Supplementary Information

Reversible Friedel–Crafts Acyl Rearrangements of Planar Polycyclic Aromatic Ketones: Dibenzofluorenones

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Table S1. Crystallographic data for compounds **DB*ah*F**, **DB*ai*F and DB*cg*F**

	DBa*h*F[a]	**DB*cg*F**[a,b]	**DB*ai*F**[c]
Temperature, K	173(1)	193(1)	293(2)
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space Group	$P2_1/c$	$P2_1/n$	P_{nma}
a, Å	13.3493(8)	16.753	13.2543(9)
b, Å	7.6721(5)	14.395	25.769(2)
c, Å	13.0564(8)	5.793	3.8521(2)
α, deg.	90	90	90
β, deg.	94.888(2)	91.0	90
γ, deg.	90	90	90
Volume, $Å^3$	1335.1(1)	1396.7	1315.7(2)
Z	4	4	4
Density (calculated) Mg/m^3	1.395	1.333	1.415
Absorption coeff. mm^{-1}	0.084	0.075	
F(000)	584	584	584
Crystal size, mm^3	0.37×0.34×0.10		
Crystal color	yellow	red	red
Theta range, deg.	3.06 to 27.00	2.5 to 27.5	3.07 to 32.9
Reflections collected	14046	3648	3713
Independent reflections (R_{int})	2809 (0.0238)	2337 (3.28)	2502 (0.018)
Absorption correction	none	none	none
Data/restraints/parameters	2909/0/199	2337/0/248	2502/0/127
Goodness-of-fit on F^2	1.107		
Final *R* indices [$I>2\sigma_I$]	R_1=0.0539	R_1=0.039	R_1=0.054
	wR_2=0.1258	wR_2=0.053	
R indices (all data)	R_1=0.0581		R_1=0.116
	wR_2=0.1286		wR_2=0.167
Largest diff. peak/hole, eA^{-3}	0.325/-0.222	0.16/-0.20	0.36/-0.24

[a] This study
[b] CCDC 801984[34]
[c] COD 2010900[33]

References

33. D. G. Morris, S. Higgins, K. S. Ryder, R. A. Howie, K. W. Muir, *Acta Cryst. C* **2000**, *56*, 570–571
34. G. L. Eakins, J. S. Alford, B. J. Tiegs, B. E. Breyfogle, C. J. Stearman, J. Phys. Org. Chem. **2011**, *24*, 1119–1128

Table S2. Total and relative B3LYP/6-311++G(*d*,*p*) energies, selected geometric parameters, HOMA and NICS indices of dibenzofluorenones

		[a]	nonbonding distances								PCM(water)[g]	
			E_{Tot}	ΔZPE	ΔG_{298}	O···H[b]	H···H[c]	HOMA5[d]	HOMA21[e]	NICS[f]	NICS+1[f]	E_{Tot}	ΔG_{298}
			Hartree	kJ/mol	kJ/mol	pm	pm					Hartree	kJ/mol
DB*bh*F	C_{2v}	M	-882.940297	0.00	0.00	293.1	266.6	-0.757	0.477	9.6	2.4	-882.951317	0.00
DB*ah*F	C_s	M	-882.938980	3.60	1.74	240.4, 293.6	261.4	-0.704	0.466	11.4	4.2	-882.948972	4.01
DB*bg*F	C_s	M	-882.935268	13.07	10.10	287.1, 290.8	191.0	-0.732	0.464	11.2	4.0		
DB*ai*F	C_{2v}	M	-882.934244	16.07	16.14	241.5	258.1	-0.819	0.437	15.3	7.9	-882.942992	21.40
DB*ag*F	C_s	M	-882.930300	26.24	23.42	238.8, 286.7	188.5	-0.822	0.431	14.8	7.3		
DB*cg*F	C_2	M	-882.919610	54.86	55.61	289.9	208.1	-0.842	0.414	14.2	5.9, 5.7		
DB*cg*F	C_{2v}	TS	-882.908904	80.71	81.86	272.7	147.2	-	-	-	-		

[a] – M: minimum; TS: transition state
[b] – the distance between the oxygen atom and the nearest aromatic hydrogen: $O^{12}\cdots H^{11}$ for **DB*bh*F**, $O^{13}\cdots H^{1}/O^{13}\cdots H^{12}$ for **DB*ah*F**, **DB*ai*F** and **DB*ag*F**, $O^{7}\cdots H^{6}/O^{7}\cdots H^{8}$ for **DB*bg*F** and **DB*cg*F**
[c] – the shortest distance between aromatic hydrogens: $H^{5}\cdots H^{6}$ for **DB*bh*F**, $H^{6}\cdots H^{7}$ for **DB*ah*F**, **DB*ai*F** and **DB*ag*F**, $H^{1}\cdots H^{13}$ for **DB*bg*F** and **DB*cg*F**
[d] – HOMA index of the five-membered ring
[e] – HOMA index of the 21-membered aromatic system
[f] – NICS values of the five-membered ring (calculated in the plane of the ring and 1 Å above it)
[g] – Self-consistent reaction field calculations using PCM model, with water as a solvent

Table S3. Total and relative B3LYP/6-311++G(*d*,*p*) energies, selected geometric parameters, HOMA and NICS indices of *O*-protonates of dibenzofluorenones

	[a]	nonbonding distances										PCM(water)[i]	
		E_{Tot}	ΔZPE	ΔG_{298}	O···H[b]	H···H[c]	OH···H[d]	Φ[e]	HOMA5[f]	HOMA21[g]	NICS[h]	NICS+1[h]	E_{Tot}	ΔG_{298}
		Hartree	kJ/mol	kJ/mol	pm	pm	pm	deg					Hartree	kJ/mol
DB*bh*FH$^+$	C_s	M	-883.301198	0.00	0.00	283.0, 302.1	273.9	237.3	0.0	0.142	0.735	10.8	6.0	-883.364740	0.00
DB*ah*FH$^+$	C_s	M	-883.299782	3.98	3.99	237.3, 301.8	265.6	235.1	0.0	0.235	0.727	15.2	9.8	-883.363154	3.78
DB*ah*FH$^+$	C_1	M	-883.297729	9.36	8.81	263.4, 282.7	265.3	177.7	3.6	0.275	0.730	14.7	9.3,9.5	-883.359430	12.82
DB*ah*FH$^+$	C_s	TS	-883.297721	7.76	10.30	264.0, 282.2	264.1	175.6	0.0	-	-	-	-		
DB*bg*FH$^+$	C_s	M	-883.297313	14.18	13.03	281.3, 297.8	194.4	231.4	0.0	0.153	0.698	15.8	10.3		
DB*bg*FH$^+$	C_s	M	-883.294546	17.01	15.87	279.0, 300.2	194.3	235.4	0.0	0.114	0.688	16.2	10.6		
DB*ai*FH$^+$	C_1	M	-883.287612	35.49	34.92	237.8, 262.6	260.9	175.6	3.2	0.157	0.691	27.7	20.6	-883.349682	38.31
DB*ai*FH$^+$	C_s	TS	-883.287565	33.75	36.14	237.1, 263.1	259.8	172.9	0.0	-	-	-	-		
DB*ag*FH$^+$	C_s	M	-883.285314	40.95	39.47	236.2, 295.5	191.8	226.3	0.0	0.012	0.653	30.3	22.7		
DB*ag*FH$^+$	C_1	M	-883.282440	48.80	47.70	262.5, 278.1	193.2	177.9	7.0	0.029	0.656	30.1	22.5,22.6		
DB*ag*FH$^+$	C_s	TS	-883.282149	47.25	48.57	262.3, 276.6	190.8	173.3	0.0	-	-	-	-		
DB*cg*FH$^+$	C_1	M	-883.273733	72.37	73.35	281.9, 300.0	210.7	233.8	26.5	-0.042	0.622	29.3	21.8		

[a] – M: minimum; TS: transition state
[b] – distance between the oxygen atom and the nearest hydrogen: $O^{12}\cdots H^{11}$ for **DB*bh*FH$^+$**, $O^{13}\cdots H^{1}$/$O^{13}\cdots H^{12}$ for **DB*ah*FH$^+$**, **DB*ai*FH$^+$** and **DB*ag*FH$^+$**, $O^{7}\cdots H^{6}$/$O^{7}\cdots H^{8}$ for **DB*bg*FH$^+$** and **DB*cg*FH$^+$**
[c] – the shortest distance between aromatic hydrogens: $H^{5}\cdots H^{6}$ for **DB*bh*FH$^+$**, $H^{6}\cdots H^{7}$ for **DB*ah*FH$^+$**, **DB*ai*FH$^+$** and **DB*ag*FH$^+$**, $H^{1}\cdots H^{13}$ for **DB*bg*FH$^+$** and **DB*cg*FH$^+$**
[d] – the distance between the hydroxyl hydrogen and the nearest aromatic hydrogen
[e] – the dihedral angle between the least-square planes of two naphthyl moieties
[f] –HOMA index of the five-membered ring
[g] – HOMA index of the 21-membered aromatic system
[f] – NICS values of the five-membered ring (calculated in the plane of the ring and 1 Å above it)
[i] – Self-consistent reaction field calculations using PCM model, with water as a solvent

Table S4. Total and relative B3LYP/6-311++G(*d*,*p*) energies and selected geometric parameters of σ-complexes of dibenzofluorenones (minima only)

					nonbonding distances			PCM(water)[e]	
		E_{Tot}	ΔZPE[a]	ΔG_{298}[a]	$\Delta\Delta G_{298}$	O···H[b]	H···H[c]	Φ[d]	E_{Tot}	$\Delta\Delta G_{298}$
		Hartree	kJ/mol	kJ/mol	kJ/mol	pm	pm	deg	Hartree	kJ/mol
σ-13a*H*-DB*ah*F$^+$	C_1	-883.274232	68.31	67.54	0.00	251.0, 295.8	25919	20.5	-883.338622	0.00
σ-12b*H*-DB*ai*F$^+$	C_1	-883.273941	69.95	69.26	1.71	241.7, 251.7	255.8	22.3	-883.337295	3.17
σ-13a*H*-DB*ag*F$^+$	C_1	-883.271048	77.62	76.93	9.39	253.8, 290.3	208.6	29.1		
σ-6a*H*-DB*bg*F$^+$	C_1	-883.262059	99.27	97.60	30.06	293.1, 294.0	196.3	21.5		
σ-12a*H*-DB*ag*F$^+$	C_1	-883.261955	100.59	99.35	31.80	240.0, 292.5	194.9	24.0		
σ-11a*H*-DB*bh*F$^+$	C_1	-883.260814	101.19	100.05	32.51	295.7, 298.9	267.7	22.4	-883.326684	28.05
σ-12a*H*-DB*ah*F$^+$	C_1	-883.260876	101.70	100.84	33.29	243.0, 298.8	263.4	23.7	-883.326512	29.58
σ-7a*H*-DB*bg*F$^+$	C_1	-883.257922	109.57	108.62	41.08	292.5, 298.2	215.0	29.8		
σ-6a*H*-DB*cg*F$^+$	C_1	-883.255427	117.72	117.90	50.36	298.5, 293.5	220.7	40.2		

[a] – relative to the respective energy of **DB*bh*FH$^+$**

[b] – the distance between the oxygen atom and the nearest hydrogen: $O^{12}\cdots H^{11}$ for **σ-11b*H*-DB*bh*F$^+$**, $O^{13}\cdots H^1/O^{13}\cdots H^{12}$ for **σ-12a*H*-DB*ah*F$^+$**, **σ-13a*H*-DB*ah*F$^+$**, **σ-12b*H*-DB*ai*F$^+$**, **σ-12a*H*-DB*ag*F$^+$** and **σ-13a*H*-DB*ag*F$^+$**, $O^7\cdots H^6/O^7\cdots H^8$ for **σ-6a*H*-DB*bg*F$^+$**, **σ-7a*H*-DB*bg*F$^+$** and **σ-6a*H*-DB*cg*F$^+$**

[c] – the shortest distance between aromatic hydrogens: $H^5\cdots H^6$ for **σ-11b*H*-DB*bh*FH$^+$**, $H^6\cdots H^7$ for **σ-12a*H*-DB*ah*FH$^+$**, **σ-13a*H*-DB*ah*FH$^+$**, **σ-12b*H*-DB*ai*FH$^+$**, **σ-12a*H*-DB*ag*FH$^+$** and **σ-12a*H*-DB*ag*FH$^+$**, $H^1\cdots H^{13}$ for **σ-6a*H*-DB*bg*F$^+$**, **σ-7a*H*-DB*bg*F$^+$** and **σ-6a*H*-DB*cg*F$^+$**

[d] – the dihedral angle between the least-square planes of two naphthyl moieties

[e] – Self-consistent reaction field calculations using PCM model, with water as a solvent

Table S5. Total and relative B3LYP/6-311++G(*d*,*p*) energies and selected geometric parameters of naphthyl naphthoylium ions, derived from the respective σ-complexes of dibenzofluorenones

naphthyl naphthoylium ion	structurally related to σ-complex	E_{Tot} Hartree	ΔZPE[a] kJ/mol	ΔG_{298}[a] kJ/mol	$\Delta\Delta G_{298}$ kJ/mol	φ[b] deg	Φ[c] deg	PCM(water)[d] E_{Tot} Hartree	PCM(water)[d] $\Delta\Delta G_{298}$ kJ/mol
αCOβN-βN$^+$	**σ-12b*H*-DB*ai*F$^+$**	-883.271506	72.89	67.73	0.00	42.0	41.5	-883.334357	0.00
αCOβN-βN$^+$	**σ-12a*H*-DB*ah*F$^+$**	-883.270720	75.03	69.84	2.11	141.3	38.3	-883.333342	0.51
αCOβN-αN$^+$	**σ-12a*H*-DB*ag*F$^+$**	-883.267219	84.21	79.05	11.32	130.3	53.9		
βCOαN-βN$^+$	**σ-13a*H*-DB*ag*F$^+$**	-883.267388	83.82	78.81	11.08	54.7	56.7		
βCOβN-βN$^+$	**σ-13a*H*-DB*ah*F$^+$**	-883.266743	84.90	79.57	11.84	45.6	45.4	-883.332306	11.64
βCOβN-βN$^+$	**σ-11a*H*-DB*bh*F$^+$**	-883.265934	87.09	81.37	13.64	134.4	45.3	-883.331668	13.96
βCOαN-βN$^+$	**σ-7a*H*-DBb*g*F$^+$**	-883.266401	86.44	81.40	13.67	123.8	56.1		
αCOβN-αN$^+$	**σ-12a*H*-DB*ag*F$^+$**	-883.265013	89.85	84.64	16.91	53.6	55.2		
βCOαN-αN$^+$	**σ-6a*H*-DB*cg*F$^+$**	-883.263872	92.88	87.78	20.05	112.8	69.5		
βCOβN-αN$^+$	**σ-6a*H*-DB*bg*F$^+$**	-883.262996	99.94	89.13	21.40	122.6	59.7		
βCOαN-αN$^+$	**σ-6a*H*-DB*cg*F$^+$**	-883.262837	95.44	87.13	19.40	74.9	76.4		
βCOβN-αN$^+$	**σ-6a*H*-DB*bg*F$^+$**	-883.262364	96.50	90.22	22.49	63.0	63.9		

[a] – relative to the respective energy of **DB*bh*FH**$^+$
[b] – the torsion angle between two naphthyl moieties (absolute value)
[c] – dihedral angle between the least-square planes of two naphthyl moieties
[d] – Self-consistent reaction field calculations using PCM model, with water as a solvent

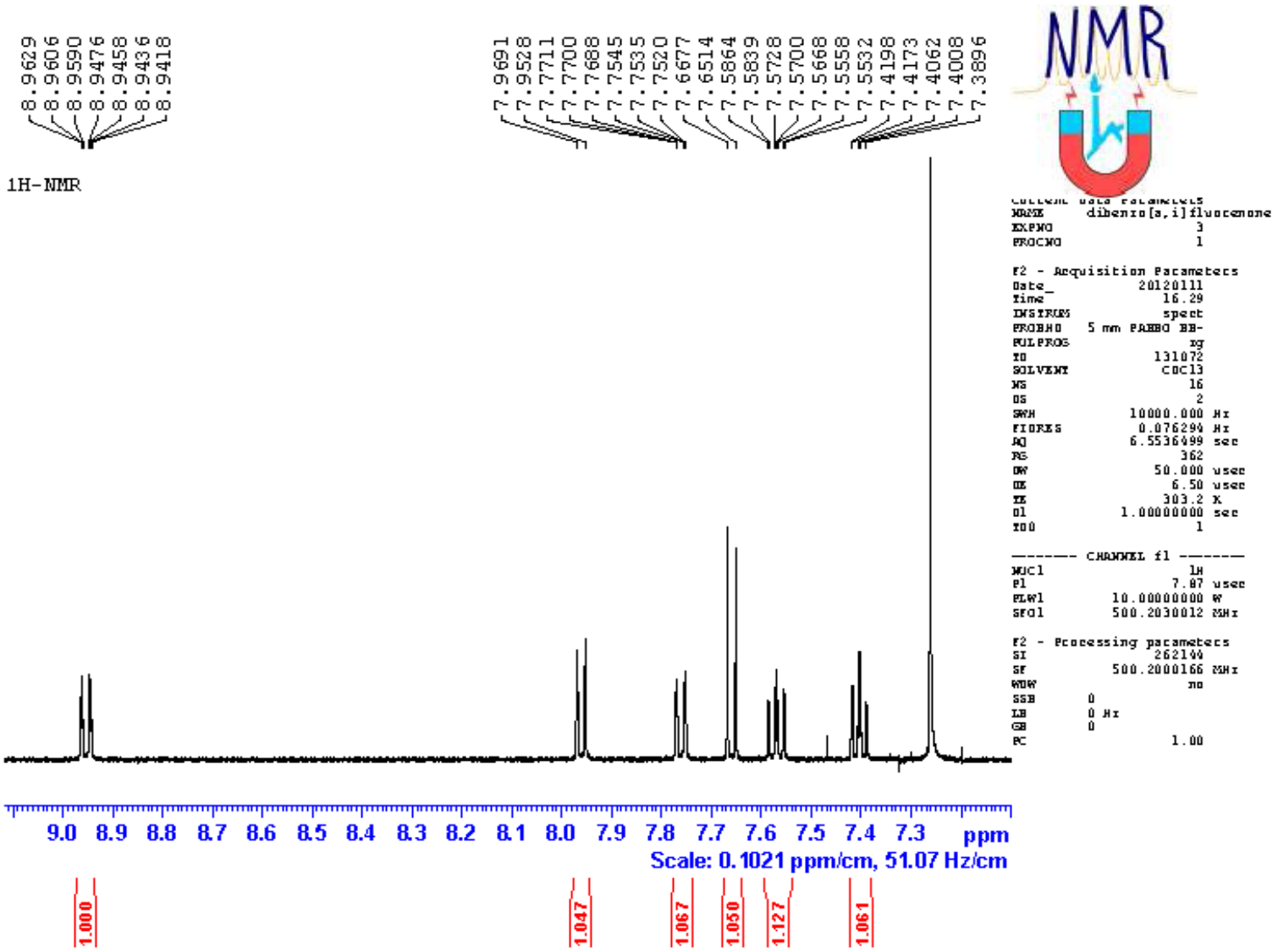


Figure S1. ^{1}H-NMR spectra of 13*H*-dibenzo[*a*,*i*]fluoren-13-one (**DB*ai*F**)

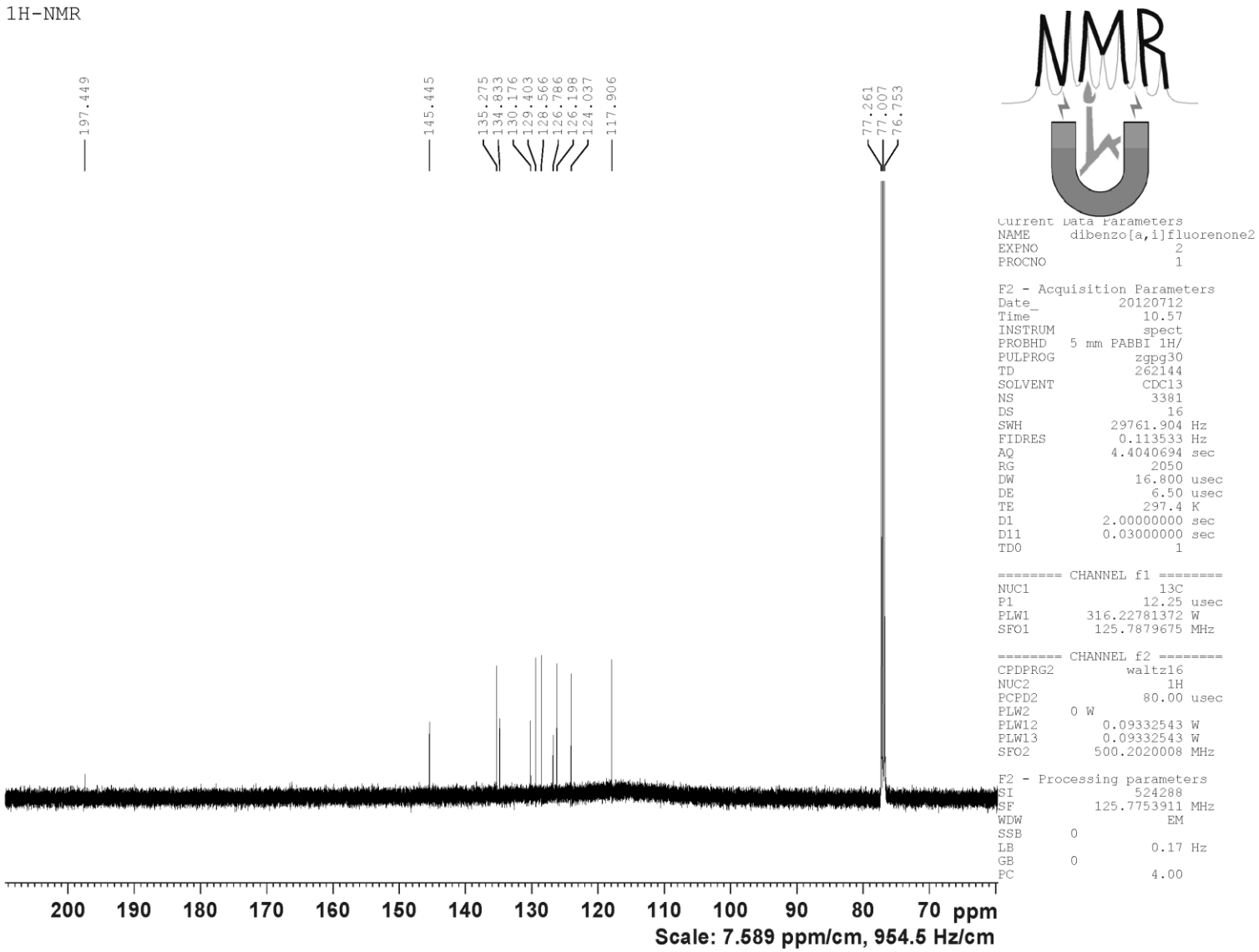


Figure S2. ^{13}C-NMR spectra of 13*H*-dibenzo[*a*,*i*]fluoren-13-one (**DB*ai*F**)

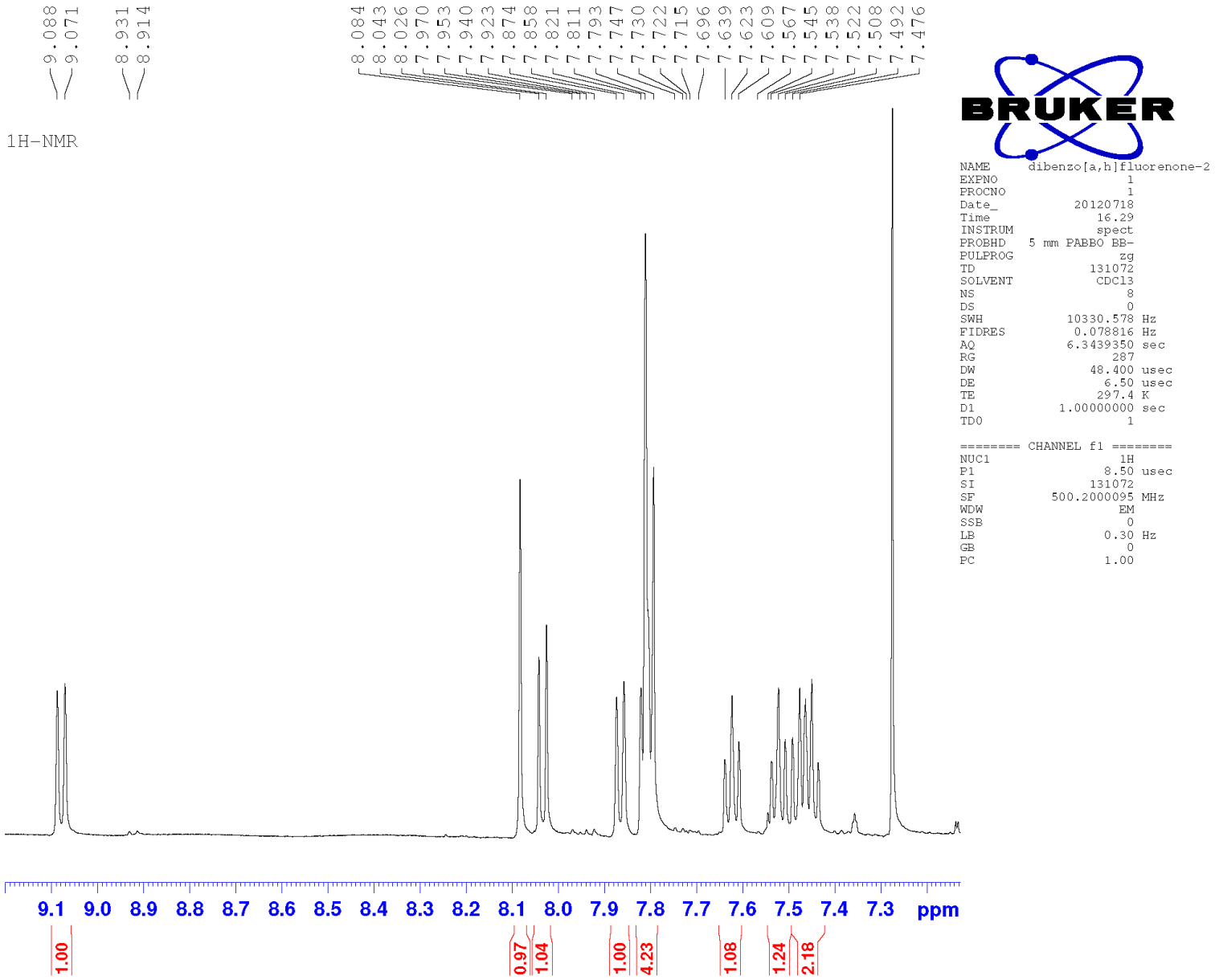
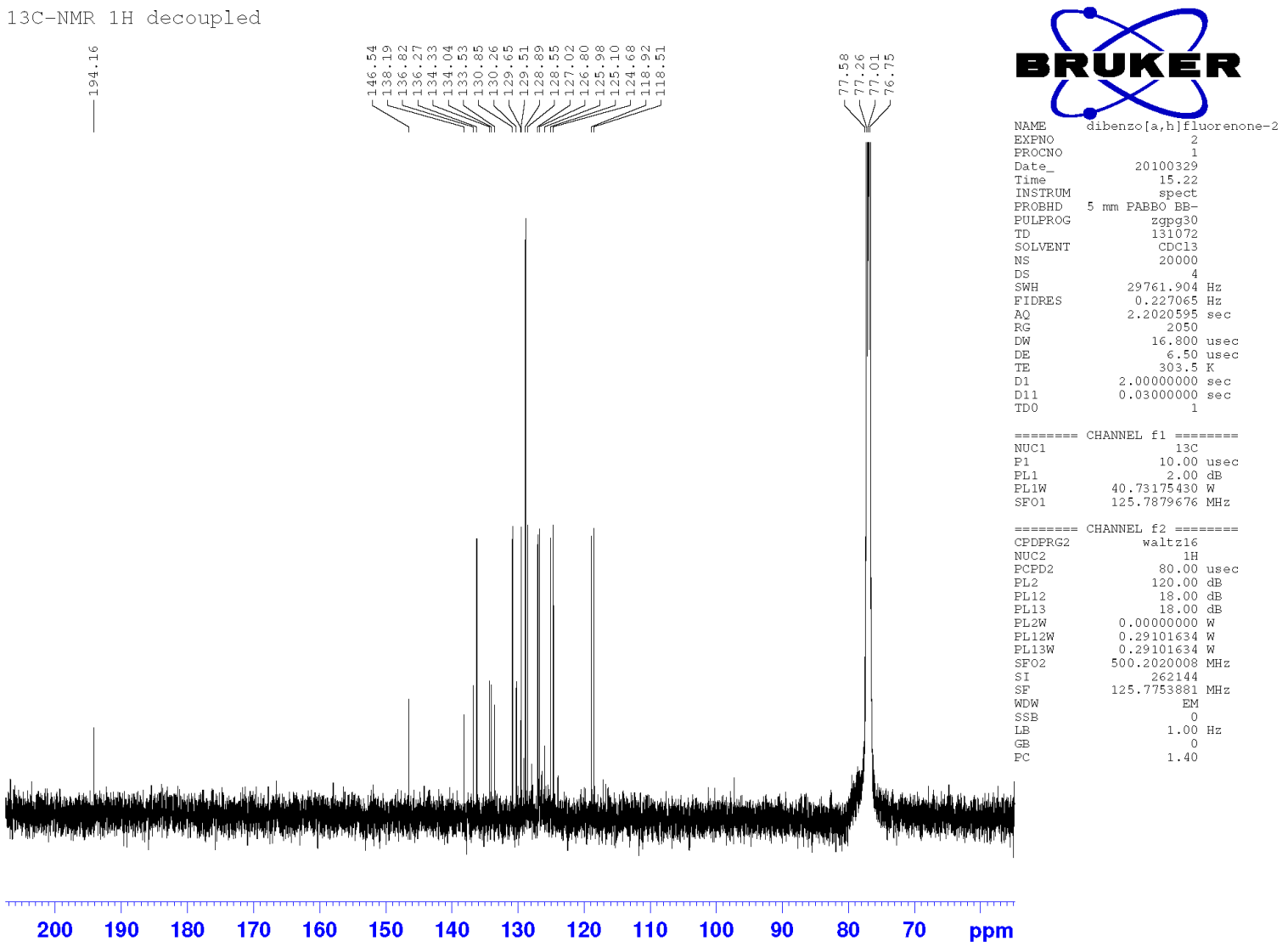


