

# Proton-Sensitive Free Radical Dimer Evolution Is a Critical Control Point for the Synthesis of $\Delta^{2,2'}$ -Bibenzothiazines.

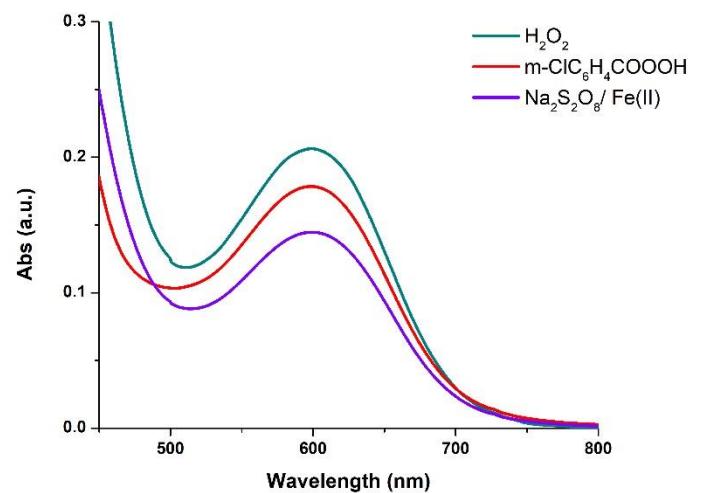
Luca Valgimigli,<sup>†\*</sup> Maria Laura Alfieri,<sup>‡</sup> Riccardo Amorati,<sup>†</sup> Andrea Baschieri,<sup>†</sup> Orlando Crescenzi,<sup>‡</sup> Alessandra Napolitano,<sup>‡\*</sup> and Marco d'Ischia<sup>‡</sup>

<sup>†</sup>Department of Chemistry “Giacomo Ciamician”, University of Bologna, I-40126 Bologna, Italy

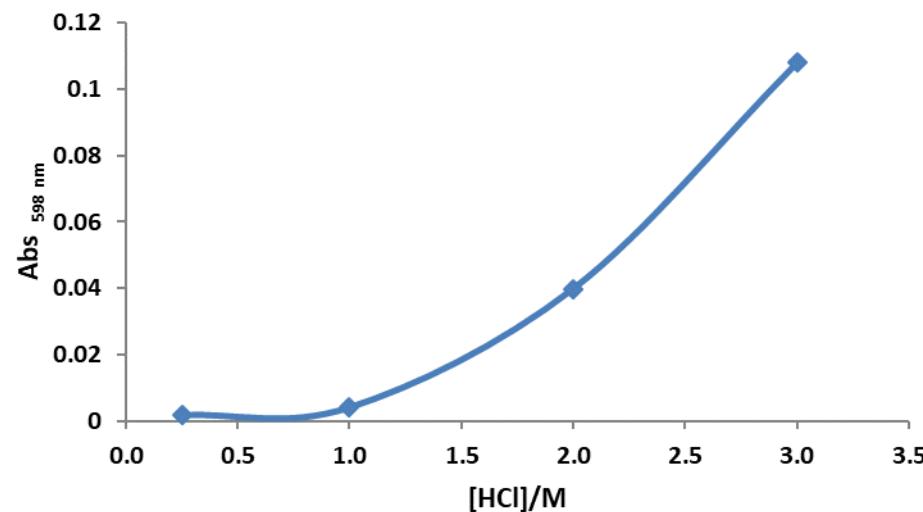
<sup>‡</sup>Department of Chemical Sciences, University of Naples Federico II, I-80126, Naples, Italy

## Supporting Information

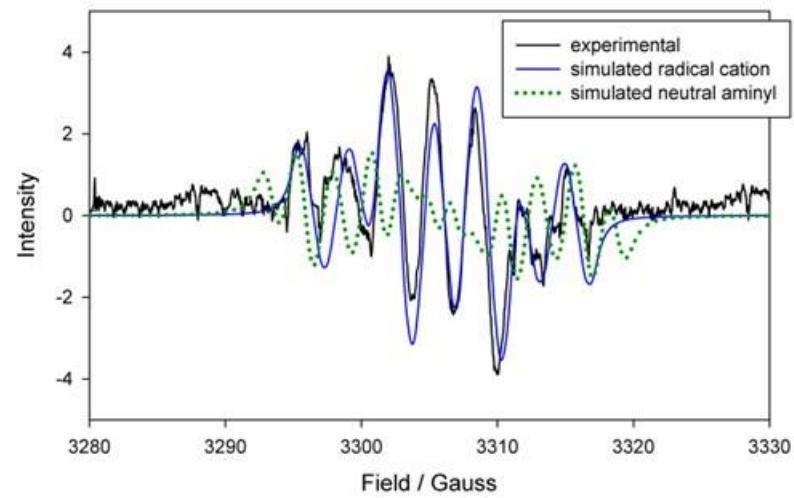
Content	Page
<b>Figure S1.</b> UV-vis analysis of the oxidation of dimer <b>2</b> with peroxides and hydroperoxides.	S2
<b>Figure S2.</b> Development of the chromophore of dimers <b>3</b> at 598 nm from <b>2</b> .	S3
<b>Figure S3.</b> EPR spectrum of a solution of <b>1</b> in acidic MeOH and simulated spectra.	S4
<b>Figure S4.</b> Control experiment of oxygen evolution from H <sub>2</sub> O <sub>2</sub> in MeOH 3 M H <sub>2</sub> SO <sub>4</sub> at 303 K.	S5
<b>Figure S5.</b> Oxygen uptake measured by incubating 6.5 $\mu$ moles of monomer <b>1</b> in 4 mL MeOH 3 M H <sub>2</sub> SO <sub>4</sub> .	S6
<b>Figure S6.</b> UV-vis absorption spectra of substituted anilines in 3:1 methanol/36%HCl.	S7
<b>Figure S7.</b> Computed free energy diagram for reagents, products and putative intermediates in the reaction pathway leading from <b>2</b> to <b>3</b> (reaction path a: see text), under different pH conditions.	S9
<b>Figure S8.</b> Computed free energy diagram for reagents, products and putative intermediates in the reaction pathway leading from <b>2</b> to <b>3</b> (reaction path b: see text) under different pH conditions.	S10
<b>Table S1.</b> EPR parameters computed for the predominant forms of <i>N</i> -monoprotonated <i>C</i> -radicals from single-bond dimers in MeOH.	S11
<b>Table S2.</b> EPR parameters computed for the predominant forms of <i>N,N'</i> -diprotonated <i>C</i> -radicals from single-bond dimers in MeOH.	S15
<b>Table S3.</b> Calculations on neutral forms in vacuo.	S19
<b>Table S4.</b> Calculations on neutral forms in methanol.	S57
<b>Table S5.</b> Calculations on monoprotonated forms in methanol.	S95
<b>Table S6.</b> Calculations on diprotonated forms in methanol.	S157
<b>Table S7.</b> p <i>K</i> <sub>a</sub> values computed in methanol at different theory levels for all bibenzothiazine derivatives examined.	S191
<b>Table S8.</b> p <i>K</i> <sub>a</sub> values computed in methanol at different theory levels for some reference nitrogen bases and corresponding experimental values.	S192



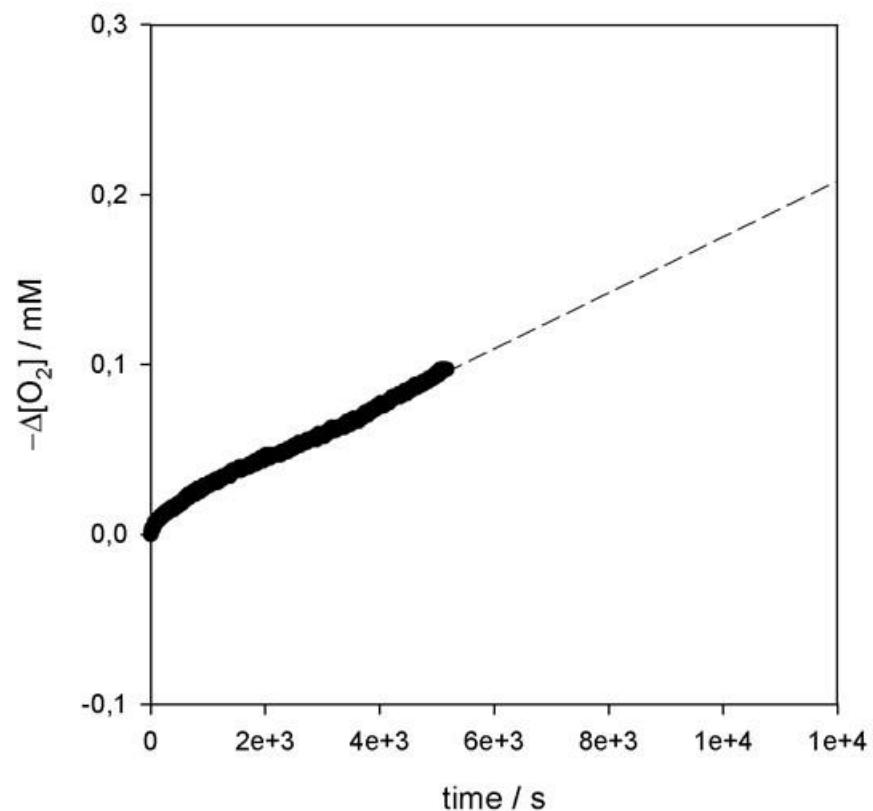
**Figure S1.** UV-vis analysis of the oxidation of dimer **2** at 50  $\mu\text{M}$  in MeOH:36% HCl 3:1 with hydrogen peroxide (0.4 equiv.), m-chloroperbenzoic acid ( $\text{m-ClC}_6\text{H}_4\text{COOOH}$ ) (0.8 equiv.) and sodium persulfate/Fe(II) (1.5 equiv) at 5 min reaction time.



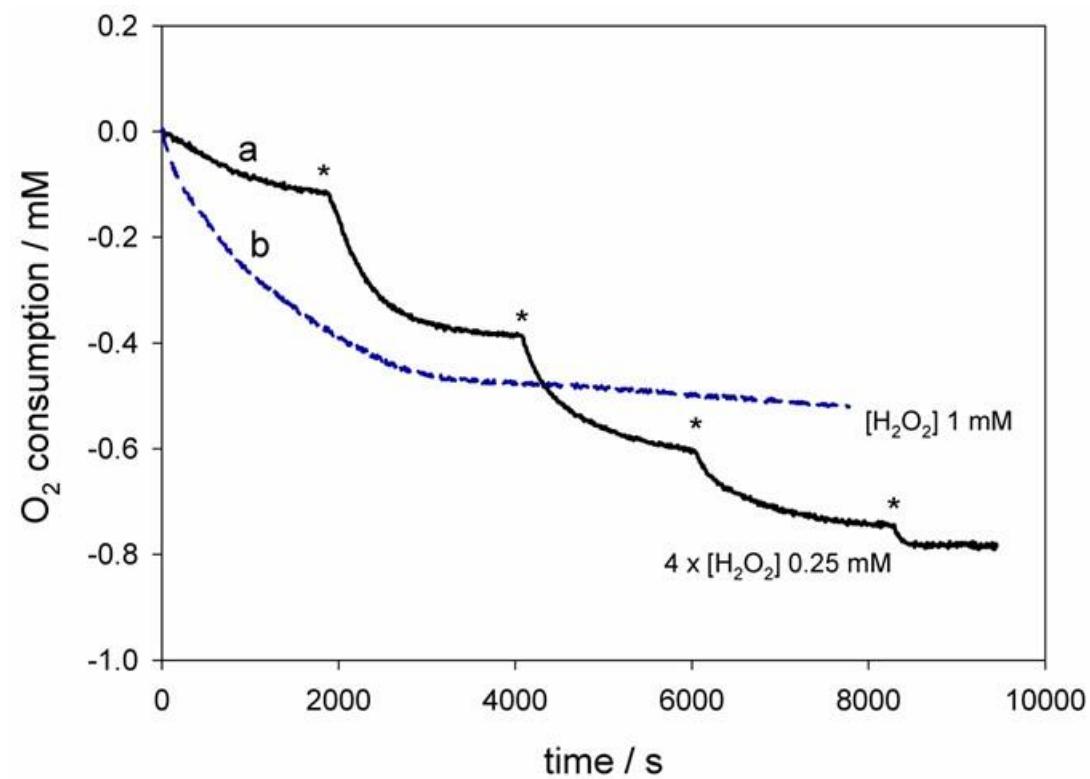
**Figure S2.** Development of the chromophore of dimers **3** at 598 nm from **2** (50  $\mu$ M) in methanol / HCl 3:1 at different final HCl concentrations in the presence of  $\text{H}_2\text{O}_2$  (500  $\mu$ M) at 30 min.



**Figure S3.** EPR spectrum of a solution of **1** in acidic MeOH and simulated spectra of the neutral and protonated free radical **1<sup>·</sup>**.

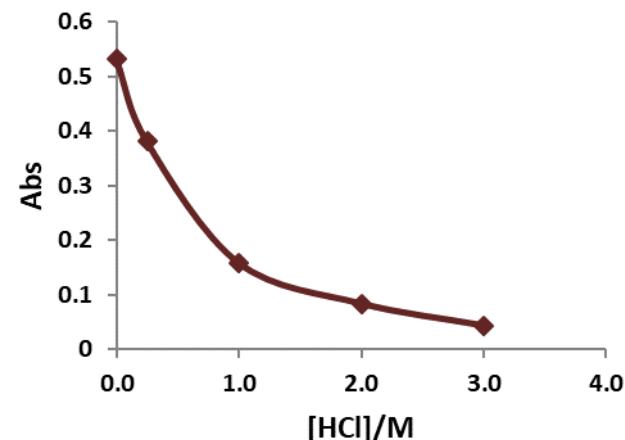
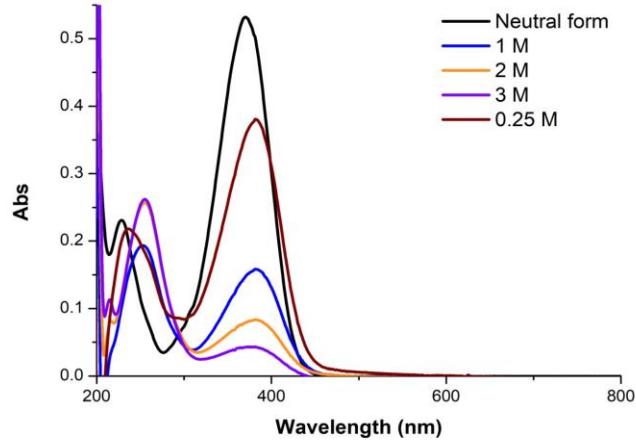


**Figure S4.** Oxygen evolution measured by adding 10 µmoles of H<sub>2</sub>O<sub>2</sub> in 4 mL MeOH 3 M H<sub>2</sub>SO<sub>4</sub> at 303 K in the absence of monomer **1** or dimer **2**.

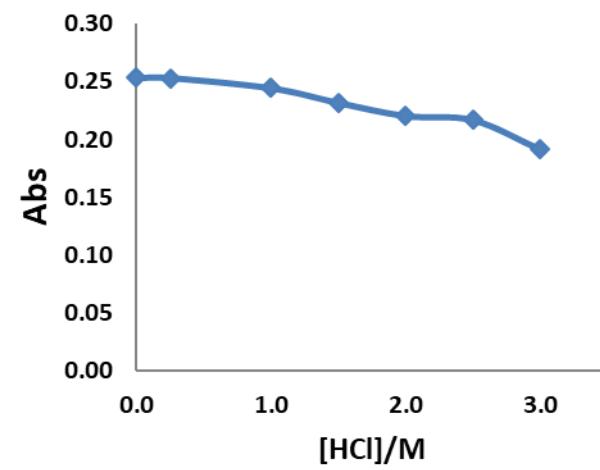
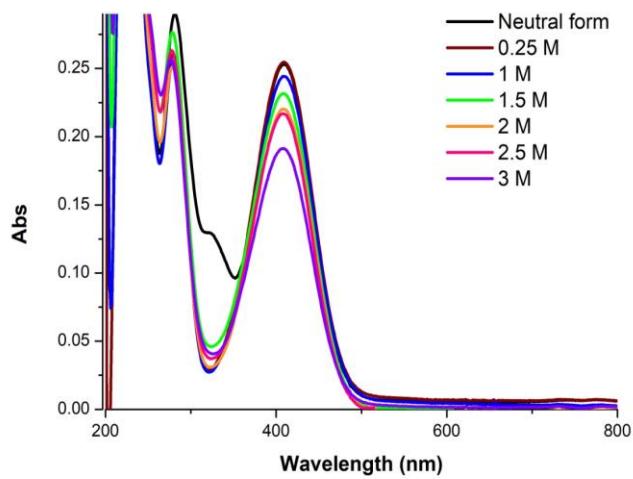


**Figure S5.** Oxygen uptake measured by incubating 6.5  $\mu$ moles of monomer **1** in 4 mL MeOH 3 M H<sub>2</sub>SO<sub>4</sub> (final conc. 1.6 mM) at 303 K with (a) addition of aliquots of 1  $\mu$ mole H<sub>2</sub>O<sub>2</sub> to the system at time points indicated by an asterisk, or (b) by single addition of 4 molar equivalents of H<sub>2</sub>O<sub>2</sub> (1 mM).

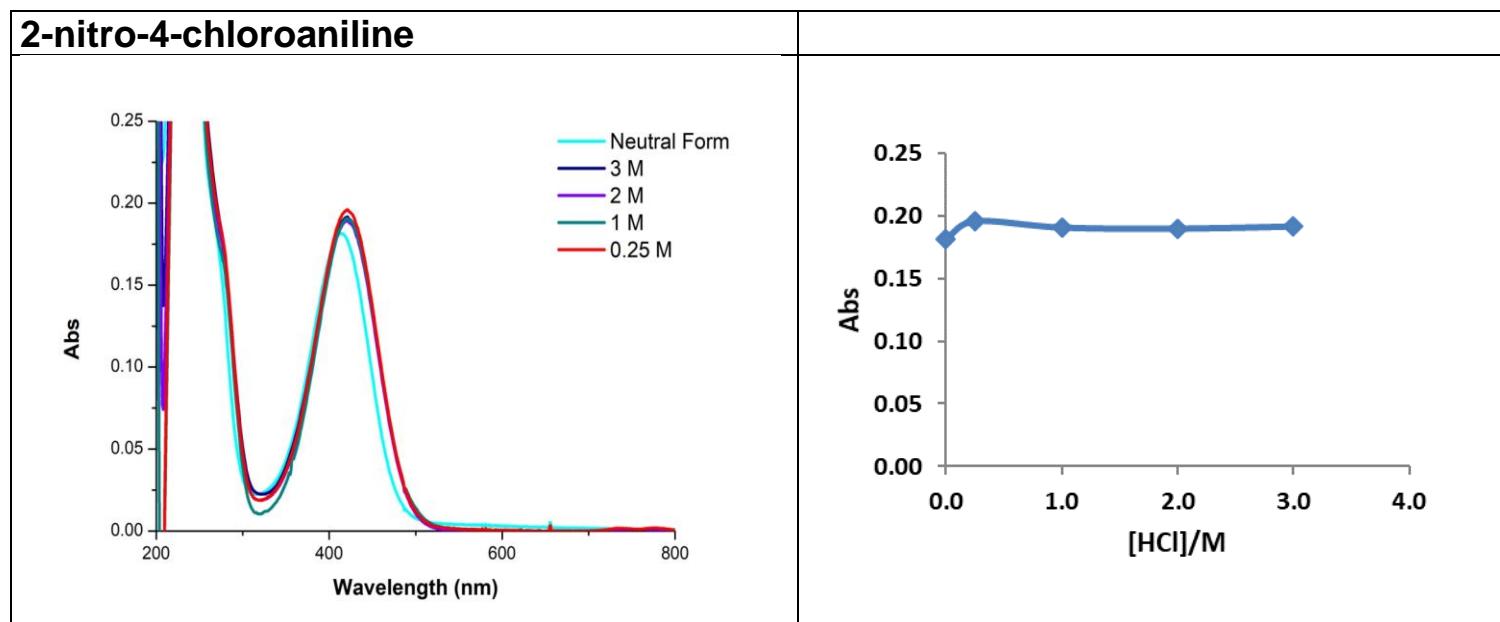
### 4-nitroaniline



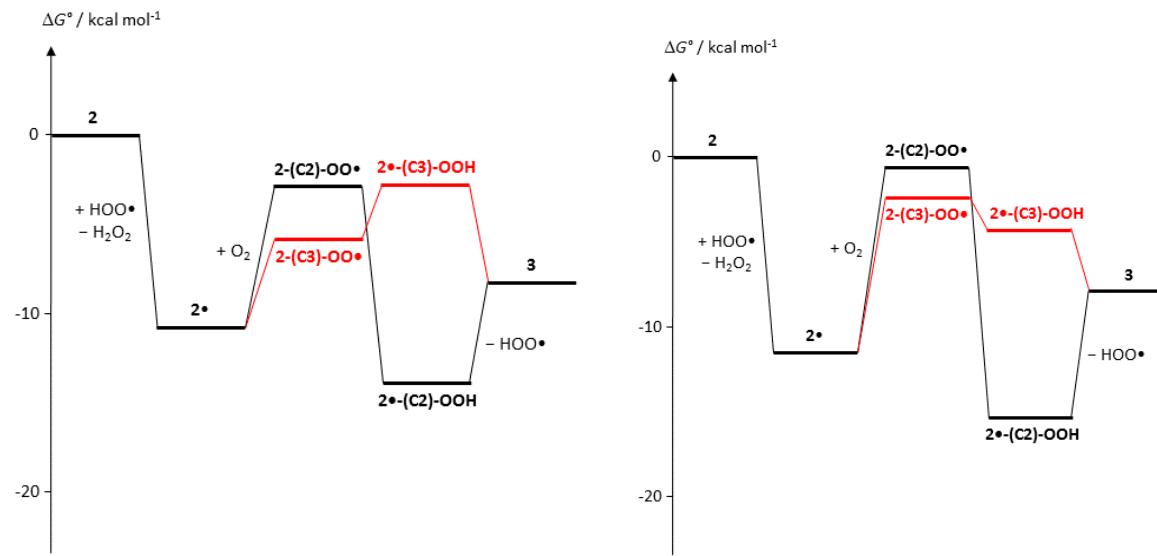
### 2-nitroaniline



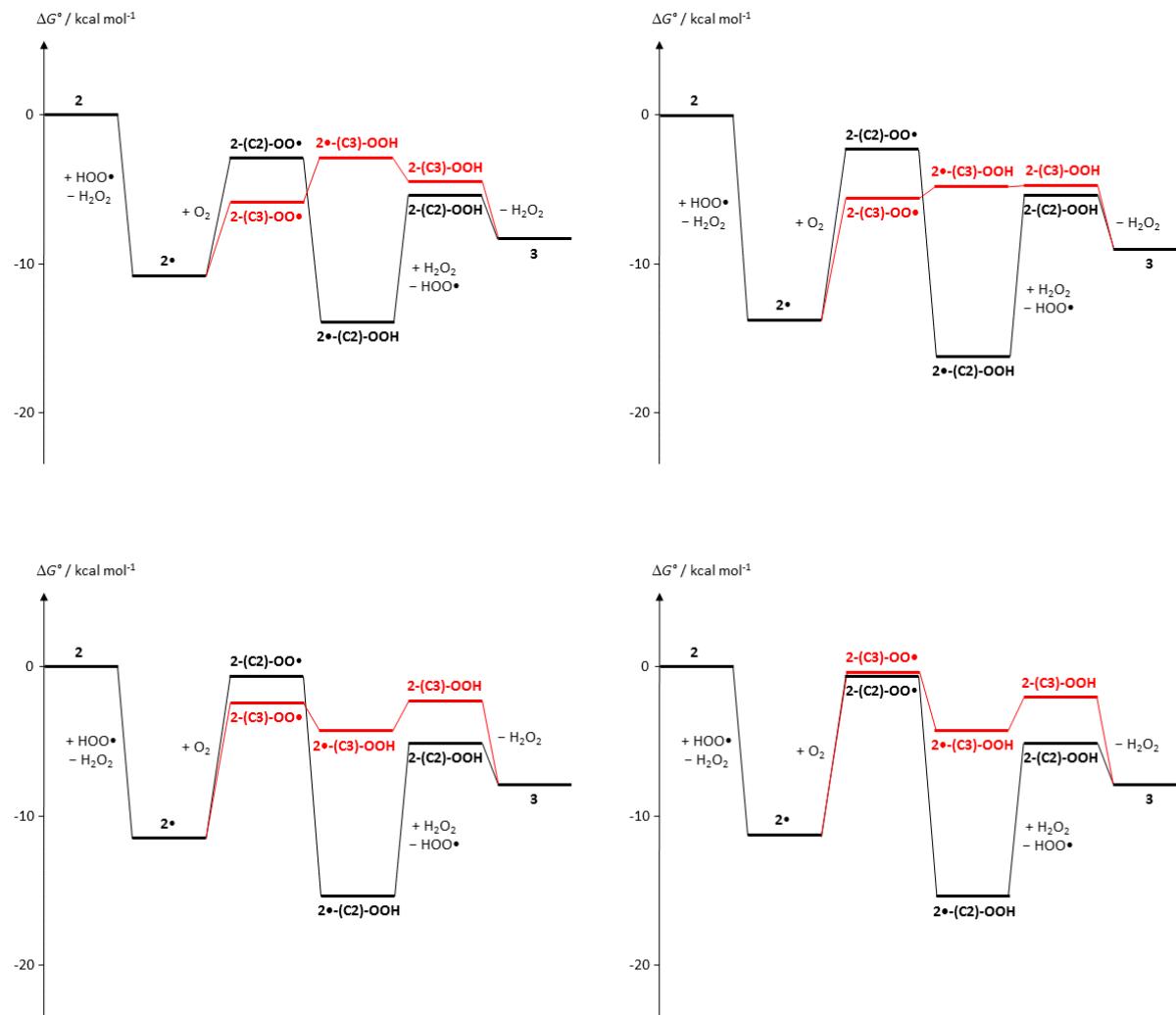
## 2-nitro-4-chloroaniline



**Figure S6.** Left: Absorption spectra of substituted anilines in 3:1 methanol/HCl at the concentrations shown. Right: Absorbance at maximum vs HCl concentration. Choice of anilines was based on their  $pK_a$ s in methanol as reported by Rived, F.; Roses, M.; Bosch, E. *Anal. Chim. Acta* **1998**, 374, 309-324.

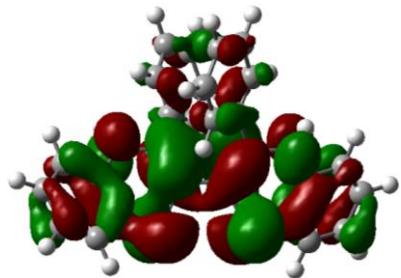
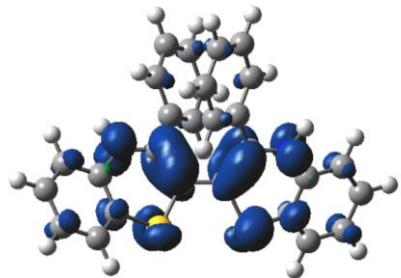


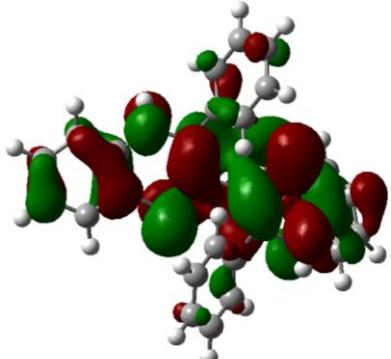
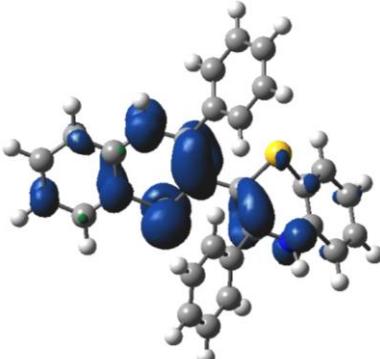
**Figure S7.** Computed free energy diagram for reagents, products and putative intermediates in the reaction pathway leading from **2** to **3** (reaction path a: see text), under different pH conditions. Left panel, pH 6.0; right panel, pH 0.0. The graphs at pH 3.0 and -1.5 are shown in the main text.

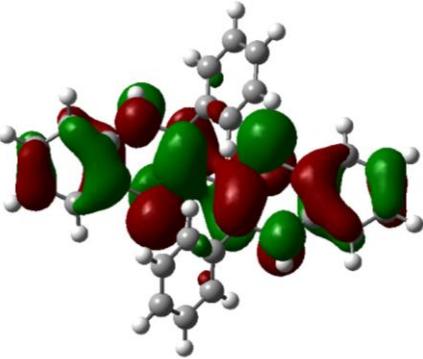
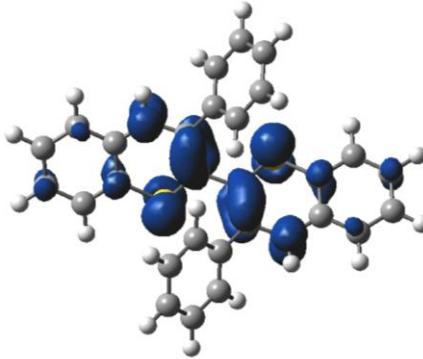


**Figure S8.** Computed free energy diagram for reagents, products and putative intermediates in the reaction pathway leading from **2** to **3** (reaction path b: see text) under different pH conditions. Top left panel, pH 6.0; top right panel, pH 3.0; bottom left panel, pH 0.0; bottom right panel, pH -1.5.

**Table S1.** EPR parameters computed for the predominant forms of *N*-monoprotonated *C*-radicals from single-bond dimers in MeOH.

