
8 H	H4	1.6766230	0.0000000	-1.2043996
9 C	C7	1.6802108	0.0000000	-3.9278317
10 H	H7	2.6821709	0.0000000	-3.4835064
11 C	C8	1.4888636	0.0000000	-5.2581857
12 H	H3	2.3117557	0.0000000	-5.9806171
13 C	C9	0.1219187	0.0000000	-5.7942032
14 O	O1	-0.2660688	0.0000000	-6.9417107
15 O	O2	-0.9769119	0.0000000	-4.9578166
16 H	H15	-2.6251205	0.0000000	-0.7597820
17 C	C10	-0.3201257	0.0000000	0.5674988
18 C	C11	-0.2045466	0.0000000	1.7570521
19 C	C12	-0.0676894	0.0000000	3.1656042
20 C	C13	0.2020284	0.0000000	5.9356325
21 C	C14	-1.2067250	0.0000000	3.9783627
22 C	C15	1.2067382	0.0000000	3.7434880
23 C	C16	1.3345882	0.0000000	5.1272993
24 C	C17	-1.0651412	0.0000000	5.3608855
25 H	H2	-2.2037160	0.0000000	3.5253046
26 H	H6	2.0974847	0.0000000	3.1065711
27 H	H5	2.3307468	0.0000000	5.5819500
28 H	H8	-1.9549073	0.0000000	5.9991622
29 H	H9	0.3081441	0.0000000	7.0254081

Optimized ground state geometry of **5**.

Energy: 38.904 kcal/mol

Cartesian Coordinates (Angstroms)				
Atom		X	Y	Z
1	H H1	-7.2181135	0.0000000	-1.7968505
2	C C1	-6.7666982	0.0000000	-0.7982725
3	C C4	-5.6014556	0.0000000	1.7581325
4	C C2	-5.3701886	0.0000000	-0.6489788
5	C C6	-7.5561708	0.0000000	0.3387974
6	C C5	-6.9772793	0.0000000	1.6120821
7	C C3	-4.7758403	0.0000000	0.6245499
8	H H6	-8.6470359	0.0000000	0.2422004
9	H H5	-7.6207629	0.0000000	2.4982116
10	H H4	-5.1472601	0.0000000	2.7558614
11	C C7	-3.3358398	0.0000000	0.7286656
12	H H7	-2.8787095	0.0000000	1.7249572
13	C C8	-2.5853073	0.0000000	-0.3991059
14	C C9	-3.2546949	0.0000000	-1.7163172
15	O O1	-2.8034613	0.0000000	-2.8394412
16	O O2	-4.6333768	0.0000000	-1.8095068
17	C C10	-1.1784327	0.0000000	-0.3522893
18	C C11	0.0160483	0.0000000	-0.2953228
19	C C12	1.4268028	0.0000000	-0.2267420
20	C C13	4.2286855	0.0000000	-0.0983986
21	C C14	2.1846268	0.0000000	-1.4030772
22	C C15	2.0745420	0.0000000	1.0132261
23	C C16	3.4582213	0.0000000	1.0808668
24	C C17	3.5681648	0.0000000	-1.3428297
25	H H2	1.6789793	0.0000000	-2.3753910
26	H H3	1.4835825	0.0000000	1.9355442
27	H H8	3.9321485	0.0000000	2.0697254
28	H H9	4.1305187	0.0000000	-2.2841613
29	N N1	5.6425642	0.0000000	-0.0353715
30	C C18	6.4633061	0.0000000	-1.2570155
31	H H11	6.2655311	0.8906926	-1.8713036
32	H H12	6.2655311	-0.8906926	-1.8713036
33	H H13	7.5285248	0.0000000	-0.9850341
34	C C19	6.3538903	0.0000000	1.2528009
35	H H10	7.4386639	0.0000000	1.0739122
36	H H14	6.1051477	-0.8904675	1.8485897
37	H H15	6.1051477	0.8904675	1.8485897

Optimized ground state geometry of **10**.