Figure S3. ^{1}H-NMR spectra of 13*H*-dibenzo[*a*,*h*]fluoren-13-one (**DB*ah*F**)



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PROCNO	1
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PL1	2.00 dB
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PL12	18.00 dB
PL13	18.00 dB
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PL13W	0.29101634 W
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SF	125.7753881 MHz
WDW	EM
SSB	0
LB	1.00 Hz
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Figure S4. ^{13}C-NMR spectra of 13*H*-dibenzo[*a*,*h*]fluoren-13-one (**DB*ah*F**)

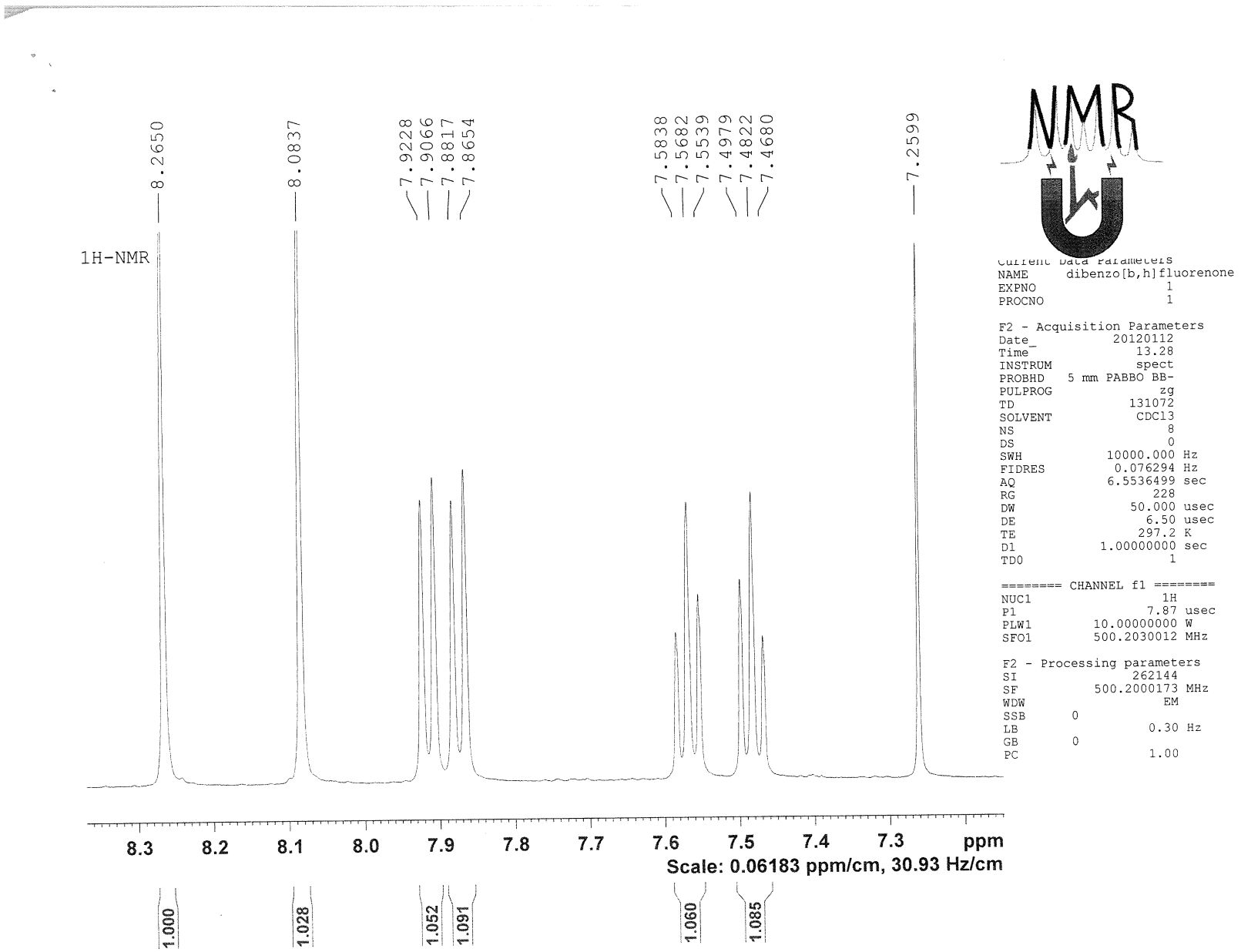


Figure S5. ^{1}H-NMR spectra of 12*H*-dibenzo[*b*,*h*]fluoren-12-one (**DB*bh*F**)

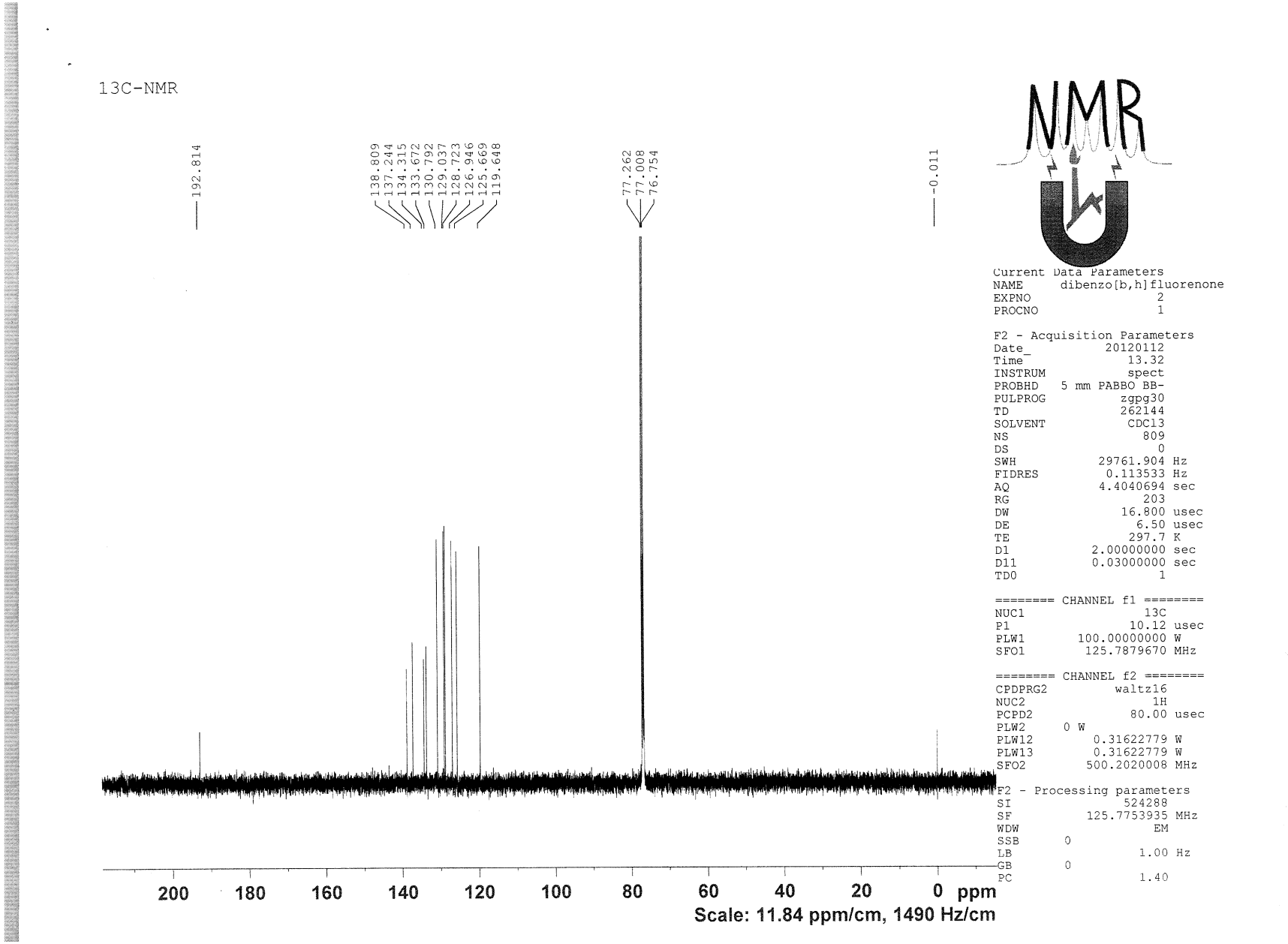


Figure S6. ^{13}C-NMR full spectra of 12*H*-dibenzo[*b*,*h*]fluoren-12-one (**DB*bh*F**)

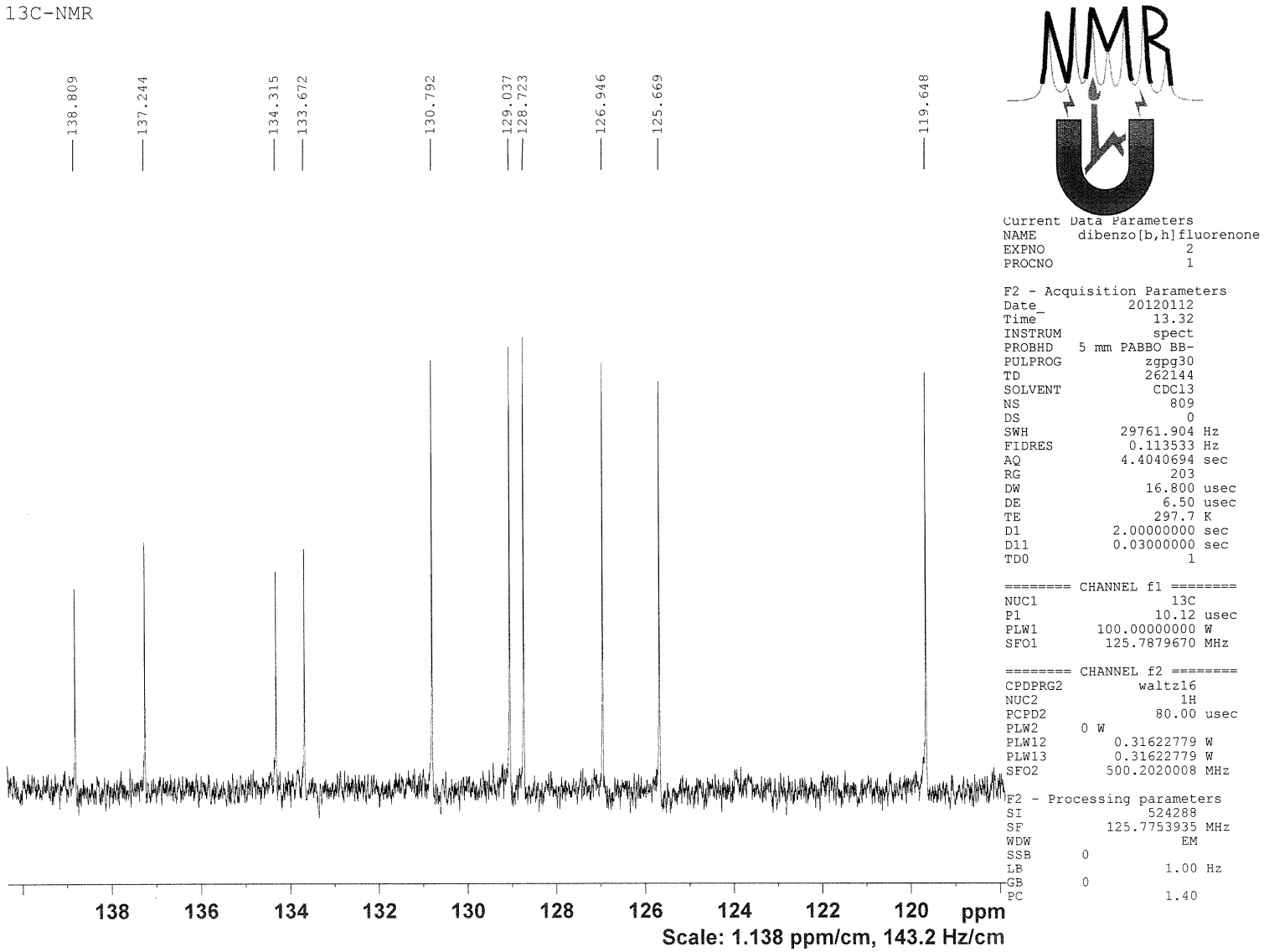
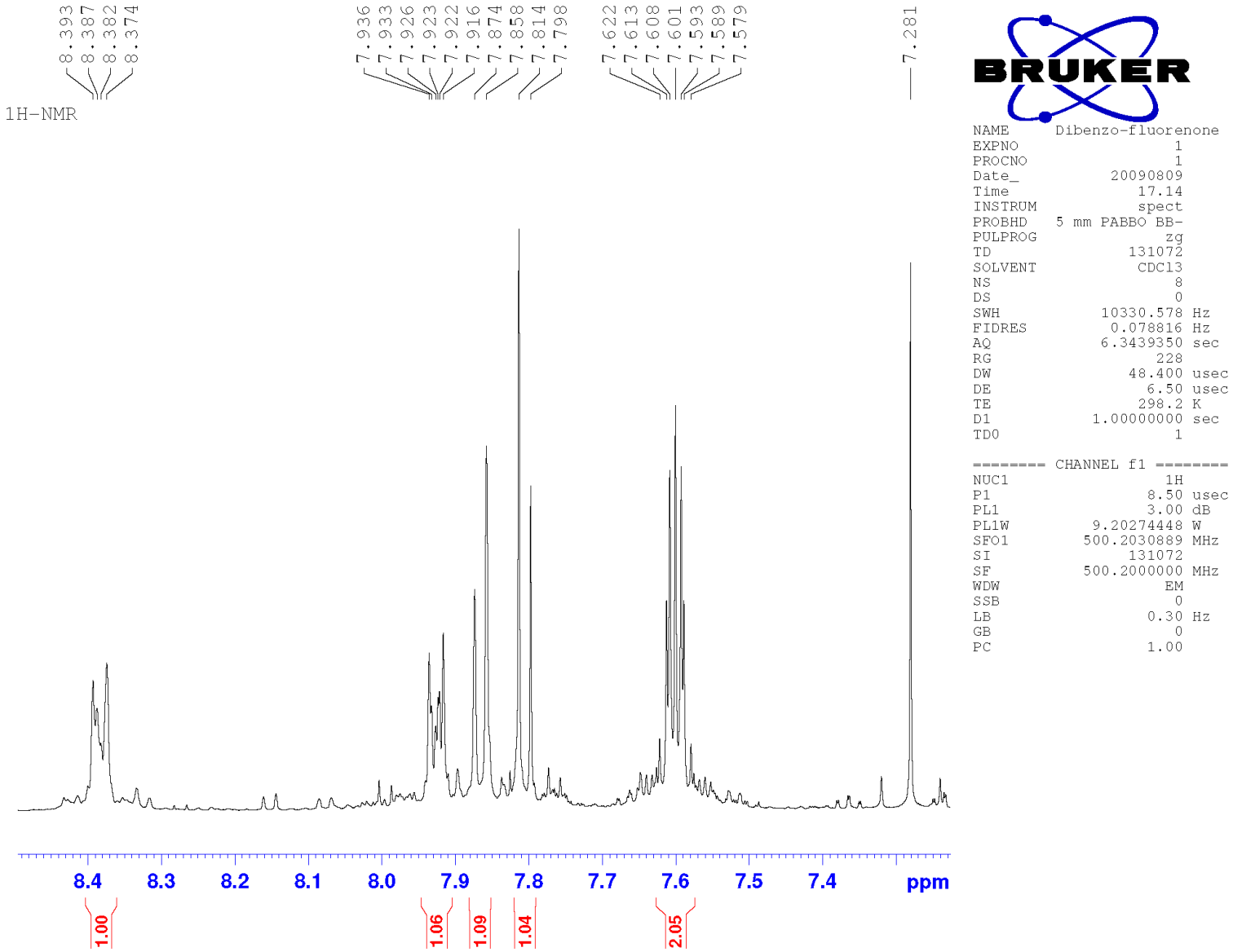


Figure S7. ^{13}C-NMR spectra (aromatic region) of 12*H*-dibenzo[*b*,*h*]fluoren-12-one (**DB*bh*F**)

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PROCNO                         1
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PULPROG                       zg
TD                        131072
SOLVENT                    CDCl3
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DS                             0
SWH                   10330.578 Hz
FIDRES                 0.078816 Hz
AQ                     6.3439350 sec
RG                           228
DW                        48.400 usec
DE                         6.50 usec
TE                        298.2 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
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P1                         8.50 usec
PL1                        3.00 dB
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SI                        131072
SF                 500.2000000 MHz
WDW                           EM
SSB                            0
LB                         0.30 Hz
GB                             0
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Figure S8. ^{1}H-NMR spectra of 7*H*-dibenzo[*c*,*g*]fluoren-7-one (**DB*cg*F**)

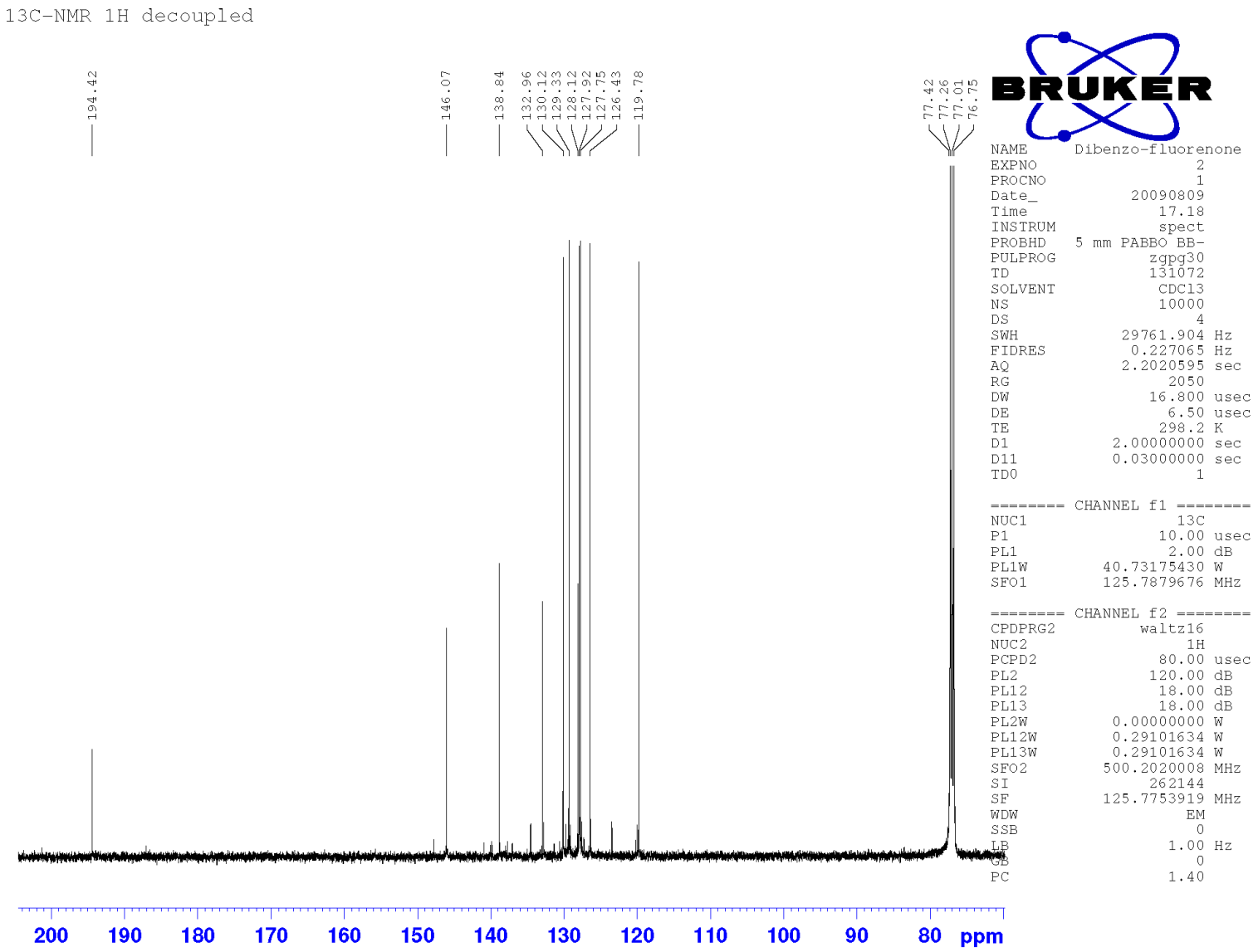

Figure S9. ^{13}C-NMR spectra of 7*H*-dibenzo[*c*,*g*]fluoren-7-one (**DB*cg*F**)

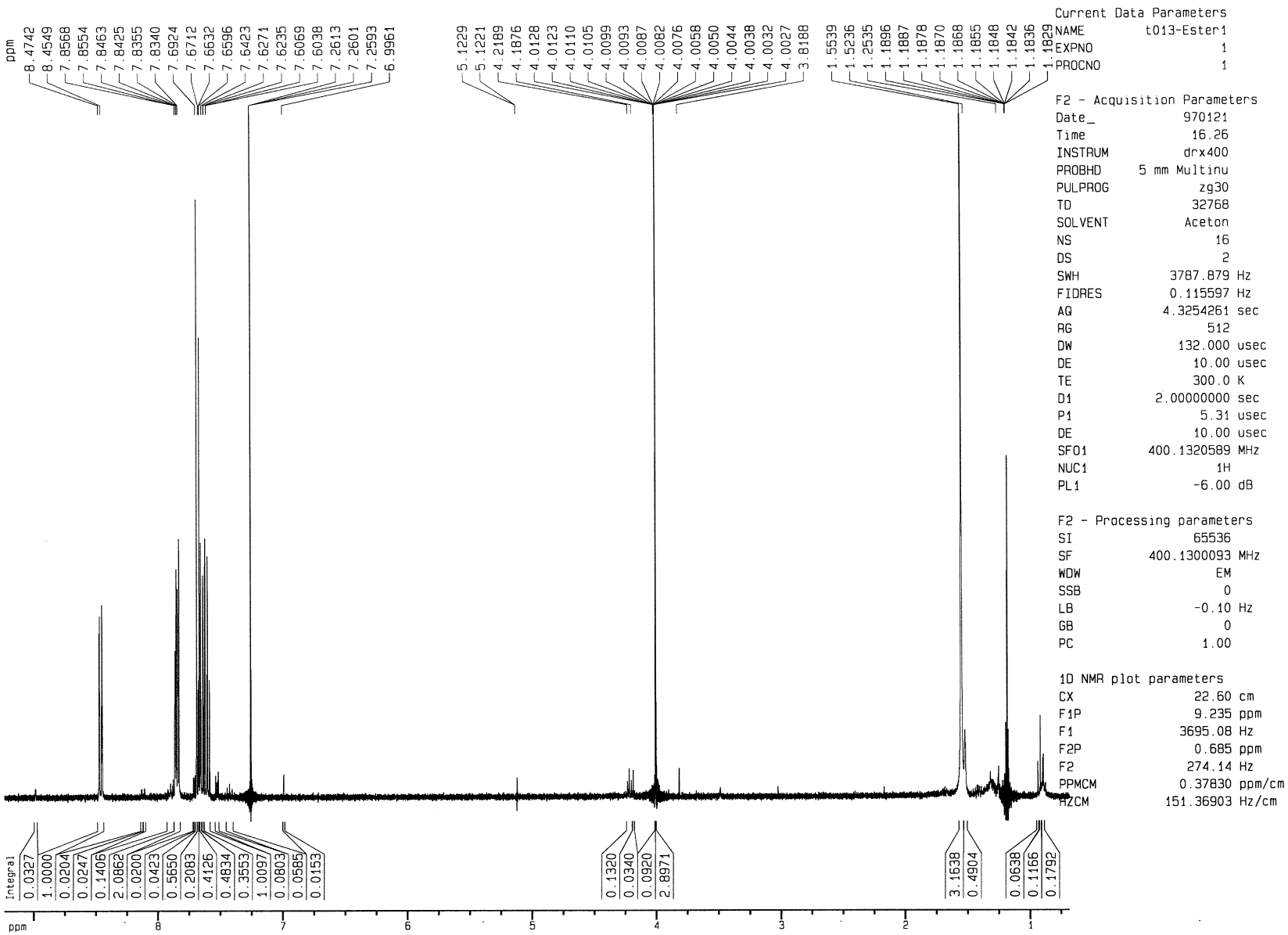

Figure S10. ^{1}H-NMR full spectra of 1-bromo-2-naphthoic acid methyl ester

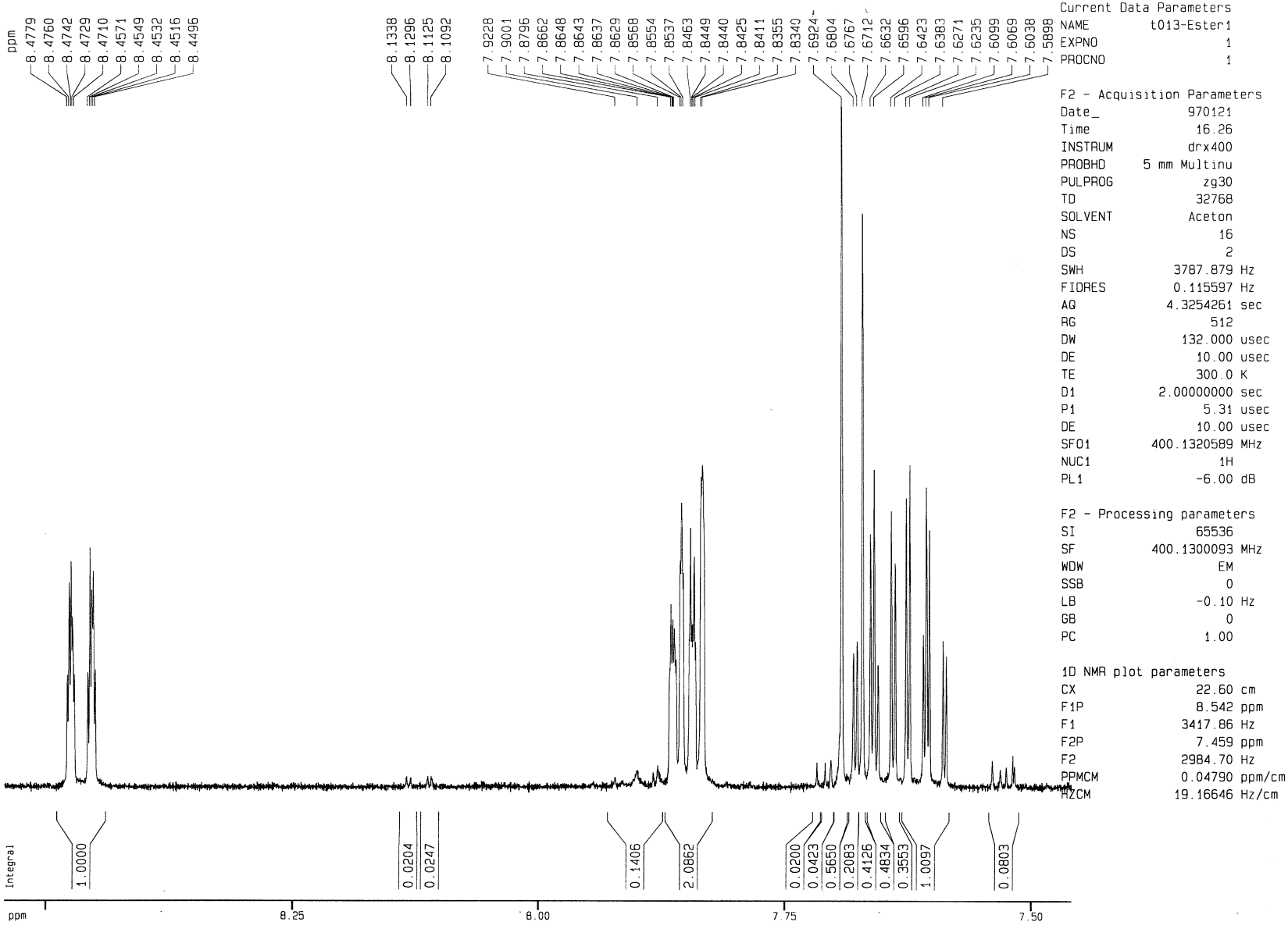

Figure S11. ^{1}H-NMR spectra (aromatic region) of 1-bromo-2-naphthoic acid methyl ester