SOMO <sup>a</sup>	Spin density <sup>b</sup>	Statistical weight	<i>hcc</i> / Gauss <sup>c</sup> B3LYP/EPR-II	<i>hcc</i> / Gauss <sup>c</sup> B3LYP/EPR-III
		0.36	S1 5.17 C2 0.25 C3 4.33 N4 1.87 C5 1.46 C6 -0.91 C7 1.51 C8 0.76 C8a 4.67 C4a -2.04 C-Ph, <i>ipso</i> -1.67 C-Ph, <i>ortho</i> 0.69 C-Ph, <i>meta</i> -0.62 C-Ph, <i>para</i> 0.67 C-Ph, <i>meta</i> -0.45 C-Ph, <i>ortho</i> 0.96 H5 -0.76 H6 0.31 H7 -0.76 H8 0.33 H-Ph, <i>ortho</i> -0.21 H-Ph, <i>para</i> -0.57 H-Ph, <i>meta</i> 0.35 H-Ph, <i>ortho</i> -0.48 H-Ph, <i>ortho</i> -0.49 S1' 5.52 C2' 0.21 C3' 4.45 C3' 4.33 N4' 1.88 C5' 1.46 C6' -0.91 C7' 1.51 C8' 0.76 C8a' 4.67 C4a' -2.04 C-Ph', <i>ipso</i> -1.67 C-Ph', <i>ortho</i> 0.69 C-Ph', <i>meta</i> -0.57	S1 5.52 C2 0.21 C3 4.45 N4 1.88 C5 1.39 C6 -0.83 C7 1.45 C8 0.87 C8a 4.52 C4a -1.85 C-Ph, <i>ipso</i> -1.56 C-Ph, <i>ortho</i> 0.66 C-Ph, <i>meta</i> -0.57 C-Ph, <i>para</i> 0.64 C-Ph, <i>meta</i> -0.43 C-Ph, <i>ortho</i> 0.96 H5 -0.72 H6 0.30 H7 -0.73 H8 0.32 H-Ph, <i>para</i> -0.56 H-Ph, <i>meta</i> 0.35 H-Ph, <i>ortho</i> -0.48 S1' 5.52 C2' 0.21 C3' 4.45 N4' 1.88 C5' 1.39 C6' -0.83 C7' 1.45 C8' 0.87 C8a' 4.52 C4a' -1.85 C-Ph', <i>ipso</i> -1.56 C-Ph', <i>ortho</i> 0.66 C-Ph', <i>meta</i> -0.57

			C-Ph', <i>meta</i> -0.62 C-Ph', <i>para</i> 0.67 C-Ph', <i>meta</i> -0.45 C-Ph', <i>ortho</i> 0.96 H5' -0.76 H6' 0.31 H7' -0.76 H8' 0.33 H-Ph', <i>ortho</i> -0.21 H-Ph', <i>para</i> -0.57 H-Ph', <i>meta</i> 0.35 H-Ph', <i>ortho</i> -0.49 H4' -3.83 H4 -3.83	C-Ph', <i>para</i> 0.64 C-Ph', <i>meta</i> -0.43 C-Ph', <i>ortho</i> 0.96 H5' -0.72 H6' 0.30 H7' -0.73 H8' 0.32 H-Ph', <i>para</i> -0.56 H-Ph', <i>meta</i> 0.35 H-Ph', <i>ortho</i> -0.48 H4' -3.75 H4 -3.75
	 	0.30	S1 3.87 C2 2.70 C3 -1.90 N4 3.60 C5 0.88 C6 -0.93 C7 1.55 C8 -1.94 C8a 1.26 C4a -2.63 C-Ph, <i>ipso</i> -1.57 C-Ph, <i>ortho</i> 0.70 C-Ph, <i>meta</i> -0.41 C-Ph, <i>para</i> 0.35 C-Ph, <i>ortho</i> 1.46 H5 -0.95 H7 -1.51 H8 0.32 H-Ph, <i>ortho</i> -0.21 H-Ph, <i>meta</i> 0.23 H-Ph, <i>para</i> -0.26 H-Ph, <i>meta</i> 0.21 H-Ph, <i>ortho</i> -0.21 S1' 2.70 C2' 2.49 C2' -1.79 C3' 2.85 N4' 1.12	S1 2.79 C2 2.61 C3 -1.64 N4 3.64 C5 0.81 C6 -0.81 C7 1.42 C8 -1.77 C8a 1.13 C4a -2.38 C-Ph, <i>ipso</i> -1.51 C-Ph, <i>ortho</i> 0.71 C-Ph, <i>meta</i> -0.40 C-Ph, <i>para</i> 0.34 C-Ph, <i>ortho</i> 1.48 H5 -0.90 H7 -1.48 H8 0.30 H-Ph, <i>meta</i> 0.24 H-Ph, <i>para</i> -0.26 H-Ph, <i>meta</i> 0.21 H-Ph, <i>ortho</i> -0.21 S1' 2.70 C2' -1.82 C3' 2.86 N4' 1.12

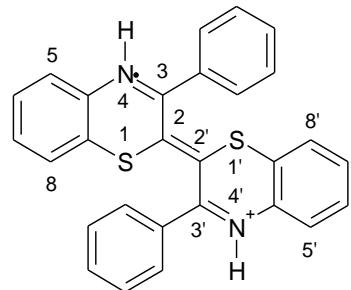
			N4' 1.15 C5' 1.09 C6' -0.51 C7' 0.83 C8' 0.27 C8a' 2.56 C4a' -0.49 C-Ph', <i>ortho</i> 0.49 C-Ph', <i>ortho</i> 0.46 H5' -0.47 H6' 0.23 H7' -0.43 H-Ph', <i>meta</i> 0.21 H4' -2.14 H4 -6.19	C5' 1.00 C6' -0.44 C7' 0.76 C8' 0.30 C8a' 2.38 C4a' -0.38 C-Ph', <i>ortho</i> 0.49 C-Ph', <i>ortho</i> 0.45 H5' -0.44 H6' 0.22 H7' -0.40 H-Ph', <i>meta</i> 0.21 H4' -2.03 H4 -6.11
		0.34	S1 2.42 C3 -0.81 N4 2.47 C5 0.76 C6 -0.67 C7 0.98 C8 -1.30 C8a 0.43 C4a -1.33 C-Ph, <i>ipso</i> -1.19 C-Ph, <i>ortho</i> 0.83 H5 -0.67 H7 -0.99 S1' 2.42 C3' -0.81 N4' 2.47 C5' 0.76 C6' -0.67 C7' 0.98 C8' -1.30 C8a' 0.43 C4a' -1.33 C-Ph, <i>ipso</i> -1.19 C-Ph, <i>ortho</i> 0.83 H5' -0.67	S1 1.59 C3 -0.62 N4 2.47 C5 0.70 C6 -0.59 C7 0.89 C8 -1.18 C8a 0.35 C4a -1.14 C-Ph, <i>ipso</i> -1.14 C-Ph, <i>ortho</i> 0.22 C-Ph, <i>ortho</i> 0.84 H5 -0.63 H7 -0.96 S1' 1.59 C3' -0.62 N4' 2.47 C5' 0.70 C6' -0.59 C7' 0.89 C8' -1.18 C8a' 0.35 C4a' -1.14 C-Ph, <i>ipso</i> -1.14 C-Ph, <i>ortho</i> 0.84

			H7' -0.99 H4' -4.19 H4 -4.19	C-Ph', <i>ortho</i> 0.22 H5' -0.63 H7' -0.96 H4' -4.10 H4 -4.10
--	--	--	------------------------------------	---

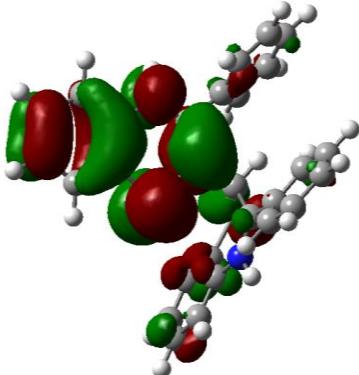
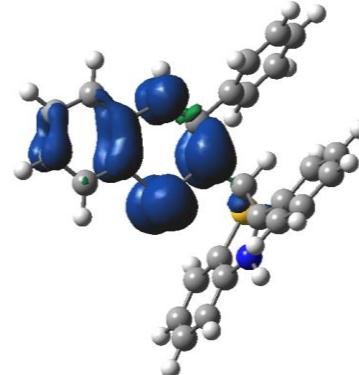
[a] Isovalue 0.02 a.u.

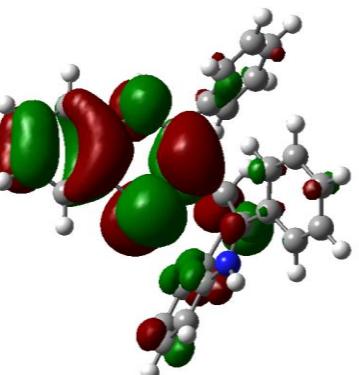
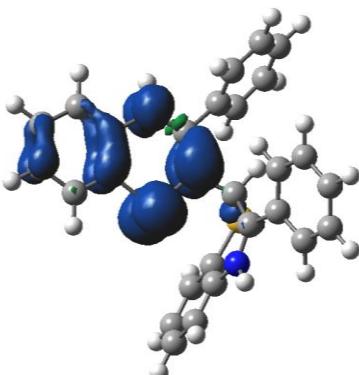
[b] Isodensity 0.002 a.u.

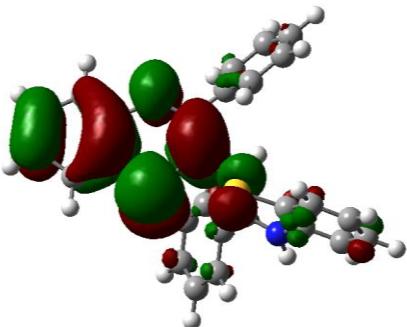
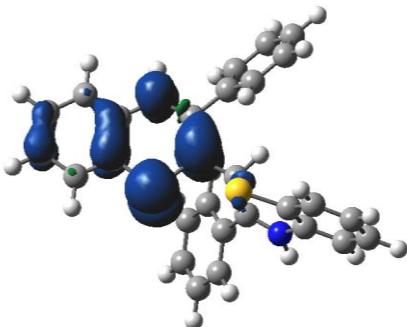
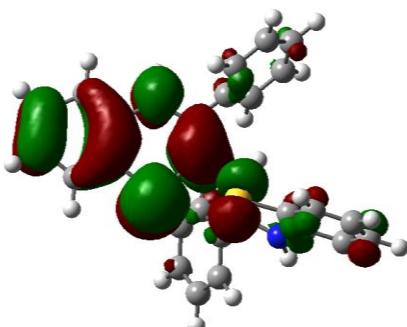
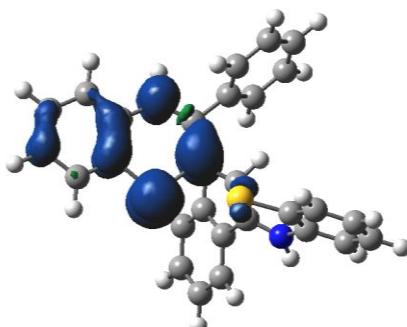
[c] Isotopes:  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{14}\text{N}$ ,  $^{33}\text{S}$ . Only couplings whose absolute value exceeds 0.2 Gauss are listed. The numbering system is shown in the following scheme:



**Table S2.** EPR parameters computed for the predominant forms of *N,N'*-diprotonated *C*-radicals from single-bond dimers in MeOH.

SOMO <sup>a</sup>	Spin density <sup>b</sup>	Statistical weight	<i>hcc</i> / Gauss <sup>c</sup> B3LYP/EPR-II	<i>hcc</i> / Gauss <sup>c</sup> B3LYP/EPR-III
		0.54	S1 6.41 C2 7.78 C3 -5.54 N4 4.11 C5 -0.41 C7 1.46 C8 -2.13 C8a 1.32 C4a -2.73 C-Ph <i>ortho</i> 0.34 C-Ph <i>ortho</i> -0.29 H4 -6.99 H5 -0.65 H6 -0.81 H7 -1.74 S1' 1.36 C2' -4.17 C3' 2.41 C5' -0.26 C6' 0.30 C7' -0.30 C8' 0.46 C8a' -0.29 C4a' 0.32 C-Ph', <i>ipso</i> -0.29 C-Ph', <i>ortho</i> 0.22 H2' 0.57 H4' 0.51 H6' -0.22 H8' -0.27	S1 4.99 C2 7.31 C3 -5.04 N4 4.10 C5 -0.42 C7 1.30 C8 -1.88 C8a 1.20 C4a -2.47 C-Ph <i>ipso</i> -0.23 C-Ph <i>ortho</i> 0.41 C-Ph <i>ortho</i> -0.22 H4 -6.83 H5 -0.59 H6 -0.85 H7 -1.67 S1' 1.14 C2' -3.86 C3' 2.31 C5' -0.26 C6' 0.29 C7' -0.28 C8' 0.43 C8a' -0.26 C4a' 0.31 C-Ph', <i>ipso</i> -0.27 C-Ph', <i>ortho</i> 0.21 H2' 0.54 H4' 0.51 H6' -0.23 H8' -0.27

		0.43	S1 6.38 C2 7.40 C3 -5.34 N4 4.09 C5 -0.39 C7 1.46 C8 -2.14 C8a 1.27 C4a -2.74 C-Ph <i>ipso</i> -0.25 C-Ph <i>ortho</i> 0.32 C-Ph <i>ortho</i> -0.27 H4 -7.00 H5 -0.66 H6 -0.81 H7 -1.74 S1' 1.71 C2' -4.18 C3' 1.61 C5' -0.32 C6' 0.32 C7' -0.31 C8' 0.46 C8a' -0.35 C4a' 0.41 C-Ph', <i>ipso</i> -0.26 C-Ph', <i>ortho</i> 0.47 C-Ph', <i>para</i> 0.21 H2' 1.10 H4' 0.59 H6' -0.22 H8' -0.26	S1 5.00 C2 6.97 C3 -4.85 N4 4.09 C5 -0.40 C7 1.30 C8 -1.89 C8a 1.15 C4a -2.49 C-Ph <i>ipso</i> -0.29 C-Ph <i>ortho</i> 0.39 H4 -6.85 H5 -0.60 H6 -0.84 H7 -1.67 S1' 1.44 C2' -3.88 C3' 1.54 C5' -0.31 C6' 0.31 C7' -0.29 C8' 0.44 C8a' -0.32 C4a' 0.39 C-Ph', <i>ipso</i> -0.23 C-Ph', <i>ortho</i> 0.47 H4' 0.58 H2' 1.06 H6' -0.22 H8' -0.26
---	--	------	---	---

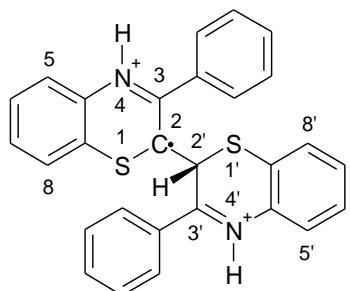
		0.02	S1 6.53 C2 6.75 C3 -5.39 N4 4.09 C5 -0.47 C7 1.46 C8 -2.10 C8a 1.31 C4a -2.66 C-Ph <i>ortho</i> -0.30 C-Ph <i>ortho</i> 0.31 H4 -7.01 H5 -0.62 H6 -0.85 H7 -1.76 S1' 0.79 C2' -3.95 C3' 2.19 C8' 0.37 C8a' -0.56 C-Ph', <i>ortho</i> 0.60 C-Ph', <i>para</i> 0.21 C-Ph', <i>ortho</i> 0.22 H2' 0.84 H4' 0.64	S1 4.88 C2 6.31 C3 -4.86 N4 4.09 C5 -0.46 C7 1.32 C8 -1.86 C8a 1.19 C4a -2.42 C-Ph <i>ortho</i> -0.23 C-Ph <i>ortho</i> 0.38 H4 -6.85 H5 -0.58 H6 -0.88 H7 -1.69 S1' 0.37 C2' -3.68 C3' 2.05 C8' 0.35 C8a' -0.55 C-Ph', <i>ortho</i> 0.59 C-Ph', <i>para</i> 0.21 C-Ph', <i>ortho</i> 0.22 H2' 0.83 H4' 0.64
		0.01	S1 6.53 C2 6.83 C3 -5.57 N4 4.06 C5 -0.47 C7 1.48 C8 -2.19 C8a 1.22 C4a -2.66 C-Ph <i>ortho</i> -0.37 C-Ph <i>ortho</i> 0.28 H4 -7.00 H5 -0.63 H6 -0.85 H7 -1.78	S1 4.95 C2 6.38 C3 -5.05 N4 4.05 C5 -0.47 C7 1.33 C8 -1.95 C8a 1.10 C4a -2.41 C-Ph <i>ipso</i> -0.24 C-Ph <i>ortho</i> -0.30 C-Ph <i>ortho</i> 0.35 H4 -6.84 H5 -0.58 H6 -0.88

		H8 0.21	H7 -1.71
		S1' 0.64	C2' -2.85
		C2' -3.09	C3' 1.88
		C3' 2.00	C5' -0.21
		C5' -0.21	C6' 0.25
		C6' 0.25	C7' -0.24
		C7' -0.24	C8' 0.36
		C8' 0.38	C8a' -0.70
		C8a' -0.71	C4a' 0.27
		C4a' 0.27	C-Ph', <i>ortho</i> 0.43
		C-Ph', <i>ortho</i> 0.46	H2' 0.44
		H2' 0.47	H4' 0.59
		H4' 0.60	

[a] Isovalue 0.02 a.u.

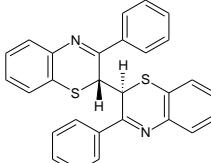
[b] Isodensity 0.002 a.u.

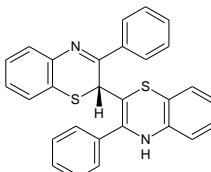
[c] Isotopes:  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{14}\text{N}$ ,  $^{33}\text{S}$ . Only couplings whose absolute value exceeds 0.2 Gauss are listed. The numbering system is shown in the following scheme:

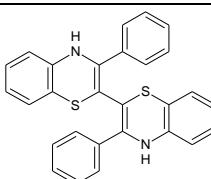


**Table S3.** Neutral forms in vacuo. For each chemical species, values are reported for the most stable conformer / geometric isomer identified.  $G_{RRHO,calc}$  [M062X / 6-311++G(2d,2p)] =  $E_{el}$  [M062X / 6-311++G(2d,2p) // PBE0 / 6-31+G(d,p)] -  $E_{el}$  [PBE0 / 6-31+G(d,p)] +  $G_{RRHO}$  [PBE0 / 6-31+G(d,p)]; and likewise for  $G_{RRHO,calc}$  [M062X / 6-31+G(d,p)]. In this and in the following tables,  $G$  values are referred to a 1 atm standard state; however, they were converted to a 1 M standard state in order to compute the reaction free energies discussed in the paper (see e.g. Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*, 2nd edition, John Wiley & Sons, Chichester, 2004, pp 378-379).

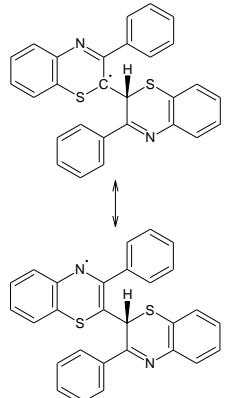
Species	PBE0 / 6-31+G(d,p)			M062X / 6-31+G(d,p)		M062X / 6-311++G(2d,2p)		
	$E_{el}$ / Ha	$H_{RRHO}$ / Ha	$G_{RRHO}$ / Ha	$E_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$E_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$\Delta G_{RRHO,calc}$ / kcal mol <sup>-1</sup>
Cartesian coordinates / Å								
Single-bond dimer								
S -1.00031 -2.46028 1.24651 C -0.10319 -0.97711 0.71763 C -0.80252 0.23685 1.30911 N -2.07630 0.40335 1.22142 C -4.19650 -0.18781 0.28865 C -5.13026 -1.12711 -0.12414 C -4.80999 -2.48689 -0.09351 C -3.54723 -2.89635 0.31990 C -2.59379 -1.95261 0.71077 C -2.91690 -0.57776 0.71628 C -0.00880 1.30619 1.95755 C -0.59399 2.57071 2.13524 C 0.10810 3.59810 2.74886 C 1.40889 3.38449 3.20787 C 1.99907 2.13502 3.04208 C 1.30022 1.10602 2.41606 H 0.89390 -1.09589 1.14423 H -4.43314 0.87212 0.31034 H -6.11371 -0.80523 -0.45354 H -5.54141 -3.22879 -0.40015 H -3.28692 -3.95129 0.32490 H -1.60597 2.72380 1.77603 H -0.35824 4.57200 2.86814 H 1.95799 4.18824 3.69027 H 3.00899 1.95545 3.39941 H 1.79088 0.14413 2.30793 S 0.89007 -2.29413 -1.55185 C 0.04076 -0.86660 -0.82290 C 0.80768 0.37981 -1.24277 N 2.08276 0.47322 -1.08572	-1983.28470	-1982.85166	-1982.93600	-1984.41474	-1984.06604	-1984.76490	-1984.41619	1.1

C 4.12949 -0.33778 -0.15019 C 5.00671 -1.36905 0.15161 C 4.63928 -2.69373 -0.10147 C 3.38228 -2.98089 -0.62153 C 2.48309 -1.94775 -0.89902 C 2.85885 -0.60279 -0.68618 C 0.09495 1.53755 -1.83178 C 0.84521 2.63946 -2.27646 C 0.22178 3.74425 -2.83744 C -1.16788 3.77610 -2.97020 C -1.92320 2.69229 -2.53340 C -1.29899 1.58212 -1.96931 H -0.95166 -0.88687 -1.27626 H 4.40384 0.70176 0.00369 H 5.98462 -1.14434 0.56707 H 5.32824 -3.50445 0.11649 H 3.08291 -4.01068 -0.79661 H 1.92392 2.60199 -2.16888 H 0.82025 4.58535 -3.17609 H -1.65605 4.64015 -3.41224 H -3.00514 2.70555 -2.62905 H -1.92341 0.76338 -1.62805								
 S 0.97930 -0.84050 -1.81970 C -0.29150 -0.38777 -0.60122 C -0.99478 -1.66771 -0.17601 N -0.32942 -2.69391 0.22759 C 1.72257 -3.72171 0.90883 C 3.07836 -3.96049 0.74071 C 3.79024 -3.27461 -0.24813 C 3.14999 -2.32358 -1.03375 C 1.79178 -2.05440 -0.84480 C 1.05021 -2.77602 0.11711 C -2.47275 -1.76654 -0.20009 C -3.08309 -2.91637 0.32966 C -4.46257 -3.06001 0.31659 C -5.26900 -2.06229 -0.23522 C -4.67814 -0.92081 -0.76753 C -3.29314 -0.77124 -0.74757 H -0.96247 0.27143 -1.15333 H 1.13963 -4.27119 1.64214 H 3.57977 -4.69513 1.36380 H 4.84716 -3.47349 -0.39976 H 3.70559 -1.76500 -1.78193	-1983.28475	-1982.85171	-1982.93580	-1984.41618	-1984.06723	-1984.76686	-1984.41791	0.0

H -2.44632 -3.68741 0.74977 H -4.91405 -3.95467 0.73620 H -6.34927 -2.17663 -0.24929 H -5.29259 -0.13674 -1.20052 H -2.87279 0.13704 -1.16533 S -0.97930 0.84050 1.81970 C 0.29150 0.38777 0.60122 C 0.99478 1.66771 0.17601 N 0.32942 2.69391 -0.22759 C -1.72257 3.72171 -0.90883 C -3.07836 3.96049 -0.74071 C -3.79024 3.27461 0.24813 C -3.14999 2.32358 1.03375 C -1.79178 2.05440 0.84480 C -1.05021 2.77602 -0.11711 C 2.47275 1.76654 0.20009 C 3.08309 2.91637 -0.32966 C 4.46257 3.06001 -0.31659 C 5.26900 2.06229 0.23522 C 4.67814 0.92081 0.76753 C 3.29314 0.77124 0.74757 H 0.96247 -0.27143 1.15333 H -1.13963 4.27119 -1.64214 H -3.57977 4.69513 -1.36380 H -4.84716 3.47349 0.39976 H -3.70559 1.76500 1.78193 H 2.44632 3.68741 -0.74977 H 4.91405 3.95467 -0.73620 H 6.34927 2.17663 0.24929 H 5.29259 0.13674 1.20052 H 2.87279 -0.13704 1.16533								
 S 1.62853 1.63209 -1.72647 C 0.46911 1.02214 -0.44100 C 1.16862 1.07328 0.91527 N 2.39692 0.75033 1.10706 C 4.42611 -0.30501 0.43460 C 5.37176 -0.64842 -0.52094 C 5.17321 -0.28852 -1.85591 C 4.01950 0.39191 -2.22947 C 3.05834 0.72289 -1.27189 C 3.25781 0.38596 0.08181 C 0.37750 1.49666 2.09772 C 1.03039 1.67220 3.32859	-1983.27699	-1982.84361	-1982.92760	-1984.40550	-1984.05610	-1984.75711	-1984.40772	6.4

C 0.32704 2.06989 4.45697 C -1.04817 2.29917 4.38509 C -1.70861 2.12476 3.17256 C -1.00351 1.72851 2.03844 H -0.30414 1.79267 -0.45408 H 4.56279 -0.55781 1.48178 H 6.26793 -1.18731 -0.22800 H 5.91283 -0.54523 -2.60873 H 3.85135 0.65832 -3.26940 H 2.09892 1.48993 3.37129 H 0.85257 2.20467 5.39833 H -1.59853 2.61174 5.26812 H -2.77912 2.29683 3.10384 H -1.55204 1.59020 1.11229 S 0.77951 -1.78109 -0.54999 C -0.18429 -0.29543 -0.74794 C -1.47375 -0.41509 -1.15100 N -2.07079 -1.67216 -1.26947 C -2.76389 -3.61792 0.02634 C -2.44187 -4.64738 0.90817 C -1.15168 -4.75472 1.42111 C -0.17542 -3.83663 1.03487 C -0.47877 -2.83810 0.11325 C -1.78212 -2.71329 -0.38081 C -2.37473 0.72162 -1.46021 C -3.62862 0.81863 -0.83776 C -4.49098 1.86787 -1.14199 C -4.11807 2.83059 -2.07936 C -2.88051 2.73599 -2.71260 C -2.01541 1.68750 -2.40925 H -3.77784 -3.51960 -0.35536 H -3.20867 -5.35757 1.20313 H -0.90175 -5.54840 2.11829 H 0.83471 -3.90566 1.42819 H -3.91476 0.08006 -0.09225 H -5.45306 1.93744 -0.64217 H -4.79177 3.64854 -2.31766 H -2.58922 3.47506 -3.45338 H -1.06207 1.59805 -2.92306 H -3.01351 -1.65951 -1.62883								
	-1983.27662	-1982.84278	-1982.92647	-1984.40714	-1984.05699	-1984.76031	-1984.41017	4.9

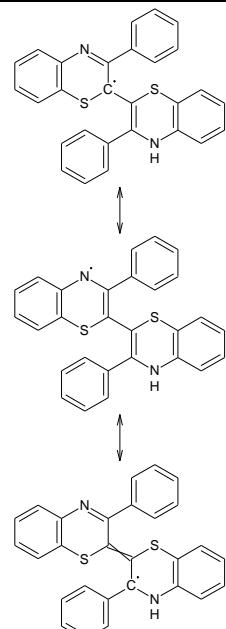
N -2.69468 -0.27251 -1.39516 C -4.56123 -1.29323 -0.20854 C -5.06618 -2.33516 0.56585 C -4.23367 -3.37595 0.97065 C -2.89484 -3.38058 0.57968 C -2.39709 -2.36969 -0.23992 C -3.22637 -1.30497 -0.61853 C -1.19810 1.63802 -1.40766 C -2.10409 2.53713 -0.82773 C -1.96100 3.90970 -1.01293 C -0.91165 4.40479 -1.78354 C -0.00545 3.51783 -2.36535 C -0.14774 2.14641 -2.18365 H -5.20529 -0.46728 -0.50245 H -6.11072 -2.32265 0.86303 H -4.62124 -4.18401 1.58343 H -2.23455 -4.18780 0.88436 H -2.90346 2.16141 -0.19325 H -2.66563 4.59226 -0.54600 H -0.80096 5.47511 -1.93325 H 0.81144 3.89494 -2.97423 H 0.55346 1.46103 -2.65035 S 2.21676 -0.86849 -1.67287 C 0.96485 -0.30855 -0.53289 C 1.31349 0.44074 0.53668 N 2.65499 0.78763 0.77789 C 4.83082 -0.15013 1.31949 C 5.86603 -1.03990 1.04411 C 5.76036 -1.93033 -0.02063 C 4.61597 -1.91585 -0.81699 C 3.59889 -0.99652 -0.57398 C 3.69388 -0.11358 0.50903 C 0.35635 0.97013 1.53438 C -0.59990 0.14077 2.13377 C -1.47207 0.64956 3.09102 C -1.39801 1.98966 3.47108 C -0.44644 2.82033 2.88413 C 0.42545 2.31533 1.92221 H 4.90506 0.52892 2.16614 H 6.74995 -1.04243 1.67503 H 6.55840 -2.63515 -0.23192 H 4.51408 -2.61033 -1.64617 H -0.64971 -0.90650 1.85168 H -2.20656 -0.00791 3.54781 H -2.07746 2.38282 4.22212 H -0.38701 3.86789 3.16613 H 1.13951 2.97954 1.44092 H 2.77666 1.27434 1.65501 H -3.35268 0.43108 -1.69456							
<b>Single-bond dimer, radical</b>							



S 0.81531 1.55945 -0.49776  
 C -0.29816 0.46535 0.27051  
 C -1.64585 0.81120 0.47341  
 N -2.25695 1.91317 0.04335  
 C -2.34973 4.02498 -1.02549  
 C -1.76603 5.09304 -1.68161  
 C -0.39273 5.08231 -1.95709  
 C 0.38143 3.99495 -1.57650  
 C -0.20808 2.91229 -0.91708  
 C -1.59021 2.90583 -0.62068  
 C -2.56351 -0.11994 1.19863  
 C -2.28781 -0.57410 2.49288  
 C -3.18908 -1.40397 3.15691  
 C -4.37264 -1.79313 2.53369  
 C -4.66050 -1.33364 1.24892  
 C -3.76711 -0.49456 0.58999  
 H -3.40974 4.00981 -0.79132  
 H -2.37306 5.94262 -1.98015  
 H 0.07103 5.91996 -2.46909  
 H 1.44677 3.97800 -1.79204  
 H -1.37796 -0.25348 2.99372  
 H -2.96686 -1.74057 4.16557  
 H -5.07242 -2.44394 3.05023  
 H -5.58752 -1.62339 0.76189  
 H -3.99593 -0.11011 -0.39971  
 S 1.27268 -0.86380 2.20445  
 C 0.28408 -0.86524 0.65524  
 C 1.09786 -1.54157 -0.44905  
 N 2.36088 -1.37692 -0.61997  
 C 4.40729 -0.21233 -0.24746  
 C 5.28995 0.48784 0.56242  
 C 4.94261 0.77258 1.88536  
 C 3.70622 0.37583 2.38214  
 C 2.80879 -0.31450 1.56373

-1982.65422 -1982.23431 -1982.31843 -1983.77875 -1983.44296 -1984.12973 -1983.79395 1.6

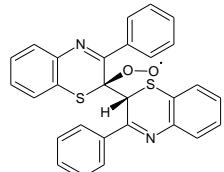
C 3.15769 -0.62840 0.23482							
C 0.37847 -2.41827 -1.40336							
C -1.01928 -2.52416 -1.42040							
C -1.65768 -3.35513 -2.33790							
C -0.91287 -4.09752 -3.24946							
C 0.47995 -4.00009 -3.24174							
C 1.11804 -3.16928 -2.33185							
H -0.54531 -1.52313 0.91714							
H 4.65844 -0.46320 -1.27375							
H 6.25222 0.80322 0.17027							
H 5.63192 1.31125 2.52900							
H 3.42416 0.61095 3.40480							
H -1.63269 -1.95457 -0.72923							
H -2.74196 -3.41988 -2.33557							
H -1.41195 -4.74910 -3.96121							
H 1.06963 -4.57745 -3.94833							
H 2.19931 -3.08318 -2.31664							



S -2.02152 -1.75477 -1.03426							
C -0.87950 -0.72579 -0.20480							
C -1.28497 0.13734 0.83058							
N -2.53795 0.34567 1.23117							
C -4.86966 -0.06272 1.27967							
C -6.00371 -0.74849 0.88393							
C -5.91045 -1.76767 -0.07181							
C -4.67808 -2.08196 -0.62932							

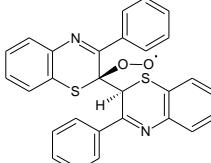
-1982.65389	-1982.23380	-1982.31803	-1983.78060	-1983.44474	-1984.13235	-1983.79650	0.0
-------------	-------------	-------------	-------------	-------------	-------------	-------------	-----

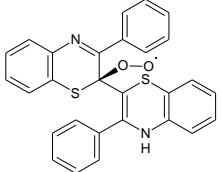
C -3.53339 -1.38219 -0.23866 C -3.60021 -0.35910 0.73623 C -0.27507 0.92668 1.59381 C 0.91433 0.35557 2.05983 C 1.81005 1.10840 2.81482 C 1.53073 2.44164 3.11171 C 0.34113 3.01297 2.66199 C -0.55909 2.25805 1.91652 H -4.91059 0.72059 2.03031 H -6.96648 -0.50019 1.32088 H -6.79627 -2.31455 -0.38040 H -4.59895 -2.86892 -1.37513 H 1.13261 -0.68710 1.84999 H 2.72435 0.64688 3.17773 H 2.23127 3.02822 3.70001 H 0.11042 4.04856 2.89697 H -1.49570 2.68916 1.57739 S 1.21124 -2.51779 -0.60589 C 0.47769 -0.87857 -0.72406 C 1.22184 0.12230 -1.25950 N 2.57414 -0.06679 -1.52617 C 4.72714 -0.54371 -0.49313 C 5.52238 -1.36633 0.30143 C 4.98130 -2.50329 0.89651 C 3.64202 -2.82591 0.67841 C 2.85750 -2.03669 -0.15937 C 3.39274 -0.87617 -0.73223 C 0.70313 1.47277 -1.56734 C -0.49084 1.63302 -2.28265 C -0.95392 2.90478 -2.60313 C -0.23091 4.03372 -2.21870 C 0.95828 3.88417 -1.50832 C 1.42406 2.61285 -1.18632 H 5.14228 0.35977 -0.93419 H 6.56398 -1.10626 0.46495 H 5.59538 -3.14022 1.52559 H 3.20634 -3.70996 1.13535 H -1.04472 0.75390 -2.59843 H -1.87801 3.01455 -3.16349 H -0.59369 5.02577 -2.47222 H 1.51914 4.75911 -1.19218 H 2.33048 2.50438 -0.59561 H 3.03228 0.71123 -1.97643							
<b>Single-bond dimer, C2-peroxy radical</b>							

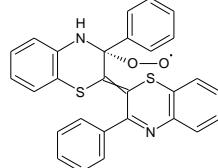


S 0.84900 -1.17925 -1.03435  
 C 0.21651 0.41704 -0.50428  
 C 1.29778 1.40208 -0.04408  
 N 2.54635 1.33177 -0.31885  
 C 4.49251 0.52500 -1.41256  
 C 5.18049 -0.42145 -2.15663  
 C 4.52604 -1.58539 -2.56756  
 C 3.19108 -1.79284 -2.24084  
 C 2.49945 -0.83561 -1.49481  
 C 3.14638 0.33320 -1.06878  
 C 0.87412 2.59208 0.74932  
 C 1.64600 2.96346 1.85732  
 C 1.31998 4.09095 2.60230  
 C 0.22399 4.87510 2.24437  
 C -0.53876 4.52545 1.13280  
 C -0.22072 3.39026 0.39024  
 H 4.96769 1.44148 -1.07611  
 H 6.22153 -0.25807 -2.41753  
 H 5.05513 -2.33351 -3.15063  
 H 2.68024 -2.69456 -2.56787  
 H 2.50194 2.35178 2.12411  
 H 1.92309 4.35845 3.46532  
 H -0.02971 5.75756 2.82475  
 H -1.37953 5.14414 0.83181  
 H -0.80273 3.15226 -0.49542  
 S -0.27547 -0.17781 2.20850  
 C -0.90441 0.21140 0.55181  
 C -1.99632 -0.77481 0.14204  
 N -1.98399 -2.02735 0.42592  
 C -0.94610 -4.03047 1.19364  
 C -0.06262 -4.71705 2.01513  
 C 0.75063 -4.00962 2.90226  
 C 0.69369 -2.62001 2.94526  
 C -0.18019 -1.92863 2.10602  
 C -1.02167 -2.63140 1.22402  
 C -3.14791 -0.27167 -0.64727  
 C -3.57959 1.06021 -0.59841  
 C -4.69056 1.47493 -1.32770  
 C -5.37893 0.57094 -2.13177  
 C -4.95487 -0.75696 -2.19322  
 C -3.85651 -1.17503 -1.45451  
 H -1.35682 1.19384 0.68854  
 H -1.60699 -4.55497 0.51007

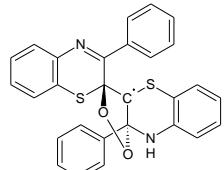
-2132.82908 -2132.39965 -2132.48817 -2134.05455 -2133.71365 -2134.45224 -2134.11133 0.4

