Supplementary Information

NMR and experimental reinvestigation of the condensation reaction between γ-methylene-α,β-unsaturated aldehydes and propargyl aldehydes

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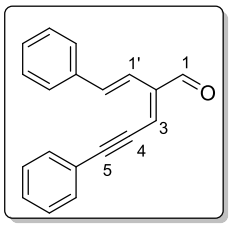
Part A

Experimental Section

Preparation of **8a** (revised as (*E*)-5-phenyl-2-((*E*)-styryl)pent-2-en-4-ynal, **9**). To a solution of phenylpropargyl aldehyde (1 mmol; 130.1 mg) in dichloromethane (3.0 mL) was added (2*E*)-4-phenyl-2-butenal (1.5 mmol; 219 mg), pyrrolidine (0.2 mmol; 0.016 mL) and K_2CO_3 (0.2 mmol; 27 mg). The reaction mixture was stirred at room temperature for 72 h and then the solvent was removed under vacuum. The residue was purified by silica gel chromatography (hexane/ethyl acetate) to yield the desired product **9a** (149 mg; 0.58 mmol, 57% yield) as a yellow liquid. All the ^{1}H and ^{13}C NMR signals were, within the experimental error, identical to the original report.



(E)-5-phenyl-2-((E)-styryl)pent-2-en-4-ynal (9a)

Yellow liquid. **IR** (film) (cm^{-1}): 3078, 3057, 3024, 2918, 2847, 2721, 2183, 1690. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 9.65 (d, *J* = 1.8 Hz, 1H, 1-H), 7.99 (d, *J* = 16.5 Hz, 1H, 2'-H), 7.60-7.52 (m, 4H, Ar-H), 7.45-7.27 (m, 6H, Ar-H), 7.25 (dd, *J* = 16.5; 1.7 Hz, 1H, 1'-H), 6.52 (s, 1H, 3-H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 193.2 (CH, C-1), 143.2 (C, C-2), 137.0 (C, Ar), 136.2 (CH, C-2'), 131.8 (2 × CH, Ar), 129.7 (CH, Ar), 128.7 (2 × CH, Ar), 128.6 (3 × CH, Ar), 127.1 (CH, C-3), 126.9 (2 × CH, Ar), 122.2 (C, Ar), 119.3 (CH, C-1'), 109.5 (C, C-5), 86.8 (C, C-4).

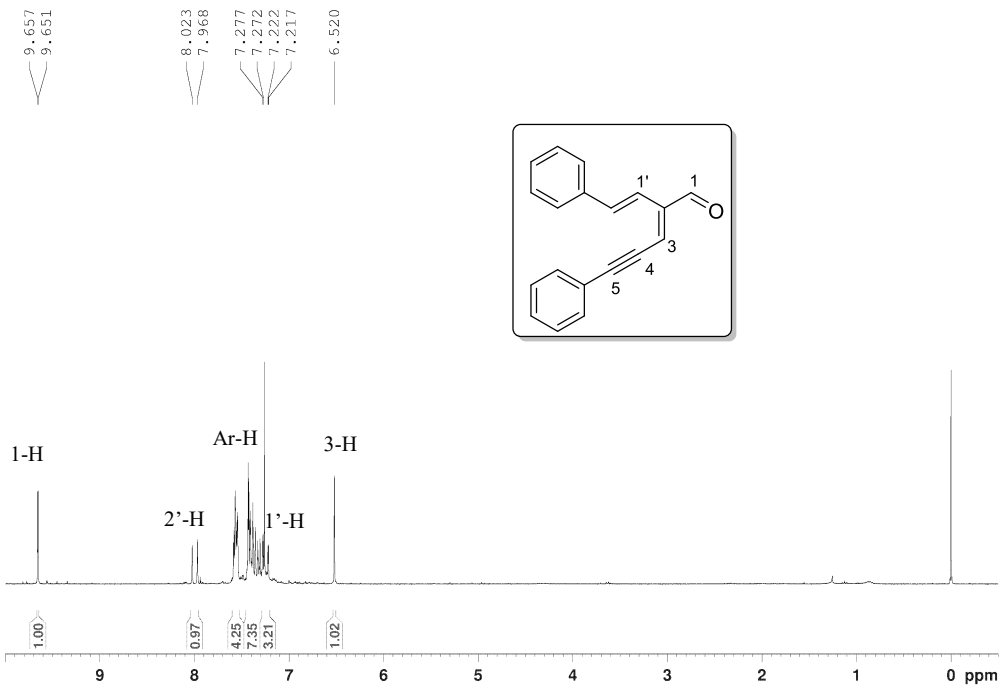


Figure S1. ^{1}H NMR Spectrum of Compound **9a** ($CDCl_3$, 300 MHz)

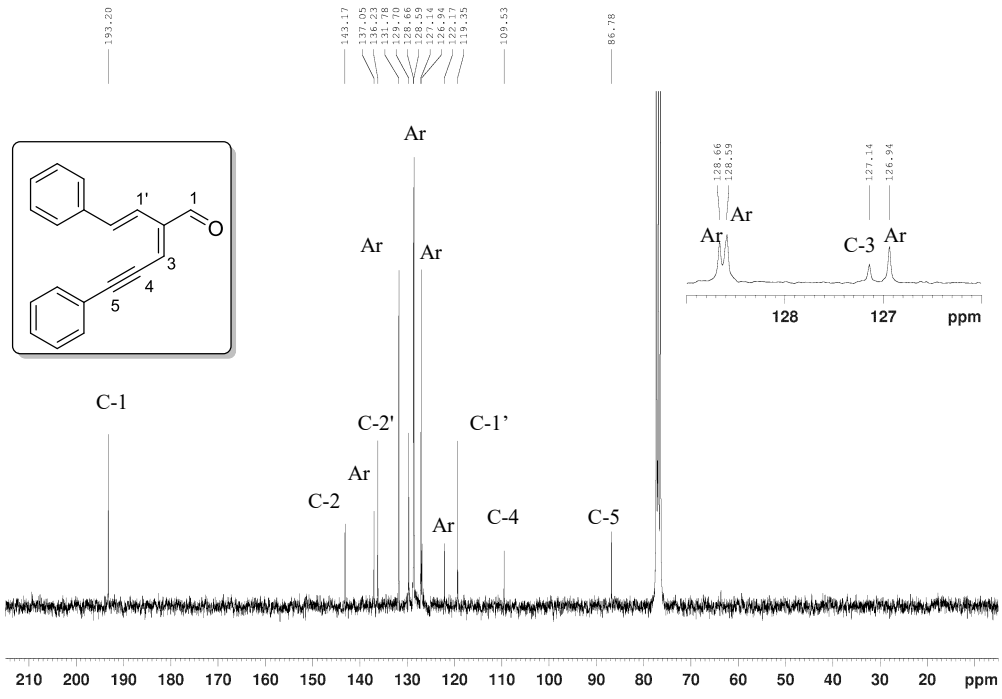


Figure S2. $^{13}C\{^{1}H\}$ NMR Spectrum of Compound **9a** ($CDCl_3$, 75 MHz)

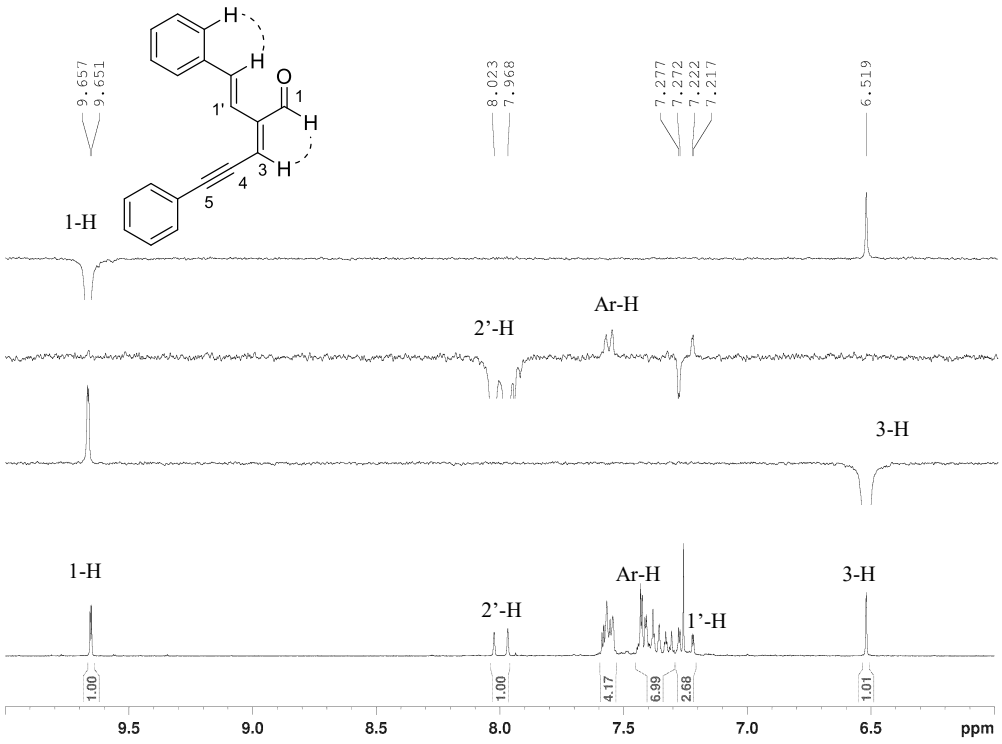


Figure S3. ^{1}H NMR NOE Spectra of Compound **9a** ($CDCl_3$, 300 MHz)

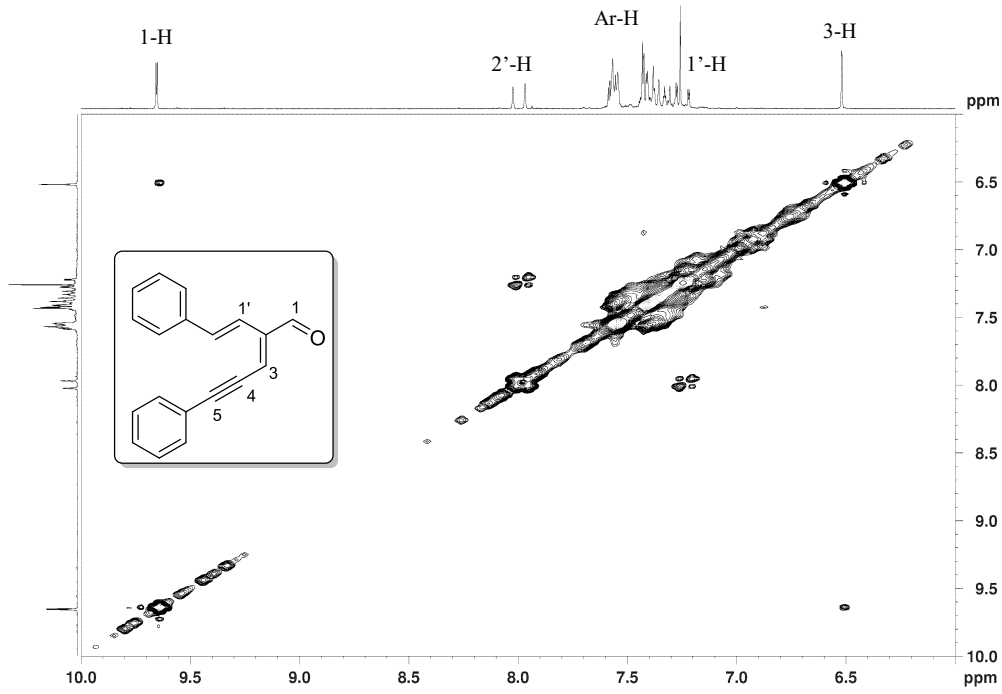


Figure S4. ROESY Spectrum of Compound **9a** ($CDCl_3$, 300 MHz)

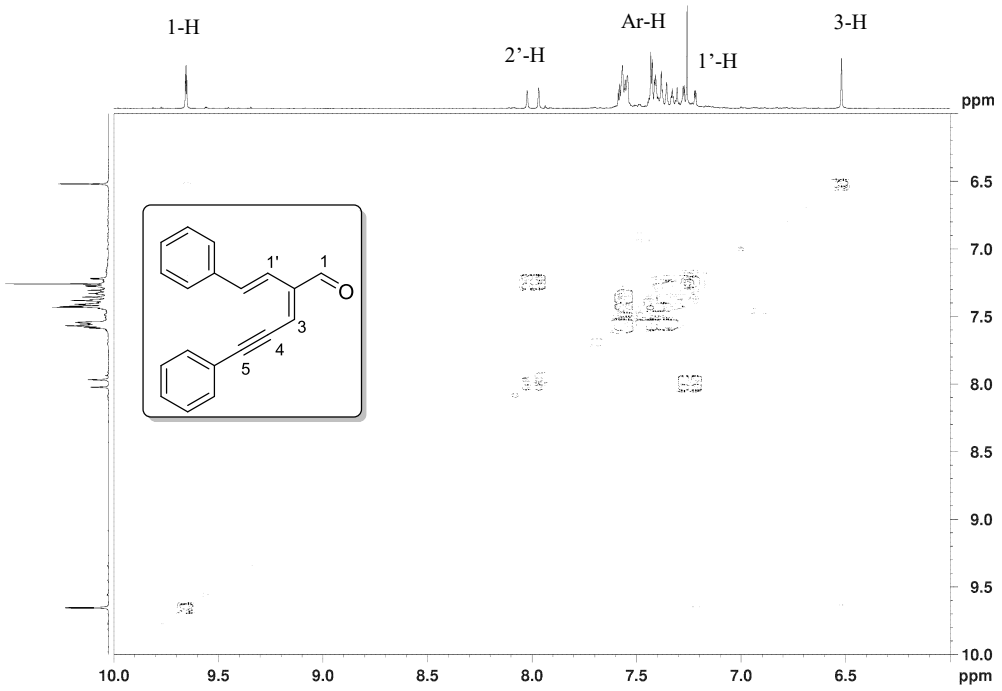


Figure S5. COSY Spectrum of Compound **9a** ($CDCl_3$, 300 MHz)

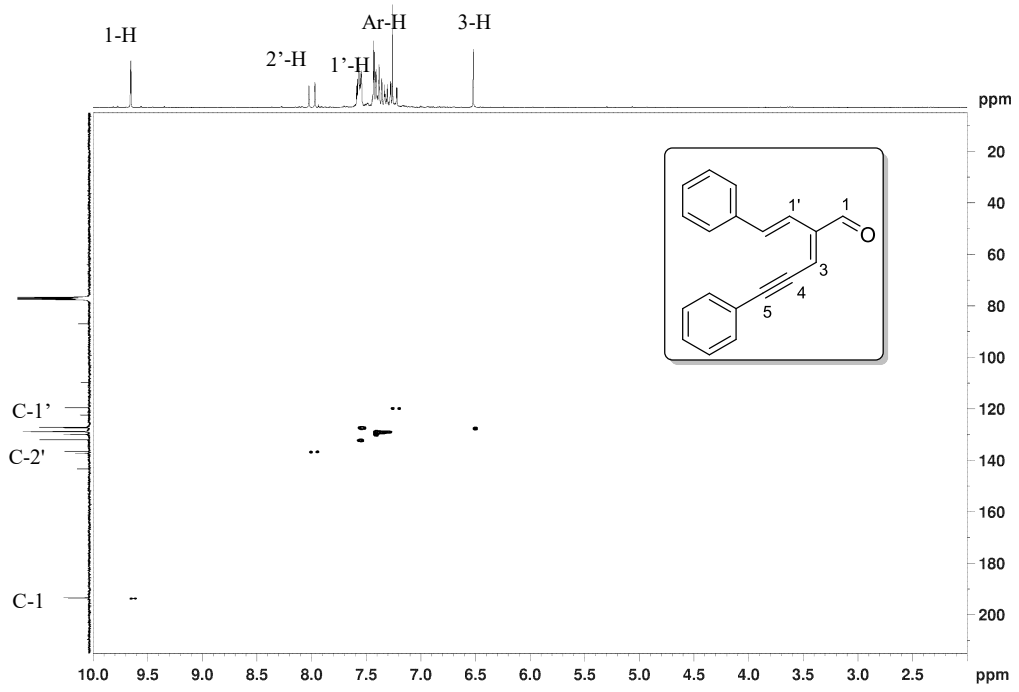


Figure S6. HSQC Spectrum of Compound **9a** ($CDCl_3$, 300 MHz)

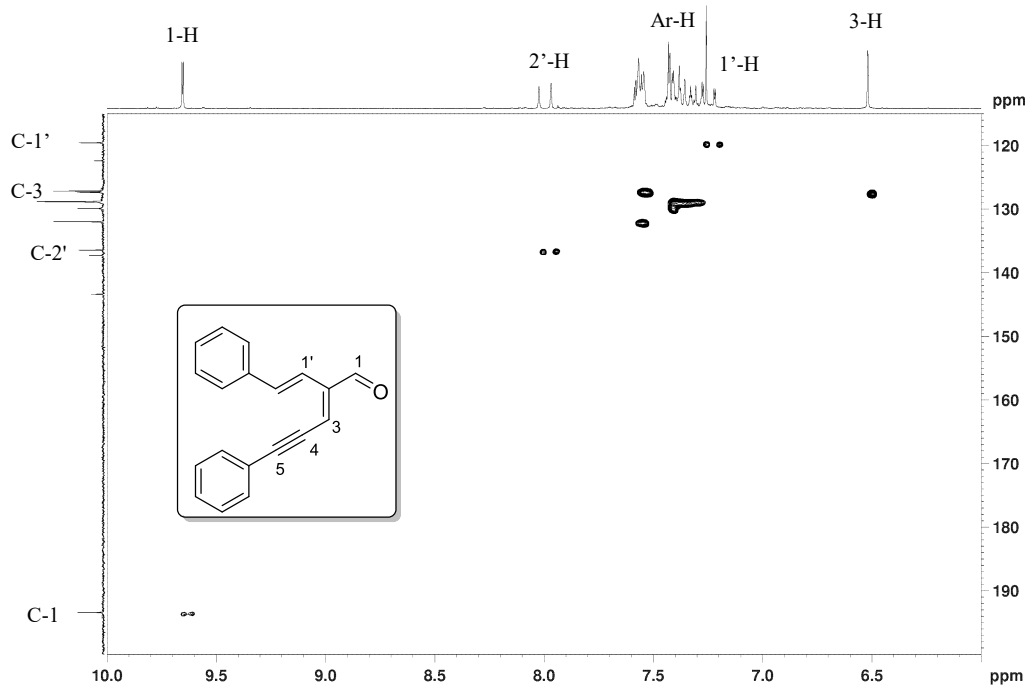


Figure S7. Partial HSQC Spectrum of Compound **9a** ($CDCl_3$, 300 MHz)

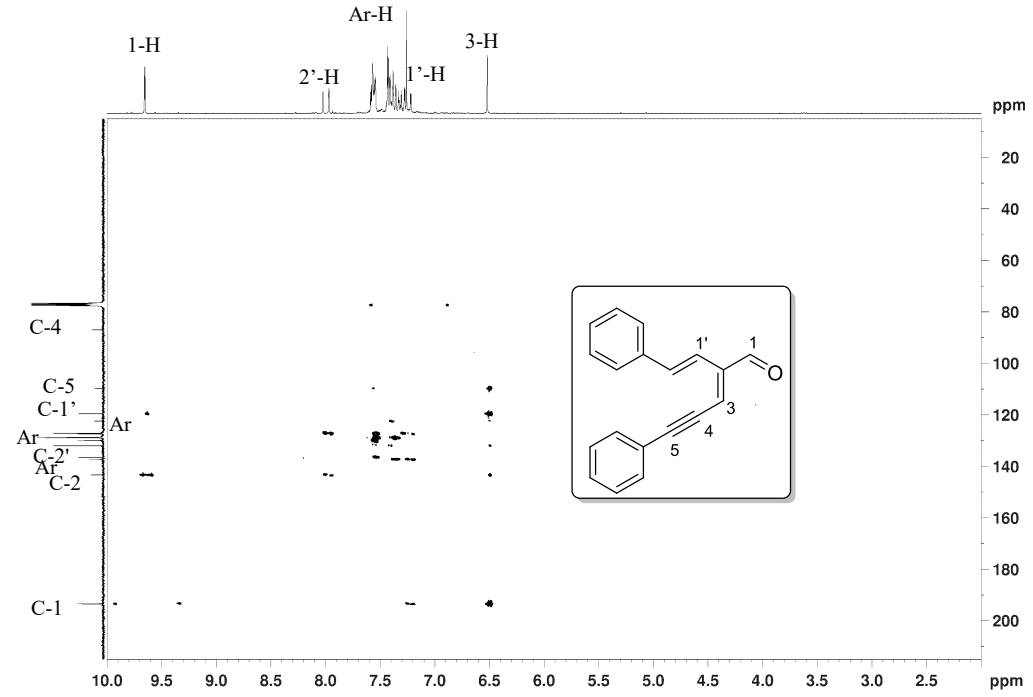


Figure S8. HMBC Spectrum of Compound **9a** ($CDCl_3$, 300 MHz)

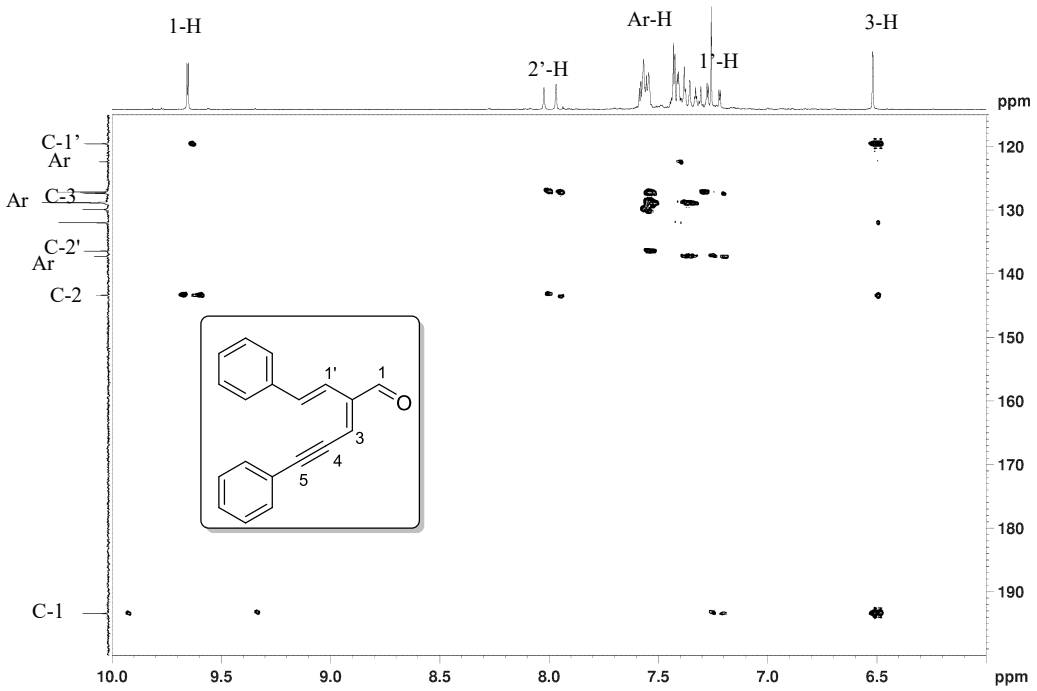


Figure S9. Partial HMBC Spectrum of Compound **9a** ($CDCl_3$, 300 MHz)

Part B

Computational Section

Computational Methods. All the quantum mechanical calculations were performed using Gaussian 09.[1] Systematic conformational searches were done for each compound in the gas phase using the MMFF and MM+ force fields, implemented in Spartan 08[2] and Hyperchem, respectively.[3] All conformers within 10 kcal/mol of the lowest energy conformer were subjected to further reoptimization at the B3LYP/6-31G* level of theory. The choice for the 10 kcal/mol of cutoff was set as a balance between reducing the overall CPU calculation time and minimizing the possibility of losing further contributing conformers. Frequency calculations were done for all optimized geometries at the B3LYP/6-31G* level to determine the nature of the stationary point found, and to compute the thermochemical properties (at 1 atm and 298.15 K). All the B3LYP/6-31G* optimized geometries were next subjected to NMR calculations. The magnetic shielding constants (σ) were computed using three different methods to solve the gauge origin problem:[4] GIAO (*gauge including atomic orbitals*),[5] CSGT (*continuous set of gauge transformations*)[6] and IGAIM (*individual gauges for atoms in molecules*).[6a,b] Appart from the well known B3LYP, mPW1PW91 and PBE0, we also tested the LC-TPSSTPSS (the long-range corrected version of the Tao-Perdew-Staroverov–Scuseria functional),[7] in combination with the 6-31+G**, 6-311+G**, cc-PVTZ and 6-311++G(3df,2pd) basis sets. The effect of the solvent was included using the polarizable continuum model, PCM,[8] with chloroform as the solvent.

The unscaled chemical shifts (δ_u) were computed using benzene as reference standard according to $\delta_u = \sigma_0 - \sigma_x + \delta_0$, where σ_x is the Boltzmann averaged shielding tensor (over all significantly populated conformations) and σ_0 is the shielding tensor of benzene computed at the same level of theory employed for σ_x, and δ_0 is the experimental NMR shift of benzene (128.37 ppm and 7.36 ppm for carbon and proton data, respectively).[9] The Boltzmann averaging was done according to eq 1:

$$\sigma^x = \frac{\sum_i \sigma_i^x e^{(-E_i/RT)}}{\sum_i e^{(-E_i/RT)}} \qquad \textit{(eq. 1)}$$

where σ_i^x is the shielding constant for nucleus *x* in conformer *i*, *R* is the molar gas constant (8.3145 J K^{-1} mol^{-1}), *T* is the temperature (298 K), and E_i is the SCF energy of conformer *i* (relative to the lowest

energy conformer), obtained at corresponding level of theory. The scaled chemical shifts (δ_s) were computed as $\delta_s = (\delta_u - b)/m$, where m and b are the slope and intercept, respectively, resulting from a linear regression calculation on a plot of δ_u against δ_{exp}.[4]

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3) Hyperchem Professional Release 7.52, Hypercube, Inc., 2005.

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8) For a review on continuum solvation models, see: Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999.

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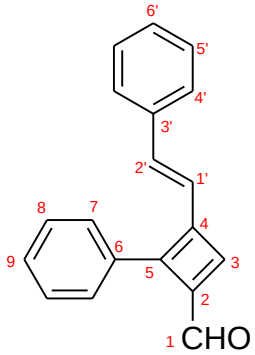
Table S1. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **8a**.



8a

δ_{exp}	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	21.6267	C-1	177.3	185.5	16.0	7.8
143.3	24.3304	C-3	174.6	181.5	31.3	38.2
137.2	38.2587	C-5	160.6	160.7	23.4	23.5
136.4	52.3405	C-2	146.5	139.7	10.1	3.3
131.9	60.5429	C-4	138.3	127.5	6.4	4.4
129.8	61.0509	C-3'	137.8	126.7	8.0	3.1
128.8	61.996	C-2'	136.9	125.3	8.1	3.5
128.7	64.69715	C-7	134.2	121.3	5.5	7.4
128.7	65.5505	C-6	133.3	120.0	4.6	8.7
127.2	68.6401	C-9	130.2	115.4	3.0	11.8
127.0	70.01075	C-5'	128.9	113.4	1.9	13.6
122.3	70.04195	C-8	128.8	113.4	6.5	8.9
119.5	70.3668	C-6'	128.5	112.9	9.0	6.6
109.6	71.53235	C-4'	127.4	111.1	17.8	1.5
86.9	81.5505	C-1'	117.3	96.2	30.4	9.3
		Average			***12.2***	***10.1***

* The assignment corresponds to the computed σ vaues.

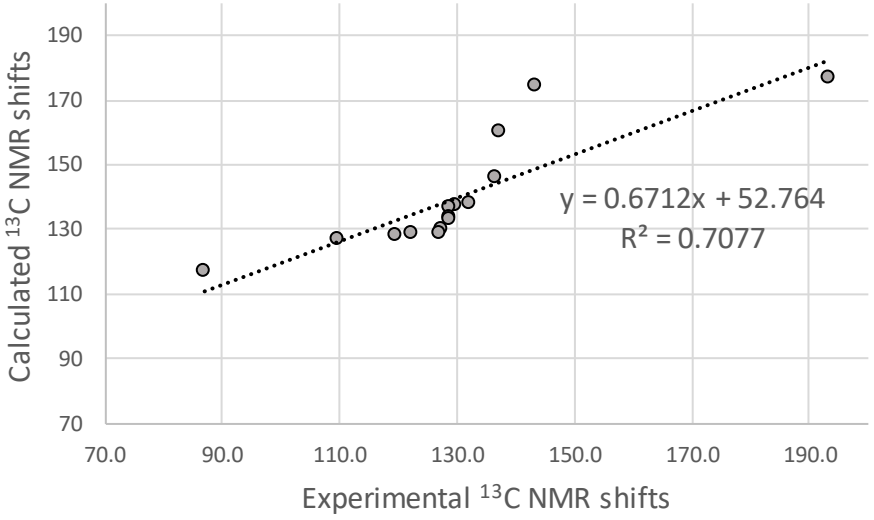
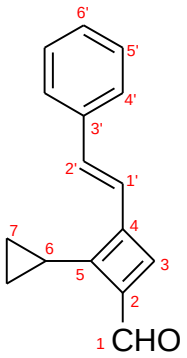


Table S2. Experimental ^{13}C NMR data of synthetic **8i** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **8i**.



8i

δ_{exp}	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.7	20.1559	C-5	178.7	172.4	15.0	21.3
142.8	24.1958	C-3	174.7	167.9	31.9	25.1
137.3	24.6250	C-1	174.3	167.4	37.0	30.1
135.3	55.4384	C-2	143.5	133.0	8.1	2.3
129.2	61.3590	C-3'	137.5	126.4	8.3	2.8
128.7	63.3999	C-4	135.5	124.1	6.8	4.6
128.5	70.5913	C-5'	128.3	116.1	0.2	12.4
126.9	72.1096	C-6'	126.8	114.4	0.1	12.5
119.5	72.5789	C-4'	126.3	113.9	6.8	5.6
116.8	72.8681	C-2'	126.0	113.6	9.2	3.2
74.2	83.4352	C-1'	115.5	101.8	41.3	27.6
10.1	176.6287	C-7	22.3	-2.2	12.2	12.3
1.5	178.4058	C-6	20.5	-4.2	19.0	5.7
		Average			***15.1***	***12.7***

* The assignment corresponds to the computed σ vaues.

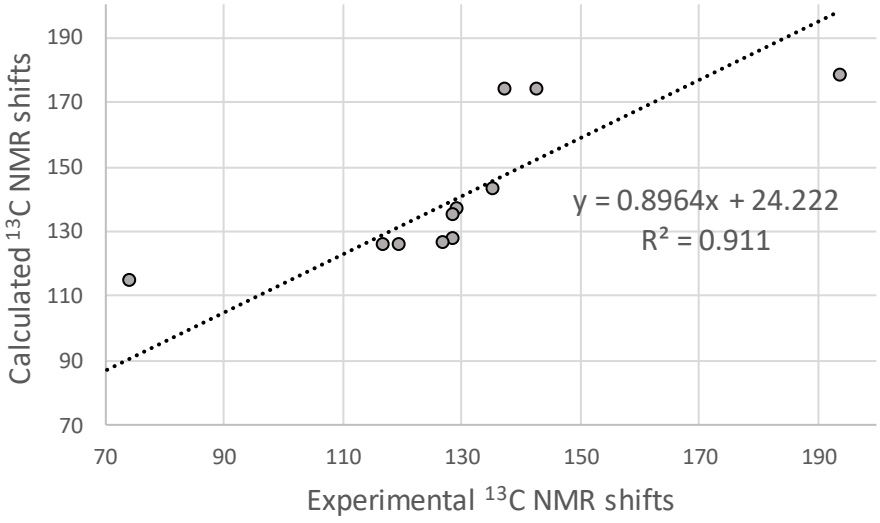
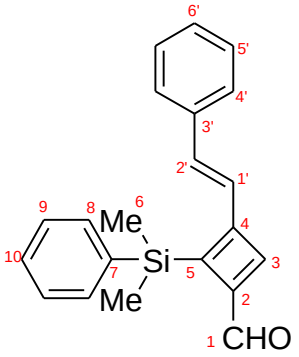


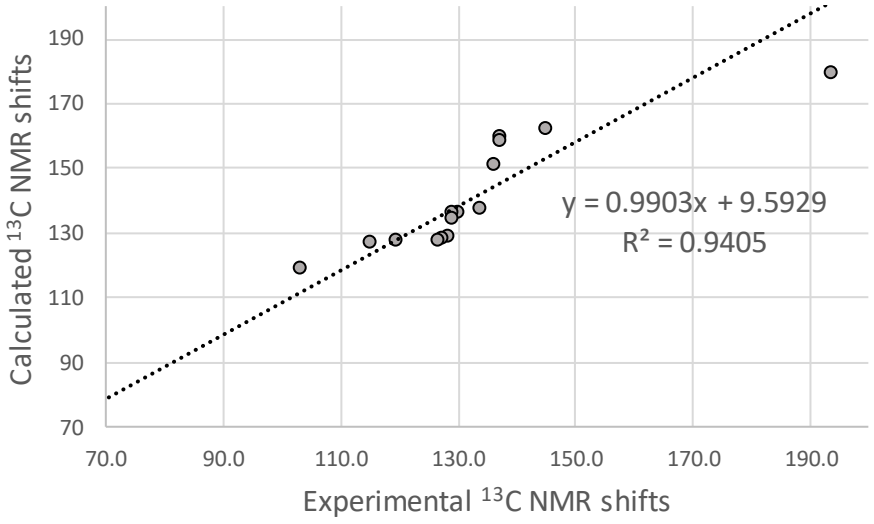
Table S3. Experimental ^{13}C NMR data of synthetic **8l** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **8l**.



8l

δ_{exp}	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.4	C-1	18.8528	180.0	172.1	13.4	21.3
144.8	C-5	36.2095	162.7	154.6	17.9	9.8
137.0	C-3	38.9379	160.0	151.8	23.0	14.8
136.8	C-4	39.8054	159.1	151.0	22.3	14.2
135.8	C-2	47.1368	151.8	143.6	16.0	7.8
133.7	C-7	60.7115	138.2	129.8	4.5	3.9
129.9	C-2'	62.4449	136.4	128.1	6.5	1.8
128.8	C-3'	62.4723	136.4	128.1	7.6	0.7
128.7	C-8	63.9494	134.9	126.6	6.2	2.1
128.2	C-10	69.3059	129.6	121.2	1.4	7.0
127.1	C-6'	69.9181	129.0	120.5	1.9	6.6
126.4	C-5'	70.5898	128.3	119.9	1.9	6.5
119.3	C-9	70.9317	128.0	119.5	8.7	0.2
114.8	C-4'	71.3287	127.6	119.1	12.8	4.3
102.8	C-1'	79.2616	119.6	111.1	16.8	8.3
1.2	C-6	197.4067	1.5	-8.2	0.3	9.4
		Average			***10.1***	***7.4***

* The assignment corresponds to the computed σ vaues.



NMR calculations of 8a at different levels of theory

On the basis of the modest match between experimental and calculated values observed for **8a** at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level of theory, we next undertook the NMR calculations at different levels of theory (pages S13-S21). From the data collected in Tables S4-S6 (Figure S10), we concluded that all the levels of theory under study afforded similar results.

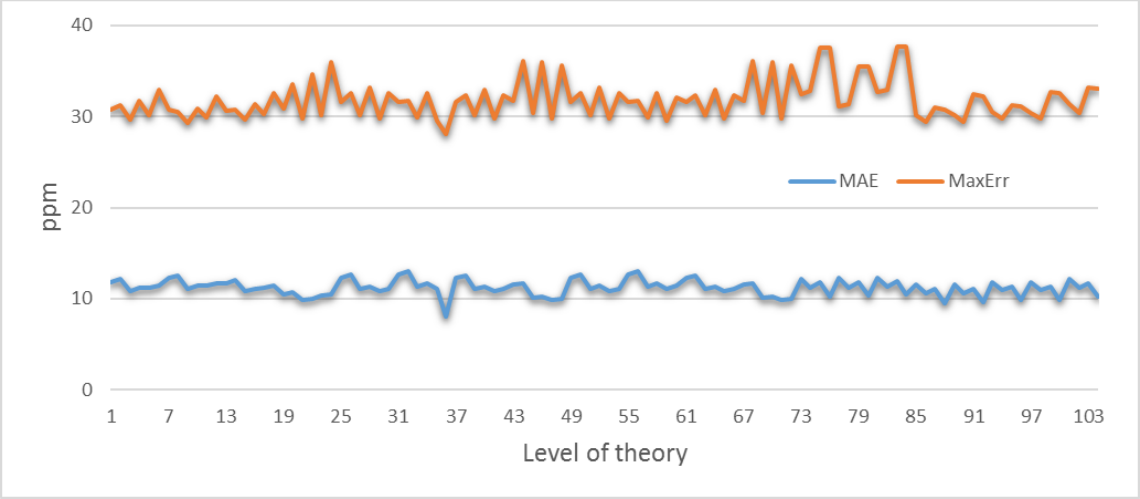


Figure S10. MAE and MaxErr values computed for **8a** at the 104 different levels of theory indicated in Table S4.

Table S4. Levels of theory used for the calculation of the NMR shifts of **8a**.

Level of theory Nº	Geom Opt.	Method	Functional	Basis set	Solvent effect
1	B3LYP/6-31G*	GIAO	mPW1PW91	6-31+G**	Gas Phase
2	B3LYP/6-31G*	GIAO	mPW1PW91	6-31+G**	PCM
3	B3LYP/6-31G*	GIAO	mPW1PW91	cc-PVTZ	Gas Phase
4	B3LYP/6-31G*	GIAO	mPW1PW91	cc-PVTZ	PCM
5	B3LYP/6-31G*	GIAO	mPW1PW91	6-311++G(3df,2pd)	Gas Phase
6	B3LYP/6-31G*	GIAO	mPW1PW91	6-311++G(3df,2pd)	PCM
7	B3LYP/6-31G*	GIAO	B3LYP	6-31+G**	Gas Phase
8	B3LYP/6-31G*	GIAO	B3LYP	6-31+G**	PCM
9	B3LYP/6-31G*	GIAO	B3LYP	cc-PVTZ	Gas Phase
10	B3LYP/6-31G*	GIAO	B3LYP	cc-PVTZ	PCM
11	B3LYP/6-31G*	GIAO	B3LYP	6-311++G(3df,2pd)	Gas Phase
12	B3LYP/6-31G*	GIAO	B3LYP	6-311++G(3df,2pd)	PCM
13	B3LYP/6-31G*	GIAO	PBE0	6-31+G**	Gas Phase
14	B3LYP/6-31G*	GIAO	PBE0	6-31+G**	PCM
15	B3LYP/6-31G*	GIAO	PBE0	cc-PVTZ	Gas Phase
16	B3LYP/6-31G*	GIAO	PBE0	cc-PVTZ	PCM
17	B3LYP/6-31G*	GIAO	PBE0	6-311++G(3df,2pd)	Gas Phase
18	B3LYP/6-31G*	GIAO	PBE0	6-311++G(3df,2pd)	PCM
19	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	6-31+G**	Gas Phase
20	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	6-31+G**	PCM
21	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	cc-PVTZ	Gas Phase
22	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	cc-PVTZ	PCM
23	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	6-311++G(3df,2pd)	Gas Phase
24	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	6-311++G(3df,2pd)	PCM
25	B3LYP/6-31G*	CSGT	mPW1PW91	6-31+G**	Gas Phase
26	B3LYP/6-31G*	CSGT	mPW1PW91	6-31+G**	PCM
27	B3LYP/6-31G*	CSGT	mPW1PW91	cc-PVTZ	Gas Phase
28	B3LYP/6-31G*	CSGT	mPW1PW91	cc-PVTZ	PCM
29	B3LYP/6-31G*	CSGT	mPW1PW91	6-311++G(3df,2pd)	Gas Phase
30	B3LYP/6-31G*	CSGT	mPW1PW91	6-311++G(3df,2pd)	PCM
31	B3LYP/6-31G*	CSGT	B3LYP	6-31+G**	Gas Phase
32	B3LYP/6-31G*	CSGT	B3LYP	6-31+G**	PCM
33	B3LYP/6-31G*	CSGT	B3LYP	cc-PVTZ	Gas Phase
34	B3LYP/6-31G*	CSGT	B3LYP	cc-PVTZ	PCM
35	B3LYP/6-31G*	CSGT	B3LYP	6-311++G(3df,2pd)	Gas Phase
36	B3LYP/6-31G*	CSGT	B3LYP	6-311++G(3df,2pd)	PCM
37	B3LYP/6-31G*	CSGT	PBE0	6-31+G**	Gas Phase
38	B3LYP/6-31G*	CSGT	PBE0	6-31+G**	PCM
39	B3LYP/6-31G*	CSGT	PBE0	cc-PVTZ	Gas Phase
40	B3LYP/6-31G*	CSGT	PBE0	cc-PVTZ	PCM
41	B3LYP/6-31G*	CSGT	PBE0	6-311++G(3df,2pd)	Gas Phase
42	B3LYP/6-31G*	CSGT	PBE0	6-311++G(3df,2pd)	PCM
43	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-31+G**	Gas Phase
44	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-31+G**	PCM
45	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	cc-PVTZ	Gas Phase
46	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
47	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-311++G(3df,2pd)	Gas Phase
48	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-311++G(3df,2pd)	PCM
49	B3LYP/6-31G*	IGAIM	mPW1PW91	6-31+G**	Gas Phase
50	B3LYP/6-31G*	IGAIM	mPW1PW91	6-31+G**	PCM
51	B3LYP/6-31G*	IGAIM	mPW1PW91	cc-PVTZ	Gas Phase
52	B3LYP/6-31G*	IGAIM	mPW1PW91	cc-PVTZ	PCM
53	B3LYP/6-31G*	IGAIM	mPW1PW91	6-311++G(3df,2pd)	Gas Phase
54	B3LYP/6-31G*	IGAIM	mPW1PW91	6-311++G(3df,2pd)	PCM
55	B3LYP/6-31G*	IGAIM	B3LYP	6-31+G**	Gas Phase
56	B3LYP/6-31G*	IGAIM	B3LYP	6-31+G**	PCM
57	B3LYP/6-31G*	IGAIM	B3LYP	cc-PVTZ	Gas Phase
58	B3LYP/6-31G*	IGAIM	B3LYP	cc-PVTZ	PCM
59	B3LYP/6-31G*	IGAIM	B3LYP	6-311++G(3df,2pd)	Gas Phase
60	B3LYP/6-31G*	IGAIM	B3LYP	6-311++G(3df,2pd)	PCM
61	B3LYP/6-31G*	IGAIM	PBE0	6-31+G**	Gas Phase
62	B3LYP/6-31G*	IGAIM	PBE0	6-31+G**	PCM

Table S4 (cont). Levels of theory used for the calculation of the NMR shifts of **8a**.