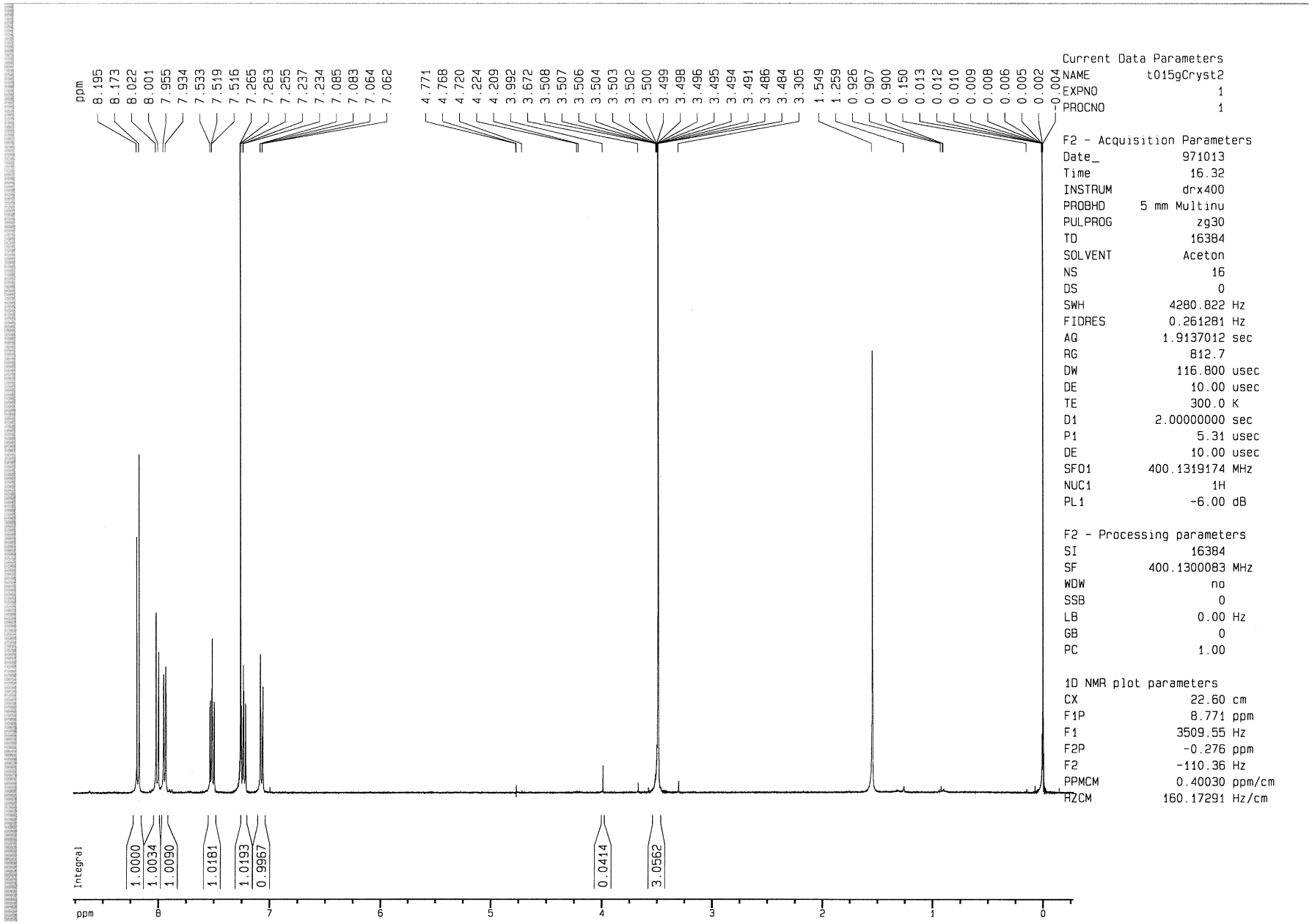

Figure S12. ^{1}H-NMR full spectra of [1,1'-binaphthalene]-2,2'-dicarboxylic acid, 2,2'-dimethyl ester

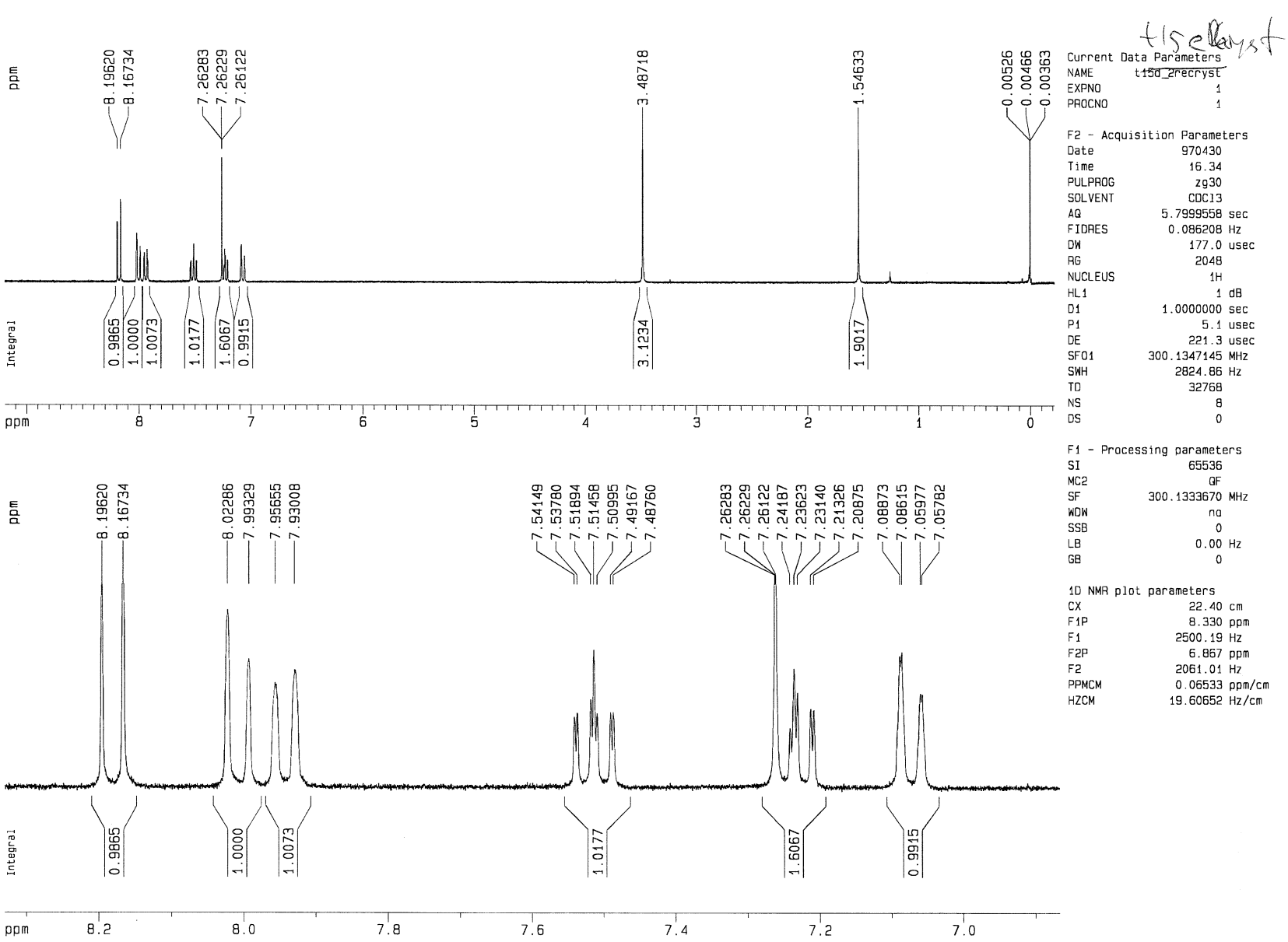

Figure S13. ^{1}H-NMR spectra (aromatic region) of [1,1'-binaphthalene]-2,2'-dicarboxylic acid, 2,2'-dimethyl ester

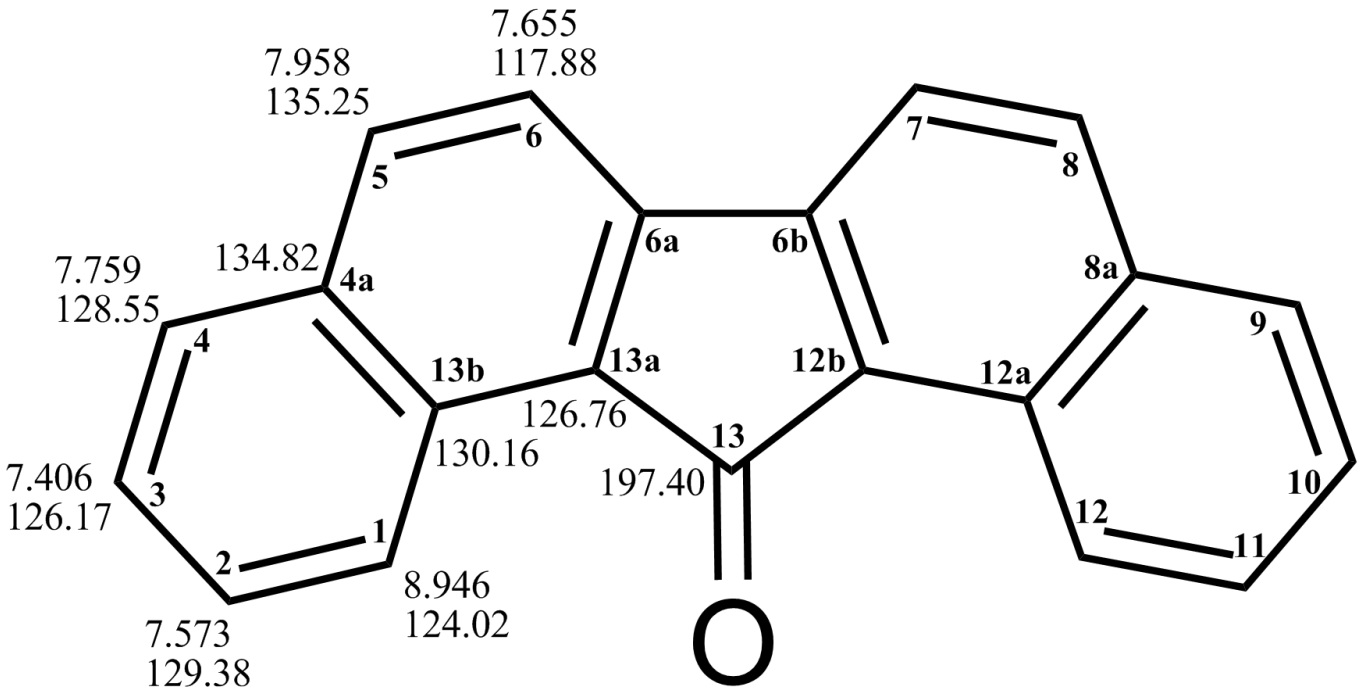

Figure S14. ^{1}H and ^{13}C chemical shifts of 13*H*-dibenzo[*a*,*i*]fluoren-13-one (**DB*ai*F**)

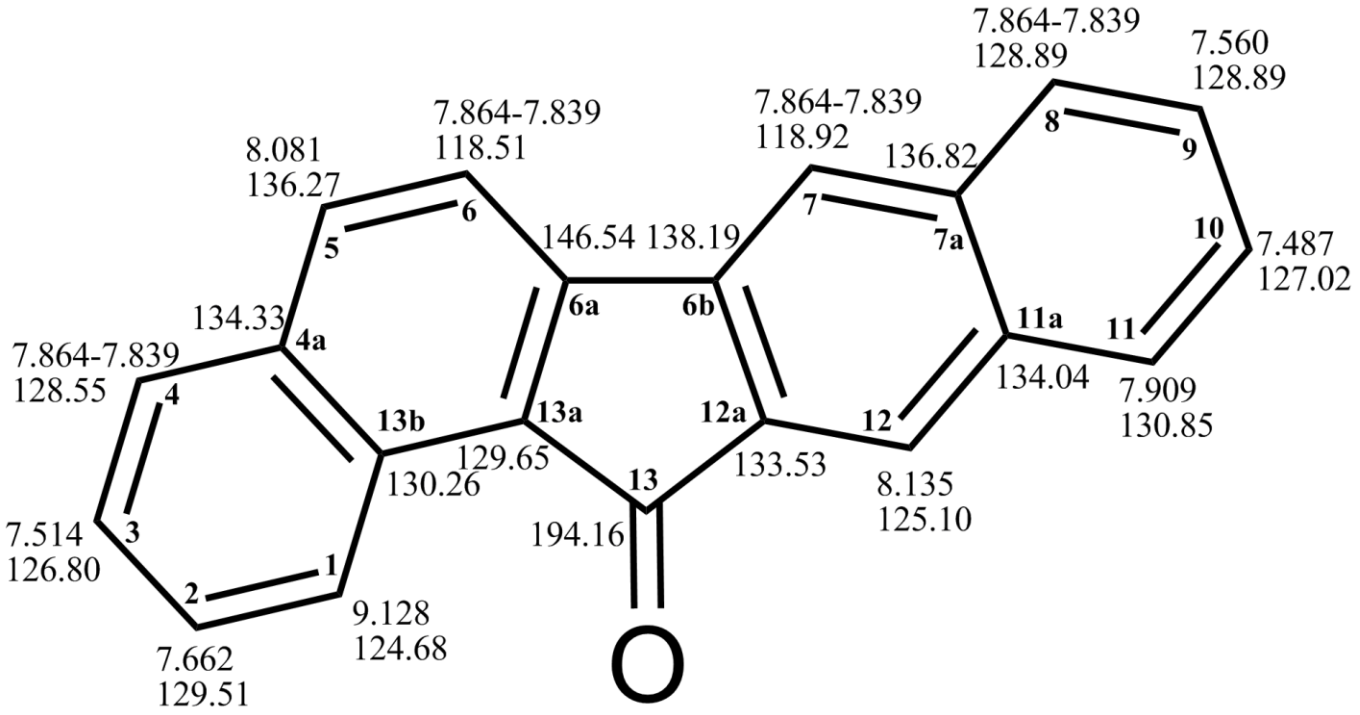

Figure S15. ^{1}H and ^{13}C chemical shifts of 13*H*-dibenzo[*a*,*h*]fluoren-13-one (**DB*ah*F**)

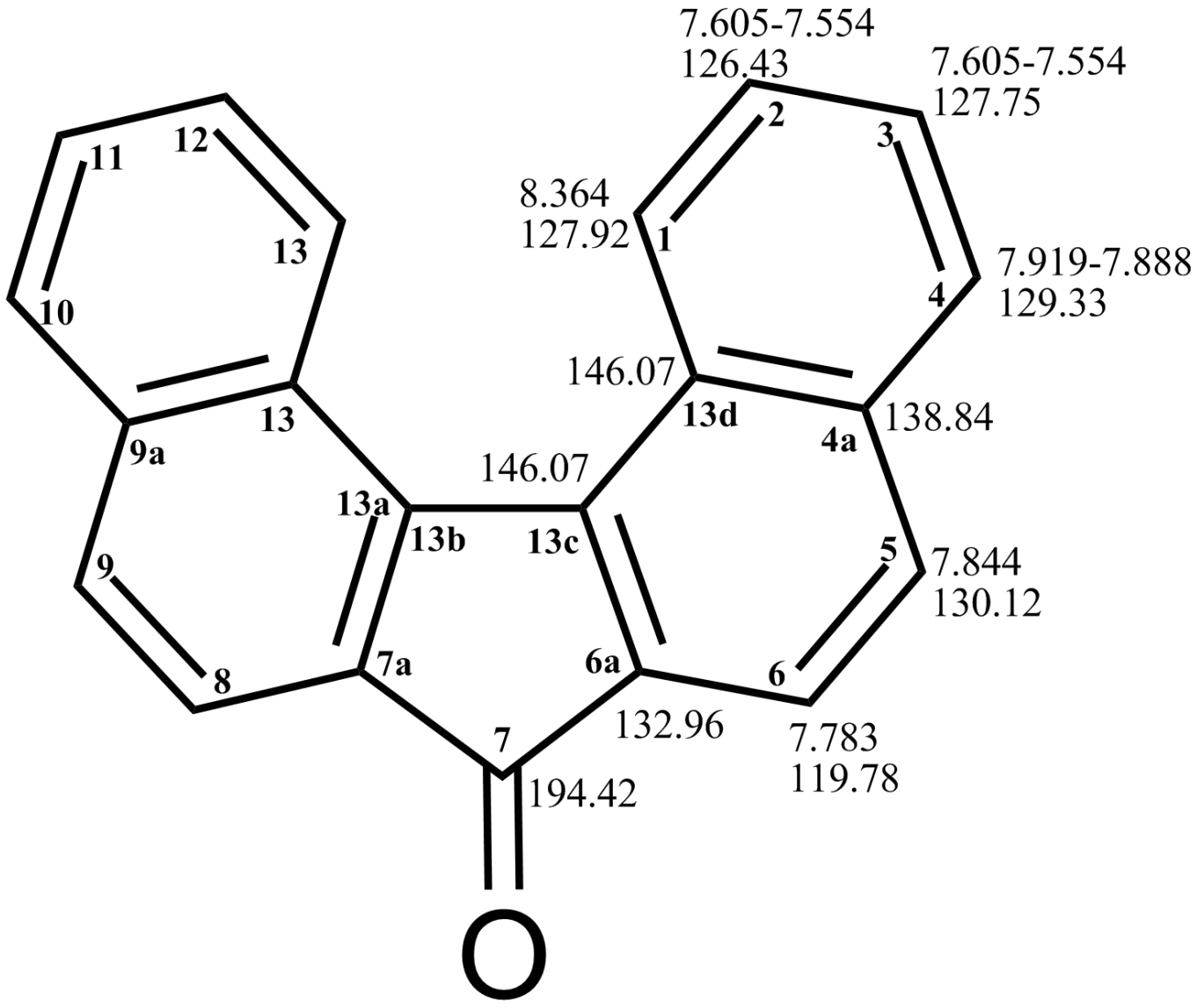

Figure S16. ^{1}H and ^{13}C chemical shifts of 7*H*-dibenzo[*c*,*g*]fluoren-7-one (**DB*cg*F**)

Synthesis of 7*H*-dibenzo[*cg*]fluoren-7-one

1-Bromo-2-naphthoic acid methyl ester: To a solution of 1-bromo-2-naphthoic acid (0.261 g, 1.04 mmol) in Et_2O (20 mL) the yellow solution of diazomethane (obtained according to a literature procedure[48] from N-nitrosomethylurea (0.428 g, 4.15 mmol)) in Et_2O (8 mL) was added dropwise at 0 °C under argon atmosphere. The reaction mixture was gradually heated to rt, and stirred for 2 h. The solvent was evaporated in vacuum to give 0.247 g (89 %) of 1-bromo-2-naphthoic acid methyl ester, mp. 60–64 °C.

^{1}H-NMR (δ, ppm): 8.465 (*d*, *J*=7.7 Hz, 1H), 7.866–7.834 (m, 2H), 7.682 (d, *J*=8.5 Hz, 1H), 7.660 (*td*, ^3J=7.6 Hz, ^4J=1.5 Hz, 1H), 7.607 (*td*, ^3J=7.4 Hz, ^4J=1.4 Hz, 1H), 4.082 (*s*, 3H).

[1,1'-Binaphthalene]-2,2'-dicarboxylic acid, 2,2'-dimethyl ester: The mixture of 1-bromo-2-naphthoic acid methyl ester (0.221 g, 0.833 mmol), copper bronze (1.03 g, 20.0 mmol) and DMF (8 mL) was refluxed for 16 h under argon atmosphere. The reaction mixture were extracted by boiling toluene (2x30 mL), the organic layer was washed with 2N HCl (4x7 mL), water (4x16 mL), and dried over anhydrous $MgSO_4$. Evaporation afforded 0.161 g of pink solid. Recrystallization from CH_3OH yielded 0.0775 g (50%) of [1,1'-binaphthalene]-2,2'-dicarboxylic acid 2,2'-dimethyl ester as white powder, mp. 155–156 °C (lit.[31] 156.5–157.5 °C).

^{1}H-NMR (δ, ppm): 8.187 (*dd*, ^3J=8.8 Hz, ^4J=3.7 Hz, 1H), 8.016 (*d*, *J*=8.7 Hz, 1H), 7.967 (*d*, *J*=6.0 Hz, 1H), 7.519 (*t*, *J*=7.2 Hz, 1H), 7.240 (*t*, *J*=7.2 Hz, 1H), 7.082 (*d*, *J*=8.4 Hz, 1H), 3.496 (*s*, CH_3).

[1,1'-Binaphthalene]-2,2'-dicarboxylic acid: The mixture of [1,1'-binaphthalene]-2,2'-dicarboxylic acid 2,2'-dimethyl ester (0.0775 g, 0.21 mmol) and KOH (0.422 g, 7.52 mmol) in CH_3OH (5 mL) was refluxed for 20 h. The solvent was removed in vacuum, the solid product was dissolved in concentrated HCl (1 mL) and the resulting amorphous white precipitate was filtered off and washed with water, yielding 0.0696 g (97%) of [1,1'-binaphthalene]-2,2'-dicarboxylic acid as white powder, mp. 275–278 °C (lit.[31] 266 °C).

7*H*-Dibenzo[*cg*]fluoren-7-one (DB*cg*F): A mixture of [1,1'-binaphthalene]-2,2'-dicarboxylic acid (0.0696 g, 0.20 mmol) and acetic anhydride (2.52 mL, 20 mmol) was refluxed for 45 m. Unreacted acetic anhydride, acetic acid and water were removed in vacuum, and the solid residue heated at 280 °C for 3 h under argon atmosphere. The resulting red melt was extracted with boiling benzene (3x10 mL) and the solvent evaporated, yielding 0.0604 g of red solid. The crude product was purified by sublimation at 5 mm Hg/130 °C, yielding 0.0236 g (41%) of **DB*cg*F** as dark red crystals, mp. 223–224 °C (lit.[31] 222–222.5 °C, lit.[34] 225–226 °C).

^{1}H-NMR (δ, ppm): 8.364 (*d*, *J*=8.2 Hz, H^1), 7.919–7.888 (*m*, H^4), 7.844 (*d*, *J*=8.0 Hz, H^5), 7.783 (*d*, *J*=8.0 Hz, H^6), 7.605–7.554 (*m*, H^2, H^3).

^{13}C-NMR (δ, ppm): 194.42 (C^7=O), 146.07 (C^{13b}), 138.84 (C^{4a}), 132.96 (C^{6a}), 130.12 (C^5), 129.33 (C^4), 128.12 (C^{13a}), 127.92 (C^1), 127.75 (C^3), 126.43 (C^2), 119.78 (C^6).

References

31. R. H. Martin, *J. Chem. Soc.* 1941, 679–685
34. G. L. Eakins, J. S. Alford, B. J. Tiegs, B. E. Breyfogle, C. J. Stearman, J. Phys. Org. Chem. 2011, **24,** 1119–1128
48. *Organic Syntheses*, Wiley & Sons, New York, 1943, Coll. Vol. 2, pp. 165–166

Cartesian coordinates

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18-Mar-2013
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16-Mar-2013
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28-Sep-2012
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10-Oct-2012
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25-Sep-2012
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C21H13O1(1+)
SERGEY
10-Oct-2012
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C -0.4810767018 0.0777318766 -0.9027644246
C 0.9326807529 -3.3846792154 1.2121385462
C -1.29527458 2.4233492666 -2.341902645
C 1.085685648 -0.9936931649 0.6906382509
C -0.8072890504 0.0184031825 -2.2671057414
C 1.5729243643 -2.118659025 1.398505562
C -1.1977280402 1.1481992438 -2.954783789
C 2.6815516127 -2.0251444874 2.2816206331
C -1.1093474423 3.8145421086 -0.3396826153
C 1.4169406227 -4.5092292587 1.9255505128
C -1.671957066 3.5717911131 -3.0806230407
C 3.1261735612 -3.1351461691 2.9605331141
C -1.482144337 4.9155979094 -1.0870858406
C 2.4883543168 -4.3857929255 2.7814184443
C -1.7654030758 4.7977725073 -2.462214542
H 3.1675270445 -1.0650586954 2.4159462318
H -0.8856706807 3.9386077927 0.7135167595
H 3.9694718106 -3.0568459483 3.6366151389
H -1.5522965246 5.884036604 -0.606789297
H 2.8515014415 -5.2518315892 3.322583823
H -2.053865086 5.6745298733 -3.0284938123
H 0.93251232 -5.4692449106 1.7857464302
H -1.8832684368 3.4654467978 -4.1380805947
H -0.6488132746 -4.430397983 0.1666208411
H -1.4211195926 1.0700332058 -4.012932395
H 1.6201136315 -0.0549391266 0.7903366576
H -0.7062443959 -0.9230562156 -2.7904496374
H -1.4540089013 -2.4571073045 -1.0467220089

Version=EM64L-G09RevC.01
State=1-A
HF=-883.334357
RMSD=4.664e-09
RMSF=1.150e-05
Dipole=-0.9913337 1.8440932 -1.2071959
Quadrupole=-15.3327258 17.3412111 -2.0084853 -10.2599616 13.8930061 -11.306736
PG=C01 [X(C21H13O1)]

αCOβN-αN from **σ-12aH-DB*ag*F**$^+$ E_{Tot}=-883.265012751 Hartree, ΔG_{298}=84.64 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
18-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK
FREQ=NORAMAN
1-Carboxy-2-(1-naphthyl)-naphthalene B3LYP/6-311++G** 6-31G* E=-883.057119131 opt+freqs
1 1
C -0.2876046866 -0.6421508877 1.4917230756
O -1.1196031976 -0.8048491066 2.2455954472
C -0.3817224713 2.792535896 -0.3320848921
C 0.7709585019 -0.4723210737 0.6446704569
C -1.5091435656 3.6306848599 -0.3755679506
C 1.9479329896 -1.3055303406 0.8422513777
C -0.5013774611 1.4159546979 -0.4759266385
C 0.7131237269 0.603480885 -0.2924657543
C -2.7569728516 3.0902288715 -0.5807805371
C 3.1001220715 -0.969780716 0.072463292
C -1.7867578161 0.8308017232 -0.7619299855
C 1.8948782631 0.8864734394 -0.9968233295
C -2.9281219128 1.6989086514 -0.7912318054
C 3.0362943316 0.129492139 -0.820035231
C -4.2092224632 1.1544492103 -1.0693051274
C 2.0052957826 -2.3912768351 1.7322363032
C -1.9807092128 -0.5370490142 -1.0964032712
C 4.2790183103 -1.7415031878 0.2190258497
C -4.3647320829 -0.1812492811 -1.3456528357
C 3.1727383497 -3.1216400713 1.85671183
C -3.2352939904 -1.027841731 -1.3767313693
C 4.3150604818 -2.7990553949 1.0986503562
H -5.0648107273 1.820363608 -1.0773850088
H 1.1395085283 -2.6717360536 2.3228344231
H -5.3462591968 -0.5844642047 -1.5633537576
H 3.2061998377 -3.9573971594 2.5454387828
H -3.3562829955 -2.071968448 -1.6407288635
H 5.2177825908 -3.3865514102 1.2105578967
H -1.1301114883 -1.2039117291 -1.1716569968
H 5.1503574613 -1.4838913234 -0.372018592
H -1.3882777467 4.6968958375 -0.2293340848
H 3.9217326566 0.369980491 -1.3995145698
H -3.6318107321 3.7306471069 -0.6019566307
H 1.8856596496 1.6935782457 -1.7181433235
H 0.5905519761 3.2255768504 -0.1262657349

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2650128
RMSD=8.044e-09
RMSF=6.184e-06
Dipole=1.4673094 -0.4784434 0.336842
PG=C01 [X(C21H13O1)]

αCOβN-αN from **σ-12aH-DB*ag*F**$^{+}$ E_{Tot}=-883.26721940 Hartree, ΔG_{298}=79.05 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
16-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
1-Carboxy-2-(1-naphthyl)-naphthalene B3LYP/6-311++G** 6-31G* E=-883.059779247 opt+freqs
1 1
C 0.1223898948 0.2419710138 2.1344980647
O -0.5087520557 0.4339208685 3.0597521671
C -0.7993344399 2.2133174273 0.1598120409
C 0.9274048352 -0.0999356376 1.081530287
C -1.8745760611 3.0979664434 -0.0349092094
C 2.1859402306 -0.77878207 1.3494252012
C -0.7919457817 0.9430882079 -0.4134735894
C 0.4114455668 0.1185415376 -0.2280788078
C -2.9446025413 2.7104225211 -0.8055853958
C 2.8796262053 -1.2885363236 0.2131604058
C -1.9118542326 0.5055657031 -1.2032568182
C 1.1360918305 -0.4341739095 -1.2978895619
C -2.9960280078 1.422475093 -1.3991437082
C 2.3240419339 -1.1016416187 -1.0797048931
C -4.1171382587 1.0184325681 -2.1674982595
C 2.7299560088 -0.9595742744 2.6316510907
C -2.0282850689 -0.797565002 -1.7494060269
C 4.1090141478 -1.9651349547 0.4029964576
C -4.1825273619 -0.2426170477 -2.7100513219
C 3.9302302854 -1.6291353311 2.7841533309
C -3.1325172588 -1.1583154315 -2.4895782742
C 4.6245066252 -2.1341678456 1.6682038491
H -4.9298488192 1.7213730089 -2.3118102433
H 2.2230877479 -0.5721793837 3.5091089766
H -5.044045434 -0.5417215887 -3.294711262
H 4.3430148063 -1.7626478289 3.7769470526
H -3.2005820038 -2.1594136804 -2.8988942226
H 5.5646496768 -2.652565789 1.8098943772
H -1.2516243772 -1.5307876432 -1.5727249169
H 4.636704377 -2.3463353995 -0.4637046402
H -1.8384530148 4.0886085983 0.4009253105
H 2.8756502816 -1.4845809016 -1.9320852756
H -3.7707624371 3.3926600706 -0.9731255018
H 0.7762903417 -0.2809633366 -2.3067728623
H 0.0749039915 2.5639805119 0.6978067008

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2672194
RMSD=4.042e-09
RMSF=8.949e-06
Dipole=1.3672476 -0.1927826 0.1931449
PG=C01 [X(C21H13O1)]

βCOαN-βN from **σ-13aH-DB*ag*F**$^{+}$ E_{Tot}=-883.266400625 Hartree, ΔG_{298}=81.40 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
21-Mar-2013
#P B3LYP/6-311++G** FOPT=(LOOSE READFC MAXCYCLE=128) GUESS=READ
2-Carboxy-1-(2-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.058449740 Loose
1 1
C 1.5975718102 -1.8359469559 1.7043485317
O 1.2644029658 -2.6910315297 2.370854359
C -1.2506155182 0.2898721511 0.2517017249
C 2.095098409 -0.784710335 0.978412949
C -2.5773149234 -0.1893347087 0.166052039
C 3.4643832464 -0.4027777663 1.2223026776
C -0.1698469725 -0.5314279881 -0.0354443881
C 1.2126712207 -0.0507467565 0.1378503376
C -2.8039149041 -1.5415841494 -0.2523316731
C 3.9222806697 0.7353932967 0.6428160055
C -0.4032916263 -1.8784693417 -0.446098961
C 1.7339204568 1.1143900838 -0.4851732969
C -1.6842867081 -2.3578052524 -0.5584285678
C 3.0891978871 1.5213435032 -0.2125042849
C -3.692303341 0.6326138127 0.4829700903
C 3.5887095874 2.6880459422 -0.8239040972
C -4.1356800355 -2.0158577688 -0.3505923913
C 0.9683306163 1.8728933862 -1.416508708
C -4.9697978765 0.140392687 0.3790451759
C 2.8039217026 3.4194694972 -1.6913625588
C -5.1928738412 -1.1929423416 -0.0418350969
C 1.4920535452 3.0014394914 -1.9994884867
H -3.5212149035 1.6536539731 0.8059540647
H 4.6048719044 2.9992442797 -0.6118356761
H -5.8163627921 0.7722138014 0.6200149838
H 3.2039831847 4.312590284 -2.1569582602
H -6.2079741399 -1.5643690325 -0.1178375364
H 0.9016694778 3.5668674612 -2.7100519959
H -4.3093714847 -3.0369733288 -0.6709106962
H -0.0271646852 1.5424158581 -1.6778292328
H -1.8520619144 -3.3726548766 -0.901609667
H 4.0895408693 -1.0066327085 1.8670883369
H 0.4330814908 -2.5064332304 -0.734398816
H 4.9421220854 1.0566802899 0.8182610671
H -1.0856232475 1.3061465437 0.5923164323