H -0.01519 -5.80110 1.97548 H 1.43659 -4.53821 3.55768 H 1.33903 -2.06629 3.62187 H -3.07272 1.78892 0.02673 H -5.01671 2.50913 -1.26611 H -6.23935 0.89819 -2.70845 H -5.48220 -1.46835 -2.82244 H -3.52203 -2.20634 -1.48908 O -0.51416 1.07875 -1.62985 O 0.24025 1.24886 -2.67681								
 S 1.16871 -1.01713 1.62206 C -0.19524 -0.46133 0.53357 C -0.94306 -1.71841 0.05564 N -0.29666 -2.68365 -0.49633 C 1.69711 -3.61312 -1.44249 C 3.06463 -3.83976 -1.40569 C 3.84635 -3.23303 -0.41778 C 3.26322 -2.36999 0.50237 C 1.89048 -2.10970 0.44762 C 1.08623 -2.75527 -0.51411 C -2.40004 -1.90643 0.25713 C -2.85544 -3.22388 0.42896 C -4.20735 -3.49379 0.59467 C -5.13425 -2.45158 0.58664 C -4.69484 -1.14184 0.41243 C -3.33971 -0.86605 0.25434 H 1.06076 -4.10413 -2.17262 H 3.52302 -4.50440 -2.13186 H 4.91469 -3.42298 -0.37235 H 3.87267 -1.87107 1.25060 H -2.12669 -4.02766 0.42997 H -4.53842 -4.51872 0.73559 H -6.19236 -2.65981 0.71881 H -5.40850 -0.32299 0.40086 H -3.02889 0.16080 0.11266 S -0.91167 0.75394 -1.93163 C 0.32506 0.40212 -0.65144 C 0.98337 1.70450 -0.21404 N 0.31860 2.77789 0.02394 C -1.71789 3.97355 0.37135 C -3.04221 4.24421 0.06093 C -3.70725 3.46643 -0.89023	-2132.83010	-2132.40039	-2132.48746	-2134.05705	-2133.71441	-2134.45456	-2134.11192	0.0

C -3.05507 2.39821 -1.49657 C -1.73165 2.10308 -1.15965 C -1.03645 2.90813 -0.23519 C 2.45453 1.76378 -0.04337 C 2.99647 2.73350 0.81487 C 4.36998 2.84910 0.97632 C 5.23415 2.00942 0.27125 C 4.70881 1.05143 -0.59098 C 3.33008 0.92310 -0.74173 H 1.05072 -0.23025 -1.16777 H -1.16837 4.58285 1.08240 H -3.55398 5.07082 0.54441 H -4.73713 3.68684 -1.15550 H -3.57483 1.77721 -2.22156 H 2.31555 3.38539 1.35158 H 4.77073 3.59689 1.65481 H 6.30953 2.10379 0.39326 H 5.37076 0.39858 -1.15276 H 2.95492 0.17143 -1.42936 O -1.07501 0.35006 1.34372 O -0.57755 0.67499 2.50626									
	S -2.11964 -0.80479 -1.30554 C -0.92046 -0.30472 -0.04453 C -1.23281 1.07975 0.55529 N -2.39361 1.62130 0.59569 C -4.75335 1.74917 0.36905 C -5.96395 1.31506 -0.15078 C -5.99238 0.21990 -0.01707 C -4.81467 -0.44120 -1.34822 C -3.59932 -0.00680 -0.81647 C -3.55285 1.10066 0.04409 C -0.13435 1.81084 1.23952 C 0.88919 1.15812 1.93806 C 1.86374 1.89377 2.60880 C 1.83759 3.28523 2.58378 C 0.81904 3.94272 1.89274 C -0.16095 3.21222 1.23298 H -4.69507 2.59940 1.04185 H -6.88418 1.82726 0.11303 H -6.93477 -0.12591 -1.43182 H -4.83678 -1.30057 -2.01313 H 0.91196 0.07507 1.98868	-2132.82692	-2132.39712	-2132.48573	-2134.05325	-2133.71206	-2134.45160	-2134.11041	0.9

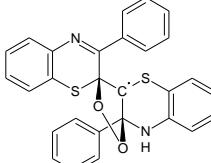
H 2.64431 1.37342 3.15671 H 2.60347 3.85545 3.10207 H 0.78835 5.02864 1.86989 H -0.96332 3.71252 0.70038 C 0.42277 -0.39909 -0.71741 S 0.73906 0.95669 -1.83358 C 2.45304 1.19697 -1.45761 C 3.23423 0.05662 -1.24072 N 2.60939 -1.19440 -1.18705 C 1.35096 -1.38151 -0.61482 C 3.03978 2.45910 -1.45936 C 4.41983 2.58644 -1.30828 C 5.20308 1.44948 -1.12232 C 4.61306 0.18895 -1.06817 C 1.20904 -2.68818 0.07575 C 0.22510 -3.60207 -0.31524 C 0.13820 -4.84628 0.30179 C 1.03283 -5.19249 1.31239 C 2.02236 -4.29104 1.70161 C 2.11608 -3.04920 1.08045 H 2.41464 3.33607 -1.59889 H 4.87822 3.57005 -1.33692 H 6.27884 1.54062 -1.00462 H 5.22231 -0.69567 -0.89672 H -0.47097 -3.33314 -1.10404 H -0.63090 -5.54741 -0.00875 H 0.96015 -6.16262 1.79549 H 2.71830 -4.55265 2.49355 H 2.87936 -2.34071 1.39427 O -0.91317 -1.24063 1.10583 O -2.10211 -1.42260 1.60316 H 3.22797 -1.98703 -1.09923								
<b>Single-bond dimer, C3-peroxyl radical</b>								
 S 1.78894 0.21387 1.46006 C 0.47250 0.63235 0.35766 C 0.46443 2.09048 0.05188 N 1.53697 2.71333 -0.30258 C 3.81536 2.67296 -1.03781 C 5.10981 2.18253 -0.95629 C 5.39854 1.11305 -0.10419 C 4.38381 0.51695 0.63589 C 3.07357 0.98730 0.52872	-2132.83405	-2132.40399	-2132.49250	-2134.05900	-2133.71744	-2134.45809	-2134.11654	0.0

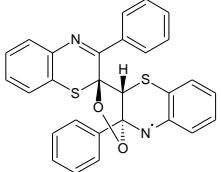
C 2.77473 2.09184 -0.29633 C -0.77134 2.88768 0.23919 C -1.78423 2.46289 1.10743 C -2.90904 3.25408 1.31744 C -3.04201 4.47328 0.65520 C -2.03600 4.90233 -0.21131 C -0.90496 4.12026 -0.41238 H 3.57315 3.52718 -1.66304 H 5.90093 2.64266 -1.54078 H 6.41376 0.73597 -0.02291 H 4.59859 -0.33168 1.27947 H -1.68727 1.51433 1.62774 H -3.68274 2.91645 2.00116 H -3.92344 5.08801 0.81530 H -2.13338 5.85158 -0.73083 H -0.11025 4.44737 -1.07489 S -1.51076 0.22077 -1.42950 C -0.38312 -0.27639 -0.16641 C -0.38737 -1.74376 0.21946 N -1.44451 -2.47714 -0.36190 C -3.85998 -2.74384 -0.07444 C -5.14228 -2.22987 -0.24438 C -5.32774 -0.93701 -0.73265 C -4.22239 -0.15448 -1.05826 C -2.93988 -0.67971 -0.91822 C -2.74897 -1.97417 -0.42213 C 0.91963 -2.47773 -0.06051 C 1.55282 -3.28483 0.88495 C 2.70305 -3.99222 0.53775 C 3.22845 -3.89670 -0.74779 C 2.59388 -3.09343 -1.69431 C 1.44165 -2.39273 -1.35446 H -3.71378 -3.74263 0.32858 H -6.00077 -2.83919 0.02219 H -6.32860 -0.53337 -0.85020 H -4.34823 0.85969 -1.42613 H 1.16606 -3.35550 1.89540 H 3.19075 -4.61537 1.28205 H 4.12800 -4.44527 -1.01237 H 2.99459 -3.01307 -2.70063 H 0.93915 -1.77730 -2.09557 H -1.38815 -3.45709 -0.11724 O -0.57200 -1.66211 1.74870 O -1.11849 -2.73128 2.23662							
<b>Single-bond dimer, dioxolane radical</b>							

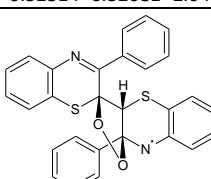


S 1.73114 -1.86805 0.37896  
 C 1.02178 -0.25027 -0.15171  
 C 1.92377 0.86398 0.39511  
 N 3.20484 0.81108 0.31545  
 C 5.23817 -0.09985 -0.53506  
 C 6.03237 -1.17276 -0.90784  
 C 5.51348 -2.47065 -0.86510  
 C 4.19658 -2.68460 -0.47881  
 C 3.38373 -1.60198 -0.12821  
 C 3.90580 -0.29351 -0.13833  
 C 1.32803 2.06325 1.02752  
 C 1.97281 2.62757 2.13678  
 C 1.46477 3.77191 2.74083  
 C 0.31423 4.37775 2.23572  
 C -0.32218 3.83313 1.12254  
 C 0.17640 2.67959 0.52379  
 H 5.62140 0.91611 -0.53279  
 H 7.05903 -1.00562 -1.21946  
 H 6.13427 -3.31703 -1.14431  
 H 3.78434 -3.68972 -0.46484  
 H 2.87330 2.15231 2.51329  
 H 1.96718 4.19217 3.60755  
 H -0.08202 5.27299 2.70693  
 H -1.20905 4.30698 0.71168  
 H -0.31850 2.28128 -0.35503  
 S -1.08425 -0.56455 1.72551  
 C -0.43368 -0.29032 0.17501  
 C -1.16868 -0.53668 -1.11699  
 N -2.01004 -1.70400 -1.05041  
 C -3.92580 -2.82108 -0.11637  
 C -4.72695 -3.18190 0.95635  
 C -4.42833 -2.72851 2.24216  
 C -3.31584 -1.92051 2.43059  
 C -2.49210 -1.56972 1.35670  
 C -2.79274 -2.00972 0.05599  
 C -1.91451 0.68876 -1.64573  
 C -1.54019 1.29815 -2.84477  
 C -2.24545 2.40394 -3.31889  
 C -3.32460 2.91123 -2.60001  
 C -3.69933 2.30633 -1.39995  
 C -2.99900 1.20261 -0.92390  
 H -4.16734 -3.17152 -1.11732  
 H -5.59338 -3.81366 0.78520

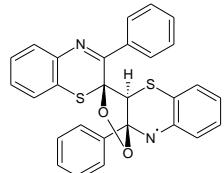
-2132.83935 -2132.40913 -2132.49602 -2134.06269 -2133.71937 -2134.46111 -2134.11778 0.4

H -5.05344 -2.99965 3.08661 H -3.06823 -1.55608 3.42456 H -0.69379 0.90648 -3.39848 H -1.94479 2.87061 -4.25275 H -3.87127 3.77390 -2.97024 H -4.53979 2.69505 -0.83171 H -3.29828 0.74361 0.01436 O 1.00825 -0.08851 -1.56350 O -0.09490 -0.89596 -2.00208 H -2.47562 -1.88741 -1.92996								
 S 1.40605 -2.05973 1.44582 C 0.93100 -0.33422 0.91842 C 2.17247 0.30805 0.29855 N 2.88500 -0.31112 -0.57233 C 3.21913 -2.06751 -2.15287 C 3.14778 -3.39931 -2.53426 C 2.55542 -4.33609 -1.68351 C 2.01132 -3.93062 -0.47019 C 2.05709 -2.58544 -0.09418 C 2.68257 -1.63752 -0.92983 C 2.56276 1.69103 0.65298 C 3.92689 2.01576 0.62333 C 4.35128 3.31010 0.89497 C 3.41761 4.30482 1.18630 C 2.06017 3.99322 1.20582 C 1.62978 2.69428 0.95010 H 3.69972 -1.32336 -2.78082 H 3.56486 -3.71355 -3.48633 H 2.50728 -5.38256 -1.97013 H 1.53325 -4.65282 0.18580 H 4.64149 1.23475 0.38420 H 5.41200 3.54420 0.88047 H 3.74782 5.31825 1.39718 H 1.32765 4.76578 1.42210 H 0.56946 2.46721 0.96630 S -0.39882 -0.00779 -1.60358 C -0.30406 -0.27925 0.07946 C -1.43801 0.08450 1.00220 N -1.79109 1.46886 0.75277 C -3.03985 2.95352 -0.69574 C -3.41905 3.38138 -1.96022 C -2.93175 2.73469 -3.09681	-2132.83913	-2132.40897	-2132.49469	-2134.06320	-2133.71875	-2134.46116	-2134.11672	1.1

C -2.04630 1.67597 -2.94773 C -1.63876 1.25545 -1.67860 C -2.15459 1.87820 -0.52676 C -2.61153 -0.88958 1.02187 C -2.37037 -2.23503 1.31982 C -3.42021 -3.14497 1.35369 C -4.72305 -2.72441 1.08454 C -4.96678 -1.38861 0.78243 C -3.91511 -0.47277 0.75199 H -3.43427 3.44983 0.18863 H -4.10670 4.21620 -2.05708 H -3.23366 3.05471 -4.08877 H -1.64682 1.17152 -3.82392 H -1.35506 -2.56062 1.52746 H -3.22151 -4.18616 1.59137 H -5.54274 -3.43691 1.10848 H -5.97673 -1.05230 0.56628 H -4.12280 0.56229 0.50143 O 0.55323 0.33447 2.10189 O -0.83737 -0.02327 2.28719 H -2.33826 1.87625 1.50111							
 S 1.47601 -1.54015 -0.00349 C 0.81952 0.13640 -0.28104 C 1.81314 1.18718 0.22911 N 3.08593 1.07535 0.11551 C 5.05913 0.12177 -0.81374 C 5.78385 -0.95016 -1.31108 C 5.18332 -2.20895 -1.40746 C 3.85861 -2.38398 -1.02733 C 3.12039 -1.29953 -0.54460 C 3.72035 -0.03358 -0.42383 C 1.30946 2.44394 0.84434 C 1.82755 2.85237 2.07821 C 1.40735 4.04535 2.65857 C 0.47646 4.85196 2.00601 C -0.02925 4.46197 0.76718 C 0.38053 3.26356 0.18907 H 5.50110 1.10811 -0.70977 H 6.81692 -0.81309 -1.61579 H 5.74677 -3.05536 -1.78926 H 3.38402 -3.35709 -1.11783 H 2.56341 2.22481 2.57182	-2132.83813	-2132.40891	-2132.49655	-2134.06012	-2133.71854	-2134.45709	-2134.11551

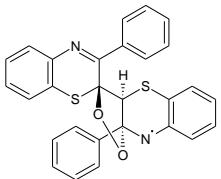
H 1.81034 4.34702 3.62125 H 0.15057 5.78427 2.45835 H -0.74145 5.09375 0.24421 H 0.00419 2.98009 -0.79059 S -1.02189 -0.48252 1.85889 C -0.62780 0.20713 0.24504 C -1.46962 -0.33074 -0.94770 N -1.93271 -1.68140 -0.95541 C -2.40810 -3.80134 -0.08357 C -2.49205 -4.70449 0.94906 C -2.11056 -4.31801 2.24659 C -1.64214 -3.02946 2.48779 C -1.55039 -2.09754 1.45551 C -1.94487 -2.46062 0.12133 C -2.64590 0.59564 -1.23208 C -2.60111 1.49068 -2.30067 C -3.66572 2.36153 -2.52707 C -4.77921 2.34321 -1.69046 C -4.82787 1.44390 -0.62636 C -3.76748 0.57103 -0.39890 H -0.86462 1.26499 0.36104 H -2.69062 -4.05985 -1.09930 H -2.84761 -5.71359 0.76458 H -2.16881 -5.02697 3.06702 H -1.33347 -2.74509 3.49041 H -1.73648 1.49142 -2.95636 H -3.62519 3.05180 -3.36520 H -5.60900 3.02094 -1.87008 H -5.69589 1.41725 0.02639 H -3.81746 -0.13388 0.42668 O 0.60380 0.46707 -1.63946 O -0.52514 -0.32081 -2.04755								
 S 1.47220 -1.26090 0.79181 C 0.87279 0.10949 -0.24436 C 1.76628 1.34817 -0.10765 N 3.02634 1.32817 0.13600 C 5.16262 0.30100 0.32478 C 5.98028 -0.79182 0.56783 C 5.40990 -2.03266 0.86695 C 4.02868 -2.17655 0.90696 C 3.20513 -1.07541 0.65447 C 3.76518 0.17852 0.36533	-2132.82898	-2132.39961	-2132.48425	-2134.05235	-2133.70762	-2134.44952	-2134.10478	8.6

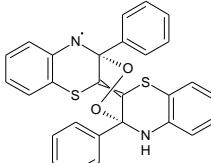
C 1.17684 2.69347 -0.35380							
C 0.36828 2.96435 -1.46670							
C -0.10991 4.25378 -1.68703							
C 0.20244 5.28222 -0.80037							
C 1.01040 5.01953 0.30499							
C 1.50087 3.73625 0.52228							
H 5.57278 1.28015 0.09666							
H 7.05982 -0.68224 0.52954							
H 6.04359 -2.89290 1.06204							
H 3.58141 -3.14260 1.12519							
H 0.13500 2.17611 -2.17687							
H -0.72425 4.45345 -2.56042							
H -0.17766 6.28521 -0.97277							
H 1.26255 5.81691 0.99843							
H 2.14480 3.52583 1.37069							
S -1.27527 0.13346 1.69026							
C -0.61027 0.30642 0.03102							
C -1.28997 -0.60683 -0.99762							
N -2.62838 -0.18434 -1.25310							
C -4.73381 0.51597 -0.50498							
C -5.63480 0.86855 0.47267							
C -5.20963 0.96540 1.80805							
C -3.87773 0.73259 2.13949							
C -2.94185 0.37921 1.16822							
C -3.36501 0.22407 -0.20769							
C -1.26669 -2.12662 -0.80621							
C -0.49247 -2.91444 -1.66323							
C -0.47950 -4.29981 -1.53150							
C -1.24242 -4.92034 -0.54552							
C -2.03275 -4.14366 0.29788							
C -2.05319 -2.75807 0.16262							
H -0.86597 1.31993 -0.29004							
H -5.02716 0.41703 -1.54549							
H -6.66982 1.06948 0.21403							
H -5.91283 1.24271 2.58756							
H -3.55093 0.84710 3.16986							
H 0.10651 -2.43732 -2.42953							
H 0.13113 -4.89449 -2.20511							
H -1.23145 -6.00186 -0.44262							
H -2.64692 -4.61510 1.05987							
H -2.69903 -2.18058 0.81378							
O 0.86422 -0.23216 -1.65434							
O -0.50502 -0.23673 -2.14061							

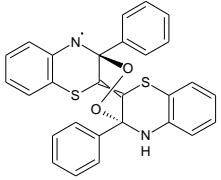


S -0.63396 -2.39255 -1.65492  
 C 0.07096 -0.82093 -0.99372  
 C 1.48718 -1.12710 -0.51021  
 N 1.70015 -2.10885 0.28989  
 C 0.92532 -3.79916 1.78965  
 C 0.06500 -4.83538 2.11963  
 C -1.00062 -5.15250 1.27315  
 C -1.21976 -4.40853 0.11936  
 C -0.37657 -3.34009 -0.19866  
 C 0.72722 -3.03734 0.62778  
 C 2.64653 -0.26768 -0.85582  
 C 3.63250 -0.08272 0.12572  
 C 4.76896 0.66932 -0.14226  
 C 4.95016 1.23792 -1.40268  
 C 3.98551 1.04679 -2.38864  
 C 2.83730 0.30671 -2.12033  
 H 1.78208 -3.55689 2.41108  
 H 0.23095 -5.40974 3.02610  
 H -1.66874 -5.97308 1.51743  
 H -2.05912 -4.63915 -0.53093  
 H 3.48692 -0.53979 1.09893  
 H 5.51589 0.81161 0.63381  
 H 5.83991 1.82404 -1.61543  
 H 4.12412 1.47469 -3.37735  
 H 2.10336 0.16453 -2.90396  
 S -0.31652 0.11893 1.75336  
 C -0.89136 -0.18401 0.07250  
 C -1.39613 1.08711 -0.66329  
 N -0.64374 2.29377 -0.52585  
 C 0.94564 3.75144 0.39010  
 C 1.82326 4.12734 1.37798  
 C 2.04292 3.27767 2.47830  
 C 1.39177 2.05042 2.56169  
 C 0.50274 1.64570 1.56779  
 C 0.23107 2.50873 0.44859  
 C -2.88128 1.33510 -0.44911  
 C -3.81273 0.42316 -0.95472  
 C -5.17288 0.62645 -0.74405  
 C -5.61244 1.73451 -0.02041  
 C -4.68502 2.64162 0.48461  
 C -3.32229 2.44701 0.26611  
 H -1.73456 -0.86322 0.20872  
 H 0.74569 4.37996 -0.47211

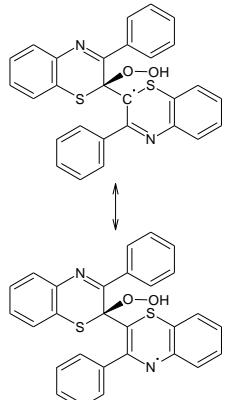
-2132.84013 -2132.41093 -2132.49703 -2134.06459 -2133.72149 -2134.46153 -2134.11844 0.0

H 2.34753 5.07570 1.31103 H 2.73446 3.56972 3.26302 H 1.58349 1.39134 3.40449 H -3.46990 -0.43692 -1.52374 H -5.89120 -0.08137 -1.14789 H -6.67463 1.89059 0.14555 H -5.02004 3.50897 1.04624 H -2.60097 3.16518 0.64233 O 0.06523 0.10404 -2.04941 O -1.25775 0.66571 -2.02745								
 S 1.83462 -1.44169 2.10873 C 0.40629 -0.89021 1.08716 C 0.20888 -1.95331 0.00307 N 1.20187 -2.28094 -0.74777 C 3.43496 -1.98967 -1.55391 C 4.78500 -1.76030 -1.33889 C 5.24589 -1.46334 -0.05311 C 4.34913 -1.36542 1.00429 C 2.98270 -1.55808 0.78510 C 2.51057 -1.89653 -0.50163 C -1.09465 -2.60193 -0.28205 C -1.34053 -3.01117 -1.60287 C -2.51917 -3.66398 -1.93697 C -3.47002 -3.93857 -0.95351 C -3.22707 -3.55459 0.36220 C -2.05384 -2.88489 0.69978 H 3.05766 -2.25973 -2.53564 H 5.48478 -1.83014 -2.16626 H 6.30446 -1.29805 0.12433 H 4.70098 -1.11466 2.00114 H -0.58774 -2.80713 -2.35732 H -2.69598 -3.96246 -2.96662 H -4.39205 -4.45188 -1.21189 H -3.95573 -3.77367 1.13731 H -1.88712 -2.59674 1.72981 S 0.99032 1.02159 -1.10701 C 0.58159 0.56559 0.59128 C -0.68615 1.25510 1.09424 N -0.45317 2.64195 1.32291 C 0.23950 4.72880 0.50515 C 0.77420 5.54915 -0.45993 C 1.30875 4.98672 -1.63202	-2132.82325	-2132.39389	-2132.47937	-2134.04843	-2133.70454	-2134.44560	-2134.10171	10.5

C 1.33105 3.60738 -1.80163 C 0.80316 2.75082 -0.83341 C 0.18981 3.30856 0.35020 C -2.03426 1.11486 0.39216 C -3.12606 1.66238 1.08112 C -4.40616 1.59864 0.54541 C -4.61750 0.98508 -0.68947 C -3.53968 0.43555 -1.37532 C -2.25299 0.50256 -0.84122 H 1.38071 0.99184 1.20745 H -0.20034 5.12618 1.41466 H 0.77939 6.62564 -0.31993 H 1.72895 5.62589 -2.40273 H 1.78870 3.18158 -2.69097 H -2.96051 2.13207 2.04557 H -5.24095 2.02570 1.09401 H -5.61800 0.93065 -1.10951 H -3.69303 -0.06001 -2.32966 H -1.43118 0.06930 -1.39665 O -0.69926 -0.78231 1.97167 O -0.76366 0.59792 2.37935								
<b>Single-bond dimer, dioxane radical</b>								
 S -1.63220 -0.04024 2.03837 C -0.71119 -0.00209 0.54479 C -1.49728 0.11437 -0.74230 N -2.48464 -0.91191 -0.89887 C -4.36331 -2.11484 -0.16206 C -5.28641 -2.45229 0.79871 C -5.13123 -1.98114 2.11592 C -4.02925 -1.20740 2.46001 C -3.07271 -0.86808 1.50239 C -3.24728 -1.26829 0.13297 C -2.13053 1.48775 -0.96249 C -1.73492 2.61017 -0.23553 C -2.30758 3.85368 -0.49670 C -3.27698 3.98409 -1.48748 C -3.66684 2.86599 -2.22445 C -3.09576 1.62446 -1.96572 H -4.46180 -2.44155 -1.19265 H -6.13766 -3.07531 0.54190 H -5.86177 -2.23838 2.87691 H -3.89381 -0.88442 3.48899	-2132.83916	-2132.40934	-2132.49572	-2134.06385	-2133.72041	-2134.46310	-2134.11967	0.0

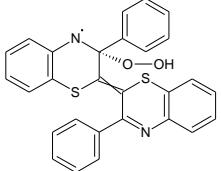
H -0.97015 2.51906 0.52958 H -1.99091 4.72136 0.07526 H -3.72384 4.95368 -1.68934 H -4.41520 2.96205 -3.00622 H -3.38737 0.75281 -2.54330 S 1.57737 -0.35275 1.98359 C 0.63285 -0.04354 0.54564 C 1.39329 0.16177 -0.74966 N 2.30204 1.26580 -0.55597 C 4.51390 1.85881 0.23029 C 5.50988 1.80674 1.19539 C 5.31987 1.06064 2.35860 C 4.11801 0.39073 2.54894 C 3.10244 0.45455 1.59167 C 3.29915 1.18152 0.40520 C 2.04220 -1.12216 -1.26777 C 3.24417 -1.06780 -1.97650 C 3.80757 -2.22450 -2.50903 C 3.17564 -3.45326 -2.33436 C 1.97980 -3.51689 -1.62281 C 1.41846 -2.35962 -1.09091 H 4.66756 2.43063 -0.68241 H 6.44084 2.34139 1.03233 H 6.09806 1.00251 3.11273 H 3.95342 -0.18370 3.45706 H 3.75772 -0.12070 -2.11133 H 4.74442 -2.16435 -3.05557 H 3.61554 -4.35707 -2.74647 H 1.47977 -4.47055 -1.47972 H 0.48546 -2.41935 -0.53994 H 2.56851 1.71446 -1.42240 O 0.49290 0.70652 -1.72044 O -0.59903 -0.19054 -1.83323								
 S -1.71914 -1.24853 -1.51695 C -0.71978 -0.41933 -0.33294 C -1.48294 0.44156 0.65047 N -2.34032 -0.36123 1.47626 C -4.04862 -1.95058 1.75734 C -4.95804 -2.85489 1.26027 C -4.92481 -3.20417 -0.10186 C -3.95176 -2.67131 -0.94139 C -3.01014 -1.76784 -0.45158	-2132.83897	-2132.40905	-2132.49509	-2134.06416	-2133.72028	-2134.46338	-2134.11951	0.1

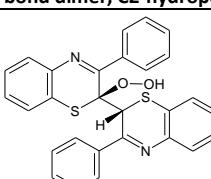
C -3.07238 -1.32689 0.91684 C -2.24283 1.58408 -0.03226 C -1.57469 2.36961 -0.97517 C -2.22882 3.42885 -1.59396 C -3.55605 3.71445 -1.27372 C -4.21917 2.94133 -0.32514 C -3.56412 1.88014 0.29874 H -4.05686 -1.64036 2.79782 H -5.70381 -3.29475 1.91537 H -5.64437 -3.91265 -0.50116 H -3.90429 -2.98273 -1.98168 H -0.53798 2.15272 -1.21748 H -1.70158 4.03289 -2.32697 H -4.06838 4.54021 -1.75961 H -5.24982 3.16386 -0.06357 H -4.07896 1.28751 1.04742 S 1.46003 -1.62566 -1.39956 C 0.61308 -0.59065 -0.26912 C 1.36307 0.09777 0.86198 N 2.32073 -0.82187 1.44313 C 4.59976 -1.60192 1.17635 C 5.59074 -2.20162 0.41186 C 5.33152 -2.57031 -0.90850 C 4.07024 -2.34306 -1.44461 C 3.06136 -1.76413 -0.67086 C 3.32016 -1.37628 0.65189 C 1.99535 1.43777 0.48872 C 2.21552 2.38456 1.49444 C 2.86579 3.57960 1.20654 C 3.30780 3.84432 -0.08966 C 3.08902 2.90676 -1.09435 C 2.43483 1.70864 -0.80781 H 4.80713 -1.29937 2.20023 H 6.57257 -2.36828 0.84467 H 6.10521 -3.02612 -1.51797 H 3.85476 -2.62487 -2.47216 H 1.84735 2.19225 2.49810 H 3.01797 4.31183 1.99461 H 3.81423 4.77875 -0.31426 H 3.42620 3.10390 -2.10816 H 2.26655 0.98960 -1.60461 H 2.66807 -0.45319 2.32070 O 0.44060 0.24998 1.93685 O -0.56258 1.15736 1.47590							
Single-bond dimer, C2-hydroperoxylalkyl radical							



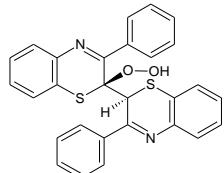
S 1.14810 -2.23257 0.28532  
 C 0.42898 -0.86376 -0.72715  
 C 1.32783 0.37573 -0.84669  
 N 2.58447 0.40924 -0.60082  
 C 4.73190 -0.38137 0.00698  
 C 5.59866 -1.34191 0.50536  
 C 5.09589 -2.57735 0.92037  
 C 3.73464 -2.84305 0.82766  
 C 2.86391 -1.87346 0.32172  
 C 3.35180 -0.62302 -0.09172  
 C 0.73389 1.60925 -1.43072  
 C -0.43092 1.61374 -2.21079  
 C -0.92026 2.80393 -2.74363  
 C -0.25887 4.00636 -2.50930  
 C 0.90568 4.01077 -1.74077  
 C 1.39680 2.82605 -1.20995  
 H 5.08920 0.58830 -0.32614  
 H 6.66204 -1.13342 0.57231  
 H 5.76394 -3.33767 1.31435  
 H 3.34218 -3.80525 1.14712  
 H -0.94612 0.68795 -2.43709  
 H -1.81908 2.78490 -3.35346  
 H -0.64447 4.93305 -2.92543  
 H 1.42966 4.94323 -1.54967  
 H 2.29627 2.82011 -0.60415  
 C -0.97164 -0.66062 -0.18026  
 S -2.10540 -1.77599 -0.91203  
 C -3.59861 -1.38023 -0.09820  
 C -3.66529 -0.32839 0.84104  
 N -2.60371 0.41562 1.27323  
 C -1.35908 0.23025 0.83715  
 C -4.73813 -2.11514 -0.43922  
 C -5.96089 -1.80824 0.14144  
 C -6.05236 -0.75964 1.06583

-2132.83944 -2132.41052 -2132.49883 -2134.06829 -2133.72768 -2134.46771 -2134.12710 0.0

C -4.92464 -0.03647 1.40845 C -0.38714 1.11705 1.54867 C -0.65610 2.49032 1.59614 C 0.16816 3.34611 2.31628 C 1.26208 2.83941 3.01867 C 1.52053 1.47180 2.99793 C 0.70099 0.61410 2.26639 H -4.66217 -2.92275 -1.16300 H -6.84282 -2.38215 -0.12634 H -7.00938 -0.51706 1.51816 H -4.96301 0.77353 2.13022 H -1.51748 2.87660 1.06031 H -0.04483 4.41135 2.33254 H 1.90392 3.50770 3.58618 H 2.35899 1.06476 3.55609 H 0.89780 -0.45283 2.27219 O 0.20686 -1.35129 -2.06063 O 1.44589 -1.70228 -2.64971 H 1.54799 -2.62223 -2.35130								
<b>Single-bond dimer, C3-hydroperoxylalkyl radical</b>								
 S 1.94447 -0.65965 1.47684 C 0.88793 0.34600 0.47371 C 1.57230 1.56860 -0.03162 N 2.75728 1.55179 -0.53943 C 4.64507 0.34913 -1.38625 C 5.54604 -0.70240 -1.31695 C 5.36697 -1.70894 -0.36366 C 4.26946 -1.67691 0.48850 C 3.33921 -0.63783 0.39700 C 3.53302 0.40452 -0.53135 C 0.91229 2.88964 0.12418 C -0.01937 3.11788 1.14527 C -0.57843 4.38078 1.31435 C -0.22637 5.42534 0.46166 C 0.70116 5.20336 -0.55689 C 1.27390 3.94761 -0.71946 H 4.78237 1.16644 -2.08807 H 6.39894 -0.73167 -1.98842 H 6.07813 -2.52656 -0.29049 H 4.11368 -2.47288 1.21183 H -0.29781 2.30758 1.81387 H -1.29060 4.54891 2.11731	-2132.82465	-2132.39596	-2132.48511	-2134.04834	-2133.70881	-2134.44844	-2134.10890	0.0