Level of theory Nº	Geom Opt.	Method	Functional	Basis set	Solvent effect
63	B3LYP/6-31G*	IGAIM	PBE0	cc-PVTZ	Gas Phase
64	B3LYP/6-31G*	IGAIM	PBE0	cc-PVTZ	PCM
65	B3LYP/6-31G*	IGAIM	PBE0	6-311++G(3df,2pd)	Gas Phase
66	B3LYP/6-31G*	IGAIM	PBE0	6-311++G(3df,2pd)	PCM
67	B3LYP/6-31G*	IGAIM	LC-TPSSTPSS	6-31+G**	Gas Phase
68	B3LYP/6-31G*	IGAIM	LC-TPSSTPSS	6-31+G**	PCM
69	B3LYP/6-31G*	IGAIM	LC-TPSSTPSS	cc-PVTZ	Gas Phase
70	B3LYP/6-31G*	IGAIM	LC-TPSSTPSS	cc-PVTZ	PCM
71	B3LYP/6-31G*	IGAIM	LC-TPSSTPSS	6-311++G(3df,2pd)	Gas Phase
72	B3LYP/6-31G*	IGAIM	LC-TPSSTPSS	6-311++G(3df,2pd)	PCM
73	PCM/B3LYP/6-31G*	GIAO	mPW1PW91	6-31+G**	PCM
74	PCM/B3LYP/6-31G*	GIAO	mPW1PW91	cc-PVTZ	PCM
75	PCM/B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-31+G**	PCM
76	PCM/B3LYP/6-31G*	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
77	B3LYP/6-311+G**	GIAO	mPW1PW91	6-31+G**	PCM
78	B3LYP/6-311+G**	GIAO	mPW1PW91	cc-PVTZ	PCM
79	B3LYP/6-311+G**	CSGT	LC-TPSSTPSS	6-31+G**	PCM
80	B3LYP/6-311+G**	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
81	PCM/B3LYP/6-311+G**	GIAO	mPW1PW91	6-31+G**	PCM
82	PCM/B3LYP/6-311+G**	GIAO	mPW1PW91	cc-PVTZ	PCM
83	PCM/B3LYP/6-311+G**	CSGT	LC-TPSSTPSS	6-31+G**	PCM
84	PCM/B3LYP/6-311+G**	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
85	M06-2X/6-31G*	GIAO	mPW1PW91	6-31+G**	PCM
86	M06-2X/6-31G*	GIAO	mPW1PW91	cc-PVTZ	PCM
87	M06-2X/6-31G*	CSGT	LC-TPSSTPSS	6-31+G**	PCM
88	M06-2X/6-31G*	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
89	PCM/M06-2X/6-31G*	GIAO	mPW1PW91	6-31+G**	PCM
90	PCM/M06-2X/6-31G*	GIAO	mPW1PW91	cc-PVTZ	PCM
91	PCM/M06-2X/6-31G*	CSGT	LC-TPSSTPSS	6-31+G**	PCM
92	PCM/M06-2X/6-31G*	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
93	M06-2X/6-311+G**	GIAO	mPW1PW91	6-31+G**	PCM
94	M06-2X/6-311+G**	GIAO	mPW1PW91	cc-PVTZ	PCM
95	M06-2X/6-311+G**	CSGT	LC-TPSSTPSS	6-31+G**	PCM
96	M06-2X/6-311+G**	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
97	PCM/M06-2X/6-311+G**	GIAO	mPW1PW91	6-31+G**	PCM
98	PCM/M06-2X/6-311+G**	GIAO	mPW1PW91	cc-PVTZ	PCM
99	PCM/M06-2X/6-311+G**	CSGT	LC-TPSSTPSS	6-31+G**	PCM
100	PCM/M06-2X/6-311+G**	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
101	MP2/6-31G*	GIAO	mPW1PW91	6-31+G**	PCM
102	MP2/6-31G*	GIAO	mPW1PW91	cc-PVTZ	PCM
103	MP2/6-31G*	CSGT	LC-TPSSTPSS	6-31+G**	PCM
104	MP2/6-31G*	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM

Table S5. Boltzmann averaged isotropic magnetic shielding values (σ) calculated at the levels of theory indicated in Table Sx for all significantly populated conformers of **8a** (arranged in ascending order of magnitude)

Level of theory N°											
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
22.7422	21.6267	3.5630	2.4127	1.9206	0.7257	21.0456	20.0861	0.0607	-0.9724	-2.0239	-3.0972
30.0966	24.3304	12.5545	6.8562	10.4777	4.5624	29.0178	23.2288	9.1900	3.4552	6.8632	0.8477
38.4408	38.2587	22.6443	22.6117	20.2886	20.2519	35.5563	35.2891	18.0605	17.9747	15.5124	15.4023
51.1349	52.3405	34.2897	35.5768	32.3133	33.7263	47.8121	48.9383	29.0380	30.2345	26.8647	28.1978
60.8708	60.5429	44.2879	44.5521	43.3606	43.6435	57.3024	56.6125	38.9052	39.1226	38.1666	38.3868
61.3708	61.0509	47.6359	46.8312	46.0071	45.8976	57.4812	57.4280	42.5995	41.7777	41.6048	40.7345
63.2213	61.9960	47.6547	48.1307	46.7366	46.4859	59.4618	58.2782	43.5016	43.9746	41.7612	42.2339
64.2996	64.6972	49.8949	50.0678	47.7793	47.9960	61.5266	61.9086	44.6224	44.7794	42.4817	42.6510
65.3867	65.5505	51.3844	50.0939	49.3007	48.0130	61.9141	62.0279	47.1169	45.8197	44.7299	43.4681
69.2857	68.6401	51.8118	51.2142	51.3999	50.7800	66.9127	66.3416	47.7745	47.2346	47.2990	46.7517
70.3278	70.0108	53.0867	52.8359	51.8289	51.5753	67.5877	67.3309	48.8116	48.6029	47.3093	47.0926
70.5032	70.0420	53.2892	52.8811	52.3448	51.6884	67.7820	67.3885	49.0040	48.6493	48.0493	47.4607
71.0469	70.3668	53.8491	53.2003	52.5205	52.1068	68.8287	68.2321	49.8309	49.2455	48.1037	47.7478
71.9916	71.5324	55.0844	54.6332	54.0833	53.6445	69.4410	69.0125	51.0018	50.5632	49.8339	49.4109
81.4643	81.5505	65.4960	65.5460	63.9048	63.9981	78.9500	79.0093	61.6039	61.6208	59.7239	59.7935

Level of theory N°											
13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
22.7935	21.6674	3.9379	2.7904	2.4261	1.2361	18.1429	15.9063	-1.7484	-4.0125	-3.4709	-5.8287
30.8329	25.0651	13.4842	7.8156	11.4788	5.5834	28.7047	22.6273	9.8365	3.8470	7.5961	1.3639
39.1689	38.9950	23.4921	23.4702	21.1544	21.1268	40.6008	40.6684	23.2023	23.4434	21.1279	21.3722
51.2808	52.4654	34.8679	36.1307	32.9335	34.3210	53.1255	54.9834	37.1077	39.1129	34.9341	37.0812
61.3556	60.9720	44.9481	45.2068	44.1936	44.4615	62.6734	62.9153	45.6192	45.9709	43.8020	44.1686
61.8079	61.5317	48.3210	47.5819	46.7074	46.6595	65.7196	66.0925	48.1470	48.6125	46.4432	46.9233
63.6520	62.4085	48.3852	48.7976	47.4954	47.1865	67.3092	66.2025	51.2704	50.7816	49.6629	48.6701
64.5761	64.9751	50.5277	50.5995	48.5846	48.5631	67.7449	67.7284	51.3060	50.8111	50.0239	49.5097
65.8231	65.9880	51.9218	50.7283	49.8501	48.7975	69.2580	68.4868	52.2340	51.0950	50.0826	49.7133
69.5757	68.9224	52.4939	51.8875	52.0798	51.4510	69.7761	68.7417	52.2541	51.3345	50.9948	49.8132
70.5295	70.2058	53.7412	53.4790	52.4776	52.2162	70.7681	70.4626	53.2852	52.7461	52.0758	51.6690
70.7182	70.2484	53.9371	53.5209	53.0058	52.3372	71.3826	70.7072	53.4325	53.0316	52.3585	51.8273
71.3253	70.6367	54.5052	53.8442	53.1687	52.7488	71.4111	70.9074	54.1769	53.7030	52.8947	52.4211
72.2002	71.7453	55.7648	55.3097	54.7619	54.3263	72.2630	71.7693	54.9681	54.4500	53.5210	53.0279
81.8588	81.9371	66.1650	66.2039	64.5808	64.6724	81.9025	82.1919	65.3758	65.6937	63.8233	64.1933

Level of theory N°											
25	**26**	**27**	**28**	**29**	**30**	**31**	**32**	**33**	**34**	**35**	**36**
19.7882	18.8981	4.5256	3.4676	2.2726	1.0639	19.1645	18.4350	1.1369	0.1974	-1.7358	1.0639
26.2097	20.3532	11.5311	5.9776	11.5368	5.6200	25.3925	19.5359	7.9091	2.3373	7.6279	5.6200
32.8813	32.7978	23.1654	23.0626	22.0323	21.9788	30.6631	30.4830	18.6127	18.4414	17.1636	21.9788
44.9138	46.0567	34.9877	36.1748	33.6151	35.0222	42.4464	43.5019	29.8881	30.9723	28.1348	35.0222
57.4626	56.7564	45.5272	45.7132	44.3082	44.5370	54.6714	53.9251	40.4074	40.5426	38.7578	44.5370
58.6104	58.7839	47.0641	46.4047	47.1598	46.6720	55.8405	55.9524	41.9410	41.2649	42.2278	46.6720
62.0278	62.4164	48.6142	49.1005	47.5183	47.6072	59.9583	60.0598	44.5081	44.9897	42.6403	47.6072
62.8120	62.6368	50.7347	49.8584	49.6954	49.0933	60.2433	60.6166	45.6242	45.5105	44.2367	49.0933
63.7994	62.9724	51.0517	50.8962	50.4015	49.8760	61.7683	60.6403	46.6706	45.7453	45.7714	49.8760
66.2640	65.6754	52.2041	51.6859	51.6834	51.0608	64.6814	64.1565	48.1678	47.7107	47.3969	51.0608
67.4380	67.0320	53.4627	53.2585	52.8083	52.5603	65.6328	65.2898	49.1824	49.0196	48.2458	52.5603
67.5088	67.2413	53.6187	53.2615	52.9768	52.5623	65.7182	65.5054	49.3213	49.0227	48.3966	52.5623
68.1456	67.5317	53.9318	53.3680	53.4977	52.8510	66.5224	65.9888	49.8365	49.3407	49.1690	52.8510
68.8013	68.3596	56.0703	55.6631	54.7405	54.2874	67.0160	66.5957	52.0281	51.6343	50.3057	54.2874
77.9631	78.0354	65.5770	65.6383	64.9537	65.0390	76.2675	76.3188	61.6480	61.6792	60.7289	65.0390

Table S5 (cont). Boltzmann averaged isotropic magnetic shielding values (σ) calculated at the levels of theory indicated in Table Sx for all significantly populated conformers of **8a** (arranged in ascending order of magnitude)

Level of theory N°											
37	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**	**46**	**48**	**48**
19.8832	18.9852	4.9100	3.8556	2.7133	1.5136	15.3583	13.3708	-0.6282	-2.7698	-3.2037	-5.5596
26.6715	20.8539	12.3266	6.8089	12.3914	6.5018	23.5941	17.5093	8.8326	2.9909	8.6966	2.4833
33.3693	33.2900	23.9969	23.9009	22.8997	22.8530	33.4866	33.6536	23.7120	23.8952	22.6584	22.8822
45.1788	46.2933	35.5812	36.7359	34.2174	35.5928	47.3499	49.1377	37.2994	39.2097	36.3985	38.5275
57.7989	57.0963	46.2604	46.4387	45.0357	45.2571	60.4234	60.3964	46.4735	46.7401	45.3994	45.7274
59.0013	59.1666	47.7681	47.1123	47.8025	47.4233	61.3367	60.6265	49.2929	49.7712	47.7180	48.1634
62.3116	62.6983	49.2464	49.7326	48.2668	48.2509	63.4763	63.8304	51.6197	50.6163	50.9760	49.9648
63.1488	62.8020	51.4248	50.3429	50.3830	49.6238	65.0064	63.8332	51.6378	50.7494	51.1117	50.4609
63.9659	63.3069	51.5357	51.5871	50.9340	50.5634	65.0446	64.9914	52.0651	51.2172	51.3689	50.9570
66.5651	65.9690	52.8512	52.3267	52.3707	51.7420	66.5727	66.0916	52.1578	52.1383	52.1435	51.1341
67.6928	67.2789	54.0886	53.8601	53.4548	53.1826	68.3598	67.9954	53.6639	53.0457	52.9648	52.4291
67.7862	67.5082	54.2240	53.8744	53.6035	53.1977	68.6381	68.0769	53.6697	53.4543	53.1140	52.7137
68.4051	67.7809	54.5314	53.9582	54.1319	53.4769	68.9070	68.4470	54.5029	54.0759	53.8114	53.3339
69.0958	68.6504	56.7239	56.3131	55.3897	54.9353	69.6034	69.1058	56.0780	55.6070	54.6727	54.1614
78.2598	78.3263	66.2181	66.2710	65.6212	65.7003	78.5865	78.8559	65.5700	65.8821	64.9488	65.3134

Level of theory N°											
49	**50**	**52**	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**
19.8002	18.9102	4.5392	3.4812	2.2770	1.0683	19.1769	18.4476	1.1509	0.2114	-1.7313	-2.8210
26.2254	20.3690	11.5415	5.9880	11.5411	5.6244	25.4088	19.5521	7.9198	2.3480	7.6323	1.6227
32.8814	32.7979	23.1679	23.0652	22.0330	21.9795	30.6638	30.4837	18.6153	18.4440	17.1646	17.0403
44.9147	46.0577	34.9914	36.1785	33.6162	35.0234	42.4479	43.5034	29.8919	30.9762	28.1361	29.4571
57.4640	56.7578	45.5307	45.7168	44.3089	44.5377	54.6734	53.9271	40.4111	40.5463	38.7586	38.9298
58.6112	58.7848	47.0673	46.4079	47.1635	46.6729	55.8420	55.9539	41.9443	41.2682	42.2289	41.3517
62.0412	62.4298	48.6242	49.1107	47.5192	47.6109	59.9611	60.0626	44.5183	45.0000	42.6441	43.0852
62.8142	62.6498	50.7380	49.8680	49.6962	49.0970	60.2572	60.6306	45.6276	45.5203	44.2376	44.3698
63.8123	62.9746	51.0613	50.8995	50.4051	49.8768	61.7817	60.6537	46.6804	45.7487	45.7752	44.4822
66.2813	65.6928	52.2162	51.6982	51.6875	51.0649	64.6992	64.1743	48.1803	47.7232	47.4011	46.8413
67.4547	67.0487	53.4746	53.2704	52.8124	52.5643	65.6499	65.3070	49.1946	49.0317	48.2500	48.0438
67.5254	67.2580	53.6306	53.2733	52.9808	52.5663	65.7353	65.5225	49.3334	49.0349	48.4007	48.0496
68.1628	67.5489	53.9440	53.3802	53.5018	52.8552	66.5401	66.0065	49.8490	49.3533	49.1732	48.5989
68.8154	68.3738	56.0810	55.6739	54.7443	54.2911	67.0306	66.6104	52.0389	51.6452	50.3096	49.8680
77.9768	78.0491	65.5868	65.6482	64.9574	65.0428	76.2816	76.3330	61.6580	61.6892	60.7327	60.7894

Level of theory N°											
61	**62**	**63**	**64**	**65**	**66**	**67**	**68**	**69**	**70**	**71**	**72**
19.8950	18.9973	4.9236	3.8692	2.7177	1.5180	15.3705	13.3832	-0.6145	-2.7560	-3.1994	-5.5552
26.6871	20.8696	12.3369	6.8193	12.3957	6.5061	23.6101	17.5253	8.8431	3.0014	8.7008	2.4876
33.3693	33.2900	23.9993	23.9033	22.9005	22.8538	33.4865	33.6535	23.7145	23.8977	22.6591	22.8830
45.1796	46.2942	35.5848	36.7395	34.2185	35.5939	47.3510	49.1388	37.3032	39.2135	36.3996	38.5285
57.8002	57.0976	46.2639	46.4421	45.0364	45.2578	60.4241	60.3978	46.4771	46.7437	45.4000	45.7281
59.0020	59.1674	47.7713	47.1154	47.8062	47.4243	61.3380	60.6273	49.3030	49.7814	47.7217	48.1670
62.3250	62.7117	49.2564	49.7425	48.2677	48.2546	63.4899	63.8440	51.6229	50.6196	50.9801	49.9684
63.1509	62.8148	51.4281	50.3525	50.3838	49.6274	65.0086	63.8461	51.6502	50.7591	51.1125	50.4650
63.9787	63.3091	51.5451	51.5903	50.9377	50.5642	65.0574	64.9935	52.0747	51.2296	51.3725	50.9579
66.5824	65.9863	52.8633	52.3388	52.3748	51.7462	66.5902	66.1092	52.1612	52.1417	52.1444	51.1348
67.7095	67.2955	54.1004	53.8718	53.4589	53.1867	68.3766	68.0128	53.6762	53.0581	52.9688	52.4333
67.8027	67.5248	54.2358	53.8863	53.6075	53.2018	68.6555	68.0938	53.6818	53.4664	53.1182	52.7177
68.4222	67.7981	54.5435	53.9703	54.1360	53.4810	68.9240	68.4640	54.5148	54.0879	53.8154	53.3379
69.1098	68.6644	56.7344	56.3237	55.3934	54.9390	69.6177	69.1200	56.0887	55.6178	54.6765	54.1651
78.2733	78.3400	66.2279	66.2807	65.6249	65.7041	78.6002	78.8696	65.5799	65.8920	64.9525	65.3170

Table S5 (cont). Boltzmann averaged isotropic magnetic shielding values (σ) calculated at the levels of theory indicated in Table Sx for all significantly populated conformers of **8a** (arranged in ascending order of magnitude)

Level of theory N°											
73	**74**	**75**	**76**	**77**	**78**	**79**	**80**	**81**	**82**	**83**	**84**
21.0979	1.7350	12.5871	-3.6336	22.5139	3.3416	14.4329	-1.6184	21.7805	2.4085	13.3569	-2.8037
23.0270	5.6061	15.8129	1.2535	25.0715	7.7182	18.5351	4.0977	23.3105	6.0210	16.2568	1.7641
37.9611	22.3174	33.2134	23.4643	39.2531	23.6704	34.7515	25.0705	38.7718	23.1896	34.0796	24.3932
52.6352	35.9016	49.3236	39.4434	51.8452	35.1347	48.5257	38.6175	52.2644	35.6066	48.8119	38.9755
60.2820	44.3872	60.1463	46.5830	60.6392	45.0083	60.4179	47.2380	60.3726	44.8383	60.1848	47.0750
60.8984	46.5582	60.4797	49.6949	61.4664	46.9186	61.0740	50.5845	61.3076	46.6678	60.9213	50.3894
61.7397	48.0678	63.6134	50.3862	62.2344	49.0382	64.0296	50.6424	61.9738	48.9572	63.8317	50.5433
64.6307	49.7878	63.7639	50.5007	65.5311	50.3235	64.6256	50.9744	65.4483	50.0365	64.5376	50.7430
65.5554	50.0686	64.9796	50.9533	66.0284	50.6189	65.4398	51.8424	66.0455	50.6076	65.4400	51.5201
68.3920	50.9654	65.8430	52.1362	69.2641	51.8269	66.6479	52.6021	68.9640	51.5168	66.3447	52.6204
69.8463	52.6596	67.8780	52.9137	70.4543	53.3015	68.4076	53.5110	70.2684	53.1020	68.2792	53.3659
69.9196	52.7513	67.9051	53.2627	70.5112	53.3723	68.4847	53.9106	70.3688	53.2188	68.2922	53.6957
70.2278	53.0510	68.3300	53.9503	70.8163	53.6792	68.8556	54.5274	70.6583	53.5095	68.7197	54.3829
71.4042	54.4934	68.9830	55.4736	72.0283	55.1607	69.5841	56.1307	71.8864	55.0052	69.4498	55.9855
81.4456	65.4189	78.7575	65.7936	81.9216	65.9576	79.2348	66.3131	81.8349	65.8474	79.1632	66.2516

Level of theory N°											
85	**86**	**87**	**88**	**89**	**90**	**91**	**92**	**93**	**94**	**95**	**96**
23.8756	4.6909	16.1173	0.2366	23.1741	3.8357	15.1182	-0.8381	23.8756	4.6909	16.1173	0.2366
28.6014	11.2062	23.3377	9.1327	27.2816	9.9243	21.7150	7.4740	28.6014	11.2062	23.3377	9.1327
43.0276	27.3630	39.3761	29.9085	42.7296	27.0565	38.9778	29.5130	43.0276	27.3630	39.3761	29.9085
51.0036	34.4298	47.8227	37.8065	51.2603	34.6950	47.9334	37.9703	51.0036	34.4298	47.8227	37.8065
61.5136	46.0360	61.3903	48.4517	61.2113	45.8260	61.1092	48.2495	61.5136	46.0360	61.3903	48.4517
62.3399	47.6891	62.1621	50.4398	62.1429	47.3886	61.9743	50.1549	62.3399	47.6891	62.1621	50.4398
62.5319	49.7741	63.4836	51.4501	62.2331	49.4565	63.2231	51.1872	62.5319	49.7741	63.4836	51.4501
66.9831	50.7455	66.2001	52.4289	66.8771	50.6391	66.1038	52.3167	66.9831	50.7455	66.2001	52.4289
67.0321	51.4150	66.2020	53.2321	66.9815	51.3408	66.1392	52.9685	67.0321	51.4150	66.2020	53.2321
70.4659	53.0232	67.9483	53.4271	70.2122	52.7660	67.7029	53.3695	70.4659	53.0232	67.9483	53.4271
70.7846	53.8652	68.9684	54.1985	70.6311	53.6505	68.7627	54.0480	70.7846	53.8652	68.9684	54.1985
70.9385	53.9267	69.0424	54.4453	70.7378	53.7603	68.9085	54.2158	70.9385	53.9267	69.0424	54.4453
71.4591	54.3019	69.2882	54.9466	71.3041	54.1336	69.1380	54.7829	71.4591	54.3019	69.2882	54.9466
73.0008	56.1333	70.5005	57.1404	72.8427	55.9627	70.3485	56.9758	73.0008	56.1333	70.5005	57.1404
82.6351	66.3425	79.8179	66.9979	82.5019	66.1873	79.6908	66.8781	82.6351	66.3425	79.8179	66.9979

Level of theory N°							
97	**98**	**99**	**100**	**101**	**102**	**103**	**104**
23.1741	3.8357	15.1182	-0.8381	18.8717	-0.5922	10.4312	-5.7874
27.2816	9.9243	21.7150	7.4740	25.9462	8.7358	20.3396	5.9467
42.7296	27.0565	38.9778	29.5130	41.2390	25.7065	37.0197	27.6887
51.2603	34.6950	47.9334	37.9703	48.4507	31.5914	45.2732	35.0344
61.2113	45.8260	61.1092	48.2495	58.4846	44.0729	57.7989	47.3566
62.1429	47.3886	61.9743	50.1549	59.9645	45.0483	61.1592	47.6338
62.2331	49.4565	63.2231	51.1872	61.5625	47.8869	61.2903	48.1608
66.8771	50.6391	66.1038	52.3167	65.6461	49.1637	64.8190	50.8718
66.9815	51.3408	66.1392	52.9685	66.1107	50.4414	65.3000	51.9180
70.2122	52.7660	67.7029	53.3695	69.0809	51.8276	66.7197	52.4096
70.6311	53.6505	68.7627	54.0480	69.7021	52.5395	67.7804	52.8440
70.7378	53.7603	68.9085	54.2158	69.7310	52.5684	67.8158	53.1342
71.3041	54.1336	69.1380	54.7829	70.1673	52.9775	68.0872	53.6327
72.8427	55.9627	70.3485	56.9758	71.4881	54.5722	69.0633	55.5749
82.5019	66.1873	79.6908	66.8781	80.6797	64.5782	77.8324	64.9732

Table S6. Unscaled chemical shifts calculated at the levels of theory indicated in Table S4 for all significantly populated conformers of **8a** (arranged in descending order of magnitude) using the Boltzmann Boltzmann averaged isotropic magnetic shielding values shown in Table S5.

Level of theory N°											
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
176.4	177.3	178.5	179.4	179.1	180.1	175.6	176.4	177.8	178.6	178.6	179.5
169.0	174.6	169.5	175.0	170.5	176.2	167.6	173.2	168.7	174.2	169.7	175.5
160.7	160.6	159.4	159.2	160.7	160.5	161.1	161.2	159.8	159.7	161.1	161.0
148.0	146.5	147.8	146.3	148.7	147.1	148.8	147.5	148.8	147.4	149.7	148.2
138.2	138.3	137.8	137.3	137.6	137.1	139.3	139.8	138.9	138.5	138.4	138.0
137.7	137.8	134.4	135.0	135.0	134.9	139.1	139.0	135.2	135.9	135.0	135.6
135.9	136.9	134.4	133.7	134.3	134.3	137.2	138.2	134.3	133.7	134.8	134.1
134.8	134.2	132.2	131.8	133.2	132.8	135.1	134.5	133.2	132.9	134.1	133.7
133.7	133.3	130.7	131.7	131.7	132.8	134.7	134.4	130.7	131.8	131.8	132.9
129.8	130.2	130.2	130.6	129.6	130.0	129.7	130.1	130.1	130.4	129.3	129.6
128.8	128.9	129.0	129.0	129.2	129.2	129.0	129.1	129.0	129.0	129.3	129.3
128.6	128.8	128.8	129.0	128.7	129.1	128.8	129.1	128.8	129.0	128.5	128.9
128.1	128.5	128.2	128.6	128.5	128.7	127.8	128.2	128.0	128.4	128.5	128.6
127.1	127.4	127.0	127.2	126.9	127.1	127.2	127.4	126.8	127.1	126.7	127.0
117.6	117.3	116.6	116.3	117.1	116.8	117.7	117.4	116.2	116.0	116.9	116.6

Level of theory N°											
13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
176.6	177.5	178.8	179.7	179.3	180.2	181.5	183.5	183.8	185.8	184.4	186.4
168.5	174.1	169.2	174.7	170.2	175.9	171.0	176.8	172.2	177.9	173.3	179.3
160.2	160.1	159.2	159.0	160.5	160.3	159.1	158.8	158.8	158.3	159.8	159.2
148.1	146.7	147.9	146.4	148.8	147.1	146.6	144.4	144.9	142.6	146.0	143.5
138.0	138.2	137.8	137.3	137.5	137.0	137.0	136.5	136.4	135.8	137.1	136.4
137.6	137.6	134.4	134.9	135.0	134.8	134.0	133.3	133.9	133.1	134.4	133.7
135.7	136.7	134.3	133.7	134.2	134.3	132.4	133.2	130.7	131.0	131.2	131.9
134.8	134.2	132.2	131.9	133.1	132.9	131.9	131.7	130.7	130.9	130.9	131.1
133.5	133.2	130.8	131.8	131.9	132.7	130.4	130.9	129.8	130.6	130.8	130.9
129.8	130.2	130.2	130.6	129.6	130.0	129.9	130.7	129.8	130.4	129.9	130.8
128.8	128.9	129.0	129.0	129.2	129.3	128.9	129.0	128.7	129.0	128.8	128.9
128.6	128.9	128.8	129.0	128.7	129.1	128.3	128.7	128.6	128.7	128.5	128.8
128.0	128.5	128.2	128.7	128.5	128.7	128.3	128.5	127.8	128.0	128.0	128.2
127.2	127.4	127.0	127.2	126.9	127.1	127.4	127.7	127.0	127.3	127.4	127.6
117.5	117.2	116.6	116.3	117.1	116.8	117.8	117.2	116.6	116.0	117.1	116.4

Level of theory N°											
25	**26**	**27**	**28**	**29**	**30**	**31**	**32**	**33**	**34**	**35**	**36**
176.7	177.3	178.1	178.9	179.4	180.4	175.6	176.1	177.3	178.0	178.9	175.9
170.3	175.9	171.1	176.4	170.1	175.8	169.3	175.0	170.5	175.9	169.5	171.3
163.6	163.4	159.4	159.3	159.6	159.5	164.1	164.0	159.8	159.8	160.0	155.0
151.5	150.2	147.6	146.2	148.1	146.4	152.3	151.0	148.5	147.3	149.0	141.9
139.0	139.5	137.1	136.7	137.4	136.9	140.1	140.6	138.0	137.7	138.4	132.4
137.9	137.4	135.5	136.0	134.5	134.8	138.9	138.6	136.4	137.0	134.9	130.3
134.4	133.8	134.0	133.3	134.2	133.8	134.8	134.5	133.9	133.2	134.5	129.3
133.6	133.6	131.9	132.6	132.0	132.4	134.5	133.9	132.8	132.7	132.9	127.9
132.7	133.3	131.5	131.5	131.3	131.6	133.0	133.9	131.7	132.5	131.4	127.1
130.2	130.6	130.4	130.7	130.0	130.4	130.0	130.4	130.2	130.5	129.8	125.9
129.0	129.2	129.1	129.2	128.9	128.9	129.1	129.2	129.2	129.2	128.9	124.4
129.0	129.0	129.0	129.2	128.7	128.9	129.0	129.0	129.1	129.2	128.8	124.4
128.3	128.7	128.7	129.0	128.2	128.6	128.2	128.5	128.6	128.9	128.0	124.1
127.7	127.9	126.5	126.7	126.9	127.2	127.7	127.9	126.4	126.6	126.8	122.7
118.5	118.2	117.0	116.8	116.7	116.4	118.5	118.2	116.7	116.6	116.4	111.9

Table S6 (cont). Unscaled chemical shifts calculated at the levels of theory indicated in Table S4 for all significantly populated conformers of **8a** (arranged in descending order of magnitude) using the Boltzmann Boltzmann averaged isotropic magnetic shielding values shown in Table S5.

Level of theory N°											
37	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**	**46**	**48**	**48**
176.9	177.5	178.3	179.2	179.6	180.6	181.8	183.5	183.2	185.1	184.8	186.9
170.1	175.7	170.9	176.2	169.9	175.6	173.6	179.4	173.7	179.3	172.9	178.9
163.4	163.2	159.2	159.1	159.4	159.2	163.7	163.2	158.8	158.4	159.0	158.5
151.6	150.2	147.6	146.3	148.1	146.5	149.8	147.7	145.2	143.1	145.2	142.8
139.0	139.4	137.0	136.6	137.3	136.8	136.7	136.5	136.1	135.6	136.2	135.6
137.7	137.3	135.5	135.9	134.5	134.7	135.8	136.2	133.3	132.5	133.9	133.2
134.4	133.8	134.0	133.3	134.1	133.8	133.7	133.0	130.9	131.7	130.7	131.4
133.6	133.7	131.8	132.7	131.9	132.5	132.1	133.0	130.9	131.6	130.5	130.9
132.8	133.2	131.7	131.5	131.4	131.5	132.1	131.9	130.5	131.1	130.3	130.4
130.2	130.5	130.4	130.7	130.0	130.4	130.6	130.8	130.4	130.2	129.5	130.2
129.1	129.2	129.1	129.2	128.9	128.9	128.8	128.9	128.9	129.3	128.7	128.9
129.0	129.0	129.0	129.2	128.7	128.9	128.5	128.8	128.9	128.9	128.5	128.6
128.3	128.7	128.7	129.1	128.2	128.6	128.2	128.4	128.0	128.2	127.8	128.0
127.7	127.9	126.5	126.7	126.9	127.2	127.6	127.8	126.5	126.7	127.0	127.2
118.5	118.2	117.0	116.8	116.7	116.4	118.6	118.0	117.0	116.4	116.7	116.0

Level of theory N°											
49	**50**	**52**	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**
176.7	177.3	178.1	178.9	179.4	180.4	175.6	176.1	177.3	178.0	178.9	179.8
170.3	175.9	171.1	176.4	170.1	175.8	169.3	175.0	170.5	175.9	169.5	175.3
163.6	163.5	159.4	159.4	159.6	159.5	164.1	164.1	159.8	159.8	160.0	159.9
151.6	150.2	147.6	146.2	148.1	146.4	152.3	151.0	148.5	147.3	149.0	147.5
139.0	139.5	137.1	136.7	137.4	136.9	140.1	140.6	138.0	137.7	138.4	138.0
137.9	137.5	135.5	136.0	134.5	134.8	138.9	138.6	136.5	137.0	134.9	135.6
134.4	133.8	134.0	133.3	134.2	133.8	134.8	134.5	133.9	133.3	134.5	133.9
133.7	133.6	131.9	132.6	132.0	132.4	134.5	133.9	132.8	132.7	132.9	132.6
132.7	133.3	131.5	131.5	131.3	131.6	133.0	133.9	131.7	132.5	131.4	132.5
130.2	130.6	130.4	130.7	130.0	130.4	130.0	130.4	130.2	130.5	129.8	130.1
129.0	129.2	129.1	129.2	128.9	128.9	129.1	129.2	129.2	129.2	128.9	128.9
129.0	129.0	129.0	129.2	128.7	128.9	129.0	129.0	129.1	129.2	128.8	128.9
128.3	128.7	128.7	129.0	128.2	128.6	128.2	128.5	128.6	128.9	128.0	128.4
127.7	127.9	126.5	126.7	126.9	127.2	127.7	127.9	126.4	126.6	126.8	127.1
118.5	118.2	117.0	116.8	116.7	116.4	118.5	118.2	116.7	116.6	116.4	116.2

Level of theory N°											
61	**62**	**63**	**64**	**65**	**66**	**67**	**68**	**69**	**70**	**71**	**72**
176.9	177.5	178.3	179.2	179.6	180.6	181.8	183.5	183.2	185.1	184.8	186.9
170.1	175.7	170.9	176.2	169.9	175.6	173.6	179.3	173.7	179.3	172.9	178.9
163.4	163.2	159.2	159.2	159.4	159.2	163.7	163.2	158.8	158.4	159.0	158.5
151.6	150.2	147.7	146.3	148.1	146.5	149.8	147.7	145.3	143.1	145.2	142.8
139.0	139.4	137.0	136.6	137.3	136.8	136.7	136.5	136.1	135.6	136.2	135.6
137.8	137.4	135.5	135.9	134.5	134.7	135.8	136.2	133.3	132.5	133.9	133.2
134.4	133.8	134.0	133.3	134.1	133.8	133.7	133.0	130.9	131.7	130.7	131.4
133.6	133.7	131.8	132.7	131.9	132.5	132.2	133.0	130.9	131.6	130.5	130.9
132.8	133.2	131.7	131.5	131.4	131.5	132.1	131.9	130.5	131.1	130.3	130.4
130.2	130.5	130.4	130.7	130.0	130.4	130.6	130.8	130.4	130.2	129.5	130.2
129.1	129.2	129.1	129.2	128.9	128.9	128.8	128.9	128.9	129.3	128.7	128.9
129.0	129.0	129.0	129.2	128.7	128.9	128.5	128.8	128.9	128.9	128.5	128.6
128.3	128.7	128.7	129.1	128.2	128.6	128.2	128.4	128.0	128.2	127.8	128.0
127.7	127.9	126.5	126.7	126.9	127.2	127.6	127.8	126.5	126.7	127.0	127.2
118.5	118.2	117.0	116.8	116.7	116.4	118.6	118.0	117.0	116.4	116.7	116.0

Table S6 (cont). Unscaled chemical shifts calculated at the levels of theory indicated in Table S4 for all significantly populated conformers of **8a** (arranged in descending order of magnitude) using the Boltzmann Boltzmann averaged isotropic magnetic shielding values shown in Table S5.

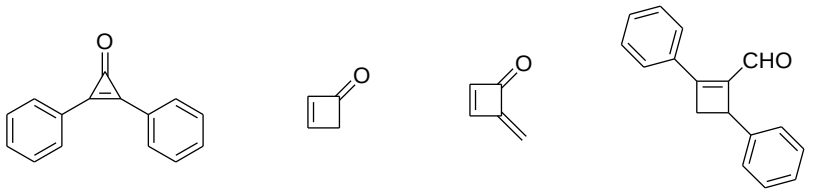
Level of theory N°											
73	**74**	**75**	**76**	**77**	**78**	**79**	**80**	**81**	**82**	**83**	**84**
177.6	179.9	184.1	185.8	176.9	179.1	182.9	184.5	177.5	179.8	183.8	185.5
175.7	176.1	180.9	180.9	174.4	174.7	178.8	178.8	175.9	176.2	180.9	180.9
160.8	159.3	163.5	158.7	160.2	158.7	162.6	157.8	160.5	159.0	163.1	158.3
146.1	145.8	147.4	142.7	147.6	147.3	148.8	144.3	147.0	146.6	148.4	143.7
138.4	137.3	136.6	135.5	138.8	137.4	137.0	135.6	138.9	137.4	137.0	135.6
137.8	135.1	136.2	132.4	138.0	135.5	136.3	132.3	137.9	135.6	136.3	132.3
137.0	133.6	133.1	131.7	137.2	133.4	133.3	132.2	137.3	133.3	133.4	132.1
134.1	131.9	132.9	131.6	133.9	132.1	132.7	131.9	133.8	132.2	132.7	131.9
133.2	131.6	131.7	131.2	133.4	131.8	131.9	131.0	133.2	131.6	131.8	131.2
130.3	130.7	130.9	130.0	130.2	130.6	130.7	130.3	130.3	130.7	130.8	130.1
128.9	129.0	128.8	129.2	129.0	129.1	129.0	129.4	129.0	129.1	128.9	129.3
128.8	128.9	128.8	128.9	128.9	129.0	128.9	129.0	128.9	129.0	128.9	129.0
128.5	128.6	128.4	128.2	128.6	128.7	128.5	128.3	128.6	128.7	128.5	128.3
127.3	127.2	127.7	126.7	127.4	127.2	127.8	126.7	127.4	127.2	127.7	126.7
117.3	116.2	117.9	116.3	117.5	116.5	118.1	116.6	117.4	116.4	118.0	116.4

Level of theory N°											
85	**86**	**87**	**88**	**89**	**90**	**91**	**92**	**93**	**94**	**95**	**96**
175.8	178.0	181.5	182.9	176.3	178.7	182.3	183.8	176.1	178.3	181.8	183.3
171.1	171.4	174.3	174.0	172.2	172.6	175.7	175.5	171.4	171.8	174.6	174.4
156.6	155.3	158.2	153.2	156.8	155.4	158.5	153.5	157.0	155.6	158.6	153.6
148.7	148.2	149.8	145.3	148.2	147.8	149.5	145.0	149.0	148.6	150.1	145.7
138.2	136.6	136.2	134.7	138.3	136.7	136.4	134.7	138.5	137.0	136.5	135.0
137.3	135.0	135.5	132.7	137.4	135.1	135.5	132.8	137.7	135.3	135.8	133.1
137.1	132.9	134.1	131.7	137.3	133.0	134.2	131.8	137.5	133.2	134.4	132.0
132.7	131.9	131.4	130.7	132.6	131.8	131.4	130.7	133.0	132.3	131.7	131.1
132.6	131.2	131.4	129.9	132.5	131.1	131.3	130.0	133.0	131.6	131.7	130.3
129.2	129.6	129.7	129.7	129.3	129.7	129.8	129.6	129.5	130.0	130.0	130.1
128.9	128.8	128.6	128.9	128.9	128.8	128.7	128.9	129.2	129.1	129.0	129.3
128.7	128.7	128.6	128.7	128.8	128.7	128.6	128.8	129.1	129.1	128.9	129.0
128.2	128.3	128.3	128.2	128.2	128.4	128.3	128.2	128.5	128.7	128.6	128.5
126.7	126.5	127.1	126.0	126.7	126.5	127.1	126.0	127.0	126.9	127.4	126.4
117.0	116.3	117.8	116.1	117.0	116.3	117.8	116.1	117.4	116.7	118.1	116.5

Level of theory N°							
97	**98**	**99**	**100**	**101**	**102**	**103**	**104**
176.7	179.0	182.6	184.1	180.0	182.4	186.4	188.1
172.5	172.9	176.0	175.8	172.9	173.1	176.5	176.4
157.1	155.8	158.8	153.8	157.6	156.1	159.8	154.6
148.6	148.1	149.8	145.3	150.4	150.2	151.6	147.3
138.6	137.0	136.6	135.1	140.4	137.8	139.1	134.9
137.7	135.4	135.8	133.1	138.9	136.8	135.7	134.7
137.6	133.4	134.5	132.1	137.3	133.9	135.6	134.1
133.0	132.2	131.7	131.0	133.2	132.7	132.0	131.4
132.8	131.5	131.6	130.3	132.8	131.4	131.6	130.4
129.6	130.1	130.1	129.9	129.8	130.0	130.1	129.9
129.2	129.2	129.0	129.3	129.2	129.3	129.1	129.5
129.1	129.1	128.8	129.1	129.2	129.3	129.0	129.2
128.5	128.7	128.6	128.5	128.7	128.9	128.8	128.7
127.0	126.9	127.4	126.3	127.4	127.3	127.8	126.7
117.3	116.6	118.1	116.4	118.2	117.3	119.0	117.3

NMR calculations of related strained strained compounds

On the basis of the modest match between experimental and calculated NMR shifts observed for **8a** at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level of theory, we undertook additional NMR calculations on related strained sp^2-carbon containing 3- or 4-membered rings (Figure S11). As can be seen it more detail in Pages S22-S26, a good overall match between experimental and calculated values were observed (Figure S12).