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2664007
RMSD=4.608e-09
RMSF=9.458e-06
Dipole=1.6642472 0.3398572 0.2199081
PG=C01 [X(C21H13O1)]

βCOαN-βN from **σ-13aH-DB*ag*F**$^+$ E_{Tot}=-883.267388159 Hartree, ΔG_{298}=78.81 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
20-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-1-(2-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* -883.059563690 opt+freqs
1 1
C 0.3887756736 1.2397178791 2.3334411656
O -0.2996588563 1.338572101 3.230311797
C -1.3764258265 0.5469775532 0.1368483219
C 1.3453374715 1.1529985497 1.3503197017
C -2.6879660523 0.0195224204 0.0646354959
C 2.6058086708 1.8157386583 1.5689259324
C -0.2618630148 -0.2832155609 0.1221288095
C 1.0830908507 0.3108427592 0.2391413115
C -2.857258254 -1.4005460993 -0.0036542416
C 3.6054758321 1.5851809675 0.6796091461
C -0.4390351792 -1.6949083963 0.0327304544
C 2.1414712224 0.0991980758 -0.6822464081
C -1.7011074552 -2.2277518438 -0.0141850809
C 3.4148981736 0.7320348937 -0.4517171209
C -3.8347148991 0.8556548621 0.0548654768
C 4.4597266387 0.5184672459 -1.3729687006
C -4.1677128194 -1.9324576288 -0.0643622689
C 1.9666450424 -0.6793131837 -1.8611892123
C -5.0934377857 0.3071146632 -0.0054977784
C 4.263483222 -0.268046081 -2.4889447964
C -5.2605323083 -1.095924793 -0.0638810874
C 3.0072464046 -0.860565361 -2.7396969667
H -3.7061092792 1.9317379243 0.097177353
H 5.4203618489 0.9884807445 -1.1978134711
H -5.9658878771 0.9495050839 -0.0105811852
H 5.0760036528 -0.4213368068 -3.1894884265
H -6.2599990159 -1.5117675239 -0.1117784053
H 2.8628287219 -1.4528814437 -3.6349484423
H -4.2992473319 -3.0075156548 -0.1138174536
H 1.0005211639 -1.1184108354 -2.0689247377
H -1.8294449331 -3.3039589576 -0.0517571435
H 2.7425095631 2.4568184496 2.4299863437
H 0.4264883321 -2.3459269279 0.0480222586
H 4.5709742842 2.0564755741 0.8205476311
H -1.2531619275 1.6258860837 0.1350683814

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2673882
RMSD=9.419e-09
RMSF=2.020e-06
Dipole=1.5271547 0.5690042 0.1974576
PG=C01 [X(C21H13O1)]

DB*ag*F E_{Tot}=-882.930299606 Hartree, ΔG_{298}=23.42 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
06-Dec-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ SCF=INTREP GEOM=CHECK FREQ=NORAMAN
Dibenzo[a g]fluorenone Cs B3LYP/6-311++G** from 6-31G* E=-882.719525713 opt+freqs
0 1
C 1.8626860785 -0.1743012118 0.1451163316
O 3.0783766693 -0.1705208137 0.1419689209
C 0.9840532396 -1.1041725133 0.9192905944
C 0.9291488929 0.7224974601 -0.6015229609
C 1.3900144008 -2.1336232753 1.7763707983
C 1.234038389 1.7836820121 -1.4850234698
C -0.3480101562 -0.8008074465 0.6667207747
C -0.3806629993 0.3513792674 -0.2925445541
C 0.4197353573 -2.883666365 2.4008271667
C 0.1294645318 2.4889767646 -2.0722241332
C -1.3722671033 -1.5587220424 1.2977306494
C -1.4529834976 1.0530924702 -0.87676336
C -0.9577584509 -2.6216761903 2.1827044543
C -1.189590034 2.0950760292 -1.7442778777
C -1.9496201571 -3.4032139319 2.8333820308
C 2.5582591788 2.1825267414 -1.8170859002
C -2.7688370587 -1.3483136819 1.1225529263
C 0.3907795505 3.5620311138 -2.9656069683
C -3.2866663481 -3.1659818125 2.6358719014
C 2.7688118721 3.2261008006 -2.6859246057
C -3.6973104102 -2.1262439434 1.7702270568
C 1.6804802406 3.9232335273 -3.2663298874
H -1.6262993501 -4.1990873922 3.4959949627
H 3.3881283647 1.6493538475 -1.3731871248
H -4.0300635538 -3.7723817113 3.1407366002
H 3.7822495815 3.522695851 -2.9328579761
H -4.7546831245 -1.9420429531 1.6168685591
H 1.8717680266 4.7433504943 -3.9491270092
H -3.1152488465 -0.5630691268 0.4687892027
H -0.4473127379 4.0916913895 -3.406581276
H 2.4465191907 -2.3196068874 1.9312134367
H -2.0164643208 2.6353379797 -2.1940787227
H 0.6933737117 -3.6902638658 3.0723685127
H -2.4815733941 0.8009462488 -0.666836336

Version=AM64L-G03RevC.02
State=1-A'
HF=-882.9302996
RMSD=2.930e-09
RMSF=6.127e-05
Dipole=0. 0.0639442 -1.3559193
PG=CS [SG(C21H12O1)]

DB*ag*FH$^+$ E_{Tot}=-883.282439697 Hartree, ΔG_{298}=47.70 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
23-Feb-2013
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ GEOM=CHECK FREQ=NORAMAN
Dibenzo[a g]fluorenone O-protonate C1 B3LYP/6-311++G** from 6-31G* E=-883.075729630 opt+freqs
1 1
C 0.1243504521 -0.131482798 1.7562145157
O 0.1484064784 -0.1326317671 3.0602798195
C 0.1208174098 -1.372577054 1.0281012994
C 0.0534954989 0.9815065454 0.8557690306
C 0.1993274814 -2.6842430785 1.5258139227
C 0.0397071931 2.3863423509 1.0970420544
C 0.0084889291 -1.0683275184 -0.3350125174
C -0.079828943 0.4276603621 -0.4428874753
C 0.1738364838 -3.7148583951 0.6146572165
C -0.2122950949 3.2293550867 -0.043520119
C -0.0011754618 -2.1039154286 -1.2858281646
C -0.3064655594 1.2672283868 -1.5258751345
C 0.0789807568 -3.4638565005 -0.7771709792
C -0.381706946 2.6428973596 -1.311840132
C 0.0616038322 -4.5414136584 -1.6985652591
C 0.2737678674 3.0170084766 2.341873297
C -0.0744079897 -1.9179744126 -2.6990734503
C -0.2714741715 4.6405665968 0.1212656532
C -0.0209578366 -4.3144844374 -3.0490828617
C 0.2122224861 4.389204172 2.465074711
C -0.0839205597 -2.9894218406 -3.5513243295
C -0.0749023605 5.2110497961 1.3528230737
H 0.1177478543 -5.553753206 -1.3154602085
H 0.5630607891 2.4543924865 3.223197868
H -0.0327356112 -5.1483812135 -3.7407764094
H 0.4014285897 4.845724276 3.4295583345
H -0.1364174787 -2.8276286203 -4.6212839532
H -0.1201727284 6.2858059978 1.4760767446
H -0.1089881663 -0.9216612546 -3.1117911618
H -0.4682367481 5.2583751813 -0.7475044466
H 0.2769815928 -2.8707524947 2.589526419
H -0.5737606669 3.2947784575 -2.1573856751
H 0.2302054654 -4.742701808 0.952868648
H -0.4474718702 0.8884430423 -2.5264134206
H 0.074326347 0.7568292262 3.4364225947

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2824397
RMSD=7.307e-09
RMSF=3.477e-06
Dipole=-0.0520404 0.7863189 0.3412477
PG=C01 [X(C21H13O1)]

DB*ag*FH$^+$ E_{Tot}=-883.285313844 Hartree, ΔG_{298}=39.47 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
28-Feb-2013
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ GEOM=CHECK FREQ=NORAMAN
Dibenzo[a g]fluorenone O-ptoronate Cs flipped B3LYP/6-311++G** from 6-31G* E=-883.078515069 opt+freqs
1 1
C 0. -0.2992145453 1.7324066159
O 0. -0.3007372129 3.040274539
C 0. -1.4673602447 0.8812306702
C 0. 0.8910058212 0.9523538738
C 0. -2.8277890603 1.2350038759
C 0. 2.2606657943 1.346998998
C 0. -1.0218314796 -0.4480573
C 0. 0.4817346812 -0.4059556517
C 0. -3.7592242415 0.2232699268
C 0. 3.2322330855 0.2827940078
C 0. -1.9555659243 -1.5006196016
C 0. 1.4404391055 -1.407280976
C 0. -3.362570236 -1.1372725851
C 0. 2.7929276214 -1.0516729717
C 0. -4.3373742055 -2.1663270897
C 0. 2.7223902469 2.681300056
C 0. -1.6214022599 -2.887909283
C 0. 4.6201086279 0.5989919793
C 0. -3.9681229082 -3.4879857798
C 0. 4.0766549933 2.9466441554
C 0. -2.5969422654 -3.8488915341
C 0. 5.034113124 1.9057045994
H 0. -5.3855463648 -1.8902925731
H 0. 2.0166885079 3.4991954281
H 0. -4.7244687547 -4.263741934
H 0. 4.4151385628 3.9767078105
H 0. -2.3220083544 -4.8967795984
H 0. 6.0896345231 2.1472390099
H 0. -0.5871644227 -3.1942061297
H 0. 5.3407437982 -0.2107323159
H 0. -3.1533142411 2.2707476334
H 0. 3.5388664889 -1.8394574712
H 0. -4.8169973783 0.4564200936
H 0. 1.1823922511 -2.4549372066
H 0. -1.1973212951 3.4092850264

Version=AM64L-G03RevC.02
State=1-A'
HF=-883.2853138
RMSD=4.980e-09
RMSF=8.147e-05
Dipole=0. -0.282742 0.4462303
PG=CS [SG(C21H13O1)]

σ-12aH-DB*ag*F^{+} E_{Tot}=-883.261954659 Hartree, ΔG_{298}=99.35 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
03-Mar-2013
0

#P B3LYP/6-311++G** GUESS=READ FOPT=READFC DENSITY=CURRENT FREQ=NORAMAN GEOM=CHECK

Benzo[a g]fluorenone Σ complex at C12a/g C1 B3LYP/6-311++G** from 6-31G* E=-883.058797294 opt+freqs

1 1
C 0.520716164 -0.2994223971 1.7752547305
O 0.5216494269 -0.3007714599 2.9734517173
C 0.5214569429 -1.5935417973 0.8792121177
C 0.5674039157 0.8257273473 0.8125279831
C -0.0668946109 -2.8450416631 1.3964642855
C 0.8458485014 2.1833694255 1.0807876398
C 0.0268943121 -1.0722947447 -0.4225031734
C 0.3482464342 0.3385773863 -0.4932688562
C -0.8237719921 -3.6063387574 0.5861805934
C 0.9139821024 3.0688536855 -0.0519899941
C -0.7537978836 -1.8927786992 -1.2616695837
C 0.4428800812 1.22426334 -1.5968362819
C -1.1474944658 -3.1914761716 -0.7604224939
C 0.7264445381 2.5466006397 -1.3631588167
C -1.920258107 -4.0253447855 -1.5810389508
C 1.0457218887 2.7041420572 2.3871455865
C -1.22783466 -1.4852050536 -2.5428647299
C 1.1722875146 4.4396896649 0.1670379534
C -2.3160360332 -3.6134974853 -2.8422998836
C 1.294174705 4.0457565566 2.557974976
C -1.9778677128 -2.3326903793 -3.3217309992
C 1.3571791874 4.9170171558 1.4464590206
H -2.2178511175 -4.9993736213 -1.211135472
H 0.9994868984 2.0364056189 3.2365818483
H -2.9107845423 -4.2758954327 -3.4607772622
H 1.4453532258 4.4425719393 3.5546610552
H -2.3182446925 -2.0153908009 -4.2994825606
H 1.5560493136 5.9702423198 1.6057406226
H -0.9963963621 -0.4990571006 -2.9133262368
H 1.222765022 5.111618595 -0.6819953145
H 0.1873255522 -3.1505382616 2.4044730634
H 0.8203500131 3.2269698839 -2.2023826239
H -1.2186290537 -4.5554647782 0.9298386668
H 0.3558380138 0.8728964737 -2.6142659257
H 1.6058573803 -1.7770051047 0.7568896607

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2619547
RMSD=9.061e-09
RMSF=1.946e-06
Dipole=-0.310885 -0.678247 -1.5548332
PG=C01 [X(C21H13O1)]

σ-13aH-DB*ag*F^{+} E_{Tot}=-883.271047513 Hartree, ΔG_{298}=76.93 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
04-Mar-2013
0

#P B3LYP/6-311++G** GUESS=READ FOPT=READFC DENSITY=CURRENT FREQ=NORAMAN GEOM=CHECK

Benzo[a g]fluorenone Σ complex at C13a/a C1 B3LYP/6-311++G** from 6-31G* E=-883.068240286 opt+freqs

1 1
C 0.4588765064 0.2236505207 1.820890935
O 0.4473756109 0.223123481 3.0199285533
C 0.4614843427 -1.0423997818 0.8956210581
C 0.5184143829 1.3795123364 0.8952199586
C -0.2268670443 -2.297429037 1.3299577525
C 0.6937964225 2.7206643163 1.2418768264
C 0.0615576924 -0.4594622446 -0.4240308689
C 0.3671086021 0.9486404899 -0.436666845
C -0.9886851785 -3.0091605661 0.3597530786
C 0.7133114837 3.6511741305 0.2220291095
C -0.6574764031 -1.2245431529 -1.3349055466
C 0.4421616234 1.8936192143 -1.5101626876
C -1.1464700191 -2.4666364346 -0.9426002305
C 0.6018246059 3.2760796252 -1.1443238098
C -0.0866633851 -2.8244197133 2.6081736508
C 0.6703483676 4.2574423882 -2.1645522447
C -1.5991537826 -4.2377093938 0.7085587715
C 0.4224499858 1.5569555124 -2.8818686136
C -0.7117583819 -4.0295336598 2.9341096889
C 0.6134818376 3.8972727701 -3.4905071187
C -1.4618680724 -4.7405172712 1.987236265
C 0.5026581994 2.5378924552 -3.8483104311
H 0.4887702574 -2.2925519816 3.3544433659
H 0.7809266231 5.2981898002 -1.8825206462
H -0.6135089879 -4.4205693476 3.9402430909
H 0.669974132 4.653557975 -4.2639286008
H -1.9318915741 -5.6769671681 2.2604954483
H 0.4883477924 2.2608713162 -4.8957832338
H -2.1782362209 -4.7725936093 -0.0357703058
H 0.3744575436 0.5208816107 -3.1876109979
H -1.7416916932 -3.0316537113 -1.653901231
H 0.7818128722 3.0106919749 2.2814635975
H -0.9440425382 -0.8293352391 -2.2991606924
H 0.8170120442 4.7049820556 0.4567743319
H 1.5378741491 -1.2770465476 0.812835257

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2710475
RMSD=7.534e-09
RMSF=2.012e-06
Dipole=-0.2899857 -0.7775531 -1.1267572
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-11aH-DB*bh*F**$^{+}$ E_{Tot}=-883.265933617 Hartree, ΔG_{298}=81.37 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
04-Oct-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ FREQ=NORAMAN GEOM=CHECK
2-Carboxy-3-(2-naphthyl)naphthalene B3LYP/6-311++G** from 6-31G* E=-883.058046591 opt+freqs
1 1
C 0.2151628547 2.6485354164 0.3896939278
O -0.4537387787 3.5629350101 0.4068129197
C -1.5888081505 0.4988272156 1.3118205298
C 1.107742918 1.6069797966 0.3284642935
C -2.9333601292 0.2338341882 1.3901808565
C 2.4762157919 1.9579899988 0.3004287685
C -0.7987263991 -0.0653644553 0.2670678683
C 0.6394864111 0.243260153 0.1812467198
C -3.5721408468 -0.6019863262 0.4383885019
C 3.4347850954 0.9675490421 0.1040940183
C -1.3987627052 -0.8980483851 -0.6622007602
C 1.6114053552 -0.7060724958 -0.0317511399
C -2.7833029252 -1.1828504584 -0.6076584614
C 2.9956905472 -0.3945106389 -0.0801253397
C -3.415810816 -2.0212862303 -1.5638122901
C 3.9759367558 -1.3924848097 -0.2828761956
C -4.9591456835 -0.8894856808 0.4943473732
C 4.828576804 1.2738969971 0.0734654984
C -4.7624570027 -2.2779316683 -1.4816762414
C 5.3124267361 -1.0623236072 -0.3071215589
C -5.5397940228 -1.7082728423 -0.4445864692
C 5.7447924846 0.2773335054 -0.1284607787
H -2.8208207197 -2.4581211342 -2.3583916676
H 3.6636504055 -2.4211591204 -0.4192062535
H -5.2380499848 -2.9205839997 -2.2130667463
H 6.0524311547 -1.838314386 -0.4651113272
H -6.6010193658 -1.9217962093 -0.3954604142
H 6.8034303851 0.5043356833 -0.1522623978
H -5.5559212162 -0.4538463929 1.2879135936
H 5.1461645319 2.3009889182 0.2121974337
H -3.5196906058 0.6466230719 2.2036350623
H 2.7777366024 2.9928181324 0.4170679946
H -0.8137522793 -1.3164673496 -1.4743826504
H 1.3122565446 -1.743309081 -0.1285947771
H -1.1159836605 1.0798194965 2.097584067

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2659336
RMSD=3.449e-09
RMSF=2.076e-05
Dipole=2.2741787 0.944546 0.0635239
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-11aH-DB*bh*F**$^{+}$ PCM E_{Tot}=-883.331668258 Hartree, ΔG_{298}=75.10 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
14-Mar-2013
0

#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=(Loose MaxStep=128)

2-Carboxy-3-(2-naphthyl)naphthalene - in Water B3LYP/6-311++G** E=-883.265933617 Loose

1 1
C 0.2399614645 2.6901260407 0.3699783503
O -0.4419457749 3.5919498632 0.3943168911
C -1.5943905532 0.489621694 1.3313991775
C 1.118630857 1.635243006 0.3097753434
C -2.9344666886 0.2033138845 1.4154811094
C 2.4851777262 1.9729686297 0.2705927427
C -0.8044530172 -0.0373931312 0.2692575722
C 0.6387381563 0.2745486324 0.1862017043
C -3.56764724 -0.6223719408 0.4503551193
C 3.4351324 0.9662532374 0.0915046372
C -1.3982559689 -0.8528735821 -0.6765798235
C 1.596185536 -0.689258696 -0.0052129484
C -2.7789049842 -1.1629899769 -0.6153025926
C 2.9854764276 -0.3915053907 -0.0617421026
C -3.4064093312 -1.9904245327 -1.5860039838
C 3.9536001836 -1.4033832611 -0.2489169875
C -4.9512619316 -0.9348050593 0.509581984
C 4.8285624807 1.2619093831 0.049186468
C -4.7487846736 -2.2729263282 -1.5005538187
C 5.2938269978 -1.0854511493 -0.2857932386
C -5.5278864106 -1.7408372464 -0.4436264411
C 5.7370660657 0.2523312335 -0.1360843282
H -2.8087267134 -2.3970520976 -2.3945838166
H 3.629452118 -2.4306637662 -0.363935553
H -5.2185959909 -2.9064806458 -2.2440043249
H 6.0260351937 -1.8709028558 -0.4315582212
H -6.5853658221 -1.9728405071 -0.3907353097
H 6.7971358683 0.4707987622 -0.1687957918
H -5.5470075362 -0.5265755586 1.3187242085
H 5.1519155179 2.2894363234 0.165321236
H -3.5209794911 0.596567651 2.2384150903
H 2.7957187188 3.0061416456 0.3645315847
H -0.8112878398 -1.2466680113 -1.4989044653
H 1.2882082432 -1.724777001 -0.0868691757
H -1.1278479013 1.0804821058 2.1122436617

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3316678
RMSD=7.864e-09
RMSF=3.617e-05
Dipole=3.1269872 1.7625573 0.2183752
Quadrupole=25.0863814 -3.7172677 -21.3691136 7.7530684 -1.6116262 8.02635
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-13aH-DB*ah*F**$^+$ E_{Tot}=-883.266743242 Hartree, ΔG_{298}=79.57 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
01-Oct-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ FREQ=NORAMAN GEOM=CHECK
2-Carboxy-3-(2-naphthyl)naphthalene B3LYP/6-311++G** from 6-31G* E=-883.058908746 opt+freqs
1 1
C 0.4188049137 1.5290777 1.6999640614
O 0.4007432881 1.5666923105 2.8331634424
C 0.3843462869 -1.3180109891 1.0725080718
C 0.4384451399 1.6319101723 0.3286511012
C 0.0436367466 -2.5371918378 1.707816236
C 0.8796705307 2.8583693643 -0.2138573792
C -0.4647452929 -0.7197255994 0.1519939696
C -0.0905355257 0.5570436442 -0.4812611523
C -1.204784345 -3.1573919356 1.3822893886
C 0.7808557936 3.0724873354 -1.5867432791
C -1.69368716 -1.3554534365 -0.1809898986
C -0.2097719334 0.8124253742 -1.8269327454
C -2.0482541016 -2.5339445336 0.4236294723
C 0.2083786009 2.0363009578 -2.4125698158
C 0.9047972837 -3.1664478073 2.6438382612
C 0.0993918712 2.2707897688 -3.8024572402
C -1.5519660229 -4.3752496884 2.0166079395
C 1.2136502348 4.2949287686 -2.1830213501
C 0.5376331163 -4.3481338419 3.2421216808
C 0.5271399725 3.4617371096 -4.3446134744
C -0.7001184018 -4.9557017822 2.927671924
C 1.0879712714 4.4816937882 -3.5330930307
H 1.8559852244 -2.7033489788 2.8835322539
H -0.3255774352 1.5018403402 -4.4368043223
H 1.1982992117 -4.8218092613 3.9584937281
H 0.4353076084 3.6276152409 -5.4117308482
H -0.9736512505 -5.8879645813 3.4074678599
H 1.415434647 5.4075595745 -3.9895990293
H -2.4976510281 -4.8458041798 1.7718624423
H 1.6401955863 5.0671469411 -1.5531008693
H -2.9958060476 -3.0013989478 0.1792102457
H 1.2732960698 3.634366362 0.4327304531
H -2.3653904793 -0.883950639 -0.8885492693
H -0.6002574064 0.0358510823 -2.4745498688
H 1.3687151212 -0.9007166272 1.2664132406

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2667432
RMSD=5.085e-09
RMSF=4.373e-05
Dipole=0.4966331 2.1149806 -0.8278482
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-13aH-DB*ah*F**$^{+}$ PCM E_{Tot}=-883.332306413 Hartree, ΔG_{298}=73.24 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
24-Mar-2013
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=(ReadFC MaxStep=64) Guess=Read Freq=NoRaman
2-Carboxy-3-(2-naphthyl)naphthalene - PCM B3LYP/6-311++G** E=-883.266743242 opt from Loose E=-883.332306443
1 1
C 0.4541286435 1.5890181153 1.7164145215
O 0.4495013874 1.6075784333 2.8475481992
C 0.3930903069 -1.3185977745 1.0911637186
C 0.4508506651 1.6650894408 0.3431379076
C 0.0419506873 -2.5460130395 1.7084052846
C 0.8750044005 2.8866897727 -0.2130369892
C -0.448386956 -0.7057414943 0.1789575047
C -0.0717459102 0.5762350173 -0.4525752346
C -1.2051038571 -3.1595009497 1.3703388972
C 0.7724256114 3.0818025749 -1.5913344802
C -1.6814296273 -1.3313165779 -0.1625791401
C -0.1878204217 0.8088092118 -1.8000519567
C -2.0448383468 -2.5185128425 0.4194850695
C 0.2176785748 2.0306604727 -2.402548105
C 0.8957065878 -3.1871934728 2.6449850815
C 0.1059741682 2.2435813918 -3.79529603
C -1.5578419492 -4.3862502324 1.989232921
C 1.1898699104 4.3014446965 -2.199029819
C 0.5244763942 -4.3760816459 3.2282083671
C 0.5184690748 3.4341389875 -4.3523732057
C -0.7127521166 -4.979959282 2.8985445525
C 1.0637728486 4.4701230056 -3.5533458838
H 1.8433103455 -2.7231140367 2.8961405978
H -0.3085800063 1.4601215805 -4.4182100324
H 1.1800053443 -4.8569743509 3.9449898923
H 0.4255701565 3.5850232283 -5.4214294294
H -0.9910864823 -5.9173199116 3.3662778312
H 1.379391223 5.3948517663 -4.0200673061
H -2.5042945903 -4.8499113294 1.7332273517
H 1.6042184761 5.0848393961 -1.5757614667
H -2.9928787912 -2.9787139293 0.1633389803
H 1.2594313794 3.6744231677 0.4228483083
H -2.3449994877 -0.8476457153 -0.8691059323
H -0.5717664559 0.0227274067 -2.4393380809
H 1.3692009013 -0.8987199133 1.3129303052

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3323064
RMSD=6.646e-09
RMSF=9.924e-06
Dipole=0.7263786 3.1842035 -0.8640715
Quadrupole=-16.8791228 14.9010356 1.9780872 12.2383978 3.4354269 -16.4988946
PG=C01 [X(C21H13O1)]

DB*ai*F E_{Tot}=-882.938979575 Hartree, ΔG_{298}=1.74 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
29-Sep-2012
#P B3LYP/6-311++G** Freq=NoRaman FOpt=ReadFC Guess=Read Geom=Check
Benzo[a h]fluorenone planar Cs B3LYP/6-311++G** from 6-31G* E=-882.728283999 opt+freqs
0 1
C 0. -0.0023068108 0.0047409075
O 0. 0.0023577801 1.2215753117
C 0. -1.2081908452 -0.8846251062
C 0. 1.1697766986 -0.9243696972
C 0. -2.5310590355 -0.5528067109
C 0. 2.5567599059 -0.624932192
C 0. -0.7712367189 -2.2426222807
C 0. 0.7053756863 -2.2385259781
C 0. -3.5096456611 -1.5919954212
C 0. 3.4676225259 -1.7346904264
C 0. -1.6809219102 -3.2635366926
C 0. 1.6042849708 -3.3220776021
C 0. -3.0781716716 -2.9601805171
C 0. 2.9564634137 -3.0615918056
C 0. -4.0595229768 -3.9799183739
C 0. 3.0789947783 0.6948704614
C 0. -4.8964796333 -1.3099657298
C 0. 4.8627395851 -1.4784437297
C 0. -5.4032409001 -3.6721256064
C 0. 4.4395381062 0.9016753624
C 0. -5.8266184447 -2.3267969761
C 0. 5.3395566893 -0.1890167756
H 0. -3.7373791619 -5.0161002357
H 0. 2.386775818 1.526334263
H 0. -6.1405791901 -4.4670517317
H 0. 4.8290272562 1.9137172223
H 0. -6.8856610118 -2.0955695288
H 0. 6.4078170998 -0.0039196019
H 0. -5.2178169214 -0.2736591723
H 0. 5.5494959171 -2.3185867067
H 0. -2.8399971718 0.4875639894
H 0. 3.6645200344 -3.8841860749
H 0. -1.371892243 -4.3038154944
H 0. 1.2420676213 -4.3436951471

Version=EM64L-G09RevC.01
State=1-A'
HF=-882.9389796
RMSD=9.918e-09
RMSF=6.056e-05
Dipole=0. -0.0079649 -1.3175546
Quadrupole=-11.6026532 13.5957137 -1.9930604 0. 0. 0.8201636
PG=CS [SG(C21H12O1)]

DB*ai*F PCM E_{Tot}=-882.948972191 Hartree, ΔG_{298}=4.01 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
11-Oct-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) Freq=NoRaman FOpt=ReadFC Guess=Read
Benzo[a h]fluorenone planar Cs solvent B3LYP/6-311++G** E=-882.938979575 opt+freqs
0 1
C 0. -0.0046836638 0.0029171618
O 0. -0.0021920886 1.2257496314
C 0. -1.2097982515 -0.8825212356
C 0. 1.166778324 -0.9188738128
C 0. -2.5339915852 -0.551341284
C 0. 2.5558623014 -0.6197558467
C 0. -0.7725084684 -2.2413842825
C 0. 0.7038391109 -2.235745122
C 0. -3.511463386 -1.5926707406
C 0. 3.4650317532 -1.7317644498
C 0. -1.6794701119 -3.2642525413
C 0. 1.6010009034 -3.3201341146
C 0. -3.078171595 -2.9606978998
C 0. 2.9538100947 -3.0593892455
C 0. -4.0573536272 -3.9827901577
C 0. 3.0852385524 0.6973884908
C 0. -4.8987744304 -1.3101511605
C 0. 4.8618501087 -1.480730214
C 0. -5.4023738714 -3.6750207351
C 0. 4.4474905014 0.9010318277
C 0. -5.8275608967 -2.3296565958
C 0. 5.344452245 -0.1925238726
H 0. -3.7342858015 -5.0182358382
H 0. 2.4007961573 1.5347266395
H 0. -6.1389479159 -4.4703512622
H 0. 4.839872322 1.9117963689
H 0. -6.8867891606 -2.1001526344
H 0. 6.4129832545 -0.010918268
H 0. -5.2219148337 -0.2746656184
H 0. 5.5444245334 -2.3237122695
H 0. -2.8518236953 0.4861327774
H 0. 3.6612342527 -3.8818688527
H 0. -1.3690397548 -4.3035064611
H 0. 1.2389323019 -4.3412561791

Version=EM64L-G09RevC.01
State=1-A'
HF=-882.9489722
RMSD=7.303e-09
RMSF=5.553e-05
Dipole=0. -0.0415723 -2.0606202
Quadrupole=-14.2959463 17.9592974 -3.6633511 0. 0. 0.8764139
PG=CS [SG(C21H12O1)]