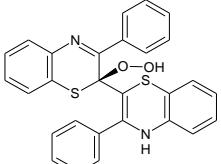
H -0.66983 6.40871 0.59127 H 0.98051 6.01344 -1.22491 H 2.00728 3.76487 -1.49827 S -1.15845 0.87391 -1.15227 C -0.39220 0.01309 0.17316 C -1.12910 -1.16021 0.80624 N -2.56042 -1.03943 0.92617 C -4.73576 -0.48970 0.22360 C -5.60853 0.11926 -0.64429 C -5.11215 0.91655 -1.69486 C -3.74533 1.11093 -1.84422 C -2.84279 0.50550 -0.96659 C -3.31646 -0.35415 0.07819 C -0.82932 -2.50148 0.13778 C -1.36224 -3.65805 0.71886 C -1.14037 -4.89976 0.13391 C -0.39131 -4.99817 -1.03848 C 0.13774 -3.84859 -1.61904 C -0.07929 -2.60278 -1.03367 H -5.08231 -1.12639 1.03180 H -6.67917 -0.01633 -0.52594 H -5.79871 1.39813 -2.38446 H -3.37146 1.75477 -2.63602 H -1.94331 -3.57294 1.63075 H -1.55164 -5.79328 0.59503 H -0.21877 -5.96848 -1.49573 H 0.72780 -3.91716 -2.52842 H 0.34682 -1.71414 -1.48838 O -0.66311 -1.32543 2.15393 O -1.14337 -0.23018 2.93327 H -2.09075 -0.44833 2.98482								
<b>Single-bond dimer, C2-hydroperoxide</b>								
 S 0.97219 -0.98771 -1.20539 C 0.09349 0.48277 -0.56585 C 1.02158 1.60405 -0.07163 N 2.28660 1.69395 -0.23996 C 4.41900 1.13096 -1.11095 C 5.29074 0.29659 -1.79414 C 4.82339 -0.91546 -2.30806 C 3.49348 -1.28137 -2.13839 C 2.61721 -0.43865 -1.44812 C 3.07287 0.78047 -0.92615	-2133.47129	-2133.02920	-2133.11856	-2134.70194	-2134.34921	-2135.10123	-2134.74850	0.6

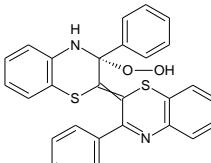
C 0.38746 2.73367 0.67067 C -0.78315 3.37198 0.23608 C -1.30071 4.45195 0.94817 C -0.66670 4.90509 2.10250 C 0.50171 4.28010 2.53654 C 1.02721 3.20849 1.82346 H 4.74416 2.08254 -0.70131 H 6.32883 0.58463 -1.92831 H 5.49581 -1.57929 -2.84368 H 3.13049 -2.22583 -2.53578 H -1.26740 3.04566 -0.67788 H -2.19857 4.94770 0.58949 H -1.07641 5.74436 2.65737 H 1.00541 4.62799 3.43404 H 1.93968 2.71978 2.14970 C -0.90055 0.04746 0.55674 S -0.08871 -0.29185 2.14231 C 0.28085 -1.99807 1.95370 C -0.50505 -2.79748 1.10344 N -1.60885 -2.33068 0.40490 C -1.84764 -1.08824 0.17898 C 1.31720 -2.56546 2.69512 C 1.59095 -3.92545 2.58535 C 0.83286 -4.72524 1.72837 C -0.21019 -4.16399 1.00434 C -3.13003 -0.75880 -0.49396 C -3.83697 -1.78813 -1.13713 C -5.05142 -1.53725 -1.75984 C -5.59577 -0.25205 -1.74748 C -4.90819 0.77650 -1.11059 C -3.68363 0.52828 -0.49567 H 1.91789 -1.93628 3.34642 H 2.40166 -4.35750 3.16467 H 1.04840 -5.78555 1.63669 H -0.83000 -4.76599 0.34658 H -3.40866 -2.78458 -1.13325 H -5.57745 -2.34670 -2.25825 H -6.54778 -0.05533 -2.23237 H -5.32246 1.78039 -1.09162 H -3.17647 1.35622 -0.01185 O -0.77911 0.98082 -1.57775 O -0.00049 1.52228 -2.63847 H 0.13812 0.73686 -3.19428 H -1.48845 0.93996 0.77497							
--	--	--	--	--	--	--	--

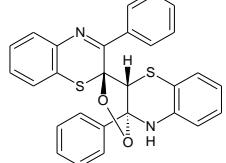


S 1.21209 -1.02602 1.60499  
 C -0.18525 -0.43917 0.54727  
 C -0.89688 -1.69819 0.02688  
 N -0.24521 -2.65603 -0.53176  
 C 1.74853 -3.56625 -1.48900  
 C 3.11536 -3.79832 -1.45948  
 C 3.89850 -3.21305 -0.46005  
 C 3.31921 -2.36584 0.47713  
 C 1.94772 -2.09621 0.42785  
 C 1.13981 -2.72351 -0.54551  
 C -2.36242 -1.89002 0.18304  
 C -3.29450 -0.83974 0.18034  
 C -4.65526 -1.10543 0.32475  
 C -5.10825 -2.41398 0.47175  
 C -4.18978 -3.46404 0.47070  
 C -2.83241 -3.20507 0.32928  
 H 1.10944 -4.04118 -2.22743  
 H 3.57095 -4.45008 -2.19888  
 H 4.96635 -3.40719 -0.41832  
 H 3.93078 -1.88459 1.23496  
 H -2.96543 0.18393 0.04609  
 H -5.36126 -0.27981 0.31447  
 H -6.16944 -2.61545 0.58750  
 H -4.53242 -4.48823 0.58777  
 H -2.10965 -4.01436 0.32855  
 C 0.34777 0.43930 -0.62047  
 S -0.87112 0.80314 -1.91743  
 C -1.69698 2.15251 -1.15159  
 C -1.00798 2.95321 -0.21882  
 N 0.34523 2.82079 0.04775  
 C 1.00460 1.74235 -0.17610  
 C -3.01721 2.45078 -1.49780  
 C -3.67386 3.51743 -0.89243  
 C -3.01519 4.29040 0.06665  
 C -1.69296 4.01699 0.38566  
 C 2.47497 1.79825 0.00766  
 C 3.35676 0.96242 -0.68865  
 C 4.73404 1.08907 -0.52440  
 C 5.25224 2.04027 0.34979  
 C 4.38198 2.87511 1.05283  
 C 3.00983 2.76153 0.87738  
 H -3.53086 1.83497 -2.23173  
 H -4.70078 3.74127 -1.16648

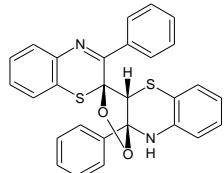
-2133.47332 -2133.03098 -2133.11679 -2134.70674 -2134.35020 -2135.10602 -2134.74949 0.0

H -3.52906 5.11676 0.54858 H -1.14775 4.62451 1.10163 H 2.98732 0.21491 -1.38382 H 5.40072 0.43976 -1.08474 H 6.32652 2.13273 0.48271 H 4.77672 3.61776 1.74053 H 2.32433 3.41084 1.41140 O -0.97837 0.41462 1.32854 O -1.38901 -0.23584 2.52803 H -2.25749 -0.59260 2.26937 H 1.07988 -0.18614 -1.13562								
 S 2.12243 0.85862 -1.31057 C 0.91154 0.36437 -0.01405 C 1.24310 -1.01923 0.58265 N 2.39829 -1.57356 0.60312 C 4.75432 -1.70527 0.36099 C 5.96626 -1.27450 -0.15866 C 5.99795 -0.17738 -1.02246 C 4.82088 0.48618 -1.35081 C 3.60249 0.05420 -0.82037 C 3.55341 -1.05399 0.04059 C 0.15277 -1.74199 1.29021 C 0.17295 -3.14353 1.29017 C -0.80514 -3.86713 1.96066 C -1.81616 -3.20223 2.65540 C -1.83546 -1.81042 2.67420 C -0.86243 -1.08132 1.99406 H 4.69387 -2.55670 1.03216 H 6.88467 -1.79136 0.10271 H 6.94046 0.16498 -1.43992 H 4.84303 1.34247 -2.02019 H 0.96877 -3.64953 0.75310 H -0.77929 -4.95335 1.94244 H -2.58091 -3.76679 3.18164 H -2.60937 -1.28449 3.22656 H -0.87206 0.00179 2.04063 C -0.41891 0.39921 -0.72893 S -0.66164 -0.97854 -1.83602 C -2.36793 -1.28993 -1.47745 C -3.20169 -0.18242 -1.28715 N -2.63168 1.09472 -1.24007 C -1.39163 1.33771 -0.64596	-2133.46708	-2133.02465	-2133.11299	-2134.69880	-2134.34471	-2135.09900	-2134.74491	2.9

C -2.89873 -2.57653 -1.46899 C -4.27402 -2.76276 -1.33629 C -5.10921 -1.65901 -1.17867 C -4.57594 -0.37309 -1.13361 C -1.32078 2.65396 0.03930 C -0.41273 3.62994 -0.38368 C -0.39726 4.88314 0.22117 C -1.28711 5.17504 1.25381 C -2.20142 4.21087 1.67419 C -2.22545 2.96028 1.06275 H -2.23339 -3.42669 -1.58675 H -4.68808 -3.76605 -1.35696 H -6.18164 -1.79584 -1.07547 H -5.22607 0.48595 -0.98329 H 0.27717 3.40020 -1.19042 H 0.30876 5.63604 -0.11783 H -1.27082 6.15265 1.72707 H -2.89418 4.43080 2.48148 H -2.93140 2.20374 1.39777 O 0.85387 1.31290 1.04124 O 2.10699 1.32953 1.71539 H 2.56869 2.03914 1.23984 H -3.28595 1.85923 -1.16172								
<b>Single-bond dimer, C3-hydroperoxide</b>								
 S 1.05816 -1.63983 1.40102 C 0.92768 -0.12860 0.49296 C 2.21933 0.24940 -0.14333 N 2.91348 -0.59594 -0.82642 C 3.14976 -2.72325 -1.89593 C 2.98326 -4.09932 -1.91335 C 2.26744 -4.72746 -0.88977 C 1.69137 -3.97188 0.12428 C 1.82449 -2.58101 0.12336 C 2.58220 -1.93911 -0.87879 C 2.77847 1.60390 0.05945 C 2.46155 2.34644 1.20509 C 3.04735 3.59200 1.41651 C 3.94006 4.11463 0.48444 C 4.25672 3.38002 -0.66048 C 3.68842 2.13047 -0.86802 H 3.73655 -2.21511 -2.65542 H 3.42602 -4.68891 -2.71062	-2133.47116	-2133.02809	-2133.11491	-2134.70234	-2134.34609	-2135.10308	-2134.74683	0.0

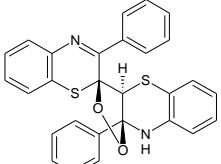
H 2.14909 -5.80707 -0.88717 H 1.11211 -4.45467 0.90666 H 1.76666 1.94368 1.93793 H 2.80327 4.15387 2.31352 H 4.38963 5.09021 0.64755 H 4.95197 3.78436 -1.39096 H 3.93526 1.54187 -1.74572 S -0.24741 2.14345 -0.41640 C -0.22437 0.57208 0.41134 C -1.48446 0.10738 1.13798 N -2.56357 1.11131 1.06241 C -4.25040 1.73643 -0.59803 C -4.56583 2.34835 -1.80737 C -3.55578 2.85029 -2.62704 C -2.22561 2.74073 -2.23005 C -1.90969 2.15659 -1.00410 C -2.92048 1.65170 -0.17992 C -2.00338 -1.24639 0.66728 C -2.66512 -2.10198 1.55393 C -3.23987 -3.28183 1.08799 C -3.17056 -3.61304 -0.26396 C -2.52149 -2.75608 -1.14975 C -1.94184 -1.57741 -0.68820 H -5.03708 1.32830 0.03246 H -5.60460 2.41854 -2.11603 H -3.79984 3.31513 -3.57717 H -1.42630 3.11444 -2.86379 H -2.70900 -1.85660 2.61033 H -3.73878 -3.94688 1.78748 H -3.61844 -4.53462 -0.62466 H -2.45998 -3.00520 -2.20519 H -1.42861 -0.91985 -1.38386 H -3.37322 0.71359 1.52963 O -1.22676 -0.02952 2.53044 O -0.75762 1.22130 3.02968 H -1.45621 1.82677 2.70908								
<b>Single-bond dimer, dioxolane</b>								
 S 2.10889 -0.43342 0.30995 C 0.53853 0.40744 -0.08206 C 0.67197 1.89970 0.25417 N 1.71856 2.58889 -0.02331 C 3.78653 2.92907 -1.16007	-2133.49066	-2133.04735	-2133.13214	-2134.71939	-2134.36087	-2135.11702	-2134.75850	1.1

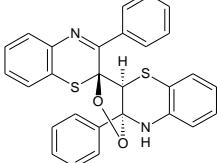
C 4.99899 2.47112 -1.65139 C 5.32972 1.11751 -1.53306 C 4.43778 0.22716 -0.94892 C 3.20262 0.68172 -0.47635 C 2.87255 2.04568 -0.56601 C -0.45020 2.63679 0.89422 C -1.73592 2.65678 0.33882 C -2.74729 3.40461 0.93657 C -2.48942 4.13227 2.09685 C -1.20991 4.12228 2.64997 C -0.19414 3.38591 2.04796 H 3.51046 3.97786 -1.21439 H 5.69404 3.16442 -2.11536 H 6.28234 0.75339 -1.90682 H 4.68426 -0.82831 -0.87291 H -1.94179 2.11128 -0.57837 H -3.73695 3.41984 0.48903 H -3.28161 4.70933 2.56548 H -1.00071 4.69226 3.55082 H 0.80927 3.38398 2.46284 S -0.37622 -1.33680 2.05133 C -0.65047 -0.37068 0.54748 C -1.21872 -1.18401 -0.66176 N -1.31501 -2.59039 -0.43390 C 0.16356 -4.53332 -0.33745 C 1.12412 -5.27258 0.34719 C 1.67521 -4.78685 1.53164 C 1.25722 -3.55599 2.03151 C 0.27420 -2.82893 1.36452 C -0.27872 -3.31126 0.17125 C -2.58190 -0.67018 -1.10787 C -3.68645 -0.85642 -0.27020 C -4.94103 -0.39018 -0.65109 C -5.10358 0.26288 -1.87321 C -4.00592 0.44405 -2.71046 C -2.74640 -0.02056 -2.33079 H -1.40080 0.35711 0.85781 H -0.25236 -4.90469 -1.27120 H 1.45280 -6.22550 -0.05709 H 2.43481 -5.35583 2.05867 H 1.68777 -3.15389 2.94431 H -3.55788 -1.37548 0.67617 H -5.79375 -0.54042 0.00507 H -6.08349 0.62481 -2.17169 H -4.12599 0.94790 -3.66546 H -1.88814 0.12071 -2.97900 O 0.22288 0.37470 -1.46757 O -0.22880 -0.96749 -1.68910 H -1.75002 -3.06640 -1.21343							
---	--	--	--	--	--	--	--

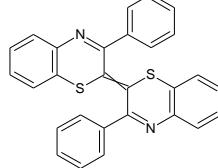


S 1.54839 -1.18692 0.81393  
 C 0.87187 0.12486 -0.25032  
 C 1.68327 1.42059 -0.12332  
 N 2.94205 1.48035 0.12040  
 C 5.13736 0.58730 0.31818  
 C 6.01984 -0.45009 0.57678  
 C 5.52589 -1.71802 0.89786  
 C 4.15598 -1.94437 0.94305  
 C 3.26708 -0.89951 0.67362  
 C 3.74988 0.38129 0.36375  
 C 1.01272 2.72444 -0.38228  
 C 0.18930 2.93491 -1.49714  
 C -0.36461 4.19118 -1.73084  
 C -0.11287 5.24581 -0.85581  
 C 0.70961 5.04341 0.25142  
 C 1.27513 3.79393 0.48207  
 H 5.48724 1.58587 0.07426  
 H 7.09073 -0.27605 0.53456  
 H 6.21070 -2.53488 1.10623  
 H 3.76786 -2.93178 1.17826  
 H 0.00243 2.12620 -2.19795  
 H -0.99107 4.34481 -2.60493  
 H -0.55240 6.22242 -1.03814  
 H 0.91363 5.86161 0.93634  
 H 1.92949 3.63095 1.33287  
 S -1.27312 0.06160 1.67976  
 C -0.62432 0.23471 0.01853  
 C -1.22777 -0.74108 -1.00365  
 N -2.58377 -0.33756 -1.21619  
 C -4.75982 0.30214 -0.44304  
 C -5.65300 0.71628 0.53311  
 C -5.20682 0.95480 1.83282  
 C -3.86290 0.77325 2.12874  
 C -2.95372 0.33774 1.15853  
 C -3.40116 0.09300 -0.15821  
 C -1.09432 -2.24539 -0.79587  
 C -0.25193 -3.00703 -1.61103  
 C -0.17490 -4.38797 -1.45135  
 C -0.93394 -5.02652 -0.47365  
 C -1.78558 -4.27567 0.33356  
 C -1.87282 -2.89573 0.16884  
 H -0.94138 1.21992 -0.33087  
 H -5.10586 0.13487 -1.46051

-2133.47442 -2133.03113 -2133.11557 -2134.70294 -2134.34409 -2135.10100 -2134.74214 11.3

H -6.69719 0.86331 0.27381 H -5.89319 1.29005 2.60372 H -3.49502 0.97020 3.13242 H 0.34905 -2.51342 -2.36593 H 0.48496 -4.96472 -2.09342 H -0.86987 -6.10369 -0.34708 H -2.39199 -4.76347 1.09147 H -2.55701 -2.33045 0.79263 O 0.90275 -0.24160 -1.65250 O -0.46341 -0.32266 -2.14631 H -3.07267 -0.92157 -1.88152								
 S -1.27128 -1.62931 -1.67307 C -0.04844 -0.56617 -0.77734 C 1.10248 -1.48767 -0.36589 N 0.84863 -2.56604 0.28495 C -0.62786 -3.96028 1.55042 C -1.85141 -4.58860 1.72783 C -2.89961 -4.34167 0.83683 C -2.72915 -3.43925 -0.20663 C -1.50895 -2.77777 -0.36927 C -0.43016 -3.05053 0.49970 C 2.52934 -1.17427 -0.62277 C 3.47598 -1.69808 0.27319 C 4.83362 -1.48828 0.07622 C 5.27692 -0.75955 -1.02802 C 4.34830 -0.24720 -1.92911 C 2.98421 -0.44576 -1.73015 H 0.21195 -4.16444 2.20762 H -1.98764 -5.28471 2.55004 H -3.85481 -4.84272 0.96277 H -3.54838 -3.22504 -0.88731 H 3.11985 -2.27072 1.12298 H 5.54953 -1.89467 0.78547 H 6.33946 -0.59582 -1.18534 H 4.68297 0.31220 -2.79799 H 2.28247 -0.04606 -2.45111 S 0.24130 0.43105 1.90729 C -0.72427 0.21776 0.38711 C -1.11601 1.56136 -0.30774 N -0.38537 2.69336 0.19022 C 1.87049 3.62190 0.09345 C 3.19391 3.59052 0.52334	-2133.49090	-2133.04761	-2133.13227	-2134.72143	-2134.36280	-2135.11882	-2134.76019	0.0

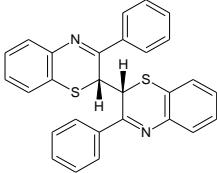
C 3.64488 2.56040 1.34665 C 2.76217 1.55828 1.74221 C 1.43012 1.60339 1.33941 C 0.97322 2.63557 0.50934 C -2.60680 1.85945 -0.24714 C -3.48507 1.36052 -1.21349 C -4.84973 1.62151 -1.11714 C -5.35148 2.36931 -0.05391 C -4.47922 2.85891 0.91545 C -3.11209 2.60897 0.81916 H -1.62414 -0.30580 0.71430 H 1.52451 4.41767 -0.56234 H 3.87907 4.36836 0.19882 H 4.68128 2.52605 1.66749 H 3.10244 0.73738 2.36639 H -3.09757 0.76956 -2.03563 H -5.52264 1.23750 -1.87867 H -6.41687 2.56885 0.01901 H -4.86073 3.43876 1.75112 H -2.42794 2.98791 1.57182 O 0.33921 0.44577 -1.66507 O -0.81334 1.30482 -1.69656 H -0.63536 3.52532 -0.33026								
 S -0.64810 -2.34049 -1.98385 C 0.18615 -0.97451 -1.08316 C 0.99182 -1.60833 0.05336 N 0.44335 -2.42608 0.87685 C -1.45678 -3.56018 1.78266 C -2.65433 -4.24257 1.63193 C -3.22619 -4.37336 0.36376 C -2.61407 -3.79323 -0.74135 C -1.42711 -3.07311 -0.58738 C -0.82125 -2.96704 0.68211 C 2.41996 -1.27261 0.27321 C 2.84456 -0.97495 1.57304 C 4.18757 -0.72881 1.83583 C 5.12647 -0.80214 0.80843 C 4.71255 -1.11618 -0.48478 C 3.36636 -1.33989 -0.75679 H -0.97171 -3.47573 2.75041 H -3.13596 -4.68969 2.49634 H -4.15614 -4.91952 0.23610	-2133.46847	-2133.02519	-2133.10885	-2134.70205	-2134.34243	-2135.10015	-2134.74053	12.3

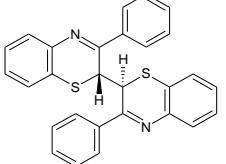
H -3.06784 -3.87439 -1.72521 H 2.10772 -0.93531 2.36900 H 4.50191 -0.48347 2.84634 H 6.17743 -0.61987 1.01546 H 5.44077 -1.19076 -1.28763 H 3.05649 -1.58874 -1.76625 S -1.48593 0.27070 0.98338 C -0.79216 0.14047 -0.66763 C -0.07162 1.41525 -1.13633 N -1.08606 2.39159 -1.38993 C -3.00376 3.66445 -0.72161 C -4.09200 3.92424 0.09691 C -4.39252 3.06407 1.15306 C -3.59172 1.95069 1.36561 C -2.47809 1.68648 0.55994 C -2.16871 2.55642 -0.50900 C 1.09520 1.99075 -0.33904 C 0.86718 2.62335 0.89017 C 1.91567 3.22114 1.58419 C 3.20427 3.21116 1.05631 C 3.43471 2.60227 -0.17402 C 2.38962 1.99680 -0.86689 H -1.64312 0.05100 -1.34986 H -2.78112 4.32575 -1.55589 H -4.71153 4.79451 -0.09789 H -5.24744 3.24961 1.79534 H -3.82254 1.26005 2.17264 H -0.13145 2.66507 1.30955 H 1.71854 3.70320 2.53764 H 4.02140 3.68005 1.59749 H 4.43399 2.59064 -0.59947 H 2.58046 1.52330 -1.82240 O 1.02876 -0.32425 -2.02556 O 0.38044 0.91128 -2.40700 H -0.71065 3.27219 -1.71741								
<b>Double-bond dimers</b>								
 C -0.98434 0.29506 4.27998 C -0.78837 0.77019 2.98157 C -0.04188 1.94568 2.75199 C 0.53261 2.59639 3.85561 C 0.36411 2.10523 5.14127 C -0.41039 0.96173 5.35642	-1982.05731	-1981.64881	-1981.73105	-1983.18691	-1982.86064	-1983.53759	-1983.21132	0.0

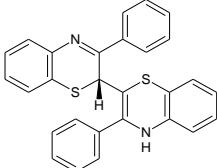
N 0.03790 2.56192 1.51437 C -0.15152 1.91638 0.41273 C -0.32267 0.43894 0.40241 S -1.49413 -0.09011 1.61496 C 0.32267 -0.43894 -0.40241 C 0.15152 -1.91638 -0.41273 N -0.03790 -2.56192 -1.51437 C 0.04188 -1.94568 -2.75199 C 0.78837 -0.77019 -2.98157 S 1.49413 0.09011 -1.61496 C 0.98434 -0.29506 -4.27998 C 0.41039 -0.96173 -5.35642 C -0.36411 -2.10523 -5.14127 C -0.53261 -2.59639 -3.85561 C 0.26997 -2.70456 0.83582 C -0.26997 2.70456 -0.83582 H 1.09834 3.50392 3.66718 H 0.81969 2.62068 5.98147 H -0.55970 0.58278 6.36318 H -1.56371 -0.61020 4.43871 H -1.09834 -3.50392 -3.66718 H -0.81969 -2.62068 -5.98147 H 0.55970 -0.58278 -6.36318 H 1.56371 0.61020 -4.43871 C 1.03885 -2.24432 1.91124 C 1.19810 -3.02795 3.04944 C 0.58124 -4.27506 3.13252 C -0.18791 -4.73908 2.06485 C -0.33607 -3.96429 0.92061 H 1.52168 -1.27294 1.85326 H 1.80509 -2.66204 3.87261 H 0.70076 -4.88423 4.02416 H -0.67210 -5.70983 2.12434 H -0.92121 -4.31860 0.07824 C 0.33607 3.96429 -0.92061 C 0.18791 4.73908 -2.06485 C -0.58124 4.27506 -3.13252 C -1.19810 3.02795 -3.04944 C -1.03885 2.24432 -1.91124 H 0.92121 4.31860 -0.07824 H 0.67210 5.70983 -2.12434 H -0.70076 4.88423 -4.02416 H -1.80509 2.66204 -3.87261 H -1.52168 1.27294 -1.85326							
<b>Oxygen species</b>							
O <sub>2</sub>							
O 0.00000 0.00000 0.60144	-150.17434	-150.16711	-150.19038	-150.26391	-150.27995	-150.31368	-150.32972
O 0.00000 0.00000 -0.60144							0.0
H <sub>2</sub> O <sub>2</sub>							
O 0.00000 0.71589 -0.05491	-151.39619	-151.36500	-151.39074	-151.48905	-151.48360	-151.54187	-151.53642
							0.0

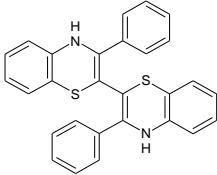
O 0.00000 -0.71589 -0.05491 H -0.81094 -0.89788 0.43932 H 0.81094 0.89788 0.43932								
H <sub>2</sub> O								
O 0.00000 0.00000 0.11621 H 0.00000 0.76535 -0.46485 H 0.00000 -0.76535 -0.46485	-76.34912	-76.32371	-76.34512			-151.54187	-151.53787	0.0
HOO·								
O 0.05526 0.71218 0.00000 O 0.05526 -0.60358 0.00000 H -0.88411 -0.86876 0.00000	-150.75733	-150.73907	-150.76503	-150.84599	-150.85368	-150.89687	-150.90456	0.0
HO·								
O 0.00000 0.00000 0.10836 H 0.00000 0.00000 -0.86687	-75.65706	-75.64516	-75.66539	-75.70173	-75.71005	-75.72841	-75.73674	0.0

**Table S4.** Neutral forms in methanol. For each chemical species, values are reported for the most stable conformer / geometric isomer identified.  $G_{RRHO,calc}$  [M062X / 6-311++G(2d,2p) / SMD] =  $G_{el}$  [M062X / 6-311++G(2d,2p) / SMD // PBE0 / 6-31+G(d,p) / PCM] -  $G_{el}$  [PBE0 / 6-31+G(d,p) / PCM] +  $G_{RRHO}$  [PBE0 / 6-31+G(d,p) / PCM]; and likewise for  $G_{RRHO,calc}$  [PBE0 / 6-31+G(d,p) / SMD] and for  $G_{RRHO,calc}$  [M062X / 6-31+G(d,p) / SMD].

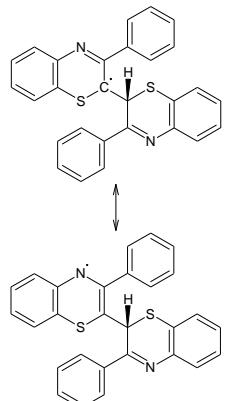
Species	PBE0 / 6-31+G(d,p) / PCM			PBE0 / 6-31+G(d,p) / SMD		M062X / 6-31+G(d,p) / SMD		M062X / 6-311++G(2d,2p) / SMD		
	$G_{el}$ / Ha	$H_{RRHO}$ / Ha	$G_{RRHO}$ / Ha	$G_{el}$ / Ha	$G_{RRHO}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$\Delta G_{RRHO,calc}$ / kcal mol <sup>-1</sup>
Cartesian coordinates / Å										
Single-bond dimer										
										
S -1.34737 1.03292 -2.39203 C -0.76722 0.11693 -0.93950 C -1.21798 0.87229 0.30123 N -1.02530 2.13869 0.43867 C 0.02861 4.17258 -0.25740 C 0.43583 5.06094 -1.24298 C 0.27026 4.73053 -2.59138 C -0.27026 3.49878 -2.94633 C -0.65567 2.58986 -1.95709 C -0.52805 2.92715 -0.59168 C -1.84818 0.13898 1.42394 C -1.86008 0.72464 2.70153 C -2.45080 0.07387 3.77661 C -3.05056 -1.17523 3.59892 C -3.05047 -1.76449 2.33710 C -2.44955 -1.11709 1.25933 H -1.26575 -0.85076 -1.00829 H 0.12159 4.42282 0.79556 H 0.86823 6.01724 -0.96444 H 0.57149 5.42798 -3.36726 H -0.38077 3.23072 -3.99341 H -1.38960 1.69333 2.83346 H -2.44033 0.53823 4.75859 H -3.51336 -1.68422 4.43952 H -3.51990 -2.73206 2.18547 H -2.48078 -1.60099 0.28861 S 1.34737 -1.03292 -2.39203 C 0.76722 -0.11693 -0.93950 C 1.21798 -0.87229 0.30123 N 1.02530 -2.13869 0.43867 C -0.02861 -4.17258 -0.25740	1983.29791	1982.86500	1982.94787	1983.31837	1982.96832	1984.44865	1984.09860	1984.79773	1984.44769	1.7

C -0.43583 -5.06094 -1.24298 C -0.27026 -4.73053 -2.59138 C 0.27026 -3.49878 -2.94633 C 0.65567 -2.58986 -1.95709 C 0.52805 -2.92715 -0.59168 C 1.84818 -0.13898 1.42394 C 1.86008 -0.72464 2.70153 C 2.45080 -0.07387 3.77661 C 3.05056 1.17523 3.59892 C 3.05047 1.76449 2.33710 C 2.44955 1.11709 1.25933 H 1.26575 0.85076 -1.00829 H -0.12159 -4.42282 0.79556 H -0.86823 -6.01724 -0.96444 H -0.57149 -5.42798 -3.36726 H 0.38077 -3.23072 -3.99341 H 1.38960 -1.69333 2.83346 H 2.44033 -0.53823 4.75859 H 3.51336 1.68422 4.43952 H 3.51990 2.73206 2.18547 H 2.48078 1.60099 0.28861										
	S 1.00027 -0.75723 -1.84385 C -0.28417 -0.36409 -0.61977 C -0.97808 -1.66332 -0.24538 N -0.31501 -2.70859 0.11063 C 1.74075 -3.75167 0.76503 C 3.10284 -3.96606 0.60781 C 3.82226 -3.22229 -0.33270 C 3.18225 -2.24109 -1.08221 C 1.81735 -1.99979 -0.90410 C 1.07044 -2.77447 0.01103 C -2.45647 -1.74638 -0.25337 C -3.09118 -2.73139 0.52202 C -4.47459 -2.85275 0.52213 C -5.25496 -2.00107 -0.26376 C -4.63712 -1.02649 -1.04339 C -3.24988 -0.89318 -1.03301 H -0.96460 0.30970 -1.14221 H 1.15801 -4.34297 1.46566 H 3.60353 -4.72340 1.20351 H 4.88445 -3.39833 -0.47411 H 3.74341 -1.64413 -1.79574 H -2.47911 -3.39044 1.12892	1983.29751	1982.86470	1982.94916	1983.31826	1982.96991	1984.44902	1984.10067	1984.79871	1984.45036

H -4.94843 -3.61177 1.13812 H -6.33686 -2.09775 -0.26610 H -5.23341 -0.36374 -1.66372 H -2.79982 -0.13185 -1.66208 S -1.00027 0.75723 1.84385 C 0.28417 0.36409 0.61977 C 0.97808 1.66332 0.24538 N 0.31501 2.70859 -0.11063 C -1.74075 3.75167 -0.76503 C -3.10284 3.96606 -0.60781 C -3.82226 3.22229 0.33270 C -3.18225 2.24109 1.08221 C -1.81735 1.99979 0.90410 C -1.07044 2.77447 -0.01103 C 2.45647 1.74638 0.25337 C 3.09118 2.73139 -0.52202 C 4.47459 2.85275 -0.52213 C 5.25496 2.00107 0.26376 C 4.63712 1.02649 1.04339 C 3.24988 0.89318 1.03301 H 0.96460 -0.30970 1.14221 H -1.15801 4.34297 -1.46566 H -3.60353 4.72340 -1.20351 H -4.88445 3.39833 0.47411 H -3.74341 1.64413 1.79574 H 2.47911 3.39044 -1.12892 H 4.94843 3.61177 -1.13812 H 6.33686 2.09775 0.26610 H 5.23341 0.36374 1.66372 H 2.79982 0.13185 1.66208										
	S -1.66149 -2.01085 -1.34836 C -0.46001 -1.13796 -0.26838 C -1.07181 -0.92777 1.11193 N -2.30503 -0.62886 1.32189 C -4.44042 0.15876 0.61134 C -5.46391 0.26499 -0.32137 C -5.32233 -0.32902 -1.57836 C -4.15016 -1.00634 -1.90085 C -3.11333 -1.10038 -0.96858 C -3.25150 -0.52301 0.30951 C -0.17371 -1.00136 2.29388 C -0.63928 -0.53127 3.53436 C 0.16228 -0.58742 4.66705	1983.29263	1982.85921	1982.94366	1983.31313	1982.96416	1984.44203	1984.09306	1984.79221	1984.44324

