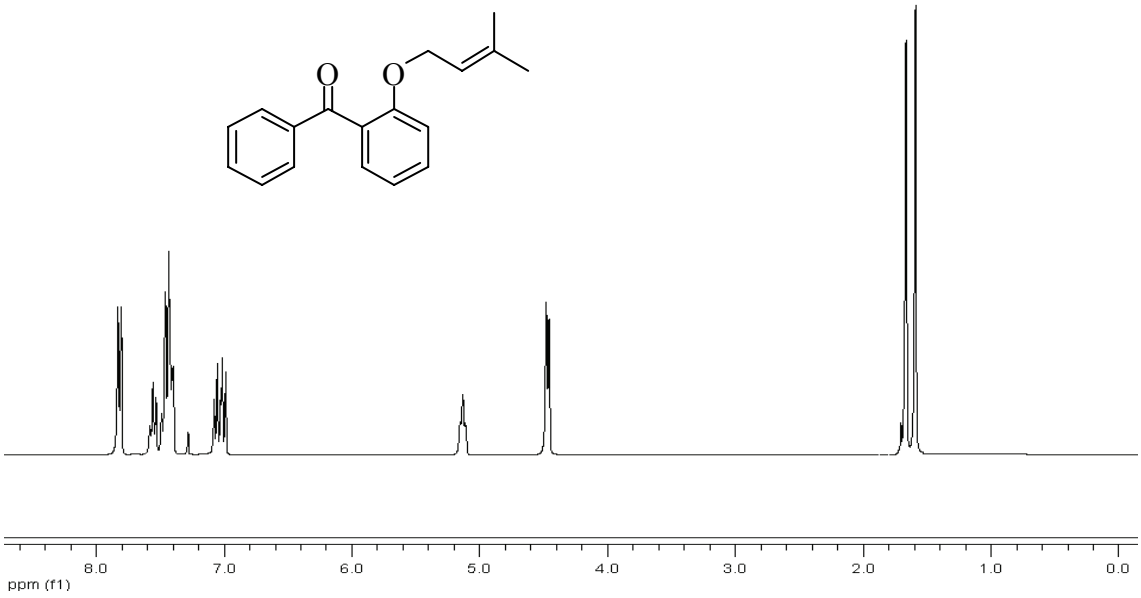
Supplementary Material (ESI) for Photochemical & Photobiological Sciences

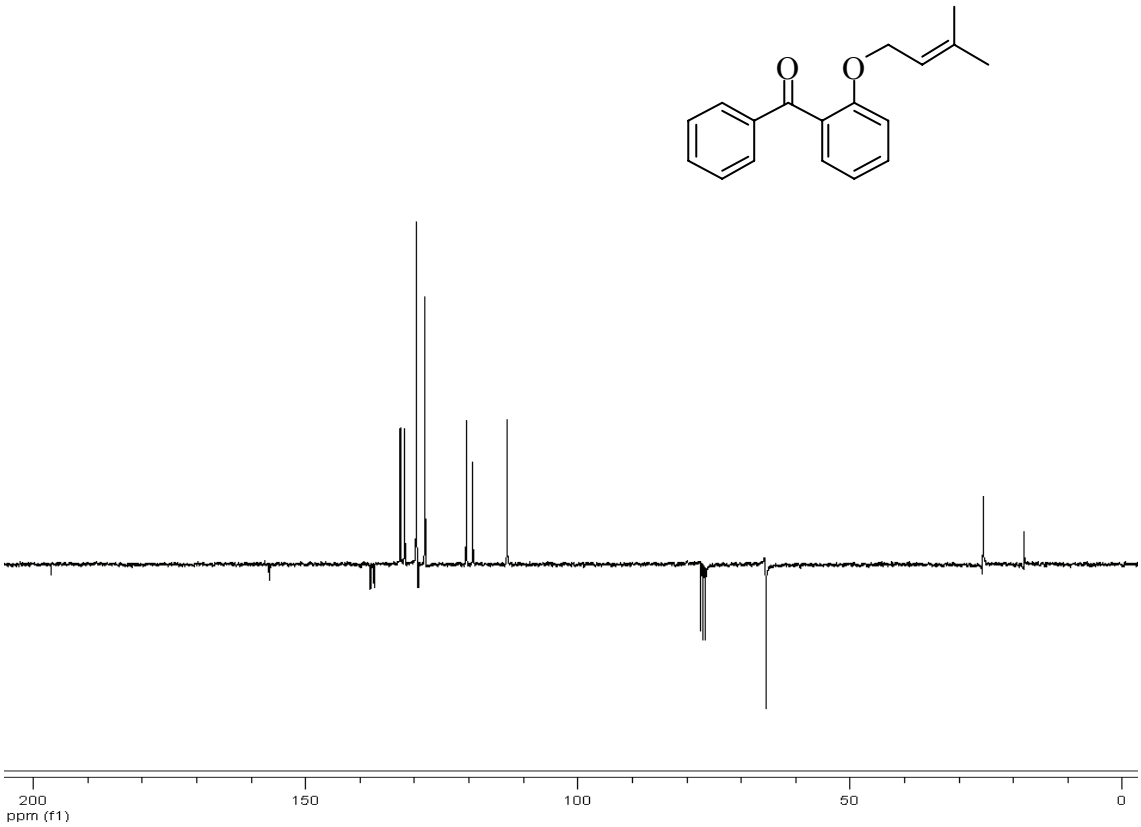
Photochemistry of Allyloxybenzophenones: a Pseudo-Paternò-Büchi Rearrangement Accompanied by H-Transfer Induced 1,5-Cyclization

Raúl Pérez-Ruiz [a], Olga Hinze [a], Jörg-M. Neudörfl [a], Dirk Blunk [a], Helmut Görner [b] and Axel G. Griesbeck [a*]

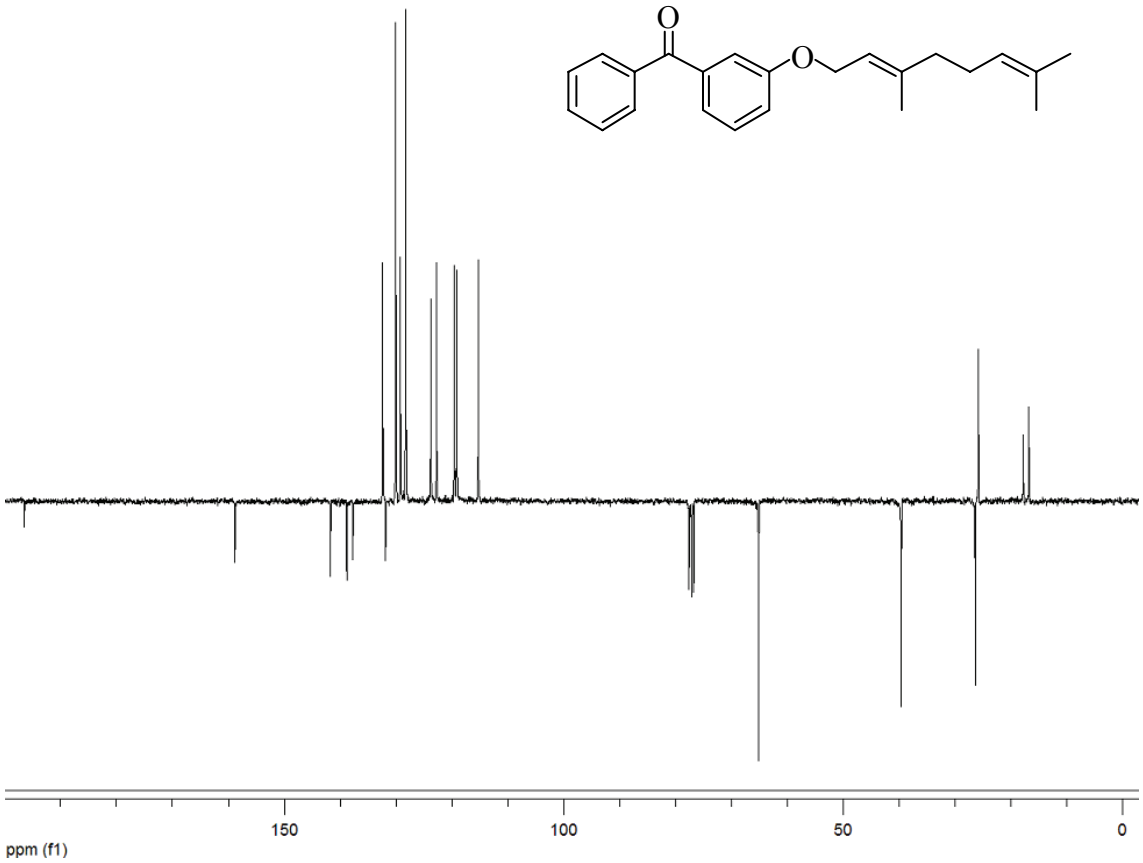
[a] *Department of Organic Chemistry, University of Cologne, Greinstrasse, 4, D-50939, Cologne, Germany. Fax:+49(0)2214705057;*
[b] *Max-Planck-Institut für Bioanorganische Chemie, D-45413, Mülheim an der Ruhr, Germany. Tel: +49(0) 2214703083*
E-mail: griesbeck@uni-koeln.de