DB*ah*FH$^+$ E_{Tot}=-883.297729154 Hartree, ΔG_{298}=8.81 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
29-Sep-2012
#P B3LYP/6-311++G** Freq=NoRaman FOpt=ReadFC Guess=Read Geom=Check
Benzo[a h]fluorenone Protonate-to-a planar Cs B3LYP/6-311++G** from 6-31G* E=-883.091008282 opt+freqs
1 1
C -0.0443331607 0.2364652411 1.3899145752
O -0.1302509433 0.2546407235 2.6981396704
C -0.0193803973 -1.0165673785 0.6780632374
C 0.007074248 1.3252542283 0.46949685
C -0.0343471216 -2.3090530535 1.1395467553
C 0.0244433048 2.746824997 0.6666396423
C 0.0134453019 -0.7069629678 -0.7213605212
C 0.0106657554 0.7569671832 -0.8350186803
C -0.0070965075 -3.3764463551 0.196066405
C -0.0278241372 3.5563754345 -0.5188499084
C 0.0342069397 -1.7059363386 -1.6458270124
C -0.012173616 1.5681307047 -1.9686096148
C 0.0281862342 -3.0759728974 -1.2070805031
C -0.0452071767 2.9406245113 -1.7977848088
C 0.0530927165 -4.1390636145 -2.1256084807
C 0.1053057594 3.4064103211 1.9114109262
C -0.015747033 -4.7247594191 0.6142100688
C -0.0409702485 4.9685876988 -0.4040018318
C 0.0443637572 -5.4545567381 -1.6859381515
C 0.0933243143 4.7863929315 1.9906155933
C 0.009759095 -5.7494521766 -0.3140127275
C 0.0093243114 5.5763292747 0.8292218449
H 0.0793086283 -3.9227952071 -3.1877264149
H 0.2197285805 2.8611183151 2.8420521516
H 0.0642671905 -6.2622153245 -2.408000668
H 0.1594426157 5.2650910091 2.9604709373
H 0.0030145603 -6.7810633189 0.0159726443
H -0.0011282893 6.6560654748 0.9105007114
H -0.0425483479 -4.948548484 1.6748431336
H -0.08537601 5.5651734896 -1.3080996547
H -0.0643219338 -2.5278166047 2.2013922745
H -0.0792009524 3.5838820454 -2.6707038019
H 0.0541670861 -1.5004262167 -2.7104821895
H -0.016523778 1.1393356958 -2.9628791242
H -0.2141088166 1.1504916846 3.052880298

Version=EM64L-G09RevC.01
State=1-A
HF=-883.2977292
RMSD=2.744e-09
RMSF=7.876e-07
Dipole=-0.0475064 0.4712209 0.1213154
Quadrupole=-33.8151559 36.8517911 -3.0366353 -0.2123921 -0.2298526 7.8014008
PG=C01 [X(C21H13O1)]

DB*ah*FH$^+$ PCM E_{Tot}=-883.359430227 Hartree, ΔG_{298}=12.82 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
28-Feb-2013
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=ReadFC Guess=Read Freq=NoRaman
Benzo[a h]fluorenone Protonate-to-a planar Cs in Water B3LYP/6-311++G** E=-883.297729154 opt+freqs
1 1
C -0.0523634035 0.2365800721 1.4001727205
O -0.1365487401 0.2422901666 2.702006325
C -0.027907933 -1.0186527021 0.6825209753
C -0.0005694036 1.32595346 0.4770062052
C -0.037215887 -2.3085972248 1.1435720868
C 0.0210566417 2.7481500536 0.6684547571
C 0.0025782547 -0.7071957128 -0.7148735734
C 0.0006786455 0.7572936146 -0.82564958
C -0.0074095244 -3.3746926212 0.1953080902
C -0.023376543 3.5531330996 -0.5204032414
C 0.0251400486 -1.7012293132 -1.6441599211
C -0.019731174 1.5624134314 -1.9636290994
C 0.02378986 -3.0713704967 -1.2063351527
C -0.0443182378 2.9349420116 -1.7984460113
C 0.0514123925 -4.1338313493 -2.1288726102
C 0.098207023 3.4107701892 1.9124049611
C -0.0084921631 -4.7241203537 0.6110560092
C -0.0279701587 4.9662647483 -0.41205353
C 0.0498045512 -5.4492090665 -1.6924077437
C 0.094912335 4.7907088808 1.9850395163
C 0.0199723141 -5.7467285922 -0.3192625284
C 0.0226035516 5.5777065535 0.8196724884
H 0.0743554134 -3.9119403923 -3.1897647279
H 0.1927286854 2.8680715025 2.8443072398
H 0.0718614126 -6.2554619453 -2.4160524873
H 0.1565304694 5.2709294693 2.9542335132
H 0.0193339868 -6.7790416581 0.0090458496
H 0.0188435545 6.6578861146 0.8971326108
H -0.0315783813 -4.9477089595 1.6715333762
H -0.06681436 5.5573302839 -1.319808982
H -0.0635116005 -2.5311147656 2.2041423733
H -0.0742714776 3.5753577125 -2.6729875719
H 0.0440805985 -1.4921185888 -2.7075250143
H -0.0272922397 1.1282765753 -2.9550235592
H -0.2059365818 1.1314806715 3.0790998621

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3594302
RMSD=4.973e-09
RMSF=4.711e-06
Dipole=-0.0620496 0.8901303 0.3999842
Quadrupole=-31.4547002 29.7620973 1.6926029 -0.2515385 -0.2550037 6.6886253
PG=C01 [X(C21H13O1)]

DB*ah*FH^{+} Cs E_{Tot}=-883.299781656 ΔG_{298}=3.99 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
09-Oct-2012
#P B3LYP/6-311++G** Freq=NoRaman FOpt=ReadFC Guess=Read
Benzo[a h]fluorenone Protonate-to-h planar Cs B3LYP/6-311++G** from 6-31G* E=-883.093001837 opt+freqs
1 1
C 0. -0.0006770773 -0.0003207134
O 0. 0.0019666741 1.3142256164
C 0. -1.1668809962 -0.8613540759
C 0. 1.1831158462 -0.7783699396
C 0. -2.5086805301 -0.5755941539
C 0. 2.5653204478 -0.3958957744
C 0. -0.6831159501 -2.2136026344
C 0. 0.7849333434 -2.1446970924
C 0. -3.4495503526 -1.6467939051
C 0. 3.5220041271 -1.4674614903
C 0. -1.5567620883 -3.2565344702
C 0. 1.7337176237 -3.1621737265
C 0. -2.9713855539 -2.9992072422
C 0. 3.0768480366 -2.812777505
C 0. -3.9078491111 -4.0473243687
C 0. 3.0353610456 0.9314744549
C 0. -4.8404674755 -1.4046773844
C 0. 4.9070853635 -1.1649805181
C 0. -5.2681874071 -3.7805142355
C 0. 4.3949214944 1.1890120284
C 0. -5.7368916208 -2.4567421531
C 0. 5.3369901114 0.1419890727
H 0. -3.5560697144 -5.0728472096
H 0. 2.3343361569 1.7539323512
H 0. -5.9766447032 -4.6003101922
H 0. 4.7408176672 2.2161336236
H 0. -6.8023265188 -2.2619141069
H 0. 6.3958310287 0.369515023
H 0. -5.2003804041 -0.3816451289
H 0. 5.6220468632 -1.9799014904
H 0. -2.8873148658 0.4431210525
H 0. 3.8268463555 -3.5969128269
H 0. -1.2150597654 -4.2857463179
H 0. 1.4400602481 -4.2043271196
H 0. -0.8917001143 1.6864835189

Version=EM64L-G09RevC.01
State=1-A'
HF=-883.2997817
RMSD=5.091e-09
RMSF=1.955e-05
Dipole=0. -0.4627349 0.2499296
Quadrupole=-33.5628361 33.2869994 0.2758367 0. 0. 6.188034
PG=CS [SG(C21H13O1)]

DB*ah*FH$^+$ Cs PCM E_{Tot}=-883.363153604 ΔG_{298}=3.78 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
06-Dec-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) Freq=NoRaman FOpt
Benzo[a h]fluorenone Protonate-to-h planar Cs in Water B3LYP/6-311++G** E=-883.299781656 opt+freqs
1 1
C 0. -0.0046701917 0.0092946579
O 0. 0.0123677188 1.314096059
C 0. -1.1708183849 -0.8547693099
C 0. 1.1811170931 -0.7781496148
C 0. -2.5116772332 -0.5699436376
C 0. 2.5618430636 -0.3987531742
C 0. -0.6850373542 -2.2063638849
C 0. 0.7829414566 -2.1388297758
C 0. -3.4474652315 -1.647779075
C 0. 3.5167872878 -1.4704331778
C 0. -1.5521550275 -3.2542078954
C 0. 1.7295873132 -3.1624154162
C 0. -2.9673019274 -2.9984695756
C 0. 3.0708116665 -2.8183636652
C 0. -3.9022451889 -4.0498947437
C 0. 3.0337826669 0.9310693344
C 0. -4.8390376313 -1.4074462661
C 0. 4.9019020214 -1.1684382471
C 0. -5.2627241102 -3.7855279169
C 0. 4.392039853 1.188291319
C 0. -5.7338277362 -2.4615161684
C 0. 5.3332050692 0.1386323219
H 0. -3.5464913742 -5.073818702
H 0. 2.3315308321 1.7523652362
H 0. -5.9696196178 -4.6067973617
H 0. 4.738518123 2.2152308561
H 0. -6.7996287444 -2.2679810706
H 0. 6.3926118428 0.3644846031
H 0. -5.1979647775 -0.3844202391
H 0. 5.6147084552 -1.9850727994
H 0. -2.8920281252 0.4458982912
H 0. 3.8200073152 -3.6026198405
H 0. -1.2052181856 -4.2811872819
H 0. 1.4299715596 -4.2024522619
H 0. -0.8735643119 1.709549389

Version=EM64L-G09RevC.01
State=1-A'
HF=-883.3631536
RMSD=4.105e-09
RMSF=2.959e-05
Dipole=0. -0.7393153 0.5457572
Quadrupole=-30.8594689 26.6028054 4.2566635 0. 0. 1.4182982
PG=CS [SG(C21H13O1)]

σ-12aH-DB*ah*F^{+} E_{Tot}=-883.260876287 Hartree ΔG_{298}=100.84 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
29-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Geom=Check Freq=NoRaman
Benzo[a h]fluorenone Σ complex at C12a C1 B3LYP/6-311++G** E=-883.057316640 opt+freqs
1 1
C -0.0018364773 -0.0019094096 0.0015307778
O 0.0029223099 -0.0010536837 1.1983042071
C 0.0008389863 -1.3376685742 -0.8922447818
C -0.0740576028 1.0917368406 -0.9824255064
C 0.64417999 -2.5584990026 -0.4273393297
C -0.3231455467 2.4672647368 -0.7328090795
C 0.3990138935 -0.8295300132 -2.2270477208
C 0.1134199963 0.5946666757 -2.2801740101
C 1.4034789531 -3.3259998239 -1.2827396168
C -0.3647190117 3.3320768325 -1.8814227891
C 1.1175847669 -1.611590064 -3.083968703
C 0.0771141052 1.4548432103 -3.3962004106
C 1.6044530544 -2.8828445731 -2.657289671
C -0.1640973771 2.7920765557 -3.1829304711
C 2.359458799 -3.7078139196 -3.5125160954
C -0.514716659 3.0180426224 0.5581461483
C 1.9771571336 -4.5689509424 -0.8495718127
C -0.5952305742 4.715066522 -1.6885697633
C 2.8857593296 -4.9002399952 -3.0559633016
C -0.7372387118 4.368857141 0.7028088608
C 2.7000131721 -5.3368495726 -1.7177888036
C -0.7779383441 5.2222398056 -0.4225937403
H 2.525968972 -3.3985944998 -4.5375786554
H -0.4841041179 2.3691462846 1.4229920137
H 3.4582486354 -5.521377021 -3.7357643628
H -0.8844690511 4.7853431277 1.6922437321
H 3.1314716792 -6.2764323445 -1.3964878123
H -0.9557185321 6.2819510787 -0.2836723287
H 1.8189326157 -4.8842584189 0.1754098329
H -0.6253479764 5.3694418669 -2.5523604779
H 0.449777089 -2.8921198215 0.5880186528
H -0.2055206477 3.469846735 -4.0286792167
H 1.4203166962 -1.2436823867 -4.0579370708
H 0.2142801321 1.0723940527 -4.4000504636
H -1.0851017575 -1.5552659126 -0.8870527168

Version=EM64L-G09RevC.01
State=1-A
HF=-883.2608763
RMSD=9.964e-09
RMSF=2.049e-06
Dipole=0.6291819 -2.0061046 -1.2242909
Quadrupole=-21.8016242 35.8316254 -14.0300012 -21.3868965 -6.2160414 4.2247667
PG=C01 [X(C21H13O1)]

σ-12aH-DB*ah*F^{+} PCM E_{Tot}=-883.326511993 Hartree ΔG_{298}=94.47 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
11-Oct-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=ReadFC Guess=Read Freq=NoRaman
Benzo[a h]fluorenone Σ complex at C12a C1 solvent B3LYP/6-311++G** E=-883.260876287 opt+freqs
1 1
C 0.0114097769 -0.0036841386 0.0049264279
O 0.0011736076 0.0163949455 1.209765909
C 0.0546108234 -1.317977618 -0.8699764621
C -0.0637366353 1.0965444479 -0.9738816474
C 0.7042276401 -2.5384202396 -0.4062204909
C -0.3264025396 2.4730805925 -0.7311698439
C 0.435759493 -0.8203077295 -2.2149645545
C 0.1440964186 0.6050042234 -2.2675192431
C 1.4237984752 -3.3226955473 -1.2803817256
C -0.3567870622 3.3370895729 -1.8775244476
C 1.1286838852 -1.6061947206 -3.081497729
C 0.1164707547 1.4641601987 -3.3855204277
C 1.6036828098 -2.8874572981 -2.6580585855
C -0.133445896 2.7995693249 -3.1778992932
C 2.3232518911 -3.7254161032 -3.5258368876
C -0.5483118947 3.024725935 0.5552388083
C 1.9814677937 -4.5726522794 -0.8526336005
C -0.6051938221 4.7192652347 -1.6893439543
C 2.8384053241 -4.9274672603 -3.0744921961
C -0.7877506763 4.3737197424 0.6980678418
C 2.6734953483 -5.3567217871 -1.7338477778
C -0.8160545617 5.2273310324 -0.4276958281
H 2.4737644544 -3.4220240127 -4.5545051962
H -0.5282772061 2.3751478401 1.4194936297
H 3.3857609984 -5.5595651387 -3.7640966955
H -0.9580819561 4.7874158685 1.685193238
H 3.0939672241 -6.3028276325 -1.4186161509
H -1.0067470784 6.2854849662 -0.2930938072
H 1.8352966893 -4.8800401241 0.1757603953
H -0.6272576846 5.3704855303 -2.5558648387
H 0.5345492761 -2.8652321695 0.6145991084
H -0.1647538894 3.4773737083 -4.0237642237
H 1.4175460337 -1.2478048886 -4.0624548381
H 0.2756928505 1.0800582916 -4.3850360307
H -1.0231627435 -1.5860486585 -0.8908733688

Version=EM64L-G09RevC.01
State=1-A
HF=-883.326512
RMSD=5.809e-09
RMSF=3.294e-06
Dipole=0.8922394 -3.278978 -1.8666939
Quadrupole=-20.6061526 34.0637871 -13.4576344 -20.0017931 -5.7061357 2.1653975
PG=C01 [X(C21H13O1)]

σ-13aH-DB*ah*F^{+} E_{Tot}=-883.274231746 Hartree, ΔG_{298}=67.54 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
29-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Geom=Check Freq=NoRaman
Benzo[a h]fluorenone Σ complex at C12a C1 B3LYP/6-311++G** E=-883.071264441 opt+freqs
1 1
C -0.0188533331 0.006336194 0.0053333641
O -0.0399091458 0.0024757388 1.2049962636
C -0.008588311 -1.2688377306 -0.9171373211
C 0.0551814126 1.1518817429 -0.9300077125
C -0.6601561887 -2.551750787 -0.5103856183
C 0.2569549361 2.4754956698 -0.6474196313
C -0.3667831785 -0.7245110452 -2.2598931453
C -0.1306568421 0.6911142343 -2.2738307656
C -1.3003233714 -3.3175533992 -1.5284963573
C 0.2886886223 3.4147074607 -1.7157929298
C -0.9542425832 -1.5355560838 -3.2206704097
C -0.1151874325 1.5882786748 -3.3311191133
C -1.3856694104 -2.8046094109 -2.8521548289
C 0.1019700486 2.9595770584 -3.0736991581
C -0.589800062 -3.0562519021 0.7829461627
C 0.1353838321 3.9109930811 -4.1282029158
C -1.8618790366 -4.5764019195 -1.2086930533
C 0.4886559126 4.7937441094 -1.4811817758
C -1.1685196883 -4.291883817 1.0771411002
C 0.3361541464 5.2439675246 -3.8609406676
C -1.7969351201 -5.0563148306 0.0846823601
C 0.5132736258 5.6873665297 -2.5303081947
H -0.107026108 -2.4813123441 1.5622218678
H -0.0019717071 3.5702525013 -5.1482126937
H -1.1301705994 -4.664712626 2.0941926159
H 0.3596675199 5.9627437067 -4.6710895579
H -2.2310777177 -6.0164891176 0.3340277784
H 0.6724019807 6.7415747606 -2.3368861856
H -2.346487901 -5.1541373739 -1.9876640543
H 0.6267925769 5.1403494029 -0.4635075398
H -1.8751940934 -3.4220593719 -3.5994396367
H 0.37941452 2.8109550128 0.3765814089
H -1.1657373974 -1.1623493542 -4.2153776695
H -0.2445793768 1.2556776029 -4.3552280396
H 1.0777715686 -1.4776694781 -0.9743629792

Version=EM64L-G09RevC.01
State=1-A
HF=-883.2742317
RMSD=8.804e-09
RMSF=2.443e-06
Dipole=-0.226744 -0.7246377 -1.4357904
Quadrupole=-26.3271784 37.0708441 -10.7436657 14.8295483 1.2877954 -12.4289469
PG=C01 [X(C21H13O1)]

σ-13aH-DB*ah*F^{+} PCM E_{Tot}=-883.338621919 Hartree, ΔG_{298}=64.89 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
11-Oct-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=ReadFC Guess=Read Freq=NoRaman
Benzo[a h]fluorenone Σ complex at C12a C1 solvent B3LYP/6-311++G** E=-883.274231746 opt+freqs
1 1
C -0.0387581899 0.0107394768 0.0055498232
O -0.0715814326 0.0165764796 1.2109308107
C -0.0243660832 -1.2597386461 -0.9077415825
C 0.0388572009 1.1569774391 -0.9264644662
C -0.6661016343 -2.5481698491 -0.5052854669
C 0.2438255398 2.4807126919 -0.6451005016
C -0.3799752373 -0.7211680505 -2.2525705609
C -0.1420385806 0.6956382031 -2.2693702312
C -1.3067747335 -3.3099880267 -1.5236217421
C 0.2837867649 3.4155151594 -1.7166819718
C -0.961683286 -1.5287134913 -3.216381443
C -0.1187140793 1.5847270089 -3.3294174618
C -1.3948648943 -2.7962648297 -2.8484783959
C 0.1024202903 2.9574947647 -3.072303865
C -0.5799398788 -3.0654328498 0.7826788935
C 0.1449846885 3.904993106 -4.1296256505
C -1.8613404749 -4.5723092605 -1.209754959
C 0.4901504791 4.7957927483 -1.4842647424
C -1.149749877 -4.3052816001 1.0731237172
C 0.3513372663 5.2385095035 -3.8655111911
C -1.785689433 -5.0622591354 0.0801146293
C 0.5244002129 5.6861678317 -2.5352508903
H -0.0838600957 -2.5001305799 1.5598213306
H 0.0103443551 3.5591577884 -5.1479335959
H -1.0967143718 -4.6880378801 2.0855676875
H 0.3821779324 5.9540544559 -4.6783112675
H -2.2142295055 -6.0261224978 0.3244100735
H 0.6873833329 6.7402264582 -2.3444474548
H -2.3462356628 -5.1451475763 -1.9913382582
H 0.6246417393 5.1425539152 -0.4663147828
H -1.8834519608 -3.413181108 -3.5955321533
H 0.3673116827 2.82329254 0.3759100463
H -1.1671932844 -1.1551960916 -4.2113437203
H -0.247655136 1.2484260367 -4.3514724147
H 1.0618584448 -1.4693237204 -0.9731672748

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3386219
RMSD=4.097e-09
RMSF=5.071e-06
Dipole=-0.2513772 -1.2838682 -2.1417539
Quadrupole=-23.7711801 33.6775298 -9.9063497 13.7967636 2.2055916 -9.0798163
PG=C01 [X(C21H13O1)]

DB*ai*F C_{2v} E_{Tot}=-882.934244142 Hartree, ΔG_{298}=16.14 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
27-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check
Benzo[a i]fluorenone B3LYP/6-311++G** from 6-31G* E=-882.724398063 opt+freqs
0 1
C 0. 0. 0.0048519949
O 0. 0. 1.2217765601
C 0. -1.1956298523 -0.9039221914
C 0. 1.1956298523 -0.9039221914
C 0. -2.5745508245 -0.5900996115
C 0. 2.5745508245 -0.5900996115
C 0. -0.7424423986 -2.2169624414
C 0. 0.7424423986 -2.2169624414
C 0. -3.4966525824 -1.6943434677
C 0. 3.4966525824 -1.6943434677
C 0. -1.6435477258 -3.2932119709
C 0. 1.6435477258 -3.2932119709
C 0. -2.9979667225 -3.0219708205
C 0. 2.9979667225 -3.0219708205
C 0. -3.0882415281 0.7353743341
C 0. 3.0882415281 0.7353743341
C 0. -4.8913962767 -1.4241304692
C 0. 4.8913962767 -1.4241304692
C 0. -4.4453140891 0.9523290865
C 0. 4.4453140891 0.9523290865
C 0. -5.3562117262 -0.1321957419
C 0. 5.3562117262 -0.1321957419
H 0. -2.3904495161 1.5620897026
H 0. 2.3904495161 1.5620897026
H 0. -4.8268991343 1.9674133513
H 0. 4.8268991343 1.9674133513
H 0. -6.4226807853 0.062840628
H 0. 6.4226807853 0.062840628
H 0. -5.5853318871 -2.2583988635
H 0. 5.5853318871 -2.2583988635
H 0. -3.7113884817 -3.839827054
H 0. 3.7113884817 -3.839827054
H 0. -1.2906981067 -4.3182175467
H 0. 1.2906981067 -4.3182175467

Version=EM64L-G09RevC.01
State=1-A1
HF=-882.9342441
RMSD=4.094e-09
RMSF=6.304e-05
Dipole=0. 0. -1.1491846
Quadrupole=-12.1690319 11.3191475 0.8498844 0. 0. 0.
PG=C02V [C2(C1O1) SGV(C20H12)]

DB*ai*F C_{2v} PCM E_{Tot}=-882.942991856 Hartree, ΔG_{298}=21.40 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
28-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check SCRF=(PCM Solvent=Water)
Benzo[a i]fluorenone B3LYP/6-311++G** from 6-31G* E=-882.724398063 opt+freqs
0 1
C 0. 0. 0.0063565593
O 0. 0. 1.2281339443
C 0. -1.1953392361 -0.8979164904
C 0. 1.1953392361 -0.8979164904
C 0. -2.576129023 -0.5856907904
C 0. 2.576129023 -0.5856907904
C 0. -0.7426938189 -2.2123914052
C 0. 0.7426938189 -2.2123914052
C 0. -3.4957347339 -1.6932377358
C 0. 3.4957347339 -1.6932377358
C 0. -1.640190625 -3.290894258
C 0. 1.640190625 -3.290894258
C 0. -2.9958615347 -3.0209499999
C 0. 2.9958615347 -3.0209499999
C 0. -3.0976925512 0.7371359336
C 0. 3.0976925512 0.7371359336
C 0. -4.8925883833 -1.4290615309
C 0. 4.8925883833 -1.4290615309
C 0. -4.4565860712 0.9498099276
C 0. 4.4565860712 0.9498099276
C 0. -5.3637497086 -0.1385315876
C 0. 5.3637497086 -0.1385315876
H 0. -2.4076073207 1.5699617111
H 0. 2.4076073207 1.5699617111
H 0. -4.8421124291 1.9632887551
H 0. 4.8421124291 1.9632887551
H 0. -6.430698422 0.0524672622
H 0. 6.430698422 0.0524672622
H 0. -5.5818685825 -2.2667402009
H 0. 5.5818685825 -2.2667402009
H 0. -3.7077975895 -3.8395134604
H 0. 3.7077975895 -3.8395134604
H 0. -1.2859575115 -4.3149001806
H 0. 1.2859575115 -4.3149001806

Version=EM64L-G09RevC.01
State=1-A1
HF=-882.9429919
RMSD=9.775e-09
RMSF=5.510e-05
Dipole=0. 0. -1.8667128
Quadrupole=-15.0935994 14.9583661 0.1352332 0. 0. 0.
PG=C02V [C2(C1O1) SGV(C20H12)]

αCOβN-βN from **σ-12bH-DB*ai*F**$^{+}$ E_{Tot}=-883.270720002 Hartree, ΔG_{298}=69.84 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
28-Sep-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ GEOM=CHECK FREQ=NORAMAN
1-Carboxy-2-(2-naphthyl)naphthalene B3LYP/6-311++G** from 6-31G* E=-883.063468755 opt+freqs
1 1
C 0.232082911 1.9971938593 0.8657677626
O 0.3759241463 2.3956739672 1.9208563208
C 0.2144129078 -2.0239183737 0.3061764881
C 0.1397183337 1.6021945093 -0.4364633302
C -0.0636711709 -2.9632282043 1.3206556676
C 0.3873661899 2.6127654332 -1.4602787339
C -0.3656480972 -0.7593400048 0.3099414178
C -0.0196303785 0.2102392418 -0.7272524224
C -0.9863105987 -2.611927845 2.3609798139
C 0.5440619841 2.1419213165 -2.7951319908
C -1.2939304885 -0.4255722448 1.3435386846
C 0.1679348791 -0.1751605703 -2.0684661507
C -1.5932267342 -1.3280668271 2.3300299278
C 0.4406952044 0.7496505444 -3.0523202968
C 0.5458741018 -4.2474621629 1.3398721713
C 0.4860745766 3.9889596915 -1.1988897097
C -1.2729139747 -3.5599117041 3.3717911778
C 0.7937710958 3.0721793493 -3.8321481067
C 0.2472084309 -5.1427137225 2.3368484992
C 0.7354445338 4.8737753794 -2.2327842403
C -0.6686097158 -4.7962025332 3.3591241628
C 0.8905925064 4.4174582844 -3.5548279832
H 1.2467325179 -4.5107206879 0.5554039866
H 0.3584208968 4.3739602076 -0.1927817131
H 0.7119883726 -6.1213009731 2.346155579
H 0.8064973344 5.9337719912 -2.0200501656
H -0.8923175528 -5.5148723961 4.138706887
H 1.0827244253 5.1269862822 -4.3499813068
H -1.9736628782 -3.2996215475 4.1569968158
H 0.9063807039 2.7076875339 -4.8467576834
H -2.3245035094 -1.0760528067 3.0898230357
H 0.5574074291 0.4092391896 -4.0759672327
H -1.8326080261 0.5149550027 1.3048527049
H 0.0419372203 -1.2171735621 -2.3314902186
H 0.9358309149 -2.2892504685 -0.4587381087

Version=AM64L-G03RevC.02
State=1-A
HF=-883.27072
RMSD=7.374e-09
RMSF=2.467e-06
Dipole=0.2670264 1.0706698 -1.0576346
PG=C01 [X(C21H13O1)]

αCOβN-βN from **σ-12bH-DB*ai*F**$^{+}$ PCM E_{Tot}=-883.333341676 Hartree, ΔG_{298}=70.83 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
10-Oct-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=ReadFC Guess=Read Freq=NoRaman
1-Carboxy-2-(2-naphthyl)naphthalene solvent calc B3LYP/6-311++G** E=-883.270720002 opt+freqs Loose E=-883.333340708
C 0.2610670382 1.9977713645 0.8709696088
O 0.4108143559 2.3678877765 1.9330953091
C 0.2398833615 -2.0020727216 0.3250004141
C 0.1539179502 1.6085187799 -0.4345193404
C -0.0499809468 -2.950795951 1.3313057104
C 0.3971212546 2.6129119127 -1.4591224603
C -0.3617595551 -0.751919357 0.321024196
C -0.0230799922 0.2233387133 -0.723504143
C -0.9984575023 -2.6174235648 2.351746531
C 0.5297194513 2.1398902482 -2.7960283136
C -1.3141129479 -0.4331438159 1.3346493325
C 0.1333680968 -0.1686778894 -2.0635029798
C -1.6206048929 -1.3416528728 2.3148624314
C 0.405139783 0.7514265192 -3.053611563
C 0.5746572753 -4.2281106557 1.3576787845
C 0.5127521003 3.9893653656 -1.1985978925
C -1.2935033681 -3.5758230796 3.3546381045
C 0.7778977375 3.0668484134 -3.8377266184
C 0.2676020505 -5.133303247 2.3444653987
C 0.7578717464 4.8691692455 -2.2359753415
C -0.6741271807 -4.804214251 3.3504929332
C 0.8929477529 4.4101688608 -3.5610689223
H 1.2942072941 -4.4763077198 0.5853838091
H 0.3999726043 4.3746269027 -0.1918166703
H 0.7453158658 -6.105942989 2.3577191332
H 0.8417454057 5.9283485884 -2.0248282395
H -0.9049200245 -5.5295504461 4.1221437366
H 1.0837659952 5.1178628343 -4.3581709707
H -2.0140228965 -3.3252023711 4.1252884809
H 0.8741273335 2.6980908164 -4.8520915363
H -2.3635616477 -1.0970906907 3.0655151191
H 0.5055085171 0.4086095049 -4.0773792743
H -1.850564971 0.5080250614 1.297231646
H -0.0038455861 -1.2099637685 -2.3221760109
H 0.9751870335 -2.2555503682 -0.4298986928

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3333417
RMSD=5.187e-09
RMSF=6.539e-06
Dipole=0.3631226 1.8903406 -1.5230903
Quadrupole=-22.1392988 17.2290719 4.9102269 2.0847096 -9.3910997 -16.1262431
PG=C01 [X(C21H13O1)]