Energy: 33.48 kcal/mol; μ = 5.61D; Pt.gp: Cs

Cartesian Coordinates (Angstroms)				
Atom		X	Y	Z
1 H	H1	2.8608857	0.0000000	-5.0593671
2 C	C1	1.8653927	0.0000000	-4.5998470
3 C	C4	-0.6993599	0.0000000	-3.4406513
4 C	C2	0.7139056	0.0000000	-5.4048193
5 C	C6	1.7210308	0.0000000	-3.2243075
6 C	C5	0.4406313	0.0000000	-2.6415537
7 C	C3	-0.5712939	0.0000000	-4.8351390
8 H	H4	-1.6972043	0.0000000	-2.9865413
9 C	C7	-1.7251349	0.0000000	-5.7099058
10 H	H7	-2.7229748	0.0000000	-5.2564469
11 C	C8	-1.5458009	0.0000000	-7.0419907
12 H	H3	-2.3750415	0.0000000	-7.7570365
13 C	C9	-0.1837467	0.0000000	-7.5900597
14 O	O1	0.1937181	0.0000000	-8.7413971
15 O	O2	0.9224728	0.0000000	-6.7640769
16 H	H15	2.6077569	0.0000000	-2.5804129
17 C	C10	0.3146516	0.0000000	-1.2319555
18 C	C11	0.2085962	0.0000000	-0.0416903
19 C	C12	0.0824045	0.0000000	1.3676750
20 C	C13	-0.1595169	0.0000000	4.1605693
21 C	C14	0.0189579	1.2092500	2.0672584
22 C	C15	0.0189579	-1.2092500	2.0672584
23 C	C16	-0.1012469	-1.2088709	3.4483596
24 C	C17	-0.1012469	1.2088709	3.4483596
25 H	H2	0.0635243	2.1589871	1.5233717
26 H	H6	0.0635243	-2.1589871	1.5233717
27 H	H5	-0.1577475	-2.1675834	3.9862436
28 H	H8	-0.1577475	2.1675834	3.9862436
29 N	N1	-0.3931496	0.0000000	5.5852641
30 C	C18	-0.0027448	-1.2252428	6.3197274
31 H	H9	-0.5230378	-1.2336918	7.2862514
32 H	H11	1.0795977	-1.2907880	6.5083936
33 H	H12	-0.3064571	-2.1225690	5.7572016
34 C	C19	-0.0027448	1.2252428	6.3197274
35 H	H10	-0.5230378	1.2336918	7.2862514
36 H	H13	-0.3064571	2.1225690	5.7572016
37 H	H14	1.0795977	1.2907880	6.5083936

Optimized ground state geometry of **10**
after planarization.

Energy: 37.82 kcal/mol; m = 7.12 D; Pt. gp.: Cs

				Cartesian Coordinates (Angstroms)			
				Atom	X	Y	Z
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1	H	H1			2.8629458	0.0000000	-5.1123388
2	C	C1			1.8755643	0.0000000	-4.6356827
3	C	C4			-0.6689360	0.0000000	-3.4328380
4	C	C2			0.7104372	0.0000000	-5.4208744
5	C	C6			1.7548656	0.0000000	-3.2579783
6	C	C5			0.4845535	0.0000000	-2.6525475
7	C	C3			-0.5647699	0.0000000	-4.8292499
8	H	H4			-1.6587409	0.0000000	-2.9617387
9	C	C7			-1.7332356	0.0000000	-5.6842598
10	H	H7			-2.7232542	0.0000000	-5.2139841
11	C	C8			-1.5767176	0.0000000	-7.0192728
12	H	H3			-2.4180741	0.0000000	-7.7199824
13	C	C9			-0.2242096	0.0000000	-7.5904635
14	O	O1			0.8958015	0.0000000	-6.7839137
15	O	O2			0.1328885	0.0000000	-8.7485060
16	H	H16			2.6524702	0.0000000	-2.6294761
17	C	C10			0.3832856	0.0000000	-1.2423970
18	C	C11			0.2985019	0.0000000	-0.0498828
19	C	C12			0.1978431	0.0000000	1.3595574
20	C	C13			-0.0028028	0.0000000	4.1590067
21	C	C14			1.3531420	0.0000000	2.1485755
22	C	C15			-1.0581216	0.0000000	1.9757335
23	C	C16			-1.1609150	0.0000000	3.3571623
24	C	C17			1.2577539	0.0000000	3.5305552
25	H	H2			2.3389528	0.0000000	1.6709333
26	H	H6			-1.9656193	0.0000000	1.3623447
27	H	H5			-2.1612155	0.0000000	3.8061200
28	H	H8			2.1837591	0.0000000	4.1176463
29	N	N1			-0.1041464	0.0000000	5.5709271
30	C	C18			1.0946431	0.0000000	6.4244471
31	H	H9			0.7946361	0.0000000	7.4818949
32	H	H11			1.7144821	0.8905913	6.2440774
33	H	H12			1.7144821	-0.8905913	6.2440774
34	C	C19			-1.4126346	0.0000000	6.2442753
35	H	H10			-1.2669760	0.0000000	7.3338046
36	H	H13			-2.0003290	-0.8905816	5.9771206
37	H	H14			-2.0003290	0.8905816	5.9771206

HOMO level of 1

LUMO level of 1

HOMO level of **6**

LUMO level of **6**

HOMO level of **6**
after planarization

LUMO level of **6**
after planarization

HOMO level of **5**

LUMO level of **5**

HOMO level of **10**

LUMO level of **10**

HOMO level of **10**
after planarization

LUMO level of **10**
after planarization