^{1}H and ^{13}C APT NMR spectra

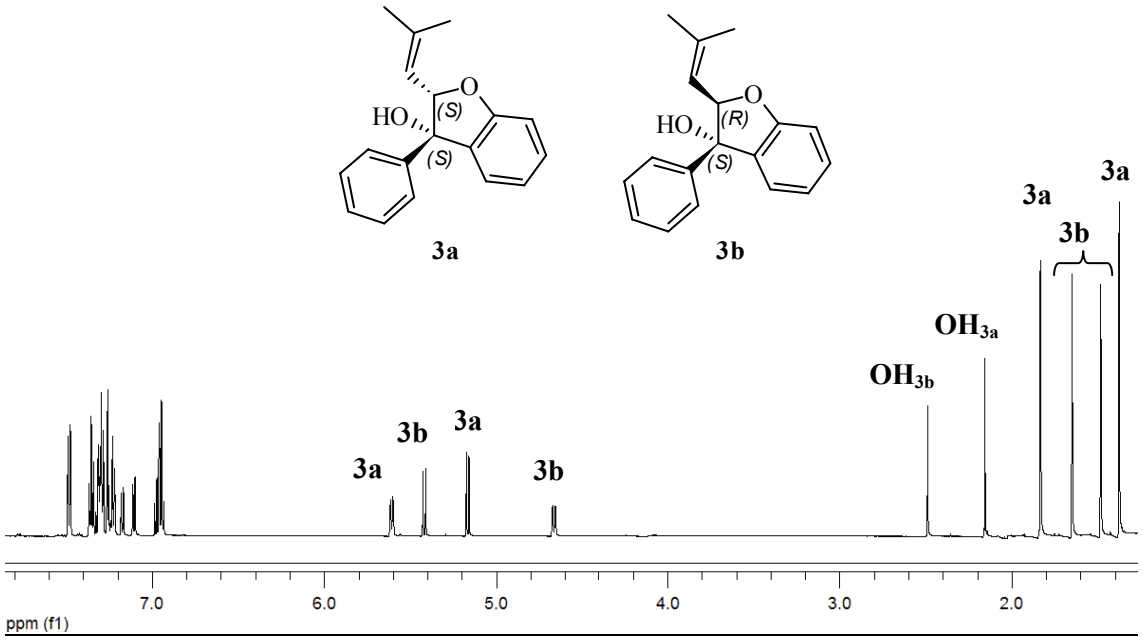


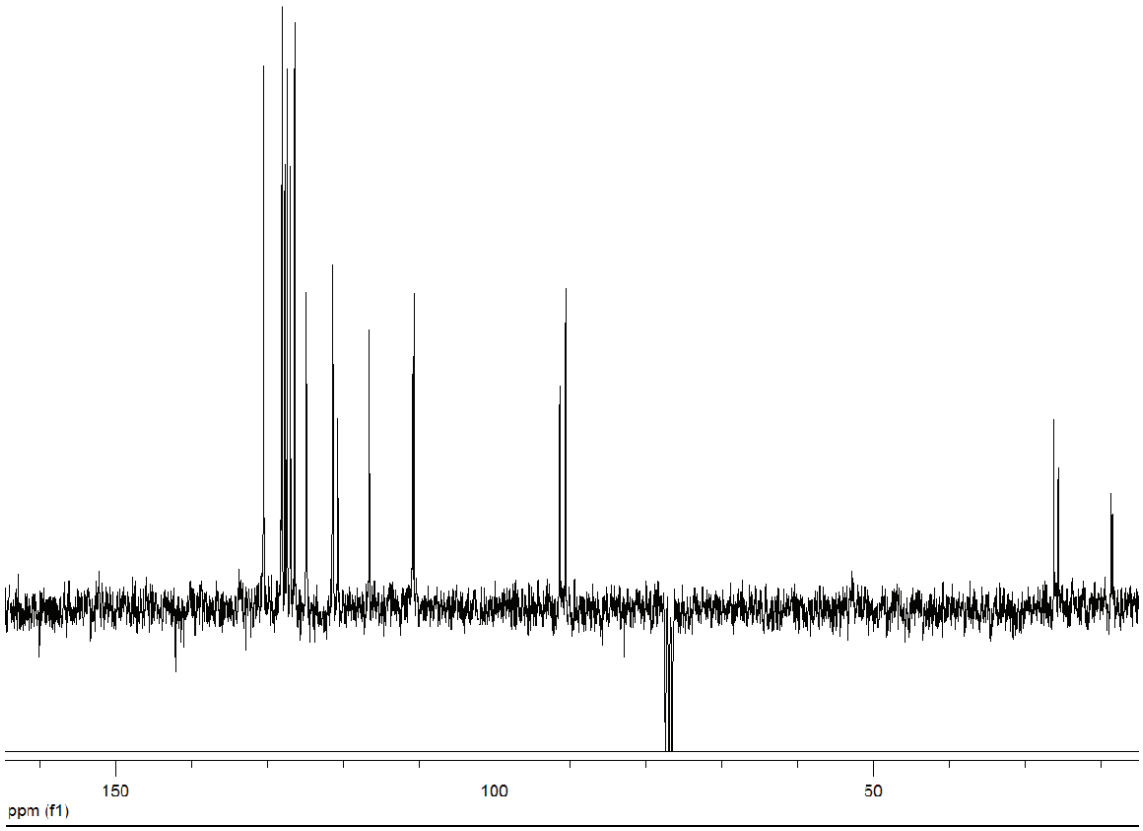


^{1}H and ^{13}C APT NMR spectra

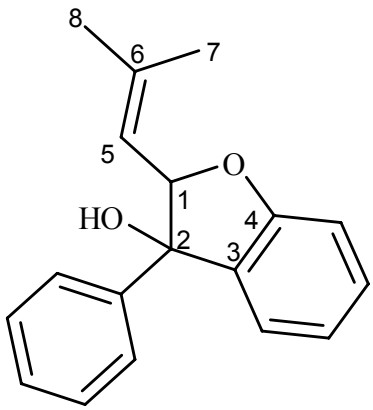


^{1}H and ^{13}C APT NMR spectra





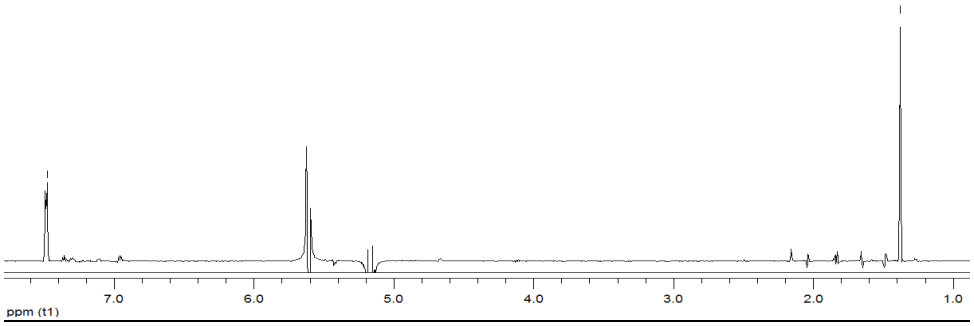
Significant correlations in the $^{1}H/^{1}H$ NMR NOEDIFF ($CDCl_3$, 600 MHz)



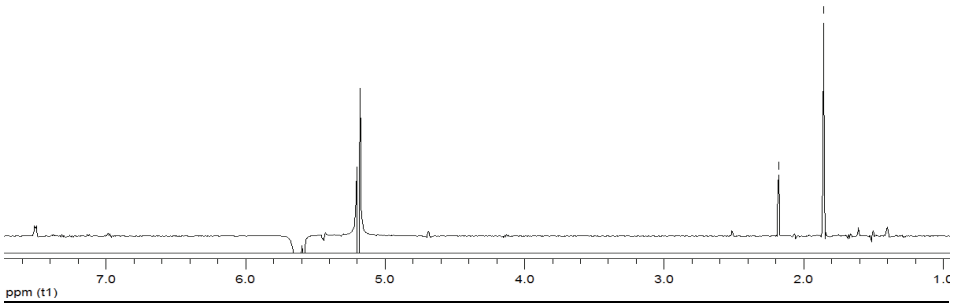
Compound	Irradiated H δ (ppm)	Observed H NOE δ (ppm)
3a	5.17 (1-H)	1.38 (7-H) 5.60 (5-H) 7.50 (Ph-2-H_{ortho})
	5.60 (5-H)	1.85 (8-H) 2.15 (OH) 5.17 (1-H)
	2.17 (OH)	5.60 (5-H) 7.50 (Ph-2-H_{ortho})
3b	4.67 (5-H)	1.48 (7-H) 5.45 (1-H)
	5.45 (1-H)	1.65 (7-H) 2.50 (OH) 4.57 (5-H)
	2.50 (OH)	5.45 (1-H) 7.19 (Ph-2-H) 7.25 (Ph-2-H)