αCOβN-βN from **σ-12bH-DB*ai*F**$^{+}$ E_{Tot}=-883.271503105 Hartree, ΔG_{298}=67.73 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
25-Sep-2012
#P B3LYP/6-311++G** FOPT=(LOOSE MAXSTEP=128 READFC) GUESS=READ
1-Carboxy-2-(2-naphthyl)naphthalene B3LYP/6-311++G** from 6-31G* E=-883.064158084 Loose
1 1
C -0.569654966 1.3526532631 1.1074331669
O -0.6130212594 1.4659092751 2.2388128155
C -0.5877297394 -2.3905593879 -0.4064776294
C -0.6268530481 1.3253261413 -0.2574502887
C -0.1372642603 -3.4842724099 0.282671856
C -0.9963856508 2.5511795662 -0.9536788655
C 0.0014735547 -1.1097432863 -0.1873055609
C -0.4887385319 0.0631680329 -0.9096546287
C 0.9395827487 -3.3866019642 1.2070679078
C -1.3063464078 2.4228794121 -2.3388245241
C 1.0682232162 -0.9939096777 0.700407921
C -0.8461620472 0.008750211 -2.2691359817
C 1.5618177026 -2.111961947 1.409022305
C -1.2339625295 1.1431007287 -2.9496643998
C 2.6599196696 -2.0098984694 2.3039045262
C -1.0754301087 3.8128261435 -0.3421281772
C 1.4273767407 -4.5067315198 1.9195562952
C -1.6828850663 3.5741842534 -3.071421546
C 3.108523636 -3.1177577107 2.9816446294
C -1.4504179777 4.918522816 -1.0841661739
C 2.4869401477 -4.3733961326 2.7890174244
C -1.7552940775 4.8024775521 -2.4533151504
H 3.1372460807 -1.046773511 2.4486790232
H -0.8345768452 3.9363419753 0.7083501615
H 3.9439171944 -3.0346076856 3.6665200141
H -1.5051281127 5.8880736814 -0.6035589314
H 2.854266151 -5.2377556121 3.3296573883
H -2.0443928512 5.6811793981 -3.0163870133
H 0.9589646161 -5.4729519836 1.7696368828
H -1.9125667194 3.4719258758 -4.1258692036
H -0.6098385694 -4.4486349289 0.1324466173
H -1.4753725354 1.0669109091 -4.0048357441
H 1.5985324214 -0.0517302813 0.7998819661
H -0.7617199394 -0.9341757841 -2.7936904389
H -1.4255588476 -2.4864899428 -1.0863518803

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2715031
RMSD=6.551e-09
RMSF=1.311e-04
Dipole=-0.5707217 1.1676094 -0.8467885
PG=C01 [X(C21H13O1)]

αCOβN-βN from **σ-12bH-DB*ai*F**$^{+}$ PCM E_{Tot}=-883.334357015 Hartree, ΔG_{298}=68.71 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
10-Oct-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt Freq=NoRaman
1-Carboxy-2-(2-naphthyl)naphthalene solvent calc B3LYP/6-311++G** E=-883.271506100 opt+freqs Loose E=-883.334356090
1 1
C -0.5844534921 1.3618652132 1.1151141124
O -0.6194574395 1.445911352 2.2464193068
C -0.6077032866 -2.3722473576 -0.3763328014
C -0.6375410945 1.333935077 -0.2522382237
C -0.1613695973 -3.472059367 0.3070638632
C -1.0099601559 2.5528262796 -0.951645723
C 0.0063731577 -1.1008517884 -0.1748671311
C -0.4810767018 0.0777318766 -0.9027644246
C 0.9326807529 -3.3846792154 1.2121385462
C -1.29527458 2.4233492666 -2.341902645
C 1.085685648 -0.9936931649 0.6906382509
C -0.8072890504 0.0184031825 -2.2671057414
C 1.5729243643 -2.118659025 1.398505562
C -1.1977280402 1.1481992438 -2.954783789
C 2.6815516127 -2.0251444874 2.2816206331
C -1.1093474423 3.8145421086 -0.3396826153
C 1.4169406227 -4.5092292587 1.9255505128
C -1.671957066 3.5717911131 -3.0806230407
C 3.1261735612 -3.1351461691 2.9605331141
C -1.482144337 4.9155979094 -1.0870858406
C 2.4883543168 -4.3857929255 2.7814184443
C -1.7654030758 4.7977725073 -2.462214542
H 3.1675270445 -1.0650586954 2.4159462318
H -0.8856706807 3.9386077927 0.7135167595
H 3.9694718106 -3.0568459483 3.6366151389
H -1.5522965246 5.884036604 -0.606789297
H 2.8515014415 -5.2518315892 3.322583823
H -2.053865086 5.6745298733 -3.0284938123
H 0.93251232 -5.4692449106 1.7857464302
H -1.8832684368 3.4654467978 -4.1380805947
H -0.6488132746 -4.430397983 0.1666208411
H -1.4211195926 1.0700332058 -4.012932395
H 1.6201136315 -0.0549391266 0.7903366576
H -0.7062443959 -0.9230562156 -2.7904496374
H -1.4540089013 -2.4571073045 -1.0467220089

Version=EM64L-G09RevC.01
State=1-A
HF=-883.334357
RMSD=4.664e-09
RMSF=1.150e-05
Dipole=-0.9913337 1.8440932 -1.2071959
Quadrupole=-15.3327258 17.3412111 -2.0084853 -10.2599616 13.8930061 -11.306736
PG=C01 [X(C21H13O1)]

DB*ai*FH^{+} E_{Tot}=-883.287612203 Hartree, ΔG_{298}=34.92 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
27-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check
Benzo[a i]fluorenone Protonate B3LYP/6-311++G** from 6-31G* E=-883.081179911 opt+freqs
1 1
C 0.0169167396 0.001719076 0.0013219314
O 0.0583333362 0.0069161804 1.3095658055
C 0.0005357838 -1.1514302524 -0.8716658379
C -0.0589481539 1.2184056271 -0.7541890317
C 0.0776367634 -2.550595802 -0.6137099186
C -0.0588806788 2.5847802721 -0.3506045197
C -0.1477447689 -0.6466149382 -2.1766078739
C -0.168841753 0.8399026251 -2.1052609685
C -0.074696633 -3.4184830769 -1.7575663133
C -0.1707411831 3.5596423552 -1.4100004816
C -0.2679761703 -1.4915829002 -3.2688041643
C -0.2806087798 1.7851623887 -3.1098970961
C -0.2426817314 -2.8659887427 -3.0440821719
C -0.2776961898 3.1346873292 -2.7480794816
C 0.306450461 -3.1569838961 0.6451422641
C 0.04656153 3.0432462108 0.9811310784
C -0.0366196889 -4.8289473869 -1.5777247184
C -0.1724990938 4.9454232855 -1.0842619633
C 0.3398686394 -4.5280912088 0.7799997361
C 0.040370172 4.3955404286 1.2528703081
C 0.1565247445 -5.3754337298 -0.335182433
C -0.0694539823 5.355209415 0.2198524265
H 0.5065159298 -2.5709637147 1.5362213957
H 0.1324120468 2.3339919206 1.791720629
H 0.5209699707 -4.9630419769 1.7558742554
H 0.1218716227 4.7308372004 2.2803667723
H 0.1848156718 -6.4499199802 -0.2044077961
H -0.0711225634 6.4101166579 0.4648723626
H -0.1574995688 -5.46634693 -2.4462622278
H -0.2566982334 5.6699626889 -1.8862538538
H -0.3498759838 -3.5439411954 -3.8838451955
H -0.3627328309 3.8896863306 -3.5223266514
H -0.3897849395 -1.104774298 -4.2728924964
H -0.3704080707 1.5010631122 -4.1510401783
H 0.0305217871 -0.8868997742 1.6807774808

Version=EM64L-G09RevC.01
State=1-A
HF=-883.2876122
RMSD=4.904e-09
RMSF=2.838e-06
Dipole=-0.0419386 -0.4980326 -0.0886431
Quadrupole=-31.8920311 32.3218526 -0.4298215 -1.5221554 3.2591859 -0.7739787
PG=C01 [X(C21H13O1)]

DB*ai*FH$^+$ E_{Tot}=-883.349681571 Hartree, ΔG_{298}=38.31 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
28-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check SCRF=(PCM Solvent=Water)
Benzo[a i]fluorenone Protonate B3LYP/6-311++G** from 6-31G* E=-883.081179911 opt+freqs
1 1
C 0.0253038299 0.0003304737 0.0122284989
O 0.0899340052 0.0271711118 1.3110086152
C -0.0019684451 -1.1532536912 -0.8614876367
C -0.0606904986 1.2190840304 -0.7529705903
C 0.0724777435 -2.5543914875 -0.6098518449
C -0.0589063881 2.5842410557 -0.353374479
C -0.1526501466 -0.6470972789 -2.1654133992
C -0.1740990378 0.838918158 -2.0983011261
C -0.0697469314 -3.4164766341 -1.7588923188
C -0.1728849112 3.5560344517 -1.4132214077
C -0.2710814498 -1.4865021506 -3.2625631317
C -0.2850980924 1.7815335534 -3.1097103359
C -0.2379100622 -2.8606038413 -3.0446497907
C -0.2814048078 3.1288539329 -2.7536475322
C 0.2869044339 -3.1657391785 0.6492681804
C 0.0478474315 3.0455759335 0.9807323862
C -0.0259458642 -4.8279299622 -1.5877933484
C -0.1751797204 4.9417496748 -1.0890520105
C 0.3255951544 -4.5371581321 0.7760189635
C 0.0406951144 4.3967798342 1.2513476961
C 0.1605806534 -5.3799724956 -0.3461573943
C -0.0711539811 5.3541735199 0.2151845171
H 0.4567470941 -2.5841254435 1.5467863143
H 0.1349843521 2.3358423148 1.7905872144
H 0.493287735 -4.9747842201 1.7528311867
H 0.1226146009 4.7336276532 2.2782565556
H 0.1934392761 -6.4551091628 -0.2209376999
H -0.0737875266 6.4098514673 0.4577627048
H -0.1384918712 -5.4589686295 -2.46177332
H -0.2610125492 5.663897216 -1.8928889131
H -0.3393522726 -3.5353925966 -3.8872480912
H -0.3663479366 3.8824438019 -3.5287064685
H -0.395109372 -1.0942569319 -4.2637337248
H -0.3731477715 1.4917800956 -4.1489767214
H 0.0903524128 -0.8538731415 1.7143895252

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3496816
RMSD=4.076e-09
RMSF=1.998e-06
Dipole=-0.0355848 -0.8629273 -0.0833301
Quadrupole=-29.7483778 26.0218617 3.7265161 -1.4658828 3.5048356 -2.2684793
PG=C01 [X(C21H13O1)]

σ-12bH-DB*ai*F^{+} E_{Tot}=-883.273940695 Hartree ΔG_{298}=69.26 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
27-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check
Benzo[a i]fluorenone Σ complex at C13a B3LYP/6-311++G** from 6-31G* E=-883.071468330 opt+freqs
1 1
C -0.0108788737 0.0025012822 0.0055485758
O -0.0301477926 0.003477546 1.207085329
C -0.0035223848 -1.2825544559 -0.8971705007
C 0.0510258055 1.1473605556 -0.9381222391
C -0.6901223126 -2.5428740914 -0.4702100402
C 0.2719529187 2.5130193377 -0.6572570819
C -0.3852492598 -0.7323769338 -2.2285118564
C -0.1384409485 0.6818125219 -2.2516496496
C -1.3720837606 -3.2936965137 -1.472451046
C 0.2832688136 3.4122157419 -1.7843601862
C -1.0081434281 -1.5288852566 -3.1781351165
C -0.137013822 1.5745609107 -3.349967052
C -1.4655241751 -2.7860310271 -2.797136108
C 0.0784071413 2.9064575413 -3.1024921002
C -0.6118963795 -3.0441862798 0.8230185689
C 0.4662573754 3.0303802009 0.6509414825
C -1.9662598876 -4.5334596884 -1.1365862214
C 0.4867832331 4.7902628686 -1.5527650768
C -1.2245354427 -4.2599569905 1.1344976132
C 0.6627333329 4.3791457817 0.8319622517
C -1.8945903456 -5.0089911175 0.1581688924
C 0.6728502314 5.2625948904 -0.2716315432
H -0.0958892628 -2.4829544591 1.5908505439
H 0.4590335277 2.3527740922 1.4937809973
H -1.178876094 -4.6290420217 2.1526267266
H 0.8131348564 4.7725364168 1.8301612965
H -2.3545707092 -5.9535648183 0.4203018339
H 0.8303825771 6.3216436168 -0.1048570557
H -2.4829387201 -5.0987475698 -1.9040127633
H 0.4940906439 5.472520533 -2.3950084593
H -1.9856623186 -3.3925032644 -3.5326706557
H 0.0950542172 3.6105709819 -3.9270421333
H -1.2326608756 -1.1497991832 -4.1675915031
H -0.2802904589 1.2162329738 -4.3616728032
H 1.0744137031 -1.5190014853 -0.9632329733

Version=EM64L-G09RevC.01
State=1-A
HF=-883.2739407
RMSD=2.892e-09
RMSF=2.569e-06
Dipole=-0.302392 -0.9414661 -1.3086329
Quadrupole=-24.7077723 32.7269762 -8.0192039 15.7493784 3.5169351 -1.9761109
PG=C01 [X(C21H13O1)]

σ-12bH-DB*ai*F^{+} PCM E_{Tot}=-883.337295026 Hartree ΔG_{298}=68.07 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
28-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check SCRF=(PCM Solvent=Water)
Benzo[a i]fluorenone Σ complex at C13a B3LYP/6-311++G** from 6-31G* E=-883.071468330 opt+freqs
1 1
C -0.0411055122 0.0059437719 0.0088764459
O -0.0929700959 0.015863924 1.2136531555
C -0.0172619512 -1.2777823474 -0.8870296945
C 0.0405546778 1.1478811111 -0.9338007328
C -0.6922847081 -2.5441604135 -0.4673193793
C 0.265320659 2.516586046 -0.6566302415
C -0.3900940627 -0.7347204962 -2.2213080901
C -0.1377964519 0.6829890292 -2.244746211
C -1.3803009722 -3.2886305888 -1.468765206
C 0.2863394196 3.4102686258 -1.7845389579
C -1.0137283751 -1.5224030722 -3.1718822834
C -0.1251268718 1.5690389806 -3.3463084183
C -1.4772095714 -2.7786782384 -2.7920067559
C 0.0893440909 2.9022671056 -3.1026078134
C -0.5967356821 -3.0597412561 0.819784513
C 0.4590912349 3.0396730624 0.6487190918
C -1.9716291024 -4.5308326773 -1.1377979852
C 0.495818222 4.7908578036 -1.5573153083
C -1.2043733747 -4.277682089 1.1278934599
C 0.6620279707 4.3884795259 0.8272953462
C -1.8875572065 -5.0166607128 0.1525822713
C 0.6792408256 5.2690102056 -0.2789228203
H -0.0642421142 -2.5104015632 1.5841865159
H 0.4489812937 2.3655732348 1.4939554153
H -1.1437048932 -4.6576244057 2.1409675589
H 0.8126940583 4.7833729947 1.8249644906
H -2.3449113894 -5.9633003059 0.4112559935
H 0.8411894217 6.3278843743 -0.1156442985
H -2.4930795927 -5.0891051654 -1.9062937873
H 0.5105588878 5.4667199817 -2.4045150048
H -2.00043726 -3.380574637 -3.5278086808
H 0.1111615214 3.6035922666 -3.9290265584
H -1.2357027934 -1.1418749667 -4.1605435269
H -0.2649503018 1.2050190137 -4.3558747228
H 1.0629711242 -1.505405485 -0.9490378333

Version=EM64L-G09RevC.01
State=1-A
HF=-883.337295
RMSD=6.791e-09
RMSF=2.393e-06
Dipole=-0.3769309 -1.6693411 -2.2197316
Quadrupole=-22.9295463 29.323256 -6.3937097 14.6939874 4.1463668 -1.3565268
PG=C01 [X(C21H13O1)]

βCOβN-αN from **σ-6aH-DB*bg*F**$^{+}$ E_{Tot}=-883.26236375 Hartree, ΔG_{298}=90.22 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
26-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-3-(1-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.053663998 opt+freqs
1 1
C -0.1065868331 -0.942382247 1.9799951551
O -0.7962954956 -1.3508061944 2.7781097771
C -1.4490770126 2.1639109445 0.2162130702
C 0.7939564081 -0.4550694244 1.06140457
C -2.8033253732 2.5565542921 0.2353006702
C 2.1402570701 -0.8410998863 1.2103726208
C -1.0908783535 0.8503900598 -0.0288271575
C 0.3426512777 0.4724902767 0.0447090467
C -3.7908720585 1.6276127589 0.016552669
C 3.1028357808 -0.3100302158 0.3509529603
C -2.0982749186 -0.1324882219 -0.3117095787
C 1.3128963245 0.9882937129 -0.7742340624
C -3.4721634017 0.2740901721 -0.2642655207
C 2.6872302135 0.6313215057 -0.6585835363
C -4.4858637802 -0.6839161696 -0.5271298276
C 3.6686901748 1.1679818367 -1.5189610823
C -1.8053619155 -1.474778813 -0.6819854182
C 4.4774281734 -0.6729689613 0.4588126758
C -4.1681252021 -1.9813264874 -0.8470390986
C 4.9897419962 0.7957240871 -1.3887311469
C -2.8144997984 -2.3740775888 -0.9386752705
C 5.3994990395 -0.1287283303 -0.3960306135
H -5.5223551625 -0.3685548488 -0.4821858579
H 3.3727334012 1.8756994436 -2.2843252782
H -4.9516262139 -2.7015410627 -1.0495780094
H 5.7322346482 1.2164395284 -2.0568763736
H -2.5705388844 -3.388925458 -1.230651241
H 6.4447704308 -0.4009570604 -0.3178648579
H -0.7753793962 -1.7892622255 -0.8063316121
H 4.7788228495 -1.3806729838 1.2226036154
H -3.0559022882 3.5897517114 0.4400140805
H 2.4298376158 -1.5365863381 1.9900503007
H -4.8342682854 1.921410425 0.0461977279
H 1.0206845476 1.6829610728 -1.5536040485
H -0.6795961656 2.8976675464 0.4288265887

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2623638
RMSD=8.378e-09
RMSF=1.988e-05
Dipole=2.1286194 -0.2313778 0.5600499
PG=C01 [X(C21H13O1)]

βCOβN-αN from **σ-6aH-DB*bg*F**$^{+}$ E_{Tot}=-883.262996055 Hartree, ΔG_{298}=89.13 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
23-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-3-(1-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.054895254 opt+freqs
1 1
C 0.3048987557 1.5714433679 2.1200240886
O -0.2112188923 2.0508884004 3.0072777876
C -1.5513351301 2.0032129688 -0.1929271715
C 1.0237663043 0.9567686315 1.1195571896
C -2.9111713431 2.3432970437 -0.3397274947
C 2.4191587754 0.8391135054 1.2854648028
C -1.1416084753 0.6777710591 -0.1340301508
C 0.3103447997 0.406233758 -0.0089851708
C -3.8552654641 1.3509558465 -0.4323855147
C 3.1582475681 0.1405263491 0.3319873066
C -2.1096516431 -0.3785371137 -0.2094744544
C 1.0600091126 -0.2967314587 -0.9188694672
C -3.4885454803 -0.0188954601 -0.3686643165
C 2.4676057111 -0.4487494378 -0.7899837996
C -4.4665635394 -1.0432830503 -0.4449423999
C 3.2277648419 -1.1528860679 -1.750956277
C -1.7810697362 -1.7552315853 -0.0984170154
C 4.5730355462 -0.0056201201 0.4474999269
C -4.1104551821 -2.3672791418 -0.3562451906
C 4.5922196992 -1.2735908465 -1.6092244505
C -2.7564741451 -2.7228786356 -0.1739447286
C 5.2713071159 -0.6987849851 -0.5045157068
H -5.5061455679 -0.7614789302 -0.5693639981
H 2.7243114692 -1.5969535657 -2.6016379984
H -4.8665588282 -3.1409252074 -0.4154440303
H 5.1617821575 -1.8175464925 -2.3537823171
H -2.485142797 -3.7684091585 -0.0858592299
H 6.345199297 -0.81111415 -0.4207199858
H -0.751966766 -2.0525910206 0.0592049732
H 5.0816465244 0.4390940868 1.295175918
H -3.1984398234 3.3857277527 -0.4011561585
H 2.9108449716 1.2772281754 2.146476021
H -4.9022539945 1.603530735 -0.5586998458
H 0.5694073476 -0.7212974187 -1.7871177098
H -0.8102413986 2.7965002285 -0.1927379722

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2629961
RMSD=8.463e-09
RMSF=1.646e-06
Dipole=2.0523734 0.3402101 0.4731649
PG=C01 [X(C21H13O1)]

DB*bg*F C_s E_{Tot}=-882.935267916 Hartree, ΔG_{298}=10.10 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
14-Nov-2012
0

#P B3LYP/6-311++G** FOPT=READFC GUESS=READ FREQ=NORAMAN GEOM=CHECK

Benzo[b g]fluorenone planar Cs B3LYP/6-311++G** from 6-31G* E=-882.723617553 opt+freqs

0 1
C 2.3878237467 -0.4078517981 0.168229118
O 3.602395603 -0.4437963694 0.1830553945
C 1.5134934299 0.7091157832 -0.2924933108
C 1.4472505659 -1.4762011587 0.6088976928
C 1.8836480295 1.922098661 -0.7928197543
C 1.789569675 -2.7350086657 1.1281257005
C 0.1431085209 0.3207365384 -0.1322961556
C 0.1290072476 -1.0566194639 0.4358302728
C 0.8791436558 2.8563940599 -1.1781942742
C 0.7791312016 -3.5941027763 1.4824814865
C -0.8404039019 1.20472359 -0.4969196847
C -0.9373462914 -1.9313094653 0.7966189909
C -0.4961282461 2.4878603613 -1.0261829325
C -0.5853892661 -3.2225882897 1.329240641
C -1.4920431665 3.418108679 -1.4098881281
C -1.6200466904 -4.1202785216 1.6995164044
C 1.1979374618 4.130951334 -1.7039186844
C -2.3171039443 -1.6180275983 0.6673977091
C -1.1510674487 4.6526721994 -1.9191160709
C -2.9432057877 -3.7791483989 1.5588083827
C 0.2045004457 5.0136315356 -2.0680031692
C -3.2923398616 -2.5142529835 1.0370692583
H -2.5360942912 3.1446164599 -1.2970791249
H 2.8343141411 -3.0015741004 1.2380775707
H -1.9276137792 5.3521435426 -2.2076312807
H -3.7208082532 -4.4774437408 1.8468385201
H 0.4614906263 5.9871401775 -2.4695522145
H -4.3376300303 -2.2483457388 0.9273888757
H 2.2421572826 4.4032132045 -1.8162201982
H -2.6141316701 -0.6589233835 0.2717901457
H 2.9345259958 2.1728513128 -0.8962492295
H 1.0048353451 -4.5749502358 1.8870576186
H -1.8930714131 0.9765264655 -0.4027938254
H -1.3443750326 -5.090304738 2.0996290324

Version=AM64L-G03RevC.02
State=1-A'
HF=-882.9352679
RMSD=1.441e-09
RMSF=5.978e-05
Dipole=0. -0.1256127 -1.574958
PG=CS [SG(C21H12O1)]

DB*bg*FH^{+} E_{Tot}=-883.295712558 Hartree, ΔG_{298}=13.03 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
18-Nov-2012
0

#P B3LYP/6-311++G** FOPT=(LOOSE READFC) GUESS=READ FREQ=NORAMAN GEOM=CHECK

Benzo[b g]fluorenone O-protonate planar Cs flipped B3LYP/6-311++G** from 6-31G* E=-883.088644411 opt+freqs

1 1
C 2.2603613587 -0.4227549024 0.09678278
O 3.5691365572 -0.3818844736 0.0874261677
C 1.4640767265 0.7389533895 -0.1691712218
C 1.4153400803 -1.5396886793 0.3524863933
C 1.8560482528 2.0212649964 -0.4627353685
C 1.7681741729 -2.8764402309 0.6585136697
C 0.0802655084 0.3417644766 -0.0782413545
C 0.0684035988 -1.1044934447 0.2528556038
C 0.8626759042 3.0132130456 -0.6898255555
C 0.7645972531 -3.7798654668 0.865338015
C -0.8834716055 1.2821871631 -0.2935356574
C -0.9764049863 -2.0328551297 0.4653887389
C -0.5180864552 2.6403206657 -0.6044579797
C -0.6071553068 -3.3949712267 0.7772228107
C -1.496428795 3.6229424426 -0.8294130701
C -1.6269833046 -4.3475055422 0.9952898718
C 1.2057616573 4.3479526253 -0.9953922241
C -2.3600488417 -1.7093972736 0.391338384
C -1.1327317427 4.928238884 -1.1282392166
C -2.9552318266 -3.9932035398 0.9141782571
C 0.2201258031 5.2933715994 -1.2118303449
C -3.3227606254 -2.6636952551 0.6098092074
H -2.5451251935 3.3543145623 -0.7679151362
H 2.8050645762 -3.1880778119 0.729857967
H -1.9007410275 5.6734293734 -1.2988383198
H -3.7253735723 -4.7363173948 1.084301949
H 0.4897838371 6.3159448739 -1.4459316734
H -4.3712871073 -2.3982986847 0.5490510288
H 2.2525671233 4.6237425956 -1.0585298007
H -2.6658195824 -0.7007172653 0.1604176902
H 2.9070474268 2.2827648952 -0.5226014683
H 0.996441879 -4.8115712779 1.1015300875
H -1.9395202465 1.0566269799 -0.2418973642
H -1.3480296721 -5.3684958955 1.2290288166
H 3.9727381447 -1.240300744 0.2839464508

Version=AM64L-G03RevC.02
State=1-A'
HF=-883.2957126
RMSD=6.322e-09
RMSF=2.940e-05
Dipole=0. 0.3439592 0.6159252
PG=CS [SG(C21H13O1)]

DB*bg*FH^{+} E_{Tot}=-883.294545652 Hartree, ΔG_{298}=15.87 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
16-Nov-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ FREQ=NORAMAN GEOM=CHECK
Benzo[b g]fluorenone O-protonate planar Cs B3LYP/6-311++G** from 6-31G* E=-883.087480187 opt+freqs
1 1
C 2.2622858965 -0.4324354907 0.1020240478
O 3.5671572218 -0.5365664276 0.1265915495
C 1.4676267244 0.7382921716 -0.1741844909
C 1.4158180418 -1.5390013846 0.3630949683
C 1.8486656482 2.0211145491 -0.4768394171
C 1.7789994263 -2.8708325892 0.6773124953
C 0.0824092364 0.3399633731 -0.0802071989
C 0.0697679023 -1.104976754 0.2606959964
C 0.8538674786 3.0109496912 -0.7103701749
C 0.7757396609 -3.7730070899 0.8901615706
C -0.8830625277 1.2765611967 -0.3011777325
C -0.9727733482 -2.0317078807 0.4793386906
C -0.5247029083 2.6336509032 -0.621354471
C -0.5974122933 -3.3915478575 0.8001642976
C -1.5067667711 3.6117734134 -0.8521218799
C -1.6151982589 -4.3447050505 1.0250416656
C 1.192737776 4.3448758044 -1.0250819514
C -2.3583239325 -1.7128072228 0.4041007958
C -1.1479874686 4.915620117 -1.1597370532
C -2.9444797298 -3.9948297138 0.9424959476
C 0.2041424993 5.2849338074 -1.2468688414
C -3.3174674733 -2.6682240316 0.6295112726
H -2.5542720352 3.3393812228 -0.7878566786
H 2.8220116845 -3.1532178654 0.7439353547
H -1.9184261913 5.657240728 -1.3347068193
H -3.7120987793 -4.7393267887 1.1181443548
H 0.4700496323 6.306841164 -1.4879663628
H -4.3670199426 -2.4071827206 0.5679240723
H 2.2382542409 4.6254371553 -1.091274494
H -2.6675813829 -0.7066051956 0.1667086162
H 2.8938686962 2.3110816937 -0.5452510587
H 1.0079549537 -4.8031809398 1.1332093971
H -1.9378023825 1.0459789336 -0.2467767031
H -1.33326815 -5.3633284024 1.2653643952
H 4.0177584091 0.2974526654 -0.0701776926

Version=AM64L-G03RevC.02
State=1-A'
HF=-883.2945457
RMSD=8.077e-09
RMSF=3.043e-05
Dipole=0. -0.6026222 0.6542759
PG=CS [SG(C21H13O1)]

σ-6aH-DB*bg*F^{+} E_{Tot}=-883.262059124 Hartree, ΔG_{298}=97.60 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
03-Dec-2012
#P B3LYP/6-311++G** GUESS=READ FOPT=READFC DENSITY=CURRENT GEOM=CHECK FREQ=NORAMAN
Benzo[b g]fluorenone Σ complex at C12a/b C1 B3LYP/6-311++G** from 6-311G** E=-883.254302580 opt+freqs
1 1
C 0.4537167686 -0.3875710285 2.3497071712
O 0.4461043259 -0.3961599662 3.5462405194
C 0.4544701666 -1.6684927547 1.431695276
C 0.5312347895 0.7393899214 1.3987537937
C -0.1205273637 -2.9375349183 1.9134574426
C 0.799663615 2.0511159239 1.6778950452
C 0.0195090314 -1.1512417632 0.1055219993
C 0.3280628558 0.2624938147 0.0565399643
C -0.8160330527 -3.7143645754 1.0628444136
C 0.9031742315 2.9818684139 0.6094382104
C -0.699460912 -1.9893462951 -0.7722239517
C 0.4517046387 1.1574609821 -0.9982667417
C -1.0832370335 -3.2996661994 -0.2951668575
C 0.7425941336 2.5171540002 -0.7454521924
C -1.7890382307 -4.152282874 -1.1580291546
C 0.8773984029 3.4478236967 -1.8105060101
C -1.1151321977 -1.5918483196 -2.075981511
C 1.1685730749 4.3509414384 0.837428763
C -2.1276437105 -3.748148537 -2.4370618598
C 1.1404680185 4.7716705291 -1.5519904388
C -1.7984852358 -2.4565184383 -2.8955560097
C 1.2847640965 5.2259712408 -0.2207929301
H -2.0780230416 -5.1354578863 -0.8059607623
H 0.7650821799 3.1004915167 -2.8314361185
H -2.6711611248 -4.423816038 -3.0874456367
H 1.2393695333 5.4751855382 -2.3698072433
H -2.0957187615 -2.1453061288 -3.8892423055
H 1.4943892308 6.2726704628 -0.0350174298
H -0.8924867336 -0.5978186709 -2.4312053478
H 1.2863381696 4.7028632159 1.8557977652
H 0.0917751082 -3.2398116141 2.9321359534
H 0.9296702295 2.378924437 2.7034598783
H -1.2035885072 -4.674728566 1.3827137052
H 0.3833788843 0.8389170435 -2.0297203822
H 1.547483706 -1.8360791271 1.3422772368