MAE 1.4 ppm
CMAE 1.3 ppm

MAE 2.1 ppm
CMAE 2.0 ppm

MAE 2.4 ppm
CMAE 1.3 ppm

MAE 2.9 ppm
CMAE 2.2 ppm

Figure S11

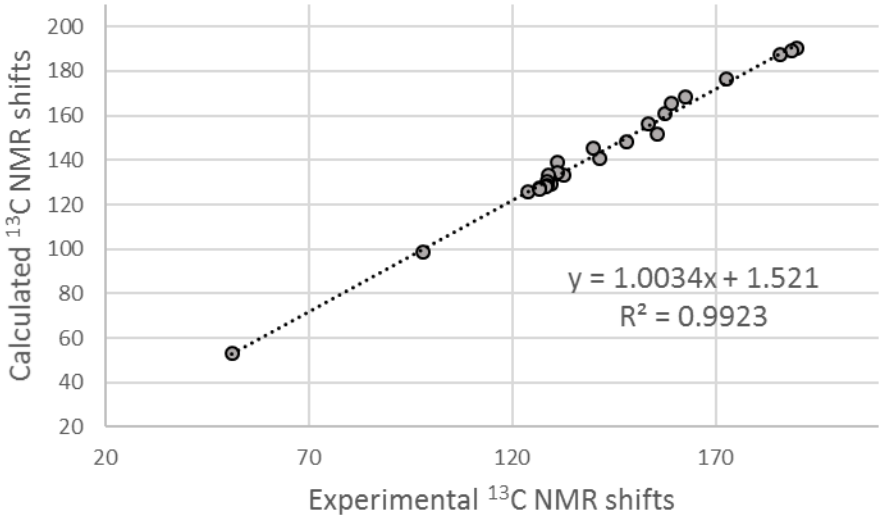
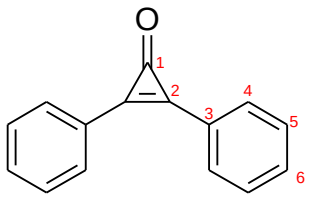


Figure S12. Correlation plot of δ_{calc} *vs* δ_{exp} obtained from the compounds depicted in Figure S11.

Table S7. Experimental ^{13}C NMR data of synthetic diphenylpropenone (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers.



δ_{exp}[a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
155.8	47.0402	C-1	151.8	154.2	4.0	1.6
148.2	50.4664	C-2	148.4	150.2	0.2	2.0
123.9	73.3499	C-3	125.5	123.5	1.6	0.4
131.5	64.9469	C-4	133.9	133.3	2.4	1.8
129.4	69.4650	C-5	129.4	128.0	0.0	1.4
132.7	65.9039	C-6	133.0	132.2	0.3	0.5
		Average			***1.4***	***1.3***

[a] Taken from "SDBS Spectral Database (http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi)
* The assignment corresponds to the computed σ vaues.

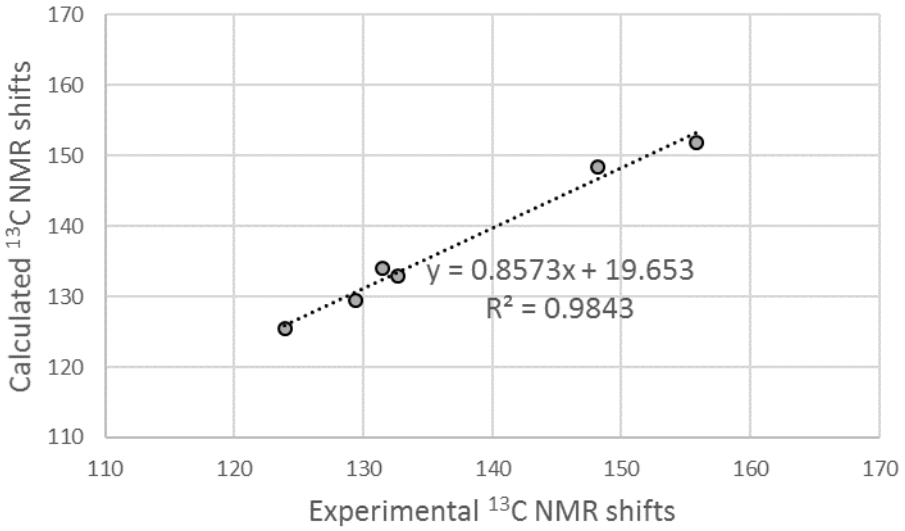
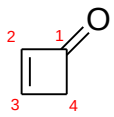


Table S8. Experimental ^{13}C NMR data of synthetic cyclobutenone (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers



δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
189.9	8.7264	C-1	190.2	188.3	0.3	1.6
162.6	30.5893	C-3	168.3	166.5	5.7	3.9
141.4	58.0184	C-2	140.9	139.0	0.5	2.4
51.1	143.5167	C-4	53.1	51.2	2.0	0.1
		Average			***2.1***	***2.0***

[a] Taken from: Ross, Audrey G.; Li, Xiaohua; Danishefsky, Samuel J. *Organic Syntheses*, **2012**, *89*, 491.
* The assignment corresponds to the computed σ vaues.

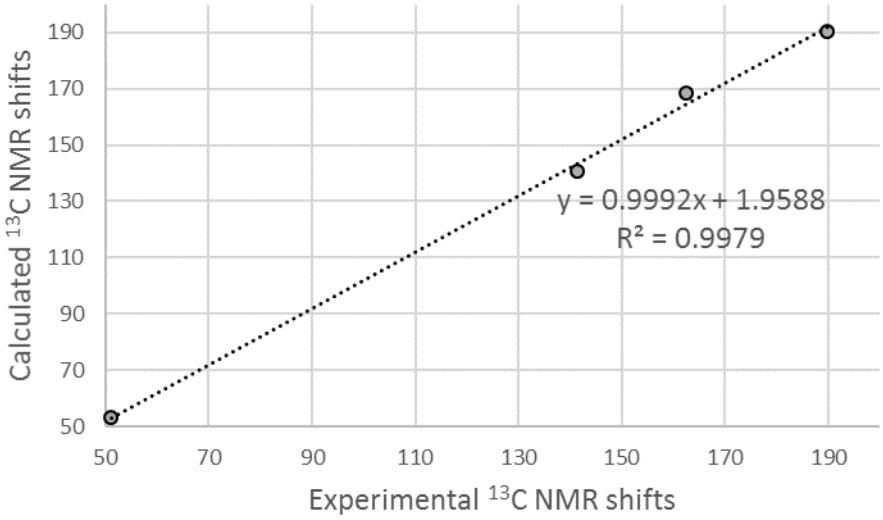
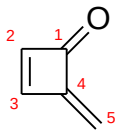


Table S9. Experimental ^{13}C NMR data of synthetic 4-methylenecyclobut-2-enone (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers



δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
157.6	38.1280	C-4	160.8	158.3	3.2	0.7
172.5	22.1290	C-3	176.8	174.1	4.3	1.6
188.6	9.8695	C-1	189.0	186.3	0.4	2.3
153.3	42.3401	C-2	156.5	154.1	3.2	0.8
98.0	99.9847	C-5	98.9	97.1	0.9	0.9
		Average			***2.4***	***1.3***

[a] Taken from: Tseng, P. W.; Kung, C. Y.; Chen, H. Y.; Chou, C. H. *J. Org. Chem.* **2011**, 76, 8440.
* The assignment corresponds to the computed σ vaues.

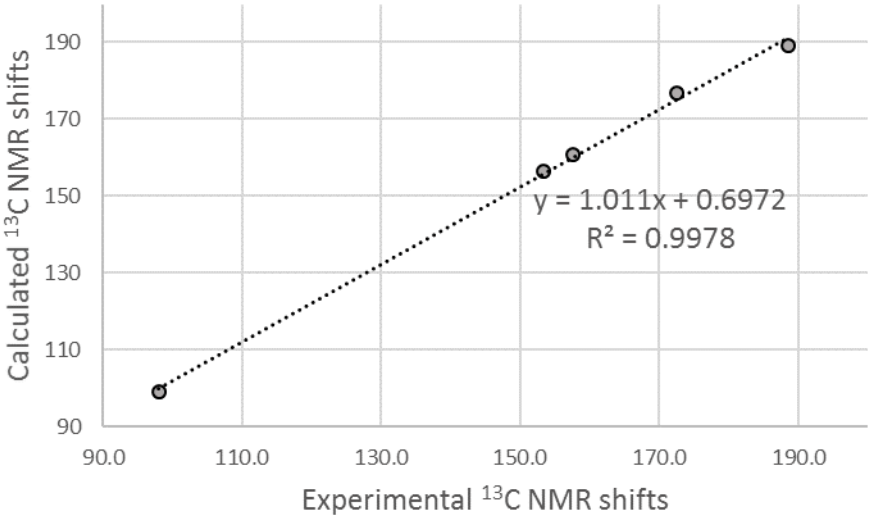
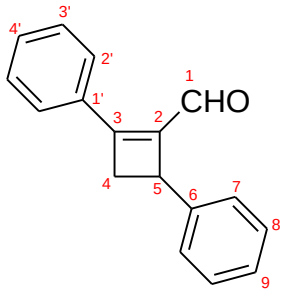
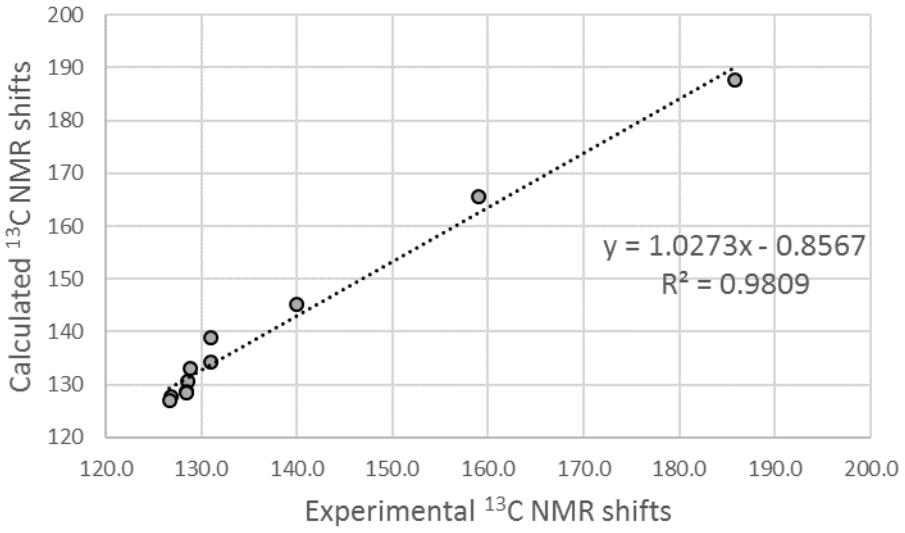


Table S10. Experimental ^{13}C NMR data of synthetic 2,4-diphenylcyclobut-1-enecarbaldehyde (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers.



δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
185.8	11.3024	C-1	187.6	183.4	1.8	2.4
131.0	60.0826	C-2	138.8	135.9	7.8	4.9
159.0	33.3695	C-3	165.5	161.9	6.5	2.9
140.0	53.7508	C-6	145.1	142.1	5.1	2.1
131.0	64.5620	C-1'	134.3	131.6	3.3	0.6
128.9	65.8447	C-4'	133.0	130.3	4.1	1.4
128.6	68.2660	C-2'	130.6	128.0	2.0	0.6
128.5	70.2480	C-8	128.6	126.1	0.1	2.4
128.4	70.5595	C-3'	128.3	125.7	0.1	2.7
126.8	71.2038	C-7	127.7	125.1	0.9	1.7
126.7	71.9139	C-9	127.0	124.4	0.3	2.3
		Average			***2.9***	***2.2***

[a] Taken from: Liu, R., Zhang, M., Winston-Mcpherson, G., Tang, W. *Chem. Commun.* **2013**, 49, 4376.
* The assignment corresponds to the computed σ vaues.



In silico screening of possible alternative structures of 8a

On the basis of the above observations, we concluded that the originally proposed structure of **8a** should be in error. Hence, in an effort to determine the real structure of **8a**, we undertook NMR calculations of the following compounds (**9a-22a**) that could have been alternatively formed. The results of these calculations are summarized in Pages S27-S41.

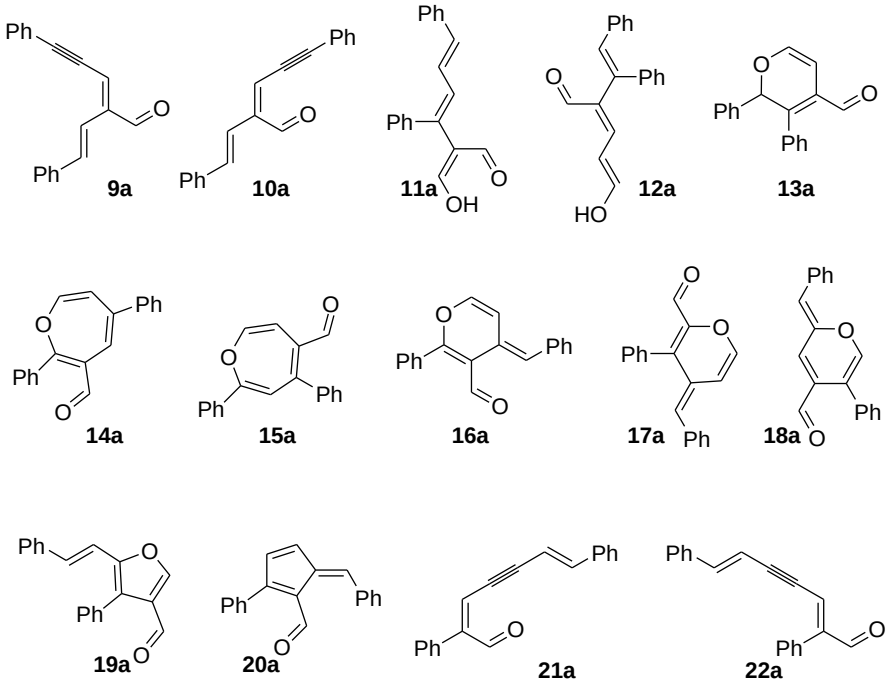
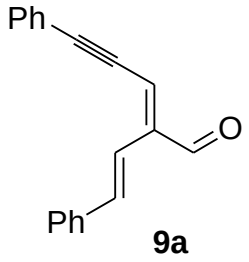


Figure S13

Table S11. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **9a**.



9a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	4.3352	194.6	195.5	1.3	2.2
143.3	55.8796	143.0	141.5	0.3	1.8
137.2	60.4520	138.4	136.7	1.2	0.5
136.4	60.9138	138.0	136.2	1.6	0.2
131.9	64.3635	134.5	132.6	2.6	0.7
129.8	66.0434	132.8	130.8	3.0	1.0
128.8	67.2368	131.7	129.6	2.9	0.8
128.7	69.7867	129.1	126.9	0.4	1.8
128.7	70.1009	128.8	126.6	0.1	2.1
127.2	70.1508	128.7	126.5	1.5	0.7
127.0	70.7129	128.2	126.0	1.2	1.0
122.3	76.0748	122.8	120.3	0.5	2.0
119.5	78.7826	120.1	117.5	0.6	2.0
109.6	79.7835	119.1	116.4	9.5	6.8
86.9	107.5555	91.3	87.3	4.4	0.4
	Average			***2.1***	***1.6***

* Arranged in ascending order of magnitude.

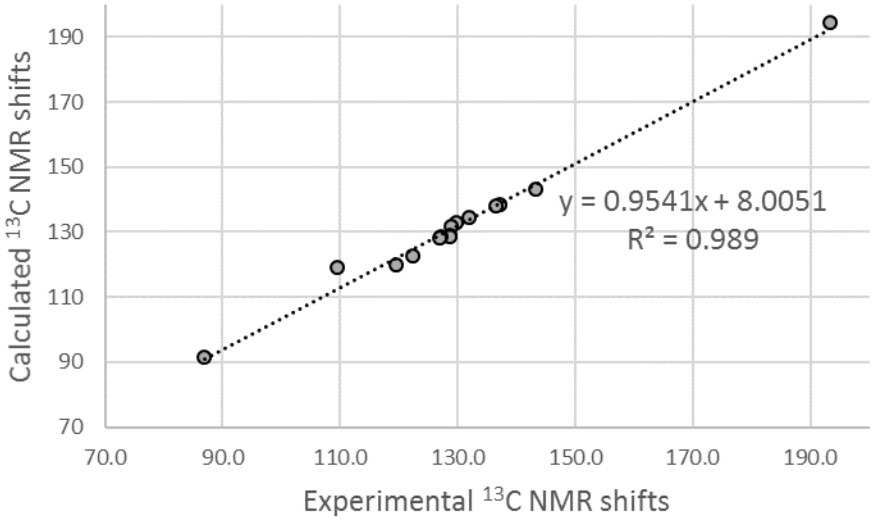
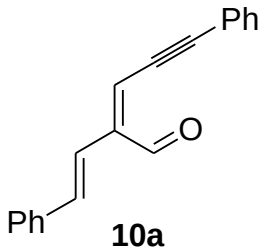


Table S12. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **10a**.



10a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	7.5858	191.3	193.8	2.0	0.5
143.3	54.7042	144.2	144.0	0.9	0.7
137.2	61.7752	137.1	136.6	0.1	0.6
136.4	63.8228	135.1	134.4	1.3	2.0
131.9	65.5454	133.3	132.6	1.4	0.7
129.8	68.5184	130.4	129.4	0.6	0.4
128.8	68.7450	130.1	129.2	1.3	0.4
128.7	69.6510	129.2	128.2	0.5	0.5
128.7	69.9306	129.0	127.9	0.3	0.8
127.2	70.6201	128.3	127.2	1.1	0.0
127.0	70.7760	128.1	127.0	1.1	0.0
122.3	75.0177	123.9	122.6	1.6	0.3
119.5	77.0222	121.9	120.4	2.4	0.9
109.6	86.6366	112.3	110.3	2.7	0.7
86.9	108.7168	90.2	86.9	3.3	0.0
	Average			***1.4***	***0.6***

* Arranged in ascending order of magnitude.

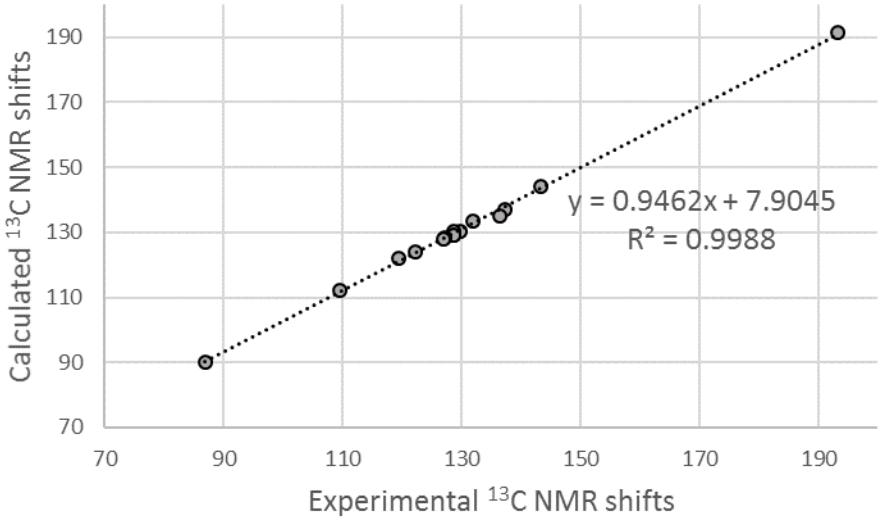
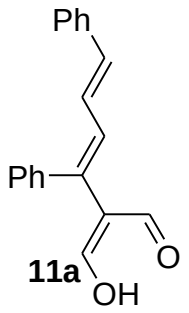


Table S13. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **11a**.



δ_{exp}	σ*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	3.9284	195.0	204.7	1.7	11.4
143.3	28.9658	169.9	172.1	26.6	28.8
137.2	57.9778	140.9	134.2	3.7	3.0
136.4	59.7988	139.1	131.8	2.7	4.6
131.9	60.6179	138.3	130.8	6.4	1.1
129.8	66.7588	132.1	122.8	2.3	7.0
128.8	67.5306	131.4	121.8	2.6	7.0
128.7	69.7928	129.1	118.8	0.4	9.9
128.7	69.9938	128.9	118.5	0.2	10.2
127.2	70.2265	128.7	118.2	1.5	9.0
127.0	70.6850	128.2	117.6	1.2	9.4
122.3	71.8063	127.1	116.2	4.8	6.1
119.5	72.1657	126.7	115.7	7.2	3.8
109.6	73.4097	125.5	114.1	15.9	4.5
86.9	74.0425	124.8	113.3	37.9	26.4
	Average			***7.7***	***9.5***

* Arranged in ascending order of magnitude.

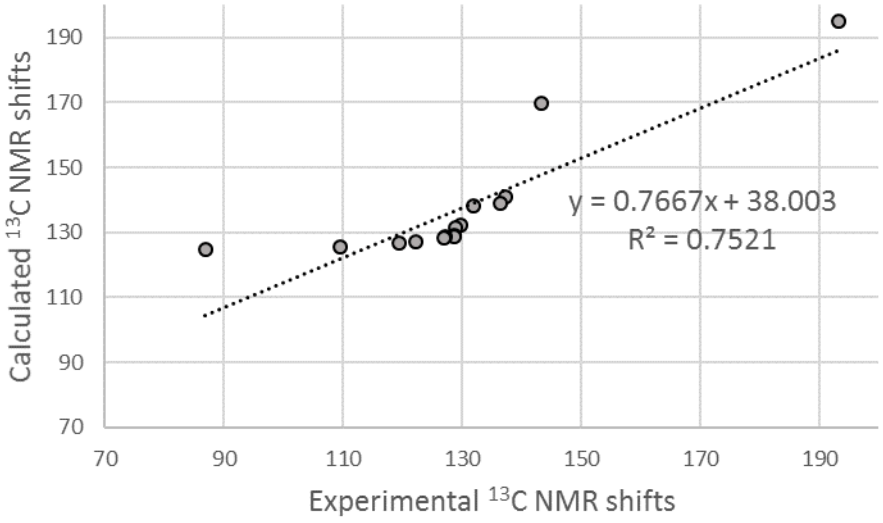
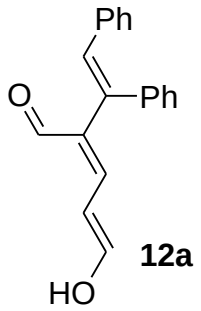


Table S14. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **12a**.



12a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	6.4468	192.4	194.6	0.9	1.3
143.3	35.9274	163.0	159.5	19.7	16.2
137.2	53.8965	145.0	138.2	7.8	1.0
136.4	54.3683	144.5	137.6	8.1	1.2
131.9	55.9345	143.0	135.7	11.1	3.8
129.8	59.7912	139.1	131.2	9.3	1.4
128.8	62.8154	136.1	127.6	7.3	1.2
128.7	68.6131	130.3	120.7	1.6	8.0
128.7	69.0882	129.8	120.1	1.1	8.6
127.2	69.1799	129.7	120.0	2.5	7.2
127.0	69.1825	129.7	120.0	2.7	7.0
122.3	70.6748	128.2	118.2	5.9	4.1
119.5	71.4631	127.4	117.3	7.9	2.2
109.6	72.5581	126.3	116.0	16.7	6.4
86.9	90.9897	107.9	94.1	21.0	7.2
	Average			***8.2***	***5.1***

* Arranged in ascending order of magnitude.

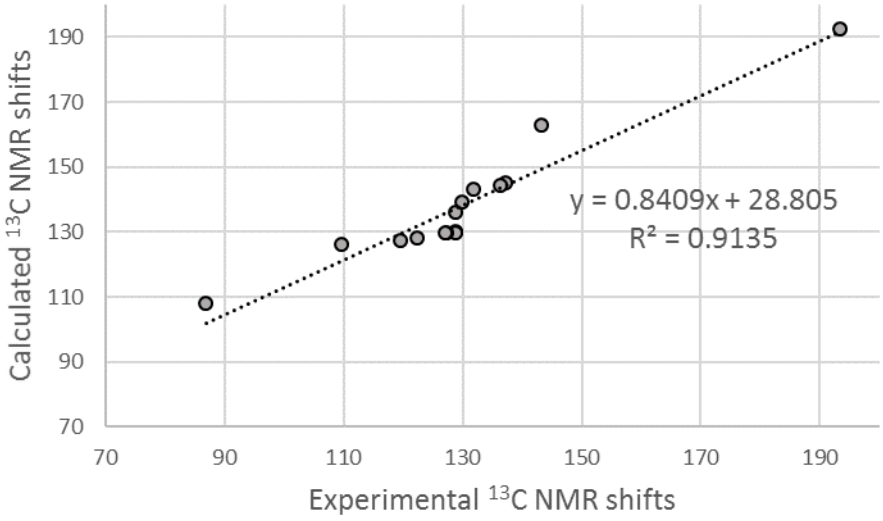
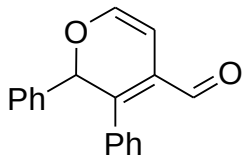


Table S15. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **13a**



13a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	9.2355	189.7	187.1	3.6	6.2
143.3	50.2240	148.7	146.6	5.4	3.3
137.2	53.4508	145.4	143.4	8.2	6.2
136.4	62.6098	136.3	134.3	0.1	2.1
131.9	63.5917	135.3	133.4	3.4	1.5
128.8	66.3139	132.6	130.7	3.8	1.9
128.7	68.2567	130.6	128.7	1.9	0.0
128.7	68.7237	130.2	128.3	1.5	0.4
127.2	69.4111	129.5	127.6	2.3	0.4
127	69.4729	129.4	127.5	2.4	0.5
122.3	70.3138	128.6	126.7	6.3	4.4
119.5	70.3159	128.6	126.7	9.1	7.2
109.6	100.7923	98.1	96.5	11.5	13.1
86.9	114.2816	84.6	83.2	2.3	3.7
	Average			***4.4***	***3.6***

* Arranged in ascending order of magnitude.

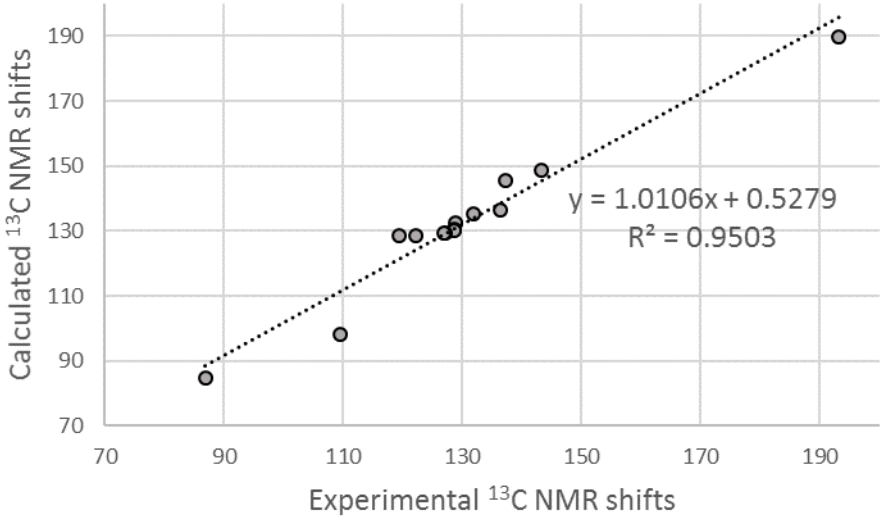
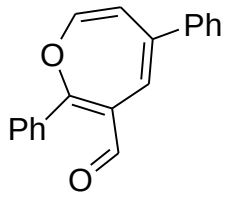


Table S16. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **14a**.



14a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	10.5849	188.3	196.2	5.0	2.9
143.3	18.9960	179.9	184.8	36.6	41.5
137.2	52.0459	146.8	140.3	9.6	3.1
136.4	56.9131	142.0	133.7	5.6	2.7
131.9	58.9001	140.0	131.0	8.1	0.9
129.8	63.7482	135.1	124.5	5.3	5.3
128.8	66.3253	132.6	121.0	3.8	7.8
128.7	66.6793	132.2	120.5	3.5	8.2
128.7	69.4192	129.5	116.8	0.8	11.9
127.2	69.7940	129.1	116.3	1.9	10.9
127.0	70.0120	128.9	116.0	1.9	11.0
122.3	70.3143	128.6	115.6	6.3	6.7
119.5	71.2525	127.6	114.4	8.1	5.1
109.6	73.4987	125.4	111.3	15.8	1.7
86.9	76.0004	122.9	108.0	36.0	21.1
	Average			***9.9***	***9.4***

* Arranged in ascending order of magnitude.

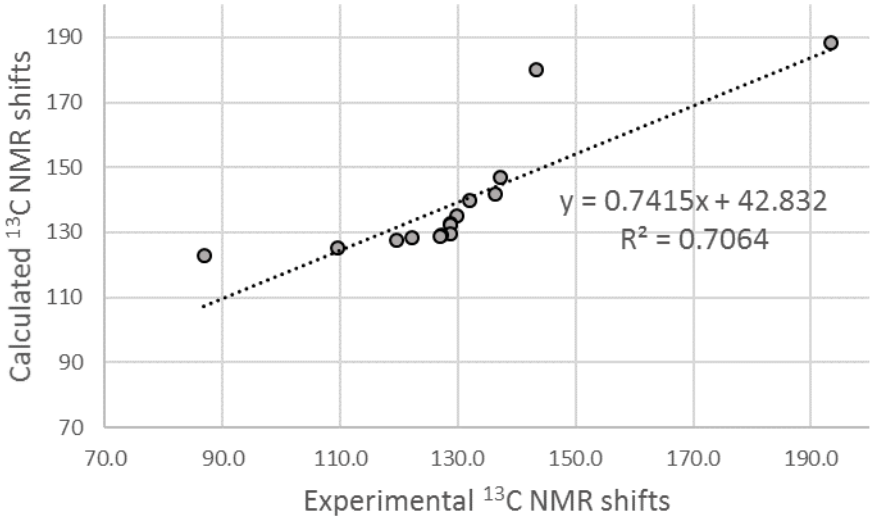
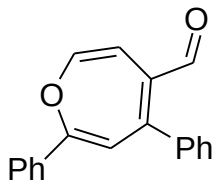


Table S17. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **15a**.



15a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	6.6883	192.2	199.8	1.1	6.5
143.3	44.2513	154.6	151.5	11.3	8.2
137.2	48.3494	150.5	146.3	13.3	9.1
136.4	55.4001	143.5	137.2	7.1	0.8
131.9	57.0700	141.8	135.1	9.9	3.2
129.8	66.1483	132.7	123.4	2.9	6.4
128.8	66.3145	132.6	123.2	3.8	5.6
128.7	66.4485	132.4	123.1	3.7	5.6
128.7	68.0873	130.8	120.9	2.1	7.8
127.2	69.7098	129.2	118.9	2.0	8.3
127.0	69.9590	128.9	118.5	1.9	8.5
122.3	70.1494	128.7	118.3	6.4	4.0
119.5	70.9381	128.0	117.3	8.5	2.2
109.6	71.4235	127.5	116.7	17.9	7.1
86.9	84.1421	114.7	100.3	27.8	13.4
	Average			***8.0***	***6.4***

* Arranged in ascending order of magnitude.

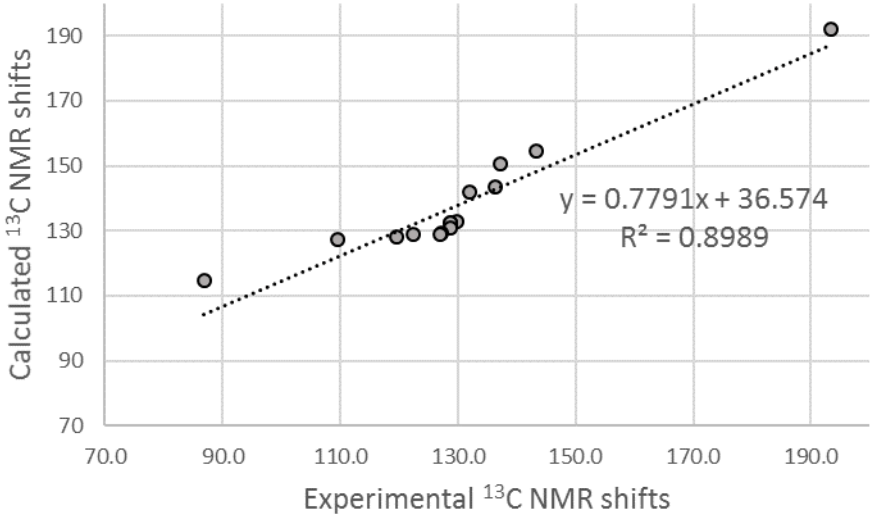
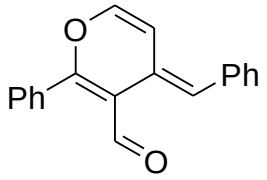


Table S18. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **16a**.



16a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	8.1183	190.8	195.3	2.5	2.0
143.3	24.2729	174.6	176.1	31.3	32.8
137.2	55.6083	143.3	138.9	6.1	1.7
136.4	59.8248	139.1	133.9	2.7	2.5
131.9	66.0456	132.8	126.5	0.9	5.4
129.8	66.0767	132.8	126.5	3.0	3.3
128.8	67.1891	131.7	125.2	2.9	3.6
128.7	70.0868	128.8	121.7	0.1	7.0
128.7	70.4705	128.4	121.3	0.3	7.4
127.2	71.0109	127.9	120.6	0.7	6.6
127.0	71.1489	127.7	120.4	0.7	6.6
122.3	72.4887	126.4	118.9	4.1	3.4
119.5	78.7222	120.2	111.5	0.7	8.0
109.6	79.3025	119.6	110.8	10.0	1.2
86.9	85.7221	113.2	103.1	26.3	16.2
	Average			***6.2***	***7.2***

* Arranged in ascending order of magnitude.

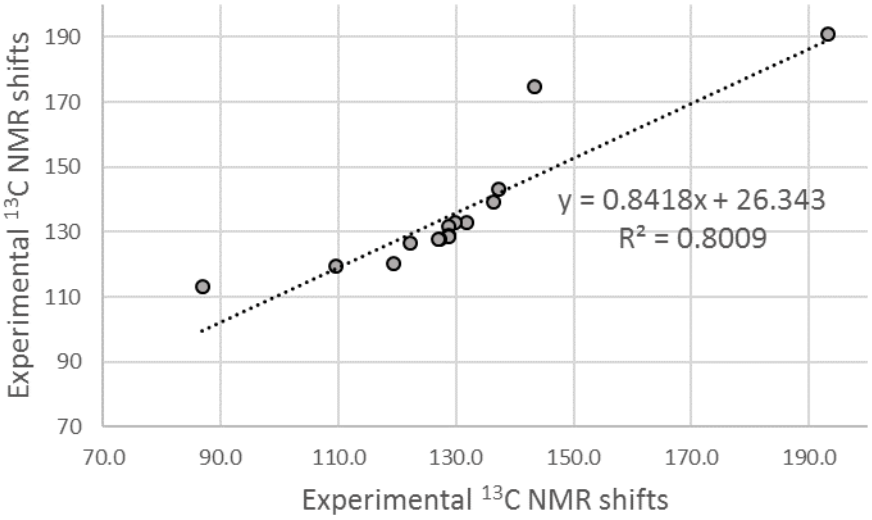
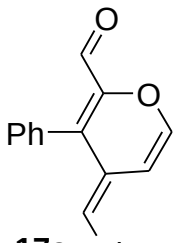


Table S19. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **17a**.



17a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error** (δ_{exp} -δ_{calc})	**Scaled Error** (δ_{exp} -δ_{scaled})
193.3	14.7577	184.1	195.2	9.2	1.9
143.3	51.1845	147.7	146.4	4.4	3.1
137.2	52.5476	146.3	144.5	9.1	7.3
136.4	53.2845	145.6	143.5	9.2	7.1
131.9	59.8642	139.0	134.7	7.1	2.8
129.8	65.6026	133.3	127.0	3.5	2.8
128.8	66.1445	132.7	126.3	3.9	2.5
128.7	67.3038	131.6	124.8	2.9	3.9
128.7	69.0864	129.8	122.4	1.1	6.3
127.2	70.1242	128.8	121.0	1.6	6.2
127.0	70.4938	128.4	120.5	1.4	6.5
122.3	70.6319	128.3	120.3	6.0	2.0
119.5	72.2984	126.6	118.1	7.1	1.4
109.6	76.6073	122.3	112.3	12.7	2.7
86.9	90.4406	108.4	93.7	21.5	6.8
	Average			***6.7***	***4.2***

* Arranged in ascending order of magnitude.

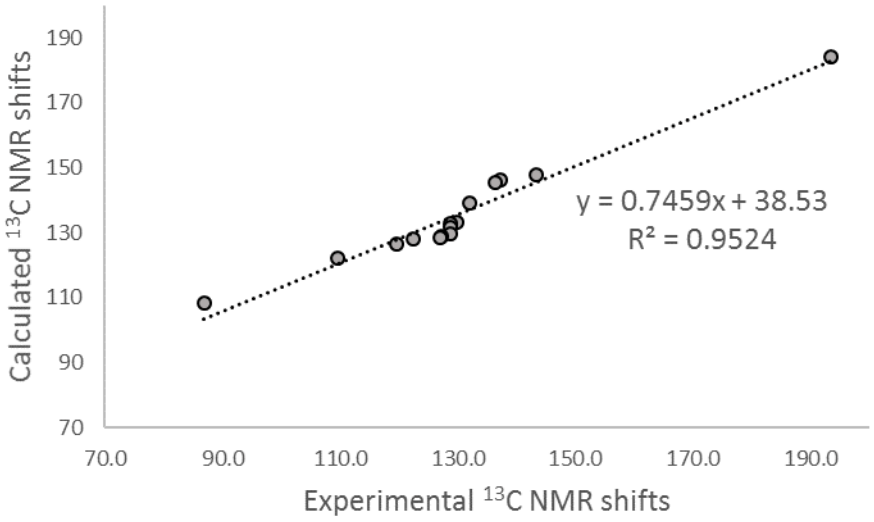
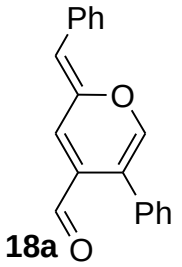


Table S20. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **18a**.



18a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	11.4602	187.4	199.8	5.9	6.5
143.3	47.2584	151.6	151.9	8.3	8.6
137.2	50.6144	148.3	147.4	11.1	10.2
136.4	61.5718	137.3	132.8	0.9	3.6
131.9	63.3524	135.5	130.4	3.6	1.5
129.8	63.5545	135.3	130.1	5.5	0.3
128.8	68.0217	130.9	124.2	2.1	4.6
128.7	69.5926	129.3	122.1	0.6	6.6
128.7	70.2196	128.7	121.2	0.0	7.5
127.2	70.6508	128.2	120.7	1.0	6.5
127.0	70.8676	128.0	120.4	1.0	6.6
122.3	71.8433	127.0	119.1	4.7	3.2
119.5	72.5306	126.4	118.1	6.9	1.4
109.6	78.6847	120.2	109.9	10.6	0.3
86.9	84.2875	114.6	102.4	27.7	15.5
	Average			***6.0***	***5.5***

* Arranged in ascending order of magnitude.