^{1}H-NMR NOE spectra of **3a**

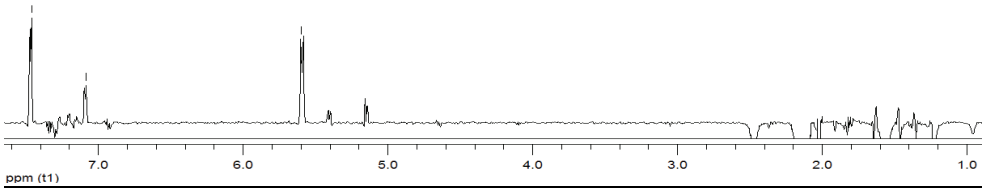
Irradiation of 1-H



Irradiation of 5-H

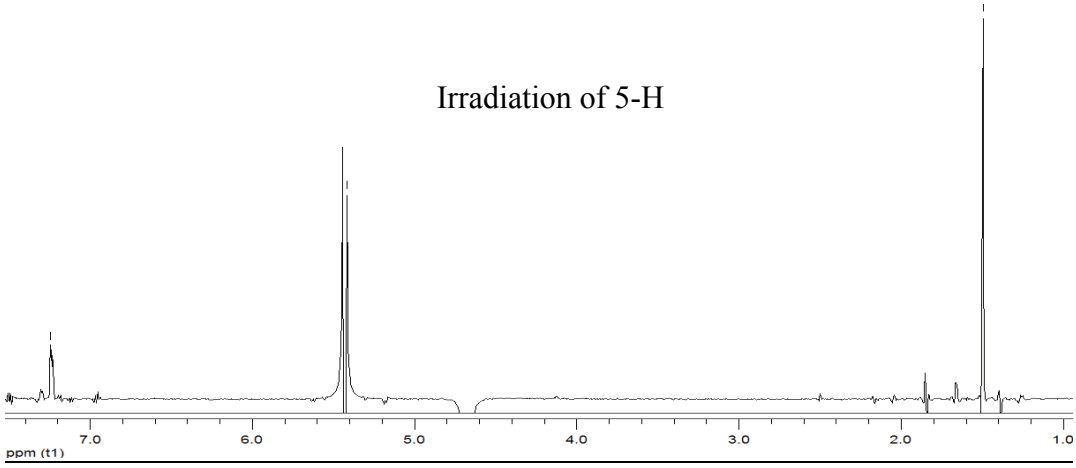


Irradiation of OH

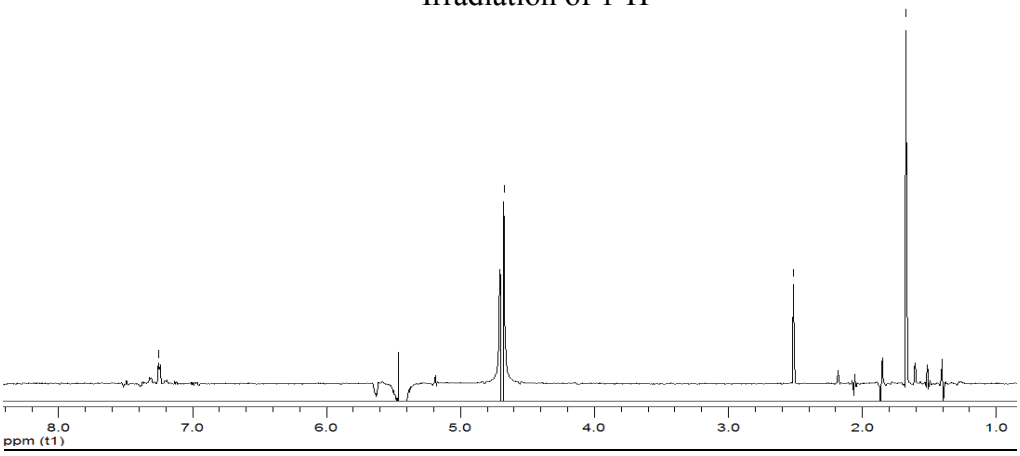


^{1}H-NMR NOE spectra of **3b**

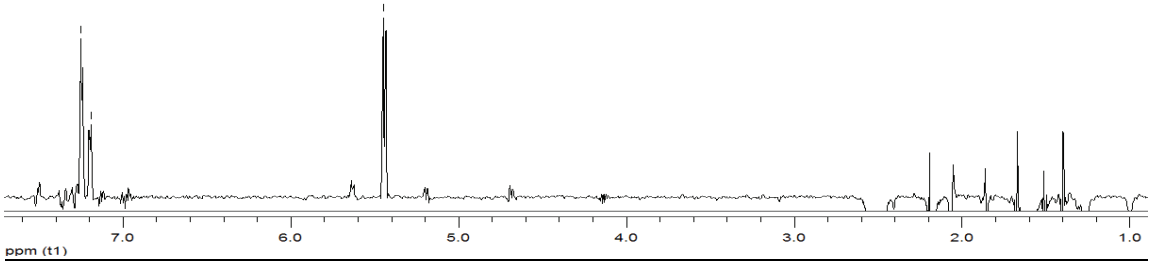