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2620591
RMSD=6.176e-09
RMSF=7.662e-07
Dipole=-0.2125643 -0.5630892 -1.6496034
PG=C01 [X(C21H13O1)]

σ-7aH-DB*bg*F^{+} E_{Tot}=-883.257921841 Hartree, ΔG_{298}=108.62 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
01-Mar-2013
#P B3LYP/6-311++G** GUESS=READ FOPT=READFC DENSITY=CURRENT FREQ=NORAMAN
Benzo[b g]fluorenone Σ complex at C13a/b C1 B3LYP/6-311++G** from 6-311G** E=-883.250181023 opt+freqs
1 1
C 0.680586629 0.3579807682 2.2900905002
O 0.6856514622 0.3567153211 3.4840474249
C 0.6745689383 -0.9598801753 1.371926184
C 0.7451811238 1.4647214253 1.3209476544
C 0.0263854997 -2.1746248229 1.8435193923
C 0.9660484512 2.8182059 1.6259631592
C 0.2531857703 -0.4210382572 0.0500489338
C 0.5826111621 0.9994283841 0.008469856
C -0.7950262298 -2.9079986036 1.0180007683
C 1.0145634256 3.7127790051 0.5827696397
C -0.5408931041 -1.1731492184 -0.7703308148
C 0.6794111115 1.9048531018 -1.0875586315
C -1.0533673334 -2.4310411688 -0.3335689795
C 0.8852618465 3.2930967993 -0.7713663993
C -1.8865404859 -3.2101497303 -1.1591640137
C 0.9755630277 4.2308598857 -1.8297505752
C -1.3856205597 -4.13949184 1.4608500084
C 0.6299643121 1.516864899 -2.4489434889
C -2.4283202889 -4.392979332 -0.6959760814
C 0.8937559454 3.8232876142 -3.1403296056
C -2.1820979299 -4.8644078366 0.6206510809
C 0.732881044 2.4554429334 -3.4505522862
H -2.1004463884 -2.8738481347 -2.1667771143
H 1.1217717188 5.2777250744 -1.5894779325
H -3.0607441541 -4.9792160556 -1.3532750097
H 0.967827873 4.5493007691 -3.9410458875
H -2.6275006128 -5.7953927495 0.9478976439
H 0.6992898567 2.1431347248 -4.4875677126
H -1.181847577 -4.4800153097 2.4695922666
H 0.5410907928 0.4707948709 -2.7098890779
H 0.2551356873 -2.5239077146 2.8463922129
H 1.0698436093 3.1356347085 2.6559519699
H -0.89316252 -0.7879581598 -1.7185308548
H 1.1551956843 4.7692431785 0.7821193281
H 1.7597201994 -1.1757761568 1.3580529626

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2579218
RMSD=6.783e-09
RMSF=4.501e-06
Dipole=-0.6060585 -1.797131 -0.7896779
PG=C01 [X(C21H13O1)]

GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
05-Oct-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ FREQ=NORAMAN GEOM=CHECK
2-Carboxy-3-(2-Napthyl)naphthalene B3LYP/6-311++G** from 6-31G* E=-883.058908850 opt+freqs
1 1
C -2.0449250238 1.1054521918 0.0467005623
O -3.0952680488 0.9318535461 0.437155933
C 0.9883906209 -1.0365341271 1.6392472051
C -0.8050485294 1.4598101186 -0.4310354078
C 0.8020349656 -2.2436151279 2.2623515294
C -0.7128154991 2.6884749774 -1.1203586426
C 0.1623675676 -0.659854085 0.543245391
C 0.3473165344 0.6449801637 -0.1155414989
C -0.2022689408 -3.151961688 1.8317130063
C 0.5398930992 3.1690127016 -1.4946194403
C -0.8140295225 -1.537424073 0.0928917276
C 1.5718007503 1.1636441336 -0.4648683109
C -1.0238576678 -2.7918126692 0.7161494286
C 1.7115258577 2.4014308229 -1.1459481511
C -2.0113321614 -3.7040798334 0.2618692718
C 2.9785524766 2.9063774492 -1.5178695397
C -0.4095428773 -4.4039486996 2.4606603272
C 0.6853297163 4.405219257 -2.1930968276
C -2.1872670021 -4.9112725533 0.8949807343
C 3.0824750191 4.1025400263 -2.1913755604
C -1.3820436488 -5.2627592445 2.0031674815
C 1.9313025136 4.85873681 -2.5325044431
H -2.6274827971 -3.4372809755 -0.5900842875
H 3.8679632509 2.340858502 -1.2660952933
H -2.9452670282 -5.6019932508 0.545194933
H 4.0609264906 4.4776395281 -2.4681419083
H -1.5329761571 -6.2189404648 2.4900463371
H 2.0460724311 5.7959764674 -3.0628275086
H 0.2112476399 -4.6778489511 3.3063644521
H -0.2011681362 4.9745478445 -2.4480936656
H 1.4223704039 -2.5142335134 3.1097208233
H -1.6056343837 3.2630872941 -1.3391264886
H -1.3877810931 -1.3112204668 -0.8017224522
H 2.4646985575 0.5880309481 -0.2495991626
H 1.7420257217 -0.3479506377 2.0025637001

Version=AM64L-G03RevC.02
State=1-A
HF=-883.266744
RMSD=6.669e-09
RMSF=6.748e-06
Dipole=0.1388554 2.1368911 -0.9037347
PG=C01 [X(C21H13O1)]

DB*bh*FH^{+} E_{Tot}=-883.301198321 Hartree, ΔG_{298}=0.0 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
29-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check
Benzo[b h]fluorenone planar Protonate B3LYP/6-311++G** from 6-31G* E=-883.094365111 opt+freqs
1 1
C 0. 0.000215376 -0.002305137
O 0. -0.0003850273 1.3083361996
C 0. -1.1254187232 -0.8930789043
C 0. 1.2096057321 -0.7591892315
C 0. -2.4836048685 -0.6313550015
C 0. 2.5259778902 -0.3312207646
C 0. -0.6121615493 -2.2410309496
C 0. 0.8578876117 -2.1563553214
C 0. -3.3960293784 -1.7094172244
C 0. 3.5575144924 -1.294637483
C 0. -1.4780913861 -3.2943099214
C 0. 1.8410264015 -3.1000386132
C 0. -2.8897237013 -3.0578423972
C 0. 3.2158496624 -2.6946524792
C 0. -3.8142955387 -4.1219503724
C 0. 4.260109455 -3.6397511533
C 0. -4.7989683326 -1.4919708018
C 0. 4.924509209 -0.9112657249
C 0. -5.1737218397 -3.8759624251
C 0. 5.5815509551 -3.2325155038
C 0. -5.6711058036 -2.5552858373
C 0. 5.9181379664 -1.8628785442
H 0. -3.4463505518 -5.141682755
H 0. 4.0176756121 -4.6964229776
H 0. -5.8693622288 -4.7069906936
H 0. 6.370957929 -3.9751304478
H 0. -6.7405404962 -2.3837493941
H 0. 6.9594247169 -1.564914795
H 0. -5.1741503095 -0.4744592542
H 0. 5.1734416349 0.1441214411
H 0. -2.8757414596 0.3820830466
H 0. 2.769319482 0.725709688
H 0. -1.1227431987 -4.318743877
H 0. 1.6121372259 -4.159911309
H 0. -0.8921881604 1.6851299533

Version=EM64L-G09RevC.01
State=1-A'
HF=-883.3011983
RMSD=6.711e-09
RMSF=2.894e-05
Dipole=0. -0.4605289 0.6498412
Quadrupole=-35.0102832 37.1178833 -2.1076001 0. 0. -1.4449301
PG=CS [SG(C21H13O1)]

DB*bh*FH^{+} PCM E_{Tot}=-883.364740499 Hartree, ΔG_{298}=0.0 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
28-Feb-2013
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=ReadFC Guess=Read Freq=NoRaman
Benzo[b h]fluorenone planar Protonate - Water B3LYP/6-311++G** E=-883.301198321 opt+freqs
1 1
C 0. -0.0034135762 0.0065571956
O 0. 0.001167225 1.3081780776
C 0. -1.127839487 -0.8887785532
C 0. 1.2095573122 -0.7560225704
C 0. -2.4839369814 -0.6267922461
C 0. 2.5220577102 -0.328042439
C 0. -0.6127236285 -2.2354942512
C 0. 0.8571404174 -2.1510111403
C 0. -3.3925094696 -1.7108525907
C 0. 3.5539449939 -1.2955746364
C 0. -1.4733366517 -3.2930435964
C 0. 1.8373758304 -3.0988690018
C 0. -2.8850562687 -3.0570532807
C 0. 3.211056384 -2.6936981377
C 0. -3.8084967699 -4.1242639355
C 0. 4.2557425497 -3.6425180749
C 0. -4.7951828238 -1.4944537973
C 0. 4.9208627907 -0.9140184074
C 0. -5.1680777925 -3.8802853373
C 0. 5.5766054671 -3.2378876814
C 0. -5.6666796315 -2.5596294019
C 0. 5.9137355831 -1.8673375621
H 0. -3.4366474473 -5.142364271
H 0. 4.0087646206 -4.6979841456
H 0. -5.8626418714 -4.7121879811
H 0. 6.365429019 -3.9809858707
H 0. -6.7362638478 -2.3887959815
H 0. 6.9552244998 -1.5698367872
H 0. -5.1681479122 -0.4765461927
H 0. 5.1693168669 0.1411442026
H 0. -2.8758474414 0.384630229
H 0. 2.7679976904 0.7276632685
H 0. -1.1152635516 -4.3160649577
H 0. 1.6052423689 -4.1574802509
H 0. -0.888397378 1.6960611407

Version=EM64L-G09RevC.01
State=1-A'
HF=-883.3647405
RMSD=3.842e-09
RMSF=7.405e-05
Dipole=0. -0.8250035 1.3271575
Quadrupole=-32.4323692 29.2278677 3.2045015 0. 0. -3.3969495
PG=CS [SG(C21H13O1)]

DB*bh*F E_{Tot}=-882.940297485 Hartree, ΔG_{298}=0.0 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
29-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check
Benzo[b h]fluorenone planar C2v B3LYP/6-311++G** from 6-31G* E=-882.728949090 opt+freqs
0 1
C 0. 0. 0.0019763844
O 0. 0. 1.2169769838
C 0. -1.1857035506 -0.9088927183
C 0. 1.1857035506 -0.9088927183
C 0. -2.5154062328 -0.587526671
C 0. 2.5154062328 -0.587526671
C 0. -0.7380958532 -2.2657568004
C 0. 0.7380958532 -2.2657568004
C 0. -3.4838033787 -1.6289606349
C 0. 3.4838033787 -1.6289606349
C 0. -1.6483331452 -3.2908104096
C 0. 1.6483331452 -3.2908104096
C 0. -3.0427194872 -2.996081277
C 0. 3.0427194872 -2.996081277
C 0. -4.0207567511 -4.0226666033
C 0. 4.0207567511 -4.0226666033
C 0. -4.8750224056 -1.3556591777
C 0. 4.8750224056 -1.3556591777
C 0. -5.3639283791 -3.7221012314
C 0. 5.3639283791 -3.7221012314
C 0. -5.7966896746 -2.3770196833
C 0. 5.7966896746 -2.3770196833
H 0. -3.6926287931 -5.0569179214
H 0. 3.6926287931 -5.0569179214
H 0. -6.0972469981 -4.5207576876
H 0. 6.0972469981 -4.5207576876
H 0. -6.8574025077 -2.1536390818
H 0. 6.8574025077 -2.1536390818
H 0. -5.2022469646 -0.3212374233
H 0. 5.2022469646 -0.3212374233
H 0. -2.8295043932 0.451285247
H 0. 2.8295043932 0.451285247
H 0. -1.3329687387 -4.3292172441
H 0. 1.3329687387 -4.3292172441

Version=EM64L-G09RevC.01
State=1-A1
HF=-882.9402975
RMSD=9.889e-09
RMSF=5.962e-05
Dipole=0. 0. -1.474421
Quadrupole=-10.829329 15.9526417 -5.1233127 0. 0. 0.
PG=C02V [C2(C1O1) SGV(C20H12)]

DB*bh*F E_{Tot}=-882.951317457 Hartree, ΔG_{298}=0.0 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
06-Dec-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=ReadFC Guess=Read Freq=NoRaman
Benzo[b h]fluorenone planar C2v in Water B3LYP/6-311++G** E=-882.940297485 opt+freqs
0 1
C 0. 0. -0.0040647738
O 0. 0. 1.2178051343
C 0. -1.1847907058 -0.9085671821
C 0. 1.1847907058 -0.9085671821
C 0. -2.5159939639 -0.5862575293
C 0. 2.5159939639 -0.5862575293
C 0. -0.7379410269 -2.2672382042
C 0. 0.7379410269 -2.2672382042
C 0. -3.4840200945 -1.6283806035
C 0. 3.4840200945 -1.6283806035
C 0. -1.6473545863 -3.2926554616
C 0. 1.6473545863 -3.2926554616
C 0. -3.0425315676 -2.9959052931
C 0. 3.0425315676 -2.9959052931
C 0. -4.0196700746 -4.023762205
C 0. 4.0196700746 -4.023762205
C 0. -4.8756179162 -1.3529837281
C 0. 4.8756179162 -1.3529837281
C 0. -5.363629873 -3.7215537763
C 0. 5.363629873 -3.7215537763
C 0. -5.7968847733 -2.3757760201
C 0. 5.7968847733 -2.3757760201
H 0. -3.691483546 -5.0576232302
H 0. 3.691483546 -5.0576232302
H 0. -6.0972533411 -4.5196439243
H 0. 6.0972533411 -4.5196439243
H 0. -6.8575566494 -2.1531695549
H 0. 6.8575566494 -2.1531695549
H 0. -5.2029958869 -0.3189382292
H 0. 5.2029958869 -0.3189382292
H 0. -2.8382782193 0.4498428277
H 0. 2.8382782193 0.4498428277
H 0. -1.3330740896 -4.3307407008
H 0. 1.3330740896 -4.3307407008

Version=EM64L-G09RevC.01
State=1-A1
HF=-882.9513175
RMSD=3.880e-09
RMSF=6.013e-05
Dipole=0. 0. -2.1749422
Quadrupole=-13.2966889 20.8805763 -7.5838874 0. 0. 0.
PG=C02V [C2(C1O1) SGV(C20H12)]

σ-11aH-DB*bh*F^{+} E_{Tot}=-883.260814236 Hartree, ΔG_{298}=100.05 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
30-Sep-2012
#P B3LYP/6-311++G** FOpt=ReadFC Guess=Read Freq=NoRaman Geom=Check
Benzo[b h]fluorenone Σ Complex at C12a B3LYP/6-311++G** from 6-31G* E=-883.056858403 opt+freqs
1 1
C 0.5239470607 0.0115073895 1.990493976
O 0.5092160163 0.0090966915 3.1854546886
C 0.5260754993 -1.3068796357 1.0771770192
C 0.6100655431 1.1132374997 1.0162701907
C -0.0923685805 -2.5482313198 1.5209950331
C 0.834340177 2.4429748173 1.276451139
C 0.1549730702 -0.8005319236 -0.2703362423
C 0.4341843681 0.6246691488 -0.317992517
C -0.807581457 -3.3313582241 0.6429828692
C 0.9025503392 3.3563632959 0.1935112333
C -0.5257198298 -1.6000659763 -1.1435399484
C 0.4906254255 1.4950143318 -1.3855372283
C -0.9904181756 -2.8831378342 -0.7329103017
C 0.7316159401 2.8731813675 -1.1541058867
C -1.7073684333 -3.7214573853 -1.6096923885
C 0.8035386992 3.8001882736 -2.2249914541
C -1.3609213255 -4.5909192981 1.055558518
C 1.1252396077 4.7393128424 0.4047690119
C -2.2143012081 -4.9281964112 -1.1723532326
C 1.0247515927 5.1357066295 -1.9820530939
C -2.0464992047 -5.3692989676 0.1675636345
C 1.185917523 5.6091035682 -0.6596350612
H -1.8595034919 -3.4088991989 -2.6360080872
H 0.6795098983 3.4416334437 -3.2406467304
H -2.757687432 -5.5581261389 -1.8677285771
H 1.0768360624 5.8344058124 -2.8085329397
H -2.4619101932 -6.3211760203 0.4735052204
H 1.3611568273 6.6643264723 -0.4876726867
H -1.2163939638 -4.9095136512 2.0815458352
H 1.2509297266 5.1023203249 1.4184805172
H 0.0836327036 -2.8782551258 2.5407774822
H 0.9496885209 2.7948851813 2.295700754
H -0.809793377 -1.239604856 -2.1260010703
H 0.373507378 1.1449367933 -2.4052954986
H 1.6171357888 -1.5079397509 1.0911326517

Version=EM64L-G09RevC.01
State=1-A
HF=-883.2608142
RMSD=3.364e-09
RMSF=3.007e-06
Dipole=-0.5054039 -1.8009946 -1.08404
Quadrupole=-23.1013698 40.146779 -17.0454092 20.6006369 3.5367917 -5.1682613
PG=C01 [X(C21H13O1)]

σ-11aH-DB*bh*F^{+} PCM E_{Tot}=-883.326684125 Hartree, ΔG_{298}=92.95 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
06-Dec-2012
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=ReadFC Guess=Read Freq=NoRaman
Benzo[b h]fluorenone Σ Complex at C12a in Water B3LYP/6-311++G** E=-883.260814236 opt+freqs
1 1
C 0.5274897515 0.0078633697 1.9858907081
O 0.5375450195 0.0245925005 3.1895613278
C 0.4797893549 -1.2883664339 1.0922793841
C 0.6101999397 1.1185769335 1.0184529835
C -0.1454448673 -2.528184633 1.5393856881
C 0.8576777982 2.4443759832 1.2769014063
C 0.1153656972 -0.7891709499 -0.2615609883
C 0.4055410575 0.6358434682 -0.3126403358
C -0.8272382983 -3.3249430274 0.6477476153
C 0.9173480123 3.3581921344 0.1936614814
C -0.5423394149 -1.5934057111 -1.1412760747
C 0.4531698466 1.5036009313 -1.3804738458
C -0.9930119344 -2.8847537743 -0.7310803691
C 0.7138593268 2.8793017241 -1.1493760414
C -1.6765440884 -3.7363562405 -1.6178296001
C 0.776570675 3.8077025475 -2.2211342728
C -1.3650094638 -4.5905907104 1.0574894663
C 1.1671371796 4.7389748878 0.4018028469
C -2.170514152 -4.9515299779 -1.1836603154
C 1.0230717465 5.1396810738 -1.9820951007
C -2.0211265673 -5.3843660095 0.1592628488
C 1.21952687 5.6096679321 -0.6618726435
H -1.8147103693 -3.4294802701 -2.6473177766
H 0.6251299691 3.4496608593 -3.2331511544
H -2.6895402205 -5.5928294179 -1.8865711615
H 1.0679903116 5.8383278389 -2.8092565319
H -2.425056744 -6.3421256056 0.4608105989
H 1.4141386172 6.6620334705 -0.4924729791
H -1.2314246709 -4.9009762846 2.0867892891
H 1.3182557525 5.0964987327 1.4139597568
H 0.0124968099 -2.8537301882 2.5623043089
H 1.0027530882 2.7963296047 2.292081134
H -0.8141001929 -1.242673973 -2.1298670839
H 0.3078105808 1.156826899 -2.3969767378
H 1.5621646752 -1.5452955181 1.0675689979

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3266841
RMSD=7.819e-09
RMSF=3.540e-06
Dipole=-0.705809 -3.0141706 -1.3664997
Quadrupole=-21.3374725 37.9367321 -16.5992597 19.2480897 3.5831436 -4.7175047
PG=C01 [X(C21H13O1)]

DB*cg*F E_{Tot}=-882.919609719 ΔG_{298}=55.61 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
08-Dec-2012
#P B3LYP/6-311++G** FOPT=(READFC LOOSE) GUESS=READ SCF=INTREP GEOM=CHECK FREQ=NORAMAN
Benzo[c g]fluorenone twisted C2 B3LYP/6-311++G** from 6-31G* E=-882.708148430 opt+freqs
0 1
C 0. 0. 2.7263563225
O 0. 0. 3.939878308
C -0.1219007229 1.1793590557 1.8190649792
C 0.1219007229 -1.1793590557 1.8190649792
C -0.2806676837 2.5207958927 2.1858262031
C 0.2806676837 -2.5207958927 2.1858262031
C -0.160240819 0.7351558963 0.4984011461
C 0.160240819 -0.7351558963 0.4984011461
C -0.5078869698 3.4476565139 1.1941686724
C 0.5078869698 -3.4476565139 1.1941686724
C -0.5725403641 1.6449980547 -0.5172305145
C 0.5725403641 -1.6449980547 -0.5172305145
C -0.6916226536 3.03671713 -0.1513179939
C 0.6916226536 -3.03671713 -0.1513179939
C -0.97551256 1.2701818235 -1.8302808437
C 0.97551256 -1.2701818235 -1.8302808437
C -1.0607881185 3.980578736 -1.1472181893
C 1.0607881185 -3.980578736 -1.1472181893
C -1.3694478421 2.2085598064 -2.7528901669
C 1.3694478421 -2.2085598064 -2.7528901669
C -1.3807108598 3.5831644193 -2.4211196032
C 1.3807108598 -3.5831644193 -2.4211196032
H -1.0162918308 0.2233146671 -2.0925366498
H 1.0162918308 -0.2233146671 -2.0925366498
H -1.6878961777 1.891771062 -3.7396890325
H 1.6878961777 -1.891771062 -3.7396890325
H -1.6746139507 4.3155229242 -3.1644879579
H 1.6746139507 -4.3155229242 -3.1644879579
H -1.1152686093 5.028033722 -0.8699242802
H 1.1152686093 -5.028033722 -0.8699242802
H -0.6033614873 4.5012820441 1.4330803601
H 0.6033614873 -4.5012820441 1.4330803601
H -0.2183053167 2.8026343453 3.230553226
H 0.2183053167 -2.8026343453 3.230553226

Version=AM64L-G03RevC.02
State=1-A
HF=-882.9196097
RMSD=2.678e-09
RMSF=6.124e-05
Dipole=0. 0. -1.5983672
PG=C02 [C2(C1O1) X(C20H12)]

DB*cg*F E_{Tot}=-882.90890351 Hartree ΔG_{298}=81.86 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H12O1
SERGEY
14-Mar-2013
#P B3LYP/6-311++G** FOPT FREQ=NORAMAN
Benzo[c g]fluorenone planar C2v B3LYP/6-311++G** from 6-31G* E=-882.697247480 opt+freqs
0 1
C 0. 0. 2.6531759538
O 0. 0. 3.8686635423
C 0. -1.1744916416 1.757692408
C 0. 1.1744916416 1.757692408
C 0. -2.4909498741 2.2259660459
C 0. 2.4909498741 2.2259660459
C 0. -0.7778983759 0.4163125724
C 0. 0.7778983759 0.4163125724
C 0. -3.5075541498 1.3103094896
C 0. 3.5075541498 1.3103094896
C 0. -1.8414675744 -0.559869223
C 0. 1.8414675744 -0.559869223
C 0. -3.2109191851 -0.0727589081
C 0. 3.2109191851 -0.0727589081
C 0. -1.7081970695 -1.9758547776
C 0. 1.7081970695 -1.9758547776
C 0. -4.2969619341 -0.9899119371
C 0. 4.2969619341 -0.9899119371
C 0. -2.7787928605 -2.8363920771
C 0. 2.7787928605 -2.8363920771
C 0. -4.0993868338 -2.3448052984
C 0. 4.0993868338 -2.3448052984
H 0. -0.7362463596 -2.4197024223
H 0. 0.7362463596 -2.4197024223
H 0. -2.5992350656 -3.905560823
H 0. 2.5992350656 -3.905560823
H 0. -4.940445719 -3.0283003761
H 0. 4.940445719 -3.0283003761
H 0. -5.3022170773 -0.582515465
H 0. 5.3022170773 -0.582515465
H 0. -4.54587943 1.6224465383
H 0. 4.54587943 1.6224465383
H 0. -2.6661699767 3.2953207491
H 0. 2.6661699767 3.2953207491

Version=AM64L-G03RevC.02
State=1-A1
HF=-882.9089035
RMSD=8.356e-09
RMSF=6.419e-05
Dipole=0. 0. -1.5260165
PG=C02V [C2(C1O1) SGV(C20H12)]

βCOαN-αN from **σ-6aH-DB*cg*F**$^+$ E_{Tot}=-883.262837344 Hartree, ΔG_{298}=87.13 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
30-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-1-(1-naphthyl)-naphthalene B3LYP/6-311G** from 6-31G* E=-883.054005639 opt+freqs
1 1
C 0.615952935 -1.275067068 2.1958673624
O 0.0348445225 -1.8474110443 2.9807249704
C -1.3379952766 1.4692615484 1.0509968322
C 1.3917872275 -0.5979565349 1.2854549981
C -2.7372712464 1.5647138645 1.1924353388
C 2.820881488 -0.7606832354 1.326315313
C -0.7600452594 0.3650208932 0.4485954821
C 0.7254551245 0.2727150096 0.3885522044
C -3.5457163732 0.5591998407 0.7195034953
C 3.5673939421 -0.0228916545 0.4622077109
C -1.5775946361 -0.6900574761 -0.0778329767
C 1.5246064691 1.0217482223 -0.5029815539
C -2.9987515272 -0.5794185852 0.0753051128
C 2.9595289672 0.8794155741 -0.4630686548
C -3.8299263496 -1.6107317004 -0.4360727611
C 3.7416900874 1.6375172466 -1.3570792234
C -1.055759928 -1.8178989274 -0.7683973781
C 0.9423612518 1.9042342465 -1.4582651
C -3.2918792651 -2.696163588 -1.0818534468
C 3.1442709161 2.4925856297 -2.259954526
C -1.8926719672 -2.7943262109 -1.2551775119
C 1.738290103 2.6231806868 -2.3147389192
H -4.9034472193 -1.5220583735 -0.3121181526
H 4.8205424222 1.5389221119 -1.3291407306
H -3.9366698476 -3.475550045 -1.4696358557
H 3.7593312951 3.0685682693 -2.9415886539
H -1.4779324164 -3.6438165375 -1.7851428623
H 1.2904925634 3.2917419444 -3.0397146594
H 0.0118967897 -1.9043555574 -0.935884697
H -0.1347599672 1.9968891538 -1.5007376774
H -3.1652553271 2.4316949518 1.680565436
H 3.2730051758 -1.4442897808 2.0329752624
H -4.6223429651 0.6276877519 0.8296336634
H 4.647000213 -0.1158791566 0.4689988222
H -0.7082569922 2.2633469313 1.4371195529

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2628373
RMSD=4.252e-09
RMSF=4.588e-06
Dipole=1.6565808 0.2554998 0.2804417
PG=C01 [X(C21H13O1)]

βCOαN-αN from **σ-6aH-DB*cg*F**$^{+}$ E_{Tot}=-883.263872357 Hartree, ΔG_{298}=87.78 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
27-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-1-(1-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.055409716 opt+freqs
1 1
C 0.4567446939 1.4253573183 2.476432186
O -0.1546057615 1.6965010381 3.3914689928
C -1.382932822 1.8916889824 0.1194523975
C 1.3014351778 1.0724400013 1.4484568094
C -2.7821560113 2.0204049224 0.0103926917
C 2.7239776626 1.133952049 1.6587572649
C -0.7795656577 0.6416635998 0.1627346022
C 0.7018705114 0.5927516306 0.2597455871
C -3.5693661321 0.896385461 -0.0425068717
C 3.5291166347 0.6844122715 0.6604802875
C -1.5791912756 -0.5497507105 0.127505245
C 1.5634977596 0.1413583408 -0.768600082
C -3.0006959351 -0.4026113952 0.0212087036
C 2.9893550836 0.1827826047 -0.5640693687
C -3.8156295684 -1.5638180096 -0.0019612229
C 3.8380244184 -0.2577602721 -1.6001946661
C -1.0400537273 -1.8580787272 0.2359342114
C 1.0581225582 -0.3102947724 -2.020524924
C -3.2598644726 -2.8168890932 0.0876600384
C 3.3129959587 -0.7073492534 -2.7934856683
C -1.8607270738 -2.9620895234 0.213887069
C 1.9164155296 -0.7268059722 -3.0074888507
H -4.8900314948 -1.4438332832 -0.0846509063
H 4.9109462037 -0.2323737968 -1.4498362783
H -3.8919484946 -3.6965626845 0.0706903853
H 3.9777266226 -1.04073549 -3.5818818402
H -1.4313806769 -3.9535597889 0.2981056846
H 1.5250441718 -1.0676121382 -3.9581850632
H 0.0294943481 -1.9946345127 0.3416152671
H -0.0108134986 -0.3178838017 -2.1868430318
H -3.2246603185 3.0074363019 -0.0428929754
H 3.1236719705 1.5177894542 2.588233404
H -4.6463112945 0.9885885568 -0.1301565314
H 4.6053221015 0.7088927887 0.7849091098
H -0.7684534251 2.7859833739 0.1162481975

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2638724
RMSD=6.641e-09
RMSF=4.398e-05
Dipole=1.4681003 0.4798404 0.2255304
PG=C01 [X(C21H13O1)]