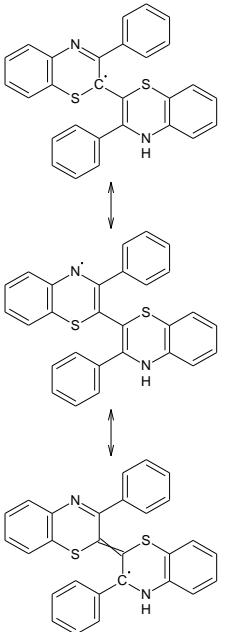
C 1.45292 -1.11572 4.58972 C 1.92999 -1.58101 3.36682 C 1.12729 -1.52157 2.22900 H 0.33813 -1.87672 -0.18689 H -4.53547 0.59943 1.59976 H -6.37425 0.80032 -0.06874 H -6.12153 -0.26078 -2.31056 H -4.03177 -1.45907 -2.88167 H -1.64147 -0.11975 3.58788 H -0.21815 -0.21489 5.61404 H 2.08076 -1.16034 5.47501 H 2.93206 -1.99341 3.29208 H 1.53851 -1.89321 1.29635 S -0.89133 1.56696 -0.95107 C 0.13687 0.11239 -0.84420 C 1.42682 0.20850 -1.25806 N 1.97314 1.44292 -1.60387 C 2.56731 3.62273 -0.68766 C 2.19028 4.78392 -0.01601 C 0.88559 4.93785 0.45099 C -0.05153 3.92827 0.22936 C 0.30919 2.78722 -0.48432 C 1.62546 2.61986 -0.93066 C 2.36966 -0.93332 -1.35224 C 3.61492 -0.87290 -0.70946 C 4.51357 -1.93108 -0.81323 C 4.18503 -3.05754 -1.56807 C 2.95504 -3.12015 -2.22156 C 2.05262 -2.06368 -2.11708 H 3.59131 3.49282 -1.02929 H 2.92632 5.56441 0.15268 H 0.59438 5.83789 0.98353 H -1.07226 4.03635 0.58517 H 3.87075 -0.00309 -0.10971 H 5.46959 -1.87754 -0.30054 H 4.88831 -3.88128 -1.65090 H 2.69984 -3.98787 -2.82276 H 1.10527 -2.10259 -2.64804 H 2.92685 1.40533 -1.93573																			
	S 1.73424 -2.47879 -0.10772 C 0.62031 -1.09302 -0.38510 C 1.00850 -0.13917 -1.26827 N 2.30226 -0.14342 -1.79089	-	1983.29245	-	1982.85882	-	1982.94278	-	1983.31390	1982.96423	-	1984.44526	-	1984.09559	-	1984.79606	-	1984.44639	2.5

C 4.64211 0.10761 -1.15274 C 5.72637 -0.30814 -0.38276 C 5.58092 -1.34203 0.54164 C 4.34543 -1.97464 0.68204 C 3.27243 -1.59583 -0.12272 C 3.40835 -0.53700 -1.02983 C 0.14608 0.97201 -1.73087 C 0.64498 2.28040 -1.79598 C -0.15363 3.32030 -2.26733 C -1.45818 3.06550 -2.68707 C -1.96021 1.76406 -2.63364 C -1.16461 0.72452 -2.16144 H 4.74937 0.93197 -1.85336 H 6.68427 0.19034 -0.49835 H 6.42258 -1.65904 1.14971 H 4.21870 -2.78354 1.39604 H 1.65442 2.49342 -1.45274 H 0.24381 4.33068 -2.30153 H -2.07987 3.87521 -3.05837 H -2.97196 1.55608 -2.97038 H -1.55167 -0.28988 -2.13674 S -1.73454 -2.47869 0.10647 C -0.62050 -1.09316 0.38455 C -1.00857 -0.13976 1.26830 N -2.30227 -0.14422 1.79105 C -4.64219 0.10721 1.15333 C -5.72655 -0.30803 0.38322 C -5.58122 -1.34136 -0.54183 C -4.34577 -1.97394 -0.68272 C -3.27268 -1.59565 0.12215 C -3.40846 -0.53735 1.02990 C -0.14599 0.97114 1.73129 C -0.64480 2.27952 1.79721 C 0.15413 3.31920 2.26851 C 1.45883 3.06415 2.68764 C 1.96069 1.76266 2.63363 C 1.16482 0.72337 2.16135 H -4.74935 0.93115 1.85447 H -6.68442 0.19042 0.49921 H -6.42296 -1.65796 -1.15001 H -4.21915 -2.78242 -1.39721 H -1.65436 2.49278 1.45447 H -0.24321 4.32959 2.30330 H 2.08075 3.87369 3.05891 H 2.97254 1.55446 2.96996 H 1.55178 -0.29106 2.13614 H 2.48712 0.57649 -2.47491 H -2.48703 0.57540 2.47541									
<b>Single-bond dimer, radical</b>									

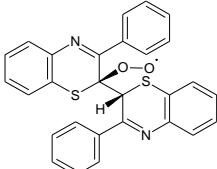


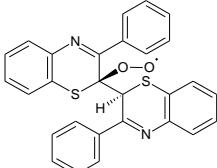
S 0.77880 1.55158 -0.55422  
 C -0.31497 0.45740 0.24075  
 C -1.66152 0.79353 0.46135  
 N -2.28451 1.89584 0.04636  
 C -2.40461 4.00511 -1.03349  
 C -1.83747 5.06933 -1.71175  
 C -0.47058 5.05768 -2.01989  
 C 0.31446 3.97400 -1.64914  
 C -0.25943 2.89635 -0.96715  
 C -1.63444 2.88941 -0.63858  
 C -2.55821 -0.14949 1.19925  
 C -2.30237 -0.52133 2.52388  
 C -3.18364 -1.36093 3.20364  
 C -4.32535 -1.84289 2.56515  
 C -4.59001 -1.47118 1.24671  
 C -3.71656 -0.62259 0.57088  
 H -3.46060 3.99656 -0.78026  
 H -2.45268 5.91535 -2.00290  
 H -0.02014 5.89133 -2.54954  
 H 1.37409 3.95834 -1.89011  
 H -1.42359 -0.13518 3.03353  
 H -2.97842 -1.63364 4.23486  
 H -5.00898 -2.50077 3.09402  
 H -5.48018 -1.83918 0.74442  
 H -3.92788 -0.31996 -0.45099  
 S 1.24613 -0.82686 2.20808  
 C 0.28123 -0.86198 0.64360  
 C 1.12573 -1.53357 -0.44012  
 N 2.38832 -1.34046 -0.59471  
 C 4.40327 -0.12259 -0.20298  
 C 5.25765 0.60463 0.61488  
 C 4.88422 0.89091 1.93110  
 C 3.64942 0.46895 2.41358  
 C 2.78020 -0.24735 1.58600

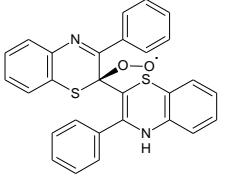
1982.66679 1982.24705 1982.33152 1982.68568 1982.35041 1983.81052 1983.47525 1984.16032 1983.82505 3.0

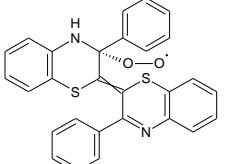
C 3.15595 -0.56389 0.26482 C 0.43987 -2.43785 -1.39317 C -0.95808 -2.52712 -1.46417 C -1.57097 -3.37626 -2.38312 C -0.79948 -4.15663 -3.24086 C 0.59396 -4.07945 -3.17712 C 1.20628 -3.22858 -2.26643 H -0.54129 -1.53092 0.90048 H 4.68026 -0.37095 -1.22350 H 6.21732 0.94041 0.23381 H 5.55130 1.44968 2.58074 H 3.35020 0.70252 3.43163 H -1.59023 -1.92911 -0.81550 H -2.65510 -3.42544 -2.42546 H -1.27828 -4.82242 -3.95310 H 1.20357 -4.68788 -3.83908 H 2.28784 -3.16371 -2.21215										
	1982.66840	1982.24840	1982.33273	1982.68839	1982.35271	1983.81521	1983.47953	1984.16556	1983.82989	0.0

C -3.54533 -1.34878 -0.26856 C -3.60292 -0.36608 0.74775 C -0.26122 0.87992 1.62136 C 0.90169 0.26559 2.10066 C 1.80579 0.97938 2.88446 C 1.56344 2.31779 3.19419 C 0.40282 2.93437 2.72660 C -0.50667 2.21731 1.95333 H -4.91116 0.66625 2.09073 H -6.96801 -0.51534 1.34079 H -6.81349 -2.25860 -0.43567 H -4.62465 -2.78140 -1.46307 H 1.09342 -0.77943 1.87562 H 2.69860 0.48575 3.25840 H 2.27179 2.87451 3.80141 H 0.20400 3.97553 2.96551 H -1.41616 2.69112 1.59631 S 1.18399 -2.49752 -0.69472 C 0.46727 -0.84644 -0.75673 C 1.22675 0.15915 -1.26808 N 2.57430 -0.04667 -1.53678 C 4.71154 -0.55878 -0.48409 C 5.48865 -1.40502 0.30435 C 4.93326 -2.55393 0.86605 C 3.59560 -2.86589 0.62151 C 2.83011 -2.04917 -0.20846 C 3.37801 -0.87927 -0.74860 C 0.72288 1.52075 -1.55240 C -0.49762 1.70674 -2.21690 C -0.95099 2.98861 -2.51282 C -0.19109 4.10295 -2.15446 C 1.02706 3.92767 -1.49941 C 1.48325 2.64592 -1.20287 H 5.13671 0.35189 -0.89832 H 6.52874 -1.15412 0.49015 H 5.53514 -3.20787 1.48947 H 3.15099 -3.75955 1.05022 H -1.08108 0.84205 -2.51855 H -1.89444 3.11766 -3.03545 H -0.54536 5.10262 -2.38902 H 1.62181 4.79002 -1.21236 H 2.42177 2.52192 -0.66871 H 3.05121 0.73100 -1.97073								
Single-bond dimer, C2-peroxy radical								

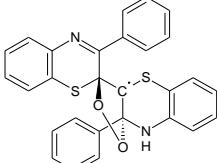
 <p>S 0.80705 -1.21254 -1.00254      C 0.22404 0.40699 -0.49018      C 1.33609 1.36571 -0.04539      N 2.57620 1.26301 -0.35351      C 4.47771 0.40512 -1.49359      C 5.12463 -0.56436 -2.24633      C 4.43498 -1.71905 -2.62675      C 3.10420 -1.89496 -2.26240      C 2.45462 -0.91338 -1.50974      C 3.13642 0.24619 -1.11227      C 0.95817 2.56189 0.75996      C 1.75818 2.91170 1.85647      C 1.47266 4.04685 2.60787      C 0.38961 4.85841 2.26801      C -0.40234 4.52792 1.17018      C -0.12462 3.38579 0.42157      H 4.98826 1.31111 -1.18069      H 6.16178 -0.42664 -2.53535      H 4.93245 -2.48509 -3.21392      H 2.56838 -2.79078 -2.56406      H 2.60008 2.27751 2.11664      H 2.09557 4.29733 3.46172      H 0.16728 5.74560 2.85377      H -1.23650 5.16309 0.88694      H -0.73498 3.16458 -0.44901      S -0.29964 -0.13344 2.22710      C -0.90871 0.24534 0.56065      C -2.01930 -0.72110 0.15409      N -2.04993 -1.96741 0.46522      C -1.07080 -3.98614 1.27669      C -0.20907 -4.68161 2.11536      C 0.61950 -3.98014 2.99404      C 0.60076 -2.58792 3.01192      C -0.25105 -1.88920 2.15515      C -1.10818 -2.58465 1.28235      C -3.13490 -0.19954 -0.67322      C -3.59151 1.12238 -0.57716      C -4.66892 1.55715 -1.34550      C -5.29461 0.68547 -2.23448      C -4.84289 -0.63100 -2.34376      C -3.77827 -1.07077 -1.56638      H -1.34360 1.23850 0.67681      H -1.73783 -4.50959 0.59783</p>	-	2132.84351	-	2132.41421	-	2132.50282	-	2132.86349	-	2132.52280	-	2134.08919	-	-	2133.74850	-	2134.48558	-	2134.14489	0.3
--	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	---	------------	---	------------	---	------------	-----

H -0.19003 -5.76691 2.09413 H 1.28751 -4.51497 3.66251 H 1.25611 -2.04118 3.68441 H -3.13719 1.82255 0.11748 H -5.01877 2.58041 -1.24611 H -6.12809 1.02940 -2.84004 H -5.31981 -1.31499 -3.03986 H -3.42199 -2.09266 -1.64602 O -0.48516 1.08164 -1.62885 O 0.27147 1.21343 -2.67804									
 S -1.17325 -1.01276 -1.59707 C 0.19088 -0.46285 -0.50778 C 0.92395 -1.72794 -0.02905 N 0.26998 -2.68568 0.52713 C -1.73741 -3.58949 1.47853 C -3.10806 -3.80024 1.43935 C -3.88125 -3.18846 0.44755 C -3.28705 -2.33544 -0.47589 C -1.91178 -2.09168 -0.41723 C -1.11600 -2.74147 0.54830 C 2.37476 -1.93639 -0.25668 C 2.79897 -3.24887 -0.52337 C 4.14465 -3.53576 -0.71996 C 5.09452 -2.51610 -0.64702 C 4.68547 -1.21078 -0.38016 C 3.33694 -0.91819 -0.19351 H -1.11343 -4.08478 2.21656 H -3.57560 -4.45519 2.16816 H -4.95157 -3.36509 0.40173 H -3.89033 -1.83849 -1.23007 H 2.05536 -4.03716 -0.58112 H 4.45209 -4.55492 -0.93554 H 6.14679 -2.73765 -0.80066 H 5.41810 -0.41156 -0.31552 H 3.04780 0.10268 0.02135 S 0.91028 0.76756 1.95074 C -0.32378 0.41798 0.66829 C -0.96402 1.72209 0.21056 N -0.28797 2.78949 -0.02890 C 1.76485 3.96273 -0.37253 C 3.09165 4.22077 -0.05745 C 3.74362 3.44124 0.90214	2132.84353	2132.41399	2132.50126	2132.86278	2132.52051	2134.08990	2133.74763	2134.48627	2134.14400

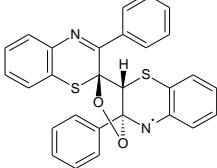
C 3.07663 2.38403 1.51327 C 1.75147 2.10092 1.17090 C 1.06940 2.90757 0.23767 C -2.43188 1.78551 0.01751 C -2.95552 2.68735 -0.92311 C -4.32754 2.80261 -1.10650 C -5.20541 2.03133 -0.34133 C -4.69717 1.14166 0.60226 C -3.32068 1.01121 0.77510 H -1.06288 -0.19744 1.18653 H 1.22942 4.57649 -1.09110 H 3.61469 5.03856 -0.54369 H 4.77483 3.65063 1.17017 H 3.58735 1.76579 2.24671 H -2.26781 3.28501 -1.51242 H -4.71540 3.49411 -1.84900 H -6.27855 2.12419 -0.48121 H -5.37143 0.54398 1.20865 H -2.95672 0.31973 1.52882 O 1.09083 0.33067 -1.31612 O 0.59786 0.68155 -2.47311										
	S -2.13102 -0.78424 -1.29878 C -0.91808 -0.29379 -0.04940 C -1.21079 1.09211 0.55749 N -2.36882 1.64186 0.61174 C -4.72987 1.80263 0.38776 C -5.94652 1.38786 -0.13567 C -5.98916 0.29868 -1.01024 C -4.81996 -0.37682 -1.34617 C -3.59905 0.03761 -0.80935 C -3.53735 1.13915 0.05875 C -0.09943 1.81013 1.23546 C 0.91377 1.14370 1.93807 C 1.89941 1.86651 2.60816 C 1.89658 3.25928 2.57577 C 0.89192 3.93091 1.87640 C -0.09987 3.21272 1.21869 H -4.66683 2.65008 1.06408 H -6.85956 1.91123 0.13060 H -6.93546 -0.03081 -1.42879 H -4.85470 -1.22908 -2.01934 H 0.92614 0.06076 1.99072	2132.84351	2132.41373	2132.50175	2132.86359	2132.52184	2134.09018	2133.74843	2134.48706	2134.14531

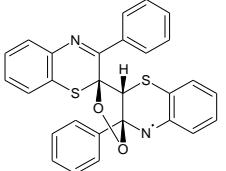
H 2.67009 1.33495 3.15905 H 2.67092 3.81936 3.09228 H 0.88298 5.01671 1.84243 H -0.88459 3.72929 0.67494 C 0.42361 -0.40797 -0.71807 S 0.75218 0.93772 -1.84434 C 2.46716 1.17529 -1.46362 C 3.23709 0.03156 -1.22322 N 2.60841 -1.21830 -1.16372 C 1.34567 -1.39829 -0.60903 C 3.06035 2.43557 -1.48144 C 4.43958 2.55579 -1.31312 C 5.21239 1.41509 -1.09706 C 4.61536 0.15798 -1.03382 C 1.17381 -2.70723 0.07062 C 0.18456 -3.60275 -0.35126 C 0.06096 -4.84913 0.25712 C 0.92361 -5.21278 1.29060 C 1.91934 -4.32929 1.70807 C 2.05154 -3.08623 1.09486 H 2.44589 3.31491 -1.65176 H 4.90527 3.53558 -1.35313 H 6.28665 1.50124 -0.96371 H 5.21525 -0.72745 -0.83957 H -0.48259 -3.32436 -1.16168 H -0.70744 -5.53860 -0.08020 H 0.82441 -6.18430 1.76608 H 2.59372 -4.60735 2.51271 H 2.82490 -2.39781 1.42635 O -0.92243 -1.22637 1.11254 O -2.11489 -1.42042 1.59248 H 3.22811 -2.01037 -1.06535									
<b>Single-bond dimer, C3-peroxy radical</b>									0.0
 S 1.79908 0.17750 1.44716 C 0.48599 0.62930 0.35134 C 0.49983 2.08997 0.06331 N 1.58308 2.70383 -0.27783 C 3.85950 2.63390 -1.02661 C 5.14628 2.11908 -0.95796 C 5.42061 1.03387 -0.12007 C 4.39878 0.44535 0.61812 C 3.09608 0.94029 0.52235	2132.84761	2132.41794	2132.50691	2132.86794	2132.52724	2134.09301	2133.75231	2134.49060	2134.14990

C 2.81261 2.06092 -0.28656 C -0.72652 2.90078 0.25612 C -1.71642 2.50397 1.16451 C -2.83264 3.30581 1.38430 C -2.98081 4.50696 0.69099 C -1.99917 4.90711 -0.21748 C -0.87583 4.11447 -0.42826 H 3.63350 3.49786 -1.64501 H 5.94184 2.57136 -1.54230 H 6.42933 0.63834 -0.04828 H 4.60492 -0.41174 1.25314 H -1.60866 1.56941 1.70767 H -3.58836 2.99114 2.09828 H -3.85636 5.12816 0.85696 H -2.11072 5.83913 -0.76433 H -0.10753 4.42047 -1.13120 S -1.51877 0.26375 -1.42417 C -0.38685 -0.26096 -0.17770 C -0.40619 -1.72972 0.19302 N -1.46823 -2.45163 -0.37465 C -3.88773 -2.71943 -0.13295 C -5.16699 -2.20016 -0.31423 C -5.34405 -0.89918 -0.78691 C -4.23306 -0.11385 -1.08753 C -2.95281 -0.64313 -0.93280 C -2.77059 -1.94406 -0.45036 C 0.89386 -2.48091 -0.06040 C 1.33236 -3.49246 0.79650 C 2.47345 -4.22916 0.48017 C 3.18078 -3.96355 -0.69018 C 2.73739 -2.96017 -1.55174 C 1.59670 -2.22575 -1.24153 H -3.74972 -3.72743 0.24868 H -6.02989 -2.81317 -0.07180 H -6.34237 -0.49267 -0.91500 H -4.35574 0.90198 -1.45187 H 0.80031 -3.70528 1.71776 H 2.81038 -5.00871 1.15727 H 4.07240 -4.53517 -0.93097 H 3.27959 -2.74767 -2.46856 H 1.25450 -1.44876 -1.91935 H -1.41109 -3.44271 -0.17871 O -0.58623 -1.63603 1.74993 O -1.27410 -2.61718 2.23538								
<b>Single-bond dimer, dioxolane radical</b>								

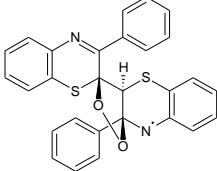
 <p> S 1.75824 -1.85592 0.45550  C 1.02793 -0.26057 -0.12216  C 1.91951 0.87372 0.39880  N 3.20116 0.83504 0.30088  C 5.23152 -0.07637 -0.56746  C 6.03136 -1.15134 -0.92565  C 5.52899 -2.45392 -0.83632  C 4.22140 -2.67233 -0.41843  C 3.40290 -1.58829 -0.08410  C 3.90860 -0.27391 -0.13977  C 1.31352 2.07172 1.02243  C 1.93291 2.63312 2.14826  C 1.41168 3.77831 2.74204  C 0.27406 4.38636 2.20938  C -0.33845 3.84251 1.08100  C 0.17222 2.68787 0.49334  H 5.60895 0.94140 -0.60368  H 7.04965 -0.98113 -1.26154  H 6.15451 -3.30073 -1.10246  H 3.82455 -3.68220 -0.36484  H 2.81882 2.15505 2.55518  H 1.89224 4.19560 3.62223  H -0.13235 5.28130 2.67189  H -1.21605 4.31829 0.65297  H -0.30633 2.28645 -0.39360  S -1.07645 -0.58082 1.74320  C -0.42941 -0.30295 0.19075  C -1.15310 -0.57761 -1.10360  N -1.99693 -1.74254 -1.02398  C -3.97382 -2.76259 -0.10004  C -4.80278 -3.07283 0.96849  C -4.50692 -2.60480 2.25093  C -3.36962 -1.83218 2.44314  C -2.51896 -1.53502 1.37282  C -2.81413 -1.99066 0.07699  C -1.88107 0.63845 -1.67461  C -1.54512 1.15884 -2.92611  C -2.24016 2.25361 -3.44081  C -3.27266 2.83765 -2.71043  C -3.61064 2.32063 -1.45872  C -2.91912 1.22883 -0.94219  H -4.21468 -3.12050 -1.09806  H -5.68993 -3.67469 0.79589 </p>	-	2132.85449	-	2132.51148	-	2132.87517	-	2132.53216	-	2134.09916	-	2133.75615	-	2134.49599	-	2134.15298	1.0
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

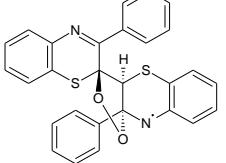
H -5.15520 -2.83501 3.09008 H -3.12703 -1.45493 3.43327 H -0.73910 0.70834 -3.49526 H -1.96924 2.65016 -4.41523 H -3.81094 3.69180 -3.11104 H -4.41294 2.77035 -0.88075 H -3.18973 0.84295 0.03701 O 1.03127 -0.14185 -1.53914 O -0.06384 -0.96602 -1.96514 H -2.46628 -1.92658 -1.90326									
<p>S 1.46007 -1.99991 1.48483 C 0.95125 -0.29546 0.92057 C 2.17882 0.35533 0.28595 N 2.90086 -0.26597 -0.57724 C 3.26179 -2.05417 -2.12169 C 3.21432 -3.39659 -2.47129 C 2.64424 -4.32492 -1.59534 C 2.09778 -3.90206 -0.38806 C 2.11983 -2.54701 -0.04536 C 2.72249 -1.60610 -0.90567 C 2.54108 1.75127 0.61959 C 3.90148 2.09282 0.65201 C 4.29580 3.40171 0.90618 C 3.33526 4.39175 1.11869 C 1.98108 4.06187 1.08004 C 1.58059 2.74947 0.84116 H 3.72418 -1.32047 -2.77551 H 3.63207 -3.72454 -3.41826 H 2.61518 -5.37843 -1.85698 H 1.63865 -4.61878 0.28695 H 4.64170 1.31706 0.48255 H 5.35277 3.64971 0.94050 H 3.64153 5.41539 1.31484 H 1.22919 4.83013 1.23640 H 0.52288 2.50798 0.81088 S -0.39249 -0.06473 -1.60369 C -0.28636 -0.27994 0.08700 C -1.42443 0.10150 0.99735 N -1.77744 1.47561 0.70713 C -3.11324 2.84790 -0.77867 C -3.53196 3.20007 -2.05442 C -3.05073 2.51228 -3.17117</p>	2132.85448	2132.42450	2132.51041	2132.87432	2132.53026	2134.09887	2133.75481	2134.49527	2134.15121

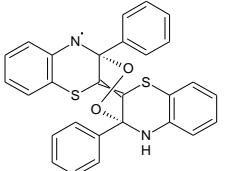
C -2.12997 1.48784 -2.99451 C -1.68282 1.14632 -1.71383 C -2.19063 1.80930 -0.58041 C -2.59210 -0.87858 1.04296 C -2.32574 -2.25044 1.11054 C -3.36978 -3.16715 1.17449 C -4.69288 -2.72207 1.16908 C -4.96282 -1.35753 1.10148 C -3.91600 -0.43716 1.03800 H -3.50572 3.37175 0.08966 H -4.24878 4.00662 -2.17561 H -3.38612 2.77340 -4.16967 H -1.73618 0.95336 -3.85515 H -1.29490 -2.59549 1.11589 H -3.15152 -4.22989 1.22659 H -5.50892 -3.43750 1.21510 H -5.98938 -1.00309 1.09524 H -4.14585 0.62155 0.97770 O 0.56878 0.39217 2.09394 O -0.82087 0.02778 2.28767 H -2.29739 1.92695 1.45050										
	S 1.44917 -1.52601 0.03215 C 0.83096 0.15454 -0.30826 C 1.84410 1.19020 0.19580 N 3.11301 1.05470 0.06109 C 5.04749 0.04345 -0.90266 C 5.74177 -1.05773 -1.38149 C 5.11989 -2.30992 -1.41796 C 3.80121 -2.45001 -1.00052 C 3.09280 -1.33562 -0.54083 C 3.71604 -0.07638 -0.47476 C 1.36235 2.44145 0.83956 C 0.52411 3.33671 0.16130 C 0.13050 4.52615 0.76987 C 0.55959 4.82805 2.06218 C 1.39677 3.94252 2.74001 C 1.80271 2.75804 2.12976 H 5.51487 1.02207 -0.84454 H 6.76891 -0.94832 -1.71546 H 5.66114 -3.17866 -1.78052 H 3.31257 -3.41940 -1.04154 H 0.20553 3.11997 -0.85514	2132.85417	2132.42510	2132.51257	2132.87505	2132.53345	2134.09824	2133.75664	2134.49366	2134.15207

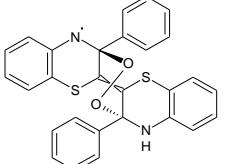
H -0.50840 5.21932 0.23055 H 0.24603 5.75307 2.53723 H 1.73691 4.17411 3.74519 H 2.45956 2.06786 2.65109 S -1.08021 -0.27648 1.81787 C -0.62362 0.28848 0.17397 C -1.44247 -0.32513 0.98951 N -1.81222 -1.70547 -0.93900 C -2.27181 -3.77611 0.06416 C -2.40203 -4.59622 1.15938 C -2.12474 -4.09404 2.44462 C -1.70665 -2.77583 2.61162 C -1.56804 -1.92830 1.51441 C -1.86800 -2.40608 0.19124 C -2.67587 0.51778 -1.29524 C -3.85773 0.31210 -0.57817 C -4.97178 1.11404 -0.81903 C -4.91556 2.12155 -1.78118 C -3.73906 2.32348 -2.50152 C -2.62179 1.52562 -2.26017 H -0.84072 1.35734 0.19985 H -2.47904 -4.13102 -0.94075 H -2.71536 -5.62794 1.03516 H -2.22300 -4.73608 3.31434 H -1.47650 -2.40554 3.60693 H -3.91740 -0.47757 0.16540 H -5.88562 0.94647 -0.25631 H -5.78583 2.74292 -1.97179 H -3.68906 3.10198 -3.25751 H -1.70826 1.67810 -2.82580 O 0.66387 0.44707 -1.68227 O -0.51039 -0.27455 -2.10411										
 S 1.50720 -1.18567 0.84387 C 0.87549 0.13592 -0.23239 C 1.73470 1.40008 -0.11194 N 3.00263 1.40653 0.09330 C 5.16224 0.40663 0.21502 C 6.00150 -0.67115 0.45606 C 5.45795 -1.90979 0.81191 C 4.08024 -2.06869 0.90707 C 3.23525 -0.98425 0.65159 C 3.76821 0.26922 0.31056	2132.84384	2132.41453	2132.49942	2132.86390	2132.51948	2134.08806	2133.74363	2134.48364	2134.13921	9.6

C 1.09852 2.72950 -0.32297									
C 0.32079 3.00885 -1.45579									
C -0.20737 4.28395 -1.64574									
C 0.02344 5.28800 -0.70595									
C 0.79728 5.01606 0.42209									
C 1.33774 3.74668 0.60909									
H 5.55907 1.38180 -0.05171									
H 7.07730 -0.55039 0.37477									
H 6.10887 -2.75634 1.00876									
H 3.65534 -3.03295 1.17193									
H 0.14932 2.23948 -2.20356									
H -0.79706 4.49262 -2.53370									
H -0.39535 6.27919 -0.85404									
H 0.98232 5.79369 1.15756									
H 1.94761 3.53195 1.48162									
S -1.30686 0.15373 1.66223									
C -0.61642 0.29501 0.01159									
C -1.25102 -0.67095 -0.99679									
N -2.59580 -0.29529 -1.29133									
C -4.73566 0.37737 -0.60591									
C -5.66187 0.73634 0.34531									
C -5.26340 0.88219 1.68516									
C -3.93158 0.69263 2.04788									
C -2.97199 0.33562 1.10325									
C -3.36485 0.12845 -0.27541									
C -1.18670 -2.18286 -0.75962									
C -0.37853 -2.97682 -1.58018									
C -0.33136 -4.35788 -1.40639									
C -1.09413 -4.96811 -0.41258									
C -1.91891 -4.18655 0.39425									
C -1.97358 -2.80573 0.21595									
H -0.89608 1.28870 -0.34889									
H -5.01483 0.24398 -1.64660									
H -6.69632 0.90428 0.06314									
H -5.98715 1.16337 2.44366									
H -3.62983 0.84279 3.08085									
H 0.22247 -2.51118 -2.35234									
H 0.30552 -4.95645 -2.05154									
H -1.05620 -6.04505 -0.27558									
H -2.53321 -4.65038 1.16061									
H -2.64625 -2.22799 0.83944									
O 0.90246 -0.23691 -1.63696									
O -0.45806 -0.31273 -2.14135									

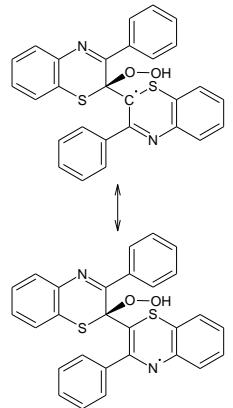
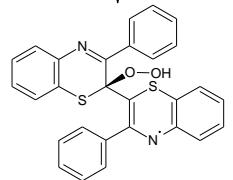
 <p>S -0.46197 -2.46280 -1.64436      C 0.12105 -0.84058 -0.99491      C 1.55271 -1.03613 -0.50365      N 1.84376 -1.99382 0.30091      C 1.19600 -3.73411 1.80972      C 0.41302 -4.83018 2.14326      C -0.62727 -5.22707 1.29798      C -0.90153 -4.50536 0.14080      C -0.13709 -3.38009 -0.17995      C 0.94102 -2.99372 0.64492      C 2.63716 -0.08837 -0.86167      C 3.52654 0.30422 0.14951      C 4.59518 1.14746 -0.13557      C 4.80164 1.59792 -1.43960      C 3.93082 1.20111 -2.45358      C 2.84960 0.37034 -2.16941      H 2.02889 -3.42844 2.43616      H 0.62004 -5.38687 3.05212      H -1.23386 -6.09294 1.54563      H -1.72180 -4.80053 -0.50734      H 3.36236 -0.05322 1.16111      H 5.26707 1.45345 0.66125      H 5.63797 2.25356 -1.66475      H 4.09271 1.53729 -3.47361      H 2.18934 0.06260 -2.97232      S -0.36625 0.07433 1.74868      C -0.89017 -0.25662 0.05685      C -1.44711 0.98749 -0.68103      N -0.73886 2.22182 -0.55126      C 0.74044 3.77000 0.40903      C 1.56168 4.19581 1.42469      C 1.78485 3.36420 2.53922      C 1.19539 2.10432 2.60901      C 0.36571 1.64963 1.58620      C 0.08780 2.49224 0.45261      C -2.94196 1.17658 -0.46997      C -3.83659 0.22489 -0.97145      C -5.20486 0.37515 -0.76394      C -5.68935 1.46920 -0.04600      C -4.79887 2.41441 0.45814      C -3.42817 2.27301 0.24238      H -1.69895 -0.97959 0.17635      H 0.54049 4.39003 -0.45955</p>	-	2132.85572	-	2132.42652	-	2132.51245	-	2132.87643	-	2132.53316	-	2134.10251	-	-	-	-	-	-	-	-	-	0.0
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	---	---	---	---	---	---	---	---	-----

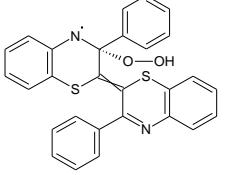
H 2.03668 5.17035 1.37098 H 2.43085 3.69604 3.34612 H 1.39214 1.46283 3.46374 H -3.46367 -0.63021 -1.52866 H -5.89309 -0.36458 -1.16244 H -6.75691 1.58314 0.11873 H -5.16810 3.26846 1.01843 H -2.73939 3.01878 0.62624 O 0.06415 0.07231 -2.06482 O -1.28809 0.56580 -2.04599											
 S 1.63281 1.69974 -2.09017 C 0.29310 0.95198 -1.07645 C -0.04651 1.96687 0.01690 N 0.88873 2.42826 0.77119 C 3.14164 2.41761 1.58454 C 4.51139 2.36028 1.37257 C 5.00986 2.13362 0.08601 C 4.13579 1.93214 -0.97708 C 2.75556 1.95044 -0.76002 C 2.24024 2.21721 0.52700 C -1.43089 2.42069 0.29427 C -1.78818 2.65952 1.63075 C -3.05285 3.13712 1.95256 C -3.97898 3.40102 0.94247 C -3.62715 3.18443 -0.38856 C -2.36550 2.69214 -0.71491 H 2.73486 2.62489 2.57000 H 5.19409 2.50820 2.20370 H 6.08111 2.10283 -0.08838 H 4.52110 1.73709 -1.97374 H -1.06313 2.45542 2.41227 H -3.31728 3.30172 2.99322 H -4.96752 3.77606 1.19171 H -4.33642 3.40136 -1.18202 H -2.10957 2.54176 -1.75689 S 1.14993 -0.89138 1.08475 C 0.65628 -0.47519 -0.60066 C -0.52111 -1.31478 -1.09353 N -0.11725 -2.65836 -1.34187 C 0.84079 -4.65302 -0.55575 C 1.48631 -5.40802 0.39483 C 1.96317 -4.79247 1.56606	-	2132.83759	2132.40829	2132.49359	2132.85778	2132.51378	2134.08388	2133.73989	2134.47958	2134.13558	11.9