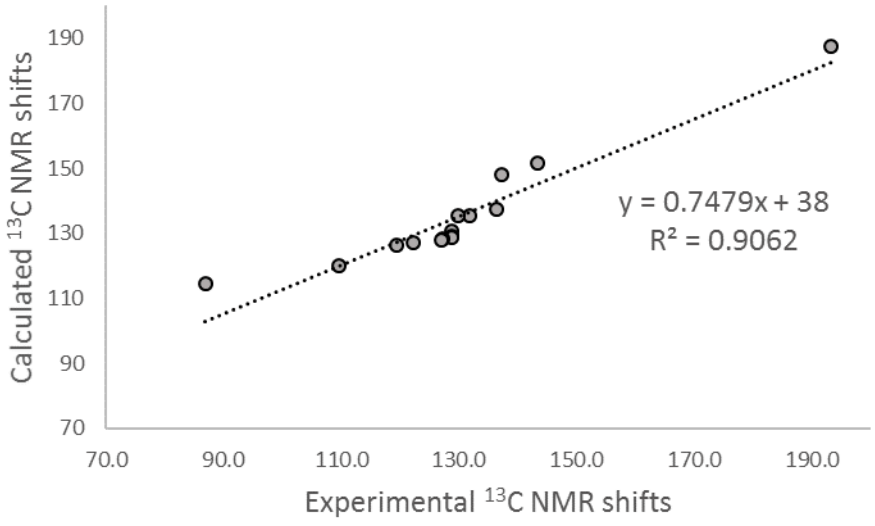
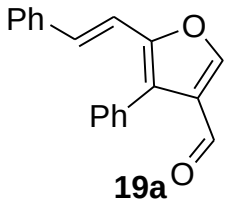


Table S21. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **19a**.



19a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	12.5173	186.4	200.1	6.9	6.8
143.3	46.0231	152.9	154.0	9.6	10.7
137.2	48.1702	150.7	151.1	13.5	13.9
136.4	61.9295	137.0	132.2	0.6	4.2
131.9	65.8043	133.1	126.8	1.2	5.1
129.8	66.5712	132.3	125.8	2.5	4.0
128.8	68.4601	130.4	123.2	1.6	5.6
128.7	69.7258	129.2	121.5	0.5	7.2
128.7	69.7855	129.1	121.4	0.4	7.3
127.2	70.8317	128.1	119.9	0.9	7.3
127.0	71.0370	127.9	119.7	0.9	7.3
122.3	71.3537	127.5	119.2	5.2	3.1
119.5	71.9170	127.0	118.4	7.5	1.1
109.6	73.1870	125.7	116.7	16.1	7.1
86.9	84.8773	114.0	100.6	27.1	13.7
	Average			***6.3***	***7.0***

* Arranged in ascending order of magnitude.

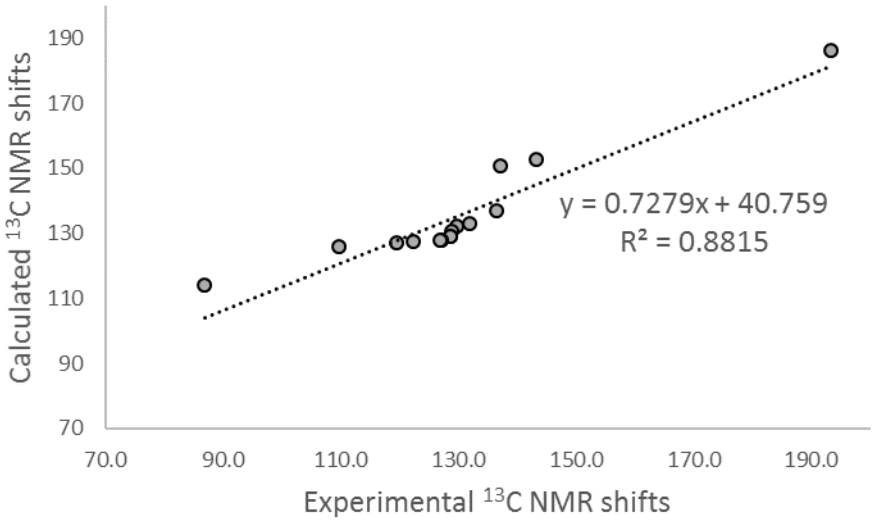
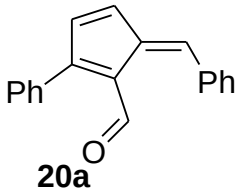


Table S22. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **20a**



20a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	16.1548	182.7	201.9	10.6	8.6
143.3	39.8766	159.0	162.7	15.7	19.4
137.2	52.1738	146.7	142.4	9.5	5.2
136.4	53.5882	145.3	140.1	8.9	3.7
131.9	61.1451	137.7	127.6	5.8	4.3
129.8	61.8193	137.1	126.5	7.3	3.3
128.8	63.0120	135.9	124.5	7.1	4.3
128.7	65.0562	133.8	121.1	5.1	7.6
128.7	66.4982	132.4	118.8	3.7	9.9
127.2	67.3034	131.6	117.4	4.4	9.8
127.0	67.6255	131.3	116.9	4.3	10.1
122.3	68.8738	130.0	114.8	7.7	7.5
119.5	69.6670	129.2	113.5	9.7	6.0
109.6	70.4977	128.4	112.2	18.8	2.6
86.9	71.6352	127.3	110.3	40.4	23.4
	Average			***10.6***	***8.4***

* Arranged in ascending order of magnitude.

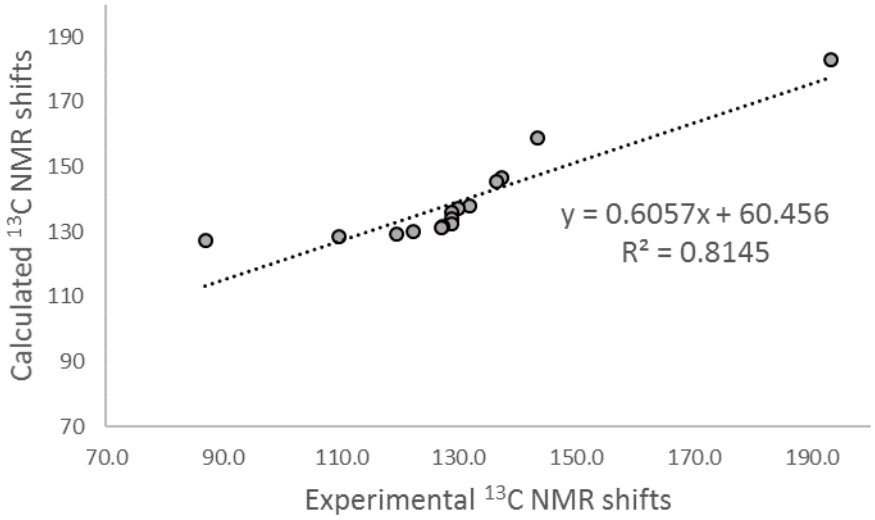
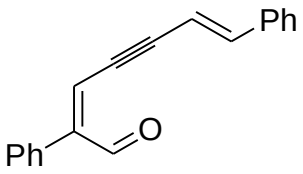


Table S23. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **21a**.



21a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	8.9857	189.9	190.2	3.4	3.1
143.3	49.0153	149.9	148.9	6.6	5.6
137.2	52.1102	146.8	145.7	9.6	8.5
136.4	62.3595	136.5	135.1	0.1	1.3
131.9	62.9663	135.9	134.5	4.0	2.6
129.8	67.1485	131.7	130.1	1.9	0.3
128.8	67.9428	130.9	129.3	2.1	0.5
128.7	69.5570	129.3	127.6	0.6	1.1
128.7	69.8601	129.0	127.3	0.3	1.4
127.2	69.9972	128.9	127.2	1.7	0.0
127.0	70.8393	128.0	126.3	1.0	0.7
122.3	70.8719	128.0	126.3	5.7	4.0
119.5	88.8079	110.1	107.8	9.4	11.7
109.6	92.4182	106.5	104.0	3.1	5.6
86.9	105.6839	93.2	90.3	6.3	3.4
	Average			***3.7***	***3.3***

* Arranged in ascending order of magnitude.

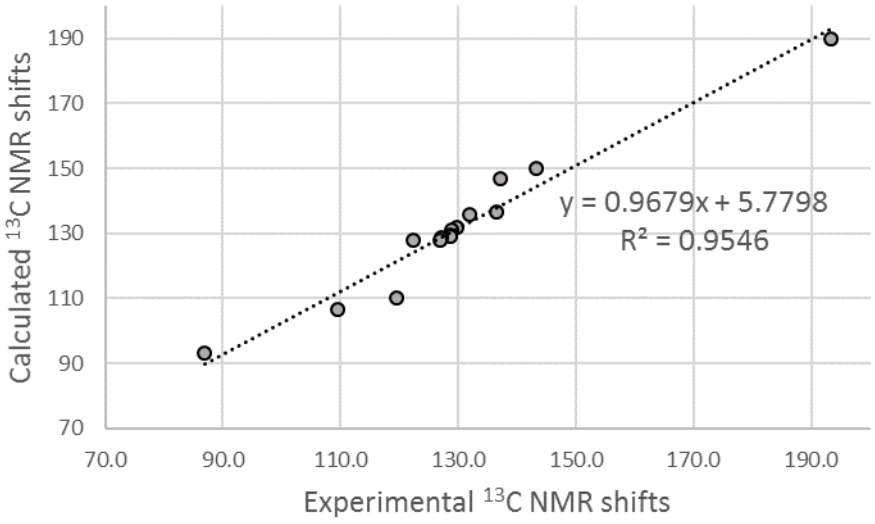
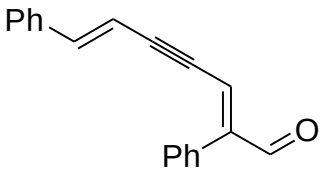


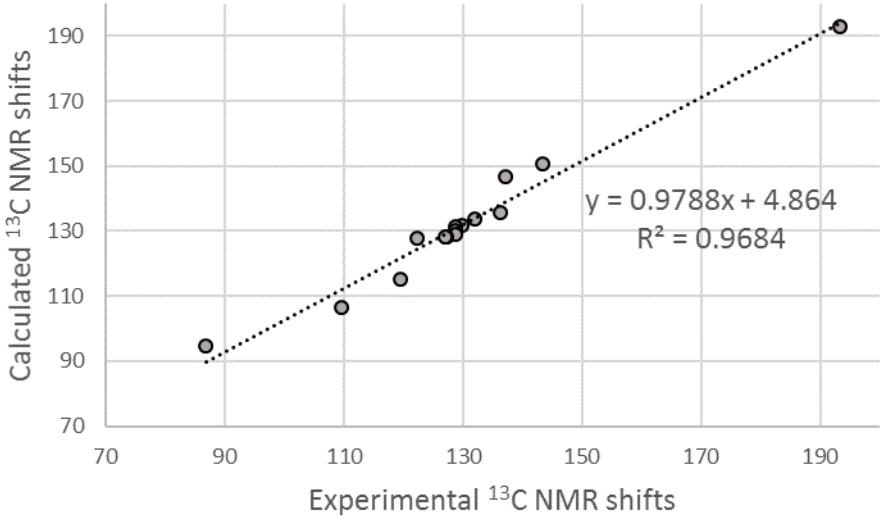
Table S24 Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **22a**.



22a

δ_{exp}	σ*	δ_{calc}	δ_{scaled}	**Unsc. Error (δ_{exp} -δ_{calc})**	**Scaled Error (δ_{exp} -δ_{scaled})**
193.3	6.0293	192.9	192.1	0.4	1.2
143.3	48.3508	150.5	148.8	7.2	5.5
137.2	52.1941	146.7	144.9	9.5	7.7
136.4	63.1932	135.7	133.7	0.7	2.7
131.9	64.9844	133.9	131.8	2.0	0.1
129.8	67.2427	131.6	129.5	1.8	0.3
128.8	67.6284	131.3	129.1	2.5	0.3
128.7	68.5851	130.3	128.2	1.6	0.5
128.7	70.0751	128.8	126.6	0.1	2.1
127.2	70.5071	128.4	126.2	1.2	1.0
127.0	70.5328	128.4	126.2	1.4	0.8
122.3	71.2073	127.7	125.5	5.4	3.2
119.5	83.8792	115.0	112.5	4.5	7.0
109.6	92.3755	106.5	103.8	3.1	5.8
86.9	104.2566	94.6	91.7	7.7	4.8
	Average			***3.3***	***2.9***

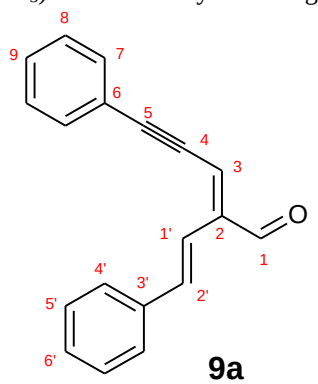
* Arranged in ascending order of magnitude.



^{1}H NMR calculations of compounds 9a and 10a

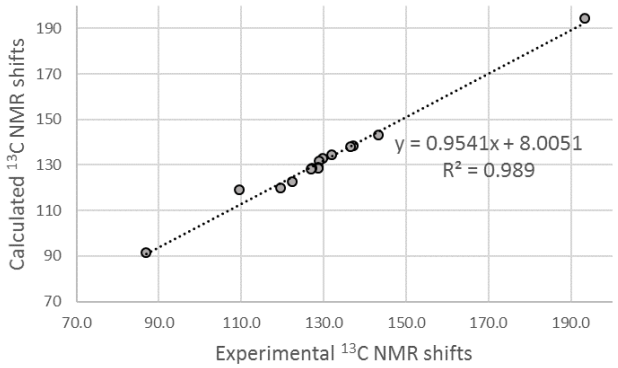
After we found compounds **9a** and **10a** as the most likely structures of **8a**, we next computed the ^{1}H NMR shifts of both compounds, for further correlation with the experimental findings. The results of these calculations are summarized Pages S42-S44.

Table S25. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **9a**.



9a

δ_{exp}	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	4.3352	C-1	194.6	195.5	1.3	2.2
143.3	55.8796	C-2	143.0	141.5	0.3	1.8
137.2	60.4520	C-2'	138.4	136.7	1.2	0.5
136.4	60.9138	C-3'	138.0	136.2	1.6	0.2
131.9	64.3635	C-7	134.5	132.6	2.6	0.7
129.8	66.0434	C-3	132.8	130.8	3.0	1.0
128.8	67.2368	C-9	131.7	129.6	2.9	0.8
128.7	69.7867	C-6'	129.1	126.9	0.4	1.8
128.7	70.1009	C-5'	128.8	126.6	0.1	2.1
127.2	70.1508	C-8	128.7	126.5	1.5	0.7
127.0	70.7129	C-4'	128.2	126.0	1.2	1.0
122.3	76.0748	C-6	122.8	120.3	0.5	2.0
119.5	78.7826	C-5	120.1	117.5	0.6	2.0
109.6	79.7835	C-1'	119.1	116.4	9.5	6.8
86.9	107.5555	C-4	91.3	87.3	4.4	0.4
		Average			***2.1***	***1.6***
9.65	21.8267	H-1	9.39	9.38	0.26	0.27
7.99	22.7579	H-2'	8.45	8.41	0.46	0.42
7.55	23.4796	H-7	7.73	7.65	0.18	0.10
7.55	23.4864	H-4'	7.73	7.64	0.18	0.09
7.25	23.5806	H-1'	7.63	7.54	0.38	0.29
7.36	23.7033	H-8	7.51	7.41	0.15	0.05
7.36	23.7752	H-9	7.44	7.34	0.08	0.02
7.36	23.8312	H-5'	7.38	7.28	0.02	0.08
7.36	23.9121	H-6'	7.30	7.19	0.06	0.17
6.52	24.9403	H-3	6.27	6.11	0.25	0.41
		Average			***0.20***	***0.19***



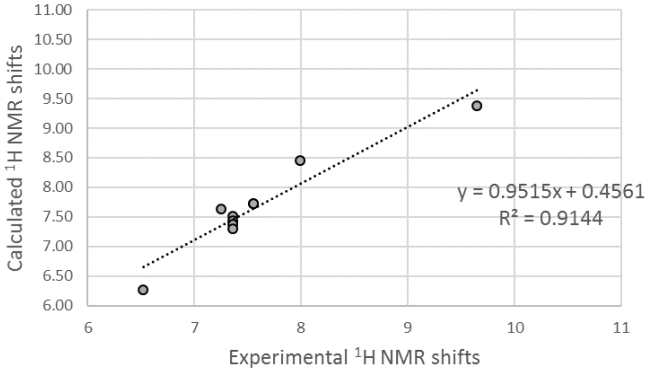
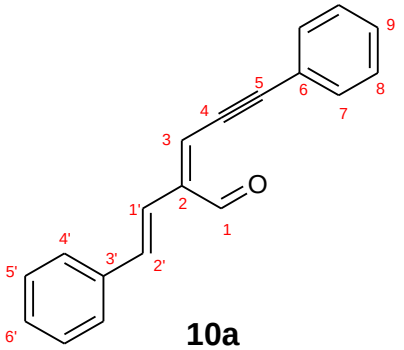
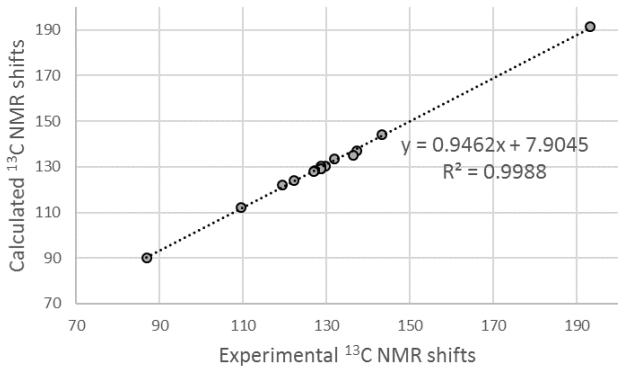


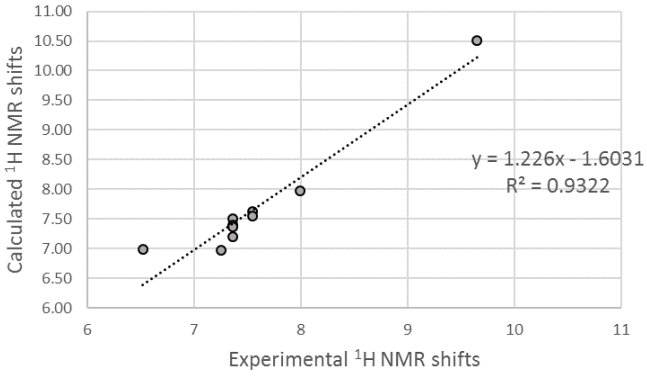
Table S26. Experimental ^{13}C NMR data of synthetic **8a** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **10a**.



10a

δ_{exp}	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.3	7.5858	C-1	191.3	193.8	2.0	0.5
143.3	54.7042	C-2	144.2	144.0	0.9	0.7
137.2	61.7752	C-3'	137.1	136.6	0.1	0.6
136.4	63.8228	C-2'	135.1	134.4	1.3	2.0
131.9	65.5454	C-7	133.3	132.6	1.4	0.7
129.8	68.5184	C-9	130.4	129.4	0.6	0.4
128.8	68.7450	C-3	130.1	129.2	1.3	0.4
128.7	69.6510	C-8	129.2	128.2	0.5	0.5
128.7	69.9306	C-6'	129.0	127.9	0.3	0.8
127.2	70.6201	C-5'	128.3	127.2	1.1	0.0
127	70.7760	C-4'	128.1	127.0	1.1	0.0
122.3	75.0177	C-6	123.9	122.6	1.6	0.3
119.5	77.0222	C-1'	121.9	120.4	2.4	0.9
109.6	86.6366	C-5	112.3	110.3	2.7	0.7
86.9	108.7168	C-4	90.2	86.9	3.3	0.0
		Average			***1.4***	***0.6***
9.65	20.7106	H-1	10.50	9.87	0.85	0.22
7.99	23.2315	H-2'	7.98	7.82	0.01	0.17
7.55	23.5895	H-7	7.62	7.52	0.07	0.03
7.55	23.6666	H-9	7.55	7.46	0.00	0.09
7.36	23.7019	H-4'	7.51	7.43	0.15	0.07
7.36	23.8216	H-8	7.39	7.34	0.03	0.02
7.36	23.8392	H-5'	7.37	7.32	0.01	0.04
7.36	24.0095	H-6'	7.20	7.18	0.16	0.18
6.52	24.2262	H-3	6.99	7.01	0.47	0.49
7.25	24.2376	H-1'	6.97	7.00	0.28	0.25
		Average			***0.20***	***0.16***





On the basis of the relatively high errors computed for some nuclei of **9a** and **10a** at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level of theory, we next undertook the NMR calculations at different levels of theory (pages S45-S50). From the data collected in Tables S27-S29 (Figure S14), we concluded that all the levels of theory under study afforded similar results. Nevertheless, we noticed an interesting dependence on the accuracy in the prediction of certain nuclei with the level fo theory employed during the NMR calculation stage.

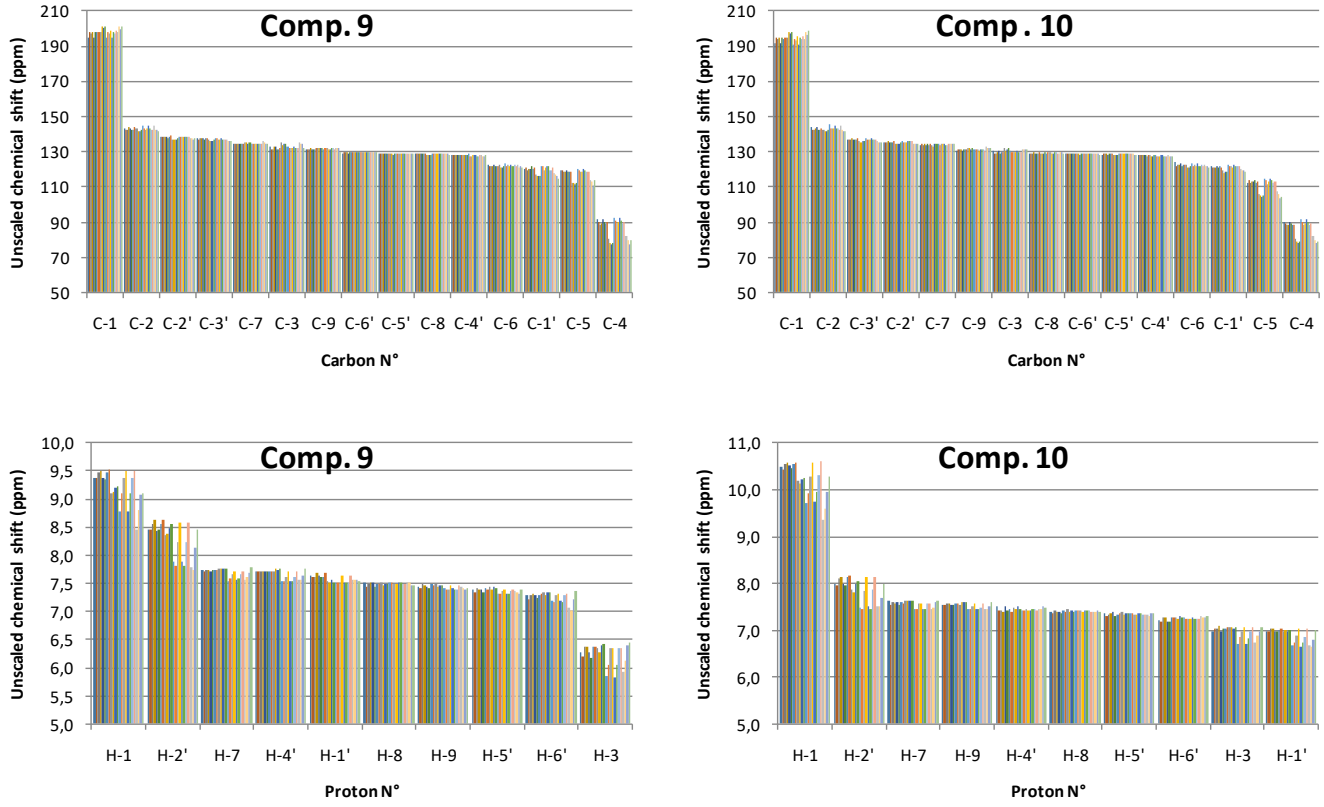


Figure S14. Unscaled chemical shifts of **9a** and **10a** computed at 24 different levels of theory.

In the case of **9a**, the carbons which showed the higher variance were C-4 (σ^2 = 30.3) and C-5 (σ^2 = 10.5). Detailed analysis of the effect of the level of theory in the accuracy of the calculations of both shifts showed an interesting trend. Whereas in the case of C-5 the best results were obtained with the functional LC-TPSSTPSS (mainly in combination with the cc-PVTZ basis set with both GIAO and CSGT methods), this functional afforded the worse results when dealing with C-4. In this regard, the shift of C-4 was nicely reproduced by mPW1PW91 and PBE0 functionals, again in combination with the cc-PVTZ basis with both GIAO and CSGT methods. When dealing with proton data, the most affected signals of **9a** with the change in the level of theory were H-1 (σ^2 = 0.08), H-2' (σ^2 = 0.094) and H-3 (σ^2 = 0.033). Here again, the optimal level of theory strongly depended on the type of nuclei. For instance, the best reproduction of the H-1 shift was achieved with mPW1PW91 or PBE0 coupled with the expensive 6-311++G(3df,2pd) basis set (both using GIAO and CSGT). In the case of H-2', the best results were obtained using CSGT and the functionals mPW1PW91 and PBE0 coupled with the much more affordable 6-31+G** basis. Finally, the H-3 signal was better simulated with the LC-TPSSTPSS functional, the 6-311++G(3df,2pd) or cc-PVTZ basis sets (both using GIAO and CSGT). In the case of **10a** similar trends were observed, both for carbon and proton NMR data. Overall, these results underscore the difficulty to correctly reproduce the experimental NMR shifts of these types of molecules using only one level of theory. As expected, in all cases the performances of the different levels of theory became more similar upon scaling.

Table S27. Levels of theory used for the calculation of the NMR shifts of **9a** and **10a**.

Level of theory Nº	Geom Opt.	Method	Functional	Basis set	Solvent effect
1	B3LYP/6-31G*	GIAO	mPW1PW91	6-31+G**	PCM
2	B3LYP/6-31G*	GIAO	mPW1PW91	6-311+G**	PCM
3	B3LYP/6-31G*	GIAO	mPW1PW91	cc-PVTZ	PCM
4	B3LYP/6-31G*	GIAO	mPW1PW91	6-311++G(3df,2pd)	PCM
5	B3LYP/6-31G*	GIAO	PBE0	6-31+G**	PCM
6	B3LYP/6-31G*	GIAO	PBE0	6-311+G**	PCM
7	B3LYP/6-31G*	GIAO	PBE0	cc-PVTZ	PCM
8	B3LYP/6-31G*	GIAO	PBE0	6-311++G(3df,2pd)	PCM
9	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	6-31+G**	PCM
10	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	6-311+G**	PCM
11	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	cc-PVTZ	PCM
12	B3LYP/6-31G*	GIAO	LC-TPSSTPSS	6-311++G(3df,2pd)	PCM
13	B3LYP/6-31G*	CSGT	mPW1PW91	6-31+G**	PCM
14	B3LYP/6-31G*	CSGT	mPW1PW91	6-311+G**	PCM
15	B3LYP/6-31G*	CSGT	mPW1PW91	cc-PVTZ	PCM
16	B3LYP/6-31G*	CSGT	mPW1PW91	6-311++G(3df,2pd)	PCM
17	B3LYP/6-31G*	CSGT	PBE0	6-31+G**	PCM
18	B3LYP/6-31G*	CSGT	PBE0	6-311+G**	PCM
19	B3LYP/6-31G*	CSGT	PBE0	cc-PVTZ	PCM
20	B3LYP/6-31G*	CSGT	PBE0	6-311++G(3df,2pd)	PCM
21	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-31+G**	PCM
22	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-311+G**	PCM
23	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	cc-PVTZ	PCM
24	B3LYP/6-31G*	CSGT	LC-TPSSTPSS	6-311++G(3df,2pd)	PCM

Table S28. Unscaled chemical shifts calculated at the levels of theory indicated in Table S27 for all significantly populated conformers of **9a** and **10a** (arranged in descending order of magnitude).

Compound 9a											
Level of theory N°											
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Carbon Shifts											
194.6	197.7	197.3	198.1	194.8	197.9	197.6	198.3	198.3	201.0	200.4	201.4
143.0	142.7	142.5	143.7	142.9	142.7	142.4	143.6	143.0	141.8	141.9	142.7
138.4	138.0	138.2	138.8	138.7	137.9	138.3	139.1	136.9	136.9	137.1	137.7
138.0	137.0	137.5	137.7	137.8	137.0	137.5	137.5	136.7	135.7	135.9	136.5
134.5	134.6	134.4	134.6	134.5	134.5	134.3	134.5	135.3	135.0	134.8	135.2
132.8	131.6	131.5	132.5	132.7	131.6	131.4	132.4	135.0	133.9	134.2	134.8
131.7	131.4	131.4	131.9	131.6	131.3	131.4	131.9	131.9	132.1	132.1	132.3
129.1	129.7	129.4	129.7	129.2	129.7	129.5	129.8	129.3	129.6	129.6	129.6
128.8	129.1	128.9	129.0	128.8	129.1	128.9	129.1	128.7	128.7	128.5	128.7
128.7	128.9	128.8	128.9	128.8	129.0	128.8	129.0	128.5	128.4	128.2	128.3
128.2	128.0	127.9	128.1	128.1	127.9	127.9	128.0	128.3	127.9	128.0	128.2
122.8	121.9	122.0	122.0	122.7	121.9	122.1	121.9	122.7	120.8	121.3	121.8
120.1	121.2	119.4	120.5	120.4	121.5	119.8	120.9	116.9	115.8	115.8	116.2
119.1	119.0	118.5	118.4	119.0	118.9	118.4	118.4	111.9	112.4	111.1	112.3
91.3	89.8	88.7	89.2	91.4	90.2	89.0	89.6	80.6	78.4	77.4	77.9
Proton Shifts											
9.39	9.36	9.48	9.51	9.38	9.35	9.48	9.51	9.09	9.12	9.20	9.22
8.45	8.46	8.55	8.64	8.44	8.45	8.55	8.63	8.36	8.39	8.47	8.54
7.73	7.72	7.74	7.73	7.73	7.73	7.73	7.73	7.77	7.76	7.76	7.76
7.73	7.71	7.73	7.72	7.72	7.71	7.72	7.72	7.72	7.75	7.74	7.76
7.63	7.61	7.61	7.69	7.64	7.63	7.62	7.70	7.53	7.50	7.55	7.52
7.51	7.43	7.49	7.51	7.51	7.43	7.49	7.50	7.51	7.46	7.48	7.48
7.44	7.42	7.48	7.46	7.44	7.42	7.48	7.46	7.49	7.45	7.46	7.45
7.38	7.35	7.41	7.40	7.39	7.35	7.41	7.40	7.44	7.40	7.43	7.42
7.30	7.23	7.30	7.32	7.30	7.23	7.30	7.31	7.35	7.28	7.35	7.34
6.27	6.19	6.37	6.37	6.27	6.19	6.37	6.37	6.34	6.29	6.41	6.42

Compound 10a											
Level of theory N°											
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Carbon Shifts											
191.3	194.6	193.9	194.8	191.4	194.8	194.2	195.0	194.8	197.8	197.0	198.2
144.2	142.8	142.5	143.3	144.1	142.7	142.5	143.2	142.4	141.2	141.3	142.1
137.1	137.0	137.2	138.0	136.9	136.9	137.2	137.8	136.4	135.3	135.8	136.4
135.1	135.6	135.3	135.6	135.5	135.5	135.4	136.0	134.7	134.8	134.5	134.9
133.3	134.5	134.1	134.4	133.3	134.5	134.0	134.3	133.5	133.2	134.1	134.7
130.4	131.1	131.0	131.0	130.5	131.0	130.9	131.1	132.1	131.7	131.7	131.9
130.1	129.2	129.3	129.8	130.3	129.2	129.5	129.9	131.7	130.4	131.1	131.7
129.2	128.9	129.2	129.3	129.3	129.2	129.2	129.4	129.2	129.2	129.2	129.4
129.0	128.9	128.9	129.0	129.0	129.0	128.9	129.1	128.6	128.7	128.4	128.8
128.3	128.9	128.6	128.6	128.3	128.9	128.7	128.7	128.4	128.4	128.2	128.3
128.1	127.9	127.7	127.8	128.1	127.8	127.7	127.8	128.1	127.6	127.7	127.8
123.9	121.5	122.2	122.8	123.7	121.5	122.2	122.6	122.9	120.8	121.3	121.8
121.9	121.3	121.3	121.1	121.9	121.3	121.4	121.3	119.6	118.1	118.6	118.7
112.3	113.9	111.9	112.6	112.6	113.9	112.2	113.0	105.5	104.8	103.9	104.7
90.2	88.9	88.2	88.5	90.3	89.3	88.4	88.8	80.8	78.8	78.1	78.5
Proton Shifts											
10.50	10.43	10.54	10.57	10.52	10.45	10.55	10.59	10.18	10.13	10.21	10.26
7.98	7.95	8.12	8.15	8.00	7.97	8.13	8.17	7.86	7.81	7.97	8.05
7.62	7.55	7.61	7.57	7.61	7.55	7.60	7.57	7.64	7.63	7.64	7.63
7.55	7.55	7.58	7.56	7.53	7.55	7.58	7.56	7.55	7.60	7.60	7.61
7.51	7.42	7.44	7.40	7.51	7.42	7.44	7.40	7.48	7.46	7.51	7.46
7.39	7.36	7.42	7.39	7.40	7.37	7.42	7.39	7.45	7.38	7.42	7.39
7.37	7.30	7.34	7.36	7.38	7.30	7.34	7.36	7.41	7.33	7.38	7.37
7.20	7.18	7.27	7.27	7.20	7.18	7.27	7.27	7.27	7.23	7.31	7.29
6.99	7.04	7.04	7.09	6.98	7.02	7.03	7.08	7.05	7.05	7.04	7.06
6.97	6.98	7.02	7.04	6.97	6.99	7.02	7.04	6.97	7.01	6.98	7.02

Table S28 (cont). Unscaled chemical shifts calculated at the levels of theory indicated in Table S27 for all significantly populated conformers of **9a** and **10a** (arranged in descending order of magnitude).

Compound 9a											
Level of theory N°											
13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
Carbon Shifts											
194.8	197.7	196.9	198.6	194.9	197.9	197.1	198.8	197.8	201.1	199.7	200.9
144.9	143.1	142.5	142.9	144.8	143.0	142.5	142.8	144.7	142.8	142.2	141.3
138.5	138.6	138.3	138.7	138.5	138.7	138.4	138.7	137.5	137.7	137.2	137.5
137.8	137.3	137.0	137.2	137.7	137.2	136.9	137.1	136.5	135.8	135.7	135.9
134.7	134.3	134.3	134.3	134.7	134.2	134.2	134.3	135.8	134.9	134.6	134.6
132.6	131.9	131.9	132.0	132.6	131.9	131.8	131.9	135.0	134.6	134.6	132.2
131.4	131.8	131.7	131.4	131.5	131.8	131.7	131.4	131.9	132.4	132.2	129.6
129.4	129.8	129.9	129.5	129.4	129.8	129.9	129.5	129.3	129.7	129.8	129.6
129.1	129.2	129.2	128.8	129.1	129.2	129.2	128.8	128.6	128.6	128.6	128.5
128.8	128.8	129.0	128.7	128.9	128.9	129.0	128.7	128.6	128.6	128.5	128.2
128.5	127.5	127.4	127.8	128.5	127.5	127.4	127.8	128.4	127.4	127.3	127.8
123.0	122.0	122.2	122.0	122.9	121.9	122.2	122.0	122.5	121.3	121.5	121.3
121.6	121.5	119.2	120.8	122.0	121.9	119.6	121.3	117.8	116.8	116.1	114.5
120.1	119.3	118.8	118.6	120.1	119.3	118.7	118.6	113.9	113.4	110.6	113.9
92.3	90.6	89.1	89.6	92.5	90.9	89.4	89.9	81.8	79.4	77.6	79.5
Proton Shifts											
8.78	9.11	9.38	9.51	8.78	9.10	9.38	9.51	8.47	8.81	9.08	9.10
7.88	7.82	8.23	8.58	7.88	7.82	8.23	8.58	7.79	7.73	8.13	8.45
7.55	7.58	7.67	7.72	7.55	7.58	7.67	7.72	7.57	7.61	7.70	7.78
7.54	7.53	7.61	7.72	7.54	7.54	7.61	7.72	7.56	7.57	7.63	7.77
7.52	7.52	7.51	7.63	7.52	7.52	7.51	7.64	7.56	7.56	7.55	7.55
7.52	7.52	7.49	7.48	7.52	7.52	7.49	7.48	7.51	7.51	7.48	7.47
7.42	7.40	7.38	7.46	7.42	7.40	7.38	7.46	7.44	7.43	7.40	7.43
7.33	7.31	7.37	7.39	7.33	7.31	7.37	7.39	7.36	7.35	7.32	7.39
7.20	7.16	7.29	7.31	7.20	7.16	7.29	7.31	7.07	7.01	7.22	7.36
5.85	6.06	6.36	6.36	5.84	6.05	6.35	6.36	5.93	6.12	6.39	6.45

Compound 10a											
Level of theory N°											
13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
Carbon Shifts											
190.9	194.3	193.4	195.2	191.1	194.5	193.6	195.5	194.0	197.7	196.2	198.6
145.2	143.2	142.8	142.8	145.1	143.1	142.8	142.7	144.4	142.2	141.8	141.6
137.4	137.1	136.8	137.0	137.4	137.0	136.7	136.9	136.1	135.6	135.5	135.6
135.8	135.5	135.6	135.6	135.9	135.7	135.8	135.8	134.8	134.4	134.4	134.5
134.5	134.0	134.1	134.1	134.5	134.0	134.0	134.1	134.2	134.1	134.2	134.3
131.0	131.3	131.2	130.9	131.0	131.3	131.2	130.8	132.6	132.0	131.8	131.7
130.5	129.4	129.5	129.8	130.6	129.6	129.7	130.0	131.6	131.3	131.2	131.6
129.0	129.4	129.5	129.0	129.0	129.4	129.5	129.1	129.0	129.4	129.5	129.2
129.0	129.1	129.1	128.7	129.0	129.1	129.1	128.7	128.6	128.6	128.7	128.4
128.8	128.8	129.0	128.7	128.8	128.8	129.0	128.7	128.5	128.5	128.5	128.1
128.2	127.2	127.1	127.5	128.2	127.2	127.1	127.5	128.1	127.1	127.1	127.5
123.0	122.0	122.2	122.0	123.1	122.1	122.2	122.0	122.5	121.4	121.6	121.3
122.9	122.0	121.7	121.3	122.8	121.9	121.9	121.4	120.5	119.3	119.0	118.6
114.3	113.5	111.7	112.7	114.6	113.8	112.0	113.0	107.2	105.9	103.6	104.6
91.4	89.8	88.2	88.9	91.5	90.0	88.5	89.1	82.2	80.0	78.1	78.7
Proton Shifts											
9.72	9.93	10.29	10.58	9.73	9.94	10.30	10.60	9.37	9.59	9.95	10.27
7.49	7.47	7.85	8.13	7.50	7.46	7.86	8.15	7.50	7.51	7.70	8.00
7.46	7.46	7.57	7.58	7.46	7.46	7.57	7.58	7.45	7.49	7.60	7.62
7.45	7.45	7.50	7.58	7.45	7.45	7.50	7.58	7.45	7.46	7.52	7.61
7.43	7.43	7.46	7.42	7.43	7.44	7.46	7.42	7.44	7.45	7.51	7.48
7.42	7.43	7.43	7.39	7.41	7.43	7.43	7.39	7.38	7.38	7.43	7.40
7.36	7.36	7.33	7.34	7.36	7.36	7.33	7.34	7.33	7.30	7.35	7.36
7.27	7.25	7.24	7.25	7.26	7.25	7.24	7.25	7.31	7.28	7.28	7.30
6.72	6.84	6.97	7.07	6.71	6.83	6.96	7.06	6.72	6.89	6.98	7.05
6.67	6.74	6.88	7.04	6.66	6.74	6.87	7.03	6.67	6.66	6.79	7.00

Table S29. Scaled chemical shifts calculated at the levels of theory indicated in Table S27 for all significantly populated conformers of **9a** and **10a** (arranged in descending order of magnitude).