DB*cg*FH$^+$ E_{Tot}=-883.273732868 Hartree, ΔG_{298}=73.35 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
21-Feb-2013
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ GEOM=CHECK FREQ=NORAMAN
Benzo[c g]fluorenone O-protonate twisted C1 B3LYP/6-311++G** from 6-31G* E=-883.066623256 opt+freqs
1 1
C -0.0167638445 -0.1385873535 2.594882576
O -0.0171697561 -0.1390502393 3.8979490233
C -0.0272023303 -1.2738550647 1.7146389726
C -0.0002668162 1.078516427 1.8415169569
C -0.0040924245 -2.6478649952 2.01921977
C -0.0310978786 2.40656231 2.3039866972
C 0.0769547023 -0.7735039214 0.3999318171
C -0.0846700078 0.726177093 0.4797051408
C 0.1554726624 -3.5376392042 0.9847940879
C -0.1778536539 3.4051510712 1.3709605875
C 0.4242483218 -1.6576856449 -0.6375541474
C -0.4163889846 1.719039137 -0.4588663175
C 0.4019096181 -3.0793821634 -0.3349976978
C -0.4017307054 3.0983275578 0.0046552136
C 0.8713341706 -1.2541300703 -1.9332157836
C -0.8426826817 1.4662153287 -1.7995716653
C 0.6824350582 -4.0019854881 -1.372102843
C -0.6664802984 4.1326924576 -0.9269709079
C 1.1760089848 -2.1824234525 -2.8929556273
C -1.1325646404 2.4974718402 -2.651996793
C 1.0479570625 -3.567994912 -2.6230852507
C -1.0103698399 3.8442153401 -2.2244152275
H 1.0176010155 -0.2047643419 -2.1414161909
H -0.9859462697 0.4477083859 -2.1285295339
H 1.533050666 -1.8590803413 -3.863366823
H -1.4742115039 2.2869020851 -3.6583433282
H 1.2743989877 -4.2870535891 -3.4014415231
H -1.2249361672 4.6469322715 -2.9199356397
H 0.6324417803 -5.0624416629 -1.1537917979
H -0.621577717 5.161312684 -0.5883842389
H 0.142762413 -4.6044190959 1.1723696757
H -0.1727049378 4.4447109768 1.6759582176
H -0.1229182368 -3.0099567208 3.0352643734
H 0.0663232678 2.6265514853 3.3597207857
H -0.0718640938 -1.0298979753 4.2769464839

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2737329
RMSD=7.657e-09
RMSF=1.355e-06
Dipole=-0.0257294 -0.5643133 0.7583041
PG=C01 [X(C21H13O1)]

σ-6aH-DB*cg*F^{+} E_{Tot}=-883.255426806 ΔG_{298}=117.90 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
06-Mar-2013
#P B3LYP/6-311++G** GUESS=READ FOPT=READFC DENSITY=CURRENT FREQ=NORAMAN GEOM=CHECK
Benzo[c g]fluorenone Σ complex at C13a/c C1 B3LYP/6-311++G** from 6-31G* E=-883.051814073 opt+freqs
1 1
C 0.6431657369 -0.0729519572 2.6015250662
O 0.6399388215 -0.0797920805 3.7952352759
C 0.6473189696 -1.3645736025 1.6748168151
C 0.7106203843 1.0579674724 1.6508279322
C 0.0701691313 -2.621891418 2.1813716389
C 0.9609421413 2.3984020895 1.9603756637
C 0.1120129452 -0.7943327994 0.4090704326
C 0.5420347993 0.5926625712 0.3310017651
C -0.7894975956 -3.3188776076 1.4164738196
C 1.0702524063 3.2900097868 0.9148504414
C -0.84895333 -1.50836882 -0.3361275828
C 0.7854447086 1.4818435915 -0.7644279998
C -1.2582788613 -2.8085115301 0.1495635734
C 1.0229335081 2.8638994103 -0.4403730633
C -2.2030353319 -3.5381845481 -0.5874369296
C 1.2695479171 3.7859837408 -1.4883735115
C -1.5140819103 -0.9714023954 -1.4781973008
C 0.9227075917 1.0750241341 -2.1130527624
C -2.7770282939 -3.0082787677 -1.7296692119
C 1.3470340529 3.3628101431 -2.7941823465
C -2.4504140599 -1.7069285284 -2.1621868054
C 1.1983277338 1.9941371433 -3.1021904001
H -2.5013253092 -4.518696606 -0.2356731895
H 1.4251611681 4.8294289918 -1.2395658982
H -3.5080570398 -3.5880147491 -2.2815455337
H 1.5494185563 4.0732878994 -3.5864539643
H -2.9454196249 -1.2867654737 -3.0288821697
H 1.3123719414 1.6613364114 -4.1271102129
H -1.2866443174 0.0323326116 -1.8036712341
H 0.846613512 0.0267098922 -2.370478033
H 0.4032234633 -2.9836275429 3.1469671679
H 1.0410996161 2.7145986779 2.9928936709
H -1.1806074157 -4.2722053995 1.7526029721
H 1.2258357623 4.3439930701 1.117131464
H 1.7314832547 -1.5246697922 1.5399473489

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2554268
RMSD=3.018e-09
RMSF=1.333e-06
Dipole=-0.3585311 -0.565672 -1.3127778
PG=C01 [X(C21H13O1)]

βCOαN-αN from **σ-6aH-DB*cg*F**$^{+}$ E_{Tot}=-883.262837344 Hartree, ΔG_{298}=87.13 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
30-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-1-(1-naphthyl)-naphthalene B3LYP/6-311G** from 6-31G* E=-883.054005639 opt+freqs
1 1
C 0.615952935 -1.275067068 2.1958673624
O 0.0348445225 -1.8474110443 2.9807249704
C -1.3379952766 1.4692615484 1.0509968322
C 1.3917872275 -0.5979565349 1.2854549981
C -2.7372712464 1.5647138645 1.1924353388
C 2.820881488 -0.7606832354 1.326315313
C -0.7600452594 0.3650208932 0.4485954821
C 0.7254551245 0.2727150096 0.3885522044
C -3.5457163732 0.5591998407 0.7195034953
C 3.5673939421 -0.0228916545 0.4622077109
C -1.5775946361 -0.6900574761 -0.0778329767
C 1.5246064691 1.0217482223 -0.5029815539
C -2.9987515272 -0.5794185852 0.0753051128
C 2.9595289672 0.8794155741 -0.4630686548
C -3.8299263496 -1.6107317004 -0.4360727611
C 3.7416900874 1.6375172466 -1.3570792234
C -1.055759928 -1.8178989274 -0.7683973781
C 0.9423612518 1.9042342465 -1.4582651
C -3.2918792651 -2.696163588 -1.0818534468
C 3.1442709161 2.4925856297 -2.259954526
C -1.8926719672 -2.7943262109 -1.2551775119
C 1.738290103 2.6231806868 -2.3147389192
H -4.9034472193 -1.5220583735 -0.3121181526
H 4.8205424222 1.5389221119 -1.3291407306
H -3.9366698476 -3.475550045 -1.4696358557
H 3.7593312951 3.0685682693 -2.9415886539
H -1.4779324164 -3.6438165375 -1.7851428623
H 1.2904925634 3.2917419444 -3.0397146594
H 0.0118967897 -1.9043555574 -0.935884697
H -0.1347599672 1.9968891538 -1.5007376774
H -3.1652553271 2.4316949518 1.680565436
H 3.2730051758 -1.4442897808 2.0329752624
H -4.6223429651 0.6276877519 0.8296336634
H 4.647000213 -0.1158791566 0.4689988222
H -0.7082569922 2.2633469313 1.4371195529

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2628373
RMSD=4.252e-09
RMSF=4.588e-06
Dipole=1.6565808 0.2554998 0.2804417
PG=C01 [X(C21H13O1)]

βCOαN-αN from **σ-6aH-DB*cg*F**$^+$ E_{Tot}=-883.263872357 Hartree, ΔG_{298}=87.78 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
27-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-1-(1-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.055409716 opt+freqs
1 1
C 0.4567446939 1.4253573183 2.476432186
O -0.1546057615 1.6965010381 3.3914689928
C -1.382932822 1.8916889824 0.1194523975
C 1.3014351778 1.0724400013 1.4484568094
C -2.7821560113 2.0204049224 0.0103926917
C 2.7239776626 1.133952049 1.6587572649
C -0.7795656577 0.6416635998 0.1627346022
C 0.7018705114 0.5927516306 0.2597455871
C -3.5693661321 0.896385461 -0.0425068717
C 3.5291166347 0.6844122715 0.6604802875
C -1.5791912756 -0.5497507105 0.127505245
C 1.5634977596 0.1413583408 -0.768600082
C -3.0006959351 -0.4026113952 0.0212087036
C 2.9893550836 0.1827826047 -0.5640693687
C -3.8156295684 -1.5638180096 -0.0019612229
C 3.8380244184 -0.2577602721 -1.6001946661
C -1.0400537273 -1.8580787272 0.2359342114
C 1.0581225582 -0.3102947724 -2.020524924
C -3.2598644726 -2.8168890932 0.0876600384
C 3.3129959587 -0.7073492534 -2.7934856683
C -1.8607270738 -2.9620895234 0.213887069
C 1.9164155296 -0.7268059722 -3.0074888507
H -4.8900314948 -1.4438332832 -0.0846509063
H 4.9109462037 -0.2323737968 -1.4498362783
H -3.8919484946 -3.6965626845 0.0706903853
H 3.9777266226 -1.04073549 -3.5818818402
H -1.4313806769 -3.9535597889 0.2981056846
H 1.5250441718 -1.0676121382 -3.9581850632
H 0.0294943481 -1.9946345127 0.3416152671
H -0.0108134986 -0.3178838017 -2.1868430318
H -3.2246603185 3.0074363019 -0.0428929754
H 3.1236719705 1.5177894542 2.588233404
H -4.6463112945 0.9885885568 -0.1301565314
H 4.6053221015 0.7088927887 0.7849091098
H -0.7684534251 2.7859833739 0.1162481975

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2638724
RMSD=6.641e-09
RMSF=4.398e-05
Dipole=1.4681003 0.4798404 0.2255304
PG=C01 [X(C21H13O1)]

βCOαN-βN from **σ-13aH-DBagF**$^{+}$ E_{Tot}=-883.266400625 Hartree, ΔG_{298}=81.40 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
21-Mar-2013
#P B3LYP/6-311++G** FOPT=(LOOSE READFC MAXCYCLE=128) GUESS=READ
2-Carboxy-1-(2-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.058449740 Loose
1 1
C 1.5975718102 -1.8359469559 1.7043485317
O 1.2644029658 -2.6910315297 2.370854359
C -1.2506155182 0.2898721511 0.2517017249
C 2.095098409 -0.784710335 0.978412949
C -2.5773149234 -0.1893347087 0.166052039
C 3.4643832464 -0.4027777663 1.2223026776
C -0.1698469725 -0.5314279881 -0.0354443881
C 1.2126712207 -0.0507467565 0.1378503376
C -2.8039149041 -1.5415841494 -0.2523316731
C 3.9222806697 0.7353932967 0.6428160055
C -0.4032916263 -1.8784693417 -0.446098961
C 1.7339204568 1.1143900838 -0.4851732969
C -1.6842867081 -2.3578052524 -0.5584285678
C 3.0891978871 1.5213435032 -0.2125042849
C -3.692303341 0.6326138127 0.4829700903
C 3.5887095874 2.6880459422 -0.8239040972
C -4.1356800355 -2.0158577688 -0.3505923913
C 0.9683306163 1.8728933862 -1.416508708
C -4.9697978765 0.140392687 0.3790451759
C 2.8039217026 3.4194694972 -1.6913625588
C -5.1928738412 -1.1929423416 -0.0418350969
C 1.4920535452 3.0014394914 -1.9994884867
H -3.5212149035 1.6536539731 0.8059540647
H 4.6048719044 2.9992442797 -0.6118356761
H -5.8163627921 0.7722138014 0.6200149838
H 3.2039831847 4.312590284 -2.1569582602
H -6.2079741399 -1.5643690325 -0.1178375364
H 0.9016694778 3.5668674612 -2.7100519959
H -4.3093714847 -3.0369733288 -0.6709106962
H -0.0271646852 1.5424158581 -1.6778292328
H -1.8520619144 -3.3726548766 -0.901609667
H 4.0895408693 -1.0066327085 1.8670883369
H 0.4330814908 -2.5064332304 -0.734398816
H 4.9421220854 1.0566802899 0.8182610671
H -1.0856232475 1.3061465437 0.5923164323

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2664007
RMSD=4.608e-09
RMSF=9.458e-06
Dipole=1.6642472 0.3398572 0.2199081
PG=C01 [X(C21H13O1)]

βCOαN-βN from **σ-13aH-DB*ag*F**$^{+}$ E_{Tot}=-883.267388159 Hartree, ΔG_{298}=78.81 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
20-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-1-(2-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* -883.059563690 opt+freqs
1 1
C 0.3887756736 1.2397178791 2.3334411656
O -0.2996588563 1.338572101 3.230311797
C -1.3764258265 0.5469775532 0.1368483219
C 1.3453374715 1.1529985497 1.3503197017
C -2.6879660523 0.0195224204 0.0646354959
C 2.6058086708 1.8157386583 1.5689259324
C -0.2618630148 -0.2832155609 0.1221288095
C 1.0830908507 0.3108427592 0.2391413115
C -2.857258254 -1.4005460993 -0.0036542416
C 3.6054758321 1.5851809675 0.6796091461
C -0.4390351792 -1.6949083963 0.0327304544
C 2.1414712224 0.0991980758 -0.6822464081
C -1.7011074552 -2.2277518438 -0.0141850809
C 3.4148981736 0.7320348937 -0.4517171209
C -3.8347148991 0.8556548621 0.0548654768
C 4.4597266387 0.5184672459 -1.3729687006
C -4.1677128194 -1.9324576288 -0.0643622689
C 1.9666450424 -0.6793131837 -1.8611892123
C -5.0934377857 0.3071146632 -0.0054977784
C 4.263483222 -0.268046081 -2.4889447964
C -5.2605323083 -1.095924793 -0.0638810874
C 3.0072464046 -0.860565361 -2.7396969667
H -3.7061092792 1.9317379243 0.097177353
H 5.4203618489 0.9884807445 -1.1978134711
H -5.9658878771 0.9495050839 -0.0105811852
H 5.0760036528 -0.4213368068 -3.1894884265
H -6.2599990159 -1.5117675239 -0.1117784053
H 2.8628287219 -1.4528814437 -3.6349484423
H -4.2992473319 -3.0075156548 -0.1138174536
H 1.0005211639 -1.1184108354 -2.0689247377
H -1.8294449331 -3.3039589576 -0.0517571435
H 2.7425095631 2.4568184496 2.4299863437
H 0.4264883321 -2.3459269279 0.0480222586
H 4.5709742842 2.0564755741 0.8205476311
H -1.2531619275 1.6258860837 0.1350683814

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2673882
RMSD=9.419e-09
RMSF=2.020e-06
Dipole=1.5271547 0.5690042 0.1974576
PG=C01 [X(C21H13O1)]

βCOβN-αN from **σ-6aH-DB*bg*F**$^{+}$ E_{Tot}=-883.26236375 Hartree, ΔG_{298}=90.22 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
26-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-3-(1-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.053663998 opt+freqs
1 1
C -0.1065868331 -0.942382247 1.9799951551
O -0.7962954956 -1.3508061944 2.7781097771
C -1.4490770126 2.1639109445 0.2162130702
C 0.7939564081 -0.4550694244 1.06140457
C -2.8033253732 2.5565542921 0.2353006702
C 2.1402570701 -0.8410998863 1.2103726208
C -1.0908783535 0.8503900598 -0.0288271575
C 0.3426512777 0.4724902767 0.0447090467
C -3.7908720585 1.6276127589 0.016552669
C 3.1028357808 -0.3100302158 0.3509529603
C -2.0982749186 -0.1324882219 -0.3117095787
C 1.3128963245 0.9882937129 -0.7742340624
C -3.4721634017 0.2740901721 -0.2642655207
C 2.6872302135 0.6313215057 -0.6585835363
C -4.4858637802 -0.6839161696 -0.5271298276
C 3.6686901748 1.1679818367 -1.5189610823
C -1.8053619155 -1.474778813 -0.6819854182
C 4.4774281734 -0.6729689613 0.4588126758
C -4.1681252021 -1.9813264874 -0.8470390986
C 4.9897419962 0.7957240871 -1.3887311469
C -2.8144997984 -2.3740775888 -0.9386752705
C 5.3994990395 -0.1287283303 -0.3960306135
H -5.5223551625 -0.3685548488 -0.4821858579
H 3.3727334012 1.8756994436 -2.2843252782
H -4.9516262139 -2.7015410627 -1.0495780094
H 5.7322346482 1.2164395284 -2.0568763736
H -2.5705388844 -3.388925458 -1.230651241
H 6.4447704308 -0.4009570604 -0.3178648579
H -0.7753793962 -1.7892622255 -0.8063316121
H 4.7788228495 -1.3806729838 1.2226036154
H -3.0559022882 3.5897517114 0.4400140805
H 2.4298376158 -1.5365863381 1.9900503007
H -4.8342682854 1.921410425 0.0461977279
H 1.0206845476 1.6829610728 -1.5536040485
H -0.6795961656 2.8976675464 0.4288265887

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2623638
RMSD=8.378e-09
RMSF=1.988e-05
Dipole=2.1286194 -0.2313778 0.5600499
PG=C01 [X(C21H13O1)]

βCOβN-αN from **σ-6aH-DB*bg*F**$^+$ E_{Tot}=-883.262996055 Hartree, ΔG_{298}=89.13 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
23-Mar-2013
#P B3LYP/6-311++G** FOPT=(READFC MAXCYCLE=64) GUESS=READ GEOM=CHECK FREQ=NORAMAN
2-Carboxy-3-(1-naphthyl)-naphthalene B3LYP/6-311++G** from 6-31G* E=-883.054895254 opt+freqs
1 1
C 0.3048987557 1.5714433679 2.1200240886
O -0.2112188923 2.0508884004 3.0072777876
C -1.5513351301 2.0032129688 -0.1929271715
C 1.0237663043 0.9567686315 1.1195571896
C -2.9111713431 2.3432970437 -0.3397274947
C 2.4191587754 0.8391135054 1.2854648028
C -1.1416084753 0.6777710591 -0.1340301508
C 0.3103447997 0.406233758 -0.0089851708
C -3.8552654641 1.3509558465 -0.4323855147
C 3.1582475681 0.1405263491 0.3319873066
C -2.1096516431 -0.3785371137 -0.2094744544
C 1.0600091126 -0.2967314587 -0.9188694672
C -3.4885454803 -0.0188954601 -0.3686643165
C 2.4676057111 -0.4487494378 -0.7899837996
C -4.4665635394 -1.0432830503 -0.4449423999
C 3.2277648419 -1.1528860679 -1.750956277
C -1.7810697362 -1.7552315853 -0.0984170154
C 4.5730355462 -0.0056201201 0.4474999269
C -4.1104551821 -2.3672791418 -0.3562451906
C 4.5922196992 -1.2735908465 -1.6092244505
C -2.7564741451 -2.7228786356 -0.1739447286
C 5.2713071159 -0.6987849851 -0.5045157068
H -5.5061455679 -0.7614789302 -0.5693639981
H 2.7243114692 -1.5969535657 -2.6016379984
H -4.8665588282 -3.1409252074 -0.4154440303
H 5.1617821575 -1.8175464925 -2.3537823171
H -2.485142797 -3.7684091585 -0.0858592299
H 6.345199297 -0.81111415 -0.4207199858
H -0.751966766 -2.0525910206 0.0592049732
H 5.0816465244 0.4390940868 1.295175918
H -3.1984398234 3.3857277527 -0.4011561585
H 2.9108449716 1.2772281754 2.146476021
H -4.9022539945 1.603530735 -0.5586998458
H 0.5694073476 -0.7212974187 -1.7871177098
H -0.8102413986 2.7965002285 -0.1927379722

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2629961
RMSD=8.463e-09
RMSF=1.646e-06
Dipole=2.0523734 0.3402101 0.4731649
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-11aH-DB*bh*F**$^{+}$ E_{Tot}=-883.265933617 Hartree, ΔG_{298}=81.37 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
04-Oct-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ FREQ=NORAMAN GEOM=CHECK
2-Carboxy-3-(2-naphthyl)naphthalene B3LYP/6-311++G** from 6-31G* E=-883.058046591 opt+freqs
1 1
C 0.2151628547 2.6485354164 0.3896939278
O -0.4537387787 3.5629350101 0.4068129197
C -1.5888081505 0.4988272156 1.3118205298
C 1.107742918 1.6069797966 0.3284642935
C -2.9333601292 0.2338341882 1.3901808565
C 2.4762157919 1.9579899988 0.3004287685
C -0.7987263991 -0.0653644553 0.2670678683
C 0.6394864111 0.243260153 0.1812467198
C -3.5721408468 -0.6019863262 0.4383885019
C 3.4347850954 0.9675490421 0.1040940183
C -1.3987627052 -0.8980483851 -0.6622007602
C 1.6114053552 -0.7060724958 -0.0317511399
C -2.7833029252 -1.1828504584 -0.6076584614
C 2.9956905472 -0.3945106389 -0.0801253397
C -3.415810816 -2.0212862303 -1.5638122901
C 3.9759367558 -1.3924848097 -0.2828761956
C -4.9591456835 -0.8894856808 0.4943473732
C 4.828576804 1.2738969971 0.0734654984
C -4.7624570027 -2.2779316683 -1.4816762414
C 5.3124267361 -1.0623236072 -0.3071215589
C -5.5397940228 -1.7082728423 -0.4445864692
C 5.7447924846 0.2773335054 -0.1284607787
H -2.8208207197 -2.4581211342 -2.3583916676
H 3.6636504055 -2.4211591204 -0.4192062535
H -5.2380499848 -2.9205839997 -2.2130667463
H 6.0524311547 -1.838314386 -0.4651113272
H -6.6010193658 -1.9217962093 -0.3954604142
H 6.8034303851 0.5043356833 -0.1522623978
H -5.5559212162 -0.4538463929 1.2879135936
H 5.1461645319 2.3009889182 0.2121974337
H -3.5196906058 0.6466230719 2.2036350623
H 2.7777366024 2.9928181324 0.4170679946
H -0.8137522793 -1.3164673496 -1.4743826504
H 1.3122565446 -1.743309081 -0.1285947771
H -1.1159836605 1.0798194965 2.097584067

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2659336
RMSD=3.449e-09
RMSF=2.076e-05
Dipole=2.2741787 0.944546 0.0635239
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-11aH-DB*bh*F**$^{+}$ PCM E_{Tot}=-883.331668258 Hartree, ΔG_{298}=75.10 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
14-Mar-2013
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=(Loose MaxStep=128)
2-Carboxy-3-(2-naphthyl)naphthalene - in Water B3LYP/6-311++G** E=-883.265933617 Loose
1 1
C 0.2399614645 2.6901260407 0.3699783503
O -0.4419457749 3.5919498632 0.3943168911
C -1.5943905532 0.489621694 1.3313991775
C 1.118630857 1.635243006 0.3097753434
C -2.9344666886 0.2033138845 1.4154811094
C 2.4851777262 1.9729686297 0.2705927427
C -0.8044530172 -0.0373931312 0.2692575722
C 0.6387381563 0.2745486324 0.1862017043
C -3.56764724 -0.6223719408 0.4503551193
C 3.4351324 0.9662532374 0.0915046372
C -1.3982559689 -0.8528735821 -0.6765798235
C 1.596185536 -0.689258696 -0.0052129484
C -2.7789049842 -1.1629899769 -0.6153025926
C 2.9854764276 -0.3915053907 -0.0617421026
C -3.4064093312 -1.9904245327 -1.5860039838
C 3.9536001836 -1.4033832611 -0.2489169875
C -4.9512619316 -0.9348050593 0.509581984
C 4.8285624807 1.2619093831 0.049186468
C -4.7487846736 -2.2729263282 -1.5005538187
C 5.2938269978 -1.0854511493 -0.2857932386
C -5.5278864106 -1.7408372464 -0.4436264411
C 5.7370660657 0.2523312335 -0.1360843282
H -2.8087267134 -2.3970520976 -2.3945838166
H 3.629452118 -2.4306637662 -0.363935553
H -5.2185959909 -2.9064806458 -2.2440043249
H 6.0260351937 -1.8709028558 -0.4315582212
H -6.5853658221 -1.9728405071 -0.3907353097
H 6.7971358683 0.4707987622 -0.1687957918
H -5.5470075362 -0.5265755586 1.3187242085
H 5.1519155179 2.2894363234 0.165321236
H -3.5209794911 0.596567651 2.2384150903
H 2.7957187188 3.0061416456 0.3645315847
H -0.8112878398 -1.2466680113 -1.4989044653
H 1.2882082432 -1.724777001 -0.0868691757
H -1.1278479013 1.0804821058 2.1122436617

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3316678
RMSD=7.864e-09
RMSF=3.617e-05
Dipole=3.1269872 1.7625573 0.2183752
Quadrupole=25.0863814 -3.7172677 -21.3691136 7.7530684 -1.6116262 8.02635
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-13aH-DB*ah*F**$^{+}$ E_{Tot}=-883.266743242 Hartree, ΔG_{298}=79.57 kJ/mol
GINC-CHIRAL
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
01-Oct-2012
#P B3LYP/6-311++G** FOPT=READFC GUESS=READ FREQ=NORAMAN GEOM=CHECK
2-Carboxy-3-(2-naphthyl)naphthalene B3LYP/6-311++G** from 6-31G* E=-883.058908746 opt+freqs
1 1
C 0.4188049137 1.5290777 1.6999640614
O 0.4007432881 1.5666923105 2.8331634424
C 0.3843462869 -1.3180109891 1.0725080718
C 0.4384451399 1.6319101723 0.3286511012
C 0.0436367466 -2.5371918378 1.707816236
C 0.8796705307 2.8583693643 -0.2138573792
C -0.4647452929 -0.7197255994 0.1519939696
C -0.0905355257 0.5570436442 -0.4812611523
C -1.204784345 -3.1573919356 1.3822893886
C 0.7808557936 3.0724873354 -1.5867432791
C -1.69368716 -1.3554534365 -0.1809898986
C -0.2097719334 0.8124253742 -1.8269327454
C -2.0482541016 -2.5339445336 0.4236294723
C 0.2083786009 2.0363009578 -2.4125698158
C 0.9047972837 -3.1664478073 2.6438382612
C 0.0993918712 2.2707897688 -3.8024572402
C -1.5519660229 -4.3752496884 2.0166079395
C 1.2136502348 4.2949287686 -2.1830213501
C 0.5376331163 -4.3481338419 3.2421216808
C 0.5271399725 3.4617371096 -4.3446134744
C -0.7001184018 -4.9557017822 2.927671924
C 1.0879712714 4.4816937882 -3.5330930307
H 1.8559852244 -2.7033489788 2.8835322539
H -0.3255774352 1.5018403402 -4.4368043223
H 1.1982992117 -4.8218092613 3.9584937281
H 0.4353076084 3.6276152409 -5.4117308482
H -0.9736512505 -5.8879645813 3.4074678599
H 1.415434647 5.4075595745 -3.9895990293
H -2.4976510281 -4.8458041798 1.7718624423
H 1.6401955863 5.0671469411 -1.5531008693
H -2.9958060476 -3.0013989478 0.1792102457
H 1.2732960698 3.634366362 0.4327304531
H -2.3653904793 -0.883950639 -0.8885492693
H -0.6002574064 0.0358510823 -2.4745498688
H 1.3687151212 -0.9007166272 1.2664132406

Version=AM64L-G03RevC.02
State=1-A
HF=-883.2667432
RMSD=5.085e-09
RMSF=4.373e-05
Dipole=0.4966331 2.1149806 -0.8278482
PG=C01 [X(C21H13O1)]

βCOβN-βN from **σ-13aH-DB*ah*F**$^+$ PCM E_{Tot}=-883.332306413 Hartree, ΔG_{298}=73.24 kJ/mol
GINC-SERGEY
FOpt
RB3LYP
6-311++G(d p)
C21H13O1(1+)
SERGEY
24-Mar-2013
#P B3LYP/6-311++G** SCRF=(PCM Solvent=Water) FOpt=(ReadFC MaxStep=64) Guess=Read Freq=NoRaman
2-Carboxy-3-(2-naphthyl)naphthalene - PCM B3LYP/6-311++G** E=-883.266743242 opt from Loose E=-883.332306443
1 1
C 0.4541286435 1.5890181153 1.7164145215
O 0.4495013874 1.6075784333 2.8475481992
C 0.3930903069 -1.3185977745 1.0911637186
C 0.4508506651 1.6650894408 0.3431379076
C 0.0419506873 -2.5460130395 1.7084052846
C 0.8750044005 2.8866897727 -0.2130369892
C -0.448386956 -0.7057414943 0.1789575047
C -0.0717459102 0.5762350173 -0.4525752346
C -1.2051038571 -3.1595009497 1.3703388972
C 0.7724256114 3.0818025749 -1.5913344802
C -1.6814296273 -1.3313165779 -0.1625791401
C -0.1878204217 0.8088092118 -1.8000519567
C -2.0448383468 -2.5185128425 0.4194850695
C 0.2176785748 2.0306604727 -2.402548105
C 0.8957065878 -3.1871934728 2.6449850815
C 0.1059741682 2.2435813918 -3.79529603
C -1.5578419492 -4.3862502324 1.989232921
C 1.1898699104 4.3014446965 -2.199029819
C 0.5244763942 -4.3760816459 3.2282083671
C 0.5184690748 3.4341389875 -4.3523732057
C -0.7127521166 -4.979959282 2.8985445525
C 1.0637728486 4.4701230056 -3.5533458838
H 1.8433103455 -2.7231140367 2.8961405978
H -0.3085800063 1.4601215805 -4.4182100324
H 1.1800053443 -4.8569743509 3.9449898923
H 0.4255701565 3.5850232283 -5.4214294294
H -0.9910864823 -5.9173199116 3.3662778312
H 1.379391223 5.3948517663 -4.0200673061
H -2.5042945903 -4.8499113294 1.7332273517
H 1.6042184761 5.0848393961 -1.5757614667
H -2.9928787912 -2.9787139293 0.1633389803
H 1.2594313794 3.6744231677 0.4228483083
H -2.3449994877 -0.8476457153 -0.8691059323
H -0.5717664559 0.0227274067 -2.4393380809
H 1.3692009013 -0.8987199133 1.3129303052

Version=EM64L-G09RevC.01
State=1-A
HF=-883.3323064
RMSD=6.646e-09
RMSF=9.924e-06
Dipole=0.7263786 3.1842035 -0.8640715
Quadrupole=-16.8791228 14.9010356 1.9780872 12.2383978 3.4354269 -16.4988946
PG=C01 [X(C21H13O1)]