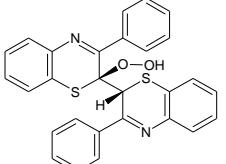
C 1.81720 -3.42128 1.75004 C 1.17431 -2.63057 0.79630 C 0.61789 -3.25032 -0.38543 C -1.87353 -1.35107 -0.38472 C -2.91204 -1.95318 -1.11147 C -4.18685 -2.06768 -0.56935 C -4.44637 -1.58366 0.71388 C -3.42187 -0.98334 1.43956 C -2.14067 -0.86878 0.89719 H 1.49246 -0.79163 -1.23347 H 0.44308 -5.10052 -1.46156 H 1.62340 -6.47413 0.24474 H 2.46971 -5.38059 2.32496 H 2.23007 -2.95211 2.63909 H -2.71515 -2.32584 -2.11192 H -4.97831 -2.53399 -1.14910 H -5.44130 -1.67087 1.14111 H -3.61351 -0.59323 2.43512 H -1.36287 -0.39951 1.48632 O -0.79606 0.71452 -1.96081 O -0.69335 -0.66207 -2.37488									
<b>Single-bond dimer, dioxane radical</b>									
 S -1.46013 -0.68729 -1.85243 C -0.49471 -0.00896 -0.55513 C -1.21344 0.19976 0.76233 N -2.34734 1.06682 0.65507 C -4.46268 1.56892 -0.25174 C -5.47647 1.34174 -1.15246 C -5.28854 0.42287 -2.20238 C -4.06882 -0.22761 -2.36095 C -3.02336 0.00210 -1.46701 C -3.21573 0.87127 -0.33787 C -1.59526 -1.12558 1.43313 C -2.63295 -1.13739 2.37149 C -2.95684 -2.31067 3.04808 C -2.24611 -3.48428 2.79651 C -1.20728 -3.47556 1.86767 C -0.88263 -2.30176 1.18909 H -4.58647 2.25086 0.58402 H -6.42334 1.86238 -1.05029 H -6.08917 0.23323 -2.91039 H -3.91952 -0.89714 -3.20366	2132.85443	2132.42486	2132.51029	2132.87617	2132.53202	2134.10095	2133.75680	2134.49778	2134.15364

H -3.18427 -0.22423 2.57312 H -3.76533 -2.30699 3.77364 H -2.49995 -4.39991 3.32311 H -0.64565 -4.38356 1.66729 H -0.06799 -2.30749 0.47145 S 1.71648 -0.15188 -2.17017 C 0.82074 0.22082 -0.69285 C 1.62557 0.72133 0.48860 N 2.89825 0.07541 0.55328 C 4.13156 -2.01565 0.48142 C 4.56263 -3.13133 -0.22904 C 4.09881 -3.37118 -1.52316 C 3.20028 -2.48032 -2.10580 C 2.79197 -1.34396 -1.40944 C 3.24655 -1.10003 -0.10220 C 1.81172 2.23858 0.54263 C 2.29089 2.80737 1.72748 C 2.52304 4.17767 1.80911 C 2.27467 4.99746 0.70773 C 1.78842 4.43634 -0.47082 C 1.55670 3.06308 -0.55289 H 4.48470 -1.83896 1.49417 H 5.25524 -3.82462 0.23914 H 4.42466 -4.24863 -0.07281 H 2.82090 -2.65673 -3.10838 H 2.46205 2.18175 2.59962 H 2.89084 4.60623 2.73710 H 2.45270 6.06707 0.77138 H 1.58291 5.06652 -1.33146 H 1.17286 2.64369 -1.47750 H 3.43887 0.30363 1.37625 O 0.91408 0.29419 1.67949 O -0.35337 0.95253 1.64279										
 S -1.71095 -1.28962 -1.50299 C -0.71379 -0.44700 -0.32693 C -1.47843 0.42389 0.64292 N -2.32938 -0.37487 1.48128 C -4.09235 -1.91359 1.75260 C -5.02512 -2.78816 1.24528 C -4.99422 -3.13272 -0.11889 C -4.00015 -2.62670 -0.95155 C -3.03586 -1.75388 -0.45037	2132.85670	2132.42678	2132.51244	2132.87835	2132.53409	2134.10427	2133.76001	2134.50154	2134.15728	0.0

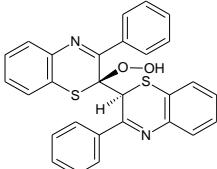
C -3.09378 -1.31579 0.91914 C -2.24541 1.56195 -0.03750 C -1.66507 2.23513 -1.11644 C -2.32659 3.30294 -1.71518 C -3.57347 3.70945 -1.23815 C -4.15014 3.04673 -0.15680 C -3.48782 1.97689 0.44543 H -4.10769 -1.60787 2.79445 H -5.78916 -3.20628 1.89309 H -5.73247 -3.81702 -0.52524 H -3.95640 -2.93725 -1.99193 H -0.69402 1.92196 -1.48976 H -1.86945 3.81638 -2.55618 H -4.09154 4.54086 -1.70762 H -5.11769 3.36150 0.22343 H -3.93764 1.46668 1.29109 S 1.47107 -1.65974 -1.37649 C 0.62011 -0.61550 -0.25819 C 1.37383 0.07954 0.86587 N 2.31858 -0.84829 1.45885 C 4.62560 -1.55592 1.17906 C 5.63039 -2.11952 0.40252 C 5.37576 -2.48493 -0.92068 C 4.10546 -2.29225 -1.45161 C 3.08481 -1.75105 -0.66483 C 3.33789 -1.36759 0.66004 C 2.01173 1.41249 0.48198 C 2.39877 2.28784 1.50323 C 3.04163 3.48360 1.19972 C 3.31155 3.81786 -0.12882 C 2.93020 2.94959 -1.14794 C 2.28154 1.75141 -0.84398 H 4.82904 -1.25550 2.20396 H 6.61922 -2.25947 0.82873 H 6.16041 -2.91113 -1.53758 H 3.89533 -2.57097 -2.48087 H 2.17942 2.04063 2.53849 H 3.32850 4.15855 2.00108 H 3.81323 4.75174 -0.36547 H 3.13253 3.20156 -2.18502 H 1.98555 1.08755 -1.65138 H 2.66818 -0.47749 2.33636 O 0.44690 0.25005 1.94036 O -0.55741 1.14985 1.46608								
<b>Single-bond dimer, C2-hydroperoxylalkyl radical</b>								

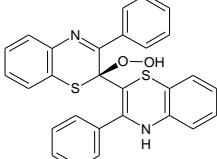
 													0.0					
S 1.12937 -2.24483 0.02122 C 0.39344 -0.79012 -0.83620 C 1.28286 0.46160 -0.85771 N 2.53938 0.48398 -0.60357 C 4.68954 -0.32636 -0.02295 C 5.56111 -1.31660 0.40510 C 5.06759 -2.59148 0.69676 C 3.71199 -2.86686 0.55404 C 2.83645 -1.86647 0.12037 C 3.31450 -0.57802 -0.17024 C 0.68481 1.73193 -1.35980 C -0.52279 1.79646 -2.07126 C -1.01473 3.01792 -2.52816 C -0.31411 4.19687 -2.28593 C 0.89164 4.14490 -1.58371 C 1.38333 2.92861 -1.12819 H 5.04419 0.67314 -0.25708 H 6.61956 -1.10113 0.51303 H 5.73894 -3.37557 1.03392 H 3.33019 -3.85939 0.77823 H -1.08031 0.89666 -2.30009 H -1.94814 3.04152 -3.08328 H -0.70115 5.14741 -2.64205 H 1.44701 5.05725 -1.38490 H 2.31405 2.88637 -0.57326 C -0.99247 -0.63453 -0.23727 S -2.17652 -1.62426 -1.05761 C -3.63521 -1.27729 -0.15992 C -3.63868 -0.36206 0.91561 N -2.53496 0.27992 1.41342 C -1.31552 0.12313 0.89969 C -4.80986 -1.91884 -0.56571 C -6.00600 -1.65113 0.08672 C -6.03539 -0.73609 1.14762	-	2132.85469	-	2132.42598	-	2132.51477	-	2132.87544	-	2132.53552	-	2134.10488	-	2133.76495	-	2134.50242	-	2134.16249

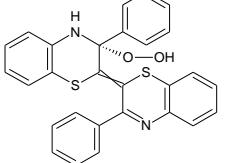
C -4.87190 -0.10675 1.55342 C -0.27917 0.87103 1.68179 C -0.37473 2.26440 1.77377 C 0.50481 2.98055 2.57983 C 1.48057 2.31077 3.31938 C 1.56702 0.92152 3.24995 C 0.69224 0.20406 2.43484 H -4.78377 -2.62202 -1.39398 H -6.91532 -2.15124 -0.23170 H -6.97127 -0.52342 1.65538 H -4.87060 0.59856 2.37909 H -1.14114 2.78390 1.20582 H 0.42690 4.06285 2.63339 H 2.16471 2.86935 3.95199 H 2.31211 0.39047 3.83571 H 0.75454 -0.87859 2.39796 O 0.13857 -1.14440 -2.20764 O 1.36470 -1.42329 -2.86079 H 1.44879 -2.38344 -2.72847										
<b>Single-bond dimer, C3-hydroperoxylalkyl radical</b>										
 S 1.98612 -0.59477 1.48809 C 0.89034 0.35096 0.46356 C 1.51765 1.60973 -0.02647 N 2.71787 1.66313 -0.49717 C 4.67806 0.56015 -1.32597 C 5.62780 -0.44900 -1.25181 C 5.48414 -1.47171 -0.30937 C 4.37310 -1.50005 0.52728 C 3.39698 -0.50441 0.42961 C 3.55271 0.55486 -0.48616 C 0.78013 2.89199 0.11317 C -0.17014 3.07287 1.12739 C -0.80340 4.30257 1.28585 C -0.50725 5.36135 0.42774 C 0.43585 5.18627 -0.58662 C 1.08135 3.96360 -0.73811 H 4.78830 1.38409 -2.02526 H 6.48903 -0.43249 -1.91280 H 6.23246 -2.25485 -0.23235 H 4.24913 -2.30782 1.24356 H -0.40898 2.25155 1.79752	2132.83987	2132.41148	2132.50132	2132.86077	2132.52223	2134.08529	2133.74674	2134.48356	2134.14501	0.0

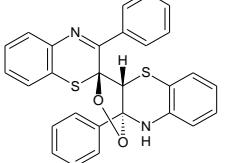
H -1.53025 4.43340 2.08246 H -1.00861 6.31754 0.54762 H 0.66742 6.00490 -1.26217 H 1.81813 3.82143 -1.52237 S -1.14052 0.74483 -1.21731 C -0.36734 -0.04457 0.14637 C -1.08097 -1.23249 0.77704 N -2.50893 -1.11304 0.92349 C -4.69867 -0.51198 0.31111 C -5.59051 0.11578 -0.52460 C -5.11762 0.89838 -1.59672 C -3.75133 1.06295 -1.80160 C -2.83264 0.44006 -0.95722 C -3.28306 -0.40721 0.10857 C -0.77571 -2.56412 0.09008 C -1.34885 -3.72598 0.62298 C -1.11416 -4.96033 0.02523 C -0.31000 -5.04645 -1.11212 C 0.26116 -3.89235 -1.64400 C 0.03142 -2.65424 -1.04507 H -5.03202 -1.13403 1.13615 H -6.65833 0.00689 -0.36336 H -5.81945 1.39372 -2.26024 H -3.39731 1.69514 -2.61127 H -1.97555 -3.65536 1.50577 H -1.55951 -5.85636 0.44789 H -0.12861 -6.00979 -1.58013 H 0.89143 -3.95121 -2.52661 H 0.48845 -1.76414 -1.46553 O -0.59483 -1.41989 2.11837 O -1.06002 -0.34182 2.93196 H -2.01314 -0.54030 2.98100									
<b>Single-bond dimer, C2-hydroperoxide</b>									0.0
 S 0.85929 -1.15570 -1.05957 C 0.17259 0.44542 -0.52240 C 1.24217 1.43586 -0.03478 N 2.49805 1.38720 -0.28790 C 4.47830 0.62291 -1.35455 C 5.19889 -0.30089 -2.09765 C 4.57467 -1.47248 -2.53562 C 3.23777 -1.70925 -2.23467 C 2.51403 -0.77520 -1.48718	2133.48695	2133.04505	2133.13369	2133.50975	2133.15649	2134.74119	2134.38793	2135.13877	2134.78551

C 3.12858 0.40297 -1.03658									
C 0.78953 2.61506 0.75897									
C -0.32135 3.39185 0.39889									
C -0.66596 4.51698 1.14622									
C 0.08517 4.87836 2.26303									
C 1.19455 4.11333 2.62528									
C 1.54625 2.99519 1.87654									
H 4.93632 1.54167 -0.99996									
H 6.24153 -0.11429 -2.33531									
H 5.12861 -2.20398 -3.11641									
H 2.75262 -2.61884 -2.57868									
H -0.89875 3.13782 -0.48446									
H -1.52125 5.11592 0.84675									
H -0.18937 5.75282 2.84595									
H 1.78597 4.38684 3.49446									
H 2.40892 2.39767 2.15479									
C -0.91531 0.17913 0.56632									
S -0.23286 -0.21150 2.20071									
C -0.10780 -1.96123 2.09227									
C -0.95279 -2.67710 1.22435									
N -1.94224 -2.08791 0.44406									
C -1.98260 -0.83418 0.16379									
C 0.79394 -2.63782 2.91500									
C 0.87642 -4.02708 2.86608									
C 0.06137 -4.74751 1.99012									
C -0.85069 -4.07485 1.18663									
C -3.14746 -0.35484 -0.62088									
C -3.78159 -1.24554 -1.50160									
C -4.88970 -0.84698 -2.23929									
C -5.39573 0.44702 -2.10176									
C -4.78004 1.33728 -1.22442									
C -3.65950 0.94406 -0.49613									
H 1.43843 -2.07566 3.58535									
H 1.58324 -4.54416 3.50816									
H 0.12981 -5.83009 1.94425									
H -1.50899 -4.61437 0.51177									
H -3.38381 -2.25006 -1.60276									
H -5.35884 -1.54563 -2.92615									
H -6.26342 0.75869 -2.67602									
H -5.17115 2.34314 -1.10302									
H -3.21249 1.65824 0.18850									
O -0.58456 1.04637 -1.57425									
O 0.29662 1.41932 -2.62905									
H 0.22946 0.65275 -3.22287									
H -1.39893 1.14358 0.72497									

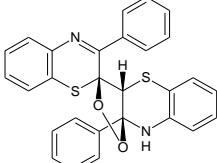
 <p> S 1.22402 -1.01892 1.58823  C -0.18098 -0.44017 0.53622  C -0.88179 -1.70551 0.01637  N -0.22000 -2.65254 -0.55117  C 1.78324 -3.53793 -1.51937  C 3.15313 -3.75577 -1.49252  C 3.93258 -3.16754 -0.49158  C 3.34606 -2.33067 0.45153  C 1.97204 -2.07652 0.40347  C 1.16735 -2.70590 -0.57060  C -2.34204 -1.91617 0.18969  C -3.29032 -0.88080 0.15505  C -4.64670 -1.16154 0.31210  C -5.07851 -2.47168 0.50797  C -4.14373 -3.50741 0.54530  C -2.79037 -3.23260 0.38893  H 1.15327 -4.01600 -2.26381  H 3.61419 -4.39779 -2.23681  H 5.00239 -3.34967 -0.45332  H 3.95477 -1.85239 1.21333  H -2.97823 0.14286 -0.01383  H -5.36627 -0.34885 0.27477  H -6.13595 -2.68504 0.63430  H -4.46974 -4.53105 0.70521  H -2.05865 -4.03307 0.42597  C 0.34191 0.45005 -0.62853  S -0.87880 0.80593 -1.92563  C -1.71966 2.14761 -1.15953  C -1.03672 2.95779 -0.23032  N 0.31982 2.83479 0.03980  C 0.98513 1.75701 -0.17684  C -3.04313 2.43254 -1.50573  C -3.70827 3.49657 -0.90337  C -3.05506 4.28072 0.05105  C -1.72913 4.01993 0.37010  C 2.45294 1.81434 0.02532  C 3.34485 1.04188 -0.73049  C 4.72053 1.16893 -0.54915  C 5.22548 2.05274 0.40195  C 4.34465 2.82163 1.16580  C 2.97329 2.71031 0.97315  H -3.55460 1.81071 -2.23570  H -4.73836 3.70746 -1.17479 </p>	-	2133.48803	-	2133.04595	-	2133.13227	-	2133.50998	-	2133.15422	-	2134.74376	-	2134.38799	-	2135.14134	-	2134.78558	-	0.0
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	-----

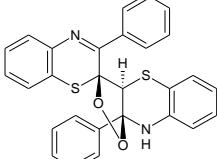
H -3.57569 5.10416 0.53047 H -1.19284 4.63755 1.08484 H 2.98337 0.35325 -1.48804 H 5.39709 0.57273 -1.15452 H 6.29800 2.14243 0.54866 H 4.72933 3.50853 1.91430 H 2.28350 3.30731 1.56076 O -0.98123 0.40497 1.32302 O -1.38921 -0.25019 2.52207 H -2.26909 -0.58883 2.27551 H 1.08438 -0.16166 -1.14588										
 S 2.12270 0.83976 -1.31425 C 0.91239 0.35841 -0.01647 C 1.23512 -1.02598 0.58224 N 2.39304 -1.57871 0.61580 C 4.75228 -1.71755 0.37450 C 5.96482 -1.29238 -0.15031 C 5.99642 -0.20128 -1.02316 C 4.81981 0.46223 -1.35600 C 3.60125 0.03586 -0.82041 C 3.55172 -1.06566 0.04975 C 0.14018 -1.74800 1.28551 C 0.15592 -3.15080 1.28729 C -0.82578 -3.87273 1.95652 C -1.83804 -3.20444 2.64797 C -1.85676 -1.81130 2.66168 C -0.87977 -1.08498 1.98244 H 4.69835 -2.56557 1.05110 H 6.88273 -1.80835 0.11409 H 6.93888 0.13756 -1.44314 H 4.84451 1.31487 -2.02940 H 0.94495 -3.66508 0.74767 H -0.80366 -4.95880 1.93648 H -2.60516 -3.76689 3.17278 H -2.63339 -1.28197 3.20667 H -0.89793 -0.00179 2.01984 C -0.42089 0.40592 -0.72490 S -0.66993 -0.96453 -1.84214 C -2.37653 -1.28093 -1.48178 C -3.20449 -0.17175 -1.27361 N -2.63396 1.10568 -1.22560 C -1.39269 1.34814 -0.63935	2133.48525	2133.04290	2133.13042	2133.50845	2133.15363	2134.74069	2134.38586	2135.13885	2134.78403	1.0

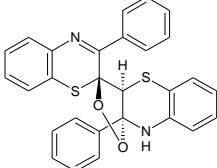
C -2.90858 -2.56833 -1.48695 C -4.28324 -2.75241 -1.33961 C -5.11348 -1.64668 -1.15728 C -4.57858 -0.36129 -1.10579 C -1.30947 2.66716 0.03918 C -0.37655 3.62391 -0.37592 C -0.34576 4.87984 0.22388 C -1.24484 5.19191 1.24392 C -2.18407 4.24649 1.65515 C -2.22417 2.99329 1.04827 H -2.24957 -3.41963 -1.63167 H -4.70060 -3.75411 -1.36988 H -6.18463 -1.78228 -1.04084 H -5.22457 0.49672 -0.93743 H 0.32022 3.38222 -1.17310 H 0.37888 5.61762 -0.10847 H -1.21755 6.17137 1.71277 H -2.88690 4.48385 2.44850 H -2.95541 2.25676 1.37206 O 0.86546 1.30178 1.04654 O 2.12615 1.31792 1.70972 H 2.55419 2.08484 1.29440 H -3.29134 1.86862 -1.14224									
<b>Single-bond dimer, C3-hydroperoxide</b>									0.0
 S 1.23021 -1.53270 1.42042 C 0.94706 -0.04531 0.50268 C 2.19551 0.46462 -0.12645 N 2.99384 -0.30590 -0.78589 C 3.47397 -2.40239 -1.84028 C 3.45452 -3.78949 -1.85283 C 2.79445 -4.48646 -0.83567 C 2.12533 -3.79242 0.16676 C 2.11021 -2.39476 0.15911 C 2.81087 -1.67996 -0.83469 C 2.59138 1.87996 0.05215 C 2.22560 2.58345 1.20854 C 2.65874 3.89363 1.39979 C 3.44339 4.52056 0.43354 C 3.80430 3.82735 -0.72480 C 3.38993 2.51417 -0.91095 H 4.01200 -1.84192 -2.59946 H 3.96700 -4.33147 -2.64185	2133.48673	2133.04405	2133.13118	2133.50926	2133.15371	2134.74078	2134.38523	2135.13967	2134.78412

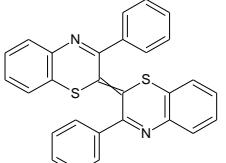
H 2.79128 -5.57233 -0.82881 H 1.59316 -4.33261 0.94503 H 1.61132 2.10033 1.96414 H 2.37974 4.42498 2.30511 H 3.77199 5.54562 0.57932 H 4.41058 4.31415 -1.48342 H 3.66940 1.96689 -1.80567 S -0.45649 2.07910 -0.43734 C -0.27173 0.53157 0.41024 C -1.48529 -0.06341 1.12446 N -2.64179 0.84566 1.09794 C -4.41947 1.35097 -0.50786 C -4.81377 1.94183 -1.70514 C -3.86899 2.52387 -2.55137 C -2.52321 2.51827 -2.19198 C -2.13168 1.95441 -0.97761 C -3.07451 1.36725 -0.12773 C -1.88022 -1.44273 0.60716 C -2.54528 -2.34555 1.44415 C -3.00176 -3.56123 0.93974 C -2.81401 -3.88091 -0.40472 C -2.16680 -2.97564 -1.24372 C -1.70152 -1.76196 -0.74137 H -5.15438 0.88476 0.14363 H -5.86336 1.93373 -1.98358 H -4.17500 2.97173 -3.49165 H -1.77530 2.95846 -2.84543 H -2.69674 -2.10609 2.49202 H -3.50518 -4.26018 1.60158 H -3.17154 -4.82900 -0.79601 H -2.01837 -3.21287 -2.29327 H -1.18934 -1.06894 -1.40264 H -3.40568 0.38689 1.58728 O -1.19664 -0.23098 2.51101 O -0.85700 1.03956 3.06573 H -1.62835 1.58028 2.79934										
<b>Single-bond dimer, dioxolane</b>										
 S -2.14628 0.25757 0.38775 C -0.51503 -0.43767 -0.04791 C -0.52544 -1.94088 0.26480 N -1.50948 -2.70604 -0.04665 C -3.53311 -3.17246 -1.22804	2133.50577	2133.06276	2133.14809	2133.52715	2133.16947	2134.75632	2134.39863	2135.15244	2134.79476	0.0

C -4.77807 -2.79719 -1.71095									
C -5.22425 -1.48263 -1.53779									
C -4.41360 -0.54478 -0.90882									
C -3.14586 -0.91385 -0.44693									
C -2.70041 -2.24087 -0.58834									
C 0.64093 -2.59039 0.91946									
C 1.92542 -2.53416 0.36235									
C 2.98347 -3.20456 0.97227									
C 2.77338 -3.92604 2.14708									
C 1.49642 -3.98752 2.70445									
C 0.43373 -3.33013 2.08988									
H -3.17500 -4.19301 -1.32765									
H -5.40897 -3.52639 -2.20989									
H -6.20302 -1.18538 -1.90237									
H -4.75303 0.48015 -0.78776									
H 2.09658 -1.98942 -0.56268									
H 3.97244 -3.16479 0.52504									
H 3.60163 -4.44163 2.62452									
H 1.32606 -4.55007 3.61787									
H -0.56433 -3.38062 2.51518									
S 0.25896 1.39179 2.05970									
C 0.61778 0.42669 0.57100									
C 1.13045 1.26584 -0.64628									
N 1.17083 2.67307 -0.42028									
C -0.40209 4.54495 -0.35940									
C -1.41259 5.23649 0.30479									
C -1.96105 4.72833 1.48247									
C -1.48995 3.52247 1.99815									
C -0.45976 2.84341 1.35010									
C 0.09066 3.34738 0.16422									
C 2.50009 0.80341 -1.12704									
C 3.60649 0.97008 -0.28718									
C 4.86978 0.55668 -0.70038									
C 5.03948 -0.02416 -1.95830									
C 3.94021 -0.18484 -2.79837									
C 2.67236 0.22770 -2.38558									
H 1.41570 -0.24089 0.89715									
H 0.01606 4.93612 -1.28354									
H -1.78015 6.17076 -0.10932									
H -2.75722 5.26093 1.99331									
H -1.91332 3.10877 2.90919									
H 3.47867 1.42933 0.68975									
H 5.72255 0.69016 -0.04096									
H 6.02513 -0.34725 -2.28090									
H 4.06472 -0.63264 -3.78019									
H 1.81712 0.10043 -3.04044									
O -0.24172 -0.36128 -1.44119									
O 0.12029 1.00880 -1.65178									
H 1.60089 3.16853 -1.19162									

 <p> S -1.58545 -1.12281 -0.84989  C -0.87575 0.14481 0.24430  C -1.64872 1.46467 0.12823  N -2.91160 1.55713 -0.08660  C -5.13174 0.70539 -0.23743  C -6.03913 -0.31122 -0.49649  C -5.57627 -1.58007 -0.86000  C -4.21145 -1.83003 -0.94466  C -3.29792 -0.80729 -0.67106  C -3.74925 0.47571 -0.32225  C -0.92941 2.74747 0.36099  C -0.14970 2.96306 1.50627  C 0.45669 4.19927 1.71809  C 0.30274 5.22672 0.78778  C -0.47181 5.01781 -0.35308  C -1.09052 3.78810 -0.56186  H -5.46462 1.70260 0.03532  H -7.10513 -0.11921 -0.42355  H -6.28050 -2.37919 -1.07109  H -3.84969 -2.81822 -1.21511  H -0.03591 2.17456 2.24495  H 1.04755 4.35949 2.61531  H 0.78236 6.18720 0.95295  H -0.59646 5.81386 -1.08151  H -1.70105 3.62283 -1.44461  S 1.28800 0.06776 -1.65893  C 0.62508 0.21794 -0.00191  C 1.19348 -0.79407 1.00604  N 2.55362 -0.42573 1.24484  C 4.75314 0.18002 0.51104  C 5.66747 0.59346 -0.44658  C 5.24459 0.86599 -1.74875  C 3.90082 0.71958 -2.06688  C 2.97100 0.28796 -1.11378  C 3.39335 0.00741 0.20406  C 1.02303 -2.28947 0.76518  C 0.15648 -3.04953 1.55685  C 0.04373 -4.42458 1.36328  C 0.79244 -5.05910 0.37373  C 1.67081 -4.31086 -0.40852  C 1.79296 -2.93734 -0.20868  H 0.96231 1.18660 0.37432  H 5.08298 -0.02069 1.52744 </p>	-	2133.48868	-	2133.04559	-	2133.13062	-	2133.50954	-	2133.15148	-	2134.73847	-	2134.38041	-	2135.13492	-	2134.77686	11.2
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	------

H 6.71130 0.71066 -0.17121 H 5.94896 1.19821 -2.50460 H 3.55324 0.93937 -3.07302 H -0.43463 -2.56314 2.32427 H -0.63386 -4.99958 1.98812 H 0.70116 -6.13066 0.22023 H 2.27222 -4.79620 -1.17187 H 2.50201 -2.37802 -0.80972 O -0.93583 -0.24341 1.63966 O 0.42101 -0.37786 2.14871 H 3.02467 -1.03015 1.90643											
	S -1.21022 -1.70238 -1.64914 C -0.02856 -0.58147 -0.76893 C 1.14602 -1.46407 -0.34584 N 0.93043 -2.53126 0.33705 C -0.51957 -3.91622 1.65217 C -1.72918 -4.56873 1.84442 C -2.77839 -4.37784 0.93994 C -2.62588 -3.50554 -0.13258 C -1.42162 -2.81850 -0.30953 C -0.34048 -3.03638 0.57278 C 2.55662 -1.12943 -0.65839 C 3.53879 -1.48310 0.28052 C 4.88440 -1.25511 0.01996 C 5.27620 -0.68120 -1.19064 C 4.31004 -0.33785 -2.13404 C 2.95861 -0.55326 -1.87182 H 0.31809 -4.07918 2.32401 H -1.85294 -5.23977 2.68898 H -3.72110 -4.89879 1.07736 H -3.44681 -3.33753 -0.82378 H 3.22826 -1.93152 1.21863 H 5.62940 -1.52309 0.76377 H 6.32805 -0.50499 -1.39704 H 4.60602 0.09681 -3.08443 H 2.22569 -0.29446 -2.62664 S 0.17297 0.43826 1.91995 C -0.74353 0.20135 0.37434 C -1.14274 1.53518 -0.33622 N -0.43003 2.67845 0.15166 C 1.80305 3.65818 0.15328 C 3.10429 3.66492 0.64901	2133.50482	2133.06177	2133.14682	2133.52549	2133.16748	2134.75598	2134.39797	2135.15202	2134.79402	0.5

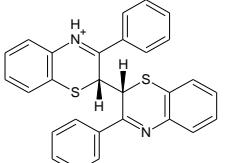
C 3.54217 2.65361 1.50473 C 2.66750 1.62987 1.86437 C 1.35672 1.63502 1.39171 C 0.91162 2.64910 0.53187 C -2.63929 1.81359 -0.30409 C -3.50218 1.22712 -1.23589 C -4.87296 1.46679 -1.16865 C -5.39761 2.28273 -0.16697 C -4.54136 2.86148 0.76765 C -3.16812 2.63158 0.69874 H -1.64232 -0.33468 0.68296 H 1.46671 4.44397 -0.51869 H 3.78232 4.46065 0.35423 H 4.56016 2.65375 1.88194 H 2.99643 0.82752 2.51850 H -3.10170 0.58339 -2.01096 H -5.53195 1.01256 -1.90308 H -6.46706 2.46589 -0.11566 H -4.93926 3.49661 1.55387 H -2.50220 3.08564 1.42529 O 0.34776 0.42570 -1.66758 O -0.82154 1.26105 -1.72260 H -0.67991 3.50807 -0.37346										
	S -0.61287 -2.33491 -1.99456 C 0.20832 -0.97440 -1.07180 C 1.00714 -1.61968 0.06238 N 0.45084 -2.45118 0.86889 C -1.46581 -3.58206 1.75245 C -2.66796 -4.25458 1.58525 C -3.23024 -4.37083 0.31063 C -2.60488 -3.78583 -0.78573 C -1.41400 -3.07546 -0.61396 C -0.81718 -2.98450 0.66116 C 2.43373 -1.28952 0.30116 C 2.84948 -1.02222 1.61224 C 4.19386 -0.79909 1.89397 C 5.14253 -0.86353 0.87327 C 4.73657 -1.14113 -0.43169 C 3.38960 -1.34198 -0.72188 H -0.99553 -3.50776 2.72862 H -3.16096 -4.70350 2.44211 H -4.16288 -4.90901 0.17078	2133.48279	2133.03970	2133.12349	2133.50415	2133.14485	2134.73721	2134.37791	2135.13376	2134.77446

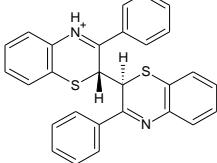
	H -3.05079 -3.85872 -1.77360 H 2.10801 -0.98551 2.40456 H 4.50108 -0.57888 2.91239 H 6.19335 -0.69864 1.09388 H 5.47095 -1.20293 -1.22969 H 3.08957 -1.56415 -1.74042 S -1.45624 0.26397 1.00695 C -0.78055 0.13113 -0.65117 C -0.08942 1.41612 -1.14085 N -1.12840 2.36260 -1.40557 C -3.04047 3.62763 -0.70381 C -4.11517 3.88364 0.13465 C -4.38577 3.03134 1.20666 C -3.56858 1.92861 1.41597 C -2.47063 1.66751 0.58686 C -2.19178 2.52766 -0.49837 C 1.07259 2.03114 -0.36514 C 0.84913 2.65845 0.86820 C 1.88972 3.29832 1.53791 C 3.16528 3.34127 0.97859 C 3.38973 2.74115 -0.25850 C 2.35379 2.08775 -0.92294 H -1.64026 0.02384 -1.31936 H -2.83657 4.28782 -1.54335 H -4.74552 4.74729 -0.05483 H -5.22786 3.21637 1.86586 H -3.77323 1.24924 2.23947 H -0.14031 2.66786 1.31038 H 1.69574 3.77427 2.49499 H 3.97472 3.84621 1.49827 H 4.37671 2.77509 -0.71117 H 2.54427 1.62075 -1.88189 O 1.05217 -0.31060 -2.00347 O 0.36956 0.89917 -2.40679 H -0.77992 3.24541 -1.75941										
<b>Double-bond dimers</b>											
	C -0.99661 0.28580 4.29094 C -0.79523 0.76007 2.99251 C -0.06062 1.94340 2.76574 C 0.50282 2.60166 3.87113 C 0.33242 2.10992 5.15730 C -0.43419 0.95991 5.36989	1982.06926	1981.66097	1981.74341	1982.08734	1981.76149	1983.21692	1982.89108	1983.56655	1983.24070	0.0

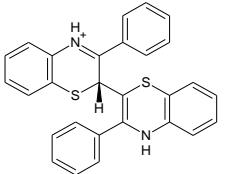
N 0.01510 2.56088 1.52588 C -0.15936 1.91126 0.42329 C -0.32068 0.43393 0.40949 S -1.48612 -0.10834 1.62205 C 0.32068 -0.43393 -0.40949 C 0.15936 -1.91126 -0.42329 N -0.01510 -2.56088 -1.52588 C 0.06062 -1.94340 -2.76574 C 0.79523 -0.76007 -2.99251 S 1.48612 0.10834 -1.62205 C 0.99661 -0.28580 -4.29094 C 0.43419 -0.95991 -5.36989 C -0.33242 -2.10992 -5.15730 C -0.50282 -2.60166 -3.87113 C 0.27665 -2.69689 0.82766 C -0.27665 2.69689 -0.82766 H 1.06536 3.51284 3.68915 H 0.78052 2.62952 5.99879 H -0.58624 0.58122 6.37615 H -1.57356 -0.62066 4.45109 H -1.06536 -3.51284 -3.68915 H -0.78052 -2.62952 -5.99879 H 0.58624 -0.58122 -6.37615 H 1.57356 0.62066 -4.45109 C 1.09922 -2.26014 1.87392 C 1.26266 -3.04220 3.01357 C 0.59567 -4.26190 3.12830 C -0.22894 -4.70075 2.09086 C -0.38115 -3.92846 0.94395 H 1.62132 -1.31090 1.79134 H 1.91192 -2.69784 3.81342 H 0.71739 -4.86778 4.02166 H -0.75509 -5.64727 2.17662 H -1.01714 -4.26493 0.13126 C 0.38115 3.92846 -0.94395 C 0.22894 4.70075 -2.09086 C -0.59567 4.26190 -3.12830 C -1.26266 3.04220 -3.01357 C -1.09922 2.26014 -1.87392 H 1.01714 4.26493 -0.13126 H 0.75509 5.64727 -2.17662 H -0.71739 4.86778 -4.02166 H -1.91192 2.69784 -3.81342 H -1.62132 1.31090 -1.79134									
<b>Oxygen species</b>									
O <sub>2</sub> O 0.00000 0.00000 0.60130 O 0.00000 0.00000 -0.60130	-150.17445	-150.16722	-150.19049	-150.17424	-150.19028	-150.26380	-150.27984	-150.31351	-150.32955 0.0
H <sub>2</sub> O <sub>2</sub> O 0.00000 0.71450 -0.06520	-151.40433	-151.37324	-151.39898	-151.41318	-151.40783	-151.50645	-151.50109	-151.55778	-151.55243 0.0

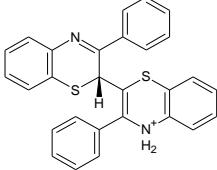
O 0.00000 -0.71450 -0.06520 H -0.74458 -0.91370 0.52162 H 0.74458 0.91370 0.52162										
H <sub>2</sub> O										
O 0.00000 0.00000 0.11750 H 0.00000 0.76275 -0.47000 H 0.00000 -0.76275 -0.47000	-76.35719	-76.33188	-76.35331	-76.36339	-76.35950					0.0
HOO·										
O 0.05522 0.71139 0.00000 O 0.05522 -0.60193 0.00000 H -0.88355 -0.87569 0.00000	-150.76380	-150.74551	-150.77146	-150.76970	-150.77736	-150.85860	-150.86626	-150.90856	-150.91622	0.0
HO·										
O 0.00000 0.00000 0.10848 H 0.00000 0.00000 -0.86783	-75.66227	-75.65038	-75.67062	-75.66470	-75.67305					0.0

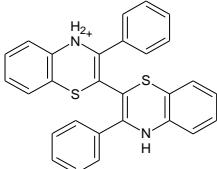
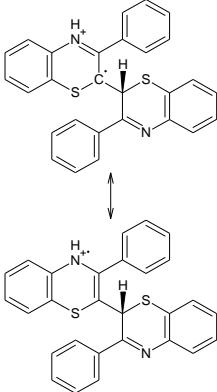
**Table S5.** Monoprotonated forms in methanol. For each chemical species, values are reported for the most stable conformer / geometric isomer identified.  $G_{RRHO,calc}$  [M062X / 6-311++G(2d,2p) / SMD] =  $G_{el}$  [M062X / 6-311++G(2d,2p) / SMD // PBE0 / 6-31+G(d,p) / PCM] -  $G_{el}$  [PBE0 / 6-31+G(d,p) / PCM] +  $G_{RRHO}$  [PBE0 / 6-31+G(d,p) / PCM]; and likewise for  $G_{RRHO,calc}$  [PBE0 / 6-31+G(d,p) / SMD] and for  $G_{RRHO,calc}$  [M062X / 6-31+G(d,p) / SMD].