Compound 9a											
Level of theory N°											
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Carbon Shifts											
195.5	196.3	195.7	195.6	195.6	196.5	195.9	195.8	192.3	192.9	192.2	192.5
141.5	140.8	140.8	141.5	141.4	140.8	140.7	141.3	141.2	140.1	140.2	140.5
136.7	136.1	136.5	136.6	137.0	136.0	136.5	136.8	135.6	135.7	136.0	136.0
136.2	135.1	135.8	135.5	136.0	135.0	135.7	135.2	135.3	134.6	134.9	135.0
132.6	132.6	132.6	132.4	132.6	132.5	132.5	132.3	134.1	134.0	133.9	133.9
130.8	129.5	129.8	130.3	130.7	129.5	129.7	130.1	133.8	133.0	133.4	133.5
129.6	129.4	129.7	129.7	129.5	129.3	129.6	129.7	131.0	131.4	131.5	131.2
126.9	127.7	127.7	127.6	127.0	127.7	127.7	127.6	128.6	129.2	129.3	128.9
126.6	127.1	127.2	126.9	126.6	127.1	127.1	126.9	127.9	128.3	128.3	128.1
126.5	126.9	127.1	126.8	126.6	126.9	127.0	126.8	127.8	128.1	128.1	127.7
126.0	125.9	126.2	126.0	125.9	125.8	126.1	125.8	127.6	127.7	127.9	127.6
120.3	119.9	120.3	119.8	120.2	119.8	120.3	119.7	122.5	121.4	121.9	121.9
117.5	119.1	117.7	118.4	117.8	119.3	118.0	118.8	117.0	116.9	117.1	117.0
116.4	116.9	116.8	116.3	116.4	116.7	116.6	116.2	112.5	113.9	112.9	113.5
87.3	87.4	87.0	87.2	87.5	87.7	87.2	87.5	83.5	83.4	82.9	83.2
Proton Shifts											
9.38	9.36	9.41	9.39	9.38	9.35	9.41	9.39	9.32	9.32	9.35	9.35
8.41	8.44	8.46	8.52	8.40	8.44	8.46	8.51	8.45	8.48	8.52	8.58
7.67	7.69	7.64	7.61	7.66	7.70	7.63	7.61	7.75	7.76	7.70	7.70
7.66	7.68	7.62	7.60	7.66	7.68	7.62	7.60	7.69	7.74	7.68	7.69
7.56	7.57	7.51	7.57	7.57	7.59	7.51	7.58	7.46	7.46	7.46	7.42
7.43	7.39	7.39	7.39	7.44	7.39	7.39	7.38	7.44	7.40	7.38	7.38
7.36	7.38	7.38	7.34	7.36	7.38	7.38	7.34	7.41	7.39	7.35	7.35
7.30	7.31	7.30	7.28	7.31	7.31	7.30	7.28	7.35	7.33	7.32	7.30
7.22	7.18	7.19	7.20	7.21	7.19	7.19	7.20	7.24	7.21	7.23	7.21
6.15	6.14	6.24	6.25	6.15	6.12	6.24	6.25	6.03	6.05	6.15	6.17

Compound 10a											
Level of theory N°											
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Carbon Shifts											
193.8	194.8	194.2	194.3	193.9	195.1	194.4	194.5	191.3	192.0	191.4	191.6
144.0	142.0	142.0	142.3	143.8	141.9	141.9	142.1	141.8	140.7	140.8	141.1
136.6	136.2	136.6	137.0	136.3	136.1	136.5	136.7	136.1	135.4	135.8	135.9
134.4	134.7	134.6	134.6	134.8	134.6	134.7	134.9	134.6	134.9	134.7	134.6
132.6	133.6	133.4	133.3	132.5	133.6	133.3	133.2	133.4	133.5	134.3	134.4
129.4	130.1	130.3	129.9	129.4	130.0	130.2	129.9	132.2	132.1	132.1	131.9
129.2	128.2	128.5	128.7	129.2	128.2	128.6	128.8	131.7	130.9	131.6	131.7
128.2	127.9	128.5	128.2	128.2	128.1	128.4	128.2	129.3	129.9	129.9	129.6
127.9	127.9	128.1	127.9	127.9	127.9	128.1	127.9	128.8	129.4	129.2	129.1
127.2	127.9	127.9	127.5	127.2	127.9	127.8	127.5	128.6	129.1	129.0	128.6
127.0	126.9	127.0	126.7	127.0	126.8	126.9	126.6	128.3	128.5	128.5	128.2
122.6	120.4	121.4	121.7	122.3	120.4	121.3	121.3	123.4	122.3	122.7	122.7
120.4	120.2	120.4	119.9	120.4	120.1	120.4	120.1	120.3	119.8	120.2	120.0
110.3	112.6	110.9	111.4	110.6	112.6	111.1	111.7	107.0	107.8	107.0	107.4
86.9	87.2	86.8	87.0	86.9	87.5	86.9	87.2	83.6	84.2	83.5	83.8
Proton Shifts											
9.88	9.89	9.87	9.88	9.88	9.89	9.87	9.88	9.88	9.89	9.85	9.85
7.83	7.84	7.92	7.94	7.85	7.85	7.93	7.95	7.77	7.75	7.85	7.91
7.54	7.51	7.51	7.48	7.54	7.51	7.50	7.48	7.57	7.58	7.55	7.54
7.48	7.51	7.49	7.47	7.47	7.51	7.49	7.47	7.49	7.55	7.52	7.52
7.45	7.40	7.37	7.34	7.45	7.40	7.37	7.34	7.43	7.42	7.44	7.39
7.36	7.36	7.36	7.33	7.36	7.36	7.36	7.33	7.40	7.36	7.36	7.33
7.34	7.30	7.30	7.31	7.35	7.30	7.30	7.31	7.36	7.31	7.32	7.31
7.20	7.20	7.23	7.24	7.20	7.20	7.24	7.23	7.24	7.22	7.26	7.24
7.03	7.09	7.05	7.09	7.03	7.07	7.05	7.09	7.04	7.05	7.01	7.04
7.02	7.04	7.04	7.05	7.02	7.05	7.03	7.05	6.97	7.01	6.97	7.00

Table S29 (cont). Scaled chemical shifts calculated at the levels of theory indicated in Table S27 for all significantly populated conformers of **9a** and **10a** (arranged in descending order of magnitude).

Compound 9a											
Level of theory N°											
13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
Carbon Shifts											
195.7	196.4	195.7	196.4	195.9	196.6	195.9	196.5	192.4	193.0	192.0	193.6
143.1	141.1	140.9	140.8	143.0	140.9	140.7	140.7	142.6	140.6	140.6	139.9
136.3	136.5	136.6	136.6	136.4	136.6	136.6	136.7	135.8	136.1	136.1	136.5
135.6	135.2	135.2	135.1	135.5	135.1	135.1	135.0	134.9	134.4	134.7	135.0
132.4	132.1	132.5	132.3	132.3	132.0	132.4	132.2	134.2	133.6	133.8	133.9
130.2	129.7	130.1	130.0	130.1	129.6	130.0	129.8	133.4	133.3	133.7	131.7
128.9	129.6	129.9	129.4	128.9	129.5	129.9	129.3	130.6	131.3	131.7	129.4
126.7	127.6	128.1	127.5	126.7	127.5	128.1	127.4	128.2	128.9	129.5	129.4
126.5	127.0	127.4	126.8	126.4	127.0	127.4	126.8	127.5	127.9	128.5	128.4
126.2	126.6	127.2	126.7	126.2	126.6	127.2	126.7	127.5	127.9	128.3	128.1
125.8	125.2	125.6	125.8	125.8	125.2	125.5	125.8	127.3	126.8	127.3	127.7
120.0	119.6	120.3	120.0	119.9	119.6	120.2	119.9	121.8	121.4	122.1	121.9
118.5	119.1	117.3	118.8	118.9	119.5	117.7	119.2	117.3	117.3	117.3	115.7
117.0	117.0	116.9	116.7	116.9	116.8	116.8	116.6	113.7	114.2	112.3	115.2
87.6	87.8	87.0	87.8	87.8	88.0	87.2	88.0	83.6	83.7	82.8	84.2
Proton Shifts											
9.24	9.43	9.48	9.41	9.24	9.43	9.47	9.41	9.13	9.35	9.41	9.33
8.13	7.97	8.25	8.48	8.14	7.98	8.25	8.48	8.15	7.96	8.27	8.55
7.73	7.71	7.66	7.62	7.73	7.71	7.66	7.62	7.83	7.80	7.75	7.74
7.72	7.65	7.59	7.62	7.71	7.65	7.60	7.61	7.81	7.74	7.67	7.73
7.69	7.63	7.49	7.53	7.69	7.63	7.49	7.54	7.81	7.73	7.57	7.46
7.69	7.63	7.46	7.38	7.69	7.63	7.46	7.38	7.73	7.67	7.48	7.36
7.56	7.50	7.35	7.36	7.57	7.50	7.35	7.36	7.63	7.56	7.38	7.31
7.45	7.40	7.34	7.29	7.45	7.40	7.34	7.29	7.52	7.46	7.29	7.28
7.30	7.23	7.25	7.21	7.30	7.23	7.25	7.21	7.10	7.02	7.17	7.23
5.63	5.99	6.26	6.26	5.62	5.98	6.26	6.25	5.43	5.86	6.16	6.14

Compound 10a											
Level of theory N°											
13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
Carbon Shifts											
193.9	194.9	193.9	194.9	194.0	195.1	194.1	195.1	191.3	192.2	191.0	192.0
144.8	142.4	142.3	142.0	144.6	142.3	142.2	141.9	143.6	141.4	141.4	140.8
136.5	136.2	136.1	136.1	136.3	136.1	136.0	136.0	135.6	135.4	135.6	135.4
134.7	134.6	134.9	134.7	134.8	134.7	135.0	134.8	134.4	134.2	134.6	134.4
133.3	133.0	133.4	133.2	133.2	132.9	133.3	133.1	133.8	133.9	134.4	134.3
129.6	130.2	130.4	130.0	129.5	130.2	130.4	129.9	132.3	132.0	132.2	131.9
129.0	128.3	128.7	128.9	129.1	128.4	128.9	129.0	131.3	131.4	131.7	131.8
127.4	128.3	128.7	128.1	127.4	128.2	128.7	128.1	128.8	129.6	130.1	129.6
127.4	128.0	128.3	127.8	127.4	127.9	128.3	127.7	128.4	128.9	129.4	129.0
127.2	127.7	128.2	127.7	127.2	127.6	128.1	127.7	128.4	128.9	129.2	128.7
126.6	126.0	126.3	126.6	126.5	125.9	126.2	126.5	128.0	127.6	127.9	128.1
121.0	120.7	121.3	121.0	121.0	120.7	121.1	120.9	122.6	122.3	122.9	122.6
120.8	120.6	120.8	120.3	120.7	120.6	120.9	120.4	120.6	120.4	120.5	120.1
111.6	112.0	110.5	111.6	111.9	112.2	110.8	111.8	107.8	108.1	106.5	107.5
87.0	87.6	86.6	87.6	87.0	87.8	86.7	87.7	83.8	84.4	83.3	84.3
Proton Shifts											
9.83	9.89	9.87	9.88	9.83	9.89	9.87	9.88	9.78	9.81	9.84	9.86
7.61	7.55	7.78	7.93	7.61	7.55	7.79	7.94	7.66	7.62	7.70	7.87
7.57	7.54	7.54	7.49	7.57	7.54	7.54	7.48	7.60	7.61	7.60	7.54
7.57	7.53	7.48	7.49	7.57	7.53	7.48	7.48	7.60	7.57	7.53	7.53
7.55	7.51	7.45	7.36	7.54	7.52	7.45	7.36	7.59	7.56	7.52	7.41
7.53	7.51	7.42	7.34	7.53	7.51	7.43	7.34	7.52	7.49	7.44	7.34
7.48	7.44	7.34	7.30	7.48	7.44	7.34	7.30	7.47	7.40	7.37	7.31
7.38	7.34	7.27	7.23	7.38	7.34	7.27	7.23	7.44	7.39	7.30	7.25
6.84	6.96	7.03	7.08	6.84	6.95	7.03	7.08	6.78	6.97	7.01	7.04
6.79	6.86	6.95	7.06	6.78	6.86	6.95	7.06	6.71	6.73	6.84	6.99

Given the high errors computed for some nuclei of **9** and **10** at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level, we also explored the performance of this level of theory in the NMR calculations of related known unsaturated analogues of **9a** and **10a** (Figure S15). The collected results provided insightful observations (Pages S53-S61). For instance, despite most carbon signals were nicely reproduced by our calculations, a systematic error in the shift reproduction of the alkyne carbon at the end of the polyene chain was noticed. In all cases, the highest ^{1}H NMR unscaled errors were computed from vinylic protons, whereas the formyl hydrogens (when corresponding) were simulated in closer agreement.

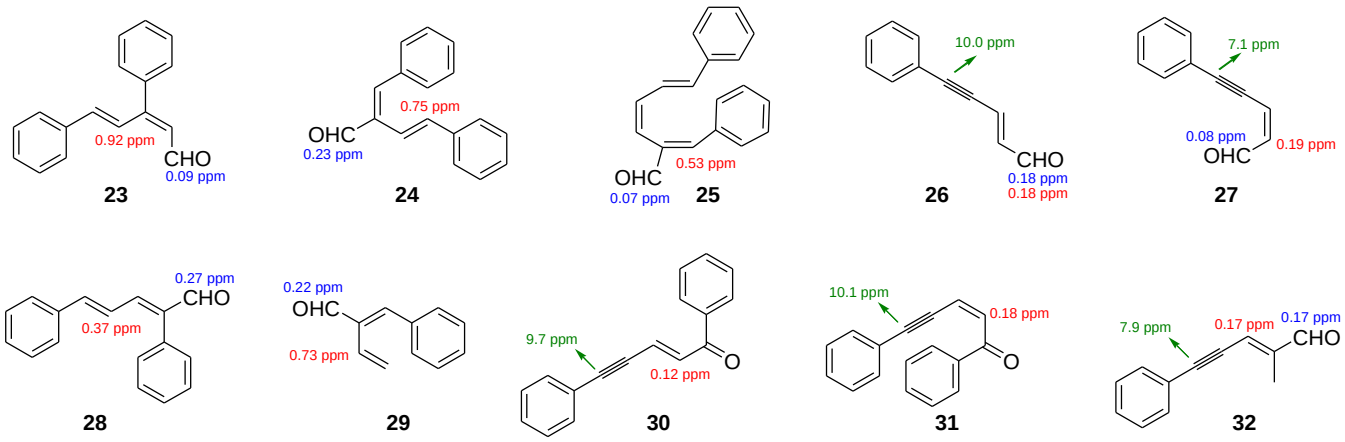


Figure S15. Known unsaturated analogues of **9a** and **10a**. The highest unscaled error ($\Delta\delta = \delta_{exp}-\delta_{calc}$) observed in proton data is given in red, whereas the $\Delta\delta$ values computed for the formyl protons and the alkyne carbon located at the end of the polyene chain are given in blue and green, respectively.

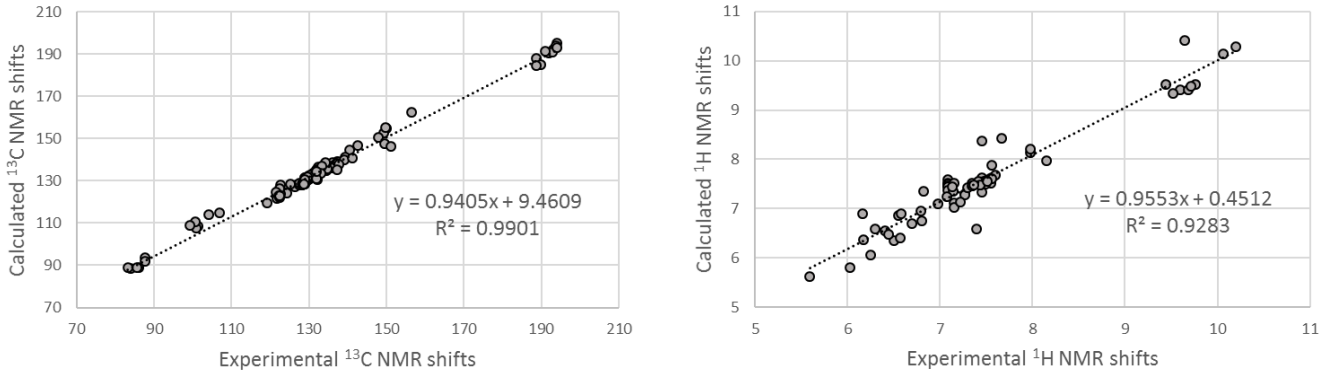
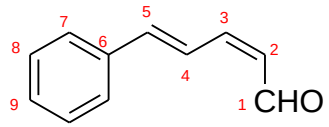


Figure S16. Correlation plot of δ_{calc} *vs* δ_{exp} obtained from the compounds depicted in Figure S15 at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level of theory.

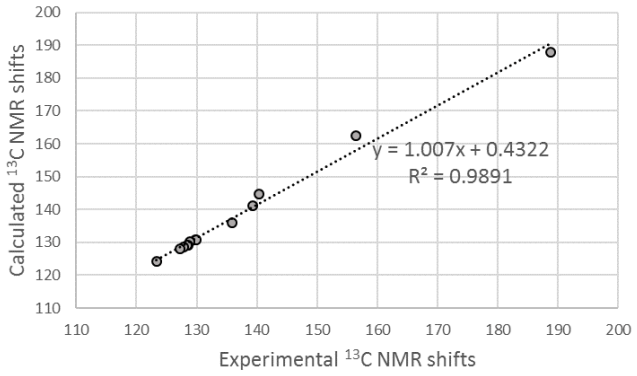
Table S30. Experimental ^{13}C NMR data of synthetic **23** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **23**



23

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
188.7	11.1197	C-1	187.8	186.0	0.9	2.7
156.4	36.3595	C-3	162.5	161.0	6.1	4.6
140.4	54.0906	C-5	144.8	143.4	4.4	3.0
139.3	57.7907	C-1'	141.1	139.7	1.8	0.4
135.9	62.9294	C-6	136.0	134.6	0.1	1.3
129.7	68.1527	C-4'	130.7	129.4	1.0	0.3
129.9	68.2289	C-9	130.7	129.3	0.8	0.6
128.9	68.5444	C-2'	130.3	129.0	1.4	0.1
128.5	69.8705	C-7	129.0	127.7	0.5	0.8
128.4	69.8759	C-8	129.0	127.7	0.6	0.7
127.9	70.3159	C-2	128.6	127.3	0.7	0.6
127.3	70.8958	C-3'	128.0	126.7	0.7	0.6
123.3	74.7441	C-4	124.1	122.9	0.8	0.4
		Average			***1.5***	***1.2***
10.06	21.0669	H-1	10.15	9.78	0.09	0.28
7.45	22.8445	H-4	8.37	8.01	0.92	0.56
7.08	23.6216	H-7'	7.59	7.24	0.51	0.16
7.08	23.6874	H-3'	7.52	7.17	0.44	0.09
7.08	23.7131	H-4'	7.50	7.15	0.42	0.07
7.08	23.7465	H-2'	7.47	7.12	0.39	0.04
7.08	23.7673	H-8	7.44	7.09	0.36	0.01
7.08	23.8409	H-9	7.37	7.02	0.29	0.06
6.55	24.3491	H-5	6.86	6.52	0.31	0.03
6.03	25.4063	H-2	5.81	5.46	0.22	0.57
		Average			***0.40***	***0.19***

[a] Taken from: Dinesh V. Vidhani, Marie E. Krafft, and Igor V. Alabugin *Org. Lett.* **2013**, *15*, 4462.
* The assignment corresponds to the computed σ vaues.



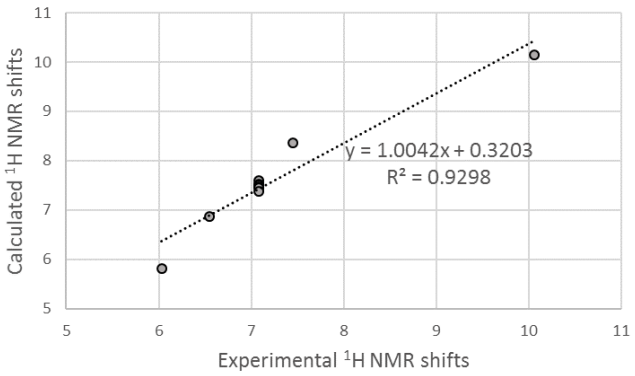
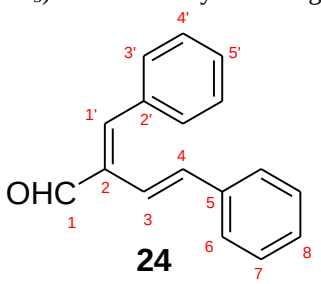


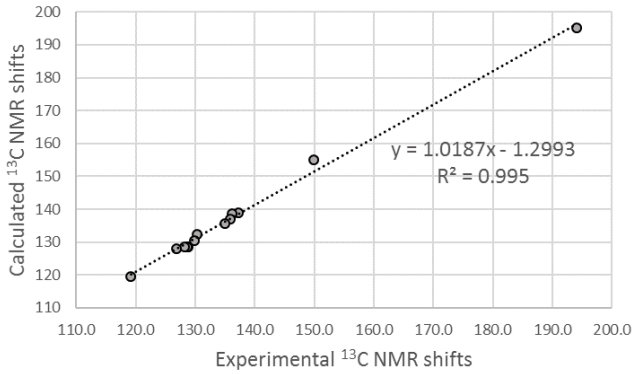
Table S31. Experimental ^{13}C NMR data of synthetic **24** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **24**



24

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
194.1	3.8520	C-1	195.0	192.7	0.9	1.4
149.9	43.9119	C-1'	155.0	153.4	5.1	3.5
137.3	59.9411	C-4	138.9	137.7	1.6	0.4
136.2	60.1973	C-5	138.7	137.4	2.5	1.2
135.9	61.7807	C-2'	137.1	135.9	1.2	0.0
135.0	63.2646	C-2	135.6	134.4	0.6	0.6
130.3	66.4771	C-3'	132.4	131.3	2.1	1.0
129.8	68.4616	C-5'	130.4	129.3	0.6	0.5
128.8	70.2527	C-7	128.6	127.6	0.2	1.2
128.6	70.3324	C-4'	128.6	127.5	0.0	1.1
128.2	70.4049	C-8	128.5	127.4	0.3	0.8
126.8	70.9315	C-6	128.0	126.9	1.2	0.1
119.2	79.2952	C-3	119.6	118.7	0.4	0.5
		Average			***1.3***	***0.9***
9.76	21.6866	H-1	9.53	9.66	0.23	0.10
7.67	22.7893	H-4	8.42	8.42	0.75	0.75
7.56	23.5811	H-6	7.63	7.53	0.07	0.03
7.45	23.5835	H-3'	7.63	7.53	0.18	0.08
7.45	23.6852	H-4'	7.53	7.41	0.08	0.04
7.45	23.7568	H-5'	7.46	7.33	0.01	0.12
7.45	23.8805	H-7	7.33	7.20	0.12	0.25
7.27	23.9066	H-3'	7.31	7.17	0.04	0.10
7.27	23.9393	H-8	7.27	7.13	0.00	0.14
6.98	24.1188	H-1'	7.09	6.93	0.11	0.05
		Average			***0.16***	***0.17***

[a] Taken from: Kobayashi, S., Kudo, K., Ito, A., Hirama, S., Otani, T., Saito, T. *Org. Biomol. Chem.* **2014**, *12*, 4061.
* The assignment corresponds to the computed σ vaues.



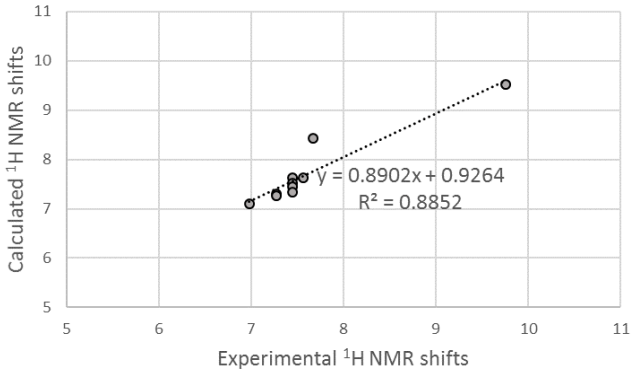
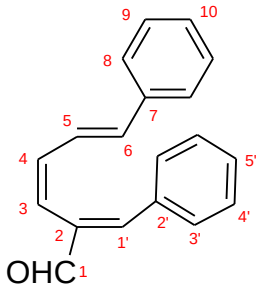


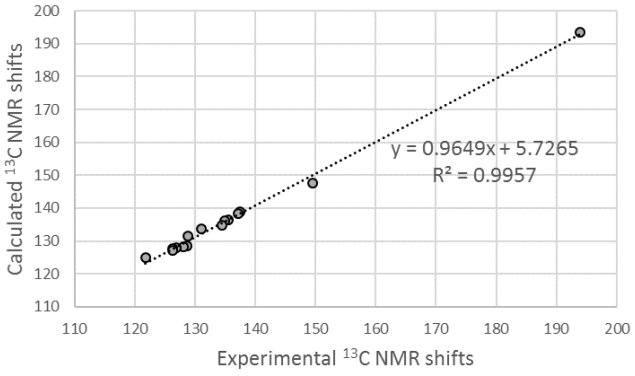
Table S32. Experimental ^{13}C NMR data of synthetic **25** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **25**



25

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.9	5.3018	C-1	193.6	194.7	0.3	0.8
149.5	51.2586	C-3'	147.6	147.1	1.9	2.4
137.5	60.0012	C-4'	138.9	138.0	1.4	0.5
137.1	60.5299	C-2'	138.4	137.5	1.3	0.4
135.5	62.5283	C-5'	136.4	135.4	0.9	0.1
134.9	62.8205	C-9	136.1	135.1	1.2	0.2
134.5	64.0961	C-7	134.8	133.8	0.3	0.7
131.1	65.2432	C-1'	133.6	132.6	2.5	1.5
128.9	67.2918	C-8	131.6	130.5	2.7	1.6
128.7	70.2923	C-2	128.6	127.3	0.1	1.4
128.1	70.6759	C-3	128.2	126.9	0.1	1.2
126.9	71.0014	C-5	127.9	126.6	1.0	0.3
126.3	71.2152	C-4	127.7	126.4	1.4	0.1
126.3	71.8114	C-6	127.1	125.8	0.8	0.5
121.8	74.0548	C-10	124.8	123.4	3.0	1.6
		Average			***1.3***	***0.9***
9.44	21.6973	H-1	9.51	9.42	0.07	0.02
7.14	23.8641	arom	7.35	7.15	0.21	0.01
6.82	23.8664	H-1'	7.35	7.15	0.53	0.33
6.70	24.5222	H-5	6.69	6.46	0.01	0.24
6.40	24.6542	H-6	6.56	6.32	0.16	0.08
6.30	24.6220	H-4	6.59	6.35	0.29	0.05
6.17	24.8386	H-3	6.37	6.13	0.20	0.04
		Average			***0.21***	***0.11***

[a] Taken from: Lee M. Bishop, Russell E. Roberson, Robert G. Bergman, Dirk Trauner. *Synthesis* **2010**, *13*, 2233.
* The assignment corresponds to the computed σ vaues.



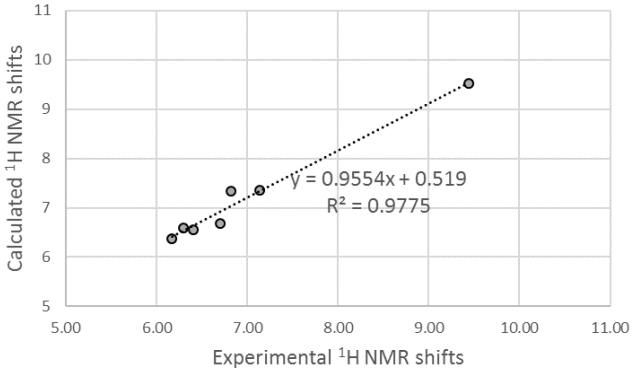
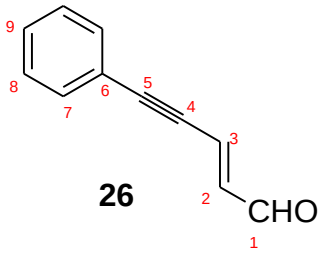


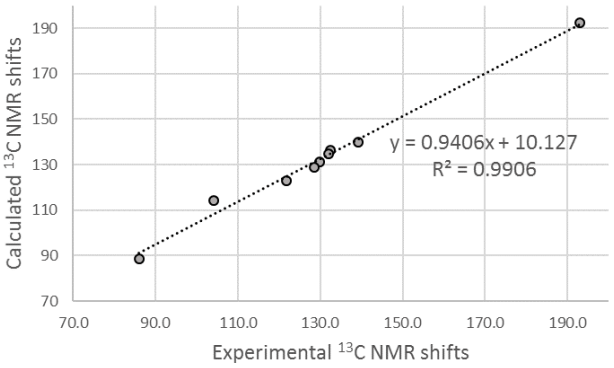
Table S33. Experimental ^{13}C NMR data of synthetic **26** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **26**



26

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.0	6.5349	C-1	192.4	193.7	0.6	0.7
139.2	59.0514	C-2	139.8	137.9	0.6	1.3
132.4	62.3790	C-3	136.5	134.4	4.1	2.0
132.1	64.2783	C-7	134.6	132.3	2.5	0.2
129.8	67.8683	C-9	131.0	128.5	1.2	1.3
128.6	69.9504	C-8	128.9	126.3	0.3	2.3
121.8	76.1355	C-6	122.8	119.7	1.0	2.1
104.2	84.7171	C-5	114.2	110.6	10.0	6.4
86.0	110.1314	C-4	88.8	83.6	2.8	2.4
		Average			***2.6***	***2.1***
9.60	21.7950	H-1	9.42	9.55	0.18	0.05
7.43	23.6901	arom	7.52	7.59	0.09	0.16
6.80	24.4606	H-3	6.75	6.80	0.05	0.00
6.50	24.8524	H-2	6.36	6.39	0.14	0.11
		Average			***0.12***	***0.08***

[a] Taken from: Jens A. John and James M. Tour *Tetrahedron* **1997**, *53*, 15515.
* The assignment corresponds to the computed σ vaues.



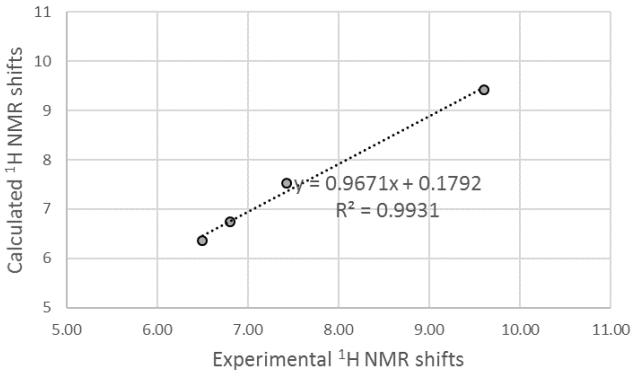
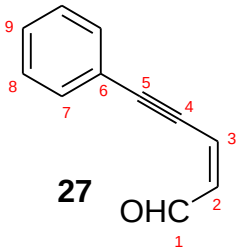
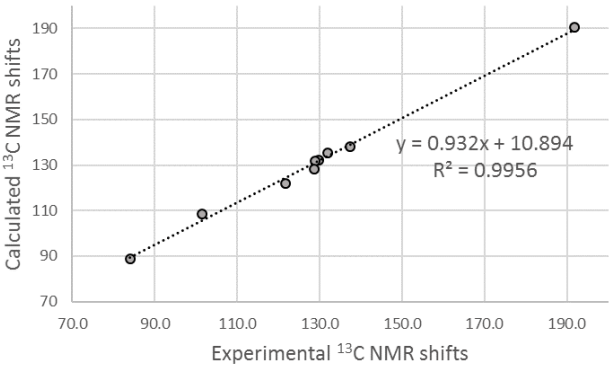


Table S34. Experimental ^{13}C NMR data of synthetic **27** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **27**



δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
191.9	8.4931	C-1	190.4	192.6	1.5	0.7
137.3	60.6453	C-2	138.2	136.6	0.9	0.7
132.0	63.5088	C-7	135.4	133.6	3.4	1.6
129.8	66.7646	C-3	132.1	130.1	2.3	0.3
128.8	67.2720	C-9	131.6	129.5	2.8	0.7
128.6	70.5835	C-8	128.3	126.0	0.3	2.6
121.7	77.1417	C-6	121.7	118.9	0.0	2.8
101.4	90.3754	C-5	108.5	104.7	7.1	3.3
84.0	110.2776	C-4	88.6	83.4	4.6	0.6
		Average			***2.6***	***1.5***
10.20	20.9314	H-1	10.28	10.15	0.08	0.05
7.35	23.7032	arom	7.51	7.46	0.16	0.11
6.79	24.2644	H-3	6.95	6.92	0.16	0.13
6.25	25.1483	H-2	6.06	6.06	0.19	0.19
		Average			***0.15***	***0.12***

[a] Taken from: Zhu, S., Huang, X., Zhao, T.-Q., Ma, T., Jiang, H. *Org. Biomol. Chem.* **2015**, *13*, 1225.
* The assignment corresponds to the computed σ vaues.



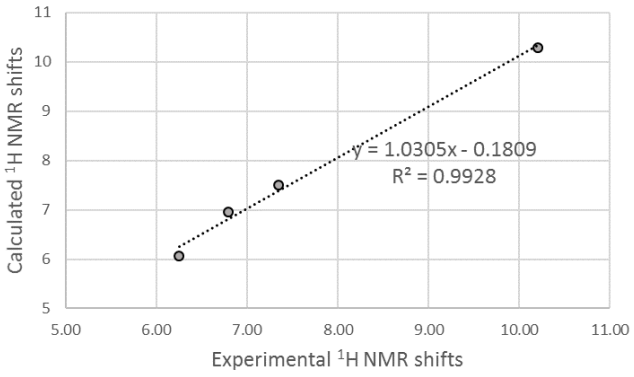
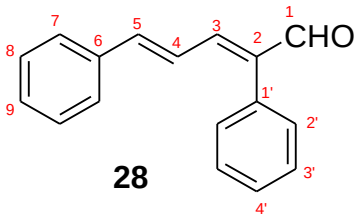


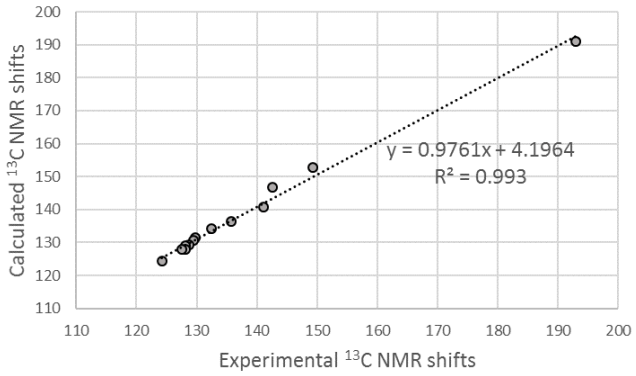
Table S35. Experimental ^{13}C NMR data of synthetic **28** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **28**



28

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
192.9	7.8605	C-1	191.0	191.4	1.9	1.5
149.3	46.2391	C-3	152.6	152.1	3.3	2.8
142.6	52.2158	C-5	146.7	146.0	4.1	3.4
141.1	58.2191	C-2	140.7	139.8	0.4	1.3
135.7	62.5937	C-6	136.3	135.3	0.6	0.4
132.5	64.7962	C-1'	134.1	133.1	1.6	0.6
129.8	67.5212	C-2'	131.4	130.3	1.6	0.5
129.4	68.2646	C-9	130.6	129.5	1.2	0.1
128.7	69.5690	C-7	129.3	128.2	0.6	0.5
128.2	69.9248	C-8	129.0	127.8	0.8	0.4
128.1	70.9370	C-4'	128.0	126.8	0.1	1.3
127.5	71.0165	C-3'	127.9	126.7	0.4	0.8
124.2	74.6277	C-4	124.3	123.0	0.1	1.2
		Average			***1.3***	***1.1***
9.68	21.8044	H-1	9.41	9.67	0.27	0.01
7.35	23.7475	arom	7.46	7.41	0.11	0.06
7.15	24.0879	H-5	7.12	7.02	0.03	0.13
7.15	24.1883	H-3	7.02	6.90	0.13	0.25
7.15	23.6960	H-4	7.52	7.47	0.37	0.32
		Average			***0.18***	***0.15***

[a] Taken from: M. J. Riveira and M. P. Mischne, *Chem. Eur. J.*, **2012**, *18*, 2382.
* The assignment corresponds to the computed σ vaues.



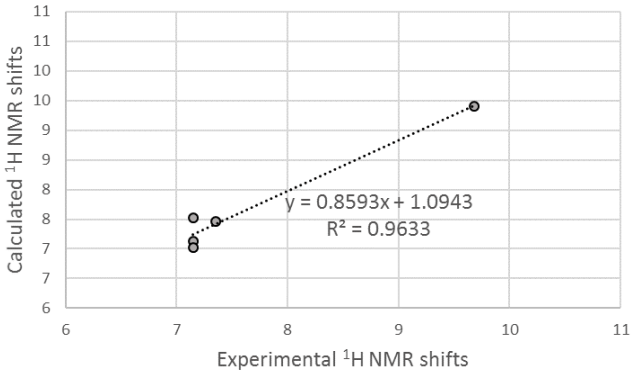
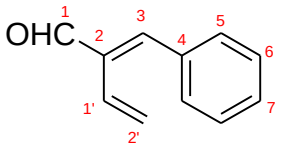


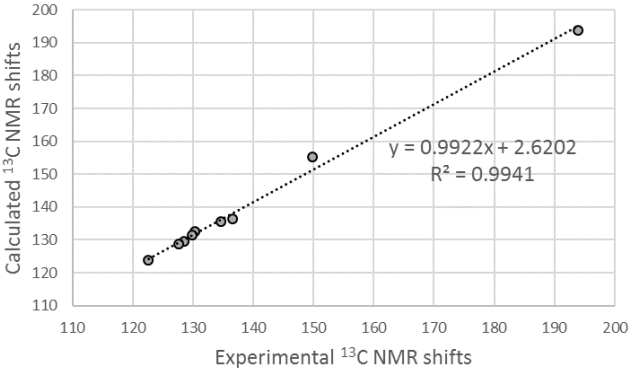
Table S36. Experimental ^{13}C NMR data of synthetic **29** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **29**



29

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.9	5.0334	C-1	193.9	192.7	0.0	1.2
149.8	43.5135	C-3	155.4	154.0	5.6	4.2
136.5	62.4931	C-4	136.4	134.8	0.1	1.7
134.6	63.2606	C-2	135.6	134.1	1.0	0.5
130.3	66.3443	C-5	132.5	130.9	2.2	0.6
129.9	67.4141	C-7	131.5	129.9	1.6	0.0
128.6	69.1850	C-1'	129.7	128.1	1.1	0.5
127.6	70.1972	C-6	128.7	127.1	1.1	0.5
122.6	74.9870	C-2'	123.9	122.2	1.3	0.4
		Average			***1.6***	***1.1***
9.71	21.7200	H-1	9.49	9.73	0.22	0.02
7.54	23.6023	H-5	7.61	7.53	0.07	0.01
7.43	23.7269	H-6,7	7.49	7.39	0.06	0.04
7.22	24.0796	H-3	7.13	6.98	0.09	0.24
6.58	24.3166	H-2'a	6.90	6.70	0.32	0.12
6.16	24.3189	H-1'	6.89	6.70	0.73	0.54
5.59	25.5911	H-2'b	5.62	5.21	0.03	0.38
		Average			***0.22***	***0.19***

[a] Taken from: Molander, G. A.; Felix, L. A. *J. Org. Chem*, **2005**, *70*, 3950.
* The assignment corresponds to the computed σ vaues.



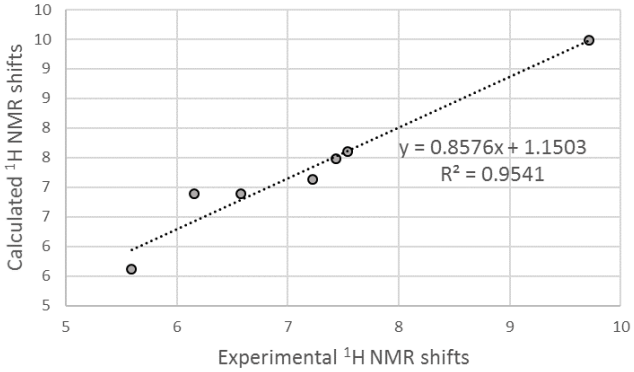
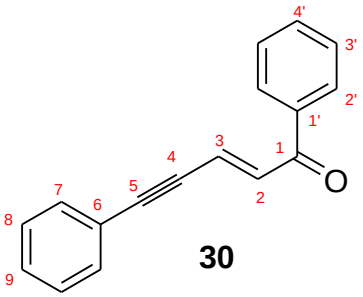


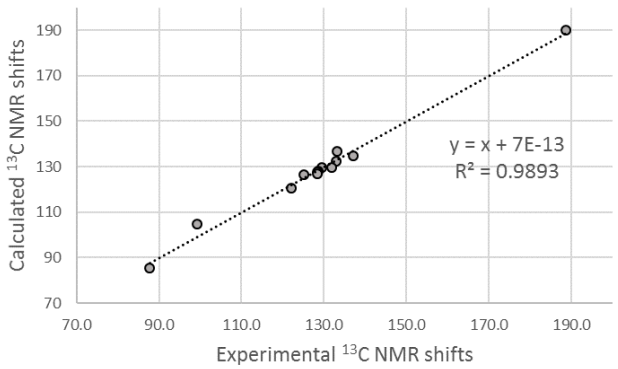
Table S37. Experimental ^{13}C NMR data of synthetic **30** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **30**



30

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
188.8	14.4593	C-1	184.4	190.2	4.4	1.4
133.2	61.8183	C-1'	137.1	136.6	3.9	3.4
137.2	63.4937	C-7	135.4	134.7	1.8	2.5
133.0	65.4227	C-4'	133.5	132.5	0.5	0.5
132.0	67.8159	C-9	131.1	129.8	0.9	2.2
129.4	67.9097	C-2	131.0	129.7	1.6	0.3
128.7	69.3455	C-2'	129.5	128.0	0.8	0.7
128.5	69.5275	C-3	129.4	127.8	0.9	0.7
128.5	70.3793	C-3'	128.5	126.9	0.0	1.6
125.1	70.6153	C-8	128.3	126.6	3.2	1.5
122.2	76.0225	C-6	122.9	120.5	0.7	1.7
99.3	89.8802	C-5	109.0	104.8	9.7	5.5
87.7	106.8531	C-4	92.0	85.6	4.3	2.1
		Average			***2.5***	***1.9***
7.98	22.9972	H-2'	8.21	8.09	0.24	0.12
7.56	23.5999	H-7	7.61	7.47	0.05	0.09
7.50	23.6457	H-3',4'	7.57	7.42	0.07	0.08
7.43	23.7352	H-2	7.48	7.33	0.05	0.10
7.35	23.7418	H-3	7.47	7.32	0.12	0.03
7.13	23.7679	H-8,9	7.44	7.30	0.31	0.17
		Average			***0.14***	***0.10***

[a] Taken from: J. Chen, G. Fan and Y. Liu, *Org. Biomol. Chem.,* **2010**, *8*, 4806-4810.
* The assignment corresponds to the computed σ vaues.