Irradiation of 5-H



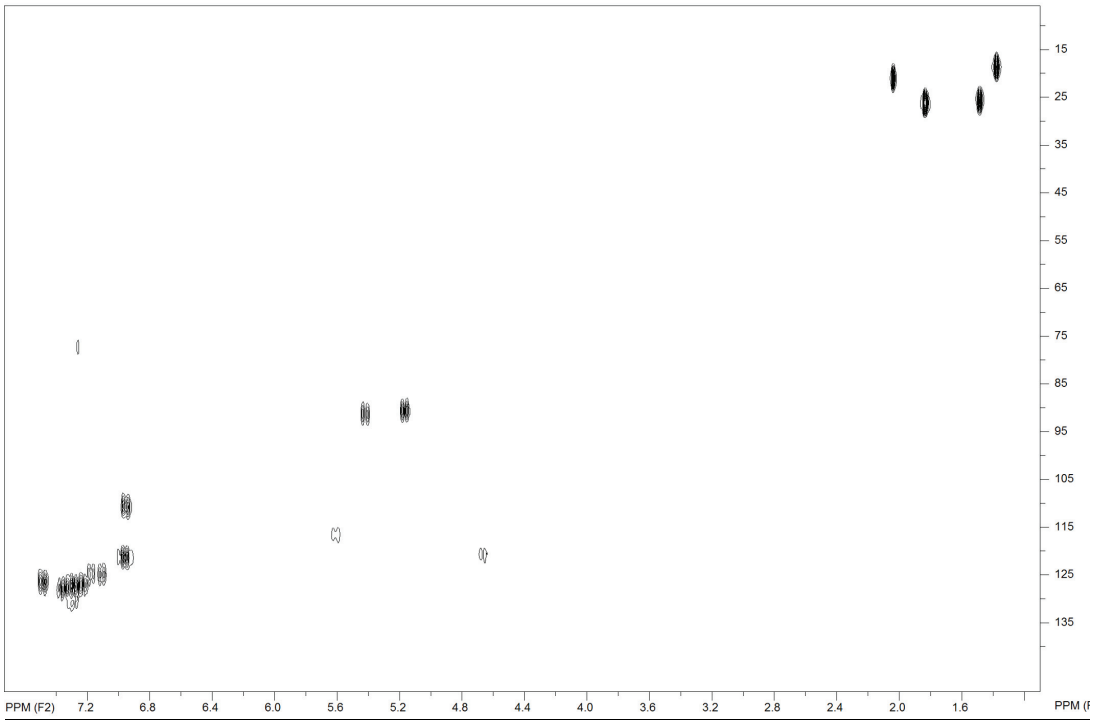
Irradiation of 1-H



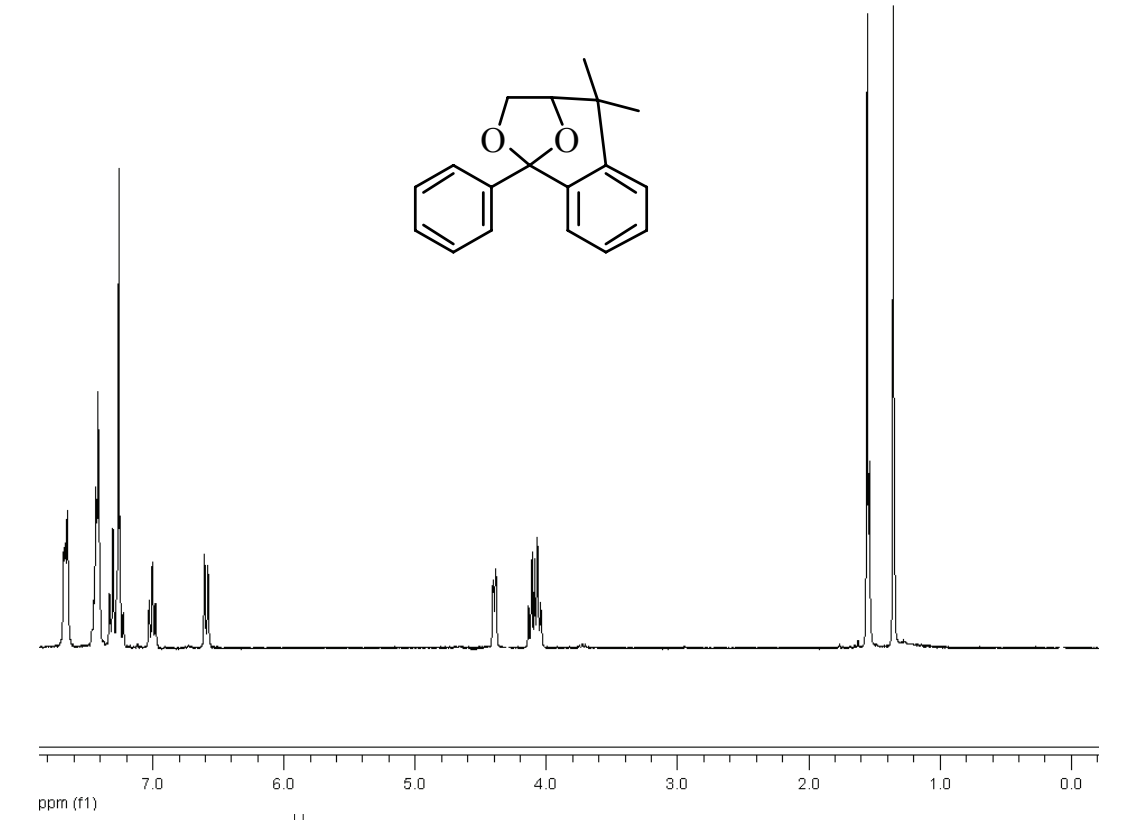
Irradiation of OH

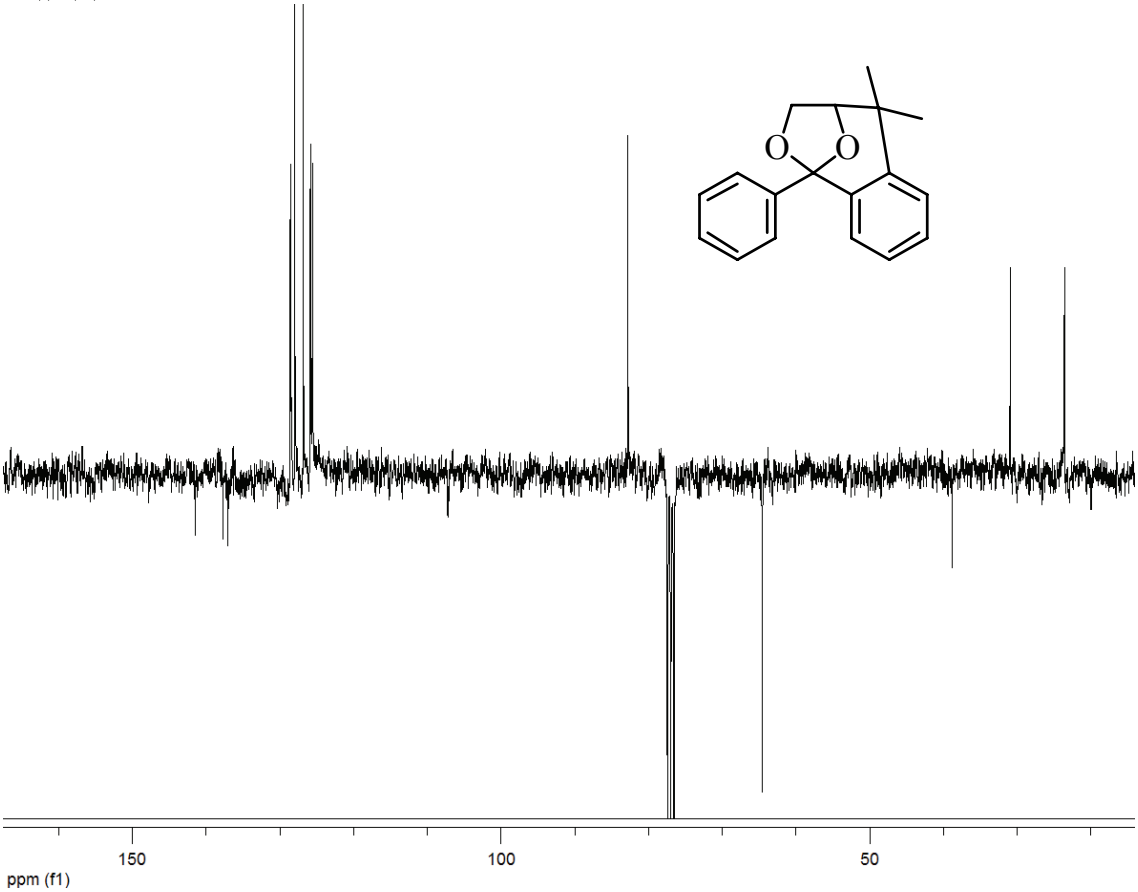


^{1}H-^{13}C correlation for a mixture of **3a** and **3b**

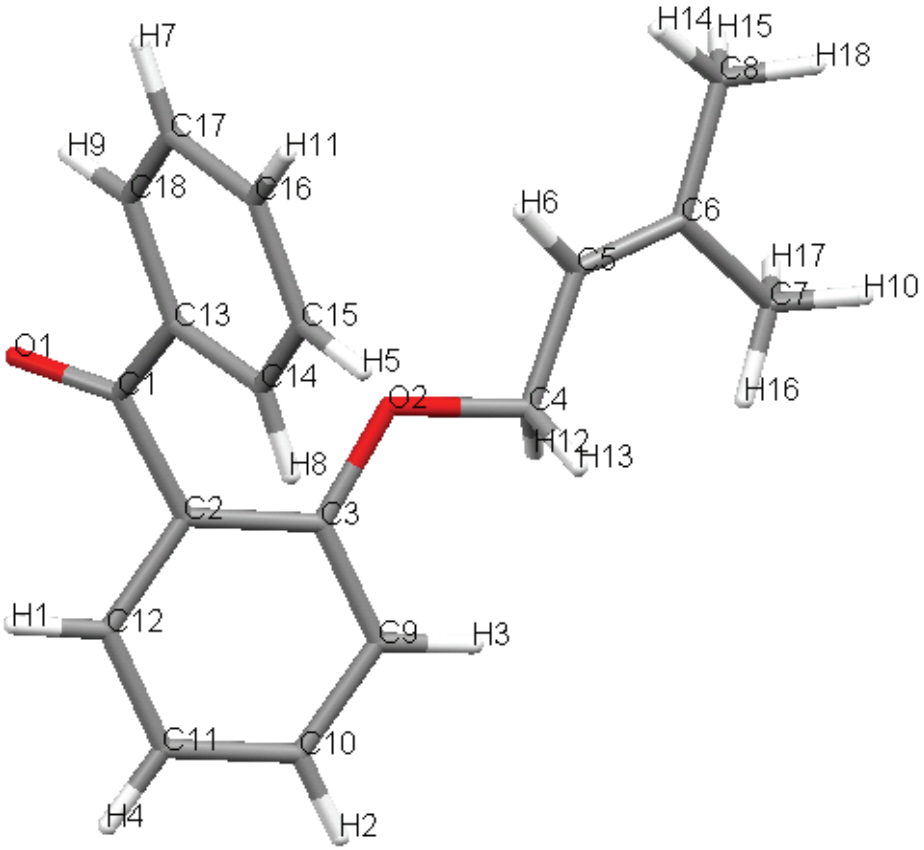