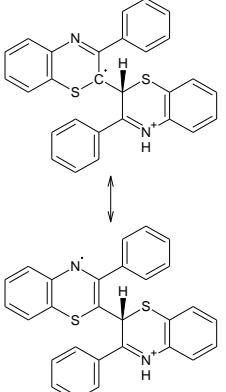
Species	PBE0 / 6-31+G(d,p) / PCM			PBE0 / 6-31+G(d,p) / SMD		M062X / 6-31+G(d,p) / SMD		M062X / 6-311++G(2d,2p) / SMD		
	$G_{el}$ / Ha	$H_{RRHO}$ / Ha	$G_{RRHO}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$\Delta G_{RRHO,calc}$ / kcal mol <sup>-1</sup>
Cartesian coordinates / Å										
Single-bond dimer										
										
S -0.95488 -2.39940 1.36073 C -0.07592 -0.94076 0.73764 C -0.74463 0.28944 1.27772 N -2.04887 0.37814 1.16827 C -4.21625 -0.24540 0.30801 C -5.12609 -1.22866 -0.05235 C -4.75783 -2.57519 0.00360 C -3.47862 -2.94394 0.40636 C -2.54964 -1.96598 0.76725 C -2.93388 -0.61683 0.71892 C 0.00878 1.40257 1.83750 C -0.48202 2.72003 1.74389 C 0.23067 3.77145 2.29882 C 1.43572 3.52827 2.96121 C 1.93178 2.22916 3.05737 C 1.23283 1.17133 2.49078 H 0.92981 -1.01639 1.15439 H -4.48875 0.80549 0.27112 H -6.12176 -0.94600 -0.37699 H -5.46992 -3.34454 -0.27726 H -3.19265 -3.99044 0.43822 H -1.38966 2.94149 1.18943 H -0.14569 4.78459 2.20245 H 1.99026 4.35397 3.39632 H 2.86496 2.03668 3.57650 H 1.62518 0.16641 2.60304 S 0.86296 -2.36672 -1.47666 C 0.04866 -0.89393 -0.81877 C 0.82305 0.33315 -1.27668 N 2.10253 0.41265 -1.15718 C 4.16894 -0.39162 -0.25717	1983.73473	1983.28790	1983.37200	1983.76701	1983.40428	1984.89083	1984.52810	1985.24033	1984.87760	0.0

C 5.03805 -1.42273 0.06968 C 4.64103 -2.75209 -0.10361 C 3.36406 -3.04418 -0.57125 C 2.47633 -2.00856 -0.87488 C 2.87789 -0.66172 -0.73977 C 0.09178 1.50240 -1.81499 C 0.73058 2.75462 -1.83650 C 0.08006 3.87481 -2.33510 C -1.22227 3.76983 -2.83030 C -1.86395 2.53414 -2.82243 C -1.21548 1.40951 -2.31562 H -0.95115 -0.91453 -1.25365 H 4.46824 0.64767 -0.15722 H 6.03086 -1.19471 0.44529 H 5.32301 -3.56265 0.13460 H 3.04597 -4.07632 -0.68824 H 1.74010 2.83049 -1.44672 H 0.58655 4.83565 -2.33469 H -1.73080 4.64661 -3.22048 H -2.87155 2.43830 -3.21574 H -1.73910 0.45945 -2.35117 H -2.49067 1.22649 1.51219										
 S 1.01274 1.00361 1.87295 C -0.23174 0.46466 0.66712 C -0.96771 1.69378 0.15153 N -0.34121 2.73491 -0.26948 C 1.67711 3.84334 -0.92896 C 3.01630 4.15116 -0.73746 C 3.73697 3.52611 0.28469 C 3.12465 2.56603 1.08301 C 1.78496 2.22692 0.86919 C 1.03351 2.88590 -0.12798 C -2.44636 1.69751 0.10235 C -3.09625 2.51660 -0.83582 C -4.48298 2.56583 -0.89177 C -5.24947 1.81039 -0.00091 C -4.61581 1.00321 0.94045 C -3.22469 0.93766 0.98659 H -0.90717 -0.17298 1.23911 H 1.09013 4.34519 -1.69268 H 3.49682 4.89169 -1.36941 H 4.77887 3.77962 0.45505 H 3.68781 2.06473 1.86559	1983.73492	1983.28791	1983.37071	1983.76576	1983.40155	1984.89051	1984.52630	1985.24064	1984.87643	0.7

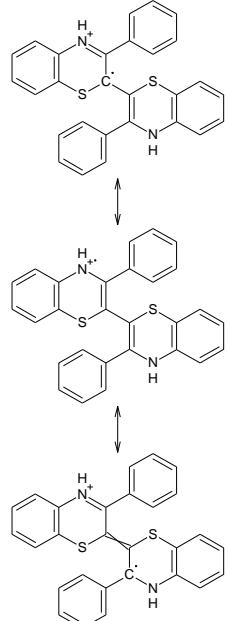
H -2.49507 3.10258 -1.52330 H -4.96983 3.19365 -1.63247 H -6.33401 1.85232 -0.04223 H -5.20253 0.41974 1.64377 H -2.76185 0.31247 1.74416 S -0.83164 -0.85422 -1.75648 C 0.38390 -0.34908 -0.49636 C 1.04255 -1.63175 -0.06598 N 0.25791 -2.56448 0.43428 C -1.85851 -3.51580 1.11681 C -3.21167 -3.70550 0.88163 C -3.84057 -3.03317 -0.17042 C -3.12781 -2.15009 -0.97297 C -1.76757 -1.93724 -0.73968 C -1.13658 -2.64352 0.29757 C 2.46431 -1.89208 -0.20014 C 2.94018 -3.21693 -0.28480 C 4.29970 -3.46602 -0.38970 C 5.20498 -2.40309 -0.41801 C 4.74456 -1.08804 -0.35554 C 3.38456 -0.82957 -0.25679 H 1.10129 0.26356 -1.04552 H -1.35415 -4.04076 1.92275 H -3.77698 -4.38111 1.51463 H -4.89883 -3.18606 -0.35648 H -3.62481 -1.61045 -1.77284 H 2.25182 -4.05598 -0.32355 H 4.65428 -4.48849 -0.46782 H 6.26905 -2.60123 -0.50329 H 5.44638 -0.26087 -0.38381 H 3.04873 0.19925 -0.19339 H 0.70234 -3.37353 0.85861										
 S -1.57116 -1.58004 -1.81520 C -0.38552 -0.98569 -0.53501 C -1.02846 -1.15763 0.81498 N -2.26553 -0.75438 0.99385 C -4.36371 0.28974 0.43861 C -5.32894 0.62760 -0.49751 C -5.13405 0.31247 -1.84550 C -3.97391 -0.33179 -2.25885 C -2.99222 -0.67913 -1.32658 C -3.20106 -0.36536 0.02389 C -0.30466 -1.72708 1.94320	1983.73393	1983.28656	1983.37001	1983.76499	1983.40107	1984.88643	1984.52250	1985.23695	1984.87302	2.9

C -1.00005 2.37185 2.98386 C -0.30801 -2.90173 4.06408 C 1.08210 -2.79856 4.12287 C 1.78155 -2.17339 3.08982 C 1.09796 -1.64624 2.00326 H 0.42103 -1.71784 -0.60530 H -4.50167 0.53195 1.48878 H -6.23197 1.13716 -0.17863 H -5.88777 0.57743 -2.58014 H -3.82002 -0.56755 -3.30726 H -2.07579 -2.51274 2.93053 H -0.85273 -3.41042 4.85282 H 1.62097 -3.21439 4.96871 H 2.86290 -2.09257 3.13309 H 1.65315 -1.14315 1.21896 S -0.82887 1.81590 -0.50748 C 0.19931 0.37902 -0.73248 C 1.50943 0.56879 -1.07523 N 2.06985 1.82801 -1.03044 C 2.60725 3.70708 0.42002 C 2.19714 4.66001 1.34962 C 0.87347 4.69786 1.78597 C -0.05062 3.78598 1.27621 C 0.34616 2.86159 0.31294 C 1.67954 2.80564 -0.10594 C 2.43795 -0.51097 -1.48840 C 3.68484 -0.64601 -0.86026 C 4.56753 -1.64529 -1.26047 C 4.22197 -2.50931 -2.29956 C 2.99140 -2.37015 -2.94023 C 2.10304 -1.37601 -2.53869 H 3.64480 3.66034 0.09966 H 2.92178 5.36688 1.74214 H 0.55699 5.43521 2.51700 H -1.08611 3.80787 1.60329 H 3.95576 0.02029 -0.04504 H 5.52502 -1.74989 -0.75903 H 4.91357 -3.28561 -2.61331 H 2.72528 -3.02946 -3.76094 H 1.15747 -1.24982 -3.05897 H 3.02105 1.89430 -1.36538 H -2.60996 -0.74449 1.95027								
	n.d.							

	n.d.											
<b>Single-bond dimer, radical</b>												
												
S 0.68112 1.46708 -0.71613 C -0.35077 0.39636 0.16684 C -1.68834 0.66978 0.40547 N -2.28857 1.79666 -0.04652 C -2.52079 3.91963 -1.14170 C -1.96143 4.96664 -1.85190 C -0.60403 4.94429 -2.19959 C 0.19187 3.86909 -1.83752 C -0.36335 2.80396 -1.12010 C -1.72415 2.82919 -0.76793 C -2.59624 -0.25865 1.12394 C -3.68868 -0.80466 0.43602 C -4.56802 -1.65827 1.09691 C -4.36984 -1.96000 2.44328 C -3.29120 -1.40619 3.13223 C -2.40278 -0.55764 2.47788 H -3.57220 3.93090 -0.87032 H -2.58181 5.80898 -2.13910 H -0.17066 5.76856 -2.75588 H 1.24301 3.84624 -2.10816 H -3.83880 -0.57769 -0.61627 H -5.40589 -2.08818 0.55688 H -5.05781 -2.62455 2.95712 H -3.14196 -1.62968 4.18402 H -1.57500 -0.11156 3.02083 S 1.14911 -0.68734 2.25571	-	1983.11486	1982.68051	1982.76494	1983.14295	1982.79303	1984.26261	-	1983.91269	1984.61340	1984.26348	4.8

C 0.29782 -0.87506 0.64538 C 1.25956 -1.51750 -0.35773 N 2.50496 -1.20900 -0.44476 C 4.36550 0.21888 -0.00421 C 5.09219 1.06242 0.82432 C 4.61149 1.37037 2.10042 C 3.39489 0.85316 2.53314 C 2.65315 0.01739 1.69372 C 3.13981 -0.32153 0.41422 C 0.71846 -2.53376 -1.28584 C -0.65959 -2.73863 -1.44823 C -1.13477 -3.68822 -2.34999 C -0.24229 -4.45514 -3.09493 C 1.13275 -4.26364 -2.93764 C 1.60820 -3.31192 -2.04592 H -0.49557 -1.58731 0.87707 H 4.72821 -0.04761 -0.99255 H 6.03757 1.47331 0.48373 H 5.18107 2.02036 2.75765 H 3.01331 1.10101 3.51954 H -1.38355 -2.15559 -0.88777 H -2.20540 -3.82722 -2.46638 H -0.61367 -5.20011 -3.79257 H 1.83469 -4.86168 -3.51144 H 2.67441 -3.15706 -1.91932 H -3.26497 1.90717 0.20545																		
 S -1.22412 1.42628 0.06639 C 0.12237 0.47012 -0.46520 C 1.40369 1.03544 -0.65451 N 1.77180 2.26308 -0.31815 C 1.44615 4.41062 0.63504 C 0.65034 5.39156 1.19761 C -0.71757 5.15890 1.39841 C -1.27606 3.93983 1.04130	-	1983.10335	-	1982.66948	-	1982.75370	-	1983.13332	1982.78368	-	1984.25136	-	1983.90171	-	1984.60140	-	1984.25175	12.2

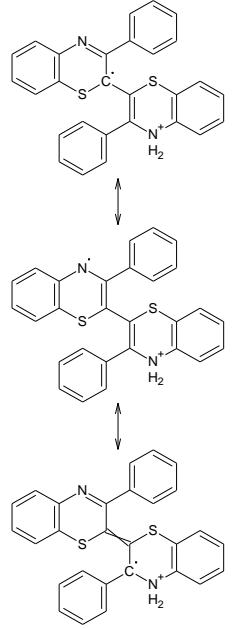
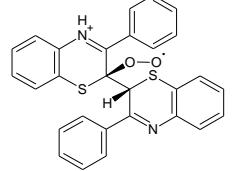
C -0.46861 2.94486 0.48119									
C 0.91037 3.16062 0.25731									
C 2.49169 0.22223 -1.27517									
C 3.70140 0.05042 -0.59334									
C 4.73870 -0.67350 -1.17570									
C 4.58330 -1.21998 -2.45007									
C 3.38665 -1.03780 -3.14163									
C 2.34336 -0.32250 -2.55625									
H 2.50585 4.57224 0.46268									
H 1.08514 6.34538 1.47984									
H -1.34552 5.92901 1.83514									
H -2.33476 3.75382 1.19938									
H 3.82172 0.48465 0.39490									
H 5.67063 -0.80929 -0.63448									
H 5.39462 -1.78101 -2.90469									
H 3.26478 -1.44626 -4.14054									
H 1.41983 -0.16558 -3.10863									
S -1.22353 -1.46182 -2.08244									
C -0.14188 -0.99628 -0.67446									
C -0.61333 -1.63759 0.60066									
N -1.89602 -1.72046 0.85284									
C -4.23271 -1.18969 0.61476									
C -5.31738 -0.85075 -0.18055									
C -5.14287 -0.66321 -1.55403									
C -3.88688 -0.80720 -2.13281									
C -2.78558 -1.15393 -1.34579									
C -2.97299 -1.34343 0.03085									
C 0.34220 -2.06626 1.61594									
C 1.57060 -2.63900 1.24308									
C 2.46086 -3.07018 2.21798									
C 2.15170 -2.91541 3.56893									
C 0.94285 -2.32994 3.94805									
C 0.03929 -1.91111 2.98195									
H 0.81491 -1.45128 -0.93489									
H -4.35347 -1.32752 1.68559									
H -6.29653 -0.72877 0.26998									
H -5.98979 -0.39586 -2.17788									
H -3.75239 -0.65398 -3.19902									
H 1.82014 -2.79169 0.19826									
H 3.39782 -3.52991 1.92065									
H 2.85552 -3.24452 4.32718									
H 0.70953 -2.18721 4.99818									
H -0.87415 -1.41297 3.29525									
H -2.15990 -2.13016 1.74586									

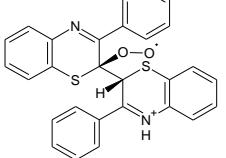


S	0.57917	1.40250	-2.45516
C	0.14075	0.69588	-0.87902
C	-0.04302	1.56078	0.20821
N	0.49387	2.79990	0.20989
C	2.22544	4.40791	-0.29719
C	3.17055	4.91918	-1.17922
C	3.36151	4.32332	-2.42609
C	2.59967	3.21758	-2.79617
C	1.63562	2.71451	-1.92403
C	1.45448	3.30414	-0.66907
C	-0.88734	1.25510	1.37990
C	-2.13536	0.63679	1.21075
C	-2.96561	0.43058	2.30619
C	-2.56471	0.83907	3.57942
C	-1.32879	1.45954	3.75299
C	-0.49387	1.67052	2.66013
H	2.08204	4.85885	0.68068
H	3.76321	5.78017	-0.88755
H	4.10405	4.71627	-3.11311
H	2.74333	2.75070	-3.76584
H	-2.46252	0.34143	0.21865
H	-3.93467	-0.03807	2.16371
H	-3.21633	0.67615	4.43272
H	-1.00761	1.77190	4.74198
H	0.48184	2.12471	2.81248

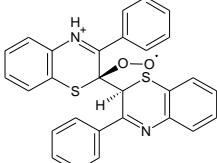
1983.12175 1982.68722 1982.77091 1983.15053 1982.79970 1984.27181 1983.92097 1984.62204 1984.27120 0.0

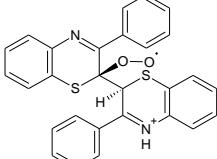
S -0.57917 -1.40250 -2.45516									
C -0.14075 -0.69588 -0.87902									
C 0.04302 -1.56078 0.20821									
N -0.49387 -2.79990 0.20989									
C -2.22544 -4.40791 -0.29719									
C -3.17055 -4.91918 -1.17922									
C -3.36151 -4.32332 -2.42609									
C -2.59967 -3.21758 -2.79617									
C -1.63562 -2.71451 -1.92403									
C -1.45448 -3.30414 -0.66907									
C 0.88734 -1.25510 1.37990									
C 2.13536 -0.63679 1.21075									
C 2.96561 -0.43058 2.30619									
C 2.56471 -0.83907 3.57942									
C 1.32879 -1.45954 3.75299									
C 0.49387 -1.67052 2.66013									
H -2.08204 -4.85885 0.68068									
H -3.76321 -5.78017 -0.88755									
H -4.10405 -4.71627 -3.11311									
H -2.74333 -2.75070 -3.76584									
H 2.46252 -0.34143 0.21865									
H 3.93467 0.03807 2.16371									
H 3.21633 -0.67615 4.43272									
H 1.00761 -1.77190 4.74198									
H -0.48184 -2.12471 2.81248									
H -0.21418 -3.40858 0.96883									
H 0.21418 3.40858 0.96883									

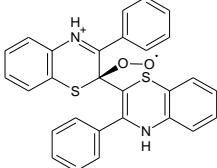
	n.d.							
<b>Single-bond dimer, C2-peroxy radical</b>  S 0.56412 -1.64020 -0.32311 C 0.35550 0.14411 -0.42588 C 1.69448 0.83128 -0.17399 N 2.73921 0.36707 -0.81219 C 3.95978 -0.94880 -2.42173 C 4.12136 -2.13779 -3.11299 C 3.19093 -3.17079 -2.95700 C 2.08919 -3.01647 -2.12429 C 1.90771 -1.81673 -1.43407 C 2.85374 -0.79546 -1.57939 C 1.92469 1.95798 0.73228 C 2.95621 1.84659 1.68086 C 3.23024 2.90834 2.53368 C 2.49801 4.09075 2.43404 C 1.49063 4.21386 1.47631 C 1.19406 3.15294 0.63014 H 4.67507 -0.13859 -2.52827		2133.27400	2132.83028	2132.91766	2133.30523	2132.94888	2134.52505	2134.16870 2134.92199 2134.56564 2.7

H 4.97252 -2.26430 -3.77306 H 3.32005 -4.10199 -3.49902 H 1.36309 -3.81594 -2.01746 H 3.50411 0.91406 1.78239 H 4.01181 2.80878 3.27999 H 2.71513 4.92010 3.10010 H 0.93862 5.14326 1.38040 H 0.44968 3.27582 -0.14893 S -0.51371 0.46052 2.25685 C -0.80871 0.62542 0.47735 C -2.16066 0.01265 0.09928 N -2.62351 -1.07001 0.60934 C -2.37443 -3.10558 1.83354 C -1.83165 -3.85120 2.87119 C -0.89664 -3.26970 3.73154 C -0.48605 -1.95510 3.53246 C -1.01477 -1.21233 2.47498 C -1.97994 -1.77689 1.61922 C -2.98200 0.70049 -0.92412 C -3.79881 -0.07187 -1.76469 C -4.59511 0.53429 -2.72894 C -4.60084 1.92380 -2.86224 C -3.80282 2.70072 -2.02475 C -2.99260 2.09467 -1.06778 H -0.86869 1.70229 0.31603 H -3.11817 -3.52986 1.16555 H -2.14452 -4.88001 3.01996 H -0.47934 -3.84204 4.55438 H 0.25336 -1.50672 4.19003 H -3.78811 -1.15162 -1.65704 H -5.21011 -0.07851 -3.38155 H -5.22419 2.39768 -3.61480 H -3.81095 3.78308 -2.11139 H -2.40426 2.73066 -0.41315 O -0.02426 0.42062 -1.83250 O 0.12247 1.68697 -2.11746 H 3.59380 0.91345 -0.71454											
	S 0.61111 -1.25397 -1.03444 C 0.22209 0.41968 -0.52035 C 1.44124 1.25833 -0.11345 N 2.64940 1.01579 -0.46426 C 4.41334 -0.04387 -1.65385	2133.27668	2132.83336	2132.92275	2133.30793	2132.95400	2134.52676	2134.17283	2134.92358	2134.56965	0.2

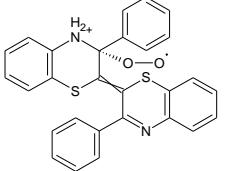
C 4.92802 -1.08146 -2.41715									
C 4.10873 -2.15917 -2.76456									
C 2.77909 -2.19276 -2.35679									
C 2.26577 -1.14286 -1.59337									
C 3.07600 -0.05834 -1.22848									
C 1.22325 2.48967 0.69617									
C 2.10096 2.75022 1.75811									
C 1.97184 3.91032 2.51306									
C 0.97055 4.83480 2.21172									
C 0.10325 4.59213 1.14875									
C 0.22412 3.42577 0.39509									
H 5.02605 0.80571 -1.36776									
H 5.96354 -1.05610 -2.74116									
H 4.50335 -2.97634 -3.36056									
H 2.14228 -3.02824 -2.63364									
H 2.87762 2.02747 1.98797									
H 2.65246 4.09297 3.33948									
H 0.87052 5.74193 2.80043									
H -0.66603 5.31525 0.89472									
H -0.43512 3.27498 -0.45442									
S -0.26303 0.03206 2.25262									
C -0.88374 0.38260 0.58146									
C -2.06209 -0.48615 0.22218									
N -2.12794 -1.72026 0.65021									
C -1.34026 -3.80971 1.54942									
C -0.49734 -4.51313 2.39882									
C 0.43895 -3.82664 3.17384									
C 0.54277 -2.44020 3.09909									
C -0.29879 -1.72275 2.24985									
C -1.23651 -2.42001 1.48112									
C -3.12733 0.00771 -0.64207									
C -3.72355 -0.85827 -1.57835									
C -4.75155 -0.40146 -2.39015									
C -5.20605 0.91257 -2.26936									
C -4.62183 1.77515 -1.34188									
C -3.57789 1.33503 -0.53946									
H -1.25407 1.40778 0.65694									
H -2.07029 -4.32872 0.93486									
H -0.56991 -5.59384 2.45429									
H 1.09970 -4.37383 3.83849									
H 1.27643 -1.91178 3.69977									
H -3.34714 -1.86833 -1.71622									
H -5.18952 -1.06695 -3.12680									
H -6.01268 1.26637 -2.90392									
H -4.98058 2.79422 -1.24168									
H -3.15564 2.01309 0.19495									
O -0.46165 1.16653 -1.62608									
O 0.22519 1.15439 -2.72922									
H -2.95716 -2.24436 0.37773									

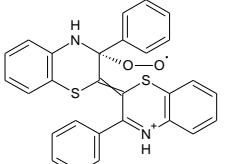
 <p> S -1.15884 -1.01830 -1.58247  C 0.17966 -0.42551 -0.48082  C 0.93007 -1.67024 -0.02813  N 0.21854 -2.59449 0.57776  C -1.78451 -3.56112 1.52670  C -3.15357 -3.76732 1.45865  C -3.90932 -3.13389 0.46777  C -3.30665 -2.27589 -0.44498  C -1.92976 -2.04963 -0.38340  C -1.17748 -2.71131 0.59809  C 2.33615 -1.94031 -0.28355  C 2.71010 -3.26258 -0.60204  C 4.04273 -3.57655 -0.82373  C 5.01807 -2.58375 -0.72360  C 4.65636 -1.27193 -0.41419  C 3.32512 -0.94177 -0.20645  H -1.18280 -4.05281 2.28511  H -3.63359 -4.42439 2.17578  H -4.98068 -3.29833 0.41496  H -3.90065 -1.76882 -1.19840  H 1.95368 -4.03132 -0.73245  H 4.31864 -4.59189 -1.08873  H 6.06105 -2.83080 -0.89677  H 5.41567 -0.50080 -0.33431  H 3.06292 0.07744 0.04696  S 0.92395 0.77480 1.96758  C -0.32880 0.45323 0.69812  C -0.94846 1.76327 0.22197  N -0.25694 2.82071 -0.00843  C 1.80583 3.97654 -0.33993  C 3.13804 4.21310 -0.03062  C 3.78617 3.41418 0.91480  C 3.10942 2.35953 1.52035  C 1.77859 2.10016 1.18380  C 1.10109 2.92387 0.26289  C -2.41022 1.82809 -0.00290  C -3.31825 1.07733 0.75598  C -4.68961 1.20525 0.54611  C -5.17171 2.06852 -0.43506  C -4.27419 2.81672 -1.20014  C -2.90726 2.70439 -0.98121  H -1.08267 -0.14126 1.21931  H 1.27387 4.60434 -1.04863 </p>	-	2133.27514	-	2132.83148	-	2132.91898	-	2133.30516	-	2132.94900	-	2134.52553	-	2134.16937	-	2134.92237	-	2134.56621	2.4
--	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

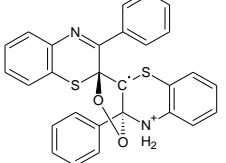
H 3.66849 5.02954 -0.51074 H 4.82167 3.60696 1.17809 H 3.61587 1.72989 2.24696 H -2.97494 0.41325 1.54369 H -5.38012 0.62834 1.15409 H -6.24079 2.15934 -0.60357 H -4.64255 3.48763 -1.97073 H -2.20404 3.28322 -1.57105 O 1.08406 0.36091 -1.28500 O 0.62538 0.62696 -2.47731 H 0.73664 -3.36435 0.99502											
	S 1.39712 -0.90659 1.65333 C -0.04818 -0.46065 0.63591 C -0.81992 -1.73380 0.26343 N -0.20853 -2.73820 -0.24701 C 1.73025 -3.76023 -1.21150 C 3.09924 -3.98327 -1.24263 C 3.93940 -3.28899 -0.36758 C 3.41286 -2.34780 0.51072 C 2.03769 -2.09829 0.52283 C 1.17693 -2.82074 -0.32823 C -2.29567 -1.82141 0.40870 C -3.02661 -2.33949 -0.67073 C -4.40446 -2.50082 -0.57839 C -5.07091 -2.16319 0.60000 C -4.34920 -1.66685 1.68383 C -2.97038 -1.48927 1.59143 H 1.05521 -4.31241 -1.85838 H 3.51351 -4.70898 -1.93546 H 5.00957 -3.47128 -0.37673 H 4.06808 -1.79231 1.17552 H -2.50274 -2.60198 -1.58433 H -4.95833 -2.89087 -1.42736 H -6.14696 -2.29086 0.67424 H -4.85780 -1.41872 2.61071 H -2.42669 -1.12180 2.45406 S -0.92562 0.45530 -1.93170 C 0.36354 0.32062 -0.66183 C 0.93238 1.67902 -0.36123 N 0.10670 2.68734 -0.22095 C -2.02540 3.75855 0.12936 C -3.39026 3.82256 -0.11217	2133.27657	2132.83300	2132.92114	2133.30743	2132.95200	2134.52854	2134.17310	2134.92541	2134.56998	0.0

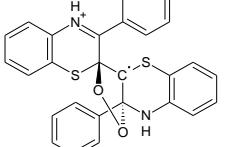
C -4.00882 2.84284 -0.89234 C -3.27073 1.79078 -1.42533 C -1.89872 1.71172 -1.18581 C -1.28478 2.70525 -0.41028 C 2.36033 1.89766 -0.18028 C 3.29234 1.14666 -0.91765 C 4.65161 1.39205 -0.77402 C 5.09790 2.36434 0.11997 C 4.17992 3.10248 0.86991 C 2.81997 2.87974 0.71900 H 1.13780 -0.28998 -1.13339 H -1.53341 4.51192 0.73800 H -3.97201 4.63544 0.30884 H -5.07633 2.89339 -1.08110 H -3.75576 1.02560 -2.02310 H 2.96605 0.40545 -1.63940 H 5.36302 0.82242 -1.36291 H 6.16200 2.54409 0.23807 H 4.52623 3.84356 1.58279 H 2.12373 3.42720 1.34841 O -0.90095 0.40237 1.41973 O -0.27803 0.98992 2.40820 H 0.52358 3.59152 -0.01263										
 S -2.10883 -0.73723 -1.35147 C -0.88997 -0.30485 -0.07852 C -1.11733 1.07876 0.52258 N -2.32938 1.57036 0.60579 C -4.71232 1.79757 0.43571 C -5.92513 1.39615 -0.10068 C -5.96849 0.32984 -1.00329 C -4.80543 -0.34077 -1.36444 C -3.57884 0.05607 -0.82912 C -3.54103 1.12993 0.06327 C -0.04589 1.82292 1.18020 C 0.95711 1.15914 1.90708 C 1.91990 1.89644 2.58682 C 1.90672 3.28929 2.53620 C 0.92107 3.95402 1.80414 C -0.05326 3.22933 1.13312 H -4.66461 2.62159 1.14220 H -6.83610 1.91110 0.18424 H -6.91723 0.01281 -1.42422	2133.27770	2132.83376	2132.92209	2133.30805	2132.95244	2134.52695	2134.17134	2134.92435	2134.56875	0.8