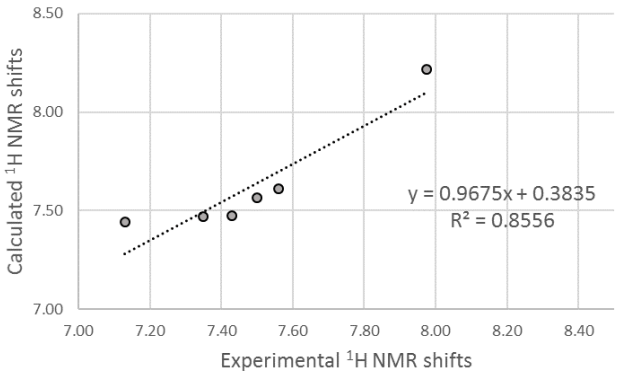
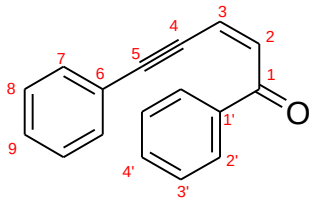


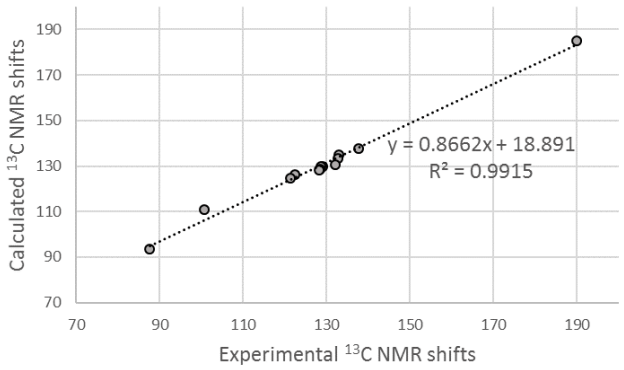
Table S38. Experimental ^{13}C NMR data of synthetic **31** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **31**



31

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
189.9	13.7980	C-1	185.1	191.9	4.8	2.0
137.7	61.1138	C-1'	137.8	137.3	0.1	0.4
132.9	63.9521	C-7	134.9	134.0	2.0	1.1
132.7	65.5495	C-4'	133.3	132.1	0.6	0.6
132.1	68.1563	C-9	130.7	129.1	1.4	3.0
129.1	69.0032	C-2	129.9	128.1	0.8	1.0
128.6	69.0881	C-2'	129.8	128.0	1.2	0.6
128.5	70.1860	C-8	128.7	126.8	0.2	1.7
128.2	70.5931	C-3'	128.3	126.3	0.1	1.9
122.5	72.6490	C-3	126.2	123.9	3.7	1.4
121.4	74.3909	C-6	124.5	121.9	3.1	0.5
100.7	88.1165	C-5	110.8	106.1	10.1	5.4
87.6	105.2389	C-4	93.6	86.3	6.0	1.3
		Average			***2.6***	***1.6***
7.98	23.0776	H-2'	8.13	7.93	0.15	0.05
7.56	23.3261	H-7	7.89	7.70	0.33	0.14
7.47	23.6538	H-3',4'	7.56	7.40	0.09	0.07
7.42	23.6641	H-3	7.55	7.39	0.13	0.02
7.30	23.7881	H-8,9	7.42	7.28	0.13	0.02
7.07	23.9643	H-2	7.25	7.12	0.18	0.05
		Average			***0.15***	***0.05***

[a] Taken from: J. Chen, G. Fan and Y. Liu, *Org. Biomol. Chem.,* **2010**, *8*, 4806-4810.
* The assignment corresponds to the computed σ vaues.



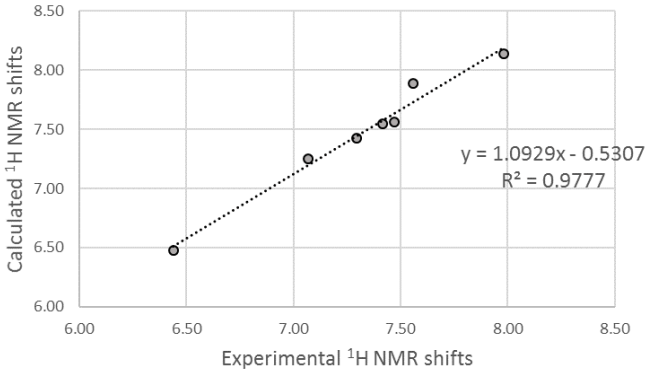
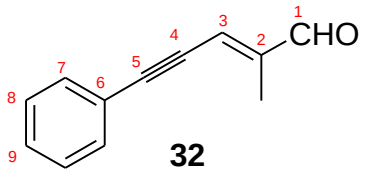


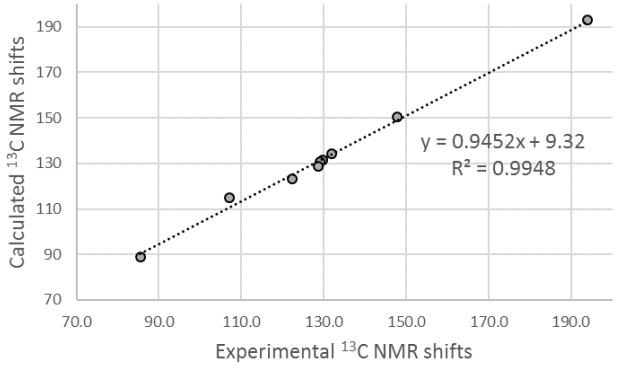
Table S39. Experimental ^{13}C NMR data of synthetic **32** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **32**

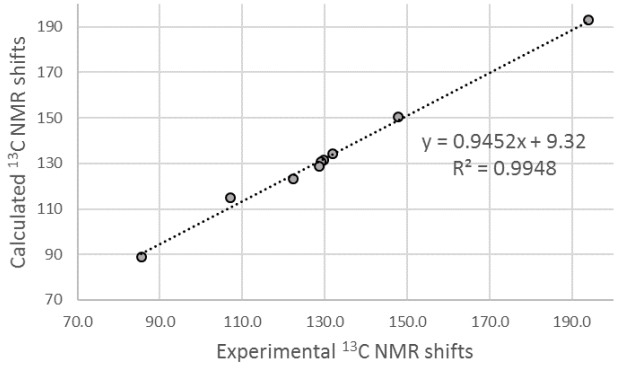


32

δ_{exp} [a]	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
194.0	5.9735	C-1	192.9	194.2	1.1	0.2
147.9	48.5463	C-2	150.3	149.2	2.4	1.3
131.9	64.5905	C-7	134.3	132.2	2.4	0.3
129.7	67.2094	C-3	131.7	129.5	2.0	0.2
129.0	68.3345	C-9	130.6	128.3	1.6	0.7
128.7	70.2913	C-8	128.6	126.2	0.1	2.5
122.4	75.8051	C-6	123.1	120.4	0.7	2.0
107.0	83.9512	C-5	114.9	111.7	7.9	4.7
85.5	109.8144	C-4	89.1	84.4	3.6	1.1
		Average			***2.4***	***1.5***
9.52	21.8669	H-1	9.35	9.45	0.17	0.07
7.51	23.6681	H-7	7.54	7.59	0.03	0.08
7.37	23.7372	H-8,9	7.47	7.52	0.10	0.15
6.57	24.8103	H-3	6.40	6.41	0.17	0.16
		Average			***0.12***	***0.11***

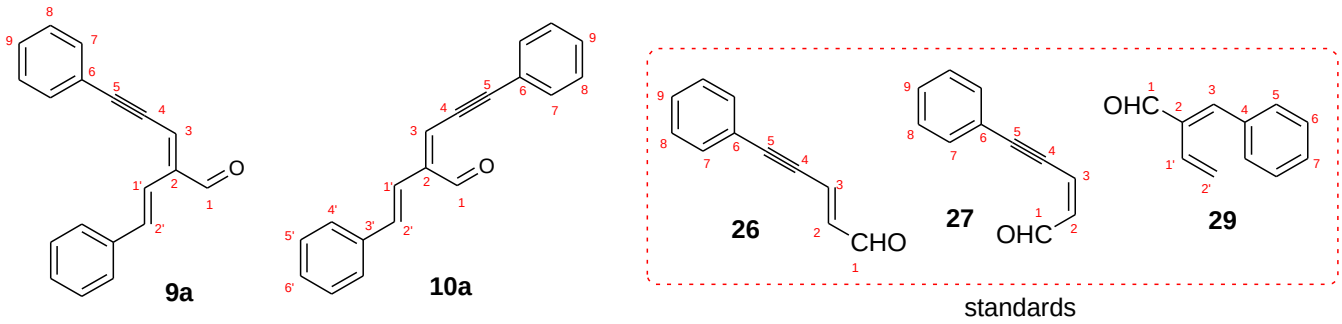
[a] This compound was prepared according to: C. F. Ingham and R. A. Massy-Westropp, *Aust. J. Chem.*, **1974**, *27*, 1491-1503.
* The assignment corresponds to the computed σ vaues.





Use of Spivey´s fragment referencing method for the calculation of the NMR shifts of 9a and 10a

To improve the accuracy in the calculations of the NMR shifts of **9a** and **10a** we employed the Spivey´s fragment referencing method. Hence, the NMR shifts of the different nuclei of **9a** and **10a** were calculated using the analogous nuclei in known compounds **26**, **27** and **29** as reference standards.



$$\delta_{calc} = \sigma_{ref} - \sigma_{calc} + \delta_{ref}$$

Compound 9a							
δ_{exp}	Nuclei	σ	Std.	σ (std)	δ_{exp} (std)	δ_{calc}	Unsc. Error (δ_{exp} -δ_{calc})
193.3	C-1	4.3352	C-1 of **26**	6.5349	193.0	195.2	1.9
143.3	C-2	55.8796	C-2 of **26**	59.0514	139.2	142.4	0.9
127.2	C-3	66.0434	C-3 of **26**	62.3790	132.4	128.7	1.5
86.9	C-4	107.5555	C-4 of **26**	110.1314	86.0	88.6	1.7
109.6	C-5	78.7826	C-5 of **26**	84.7171	104.2	110.1	0.5
119.4	C-1’	79.7835	C-1’ of **29**	69.1850	128.6	118.0	1.4
136.6	C-2’	60.4520	C-2’ of **29**	74.9870	122.6	137.1	0.5
			Average				***1.2***
9.65	H-1	21.8267	H-1 of **29**	21.7200	9.71	9.60	0.05
6.52	H-3	24.9403	H-3 of **29**	24.0796	7.22	6.36	0.16
7.25	H-1’	23.5806	H-1’ of **29**	24.3189	6.16	6.90	0.35
7.99	H-2’	22.7579	H-2’a of **29**	24.3166	6.58	8.14	0.15
			Average				***0.18***

Compound 10a							
δ_{exp}	Nuclei	σ	Std.	σ (std)	δ_{exp} (std)	δ_{calc}	Unsc. Error (δ_{exp} -δ_{calc})
193.3	C-1	7.5858	C-1 of **27**	8.4931	191.9	192.8	0.5
143.3	C-2	54.7042	C-2 of **27**	60.6453	137.3	143.2	0.1
127.2	C-3	68.7450	C-3 of **27**	66.7646	129.8	127.8	0.6
86.9	C-4	108.7168	C-4 of **27**	110.2776	84.0	85.6	1.3
109.6	C-5	86.6366	C-5 of **27**	90.3754	101.4	105.1	4.5
119.4	C-1’	77.0222	C-1’ of **29**	69.1850	128.6	120.8	1.4
136.6	C-2’	63.8228	C-2’ of **29**	74.9870	122.6	133.8	2.8
			Average				***1.6***
9.65	H-1	20.7106	H-1 of **29**	21.7200	9.71	10.72	1.07
6.52	H-3	24.2262	H-3 of **29**	24.0796	7.22	7.07	0.55
7.25	H-1’	24.2376	H-1’ of **29**	24.3189	6.16	6.24	1.01
7.99	H-2’	23.2315	H-2’a of **29**	24.3166	6.58	7.67	0.32
			Average				***0.74***

NMR calculations of the revised structures of 8i and 8l (compounds 9i and 9l, respectively)

Finally, to validate our assignemtn, we computed the NMR shifts of the revised structures of **8i** and **8l** (**9i** and **9l**, respectively) at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level of theory. The collected results (shown in Pages S64 and S65) indicate that a very good match between experimental and calculated values were observed in both cases.

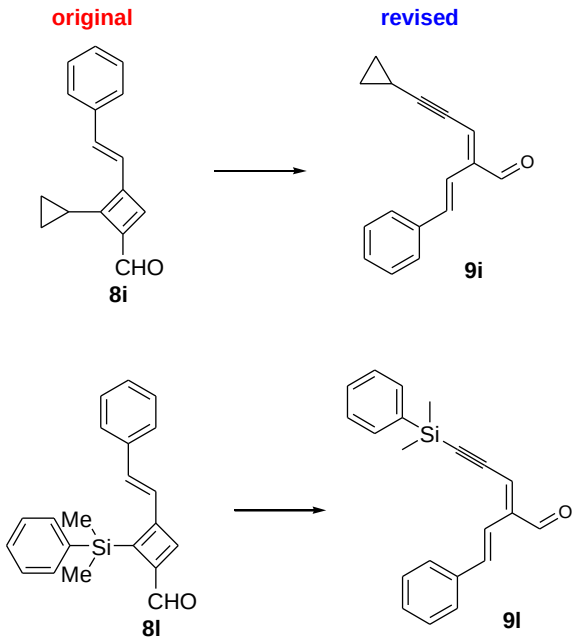
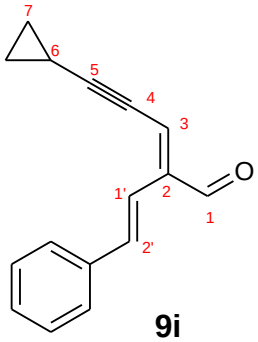


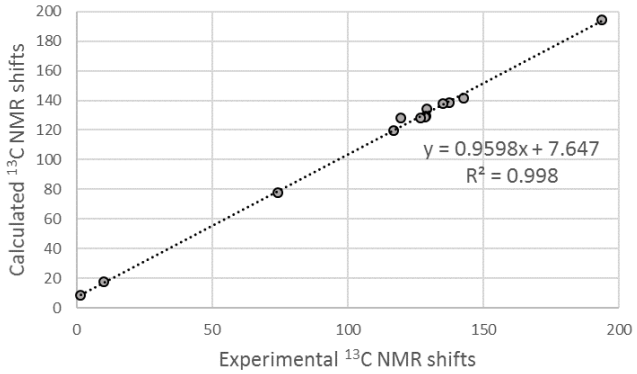
Table S40. Experimental ^{13}C NMR data of synthetic **8i** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **9i**



9i

δ_{exp}	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.7	4.4381	C-1	194.5	194.6	0.8	0.9
142.8	57.2961	C-2	141.6	139.6	1.2	3.2
137.3	60.4384	C-3'	138.5	136.3	1.2	1.0
135.3	61.2348	C-2'	137.7	135.5	2.4	0.2
129.2	64.4239	C-3	134.5	132.1	5.3	2.9
128.7	69.2076	C-5	129.7	127.1	1.0	1.6
128.5	70.2275	C-5'	128.7	126.1	0.2	2.4
126.9	70.4612	C-6'	128.4	125.8	1.5	1.1
119.5	70.8851	C-4'	128.0	125.4	8.5	5.9
116.8	78.9838	C-1'	119.9	117.0	3.1	0.2
74.2	120.8406	C-4	78.0	73.3	3.8	0.9
10.1	180.9060	C-7	18.0	10.8	7.9	0.7
1.5	190.3922	C-6	8.5	0.9	7.0	0.6
		Average			***3.4***	***1.6***
9.56	21.8835	H-1	9.33	9.33	0.23	0.23
7.91	23.0313	H-1'	8.18	8.20	0.27	0.29
7.52	23.6940	H-3'	7.52	7.55	0.00	0.03
7.38	23.8682	H-4'	7.34	7.38	0.04	0.00
7.31	23.9394	H-5'	7.27	7.31	0.04	0.00
7.11	23.9696	H-2'	7.24	7.28	0.13	0.17
6.29	25.1828	H-3	6.03	6.08	0.26	0.21
1.63	29.7905	H-6	1.42	1.56	0.21	0.07
1.08	30.2985	H-7b	0.91	1.06	0.17	0.02
0.97	30.3352	H-7a	0.88	1.02	0.09	0.05
9.56	21.8835	H-1	9.33	9.33	0.23	0.23
		Average			***0.14***	***0.11***

* The assignment corresponds to the computed σ vaues.



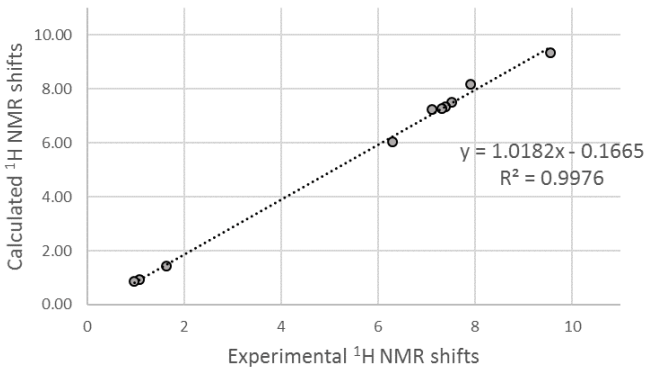
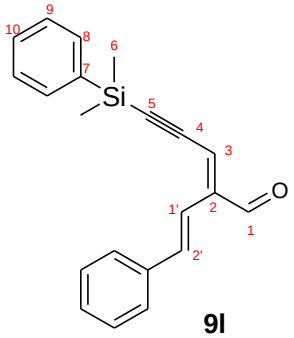


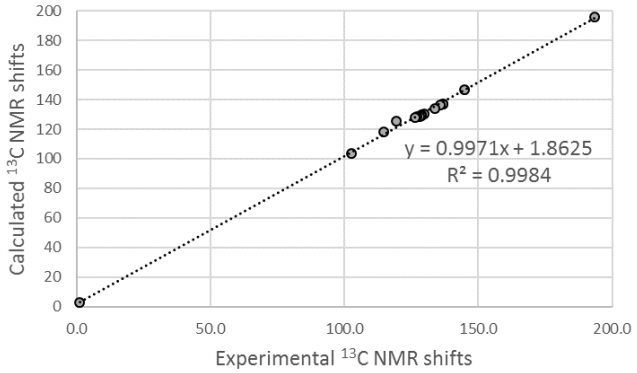
Table S41. Experimental ^{13}C NMR data of synthetic **8i** (as provided in the original reference), and Boltzmann averaged isotropic magnetic shielding values (σ), unscaled and scaled ^{13}C NMR shifts calculated at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* (solvent: $CHCl_3$) level of theory for all significantly populated conformers of **9l**

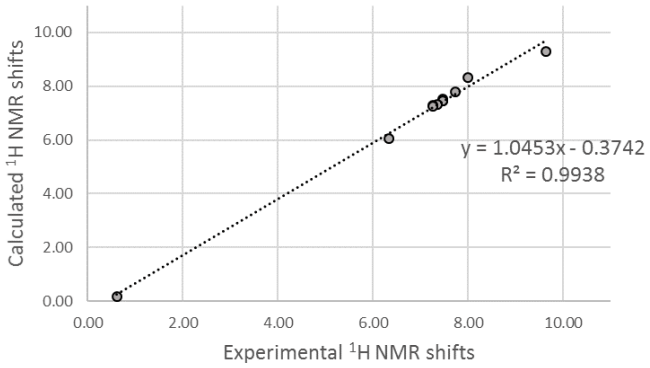


9l

δ_{exp}	σ	Nuclei*	δ_{calc}	δ_{scaled}	Unsc. Error (δ_{exp} -δ_{calc})	Scaled Error (δ_{exp} -δ_{scaled})
193.4	2.9464	C-1	195.9	194.6	2.5	1.2
144.8	52.3191	C-2	146.6	145.1	1.8	0.3
137.0	61.6913	C-7	137.2	135.7	0.2	1.3
136.8	61.7067	C-2'	137.2	135.7	0.4	1.1
135.8	62.3011	C-3'	136.6	135.1	0.8	0.7
133.7	64.8052	C-8	134.1	132.6	0.4	1.1
129.9	68.3422	C-3	130.5	129.1	0.6	0.8
128.8	68.9945	C-10	129.9	128.4	1.1	0.4
128.7	69.6459	C-6'	129.2	127.8	0.5	0.9
128.2	70.2473	C-5'	128.6	127.1	0.4	1.1
127.1	70.4756	C-4'	128.4	126.9	1.3	0.2
126.4	70.8562	C-9	128.0	126.5	1.6	0.1
119.3	73.4355	C-5	125.5	123.9	6.2	4.6
114.8	80.9428	C-1'	117.9	116.4	3.1	1.6
102.8	95.0462	C-4	103.8	102.3	1.0	0.5
1.2	195.8031	C-6	3.1	1.2	1.9	0.0
		Average			***1.5***	***1.0***
9.64	21.9200	H-1	9.29	9.25	0.35	0.39
8.00	22.8775	H-2'	8.33	8.33	0.33	0.33
7.74	23.4337	H-8	7.78	7.80	0.04	0.06
7.47	23.7014	H-10	7.51	7.54	0.04	0.07
7.47	23.7512	H-1'	7.46	7.50	0.01	0.03
7.47	23.7607	H-9	7.45	7.49	0.02	0.02
7.35	23.8809	H-3'	7.33	7.37	0.02	0.02
7.26	23.9313	H-4'	7.28	7.32	0.02	0.06
7.26	23.9462	H-5'	7.27	7.31	0.01	0.05
6.34	25.1457	H-3	6.07	6.16	0.27	0.18
0.61	31.0224	H-6	0.19	0.54	0.42	0.07
		Average			***0.14***	***0.11***

* The assignment corresponds to the computed σ vaues.





Cartesian Coordinates of all significant conformers found at the B3LYP/6-31G* level of theory for isomers **1**, **5**, **6**, **19**-**23**.

8a
B3LYP/6-31G* Geometry
C 0.657045 -2.331766 0.000044
C 0.303743 -0.853483 -0.000185
C 1.985827 -2.072492 0.000109
C 1.650619 -0.536537 -0.000178
H 0.078586 -3.250738 0.000107
C 3.106704 -2.981195 0.000047
H 2.792621 -4.048207 0.000090
O 4.298140 -2.687144 -0.000038
C 2.472627 0.637911 -0.000133
C 4.133264 2.914232 0.000124
C 1.918855 1.942384 -0.000571
C 3.881499 0.506512 0.000363
C 4.694967 1.635831 0.000511
C 2.740084 3.060390 -0.000440
H 0.842124 2.072254 -0.001055
H 4.316797 -0.489123 0.000583
H 5.774945 1.515985 0.000923
H 2.297709 4.053013 -0.000786
H 4.772216 3.793132 0.000229
C -0.946121 -0.179218 -0.000174
H -0.923689 0.906995 -0.000234
C -2.146624 -0.824050 -0.000083
H -2.135807 -1.913530 -0.000107
C -3.474539 -0.225201 0.000009
C -6.099584 0.822831 0.000171
C -3.702605 1.167701 0.000263
C -4.601555 -1.072781 -0.000156
C -5.895110 -0.558126 -0.000076
C -4.994647 1.680829 0.000339
H -2.861340 1.854557 0.000425
H -4.450151 -2.149904 -0.000354
H -6.744733 -1.235795 -0.000212
H -5.143654 2.757439 0.000542
H -7.107435 1.228425 0.000240
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.418045483
Number of imaginary frequencies = 0

8i
B3LYP/6-31G* Geometry
C -1.488167 -1.715686 -0.000142
C -0.854216 -0.328269 -0.000004
C -2.741978 -1.199780 -0.000225
C -2.108264 0.231863 -0.000115
H -1.099410 -2.730052 -0.000099
C -4.055544 -1.779112 0.000097
H -4.065925 -2.890414 0.000091
O -5.107236 -1.139892 0.000354
C 0.486846 0.147998 0.000066
H 0.604544 1.230505 0.000289
C 1.585158 -0.652783 -0.000096
H 1.425929 -1.731027 -0.000242
C 2.984645 -0.239963 -0.000049
C 5.729173 0.442739 0.000119
C 3.986590 -1.231422 -0.000045
C 3.400092 1.108410 -0.000015
C 4.750172 1.441754 0.000077
C 5.338534 -0.897268 0.000040
H 3.690767 -2.278270 -0.000097
H 2.659795 1.903241 -0.000090
H 5.043373 2.488511 0.000102
H 6.087966 -1.684498 0.000052
H 6.782747 0.708080 0.000197
C -2.656223 1.566838 -0.000213
C -3.965885 1.883465 -0.742708
C -3.965644 1.883618 0.742737
H -1.915539 2.363129 -0.000390
H -4.467377 1.054508 -1.230549
H -3.987121 2.828006 -1.279082
H -4.466941 1.054742 1.230913
H -3.986656 2.828260 1.278938
SCF Energy (PCM/mPW1PW91/6-31+G**)= -693.087003087
Number of imaginary frequencies = 0

8l_c1
B3LYP/6-31G* Geometry
C -0.932152 -2.992406 0.000796
C -0.451560 -1.523202 -0.001211
C -2.214533 -2.570017 0.002392
C -1.746816 -1.072275 0.000413
H -0.454053 -3.968109 0.000738
C -3.491069 -3.244515 0.003749
H -3.438025 -4.354655 0.004664
O -4.573045 -2.666079 0.003756
C 0.841217 -0.928467 -0.003623
H 0.865104 0.158152 -0.004226
C 1.993551 -1.649852 -0.005394
H 1.912093 -2.736671 -0.006843
C 3.357942 -1.134232 -0.006808
C 6.038320 -0.247168 -0.012296
C 4.429902 -2.048869 -0.022073
C 3.666146 0.242846 0.006766
C 4.987366 0.676090 0.003835
C 5.752510 -1.613378 -0.025034
H 4.213359 -3.114772 -0.032226
H 2.867056 0.978077 0.021044
H 5.201692 1.741558 0.014564
H 6.560193 -2.340393 -0.037239
H 7.068784 0.097319 -0.014457
Si -2.670575 0.554724 -0.002593
C -3.767067 0.633542 1.534977
H -4.461395 -0.214083 1.525898
H -4.355664 1.558788 1.548560
H -3.189995 0.586387 2.465259
C -3.754882 0.634108 -1.548571
H -4.457697 -0.206496 -1.536183
H -3.172428 0.570891 -2.474502
H -4.334970 1.564440 -1.575085
C -1.398378 1.958823 0.005360
C 0.566340 3.995281 0.019520
C -0.941615 2.542891 -1.190968
C -0.846260 2.434620 1.209970
C 0.124949 3.437419 1.221391
C 0.028664 3.546987 -1.188505
H -1.347188 2.210771 -2.143925
H -1.176280 2.016231 2.158320
H 0.533872 3.786030 2.166554
H 0.362684 3.980784 -2.127805
H 1.319830 4.778887 0.025024
SCF Energy (PCM/mPW1PW91/6-31+G**)= -1176.75423747
Number of imaginary frequencies = 0

8l_c2
B3LYP/6-31G* Geometry
C 0.310617 2.504892 -0.683510
C 0.597219 1.141099 -0.024868
C -0.988208 2.406917 -0.328073
C -0.716372 1.012904 0.349446
H 0.897108 3.253997 -1.208560
C -2.115956 3.289484 -0.507206
H -1.884566 4.226108 -1.058957
O -3.252100 3.069620 -0.098086
C 1.789307 0.375398 0.111912
H 1.697045 -0.569153 0.642887
C 2.990983 0.776592 -0.381781
H 3.026792 1.730824 -0.906683
C 4.266475 0.074642 -0.296942
C 6.786606 -1.195072 -0.193244
C 5.404362 0.660578 -0.886822
C 4.426952 -1.169234 0.348866
C 5.668745 -1.792553 0.398707
C 6.647766 0.035780 -0.836731
H 5.302734 1.619532 -1.389954
H 3.572988 -1.651022 0.815676
H 5.768122 -2.750660 0.901967
H 7.508776 0.509892 -1.300229
H 7.754954 -1.685914 -0.151934
Si -1.802328 -0.219809 1.253303
C -2.763480 0.717225 2.582668

H -2.086508 1.139376 3.335090
H -3.469172 0.053150 3.095949
H -3.329309 1.541230 2.135375
C -0.709297 -1.548674 2.044550
H 0.007686 -1.096613 2.739645
H -0.143749 -2.125442 1.303807
H -1.318942 -2.257344 2.617901
C -2.995880 -1.016214 0.019298
C -4.799070 -2.201775 -1.804882
C -3.986907 -0.250004 -0.625988
C -2.933515 -2.389619 -0.279047
C -3.823866 -2.979007 -1.179106
C -4.877709 -0.835567 -1.526335
H -4.060061 0.816915 -0.428624
H -2.183170 -3.016272 0.197420
H -3.756028 -4.043556 -1.390119
H -5.634412 -0.223743 -2.011396
H -5.493525 -2.657679 -2.506288
SCF Energy (PCM/mPW1PW91/6-31+G**)= -1176.75344485
Number of imaginary frequencies = 0

4-methylenecyclobut-2-enone
B3LYP/6-31G* Geometry
C -0.760327 0.020978 -0.000010
C -0.266364 1.418212 -0.000176
C 0.723995 -0.381989 -0.000121
C 1.053084 1.091133 0.000184
O 1.334979 -1.418736 -0.000036
C -1.923793 -0.626120 0.000090
H -0.787926 2.369282 -0.000220
H 1.972707 1.664418 0.000443
H -2.877412 -0.105242 0.000101
H -1.946771 -1.711852 0.000152
SCF Energy (PCM/mPW1PW91/6-31+G**)= -268.030388373
Number of imaginary frequencies = 0

cyclobutenone
B3LYP/6-31G* Geometry
C 0.484778 1.082388 -0.000006
C 1.425154 -0.118686 0.000004
C -0.615425 -0.037690 0.000022
C 0.466793 -1.068953 -0.000007
O -1.819479 -0.031379 -0.000008
H 0.501608 1.717902 -0.893357
H 0.501621 1.717878 0.893368
H 2.509089 -0.173052 -0.000020
H 0.475712 -2.154049 -0.000001
SCF Energy (PCM/mPW1PW91/6-31+G**)= -229.954864981
Number of imaginary frequencies = 0

diphenylcyclopropenone
B3LYP/6-31G* Geometry
C 0.000000 2.074773 -0.000021
C 0.685905 0.818423 0.000018
C -0.685906 0.818423 0.000019
O 0.000000 3.292119 -0.000059
C 1.937784 0.092246 0.000009
C 4.416418 -1.216382 -0.000018
C 2.001217 -1.313161 0.000030
C 3.135650 0.832296 -0.000027
C 4.365403 0.180009 -0.000040
C 3.232950 -1.960834 0.000017
C -1.937784 0.092246 0.000019
C -4.416418 -1.216382 0.000007
C -2.001217 -1.313160 0.000169
C -3.135650 0.832297 -0.000131
C -4.365404 0.180009 -0.000140
C -3.232950 -1.960834 0.000164
H 5.376632 -1.725025 -0.000028
H 1.083392 -1.892687 0.000051
H 3.081802 1.917008 -0.000043
H 5.284633 0.758930 -0.000067
H 3.273213 -3.046614 0.000032
H -5.376632 -1.725025 0.000002
H -1.083392 -1.892687 0.000301
H -3.081802 1.917008 -0.000240
H -5.284634 0.758930 -0.000260
H -3.273213 -3.046614 0.000283
SCF Energy (PCM/mPW1PW91/6-31+G**)= -652.671263331
Number of imaginary frequencies = 0

2,4-diphenylcyclobut-1-enecarbaldehyde
B3LYP/6-31G* Geometry
C 1.157227 -0.070253 -1.135620
C 0.087072 -1.220050 -0.985341
C 0.055756 0.845327 -0.602205
C -0.880998 -0.151540 -0.505330
C 0.111836 2.279035 -0.346989
O -0.805471 2.985624 0.053143
C -2.278056 -0.282427 -0.132154
C -4.976214 -0.627272 0.568732
C -2.877198 -1.557746 -0.177049
C -3.057544 0.821448 0.272861
C -4.393858 0.642632 0.618515
C -4.213922 -1.728344 0.169833
C 2.445386 -0.199531 -0.354463
C 4.853145 -0.480933 1.079758
C 2.443968 -0.254088 1.047804
C 3.673803 -0.283239 -1.022135
C 4.868783 -0.423489 -0.314030
C 3.635006 -0.395485 1.758418
H 1.393801 0.116101 -2.191101
H 0.354603 -1.973657 -0.236325
H -0.186332 -1.730185 -1.917332
H 1.106688 2.730072 -0.550181
H -6.020311 -0.759082 0.840306
H -2.286098 -2.415791 -0.485513
H -2.596810 1.803338 0.309881
H -4.985882 1.499325 0.929032
H -4.661953 -2.717496 0.130369
H 5.781848 -0.587377 1.633902
H 1.501666 -0.177541 1.585341
H 3.693617 -0.237772 -2.109061
H 5.810983 -0.484948 -0.852552
H 3.612783 -0.434266 2.844487
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.298230851
Number of imaginary frequencies = 0

20
B3LYP/6-31G* Geometry
C 0.727022 1.445538 -0.062333
C -0.095883 2.618313 -0.343130
C -1.393193 2.231006 -0.408971
C -1.497249 0.796779 -0.127296
C -0.207845 0.307925 0.096576
H 0.304580 3.603540 -0.553101
H -2.237297 2.858378 -0.667620
C 2.089262 1.532765 -0.063006
H 2.483486 2.549659 -0.085822
C 3.123365 0.501501 -0.068192
C 5.209851 -1.389835 -0.093178
C 4.383225 0.803722 0.488405
C 2.947492 -0.759331 -0.674000
C 3.980117 -1.693072 -0.682693
C 5.409384 -0.135708 0.490496
H 4.543073 1.781740 0.935985
H 2.009298 -0.988019 -1.168165
H 3.826769 -2.657360 -1.158830
H 6.367408 0.110991 0.939708
H 6.013297 -2.121175 -0.101498
C -2.803316 0.127793 -0.062472
C -5.364622 -1.051384 0.007434
C -2.988903 -1.217212 -0.436504
C -3.935981 0.867139 0.340787
C -5.198103 0.283497 0.384636
C -4.256735 -1.794172 -0.403367
H -2.132775 -1.804278 -0.737796
H -3.818229 1.901465 0.650033
H -6.052086 0.869810 0.713333
H -4.377560 -2.832499 -0.700263
H -6.350666 -1.507753 0.034476
C 0.179774 -0.950363 0.730800

H 1.143469 -0.891576 1.275856
O -0.446093 -2.002791 0.742470
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.495086689
Number of imaginary frequencies = 0

9_c1
B3LYP/6-31G* Geometry
C 1.526752 0.156467 0.119638
H 0.465026 0.019627 0.305583
C 2.004765 1.413177 -0.026760
H 3.070553 1.575812 -0.167543
C 2.307041 -1.081155 0.077831
C 3.706769 -3.531916 0.038425
C 1.665040 -2.293127 0.397145
C 3.672281 -1.130215 -0.269539
C 4.360292 -2.338685 -0.287147
C 2.354124 -3.503701 0.380492
H 0.612176 -2.275443 0.670549
H 4.195430 -0.216668 -0.535084
H 5.412350 -2.352852 -0.559413
H 1.835512 -4.424371 0.634632
H 4.248348 -4.473746 0.021907
C 1.250925 2.654061 0.018778
C -0.105362 2.858125 0.062496
H -0.437019 3.897158 0.109291
C 2.059005 3.901391 -0.000496
H 1.461772 4.838373 0.053300
O 3.272477 3.944148 -0.074237
C -1.136394 1.908963 0.038086
C -2.083889 1.138919 0.004781
C -3.175159 0.229921 -0.036899
C -5.334095 -1.562988 -0.116354
C -4.489282 0.679224 0.211870
C -2.963468 -1.134181 -0.329004
C -4.036893 -2.018410 -0.367887
C -5.555489 -0.213661 0.172995
H -4.655617 1.728312 0.435738
H -1.955136 -1.482631 -0.530785
H -3.862455 -3.066246 -0.595890
H -6.563008 0.143077 0.367911
H -6.169536 -2.256841 -0.147008
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.446871032
Number of imaginary frequencies = 0

9_c2
B3LYP/6-31G* Geometry
C 2.629717 0.750738 0.000006
H 3.363819 1.549803 0.000038
C 1.319324 1.091028 -0.000018
H 0.560387 0.311331 -0.000044
C 3.173477 -0.608244 0.000011
C 4.355232 -3.172435 0.000009
C 4.572772 -0.766809 0.000018
C 2.379663 -1.773046 0.000004
C 2.963154 -3.035454 0.000002
C 5.158070 -2.031006 0.000019
H 5.201472 0.120321 0.000022
H 1.296747 -1.690434 0.000003
H 2.331064 -3.919755 -0.000007
H 6.240788 -2.124610 0.000027
H 4.806991 -4.160686 0.000006
C 0.782555 2.440133 -0.000003
C -0.568800 2.694053 0.000012
H -0.887884 3.736759 0.000014
C 1.625453 3.660483 -0.000010
H 1.033692 4.603274 0.000018
O 2.841989 3.708457 -0.000041
C -1.595873 1.738978 0.000012
C -2.513092 0.933227 0.000001
C -3.583436 -0.001082 -0.000006
C -5.700678 -1.844901 -0.000005
C -4.922039 0.444968 0.000046
C -3.325953 -1.388186 -0.000050
C -4.378549 -2.297852 -0.000051
C -5.967533 -0.472913 0.000045
H -5.123648 1.511606 0.000085
H -2.297305 -1.735058 -0.000085
H -4.168312 -3.363767 -0.000087
H -6.994452 -0.118169 0.000083
H -6.520036 -2.558348 -0.000003
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.448320279
Number of imaginary frequencies = 0

10_c1
B3LYP/6-31G* Geometry
C -6.388578 0.593165 0.001214
C -6.997450 -0.666398 0.000099
C -6.202942 -1.813503 -0.001043
C -4.814501 -1.699785 -0.001086
C -4.183781 -0.440811 -0.000012
C -5.002859 0.706791 0.001177
C -2.721739 -0.386546 -0.000168
C -1.950987 0.723566 0.000120
C -0.495969 0.783078 0.000022
C 0.342716 -0.302531 0.000540
C 0.097922 2.144212 -0.000562
O -0.554835 3.173292 -0.000862
C 1.747592 -0.278553 0.000358
C 2.967161 -0.339255 0.000257
C 4.386934 -0.385547 0.000138
C 5.063340 -1.623850 0.000703
C 6.454001 -1.663870 0.000584
C 7.193212 -0.477688 -0.000091
C 6.533475 0.754465 -0.000651
C 5.143236 0.805729 -0.000543
H -6.999924 1.491691 0.002142
H -8.080757 -0.749856 0.000144
H -6.663858 -2.797657 -0.001899
H -4.200477 -2.597694 -0.001987
H -4.551035 1.693942 0.002121
H -2.240374 -1.364793 -0.000662
H -2.414504 1.706427 0.000323
H -0.099416 -1.298493 0.001195
H 1.204500 2.174232 -0.000721
H 4.484714 -2.542351 0.001231
H 6.964216 -2.623099 0.001022
H 8.279056 -0.513402 -0.000179
H 7.105298 1.678249 -0.001177
H 4.626544 1.760439 -0.000981
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.444567269
Number of imaginary frequencies = 0