^{1}H and ^{13}C APT NMR spectra

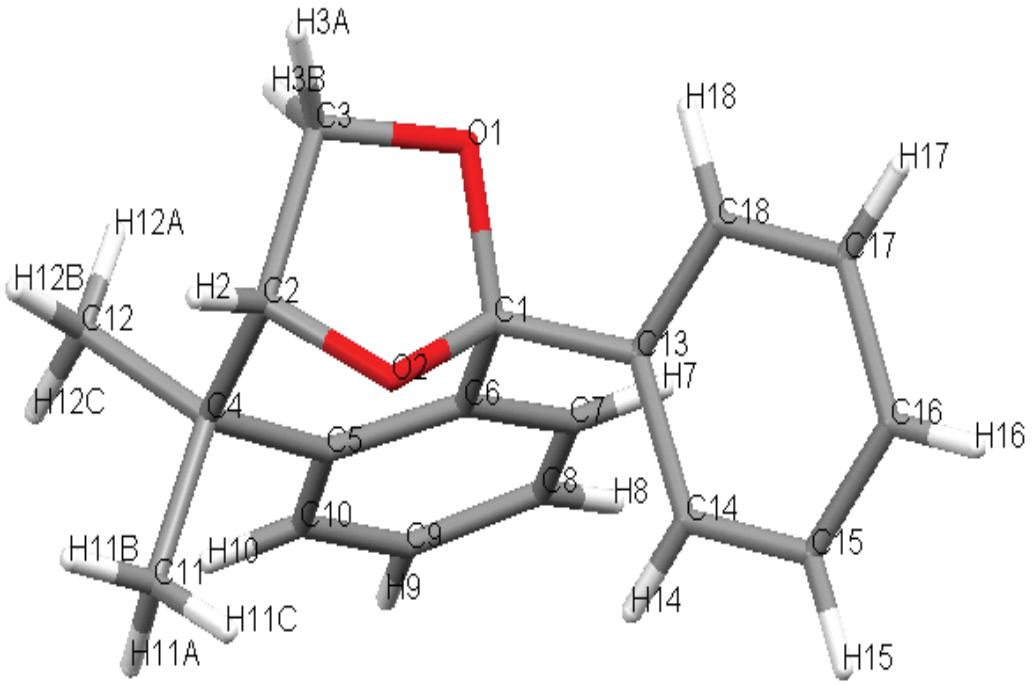




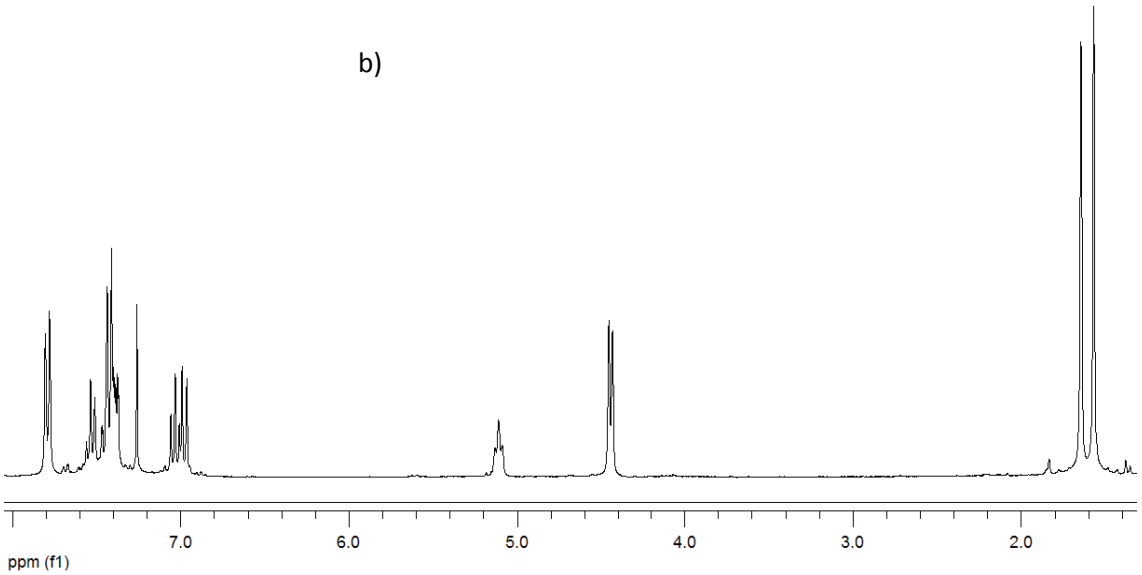
X-Ray structure of **1**



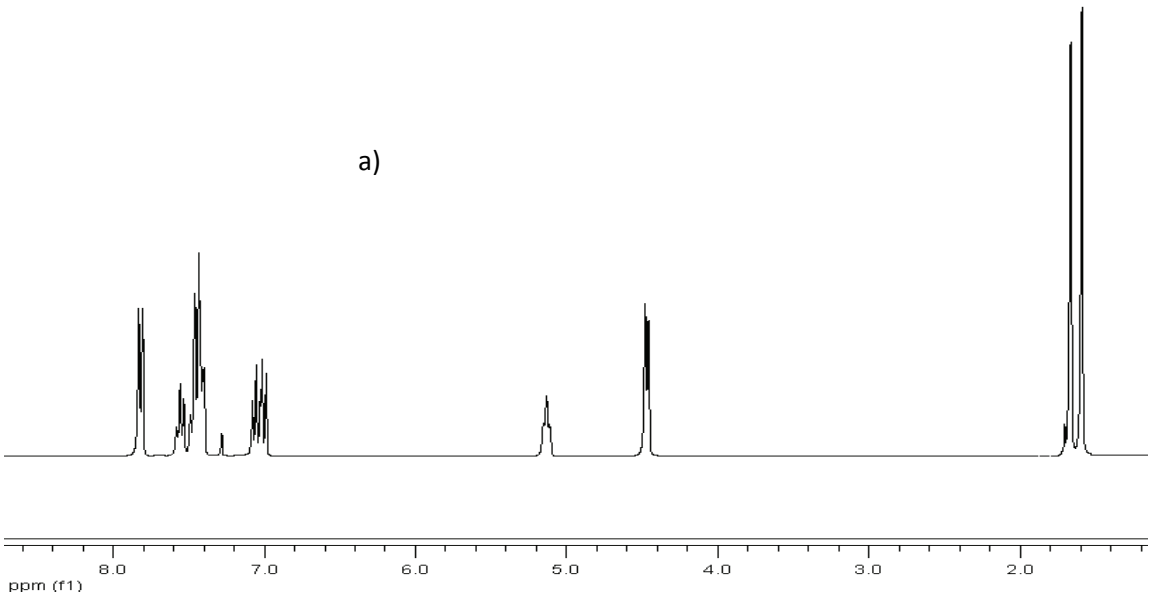
X-Ray structure of **4**

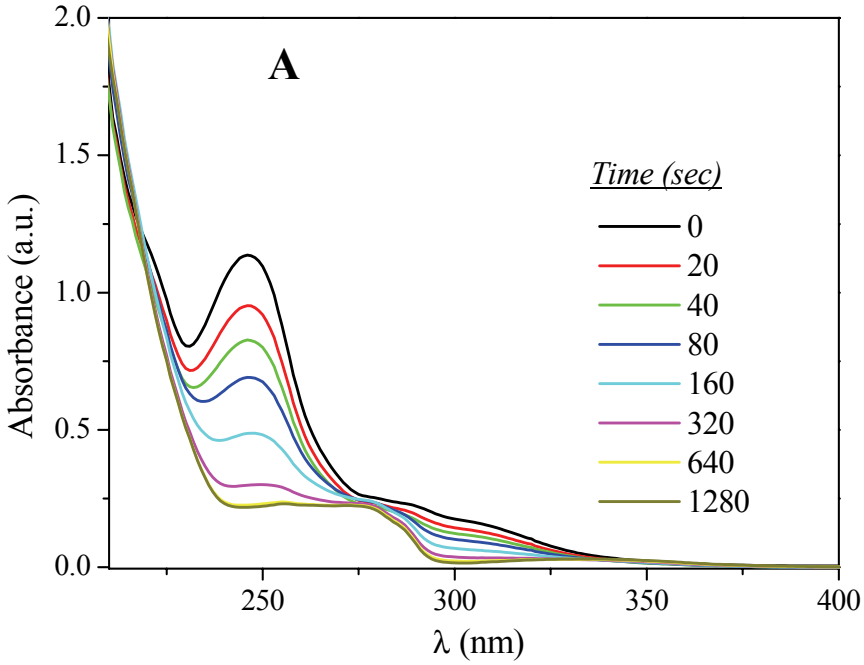


b)



a)