10_c2
B3LYP/6-31G* Geometry
C 6.719207 0.651086 0.001074
C 7.081996 -0.696443 0.000325
C 6.085334 -1.677911 -0.000670
C 4.741972 -1.317953 -0.000879
C 4.355231 0.037699 -0.000068
C 5.373429 1.010852 0.000857
C 2.963784 0.491691 -0.000156
C 1.861717 -0.294696 -0.000002
C 0.476030 0.143553 -0.000081
C -0.526962 -0.798249 0.000102
C 0.073176 1.572244 -0.000340
O 0.826130 2.530890 -0.000511
C -1.914020 -0.574866 0.000070
C -3.129982 -0.463670 0.000064
C -4.542632 -0.312942 0.000054
C -5.127350 0.971228 -0.000079
C -6.511457 1.111900 -0.000089
C -7.334643 -0.017597 0.000032
C -6.765983 -1.294359 0.000164
C -5.383079 -1.446251 0.000177
H 7.484215 1.422957 0.001816
H 8.130326 -0.982299 0.000474
H 6.359560 -2.729698 -0.001322
H 3.986649 -2.098385 -0.001762
H 5.094619 2.061806 0.001441
H 2.819631 1.566866 -0.000269
H 1.982721 -1.377921 0.000256
H -0.228008 -1.847347 0.000293
H -1.023764 1.726921 -0.000360
H -4.483955 1.845596 -0.000172

H -6.950554 2.105663 -0.000191
H -8.415061 0.096674 0.000023
H -7.403496 -2.174159 0.000258
H -4.936511 -2.435698 0.000279
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.445507379
Number of imaginary frequencies = 0

11_c1
B3LYP/6-31G* Geometry
H 3.055256 1.340576 0.527104
C 3.848526 0.628286 0.320036
C 5.917963 -1.171658 -0.191164
C 3.526828 -0.692338 -0.055469
C 5.173219 1.036159 0.434738
C 6.216517 0.140109 0.179827
C 4.591126 -1.580220 -0.306020
H 5.395724 2.059336 0.726461
H 7.249944 0.462894 0.271388
H 4.365714 -2.604067 -0.596128
H 6.719031 -1.878417 -0.391264
C 2.155249 -1.178385 -0.195722
H 2.068009 -2.231294 -0.467168
C 1.008829 -0.474691 -0.032123
H 1.053207 0.578479 0.232058
C -0.300433 -1.066737 -0.168569
H -0.312289 -2.144882 -0.328637
C -1.509376 -0.437780 -0.082735
C -1.655519 1.041861 -0.019045
C -1.965049 3.842359 0.101794
C -0.966339 1.884429 -0.910341
C -2.518307 1.634612 0.921619
C -2.665306 3.018871 0.986423
C -1.118442 3.269338 -0.848923
H -0.326224 1.442678 -1.668244
H -3.064027 1.000104 1.614506
H -3.328366 3.455523 1.728587
H -0.582287 3.900612 -1.552685
H -2.084922 4.921346 0.147940
C -2.753590 -1.238525 -0.035235
C -2.842874 -2.388224 0.719271
H -2.022515 -2.720980 1.352497
C -3.925963 -0.846467 -0.797946
H -3.855461 0.086241 -1.382506
O -4.981283 -1.500748 -0.834015
O -3.899710 -3.177957 0.771744
H -4.585199 -2.764495 0.161766
SCF Energy (PCM/mPW1PW91/6-31+G**)= -883.919033724
Number of imaginary frequencies = 0

11_c2
B3LYP/6-31G* Geometry
H 3.040522 1.345113 0.476348
C 3.833368 0.626140 0.291950
C 5.901653 -1.189800 -0.163085
C 3.510669 -0.703541 -0.049146
C 5.158298 1.034874 0.400982
C 6.201165 0.130828 0.174168
C 4.574564 -1.599205 -0.272222
H 5.381273 2.065190 0.666099
H 7.234789 0.454287 0.261125
H 4.348664 -2.630135 -0.535672
H 6.702222 -1.902994 -0.341282
C 2.138681 -1.191334 -0.180181
H 2.050811 -2.249971 -0.428129
C 0.993076 -0.482875 -0.033035
H 1.038584 0.575840 0.207578
C -0.317390 -1.074252 -0.160596
H -0.325208 -2.153917 -0.308955
C -1.523244 -0.438589 -0.083454
C -1.644072 1.045654 -0.022963
C -1.886546 3.853077 0.088575
C -0.989201 1.865137 -0.959214
C -2.436900 1.664475 0.961213
C -2.550184 3.051952 1.021238
C -1.108853 3.254199 -0.903473
H -0.397488 1.402749 -1.743842
H -2.955290 1.048271 1.690488
H -3.157579 3.509049 1.797965
H -0.599726 3.867544 -1.642280
H -1.980657 4.934746 0.131715
C -2.774063 -1.228664 -0.054749
C -3.933272 -0.772169 -0.648559
H -3.979110 0.191325 -1.151472
C -2.840370 -2.511300 0.621591
H -1.938170 -2.835784 1.167904
O -3.848452 -3.237892 0.644469
O -5.076262 -1.428498 -0.673228
H -4.910189 -2.297846 -0.191761
SCF Energy (PCM/mPW1PW91/6-31+G**)= -883.918591606
Number of imaginary frequencies = 0

12_c1
B3LYP/6-31G* Geometry
C -0.411190 -1.110253 0.406792
H 0.230237 -1.918701 0.756508
C 0.188859 0.102372 0.271105
C -1.799035 -1.528266 0.155675
C -4.417556 -2.490147 -0.288047
C -2.295801 -2.644274 0.856850
C -2.642238 -0.921358 -0.795894
C -3.933307 -1.396546 -1.011110
C -3.589983 -3.115099 0.646376
H -1.653292 -3.140282 1.581037
H -2.276055 -0.083400 -1.378305
H -4.563183 -0.915118 -1.754780
H -3.949966 -3.973311 1.207884
H -5.425761 -2.857380 -0.459971
C -0.541303 1.378890 0.014207
C -1.865078 3.822472 -0.445790
C -1.635324 1.765279 0.807911
C -0.113537 2.249918 -1.002314
C -0.774679 3.456035 -1.236211
C -2.289957 2.973986 0.579876
H -1.965089 1.110414 1.608811
H 0.738934 1.971907 -1.616314
H -0.433775 4.111206 -2.033584
H -3.130407 3.257276 1.208103
H -2.375901 4.765315 -0.621930
C 1.667302 0.202068 0.405585
C 2.193661 1.310492 1.229875
H 1.411074 1.962938 1.666214
C 2.483492 -0.720880 -0.199016
H 1.988602 -1.470978 -0.816529
O 3.371781 1.540910 1.471192
C 3.913149 -0.812909 -0.132526
H 4.449065 -0.088703 0.473391
C 4.576481 -1.776441 -0.812544
H 4.074559 -2.515421 -1.432145
O 5.911228 -1.965550 -0.824731
H 6.333150 -1.290685 -0.264868
SCF Energy (PCM/mPW1PW91/6-31+G**)= -883.901520785
Number of imaginary frequencies = 0

12_c2
B3LYP/6-31G* Geometry
C -0.983114 -1.310334 -0.063978
H -0.736085 -2.360453 -0.215119
C 0.065747 -0.460535 0.105468
C -2.430826 -1.051054 -0.095625
C -5.236151 -0.722548 -0.185436
C -3.058067 0.014056 0.580466
C -3.251584 -1.958809 -0.793400
C -4.633705 -1.793788 -0.847310
C -4.440650 0.173679 0.533239
H -2.460146 0.709282 1.158576
H -2.790213 -2.800887 -1.304666
H -5.240502 -2.505665 -1.400917
H -4.901119 1.000109 1.068606
H -6.314558 -0.593026 -0.219384
C -0.080485 1.026959 0.116788
C -0.317404 3.833525 0.110778
C 0.390498 1.791018 1.197879
C -0.654802 1.697624 -0.975190
C -0.771463 3.087604 -0.978636

C 0.263784 3.179952 1.199828
H 0.851904 1.287645 2.043192
H -1.011463 1.119022 -1.822223
H -1.216312 3.588067 -1.834774
H 0.622028 3.752397 2.051547
H -0.410544 4.916269 0.109323
C 1.441469 -1.006814 0.235396
C 1.605466 -2.285861 0.960513
H 0.684227 -2.638224 1.467770
C 2.519390 -0.315381 -0.261781
H 2.304968 0.640450 -0.739294
O 2.636311 -2.937328 1.067858
C 3.900882 -0.692063 -0.234832
H 4.172538 -1.642683 0.213468
C 4.844822 0.117701 -0.770105
H 4.610729 1.072927 -1.233259
O 6.169121 -0.126258 -0.812125
H 6.348245 -0.986128 -0.393088
SCF Energy (PCM/mPW1PW91/6-31+G**)= -883.901186384
Number of imaginary frequencies = 0

13
B3LYP/6-31G* Geometry
O -1.238473 1.531603 -1.768331
C 0.614303 0.597930 -0.411745
C -0.157290 2.900394 -0.154340
C 0.822471 1.848327 0.091175
C -1.101338 2.697433 -1.086066
C -0.693168 0.334258 -1.146993
H -1.805112 3.449280 -1.429182
H -0.502525 -0.322295 -2.000595
H -0.041067 3.857614 0.336825
C -1.759377 -0.333578 -0.282680
C -3.807669 -1.540304 1.211685
C -2.633138 -1.251460 -0.879127
C -1.922940 -0.027931 1.074396
C -2.942761 -0.625918 1.815533
C -3.650583 -1.853583 -0.139755
H -2.515042 -1.493753 -1.933074
H -1.252021 0.678355 1.552787
H -3.059684 -0.378695 2.867361
H -4.316602 -2.567978 -0.616264
H -4.598010 -2.008837 1.792105
C 1.517451 -0.564800 -0.242277
C 3.205028 -2.801479 0.068487
C 1.934026 -1.316333 -1.356886
C 1.952324 -0.970617 1.032518
C 2.789386 -2.075164 1.185155
C 2.774203 -2.416966 -1.203161
H 1.623515 -1.017204 -2.354504
H 1.606544 -0.429035 1.908104
H 3.109306 -2.372334 2.180144
H 3.095989 -2.973527 -2.079251
H 3.855442 -3.663527 0.187645
C 2.069724 2.233764 0.793586
H 2.885097 1.486900 0.783421
O 2.219754 3.312296 1.341761
SCF Energy (PCM/mPW1PW91/6-31+G**)= -844.602309495
Number of imaginary frequencies = 0

14
B3LYP/6-31G* Geometry
C -0.039051 -2.051266 -0.533342
H -0.396593 -2.961601 -1.007420
O -0.984337 -1.514052 0.342090
C -1.460027 -0.248146 0.055535
C -0.610136 0.803971 -0.152780
C 1.681113 -0.277927 -0.195347
C 1.180842 -1.551452 -0.732479
H 1.837476 -2.112375 -1.393761
C 0.841250 0.758287 0.042675
H 1.257241 1.710229 0.360349
C 3.148275 -0.146505 -0.003050
C 5.932323 0.067215 0.393528
C 3.910886 -1.260108 0.390311
C 3.815342 1.074492 -0.208567
C 5.189785 1.180223 -0.008176
C 5.286741 -1.154215 0.590291
H 3.414514 -2.211307 0.563493
H 3.255461 1.938604 -0.553913
H 5.684982 2.132450 -0.179268
H 5.853531 -2.026848 0.904383
H 7.005162 0.150566 0.544844
C -2.933069 -0.195673 0.127693
C -5.739475 -0.169155 0.290003
C -3.604909 0.860294 0.769965
C -3.692997 -1.257619 -0.397332
C -5.082167 -1.237474 -0.327178
C -4.996979 0.874108 0.844133
H -3.032705 1.648660 1.248323
H -3.184482 -2.092083 -0.868901
H -5.654784 -2.057942 -0.750702
H -5.499181 1.693562 1.350479
H -6.824225 -0.158848 0.350943
C -1.138221 2.122500 -0.574245
H -2.183815 2.134622 -0.934130
O -0.474380 3.146930 -0.575159
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.682947627
Number of imaginary frequencies = 0

15
B3LYP/6-31G* Geometry
C 0.364842 1.456731 -0.177763
H 0.782259 2.426390 0.083972
O 1.132726 0.686899 -1.021895
C 1.683437 -0.397487 -0.307328
C 0.852403 -1.396108 0.079293
C -1.399066 -0.280252 0.027964
C -0.851872 1.065487 0.261927
C -0.585594 -1.376990 -0.032824
H -1.063804 -2.349784 -0.128748
C 3.143956 -0.351182 -0.155418
C 5.949627 -0.274546 0.065357
C 3.819645 -1.201178 0.741508
C 3.902036 0.547343 -0.927823
C 5.290524 0.581996 -0.817518
C 5.206471 -1.165464 0.845164
H 3.255223 -1.876809 1.377053
H 3.390867 1.210220 -1.616564
H 5.858999 1.280959 -1.425078
H 5.709044 -1.825834 1.546691
H 7.032199 -0.244381 0.152602
H 1.302967 -2.303263 0.472560
C -2.874186 -0.435556 -0.079205
C -5.663385 -0.737036 -0.358820
C -3.549022 -1.509090 0.528538
C -3.630818 0.490556 -0.819991
C -5.009618 0.339797 -0.960273
C -4.927128 -1.659991 0.387203
H -2.989320 -2.214506 1.136258
H -3.126866 1.320528 -1.308150
H -5.572576 1.062436 -1.544891
H -5.429219 -2.493346 0.871566
H -6.738475 -0.853050 -0.465189
C -1.589548 2.032670 1.126031
H -2.524368 1.641624 1.573384
O -1.218121 3.168180 1.361695
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.683607080
Number of imaginary frequencies = 0

16
B3LYP/6-31G* Geometry
C 0.173397 -2.285236 -0.535081
C 1.639409 -0.496839 -0.085224
C -0.810569 -0.102843 -0.028501
C 0.591036 0.364133 0.131518
C -0.908745 -1.516915 -0.380664
O 1.459244 -1.815202 -0.386193
H 0.177813 -3.330010 -0.817349
H -1.879063 -1.959025 -0.566842
C -1.894517 0.712706 0.104839
H -1.699178 1.769799 0.236091
C -3.315222 0.336827 0.055970
C -6.083577 -0.240019 -0.048868

C -3.839957 -0.830423 0.645668
C -4.225450 1.223413 -0.554643
C -5.586561 0.936648 -0.615092
C -5.203731 -1.116227 0.588812
H -3.178936 -1.498155 1.190279
H -3.846681 2.143141 -0.993793
H -6.262806 1.635075 -1.101601
H -5.581866 -2.020614 1.059140
H -7.146268 -0.463194 -0.090662
C 3.086125 -0.186216 -0.058488
C 5.846635 0.321582 -0.046269
C 3.605736 0.948222 -0.703468
C 3.973242 -1.078154 0.569460
C 5.340898 -0.819397 0.582467
C 4.977032 1.200628 -0.692820
H 2.936283 1.615962 -1.236669
H 3.581110 -1.966937 1.052984
H 6.014286 -1.509504 1.083050
H 5.364671 2.079809 -1.199475
H 6.915021 0.518998 -0.039050
C 0.922890 1.706795 0.655112
H 1.960731 1.814056 1.020044
O 0.155313 2.652513 0.748127
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.698036598
Number of imaginary frequencies = 0

17
B3LYP/6-31G* Geometry
C 0.306067 -3.121379 -0.225231
C 2.040608 -1.571580 -0.029740
C -0.281059 -0.753470 -0.066979
C 1.172465 -0.517964 -0.020252
C -0.633557 -2.165053 -0.189800
O 1.640809 -2.880867 -0.119349
H 0.109791 -4.179630 -0.347563
H -1.667197 -2.458852 -0.316870
C -1.172652 0.283110 -0.057686
H -0.756169 1.284628 -0.114683
C -2.636157 0.239562 -0.028236
C -5.465682 0.303575 -0.009501
C -3.384110 -0.746453 0.648302
C -3.351295 1.277046 -0.663162
C -4.742658 1.305208 -0.662354
C -4.777496 -0.715066 0.652463
H -2.870574 -1.517583 1.213466
H -2.796152 2.061520 -1.172209
H -5.265155 2.112204 -1.169604
H -5.328132 -1.483856 1.188656
H -6.551981 0.325138 -0.004522
C 3.510092 -1.459296 0.105280
H 3.885186 -0.431826 0.255794
C 1.700232 0.879340 0.042030
C 2.676154 3.511038 0.156039
C 2.312049 1.462298 -1.077257
C 1.574255 1.636372 1.217466
C 2.063866 2.940753 1.274566
C 2.797431 2.769939 -1.019930
H 2.403948 0.886536 -1.994147
H 1.097151 1.195077 2.087930
H 1.968924 3.511138 2.194520
H 3.271527 3.206559 -1.894690
H 3.056265 4.527891 0.201787
O 4.258097 -2.417486 0.068854
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.696581030
Number of imaginary frequencies = 0

18_c1
B3LYP/6-31G* Geometry
C -1.599182 -0.035866 -0.049715
O 0.734596 -0.617918 -0.018233
C 0.106554 1.700460 -0.103105
C 1.139841 0.713146 -0.043818
C -1.219147 1.380270 -0.120196
C -0.590646 -0.932214 -0.004675
H -0.730972 -2.003715 0.071732
H 0.394260 2.745493 -0.163188
C 2.469151 1.022155 -0.026549
H 2.667805 2.090194 -0.058827
C 3.647855 0.175614 0.025531
C 6.052569 -1.313740 0.124157
C 4.910391 0.812080 0.026317
C 3.628195 -1.237090 0.076166
C 4.815577 -1.962657 0.124616
C 6.092337 0.082162 0.074497
H 4.951182 1.898309 -0.011844
H 2.681283 -1.760179 0.077253
H 4.773633 -3.048301 0.163146
H 7.046814 0.602070 0.073501
H 6.974113 -1.888124 0.162023
C -3.004665 -0.518166 0.007756
C -5.636700 -1.507475 0.165453
C -3.900972 -0.027484 0.973385
C -3.454184 -1.510521 -0.877847
C -4.756571 -2.004755 -0.796031
C -5.204207 -0.515675 1.049093
H -3.566479 0.725661 1.682341
H -2.779486 -1.881764 -1.644461
H -5.085269 -2.771607 -1.492363
H -5.880601 -0.126209 1.805172
H -6.653058 -1.886800 0.225254
C -2.199715 2.478477 -0.294266
H -3.247985 2.165814 -0.458386
O -1.900112 3.661271 -0.283764
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.699151613
Number of imaginary frequencies = 0

18_c2
B3LYP/6-31G* Geometry
C -1.550570 0.064819 -0.033940
O 0.789102 -0.530394 -0.006790
C 0.173158 1.784502 -0.095344
C 1.204819 0.792768 -0.038161
C -1.157417 1.479800 -0.104336
C -0.540473 -0.831077 0.010490
H -0.687400 -1.901688 0.083113
H 0.492370 2.821998 -0.154747
C 2.535042 1.095747 -0.026146
H 2.741388 2.162509 -0.060380
C 3.709290 0.242111 0.021772
C 6.103913 -1.262582 0.111973
C 4.975539 0.870601 0.019134
C 3.680013 -1.170277 0.071328
C 4.862773 -1.903563 0.115595
C 6.152938 0.132964 0.063289
H 5.023500 1.956630 -0.018390
H 2.729660 -1.687098 0.074672
H 4.813857 -2.988876 0.153222
H 7.110825 0.646487 0.059789
H 7.021735 -1.843041 0.146588
C -2.946544 -0.451139 0.013840
C -5.520432 -1.577195 0.176121
C -3.861332 -0.010655 0.983843
C -3.346672 -1.461153 -0.874184
C -4.622622 -2.021712 -0.793259
C -5.134339 -0.568259 1.062881
H -3.571975 0.769915 1.679860
H -2.657303 -1.793544 -1.645794
H -4.914425 -2.798812 -1.494795
H -5.828406 -0.214625 1.820610
H -6.516145 -2.007920 0.238863
C -2.082273 2.621652 -0.261865
H -1.555402 3.602989 -0.274706
O -3.290495 2.569264 -0.386472
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.698006005
Number of imaginary frequencies = 0

19_c1
B3LYP/6-31G* Geometry
O -0.453682 -2.389123 0.024658
C -0.425038 -1.007643 0.033400
C -1.718661 -0.522499 0.034215
C -2.578098 -1.688072 0.015432
C -1.743378 -2.774571 0.013991
H -1.937135 -3.836276 0.024521

C -4.041926 -1.771875 0.078458
H -4.570972 -0.804349 0.191862
C 0.856869 -0.357770 -0.013697
H 0.803755 0.724150 -0.093271
C 2.049985 -0.992576 0.028994
H 2.045896 -2.076541 0.126433
O -4.662276 -2.820706 0.025268
C 3.375281 -0.377652 -0.035934
C 5.984757 0.697092 -0.136936
C 4.508965 -1.199375 0.113154
C 3.584776 1.000790 -0.243157
C 4.870669 1.528521 -0.291445
C 5.797083 -0.670870 0.064888
H 4.369025 -2.266363 0.270779
H 2.735378 1.664794 -0.375525
H 5.007187 2.594474 -0.454090
H 6.654299 -1.328155 0.184175
H 6.987573 1.113326 -0.176851
C -2.131355 0.893500 0.042446
C -2.916745 3.598852 0.050070
C -1.580121 1.800822 0.964208
C -3.087775 1.368722 -0.872680
C -3.476774 2.707253 -0.867152
C -1.966626 3.140750 0.964345
H -0.863215 1.443429 1.697894
H -3.509033 0.687498 -1.606915
H -4.213931 3.055300 -1.585699
H -1.531922 3.824962 1.688173
H -3.220570 4.642000 0.053505
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.716540111
Number of imaginary frequencies = 0

19_c2
B3LYP/6-31G* Geometry
O -0.348963 -2.495779 0.043228
C -0.393856 -1.112515 0.033459
C -1.708825 -0.686335 0.026811
C -2.508838 -1.898576 0.015119
C -1.617341 -2.939415 0.036011
H -1.750458 -4.011871 0.050615
C -3.955576 -2.124829 0.027739
H -4.230445 -3.201995 0.094016
C 0.858835 -0.407620 -0.024898
H 0.759564 0.666975 -0.143147
C 2.077402 -0.989296 0.046770
H 2.119406 -2.068103 0.184401
O -4.823310 -1.272963 -0.027949
C 3.375878 -0.321330 -0.034510
C 5.938186 0.858605 -0.159815
C 4.542331 -1.089429 0.144598
C 3.528006 1.057569 -0.284466
C 4.790899 1.637085 -0.344522
C 5.807376 -0.509074 0.084314
H 4.446631 -2.155868 0.335606
H 2.652121 1.680781 -0.440013
H 4.883316 2.702266 -0.539834
H 6.690883 -1.125526 0.227428
H 6.922754 1.315436 -0.209132
C -2.157475 0.719701 0.053045
C -2.944249 3.423353 0.079433
C -1.564340 1.635095 0.940852
C -3.164228 1.182442 -0.811248
C -3.549567 2.520783 -0.798092
C -1.952398 2.974682 0.951968
H -0.814116 1.285588 1.644382
H -3.649117 0.487849 -1.486931
H -4.328842 2.859504 -1.475452
H -1.486140 3.663577 1.651444
H -3.250682 4.465924 0.088977
SCF Energy (PCM/mPW1PW91/6-31+G**)= -882.715665323
Number of imaginary frequencies = 0

21
B3LYP/6-31G* Geometry
C 6.731576 -1.039048 -0.227768
C 5.218151 1.237639 0.294766
C 7.371992 0.173424 0.049845
C 5.343438 -1.114190 -0.243610
C 4.555954 0.025506 0.019105
C 6.608756 1.312222 0.311099
C 3.096456 0.013868 0.019014
C 2.283219 -1.052487 -0.193035
C 0.877853 -0.969518 -0.177385
C -0.343134 -0.908449 -0.167507
C -1.749055 -0.922465 -0.169743
C -2.590450 0.150013 -0.023374
C -4.058395 -0.031014 0.008359
C -6.847891 -0.440317 0.026224
C -4.620142 -1.174336 0.607393
C -4.928708 0.915216 -0.565169
C -6.306510 0.705592 -0.558900
C -5.997702 -1.379242 0.613672
C -1.985274 1.496746 0.105829
O -2.599511 2.544979 0.204446
H 7.319954 -1.929124 -0.433674
H 4.627117 2.127330 0.498662
H 8.457041 0.227244 0.060758
H 4.866753 -2.064655 -0.464193
H 7.095990 2.259016 0.527246
H 2.622214 0.974117 0.214275
H 2.706711 -2.036787 -0.387174
H -7.923336 -0.596278 0.032974
H -3.971225 -1.894519 1.098302
H -4.521176 1.811804 -1.014224
H -6.960437 1.444484 -1.014444
H -6.407552 -2.266772 1.088506
H -0.877321 1.492229 0.106887
H -2.199457 -1.902883 -0.322353
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.442503199
Number of imaginary frequencies = 0

22_c1
B3LYP/6-31G* Geometry
C -5.497582 1.472114 -0.156847
C -4.627968 -1.177390 -0.012128
C -6.430585 0.435777 -0.099712
C -4.135065 1.184234 -0.141589
C -3.670697 -0.143535 -0.068208
C -5.988020 -0.889460 -0.027672
C -2.230377 -0.377470 -0.052745
C -1.592145 -1.574280 0.019864
C -0.190318 -1.694919 0.028491
C 1.028114 -1.797150 0.040104
C 2.418953 -1.963435 0.039528
C 3.373742 -0.985562 0.020772
C 3.120359 0.470641 0.053910
C 2.685735 3.254534 0.118670
C 2.159778 1.030401 0.915646
C 3.862696 1.337698 -0.769071
C 3.644469 2.714459 -0.739741
C 1.945656 2.406741 0.946235
C 4.786516 -1.452174 -0.020741
O 5.133429 -2.619164 -0.079318
H -5.830735 2.504779 -0.213671
H -4.306143 -2.213064 0.043202
H -7.494468 0.655703 -0.111640
H -3.410958 1.994253 -0.186858
H -6.709273 -1.701044 0.016128
H -1.609839 0.515376 -0.107097
H -2.161943 -2.500671 0.072875
H 2.796096 -2.986769 0.031778
H 2.518240 4.327904 0.145023
H 1.593613 0.380263 1.574303
H 4.596474 0.928538 -1.458371
H 4.222007 3.364486 -1.391552
H 1.204938 2.820001 1.625964
H 5.544987 -0.643789 0.025856
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.442687108
Number of imaginary frequencies = 0

22_c2
B3LYP/6-31G* Geometry
C -5.768651 1.575294 -0.145637
C -5.234139 -1.151722 0.012254

C -6.826249 0.660827 -0.094425
C -4.451813 1.130432 -0.117822
C -4.156508 -0.246074 -0.037854
C -6.553085 -0.705524 -0.015495
C -2.797767 -0.777641 -0.004488
C -1.637952 -0.071919 -0.036932
C -0.366835 -0.674373 0.004535
C 0.758176 -1.152784 0.039615
C 2.007849 -1.785449 0.072226
C 3.243736 -1.202511 0.050286
C 3.517797 0.250009 0.039409
C 4.090210 3.009779 0.021515
C 2.789729 1.142613 0.846428
C 4.542749 0.771028 -0.772302
C 4.823077 2.136603 -0.783574
C 3.073112 2.506499 0.835944
C 4.403558 -2.135846 0.056727
O 4.319938 -3.351646 0.033120
H -5.974490 2.640458 -0.207794
H -5.025486 -2.217139 0.073822
H -7.853712 1.013261 -0.116228
H -3.645889 1.857055 -0.159215
H -7.367057 -1.424150 0.024444
H -2.721443 -1.861968 0.054241
H -1.657410 1.015348 -0.096248
H 2.006755 -2.875851 0.098629
H 4.310378 4.073881 0.015674
H 2.009273 0.757927 1.494417
H 5.106021 0.106363 -1.421855
H 5.612278 2.518186 -1.425835
H 2.502730 3.178185 1.472205
H 5.396584 -1.643838 0.106312
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.442606622
Number of imaginary frequencies = 0

22_c3
B3LYP/6-31G* Geometry
C -6.039043 -0.774893 -0.035771
C -4.112058 1.230683 -0.149963
C -6.433150 0.565469 -0.109848
C -4.690291 -1.111568 -0.018162
C -3.696398 -0.112939 -0.074104
C -5.463326 1.567410 -0.167203
C -2.265463 -0.398758 -0.055364
C -1.671343 -1.617454 0.024609
C -0.274137 -1.785849 0.037565
C 0.940658 -1.919952 0.054482
C 2.328060 -2.122489 0.054820
C 3.318779 -1.177660 0.025059
C 3.107861 0.285399 0.065432
C 2.696372 3.070390 0.139050
C 2.123411 0.847244 0.898616
C 3.894582 1.149272 -0.718745
C 3.682154 2.526262 -0.685937
C 1.921222 2.225176 0.935619
C 4.689447 -1.737265 -0.054160
O 5.723296 -1.101559 -0.141610
H -6.789256 -1.559766 0.008010
H -3.359125 2.013905 -0.195227
H -7.488357 0.823763 -0.123342
H -4.406131 -2.158165 0.038689
H -5.758961 2.611312 -0.225795
H -1.612594 0.470545 -0.112409
H -2.273493 -2.522810 0.081509
H 2.646842 -3.166820 0.055106
H 2.538640 4.145393 0.167241
H 1.528969 0.199678 1.534178
H 4.671105 0.738488 -1.351835
H 4.293980 3.176598 -1.305431
H 1.163065 2.639708 1.595123
H 4.714929 -2.850224 -0.028921
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.444167913
Number of imaginary frequencies = 0

22_c4
B3LYP/6-31G* Geometry
C 5.805614 1.566075 -0.184013
C 5.306067 -1.163116 0.038219
C 6.874797 0.666882 -0.108969
C 4.494583 1.104949 -0.147785
C 4.217056 -0.272911 -0.035287
C 6.619209 -0.700606 0.002230
C 2.864984 -0.820827 0.007798
C 1.696836 -0.130207 -0.036781
C 0.432063 -0.745835 0.014906
C -0.689861 -1.229514 0.058332
C -1.936351 -1.871492 0.094587
C -3.184612 -1.309982 0.059552
C -3.474281 0.139854 0.050658
C -4.016636 2.903387 0.030332
C -4.528646 0.660087 -0.723009
C -2.708875 1.031010 0.824347
C -2.978228 2.397631 0.814782
C -4.788620 2.029093 -0.736538
C -4.290041 -2.298626 0.033085
O -5.478723 -2.050279 -0.042551
H 5.997743 2.631980 -0.271641
H 5.111093 -2.229419 0.124843
H 7.897657 1.031953 -0.137503
H 3.679497 1.819872 -0.208704
H 7.442357 -1.407401 0.060814
H 2.802702 -1.904867 0.086048
H 1.702098 0.955992 -0.114269
H -1.892734 -2.961865 0.132884
H -4.226423 3.969773 0.021894
H -5.142184 -0.010607 -1.311282
H -1.910798 0.645638 1.449730
H -2.379855 3.067556 1.426789
H -5.601733 2.412801 -1.346997
H -3.939994 -3.354293 0.089121
SCF Energy (PCM/mPW1PW91/6-31+G**)= -807.444029731
Number of imaginary frequencies = 0

23_c1
B3LYP/6-31G* Geometry
C 4.428762 -1.536286 -0.497706
C 5.212449 -0.457239 -0.086869
C 3.039923 -1.428719 -0.496627
C 2.399645 -0.242608 -0.089658
C 4.594029 0.727668 0.325497
C 3.207517 0.835053 0.325542
C 0.937103 -0.195262 -0.117876
C 0.150331 0.873611 0.146977
C -1.309205 0.878011 0.082174
C -2.041752 2.032986 0.039047
C -2.048038 -0.418438 0.068763
C -3.062671 -0.645238 -0.875833
C -3.790201 -1.834680 -0.870176
C -3.523428 -2.815682 0.086348
C -2.520211 -2.601459 1.033855
C -1.784121 -1.417562 1.021692
H 4.898470 -2.462111 -0.818511
H 6.296010 -0.536705 -0.084830
H 2.433039 -2.271966 -0.818093
H 5.197741 1.570730 0.650512
H 2.748960 1.761941 0.656776
H 0.457210 -1.129467 -0.400855
H 0.622439 1.818903 0.394956
H -3.266690 0.112544 -1.626859
H -4.564613 -1.995202 -1.615394
H -4.092585 -3.741292 0.093334
H -2.311791 -3.356137 1.787520
H -1.012575 -1.252515 1.767688
C -1.527446 3.399390 -0.027198
O -2.253603 4.382640 -0.046780
H -3.126927 1.970898 0.049812
H -0.425981 3.527994 -0.069532
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.307055573
Number of imaginary frequencies = 0

23_c2
B3LYP/6-31G* Geometry
C -4.160961 -1.952173 -0.360034
C -5.043779 -0.904914 -0.092380

C -2.787154 -1.722406 -0.354316
C -2.262124 -0.444306 -0.082357
C -4.540096 0.371539 0.180202
C -3.168849 0.601696 0.186086
C -0.810728 -0.267093 -0.092928
C -0.139236 0.891505 0.116126
C 1.308166 1.033638 0.063824
C 1.916316 2.263008 0.030590
C 2.183479 -0.174772 0.048724
C 2.050114 -1.179834 1.022239
C 2.907632 -2.279266 1.032035
C 3.904950 -2.402283 0.062547
C 4.043361 -1.414487 -0.914104
C 3.194059 -0.308542 -0.917571
H -4.541874 -2.947273 -0.573518
H -6.116323 -1.079092 -0.095790
H -2.101821 -2.540381 -0.564677
H -5.222371 1.191257 0.388649
H -2.797587 1.599535 0.397931
H -0.243034 -1.170180 -0.308095
H -0.678395 1.817375 0.278390
H 1.284378 -1.083827 1.786162
H 2.798271 -3.039244 1.801162
H 4.568876 -3.262495 0.067770
H 4.812049 -1.505101 -1.676943
H 3.297090 0.453573 -1.684831
C 1.281351 3.581663 0.027936
O 0.082958 3.837342 0.050847
H 3.003528 2.291357 0.026917
H 2.014537 4.417917 0.010370
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.306247128
Number of imaginary frequencies = 0

23_c3
B3LYP/6-31G* Geometry
C -4.869717 -0.326834 -0.870165
C -5.159007 -1.206939 0.173516
C -3.586359 0.199118 -1.002765
C -2.562451 -0.145170 -0.101159
C -4.155747 -1.552007 1.084737
C -2.874753 -1.026217 0.952580
C -1.229070 0.430296 -0.297393
C -0.084073 0.061723 0.318811
C 1.228986 0.676444 0.085268
C 1.412686 2.021893 -0.055900
C 2.386353 -0.253351 -0.004348
C 3.664051 0.126509 0.444459
C 4.743153 -0.748916 0.349470
C 4.568467 -2.024189 -0.193267
C 3.304850 -2.418653 -0.636271
C 2.223966 -1.544108 -0.537856
H -5.643498 -0.047767 -1.580084
H -6.159373 -1.616711 0.282301
H -3.365192 0.885084 -1.817098
H -4.377018 -2.228262 1.906096
H -2.113594 -1.290072 1.681065
H -1.170197 1.208267 -1.057156
H -0.090294 -0.792572 0.993833
H 3.802104 1.105159 0.894303
H 5.720512 -0.438975 0.709374
H 5.410592 -2.707140 -0.265094
H 3.160395 -3.407694 -1.062711
H 1.246692 -1.851153 -0.899511
C 0.434169 3.068472 0.249258
O 0.626387 4.251411 0.007032
H 2.385885 2.400495 -0.359150
H -0.491129 2.741623 0.763715
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.306108166
Number of imaginary frequencies = 0

23_c4
B3LYP/6-31G* Geometry
C -4.980573 -0.110256 0.164742
C -5.035171 -1.464523 -0.167927
C -3.750321 0.537925 0.244190
C -2.545466 -0.148733 -0.004895
C -3.849678 -2.162925 -0.421773
C -2.621582 -1.515791 -0.342314
C -1.295581 0.602796 0.103335
C -0.045974 0.101413 -0.062899
C 1.235345 0.791215 0.031233
C 1.518106 2.136844 0.107713
C 2.420137 -0.125558 0.024570
C 2.427672 -1.288393 0.814555
C 3.535492 -2.134335 0.831632
C 4.651816 -1.846435 0.044168
C 4.653208 -0.702734 -0.756159
C 3.550712 0.150417 -0.762791
H -5.895830 0.441445 0.361422
H -5.992621 -1.974449 -0.231577
H -3.708572 1.593261 0.501230
H -3.886354 -3.216878 -0.684441
H -1.714563 -2.076356 -0.547976
H -1.397572 1.658582 0.330874
H 0.056178 -0.956182 -0.293055
H 1.569559 -1.514135 1.441452
H 3.526895 -3.018587 1.463338
H 5.511871 -2.510484 0.051030
H 5.511350 -0.476906 -1.383526
H 3.550102 1.026133 -1.405226
C 0.683816 3.331508 0.065226
O -0.538545 3.432876 0.090677
H 2.573602 2.386848 0.190264
H 1.292560 4.260081 0.005131
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.298908779
Number of imaginary frequencies = 0

24_c1
B3LYP/6-31G* Geometry
C 2.149512 1.431098 -0.050503
C 0.815911 1.734246 -0.058760
C -0.256256 0.746948 -0.133480
C -1.568412 0.965807 0.110013
C -2.646260 -0.020213 -0.010443
C -2.471717 -1.312195 -0.545603
C -3.933842 0.339702 0.430581
C -5.000978 -0.552859 0.354334
C -4.806987 -1.830729 -0.171734
C -3.536725 -2.203832 -0.622646
C 0.536268 3.195101 -0.054010
O -0.554544 3.728780 0.020074
H 0.063069 -0.245298 -0.442251
H -1.874331 1.955507 0.432022
H -1.497553 -1.618731 -0.915545
H -4.089560 1.334875 0.840147
H -5.984309 -0.249513 0.703898
H -5.636782 -2.529384 -0.235699
H -3.378723 -3.194283 -1.041697
H 1.455883 3.819866 -0.113446
H 2.830248 2.279141 -0.137530
C 2.827265 0.139794 0.043829
C 2.289956 -0.978554 0.714334
C 2.999045 -2.175607 0.782229
C 4.256771 -2.288152 0.185453
C 4.814073 -1.183902 -0.464596
C 4.113476 0.016685 -0.522099
H 1.333495 -0.894280 1.218371
H 2.571303 -3.021711 1.313218
H 4.805143 -3.224576 0.239180
H 5.797971 -1.257482 -0.919758
H 4.553905 0.875613 -1.022895
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.307633707
Number of imaginary frequencies = 0

24_c2
B3LYP/6-31G* Geometry
C -2.134342 1.351249 -0.180592
C -0.923541 1.966606 -0.052978
C 0.421934 1.422729 0.144753
C 0.886890 0.240259 -0.307826
C 2.254925 -0.271961 -0.187214
C 2.566626 -1.507176 -0.785593
C 3.281010 0.405218 0.501532
C 4.561140 -0.132531 0.581301

C 4.853213 -1.360782 -0.021183
C 3.849060 -2.046470 -0.705368
C -0.982307 3.452463 -0.124738
O -0.042127 4.197241 0.078325
H 1.105605 2.132527 0.604267
H 0.201809 -0.420259 -0.836248
H 1.787798 -2.045064 -1.321491
H 3.074615 1.358143 0.979381
H 5.337211 0.407542 1.117238
H 5.854715 -1.777171 0.044202
H 4.063559 -3.001656 -1.177334
H -1.988387 3.863282 -0.364718
H -2.954166 2.022276 -0.445199
C -2.575075 -0.034221 -0.001982
C -3.767900 -0.434716 -0.636317
C -4.271200 -1.723972 -0.480047
C -3.607625 -2.636382 0.341622
C -2.439666 -2.246130 1.004413
C -1.924829 -0.965057 0.832826
H -4.297659 0.278149 -1.263995
H -5.185907 -2.012306 -0.990746
H -4.000920 -3.640650 0.473341
H -1.928512 -2.944730 1.661353
H -1.022617 -0.672766 1.357701
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.304244815
Number of imaginary frequencies = 0

24_c3
B3LYP/6-31G* Geometry
C 2.141858 1.272965 0.040353
C 0.830760 1.644876 0.101280
C -0.304659 0.732054 0.218601
C -1.567087 0.993317 -0.188930
C -2.737762 0.124540 -0.031359
C -2.741287 -1.030774 0.774973
C -3.923305 0.453916 -0.714517
C -5.061861 -0.342645 -0.612482
C -5.043833 -1.489353 0.182564
C -3.877775 -1.826824 0.876751
C 0.570743 3.114377 0.168811
O 1.416973 3.979839 0.038198
H -0.091718 -0.225767 0.689143
H -1.763499 1.921516 -0.723931
H -1.852613 -1.299954 1.338431
H -3.943562 1.345320 -1.337415
H -5.963350 -0.066663 -1.153009
H -5.930330 -2.111780 0.267571
H -3.857949 -2.711982 1.507172
H -0.482499 3.391182 0.379690
H 2.850142 2.099288 0.088791
C 2.737290 -0.054107 -0.063221
C 2.077697 -1.173612 -0.613693
C 2.714448 -2.410034 -0.686197
C 4.020129 -2.561983 -0.213341
C 4.696787 -1.459831 0.316123
C 4.067597 -0.220814 0.377588
H 1.079868 -1.061431 -1.023148
H 2.192653 -3.256877 -1.123738
H 4.512386 -3.528974 -0.270404
H 5.717571 -1.566054 0.672984
H 4.598678 0.637067 0.782456
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.305261733
Number of imaginary frequencies = 0