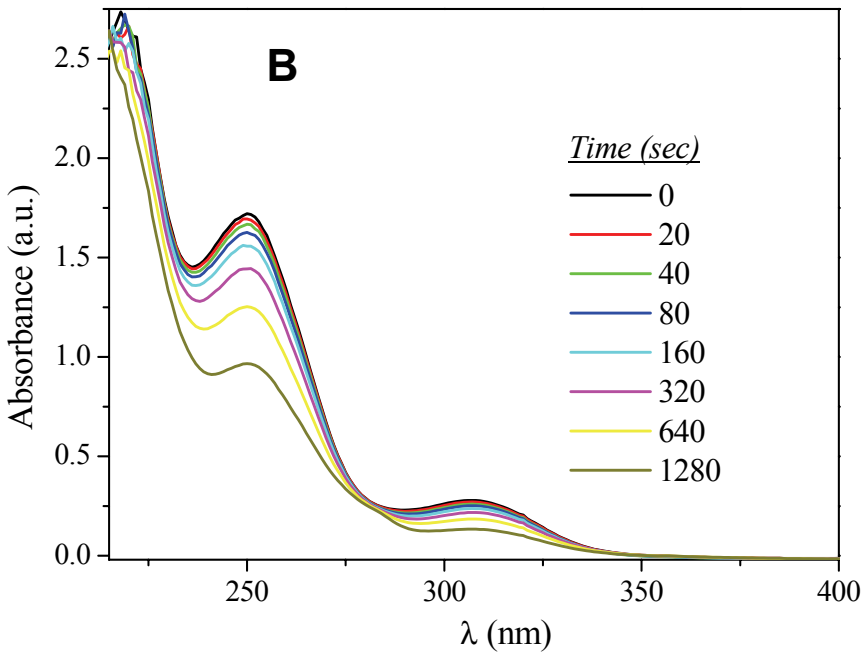


Table 1. Crystal data and structure refinement for **1**.

Empirical formula	C18 H18 O2
Formula weight	266.32
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P21/c
Unit cell dimensions	a = 8.8321(9) A alpha = 90 deg.
	b = 11.3213(6) A beta = 102.528(4) deg.
	c = 14.976(2) A gamma = 90 deg.
Volume	1461.8(3) A^3
Z, Calculated density	4, 1.210 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	568
Crystal size.	3 x .3 x .1 mm
Theta range for data collection	2.28 to 27.00 deg.
Limiting indices	-10<=h<=11, -14<=k<=11, -11<=l<=19
Reflections collected / unique	6715 / 3178 [R(int) = 0.0541]
Reflection observed [I>2sigma(I)]	1878
Completeness to theta =	27.00 99.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3178 / 0 / 253
Goodness-of-fit on F^2	0.888
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.0832
R indices (all data)	R1 = 0.0947, wR2 = 0.0951
Largest diff. peak and hole	0.169 and -0.184 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	2712(1)	3895(1)	3530(1)	29(1)
O(2)	712(1)	1679(1)	1763(1)	24(1)
C(1)	2782(2)	3007(1)	3069(1)	22(1)
C(2)	2031(2)	1886(1)	3293(1)	20(1)
C(3)	1054(2)	1208(1)	2622(1)	20(1)
C(4)	-326(2)	1016(1)	1060(1)	24(1)
C(5)	-609(2)	1750(1)	216(1)	22(1)
C(6)	-1842(2)	1684(1)	-472(1)	22(1)
C(7)	-3136(2)	802(2)	-508(2)	33(1)
C(8)	-2024(2)	2467(2)	-1293(1)	35(1)
C(9)	455(2)	145(1)	2861(1)	24(1)
C(10)	795(2)	-220(1)	3765(1)	30(1)
C(11)	1710(2)	459(1)	4441(1)	30(1)
C(12)	2315(2)	1511(1)	4199(1)	25(1)
C(13)	3706(2)	3004(1)	2352(1)	21(1)
C(14)	4256(2)	1959(1)	2045(1)	23(1)
C(15)	5243(2)	1982(1)	1445(1)	28(1)
C(16)	5684(2)	3057(1)	1133(1)	32(1)
C(17)	5116(2)	4102(1)	1418(1)	33(1)
C(18)	4146(2)	4079(1)	2024(1)	27(1)

Table 3. Anisotropic displacement parameters (A^2 x 10^3) for **1**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	26(1)	25(1)	35(1)	-10(1)	2(1)	2(1)
O(2)	23(1)	25(1)	21(1)	1(1)	-4(1)	-7(1)
C(1)	15(1)	21(1)	25(1)	-3(1)	-8(1)	3(1)
C(2)	16(1)	20(1)	23(1)	-2(1)	2(1)	4(1)
C(3)	17(1)	22(1)	21(1)	2(1)	3(1)	3(1)
C(4)	21(1)	22(1)	25(1)	-5(1)	-1(1)	-5(1)
C(5)	21(1)	20(1)	24(1)	-3(1)	4(1)	-3(1)
C(6)	21(1)	24(1)	22(1)	-2(1)	4(1)	0(1)
C(7)	29(1)	38(1)	28(1)	-1(1)	-1(1)	-10(1)
C(8)	31(1)	42(1)	27(1)	4(1)	-3(1)	-7(1)
C(9)	21(1)	23(1)	28(1)	-1(1)	4(1)	0(1)
C(10)	26(1)	25(1)	38(1)	7(1)	8(1)	3(1)
C(11)	30(1)	35(1)	25(1)	6(1)	8(1)	8(1)
C(12)	20(1)	28(1)	25(1)	-2(1)	1(1)	5(1)
C(13)	15(1)	21(1)	23(1)	-3(1)	-4(1)	-2(1)
C(14)	20(1)	23(1)	23(1)	1(1)	-1(1)	-2(1)
C(15)	25(1)	29(1)	29(1)	-6(1)	2(1)	-3(1)
C(16)	27(1)	39(1)	29(1)	-6(1)	5(1)	-10(1)
C(17)	34(1)	28(1)	34(1)	0(1)	5(1)	-12(1)
C(18)	26(1)	23(1)	31(1)	-4(1)	-1(1)	-4(1)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(1)	2922(15)	2003(10)	4666(10)	17(4)
H(2)	367(16)	-963(13)	3924(11)	36(5)
H(3)	-174(17)	-324(11)	2375(11)	31(4)
H(4)	1867(18)	228(13)	5081(12)	34(5)
H(5)	5644(16)	1234(12)	1243(11)	31(4)
H(6)	237(16)	2325(11)	200(10)	23(4)
H(7)	5416(16)	4856(12)	1180(11)	30(4)
H(8)	3963(15)	1225(12)	2285(10)	29(4)
H(9)	3765(16)	4807(12)	2242(11)	32(5)
H(10)	-3168(19)	305(14)	-1087(13)	54(6)
H(11)	6346(18)	3070(12)	692(12)	35(5)
H(12)	-1316(18)	858(11)	1310(11)	30(4)
H(13)	146(17)	234(13)	968(11)	35(5)
H(14)	-1140(20)	3027(13)	-1230(12)	48(5)
H(15)	-2970(20)	2941(13)	-1353(12)	47(5)
H(16)	-2952(18)	255(13)	35(12)	40(5)
H(17)	-4160(20)	1237(14)	-568(13)	61(6)
H(18)	-2124(19)	2015(14)	-1903(13)	49(5)

Table 5. Crystal data and structure refinement for **4**.

Empirical formula	C36 H36 O4
Formula weight	532.65
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P21
Unit cell dimensions	a = 8.2702(10) A alpha = 90 deg.
	b = 7.8909(5) A beta = 95.892(4) deg.
	c = 10.7596(14) A gamma = 90 deg.
Volume	698.45(13) A^3
Z, Calculated density	1, 1.266 Mg/m^3
Absorption coefficient	0.081 mm^-1
F(000)	284
Crystal size	.2 x .03 x .03 mm
Theta range for data collection	2.48 to 26.99 deg.
Limiting indices	-10<=h<=9, -10<=k<=6, -13<=l<=13
Reflections collected / unique	3314 / 1592 [R(int) = 0.0361]
Reflection observed [I>2sigma(I)]	1160
Completeness to theta =	26.99 97.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1592 / 1 / 195
Goodness-of-fit on F^2	0.957
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0612
R indices (all data)	R1 = 0.0703, wR2 = 0.0670
Absolute structure parameter	1.4(14)
Largest diff. peak and hole	0.183 and -0.184 e.A^-3

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	2265(2)	1373(2)	3887(2)	22(1)
O(2)	4569(2)	2845(2)	3742(2)	20(1)
C(1)	3005(3)	2520(3)	3091(2)	18(1)
C(2)	5136(3)	1149(3)	4066(3)	21(1)
C(3)	3579(3)	287(3)	4410(3)	21(1)
C(4)	5869(3)	412(3)	2937(2)	20(1)
C(5)	4628(3)	622(3)	1799(2)	18(1)
C(6)	3239(3)	1624(3)	1864(2)	18(1)
C(7)	2037(3)	1700(3)	854(2)	21(1)
C(8)	2232(3)	821(3)	-243(3)	24(1)
C(9)	3642(3)	-105(3)	-334(2)	23(1)
C(10)	4807(3)	-210(3)	670(2)	22(1)
C(11)	7457(3)	1370(3)	2767(3)	28(1)
C(12)	6300(3)	-1470(3)	3173(3)	23(1)
C(13)	2091(3)	4185(3)	2977(2)	17(1)
C(14)	2581(3)	5443(3)	2191(3)	23(1)
C(15)	1849(3)	7021(3)	2154(3)	26(1)
C(16)	626(3)	7360(3)	2899(3)	24(1)
C(17)	114(3)	6106(3)	3666(2)	21(1)
C(18)	845(3)	4524(3)	3709(2)	21(1)

Table 7. Anisotropic displacement parameters (A^2 x 10^3) for **4**.