24_c4
B3LYP/6-31G* Geometry
C -2.141029 1.166241 -0.098107
C -0.993118 1.887551 0.048389
C 0.394497 1.451371 0.232736
C 0.977106 0.358516 -0.303421
C 2.380370 -0.045560 -0.181664
C 3.302817 0.590855 0.672630
C 2.838464 -1.129341 -0.954379
C 4.163641 -1.554962 -0.889330
C 5.064931 -0.907321 -0.043667
C 4.625931 0.166698 0.737431
C -1.161232 3.372423 -0.019597
O -2.201679 3.960550 -0.247476
H 1.019464 2.158614 0.779494
H 0.364116 -0.302635 -0.913446
H 2.980165 1.417413 1.299049
H 2.140905 -1.636731 -1.616812
H 4.491680 -2.392731 -1.498884
H 6.098824 -1.236737 0.011626
H 5.319396 0.672172 1.404392
H -0.225538 3.946430 0.161228
H -3.003250 1.787443 -0.342417
C -2.455103 -0.255378 0.039565
C -1.701897 -1.168002 0.806447
C -2.108348 -2.491752 0.937344
C -3.266897 -2.945402 0.298097
C -4.030999 -2.054392 -0.456948
C -3.637205 -0.723325 -0.569988
H -0.805214 -0.829437 1.312441
H -1.519333 -3.175364 1.542982
H -3.574561 -3.982845 0.396833
H -4.939591 -2.392442 -0.947708
H -4.245207 -0.026876 -1.142195
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.300344374
Number of imaginary frequencies = 0

25_c1
B3LYP/6-31G* Geometry
C 0.983816 -1.978435 1.030341
C 2.300118 -1.804306 0.757427
C -0.141672 -1.357293 0.372063
C -1.422672 -1.580625 0.749122
C -2.636470 -1.018989 0.158010
C -3.887734 -1.490898 0.598774
C -5.075904 -0.996945 0.065040
C -5.041663 -0.011495 -0.922578
C -3.808024 0.475741 -1.366536
C -2.621544 -0.017523 -0.834172
H 0.735386 -2.690738 1.817410
H 0.071945 -0.703298 -0.467969
H -1.591276 -2.261161 1.584927
H -3.920342 -2.259843 1.367379
H -6.028248 -1.381064 0.420819
H -5.965877 0.378085 -1.340515
H -3.772822 1.249100 -2.129435
H -1.675189 0.387151 -1.180312
C 2.923033 -0.977165 -0.282494
C 2.700951 0.314324 -0.662621
C 1.884373 1.393459 -0.109506
H 3.005016 -2.452051 1.273744
H 3.277507 0.630474 -1.534524
C 1.660923 2.527161 -0.918367
C 1.361051 1.401030 1.199586
C 0.922424 3.612032 -0.454145
C 0.407527 3.599353 0.843734
C 0.638720 2.494290 1.667951
H 2.073836 2.547467 -1.924426
H 1.537560 0.552963 1.849950
H 0.756741 4.469730 -1.100325
H -0.164710 4.445914 1.213088
H 0.250778 2.483494 2.682830
C 4.034011 -1.647607 -1.013088
O 4.482131 -2.745787 -0.744788
H 4.465050 -1.046586 -1.845582
SCF Energy (PCM/mPW1PW91/6-31+G**)= -808.695537367
Number of imaginary frequencies = 0

25_c2
B3LYP/6-31G* Geometry
C 0.732023 -2.074720 1.219192
C 2.067211 -2.022583 0.986417
C -0.309991 -1.395468 0.486307
C -1.618931 -1.498609 0.817445
C -2.758257 -0.868881 0.151989
C -2.620328 0.092185 -0.870036
C -3.739547 0.653679 -1.475309
C -5.025964 0.276487 -1.076138
C -5.181491 -0.666947 -0.059510
C -4.060709 -1.229051 0.547443

H 0.396648 -2.716778 2.033948
H -0.008201 -0.798822 -0.369586
H -1.875375 -2.126094 1.672306
H -1.630362 0.411900 -1.181141
H -3.609968 1.394373 -2.260030
H -5.897354 0.719026 -1.550937
H -6.175978 -0.964910 0.261868
H -4.187630 -1.964792 1.338459
C 2.795477 -1.307516 -0.070809
C 2.720074 -0.014555 -0.497554
C 2.017519 1.165195 -0.002319
H 2.688506 -2.686867 1.588767
H 3.351786 0.181124 -1.364561
C 1.995135 2.302667 -0.837551
C 1.416404 1.268777 1.269594
C 1.378275 3.483858 -0.435624
C 0.785439 3.565333 0.826006
C 0.816266 2.456277 1.676672
H 2.471374 2.247180 -1.813473
H 1.437934 0.419968 1.942017
H 1.368448 4.342533 -1.101427
H 0.307644 4.486837 1.147354
H 0.366776 2.517309 2.664135
C 3.807971 -2.152720 -0.778448
O 4.471178 -1.811139 -1.740129
H 3.926860 -3.173329 -0.353281
SCF Energy (PCM/mPW1PW91/6-31+G**)= -808.692126181
Number of imaginary frequencies = 0

25_c3
B3LYP/6-31G* Geometry
C -0.196372 -0.460296 1.343200
C 1.047168 0.066875 1.214340
C -1.408316 -0.131607 0.630057
C -2.566444 -0.801680 0.833754
C -3.851463 -0.558379 0.178639
C -4.110847 0.587498 -0.600393
C -5.346517 0.767024 -1.213637
C -6.358644 -0.186440 -1.063051
C -6.123338 -1.320902 -0.284878
C -4.886381 -1.500666 0.330390
H -0.292951 -1.278654 2.057862
H -1.368229 0.678039 -0.088400
H -2.561041 -1.623825 1.550973
H -3.345842 1.350913 -0.706335
H -5.526090 1.660242 -1.806393
H -7.323173 -0.040507 -1.541794
H -6.904216 -2.065709 -0.154995
H -4.708447 -2.387041 0.935360
C 1.524121 1.186837 0.394574
C 2.760740 1.237743 -0.184240
C 3.803988 0.222381 -0.290730
H 1.829389 -0.402448 1.809091
H 3.033110 2.191820 -0.637771
C 5.120273 0.652578 -0.562303
C 3.571810 -1.164435 -0.175534
C 6.167535 -0.255854 -0.674664
C 5.921306 -1.624670 -0.540889
C 4.620029 -2.072573 -0.300942
H 5.314867 1.716696 -0.673754
H 2.562457 -1.527657 -0.020174
H 7.174316 0.101314 -0.873100
H 6.735735 -2.337767 -0.634653
H 4.418454 -3.137165 -0.218449
C 0.745964 2.446270 0.257565
O -0.367043 2.665637 0.694968
H 1.290341 3.238428 -0.304750
SCF Energy (PCM/mPW1PW91/6-31+G**)= -808.695203887
Number of imaginary frequencies = 0

25_c4
B3LYP/6-31G* Geometry
C 0.260651 -0.785257 1.417298
C -0.995338 -0.272324 1.367671
C 1.421694 -0.335967 0.681512
C 2.647394 -0.891250 0.833044
C 3.882396 -0.539066 0.134397
C 3.968745 0.502019 -0.812377
C 5.171625 0.790463 -1.447988
C 6.322643 0.050830 -1.157216
C 6.257071 -0.981846 -0.220875
C 5.052162 -1.270934 0.415602
H 0.415607 -1.659560 2.049621
H 1.276858 0.461743 -0.043633
H 2.745508 -1.701883 1.556330
H 3.089256 1.092696 -1.050943
H 5.214005 1.598292 -2.173741
H 7.260396 0.280340 -1.655666
H 7.144714 -1.563000 0.014589
H 5.007281 -2.077413 1.144100
C -1.426706 0.955163 0.691729
C -2.625754 1.140630 0.069094
C -3.692940 0.191795 -0.220743
H -1.771170 -0.807308 1.913785
H -2.816397 2.164848 -0.249620
C -4.972443 0.708436 -0.518380
C -3.521670 -1.208806 -0.252299
C -6.043783 -0.134052 -0.795740
C -5.858692 -1.519040 -0.804518
C -4.593304 -2.049560 -0.540683
H -5.116903 1.785984 -0.518247
H -2.538007 -1.632520 -0.084653
H -7.021608 0.287542 -1.011882
H -6.691913 -2.179879 -1.027535
H -4.438506 -3.124806 -0.569060
C -0.566318 2.170510 0.826131
O -0.772688 3.236917 0.275279
H 0.297783 2.049124 1.510363
SCF Energy (PCM/mPW1PW91/6-31+G**)= -808.695206835
Number of imaginary frequencies = 0

25_c5
B3LYP/6-31G* Geometry
C 0.176406 -1.766173 -1.635421
C -0.952572 -1.645562 -0.894291
C 1.521453 -1.285850 -1.345275
C 1.838569 -0.202906 -0.597313
C 3.180675 0.305171 -0.307802
C 4.360926 -0.401704 -0.613204
C 5.610344 0.137339 -0.324879
C 5.716968 1.392947 0.281875
C 4.558657 2.102828 0.600936
C 3.307474 1.563174 0.311204
H 0.073442 -2.275342 -2.593963
H 2.321645 -1.830823 -1.845178
H 1.024722 0.390160 -0.183982
H 4.299671 -1.386539 -1.067067
H 6.507287 -0.426657 -0.567128
H 6.694764 1.808763 0.509003
H 4.628768 3.076634 1.078115
H 2.408043 2.119874 0.563457
C -1.064858 -1.187902 0.494731
C -2.092818 -0.464736 1.018597
C -3.229784 0.166851 0.358738
H -1.881885 -1.978382 -1.356343
H -2.063663 -0.354804 2.102074
C -4.339455 0.526438 1.153077
C -3.280411 0.465220 -1.019543
C -5.464945 1.122447 0.593434
C -5.503413 1.394094 -0.776597
C -4.404232 1.070460 -1.576036
H -4.309828 0.320935 2.220297
H -2.422525 0.250868 -1.647188
H -6.310322 1.381103 1.225246
H -6.378605 1.864922 -1.216000
H -4.419199 1.299026 -2.638396
C -0.062686 -1.719166 1.474011
O -0.007317 -1.402476 2.647654
H 0.628431 -2.477755 1.058370
SCF Energy (PCM/mPW1PW91/6-31+G**)= -808.689954450
Number of imaginary frequencies = 0

26_c1
B3LYP/6-31G* Geometry

C 3.491591 1.404943 0.000044
C 4.365440 0.314273 -0.000216
C 3.857214 -0.987600 -0.000304
C 2.482557 -1.203269 -0.000173
C 1.592278 -0.109703 0.000055
C 2.115370 1.199939 0.000174
C 0.186309 -0.323174 0.000205
C -1.021003 -0.489874 0.000395
C -2.410614 -0.717296 0.000459
C -3.365036 0.244315 0.000260
C -4.784353 -0.117247 -0.000027
O -5.699889 0.686419 -0.000634
H 3.884649 2.417732 0.000148
H 5.439451 0.478281 -0.000319
H 4.535062 -1.836616 -0.000478
H 2.081826 -2.212133 -0.000217
H 1.431058 2.042562 0.000386
H -2.731947 -1.761128 0.000202
H -3.115863 1.301752 0.000217
H -4.983648 -1.213637 -0.000088
SCF Energy (PCM/mPW1PW91/6-31+G**)= -499.037848693
Number of imaginary frequencies = 0

26_c2
B3LYP/6-31G* Geometry
C -3.726246 -1.150749 -0.000095
C -4.351879 0.099012 -0.000129
C -3.581800 1.265321 -0.000059
C -2.192568 1.187672 0.000029
C -1.551086 -0.068362 0.000057
C -2.337682 -1.238995 -0.000007
C -0.131925 -0.154608 0.000216
C 1.085532 -0.221097 0.000235
C 2.487104 -0.338807 0.000281
C 3.360689 0.697584 -0.000244
C 4.812759 0.456451 0.000139
O 5.332305 -0.647856 -0.000439
H -4.323176 -2.058479 -0.000148
H -5.436422 0.163916 -0.000208
H -4.066503 2.237642 -0.000062
H -1.588571 2.089651 0.000094
H -1.845443 -2.206468 0.000043
H 2.910167 -1.344087 0.000948
H 3.013175 1.727502 -0.000797
H 5.440941 1.372645 0.001097
SCF Energy (PCM/mPW1PW91/6-31+G**)= -499.034832742
Number of imaginary frequencies = 0

27_c1
B3LYP/6-31G* Geometry
C -3.018633 1.538251 0.000143
C -4.035974 0.580086 -0.000097
C -3.714070 -0.779859 -0.000261
C -2.382778 -1.184591 -0.000183
C -1.348867 -0.225839 0.000038
C -1.684227 1.143825 0.000203
C 0.013533 -0.635494 0.000104
C 1.186192 -0.967505 0.000156
C 2.519777 -1.433580 0.000082
C 3.640671 -0.669377 0.000241
C 3.630259 0.797209 0.000357
O 4.643510 1.476137 -0.000732
H -3.266739 2.595937 0.000262
H -5.076595 0.892370 -0.000141
H -4.503407 -1.526340 -0.000434
H -2.126374 -2.239433 -0.000328
H -0.889766 1.883542 0.000388
H 2.636395 -2.517476 -0.000189
H 4.618324 -1.143224 0.000053
H 2.624794 1.266770 0.001545
SCF Energy (PCM/mPW1PW91/6-31+G**)= -499.035460248
Number of imaginary frequencies = 0

27_c2
B3LYP/6-31G* Geometry
C -3.540987 -0.845294 0.000121
C -3.830074 0.522245 0.000075
C -2.791322 1.458121 -0.000043
C -1.466468 1.033777 -0.000111
C -1.165771 -0.345020 -0.000045
C -2.219269 -1.280967 0.000067
C 0.192793 -0.760078 -0.000135
C 1.389749 -0.990414 -0.000140
C 2.750255 -1.342531 -0.000069
C 3.807650 -0.488134 0.000062
C 3.709279 0.977658 0.000183
O 2.672564 1.621521 -0.000047
H -4.348494 -1.572221 0.000204
H -4.863524 0.858105 0.000120
H -3.016327 2.521058 -0.000093
H -0.646918 1.745650 -0.000227
H -1.986538 -2.341430 0.000102
H 2.963382 -2.412047 -0.000065
H 4.811258 -0.906615 0.000124
H 4.691638 1.499152 0.000426
SCF Energy (PCM/mPW1PW91/6-31+G**)= -499.031225712
Number of imaginary frequencies = 0

28_c1
B3LYP/6-31G* Geometry
C -5.461469 -0.389710 0.023849
C -5.456583 0.988301 -0.197556
C -4.237908 1.662983 -0.327060
C -3.036217 0.969668 -0.236070
C -3.021409 -0.422568 -0.011942
C -4.258027 -1.084720 0.115096
C -1.792991 -1.204337 0.093397
C -0.515123 -0.755554 0.014610
C 0.614822 -1.640700 0.108220
C 1.942065 -1.318188 0.075981
H -6.402474 -0.923429 0.125441
H -6.393079 1.534343 -0.269728
H -4.227031 2.735596 -0.500942
H -2.101245 1.511569 -0.341767
H -4.266567 -2.158413 0.288126
H -1.942086 -2.272290 0.257732
H -0.312288 0.299801 -0.142215
H 0.372955 -2.703246 0.176582
C 2.484714 0.060886 0.061655
C 2.008029 1.029653 0.962749
C 2.517945 2.327456 0.955279
C 3.519300 2.680661 0.049562
C 4.012519 1.723935 -0.840191
C 3.507975 0.424898 -0.831521
C 2.874168 -2.467399 0.052088
O 4.085113 -2.407122 -0.060264
H 1.251314 0.752360 1.691312
H 2.139545 3.058766 1.664784
H 3.919233 3.691150 0.043151
H 4.798071 1.988524 -1.543048
H 3.905953 -0.314538 -1.516481
H 2.365939 -3.454804 0.140283
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.312226300
Number of imaginary frequencies = 0

28_c2
B3LYP/6-31G* Geometry
C -5.392710 0.304118 0.017796
C -5.385666 -1.079534 -0.165498
C -4.165970 -1.755434 -0.278145
C -2.965477 -1.057675 -0.207957
C -2.952662 0.340330 -0.022073
C -4.190512 1.003579 0.088070
C -1.726168 1.126968 0.060717
C -0.446262 0.679057 -0.003772
C 0.675333 1.573163 0.071653
C 2.002156 1.253886 0.051766
H -6.334561 0.838761 0.105851
H -6.321304 -1.629006 -0.221274
H -4.153568 -2.832437 -0.422547
H -2.029563 -1.600411 -0.300481
H -4.200414 2.081595 0.231063
H -1.875122 2.198972 0.193309
H -0.241453 -0.380621 -0.129945

H 0.453763 2.639330 0.118393
C 2.557279 -0.120389 0.043562
C 3.559450 -0.477711 -0.876644
C 4.107109 -1.760103 -0.877491
C 3.668863 -2.711888 0.045031
C 2.681316 -2.370164 0.971111
C 2.135031 -1.087378 0.973839
C 2.966691 2.384639 0.052833
O 2.662646 3.565812 0.055524
H 3.894070 0.249145 -1.612321
H 4.874308 -2.016877 -1.603139
H 4.096965 -3.710612 0.045433
H 2.343229 -3.100406 1.701733
H 1.390703 -0.817840 1.717759
H 4.034970 2.081126 0.063184
SCF Energy (PCM/mPW1PW91/6-31+G**)= -731.310475980
Number of imaginary frequencies = 0

29_c1
B3LYP/6-31G* Geometry
C -1.328359 0.893842 -0.453476
C -2.655733 1.313508 -0.401995
C -3.659571 0.435207 0.011945
C -3.330107 -0.878308 0.355869
C -2.006814 -1.303506 0.291945
C -0.975146 -0.421533 -0.090051
C 0.394035 -0.934373 -0.135132
C 1.585507 -0.288620 0.021049
C 2.776023 -1.151167 -0.198413
O 3.939575 -0.797237 -0.192798
C 1.726572 1.112556 0.432871
C 2.828287 1.871337 0.331639
H -0.564976 1.574788 -0.813268
H -2.908224 2.328639 -0.696051
H -4.693248 0.767398 0.052567
H -4.106281 -1.572487 0.666103
H -1.755744 -2.328726 0.553441
H 0.455556 -2.009182 -0.313637
H 2.519331 -2.217041 -0.394689
H 0.840866 1.545770 0.893048
H 2.821623 2.891829 0.705271
H 3.746340 1.503242 -0.107903
SCF Energy (PCM/mPW1PW91/6-31+G**)= -500.283862135
Number of imaginary frequencies = 0

29_c2
B3LYP/6-31G* Geometry
C -1.844575 -1.323775 0.245223
C -3.193452 -0.986030 0.284199
C -3.595135 0.320293 -0.006931
C -2.637327 1.279821 -0.343582
C -1.285232 0.947173 -0.370696
C -0.859185 -0.361001 -0.059353
C 0.536091 -0.788004 -0.067200
C 1.677244 -0.061621 0.086626
C 2.959333 -0.820904 -0.003782
O 3.056109 -1.993595 -0.316983
C 1.743026 1.364203 0.433146
C 2.732404 2.206914 0.100456
H -1.534523 -2.342501 0.464490
H -3.933148 -1.741995 0.533207
H -4.648777 0.585046 0.014365
H -2.946047 2.290612 -0.596410
H -0.556971 1.691902 -0.672117
H 0.695492 -1.857002 -0.206032
H 3.863361 -0.236746 0.264384
H 0.919649 1.745409 1.035800
H 2.724185 3.239384 0.437316
H 3.568743 1.912236 -0.527783
SCF Energy (PCM/mPW1PW91/6-31+G**)= -500.281871838
Number of imaginary frequencies = 0

29_c3
B3LYP/6-31G* Geometry
C -1.269882 0.799730 -0.542838
C -2.623704 1.116486 -0.591880
C -3.582128 0.212439 -0.123211
C -3.175419 -1.024598 0.378605
C -1.821666 -1.350513 0.409927
C -0.840403 -0.440396 -0.030443
C 0.557670 -0.878827 -0.001003
C 1.744245 -0.212287 -0.020618
C 2.941651 -1.081210 -0.165187
O 4.081011 -0.677731 -0.303772
C 2.042169 1.227669 0.073137
C 1.405882 2.132303 0.826121
H -0.537750 1.507856 -0.912330
H -2.934773 2.074281 -1.000254
H -4.637509 0.468554 -0.157387
H -3.911745 -1.739442 0.735487
H -1.510627 -2.322517 0.785724
H 0.654453 -1.966601 0.016974
H 2.722967 -2.172722 -0.158311
H 2.947435 1.521643 -0.454202
H 1.753981 3.160481 0.872056
H 0.534992 1.885533 1.426749
SCF Energy (PCM/mPW1PW91/6-31+G**)= -500.280490161
Number of imaginary frequencies = 0

30_c1
B3LYP/6-31G* Geometry
C 3.064232 -5.494496 0.000000
C 4.366364 -4.987046 0.000000
C 4.576403 -3.605384 0.000000
C 3.493189 -2.731844 0.000000
C 2.175044 -3.233105 0.000000
C 1.974579 -4.629023 0.000000
C 1.063550 -2.345503 0.000000
C 0.115389 -1.579340 0.000000
C -1.008748 -0.730868 0.000000
C -0.960117 0.621735 0.000000
C -2.219525 1.404836 0.000000
O -3.309234 0.833579 0.000000
C -2.159012 2.905199 0.000000
C -3.381281 3.598504 0.000000
C -3.409885 4.988848 0.000000
C -2.213862 5.713160 0.000000
C -0.993076 5.037248 0.000000
C -0.964291 3.642594 0.000000
H 2.898457 -6.568249 0.000000
H 5.214591 -5.666039 0.000000
H 5.587856 -3.208585 0.000000
H 3.649798 -1.657655 0.000000
H 0.960780 -5.017014 0.000000
H -1.995658 -1.193735 0.000000
H 0.000000 1.124318 0.000000
H -4.296499 3.016127 0.000000
H -4.362729 5.511304 0.000000
H -2.234090 6.799797 0.000000
H -0.060696 5.595209 0.000000
H -0.001651 3.142818 0.000000
SCF Energy (PCM/mPW1PW91/6-31+G**)= -730.059503979
Number of imaginary frequencies = 0

30_c2
B3LYP/6-31G* Geometry
C 6.261812 -0.584110 -0.041476
C 6.579759 0.774266 0.041268
C 5.559014 1.726656 0.105607
C 4.225996 1.327793 0.087398
C 3.893852 -0.040229 0.003727
C 4.931818 -0.992815 -0.060443
C 2.533325 -0.454495 -0.016466
C 1.365136 -0.802454 -0.033729
C 0.029268 -1.247940 -0.056641
C -1.058275 -0.444040 -0.002529
C -2.417103 -1.038214 -0.022521
O -2.565894 -2.259309 -0.039072
C -3.616278 -0.135393 -0.008735
C -3.547016 1.258105 -0.164072
C -4.708788 2.030108 -0.151111
C -5.952578 1.421502 0.021834
C -6.033115 0.033934 0.174905
C -4.875463 -0.736571 0.155565

H 7.053519 -1.326500 -0.091429
H 7.619408 1.089614 0.055695
H 5.803715 2.783274 0.170350
H 3.428722 2.062847 0.137183
H 4.678514 -2.046399 -0.124895
H -0.148096 -2.321536 -0.122015
H -0.931153 0.629816 0.072179
H -2.593236 1.753394 -0.312211
H -4.641401 3.107239 -0.277296
H -6.856303 2.025076 0.035489
H -6.999999 -0.443907 0.307905
H -4.914721 -1.815069 0.266122
SCF Energy (PCM/mPW1PW91/6-31+G**)= -730.059602616
Number of imaginary frequencies = 0

31_c1
B3LYP/6-31G* Geometry
C 3.009277 -5.037573 0.000000
C 4.153803 -4.235470 0.000000
C 4.031984 -2.842705 0.000000
C 2.773525 -2.249357 0.000000
C 1.612336 -3.051086 0.000000
C 1.745656 -4.454059 0.000000
C 0.333584 -2.431220 0.000000
C -0.702187 -1.788673 0.000000
C -1.962385 -1.163204 0.000000
C -2.230789 0.167840 0.000000
C -1.197476 1.225120 0.000000
O 0.000000 0.944728 0.000000
C -1.625138 2.668879 0.000000
C -0.606588 3.636779 0.000000
C -0.912112 4.993607 0.000000
C -2.246649 5.410137 0.000000
C -3.268653 4.460238 0.000000
C -2.961556 3.099327 0.000000
H 3.103257 -6.120070 0.000000
H 5.138598 -4.694845 0.000000
H 4.921520 -2.218722 0.000000
H 2.661136 -1.169709 0.000000
H 0.852170 -5.070898 0.000000
H -2.816256 -1.841803 0.000000
H -3.275923 0.454014 0.000000
H 0.421730 3.291409 0.000000
H -0.112112 5.729138 0.000000
H -2.488181 6.469797 0.000000
H -4.308011 4.777330 0.000000
H -3.777722 2.385042 0.000000
SCF Energy (PCM/mPW1PW91/6-31+G**)= -730.055177757
Number of imaginary frequencies = 0

31_c2
B3LYP/6-31G* Geometry
C 4.534582 -1.900634 0.132926
C 5.781124 -1.267590 0.146973
C 5.857936 0.126817 0.092298
C 4.695879 0.889837 0.024152
C 3.434739 0.261074 0.009531
C 3.366896 -1.147316 0.064811
C 2.232946 1.016100 -0.060070
C 1.139054 1.550361 -0.119064
C -0.064395 2.275603 -0.189474
C -1.329333 1.782349 -0.188947
C -1.665362 0.342855 -0.135943
O -0.795834 -0.524396 -0.194813
C -3.112538 -0.053599 -0.030973
C -4.136940 0.829188 0.345051
C -5.455542 0.383927 0.441089
C -5.768422 -0.945564 0.154553
C -4.754844 -1.834162 -0.216988
C -3.438369 -1.392585 -0.301628
H 4.474304 -2.984711 0.175123
H 6.690773 -1.859656 0.200433
H 6.826393 0.619390 0.103078
H 4.748054 1.973484 -0.018465
H 2.390941 -1.622405 0.052173
H 0.047655 3.358986 -0.246632
H -2.139203 2.500066 -0.257747
H -3.912970 1.862245 0.590796
H -6.237710 1.075796 0.741680
H -6.797094 -1.289498 0.223627
H -4.994074 -2.870966 -0.437973
H -2.634868 -2.067520 -0.577390
SCF Energy (PCM/mPW1PW91/6-31+G**)= -730.055310727
Number of imaginary frequencies = 0

31_c3
B3LYP/6-31G* Geometry
C -4.730889 -0.582767 -0.058305
C -4.693589 0.777826 -0.374651
C -3.464060 1.425415 -0.522871
C -2.274657 0.721605 -0.358376
C -2.302474 -0.652110 -0.039723
C -3.547517 -1.295925 0.109638
C -1.087049 -1.373178 0.128220
C -0.018896 -1.942259 0.263944
C 1.171127 -2.685897 0.434768
C 2.446100 -2.295933 0.196063
C 2.938916 -1.022597 -0.403730
O 3.853607 -1.097414 -1.218945
C 2.371285 0.307437 -0.020198
C 2.543398 1.379784 -0.909420
C 2.078462 2.649311 -0.578968
C 1.460692 2.867032 0.657148
C 1.306969 1.810318 1.557316
C 1.753881 0.533354 1.218126
H -5.685295 -1.088990 0.057581
H -5.619467 1.331277 -0.505339
H -3.432744 2.483374 -0.768704
H -1.316390 1.219218 -0.468982
H -3.570601 -2.353236 0.355052
H 1.025488 -3.716000 0.762585
H 3.227259 -3.045686 0.292580
H 3.045643 1.193437 -1.853198
H 2.203759 3.472221 -1.277549
H 1.106742 3.860512 0.920411
H 0.839421 1.980361 2.523238
H 1.637122 -0.285669 1.920009
SCF Energy (PCM/mPW1PW91/6-31+G**)= -730.052834884
Number of imaginary frequencies = 0

32_c1
B3LYP/6-31G* Geometry
C 4.171109 -0.999990 -0.000004
C 4.645384 0.314561 -0.000017
C 3.742593 1.381297 -0.000017
C 2.372211 1.139922 -0.000002
C 1.883099 -0.182664 0.000008
C 2.802553 -1.251868 0.000004
C 0.483032 -0.434826 0.000022
C -0.717732 -0.645433 0.000027
C -2.098032 -0.926728 0.000007
C -3.103532 -0.011566 -0.000005
C -4.480475 -0.535428 -0.000018
O -5.478063 0.164326 -0.000027
C -2.923891 1.477217 0.000021
H 4.870879 -1.831295 -0.000002
H 5.714789 0.506936 -0.000025
H 4.108479 2.404449 -0.000028
H 1.666258 1.964781 0.000002
H 2.428513 -2.271106 0.000011
H -2.372108 -1.983428 -0.000005
H -4.561561 -1.645612 -0.000036
H -3.410455 1.920150 0.877108
H -1.867040 1.753299 -0.000363
H -3.411168 1.920259 -0.876609
SCF Energy (PCM/mPW1PW91/6-31+G**)= -538.353225250
Number of imaginary frequencies = 0

32_c2
B3LYP/6-31G* Geometry
C 4.171426 -0.999863 -0.000019
C 4.645573 0.314726 0.000010
C 3.742693 1.381383 0.000037
C 2.372333 1.139837 0.000013

C 1.883107 -0.182785 -0.000010
C 2.802878 -1.251828 -0.000075
C 0.483212 -0.434974 -0.000026
C -0.717619 -0.645427 0.000019
C -2.098053 -0.926893 0.000083
C -3.103293 -0.011528 -0.000025
C -4.480902 -0.535372 0.000090
O -5.478338 0.164324 -0.000120
C -2.924504 1.477156 -0.000054
H 4.871189 -1.830978 -0.000041
H 5.714854 0.507156 0.000023
H 4.108435 2.404423 0.000071
H 1.666594 1.964690 0.000020
H 2.429228 -2.271056 -0.000111
H -2.372537 -1.983347 0.000208
H -4.561304 -1.645792 0.000257
H -3.407998 1.919478 0.878863
H -1.867950 1.754099 -0.003868
H -3.414905 1.920155 -0.874723
SCF Energy (PCM/mPW1PW91/6-31+G**)= -538.353219922
Number of imaginary frequencies = 0

9i_c1
B3LYP/6-31G* Geometry
C -0.539959 0.357275 -0.000168
H 0.316529 -0.311269 -0.000421
C -0.323842 1.691681 0.000056
H -1.167642 2.377394 0.000298
C -1.842375 -0.312877 -0.000100
C -4.291157 -1.719729 0.000070
C -1.876284 -1.720417 -0.000084
C -3.073449 0.373847 -0.000050
C -4.278168 -0.320963 0.000038
C -3.082684 -2.417281 0.000003
H -0.937306 -2.270061 -0.000133
H -3.087278 1.459382 -0.000094
H -5.214755 0.230449 0.000080
H -3.078940 -3.504142 0.000021
H -5.235072 -2.257937 0.000134
C 0.953961 2.385835 -0.000027
C 2.229146 1.883387 -0.000109
H 3.037180 2.617773 -0.000177
C 0.880019 3.869322 0.000027
H 1.868849 4.379498 -0.000053
O -0.149823 4.517287 0.000165
C 2.653124 0.544825 -0.000099
C 3.098286 -0.590660 -0.000057
C 3.611397 -1.927128 0.000050
C 2.867927 -3.034132 0.747583
C 2.868041 -3.034206 -0.747381
H 4.696783 -2.004617 0.000145
H 1.957604 -2.750639 1.266222
H 3.480425 -3.762891 1.270417
H 1.957776 -2.750827 -1.266195
H 3.480535 -3.763076 -1.270075
SCF Energy (PCM/mPW1PW91/6-31+G**)= -693.116214659
Number of imaginary frequencies = 0

9i _c2
B3LYP/6-31G* Geometry
C 1.488490 0.999271 -0.000695
H 2.005586 1.953275 0.002255
C 0.135593 1.008994 -0.002449
H -0.409669 0.067193 -0.003659
C 2.348230 -0.186477 -0.001267
C 4.120301 -2.385245 0.000207
C 3.743728 0.000842 0.013591
C 1.863120 -1.509743 -0.016291
C 2.736950 -2.591826 -0.015441
C 4.619907 -1.082397 0.014636
H 4.136934 1.014532 0.024726
H 0.792796 -1.693476 -0.029688
H 2.339723 -3.603621 -0.027400
H 5.692698 -0.908854 0.026524
H 4.799661 -3.233339 0.000696
C -0.717827 2.186108 -0.002181
C -2.088087 2.097686 -0.001635
H -2.655200 3.029233 -0.001965
C -0.201434 3.574884 -0.002541
H -1.007165 4.343285 -0.003081
O 0.965991 3.921440 -0.002193
C -2.850648 0.917076 -0.000374
C -3.540187 -0.088022 0.001163
C -4.351640 -1.267995 0.003182
C -3.888270 -2.518902 -0.742354
C -3.888156 -2.516302 0.752985
H -5.424984 -1.089113 0.002947
H -2.935744 -2.458347 -1.258975
H -4.653805 -3.085229 -1.264718
H -2.935561 -2.453961 1.269266
H -4.653619 -3.080820 1.277414
SCF Energy (PCM/mPW1PW91/6-31+G**)= -693.117443912
Number of imaginary frequencies = 0

9l_c1
B3LYP/6-31G* Geometry
C -2.021998 -0.089142 0.090254
H -0.949358 -0.258961 0.123186
C -2.846870 -1.144825 -0.098892
H -3.921832 -0.991390 -0.150056
C -2.426156 1.308531 0.252802
C -3.078113 4.035890 0.561602
C -3.770381 1.729415 0.311450
C -1.421127 2.289678 0.356656
C -1.741957 3.637101 0.507772
C -4.089547 3.074312 0.462944
H -4.570608 0.998924 0.242733
H -0.378328 1.985823 0.309268
H -0.947319 4.374563 0.583524
H -5.132536 3.376714 0.506881
H -3.332620 5.085552 0.681157
C -2.476669 -2.539690 -0.264309
C -1.245945 -3.140730 -0.233894
H -1.227616 -4.221087 -0.388958
C -3.607134 -3.481118 -0.500942
H -3.303121 -4.543418 -0.627940
O -4.778246 -3.161009 -0.557054
C 0.014260 -2.552313 -0.023095
C 1.140173 -2.103867 0.158277
Si 2.835688 -1.441441 0.449617
C 3.191091 -1.493527 2.303634
H 4.201341 -1.128011 2.524206
H 3.121911 -2.520315 2.680079
H 2.479470 -0.879323 2.865448
C 4.065230 -2.530549 -0.483947
H 3.857321 -2.531539 -1.559417
H 4.023212 -3.566962 -0.129477
H 5.089399 -2.164967 -0.341942
C 2.885574 0.333784 -0.192474
C 3.031216 2.970008 -1.200412
C 3.787874 1.270736 0.344295
C 2.056161 0.757049 -1.247637
C 2.125894 2.058946 -1.747845
C 3.863155 2.573278 -0.152021
H 4.442153 0.987777 1.166393
H 1.339621 0.062630 -1.680690
H 1.472424 2.361688 -2.562003
H 4.567669 3.278567 0.281641
H 3.086777 3.984177 -1.587555
SCF Energy (PCM/mPW1PW91/6-31+G**)= -1176.79618077
Number of imaginary frequencies = 0

9l_c2
B3LYP/6-31G* Geometry
C 3.079709 0.823445 0.030451
H 3.961158 1.452910 -0.036357
C 1.865131 1.420969 0.029808
H 0.967114 0.811074 0.096988
C 3.332178 -0.616313 0.112172
C 3.957901 -3.364378 0.258177
C 4.667822 -1.061671 0.092441
C 2.314070 -1.587040 0.208021
C 2.624849 -2.940740 0.279731
C 4.979036 -2.417796 0.164199

H 5.465838 -0.326669 0.019432
H 1.270977 -1.285886 0.226719
H 1.822170 -3.669794 0.354214
H 6.018342 -2.735006 0.147087
H 4.196019 -4.423133 0.315097
C 1.606404 2.847724 -0.053545
C 0.333084 3.360384 -0.066611
H 0.214587 4.442315 -0.128022
C 2.674556 3.877374 -0.131515
H 2.280431 4.916898 -0.183424
O 3.875118 3.681715 -0.142758
C -0.852339 2.602848 -0.008809
C -1.883776 1.944666 0.042119
Si -3.403198 0.905488 0.127466
C -4.218301 1.160563 1.811195
H -5.150966 0.589441 1.893671
H -4.464942 2.217706 1.960852
H -3.557565 0.849875 2.627489
C -4.571934 1.444614 -1.255814
H -4.107957 1.318539 -2.240037
H -4.852980 2.498484 -1.146493
H -5.490122 0.845175 -1.239578
C -2.870170 -0.892442 -0.096991
C -2.115609 -3.587361 -0.489248
C -3.530904 -1.938583 0.571669
C -1.816903 -1.235284 -0.965606
C -1.442202 -2.565476 -1.162614
C -3.161048 -3.271381 0.379387
H -4.344186 -1.716468 1.259292
H -1.275484 -0.451614 -1.491354
H -0.625104 -2.803489 -1.839001
H -3.686648 -4.061469 0.909771
H -1.826177 -4.624185 -0.640518
SCF Energy (PCM/mPW1PW91/6-31+G**)= -1176.79724524
Number of imaginary frequencies = 0

9l_c3
B3LYP/6-31G* Geometry
C 1.951324 -0.133681 0.037543
H 0.882528 -0.327633 0.045221
C 2.806626 -1.180905 -0.013706
H 3.879553 -1.006759 -0.025164
C 2.315157 1.283259 0.083971
C 2.885683 4.044280 0.173954
C 1.281083 2.238287 0.128639
C 3.646314 1.747516 0.085767
C 3.925400 3.109006 0.130137
C 1.562198 3.602166 0.172955
H 0.247586 1.901429 0.127172
H 4.467941 1.038523 0.052305
H 4.958888 3.445418 0.130702
H 0.744811 4.317546 0.205944
H 3.108953 5.107269 0.208610
C 2.471825 -2.593564 -0.060060
C 1.250703 -3.215141 -0.054228
H 1.258307 -4.305852 -0.096220
C 3.629900 -3.528455 -0.122322
H 3.351575 -4.604814 -0.157318
O 4.797252 -3.190078 -0.135614
C -0.027872 -2.631976 0.000636
C -1.166834 -2.182276 0.047888
Si -2.874471 -1.493442 0.123833
C -3.875980 -2.245183 -1.289457
H -4.906591 -1.871074 -1.271522
H -3.909829 -3.337312 -1.205198
H -3.447672 -2.001100 -2.267666
C -3.629598 -1.961626 1.789376
H -3.035468 -1.589047 2.630755
H -3.689710 -3.051520 1.885620
H -4.645315 -1.559630 1.885291
C -2.785125 0.383736 -0.067110
C -2.663775 3.190216 -0.378168
C -2.985734 1.247039 1.024985
C -2.520490 0.968298 -1.320537
C -2.458888 2.353256 -1.477830
C -2.926277 2.634442 0.874972
H -3.193796 0.836072 2.009940
H -2.358312 0.336066 -2.191051
H -2.253150 2.779612 -2.456255
H -3.087161 3.279724 1.734831
H -2.622415 4.269728 -0.499178
SCF Energy (PCM/mPW1PW91/6-31+G**)= -1176.79642311
Number of imaginary frequencies = 0

9l_c4
B3LYP/6-31G* Geometry
C -2.507325 0.173724 -0.006660
H -1.472980 -0.056413 0.233421
C -2.883247 1.469749 -0.101164
H -3.912636 1.720354 -0.344314
C -3.367329 -0.994741 -0.201289
C -4.920582 -3.323885 -0.555895
C -2.798477 -2.276565 -0.074127
C -4.740100 -0.909807 -0.510644
C -5.503579 -2.058797 -0.685051
C -3.563224 -3.427815 -0.249217
H -1.741132 -2.362352 0.165737
H -5.212991 0.061809 -0.615316
H -6.560184 -1.969744 -0.923260
H -3.099486 -4.405241 -0.146140
H -5.521362 -4.218764 -0.693405
C -2.053659 2.647783 0.084518
C -0.726017 2.755680 0.403787
H -0.325822 3.767829 0.487400
C -2.744387 3.955472 -0.097470
H -2.092757 4.845063 0.047220
O -3.919034 4.087199 -0.380100
C 0.206074 1.729882 0.645233
C 1.065776 0.885779 0.868493
Si 2.354978 -0.383987 1.222460
C 3.093351 -0.025217 2.923935
H 3.888821 -0.742120 3.161064
H 2.330776 -0.097427 3.707872
H 3.526609 0.979913 2.962834
C 1.541767 -2.089968 1.213322
H 1.074546 -2.298081 0.244286
H 0.770508 -2.162533 1.988984
H 2.279852 -2.878848 1.402213
C 3.673890 -0.273230 -0.122732
C 5.681807 -0.149390 -2.104964
C 3.641225 0.707427 -1.129383
C 4.741255 -1.191693 -0.137674
C 5.734879 -1.133069 -1.114998
C 4.632936 0.770714 -2.110372
H 2.828551 1.429157 -1.147942
H 4.803759 -1.968565 0.622826
H 6.548796 -1.853664 -1.105400
H 4.585267 1.537689 -2.879316
H 6.454228 -0.102047 -2.868289
SCF Energy (PCM/mPW1PW91/6-31+G**)= -1176.79586276
Number of imaginary frequencies = 0