The anisotropic displacement factor exponent takes the form:

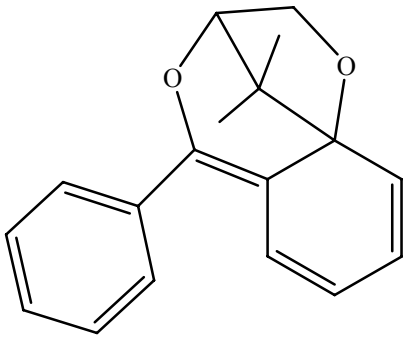
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

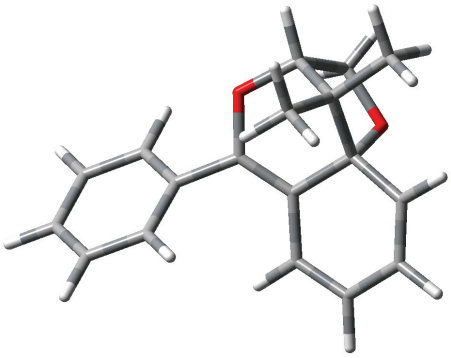
	U11	U22	U33	U23	U13	U12
O(1)	24(1)	20(1)	21(1)	6(1)	6(1)	3(1)
O(2)	20(1)	16(1)	22(1)	-1(1)	0(1)	2(1)
C(1)	16(2)	19(2)	20(2)	1(1)	1(1)	-1(1)
C(2)	21(2)	20(2)	20(2)	0(1)	-4(1)	5(1)
C(3)	25(2)	21(2)	17(2)	5(1)	2(1)	5(1)
C(4)	16(2)	25(2)	18(2)	1(1)	3(1)	2(1)
C(5)	17(2)	17(1)	20(2)	0(1)	5(1)	-4(1)
C(6)	21(2)	14(2)	20(2)	2(1)	3(1)	0(1)
C(7)	19(2)	19(2)	25(2)	1(1)	1(1)	1(1)
C(8)	26(2)	26(2)	18(2)	2(1)	-4(1)	-4(1)
C(9)	30(2)	22(2)	18(2)	-2(1)	3(1)	-3(1)
C(10)	22(2)	22(2)	23(2)	1(1)	7(1)	-1(1)
C(11)	26(2)	28(2)	31(2)	3(1)	2(1)	1(1)
C(12)	24(2)	22(2)	24(2)	3(1)	4(1)	5(1)
C(13)	16(2)	17(1)	19(2)	-2(1)	0(1)	0(1)
C(14)	20(2)	23(2)	28(2)	-3(1)	9(1)	2(1)
C(15)	26(2)	19(2)	32(2)	3(1)	3(1)	-2(1)
C(16)	20(2)	17(2)	33(2)	-2(1)	1(1)	3(1)
C(17)	18(2)	25(2)	21(2)	-4(1)	3(1)	5(1)
C(18)	20(2)	21(2)	21(2)	1(1)	0(1)	0(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(2)	6000(30)	1260(30)	4790(20)	17(6)
H(3A)	3500(30)	230(30)	5340(20)	20(7)
H(3B)	3460(30)	-940(30)	4050(20)	26(7)
H(7)	1083	2353	916	25
H(8)	1405	855	-924	29
H(9)	3801	-668	-1092	28
H(10)	5758	-862	596	26
H(11A)	7850	1034	1974	42
H(11B)	8280	1091	3458	42
H(11C)	7251	2593	2761	42
H(12A)	5298	-2137	3154	35
H(12B)	6924	-1591	3993	35
H(12C)	6951	-1878	2523	35
H(14)	3423	5217	1677	28
H(15)	2189	7873	1614	31
H(16)	138	8451	2885	28
H(17)	-743	6331	4167	26
H(18)	490	3670	4241	25

Compiled Results of DFT-Calculations





5

Functional: B3LYP

Basis set: 6-311+G(d)

Calculation type: unrestricted

E(UB+HF-LYP) = -847.355646077

Nuclear repulsion energy 1576.9950563572 Hartrees.

Zero-point correction = 0.313821(Hartree/Particle)

Thermal correction to Energy = 0.330082

Thermal correction to Enthalpy = 0.331026

Thermal correction to Gibbs Free Energy = 0.271002

Variational PCM results

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<psi(f)| H |psi(f)> (a.u.) = -847.336960

<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -847.355646

Total free energy in solution:

with all non electrostatic terms (a.u.) = -847.334352

(Polarized solute)-Solvent (kcal/mol) = -11.73

Cavitation energy (kcal/mol) = 29.65

Dispersion energy (kcal/mol) = -17.33

Repulsion energy (kcal/mol) = 1.04

Total non electrostatic (kcal/mol) = 13.36

After PCM corrections, the SCF energy is -847.355646077 a.u.

GePol: Number of tesserae being generated = 2527

GePol: Average area of tesserae = 0.12 Ang**2

GePol: Minimum area of tessera = 0.10D-02 Ang**2

GePol: Maximum area of tessera = 0.32312 Ang**2

GePol: Number of small tesserae = 6

GePol: Fraction of small tesserae (<1% of avg) = 0.24%

GePol: Total count of vertices = 9067

GePol: Maximum number of vertices in a tessera = 8

GePol: Cavity surface area = 296.429 Ang**2

GePol: Cavity volume = 370.815 Ang**3

GePol: Maximum number of non-zero 1st derivatives = 677

Sum of electronic, zero-point and PCM Energies = -847.041825077

Sum of electronic, thermal and PCM Energies = -847.025564077

Sum of electronic, thermal and PCM Enthalpies = -847.024620077

Sum of electronic, thermal Free and PCM Energies = -847.084644077

Cartesian coordinates in standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.069282	0.895520	0.886349

2	6	0	2.680217	0.794769	0.821075
3	6	0	2.073791	-0.179312	0.013617
4	6	0	2.891228	-1.063558	-0.709866
5	6	0	4.278174	-0.954769	-0.649705
6	6	0	4.872099	0.026189	0.147451
7	1	0	4.523928	1.650805	1.523799
8	1	0	2.067011	1.461180	1.420390
9	1	0	2.437057	-1.832229	-1.328920
10	1	0	4.897673	-1.638730	-1.225930
11	1	0	5.955880	0.106987	0.197867
12	6	0	0.602398	-0.319448	-0.055892
13	6	0	-0.311719	0.680106	-0.222848
14	6	0	-1.799640	0.300991	-0.222472
15	6	0	0.056237	2.055975	-0.475122
16	6	0	-2.705971	1.482460	-0.052153
17	6	0	-0.869104	3.045277	-0.466747
18	1	0	1.094228	2.291789	-0.687392
19	6	0	-2.263047	2.745580	-0.188781
20	1	0	-3.758908	1.281664	0.125431
21	1	0	-0.577635	4.074212	-0.662402
22	1	0	-2.964482	3.574183	-0.100921
23	8	0	0.228215	-1.625990	0.079348
24	6	0	-2.029121	-0.906867	0.747105
25	6	0	-1.193590	-1.916678	-0.055106
26	1	0	-1.291559	-2.955291	0.267956
27	6	0	-1.638154	-1.668544	-1.496640
28	1	0	-0.809185	-1.796700	-2.198944
29	1	0	-2.453216	-2.334815	-1.793988
30	8	0	-2.115536	-0.303563	-1.528874

31	6	0	-3.500614	-1.358164	0.783917
32	1	0	-3.577541	-2.342888	1.254640
33	1	0	-4.099547	-0.667370	1.382313
34	1	0	-3.953518	-1.419170	-0.206056
35	6	0	-1.553595	-0.682415	2.185799
36	1	0	-2.133229	0.121684	2.648803
37	1	0	-1.711316	-1.586973	2.780630
38	1	0	-0.500302	-0.414600	2.259053

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Excited states from <AA,BB:AA,BB> singles matrix:

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Excitation energies and oscillator strengths:

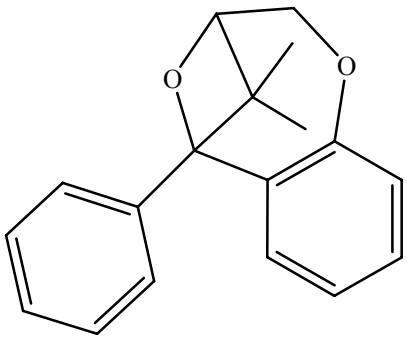
Excited State 1:	Triplet-A	1.7784 eV	697.18 nm	f=0.0000
Excited State 2:	Singlet-A	3.1224 eV	397.08 nm	f=0.2807
Excited State 3:	Triplet-A	3.2397 eV	382.70 nm	f=0.0000
Excited State 4:	Triplet-A	3.7095 eV	334.24 nm	f=0.0000
Excited State 5:	Triplet-A	4.0114 eV	309.08 nm	f=0.0000
Excited State 6:	Triplet-A	4.0954 eV	302.74 nm	f=0.0000
Excited State 7:	Singlet-A	4.1395 eV	299.52 nm	f=0.0107
Excited State 8:	Singlet-A	4.2164 eV	294.05 nm	f=0.0013
Excited State 9:	Triplet-A	4.2715 eV	290.26 nm	f=0.0000
Excited State 10:	Singlet-A	4.3830 eV	282.87 nm	f=0.0205
Excited State 11:	Triplet-A	4.4342 eV	279.61 nm	f=0.0000
Excited State 12:	Triplet-A	4.5088 eV	274.98 nm	f=0.0000
Excited State 13:	Singlet-A	4.6803 eV	264.91 nm	f=0.0306
Excited State 14:	Singlet-A	4.7530 eV	260.86 nm	f=0.0995
Excited State 15:	Triplet-A	4.7897 eV	258.86 nm	f=0.0000
Excited State 16:	Singlet-A	4.8151 eV	257.49 nm	f=0.0055

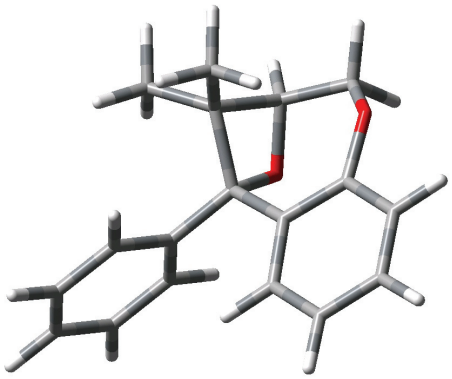
Excited State 17: Triplet-A 4.8542 eV 255.42 nm f=0.0000

Excited State 18: Singlet-A 5.0022 eV 247.86 nm f=0.0476

Excited State 19: Triplet-A 5.0677 eV 244.65 nm f=0.0000

Excited State 20: Triplet-A 5.0797 eV 244.08 nm f=0.0000





6

Functional: B3LYP

Basis set: 6-311+G(d)

Calculation type: unrestricted

E(UB+HF-LYP) = -847.364437865 (after PCM corrections

Nuclear repulsion energy 1586.3498042676 Hartrees.

Zero-point correction = 0.313738(Hartree/Particle)

Thermal correction to Energy = 0.330085

Thermal correction to Enthalpy = 0.331029

Thermal correction to Gibbs Free Energy = 0.270826

Variational PCM results

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<psi(f)| H |psi(f)> (a.u.) = -847.348183

<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -847.364438

Total free energy in solution:

with all non electrostatic terms (a.u.) = -847.343588

(Polarized solute)-Solvent (kcal/mol) = -10.20

Cavitation energy (kcal/mol) = 29.25

Dispersion energy (kcal/mol) = -17.21

Repulsion energy (kcal/mol) = 1.05

Total non electrostatic (kcal/mol) = 13.08

After PCM corrections, the SCF energy is -847.364437865 a.u.

GePol: Number of tesserae being generated = 2452

GePol: Average area of tesserae = 0.12 Ang**2

GePol: Minimum area of tessera = 0.10D-02 Ang**2

GePol: Maximum area of tessera = 0.32312 Ang**2

GePol: Number of small tesserae = 11

GePol: Fraction of small tesserae (<1% of avg) = 0.45%

GePol: Total count of vertices = 8713

GePol: Maximum number of vertices in a tessera = 7

GePol: Cavity surface area = 292.743 Ang**2

GePol: Cavity volume = 368.529 Ang**3

GePol: Maximum number of non-zero 1st derivatives = 635

Sum of electronic, zero-point and PCM Energies = -847.050699865

Sum of electronic, thermal and PCM Energies = -847.034352865

Sum of electronic, thermal and PCM Enthalpies = -847.033408865

Sum of electronic, thermal Free and PCM Energies = -847.093611865

Cartesian coordinates in standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.675950	0.610677	-1.268965
2	6	0	2.350916	0.170779	-1.315965
3	6	0	1.586033	0.094317	-0.149627
4	6	0	2.172681	0.462814	1.068528
5	6	0	3.496147	0.896893	1.117592
6	6	0	4.253675	0.974006	-0.053146
7	1	0	4.256760	0.665844	-2.187490
8	1	0	1.911787	-0.120509	-2.265218
9	1	0	1.595259	0.419296	1.989537
10	1	0	3.936296	1.175840	2.072743
11	1	0	5.286666	1.313314	-0.015709
12	6	0	0.151840	-0.389014	-0.192435
13	6	0	-0.883442	0.728125	-0.019203
14	6	0	-2.277228	0.486657	-0.092622
15	6	0	-0.482257	2.067309	0.117082
16	6	0	-3.187117	1.547593	-0.005910
17	6	0	-1.386415	3.122013	0.206066
18	1	0	0.575520	2.294757	0.151232
19	6	0	-2.753031	2.858126	0.146445
20	1	0	-4.247464	1.312338	-0.057845
21	1	0	-1.020619	4.140265	0.313791
22	1	0	-3.479705	3.665241	0.209685
23	8	0	-0.163226	-1.071947	-1.459182
24	6	0	-0.157229	-1.749093	0.576004

25	6	0	-0.886334	-2.112809	-0.742951
26	1	0	-0.659791	-3.103461	-1.158081
27	6	0	-2.372857	-1.882112	-0.844308
28	1	0	-2.640924	-1.791315	-1.904541
29	1	0	-2.918026	-2.731490	-0.424367
30	8	0	-2.888170	-0.743283	-0.140543
31	6	0	-0.904490	-1.724457	1.907506
32	1	0	-1.264662	-2.729392	2.151792
33	1	0	-0.225520	-1.426039	2.712143
34	1	0	-1.759933	-1.053692	1.922465
35	6	0	1.084375	-2.640710	0.715511
36	1	0	1.749833	-2.285768	1.505214
37	1	0	0.768841	-3.656245	0.975694
38	1	0	1.659543	-2.693839	-0.210862

Excited states from <AA,BB:AA,BB> singles matrix:

****

Excitation energies and oscillator strengths:

Excited State	1:	Triplet-A	3.6227 eV	342.24 nm	f=0.0000
Excited State	2:	Triplet-A	3.7391 eV	331.59 nm	f=0.0000
Excited State	3:	Triplet-A	4.1533 eV	298.52 nm	f=0.0000
Excited State	4:	Triplet-A	4.4409 eV	279.18 nm	f=0.0000
Excited State	5:	Triplet-A	4.6029 eV	269.36 nm	f=0.0000
Excited State	6:	Triplet-A	4.6169 eV	268.54 nm	f=0.0000
Excited State	7:	Singlet-A	4.8962 eV	253.23 nm	f=0.0451
Excited State	8:	Triplet-A	4.9642 eV	249.76 nm	f=0.0000
Excited State	9:	Triplet-A	5.0382 eV	246.09 nm	f=0.0000
Excited State	10:	Singlet-A	5.1696 eV	239.83 nm	f=0.0141

Excited State 11: Triplet-A 5.2242 eV 237.33 nm f=0.0000

Excited State 12: Singlet-A 5.2463 eV 236.33 nm f=0.0020

Excited State 13: Singlet-A 5.3183 eV 233.13 nm f=0.0092

Excited State 14: Triplet-A 5.3926 eV 229.92 nm f=0.0000

Excited State 15: Triplet-A 5.4397 eV 227.92 nm f=0.0000

Excited State 16: Singlet-A 5.5164 eV 224.75 nm f=0.0069

Excited State 17: Singlet-A 5.5668 eV 222.72 nm f=0.0244

Excited State 18: Triplet-A 5.6346 eV 220.04 nm f=0.0000

Excited State 19: Singlet-A 5.6749 eV 218.48 nm f=0.0242

Excited State 20: Triplet-A 5.7261 eV 216.52 nm f=0.0000