H -4.84568 -1.17492 -2.05799 H 0.96079 0.07812 1.97993 H 2.68020 1.37801 3.16226 H 2.66688 3.85851 3.06247 H 0.91935 5.03771 1.74592 H -0.78582 3.75586 0.52680 C 0.45528 -0.43815 -0.71675 S 0.78898 0.90172 -1.84163 C 2.50106 1.13413 -1.44575 C 3.26450 -0.00675 -1.17156 N 2.64100 -1.25799 -1.08177 C 1.36754 -1.43920 -0.58086 C 3.09794 2.39233 -1.48834 C 4.47409 2.51219 -1.30324 C 5.24090 1.37443 -1.05188 C 4.64076 0.12073 -0.97021 C 1.15440 -2.74719 0.08510 C 0.14958 -3.61426 -0.35922 C -0.01680 -4.85835 0.24270 C 0.81656 -5.24547 1.29162 C 1.82645 -4.38946 1.73143 C 2.00307 -3.14896 1.12509 H 2.48890 3.26882 -1.68913 H 4.94319 3.48937 -1.35943 H 6.31336 1.46091 -0.90640 H 5.23584 -0.76137 -0.74898 H -0.49177 -3.32001 -1.18470 H -0.79474 -5.52779 -0.11203 H 0.68343 -6.21526 1.76208 H 2.47717 -4.68696 2.54827 H 2.78599 -2.48102 1.47531 O -0.95582 -1.22351 1.08949 O -2.16724 -1.36707 1.54114 H 3.25814 -2.05274 -0.98775 H -2.41129 2.41434 1.17016									
	n.d.								
Single-bond dimer, C3-peroxyl radical									

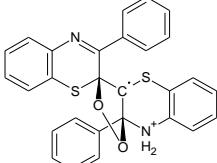
 <p>S 0.84173 -1.74644 1.44341      C 0.93420 -0.22921 0.54895      C 2.25263 -0.02750 -0.11285      N 2.82105 -0.97043 -0.78398      C 2.80351 -3.12853 -1.81763      C 2.46371 -4.47278 -1.81637      C 1.66437 -4.99113 -0.79218      C 1.17845 -4.15620 0.20775      C 1.48892 -2.79442 0.18362      C 2.32908 -2.26464 -0.81667      C 2.96781 1.25823 0.03482      C 2.85356 2.00939 1.21329      C 3.57610 3.19039 1.36600      C 4.40554 3.64026 0.34062      C 4.52207 2.89643 -0.83634      C 3.81671 1.70877 -0.98640      H 3.45245 -2.71317 -2.58295      H 2.83405 -5.12516 -2.60102      H 1.41026 -6.04654 -0.77714      H 0.54058 -4.55293 0.99243      H 2.21900 1.65983 2.02351      H 3.49030 3.75718 2.28830      H 4.96130 4.56620 0.45630      H 5.16522 3.24573 -1.63888      H 3.90315 1.12423 -1.89681      S 0.06414 2.23370 -0.27165      C -0.10715 0.63433 0.49734      C -1.42552 0.29643 1.16790      N -2.33446 1.51898 1.15262      C -3.95522 2.07256 -0.64480      C -4.16952 2.56353 -1.93110      C -3.09029 2.94751 -2.72629      C -1.78160 2.83613 -2.25939      C -1.55709 2.35328 -0.97199      C -2.64962 1.99636 -0.18936      C -2.17701 -0.89197 0.62506      C -3.08784 -1.57012 1.44326      C -3.83198 -2.62373 0.92059      C -3.68057 -2.99488 -0.41469      C -2.78185 -2.31018 -1.23079      C -2.02934 -1.25933 -0.71515      H -4.78777 1.77184 -0.01635      H -5.18282 2.64186 -2.30991</p>	2133.25900	-	2133.29152	-	-	2134.91265	
--	------------	---	------------	---	---	------------	--

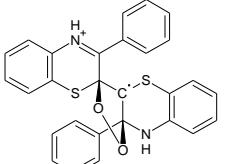
H -3.26602 3.32574 -3.72822 H -0.94232 3.11518 -2.88793 H -3.20661 -1.29934 2.48798 H -4.52823 -3.15578 1.56117 H -4.26262 -3.81772 -0.81861 H -2.66150 -2.59410 -2.27153 H -1.32580 -0.73508 -1.35451 H -3.19625 1.28460 1.65834 O -1.21356 0.05710 2.60400 O -0.81852 1.13348 3.22903 H -1.85201 2.25301 1.69983										
 S 1.85695 0.10977 1.41054 C 0.51650 0.59701 0.35585 C 0.50144 2.04265 0.11895 N 1.64161 2.63009 -0.17374 C 3.91830 2.64142 -0.99040 C 5.18675 2.07789 -1.00444 C 5.43759 0.90082 -0.29585 C 4.42221 0.27474 0.42081 C 3.14239 0.82913 0.43882 C 2.90079 2.01618 -0.26758 C -0.68991 2.87460 0.29368 C -1.63609 2.51430 1.26654 C -2.73789 3.32746 1.49366 C -2.91495 4.49251 0.74611 C -1.98185 4.84944 -0.22832 C -0.86843 4.05028 -0.45303 H 3.70995 3.55597 -1.53779 H 5.98012 2.55647 -1.56855 H 6.43015 0.46187 -0.30599 H 4.61719 -0.64451 0.96394 H -1.49351 1.61229 1.85334 H -3.45982 3.05259 2.25603 H -3.78305 5.12113 0.91965 H -2.12752 5.74597 -0.82231 H -0.17450 4.31836 -1.24519 S -1.51416 0.30213 -1.39231 C -0.40579 -0.26065 -0.16349 C -0.46413 -1.72611 0.22204 N -1.53199 -2.42771 -0.35070 C -3.96156 -2.65840 -0.19492 C -5.22393 -2.11632 -0.41873	2133.28525	2132.84164	2132.93092	2133.31535	2132.96102	2134.53307	2134.17874	2134.93112	2134.57678	0.0

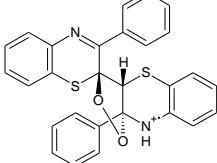
C -5.36475 -0.81150 -0.89367 C -4.23289 -0.04363 -1.15486 C -2.96959 -0.59753 -0.95430 C -2.82142 -1.90084 -0.47029 C 0.82447 -2.50162 -0.01734 C 1.30210 -3.43581 0.90351 C 2.43163 -4.19482 0.60005 C 3.08815 -4.02537 -0.61680 C 2.60605 -3.09716 -1.53966 C 1.47468 -2.34252 -1.24486 H -3.85441 -3.66923 0.18849 H -6.10446 -2.71547 -0.20780 H -6.35135 -0.38896 -1.05448 H -4.32609 0.97469 -1.52044 H 0.81145 -3.57024 1.86130 H 2.79953 -4.91626 1.32361 H 3.97117 -4.61442 -0.84659 H 3.10854 -2.96146 -2.49276 H 1.09807 -1.62905 -1.97288 H -1.48871 -3.42258 -0.17257 H 1.63260 3.64210 -0.26611 O -0.64863 -1.59650 1.77337 O -1.36719 -2.55017 2.26633									
<b>Single-bond dimer, dioxolane radical</b>									15.0
 S -1.86074 -1.67129 -0.73770 C -1.13510 -0.20988 0.10870 C -2.04890 0.99797 -0.13690 N -3.32518 0.91466 -0.02294 C -5.32342 -0.17916 0.69095 C -6.09712 -1.31733 0.86281 C -5.57810 -2.57192 0.52743 C -4.27810 -2.68712 0.04821 C -3.48887 -1.54344 -0.10044 C -4.00924 -0.27036 0.20594 C -1.45758 2.30356 -0.49986 C -2.09324 3.08203 -1.47689 C -1.58381 4.32946 -1.82233 C -0.44255 4.81943 -1.18618 C 0.18625 4.05682 -0.20234 C -0.31318 2.80206 0.13637 H -5.71368 0.80725 0.92294 H -7.10940 -1.23110 1.24523	2133.27135	2132.82676	2132.91260	2133.30425	2132.94549	2134.52562	2134.16687	2134.92276	2134.56401

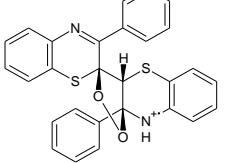
H -6.18466 -3.46431 0.64792 H -3.86833 -3.66198 -0.19946 H -2.98087 2.69297 -1.96627 H -2.07617 4.91900 -2.59010 H -0.04576 5.79421 -1.45462 H 1.06475 4.44033 0.30815 H 0.17042 2.23133 0.92306 S 0.89455 -0.13396 -1.86725 C 0.31265 -0.16308 -0.25821 C 1.06544 -0.74832 0.89592 N 1.71674 -2.06117 0.42475 C 3.91040 -2.55770 -0.56135 C 4.83874 -2.41717 -1.58810 C 4.55191 -1.59247 -2.67458 C 3.34883 -0.89837 -2.73764 C 2.40418 -1.03896 -1.71709 C 2.70294 -1.87956 -0.64314 C 2.09784 0.10294 1.59947 C 2.34569 -0.13442 2.95629 C 3.31491 0.60818 3.62399 C 4.03714 1.58831 2.94418 C 3.78514 1.82962 1.59507 C 2.81620 1.09096 0.92071 H 4.12108 -3.19904 0.28995 H 5.78264 -2.94821 -1.53323 H 5.27461 -1.47607 -3.47551 H 3.14013 -0.23995 -3.57533 H 1.77158 -0.88259 3.49459 H 3.49952 0.42451 4.67783 H 4.79047 2.16914 3.46787 H 4.33743 2.59880 1.06423 H 2.61847 1.30360 -0.12518 O -1.07438 -0.35515 1.52443 O 0.04808 -1.21734 1.76582 H 0.95411 -2.68709 0.12938 H 2.16803 -2.51387 1.22691										
 S -1.69709 -1.84289 -0.66339 C -0.96045 -0.30932 0.07640 C -1.83639 0.83670 -0.39086 N -3.12654 0.73429 -0.15910 C -5.14513 -0.24371 0.72623 C -5.90301 -1.36832 1.00768	2133.28881	2132.84465	2132.93168	2133.31948	2132.96236	2134.53613	2134.17901	2134.93348	2134.57636	7.3

C -5.37450 -2.64371 0.78035									
C -4.08525 -2.80004 0.28754									
C -3.30401 -1.67518 0.00634									
C -3.85044 -0.40053 0.22086									
C -1.34508 2.03200 -1.05475									
C -2.10799 2.59916 -2.09449									
C -1.67835 3.76441 -2.71359									
C -0.49715 4.38048 -2.29754									
C 0.26062 3.82582 -1.26531									
C -0.14986 2.65165 -0.64902									
H -5.54379 0.75265 0.89383									
H -6.90665 -1.25502 1.40310									
H -5.96979 -3.52393 1.00104									
H -3.67426 -3.79167 0.12750									
H -3.00475 2.10066 -2.45210									
H -2.25780 4.18539 -3.52870									
H -0.16365 5.29262 -2.78299									
H 1.17359 4.31140 -0.93599									
H 0.43260 2.24022 0.16748									
S 1.16265 -0.57083 -1.75296									
C 0.49987 -0.30711 -0.20843									
C 1.19076 -0.59721 1.10286									
N 2.11533 -1.69043 1.01880									
C 4.15446 -2.59225 0.11075									
C 5.01451 -2.83952 -0.94928									
C 4.71256 -2.37187 -2.23062									
C 3.53679 -1.66294 -2.43174									
C 2.65637 -1.43126 -1.36906									
C 2.95603 -1.88511 -0.07494									
C 1.79311 0.64592 1.75350									
C 1.31907 1.13511 2.97228									
C 1.90638 2.26107 3.54978									
C 2.96536 2.90591 2.91491									
C 3.44067 2.41961 1.69600									
C 2.85778 1.29667 1.11659									
H 4.40137 -2.94860 1.10756									
H 5.93178 -3.39222 -0.77055									
H 5.38583 -2.55361 -3.06172									
H 3.28711 -1.28676 -3.42038									
H 0.49479 0.63631 3.47034									
H 1.53165 2.63283 4.49908									
H 3.41985 3.78326 3.36577									
H 4.26671 2.91538 1.19451									
H 3.23786 0.93054 0.16633									
O -1.02292 -0.29641 1.49016									
O 0.08849 -1.10206 1.89418									
H 2.58175 -1.85865 1.90264									
H -3.67966 1.57087 -0.33254									

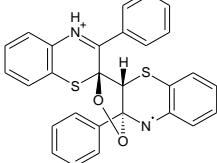
 <p> S 1.21067 -1.98723 1.65200  C 1.04307 -0.28421 0.95210  C 2.34614 0.07651 0.24084  N 2.85313 -0.72899 -0.61848  C 2.74491 -2.65845 -2.02683  C 2.41669 -3.98718 -2.25442  C 1.74150 -4.71601 -1.27142  C 1.36758 -4.10477 -0.07917  C 1.66880 -2.75826 0.14068  C 2.38241 -2.02252 -0.82929  C 2.97515 1.40471 0.42366  C 3.42790 2.08011 -0.71945  C 4.06309 3.31202 -0.60493  C 4.26863 3.87835 0.65335  C 3.83376 3.20618 1.79496  C 3.18333 1.97984 1.68514  H 3.29691 -2.08230 -2.76348  H 2.69906 -4.46198 -3.18887  H 1.49449 -5.76016 -1.43732  H 0.82552 -4.66459 0.67744  H 3.26811 1.63099 -1.69471  H 4.39726 3.83040 -1.49890  H 4.76826 4.83848 0.74409  H 4.00407 3.63485 2.77811  H 2.86672 1.46290 2.58467  S -0.21180 0.10097 -1.58931  C -0.18583 -0.13143 0.10490  C -1.25243 0.36590 1.02151  N -1.54316 1.83976 0.60300  C -3.21757 2.78242 -0.93067  C -3.78114 2.88076 -2.19931  C -3.26346 2.12492 -3.24950  C -2.18987 1.26653 -3.03964  C -1.60765 1.16830 -1.77295  C -2.13414 1.93882 -0.73279  C -2.55964 -0.37589 1.13944  C -2.79624 -1.52316 0.38155  C -3.99818 -2.21188 0.52765  C -4.95705 -1.76306 1.43324  C -4.71478 -0.62340 2.20001  C -3.51856 0.07142 2.05591  H -3.61630 3.36313 -0.10360  H -4.62584 3.54164 -2.36004 </p>	-	2133.27033	-	2132.82582	-	2132.91278	-	2133.30482	-	2132.94727	-	2134.52567	-	2134.16811	-	2134.92295	-	2134.56539	14.2
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	------

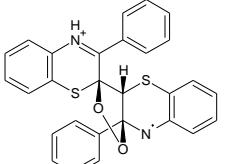
H -3.70336 2.19360 -4.23901 H -1.80056 0.66742 -3.85691 H -2.04745 -1.88152 -0.31785 H -4.18145 -3.10114 -0.06720 H -5.89259 -2.30261 1.54551 H -5.45440 -0.27581 2.91429 H -3.33955 0.94554 2.67763 O 0.77037 0.59487 2.02939 O -0.64476 0.39757 2.28157 H -2.17343 2.26255 1.29144 H -0.66058 2.36433 0.66508										
 S -1.49315 1.98456 1.51785 C -0.92263 0.29683 0.94906 C -2.10927 -0.38806 0.32370 N -2.77352 0.27918 -0.59261 C -3.20616 2.07071 -2.14611 C -3.18414 3.42132 -2.45688 C -2.63069 4.33671 -1.55690 C -2.08740 3.90481 -0.35263 C -2.09907 2.54628 -0.02573 C -2.67051 1.63777 -0.92917 C -2.52062 -1.74640 0.63734 C -3.89446 -2.05718 0.63984 C -4.31090 -3.35849 0.88192 C -3.36727 -4.36098 1.11016 C -2.00485 -4.05844 1.10803 C -1.57379 -2.75791 0.88552 H -3.63311 1.34946 -2.83697 H -3.59713 3.76191 -3.40029 H -2.61205 5.39409 -1.80078 H -1.64629 4.61598 0.33842 H -4.63525 -1.27348 0.50723 H -5.37114 -3.58842 0.90419 H -3.69511 -5.37916 1.29672 H -1.27316 -4.84136 1.28005 H -0.51304 -2.53034 0.87083 S 0.42342 0.16041 -1.58520 C 0.30685 0.29205 0.10686 C 1.44115 -0.13523 1.00425 N 1.75209 -1.50747 0.67281 C 3.04460 -2.86580 -0.86372 C 3.46255 -3.17253 -2.15065	2133.29006	2132.84595	2132.93167	2133.31955	2132.96116	2134.53719	2134.17880	2134.93405	2134.57566	7.7

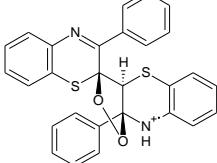
C 3.01757 -2.41839 -3.23992 C 2.13058 -1.37271 -3.02700 C 1.68341 -1.07696 -1.73456 C 2.15816 -1.80449 -0.62655 C 2.62647 0.81974 1.06345 C 2.38684 2.19129 1.20100 C 3.44996 3.08408 1.28058 C 4.76309 2.61401 1.22124 C 5.00513 1.24947 1.08444 C 3.93993 0.35229 1.00538 H 3.41303 -3.43987 -0.01706 H 4.15300 -3.99649 -2.30268 H 3.35503 -2.64618 -4.24565 H 1.76361 -0.78715 -3.86573 H 1.36462 2.55774 1.24799 H 3.25451 4.14695 1.38756 H 5.59388 3.31115 1.27991 H 6.02404 0.87703 1.03702 H 4.14691 -0.70677 0.89254 O -0.54846 -0.39949 2.11442 O 0.84564 -0.06995 2.29826 H 2.25293 -2.00226 1.40207 H -3.46420 -0.25161 -1.11811										
 S 1.66818 -0.92468 1.40540 C -0.01732 -0.75034 0.74792 C -0.55836 -2.09554 0.25527 N 0.15963 -2.91742 -0.41933 C 2.11565 -3.54843 -1.63166 C 3.48800 -3.52545 -1.83882 C 4.30420 -2.72910 -1.02984 C 3.74210 -1.93513 -0.03708 C 2.35606 -1.93189 0.14689 C 1.52415 -2.75719 -0.63673 C -2.00233 -2.40295 0.40321 C -2.70438 -2.25853 1.60935 C -4.04867 -2.61536 1.68195 C -4.71317 -3.10123 0.55706 C -4.02252 -3.24609 -0.64646 C -2.67600 -2.90788 -0.72096 H 1.46805 -4.18523 -2.22663 H 3.92736 -4.14011 -2.61817 H 5.37963 -2.72006 -1.17743	2133.29740	2132.85434	2132.94151	2133.32688	2132.97099	2134.54813	2134.19224	2134.94386	2134.58796	0.0

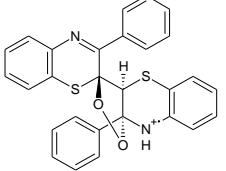
H 4.37167 -1.30430 0.58400 H -2.20012 -1.89307 2.49520 H -4.57707 -2.51456 2.62542 H -5.76413 -3.36876 0.61818 H -4.53268 -3.62326 -1.52796 H -2.13104 -3.02476 -1.65261 S 1.11160 0.77007 -1.43951 C -0.25549 0.33852 -0.36730 C -0.85942 1.50070 0.42975 N 0.17423 2.28729 1.07869 C 2.33307 3.09260 1.67458 C 3.65942 3.24431 1.37664 C 4.21442 2.64780 0.21452 C 3.42787 1.88580 -0.62338 C 2.06781 1.69213 -0.33593 C 1.48944 2.33392 0.81557 C -1.86216 2.35387 -0.32036 C -1.54188 3.65569 -0.70768 C -2.46515 4.41349 -1.42628 C -3.70653 3.87588 -1.75624 C -4.02576 2.57379 -1.36943 C -3.10793 1.81045 -0.65528 H -1.03353 -0.02931 -1.04211 H 1.90097 3.55158 2.55831 H 4.29464 3.82712 2.03516 H 5.26824 2.77893 -0.00656 H 3.85565 1.40968 -1.49987 H -0.57678 4.08453 -0.45730 H -2.20936 5.42509 -1.72605 H -4.42531 4.46867 -2.31409 H -4.99299 2.15040 -1.62237 H -3.36469 0.79978 -0.35247 O -0.69515 -0.22414 1.88770 O -1.58536 0.80827 1.42686 H -0.15848 2.83626 1.86547																	
 S 1.57488 -1.16652 0.78100 C 0.88913 0.14267 -0.26770 C 1.68446 1.44893 -0.14384 N 2.94350 1.51659 0.09129 C 5.15005 0.64162 0.28415 C 6.03992 -0.38970 0.54471 C 5.55606 -1.66060 0.87099	-	2133.27747	2132.83413	-	2132.92007	-	2133.30741	2132.95001	-	2134.52693	-	2134.16953	-	2134.92316	-	2134.56577	13.9

C 4.18735 -1.89918 0.91899									
C 3.29348 -0.86025 0.64585									
C 3.76395 0.42432 0.33212									
C 0.97863 2.73946 -0.37188									
C 0.22418 2.97996 -1.52931									
C -0.37843 4.22061 -1.72610									
C -0.24430 5.22667 -0.76995									
C 0.50656 4.99306 0.38186									
C 1.12003 3.75877 0.57775									
H 5.49893 1.63993 0.03736									
H 7.10914 -0.20786 0.50095									
H 6.24708 -2.47091 1.08231									
H 3.80981 -2.88856 1.16142									
H 0.13299 2.21197 -2.29221									
H -0.94786 4.40180 -2.63297									
H -0.71941 6.19102 -0.92452									
H 0.61689 5.77345 1.12911									
H 1.71120 3.57383 1.46966									
S -1.27170 0.16470 1.65035									
C -0.60729 0.24581 -0.01176									
C -1.18990 -0.77713 -0.99269									
N -2.57858 -0.40295 -1.18132									
C -4.76429 0.23298 -0.51864									
C -5.64990 0.61188 0.44961									
C -5.20702 0.83543 1.77782									
C -3.87274 0.69378 2.10984									
C -2.92813 0.32815 1.14335									
C -3.38375 0.05766 -0.20669									
C -1.07794 -2.27662 -0.75348									
C -0.24972 -3.04274 -1.58013									
C -0.14823 -4.41770 -1.38840									
C -0.87261 -5.04100 -0.37447									
C -1.71416 -4.28404 0.43946									
C -1.82449 -2.91014 0.24691									
H -0.92456 1.21582 -0.40764									
H -5.09259 0.04979 -1.53701									
H -6.69808 0.73954 0.20244									
H -5.91862 1.13685 2.53897									
H -3.53993 0.88859 3.12430									
H 0.32083 -2.56330 -2.36687									
H 0.50027 -5.00094 -2.03511									
H -0.79155 -6.11362 -0.22533									
H -2.29524 -4.76219 1.22195									
H -2.50484 -2.35189 0.88077									
O 0.89805 -0.20259 -1.68428									
O -0.47126 -0.37890 -2.15151									
H -3.01967 -0.71367 -2.04291									

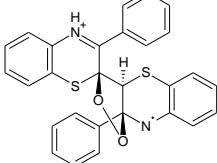
 <p> S -1.29324 -1.48746 -1.41753  C 0.22379 -0.72556 -0.75396  C 1.20620 -1.78487 -0.28221  N 0.75496 -2.82253 0.36877  C -0.82349 -4.18091 1.58096  C -2.12177 -4.63025 1.77494  C -3.16006 -4.11252 0.99785  C -2.91061 -3.13611 0.03863  C -1.61098 -2.66745 -0.15751  C -0.57569 -3.20465 0.61448  C 2.65681 -1.63561 -0.40791  C 3.45567 -1.90366 0.72108  C 4.83776 -1.80654 0.63431  C 5.43831 -1.46400 -0.57701  C 4.65215 -1.20707 -1.69994  C 3.26688 -1.27726 -1.62252  H -0.00365 -4.57893 2.17223  H -2.32294 -5.38447 2.52790  H -4.17615 -4.46396 1.14573  H -3.72351 -2.72828 -0.55384  H 2.99733 -2.13777 1.67824  H 5.44406 -1.99131 1.51517  H 6.51968 -1.39446 -0.64467  H 5.11942 -0.95096 -2.64542  H 2.66433 -1.08923 -2.50115  S -1.39237 0.40730 1.38388  C 0.07060 0.38153 0.34505  C 0.28783 1.67483 -0.47525  N -0.83092 2.16132 -1.21328  C -3.10309 2.53237 -1.66475  C -4.43639 2.43985 -1.34611  C -4.83145 1.74341 -0.18829  C -3.88184 1.12778 0.62545  C -2.52670 1.20504 0.31745  C -2.08801 1.94656 -0.83699  C 0.97166 2.77592 0.32228  C 0.27891 3.93809 0.66316  C 0.90347 4.92593 1.42348  C 2.22336 4.76294 1.83752  C 2.91948 3.60471 1.49128  C 2.29720 2.61171 0.73984  H 0.90270 0.28549 1.04820  H -2.76330 3.06988 -2.54466 </p>	-	2133.28874	-	2132.84569	-	2132.93266	-	2133.32040	-	2132.96432	-	2134.53974	-	2134.18366	-	2134.93534	-	2134.57926	5.5
--	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

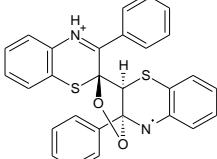
H -5.18359 2.90268 -1.98274 H -5.88300 1.66796 0.07017 H -4.20313 0.57090 1.50130 H -0.74549 4.07925 0.33467 H 0.35494 5.82527 1.68738 H 2.70979 5.53528 2.42612 H 3.95050 3.47228 1.80571 H 2.85004 1.71645 0.47041 O 0.71249 -0.03392 -1.89079 O 1.26442 1.20698 -1.41469 H 1.45815 -3.48482 0.69114										
	S 1.43207 -1.18400 0.91914 C 0.83659 0.11547 -0.20068 C 1.70341 1.35839 -0.11917 N 2.99685 1.24117 0.04044 C 5.15994 0.19495 0.15022 C 5.93996 -0.91797 0.41572 C 5.33657 -2.11754 0.80851 C 3.95593 -2.21118 0.92810 C 3.15808 -1.09497 0.66261 C 3.77007 0.10242 0.28057 C 1.18082 2.71476 -0.30072 C 0.34900 3.02791 -1.38967 C -0.07787 4.33711 -1.57072 C 0.29965 5.33233 -0.66788 C 1.12100 5.02314 0.41513 C 1.57214 3.72073 0.59772 H 5.61422 1.13102 -0.16144 H 7.01798 -0.85511 0.31513 H 5.94840 -2.98974 1.01490 H 3.49029 -3.14599 1.22399 H 0.07706 2.26506 -2.11323 H -0.70328 4.58175 -2.42324 H -0.04767 6.35102 -0.81027 H 1.40837 5.79405 1.12277 H 2.19158 3.47658 1.45647 S -1.36505 0.18527 1.67276 C -0.65145 0.32214 0.03160 C -1.28823 -0.62774 -0.99468 N -2.61638 -0.22524 -1.30720 C -4.75742 0.46877 -0.64817 C -5.69212 0.83158 0.29321	2133.27750	2132.83388	2132.91852	2133.30840	2132.94942	2134.52541	2134.16643	2134.92144	2134.56246

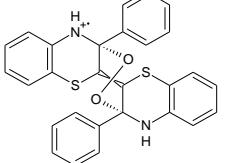
C -5.31095 0.96158 1.63929 C -3.98649 0.75234 2.02026 C -3.02047 0.38904 1.08637 C -3.39535 0.19889 -0.29935 C -1.24524 -2.14149 -0.76946 C -0.45670 -2.94458 -1.60063 C -0.43292 -4.32699 -1.43377 C -1.19954 -4.92859 -0.43794 C -2.00594 -4.13739 0.37781 C -2.03790 -2.75520 0.20745 H -0.90214 1.32335 -0.32791 H -5.02284 0.34747 -1.69379 H -6.72021 1.01479 -0.00190 H -6.04165 1.24576 2.38981 H -3.69841 0.89096 3.05858 H 0.14542 -2.48952 -2.37799 H 0.18804 -4.93304 -2.08713 H -1.17964 -6.00663 -0.30689 H -2.62416 -4.59440 1.14489 H -2.69834 -2.17049 0.83713 O 0.88204 -0.27883 -1.59039 O -0.46347 -0.26663 -2.12268 H 3.52524 2.10759 -0.04878									
 S 0.85855 2.29919 -1.63638 C -0.01408 0.82983 -0.96715 C -1.39243 1.28605 -0.49097 N -1.49659 2.28338 0.31023 C -0.52271 3.86502 1.82185 C 0.45994 4.78682 2.15290 C 1.55594 4.97472 1.30560 C 1.68350 4.21556 0.14742 C 0.71352 3.26165 -0.17127 C -0.41812 3.09042 0.65583 C -2.62611 0.55295 -0.86212 C -2.88725 0.11228 -2.16775 C -4.09339 -0.51596 -2.46615 C -5.04491 -0.72648 -1.46903 C -4.79260 -0.29001 -0.16827 C -3.59676 0.35316 0.13152 H -1.39773 3.72673 2.44986 H 0.36738 5.37238 3.06230 H 2.31954 5.70572 1.55302	2133.29667	2132.85321	2132.94012	2133.32677	2132.97021	2134.54763	2134.19108	2134.94367	2134.58711

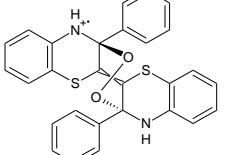
H 2.54400 4.34601 -0.50223 H -2.16722 0.28186 -2.96040 H -4.28995 -0.83841 -3.48435 H -5.98041 -1.22519 -1.70534 H -5.52844 -0.44983 0.61444 H -3.39838 0.70199 1.14013 S 0.19779 -0.16490 1.76624 C 0.87491 0.10216 0.11554 C 1.32759 -1.16461 -0.63896 N 0.45392 -2.30955 -0.42524 C -1.29347 -3.69985 0.39029 C -2.21848 -3.97857 1.35558 C -2.41059 -3.09210 2.44922 C -1.68012 -1.92508 2.54857 C -0.73243 -1.59988 1.56847 C -0.50786 -2.51260 0.47923 C 2.78566 -1.53435 -0.45328 C 3.77045 -0.75441 -1.06951 C 5.11365 -1.06226 -0.87909 C 5.48022 -2.13909 -0.07117 C 4.49843 -2.90983 0.54613 C 3.15011 -2.61157 0.35521 H 1.75913 0.71380 0.30404 H -1.13278 -4.37121 -0.44754 H -2.81263 -4.88348 1.28866 H -3.15058 -3.32749 3.20664 H -1.84505 -1.24222 3.37580 H 3.49059 0.08606 -1.69737 H 5.87502 -0.45875 -1.36364 H 6.52982 -2.37512 0.07638 H 4.77656 -3.74739 1.17832 H 2.39414 -3.21990 0.84174 O -0.11465 -0.11873 -2.00055 O 1.16078 -0.78273 -1.99530 H 0.57939 -3.03313 -1.12800											
 S -0.52250 -2.36475 -1.99714 C 0.25181 -0.97843 -1.08469 C 1.06929 -1.57867 0.06119 N 0.51254 -2.39504 0.88336 C -1.40753 -3.51248 1.77816 C -2.60040 -4.19939 1.61389 C -3.14636 -4.35611 0.33554	-	2133.27222	2132.82877	2132.91361	2133.30226	2132.94365	2134.52574	2134.16713	2134.92221	2134.56360	15.3

C -2.51527 -3.79650 -0.76967									
C -1.33240 -3.07118 -0.60333									
C -0.74967 -2.93993 0.67716									
C 2.49066 -1.22793 0.28398									
C 2.91992 -0.98713 1.59660									
C 4.26173 -0.73616 1.86332									
C 5.19463 -0.74450 0.82606									
C 4.77619 -0.99802 -0.47962									
C 3.43122 -1.22870 -0.75508									
H -0.94920 -3.40784 2.75703									
H -3.10018 -4.62966 2.47613									
H -4.07198 -4.90712 0.20046									
H -2.94864 -3.90186 -1.75996									
H 2.19053 -0.99307 2.40072									
H 4.57960 -0.53659 2.88257									
H 6.24377 -0.55596 1.03493									
H 5.49915 -1.01861 -1.28984									
H 3.12478 -1.43536 -1.77489									
S -1.54439 0.16503 0.94724									
C -0.78041 0.08982 -0.67503									
C -0.10507 1.39406 -1.11402									
N -1.17744 2.34151 -1.32966									
C -3.14246 3.54191 -0.75229									
C -4.20150 3.75847 0.08377									
C -4.43690 2.89780 1.18626									
C -3.61521 1.81510 1.41810									
C -2.52826 1.54446 0.57149									
C -2.25902 2.44801 -0.53007									
C 1.02026 2.05015 -0.32242									
C 0.78556 2.62491 0.93347									
C 1.81267 3.27109 1.61406									
C 3.08052 3.37018 1.04290									
C 3.31216 2.82296 -0.21639									
C 2.29012 2.16636 -0.89680									
H -1.61331 -0.03109 -1.37670									
H -2.95021 4.20133 -1.59303									
H -4.86527 4.59750 -0.09476									
H -5.27976 3.08279 1.84346									
H -3.81325 1.14645 2.24986									
H -0.19421 2.59191 1.39604									
H 1.61515 3.70635 2.58888									
H 3.87933 3.88010 1.57325									
H 4.29250 2.90310 -0.67622									
H 2.48338 1.74372 -1.87526									
O 1.06323 -0.26640 -2.01674									
O 0.35089 0.93654 -2.38652									
H -0.96831 3.13208 -1.93321									

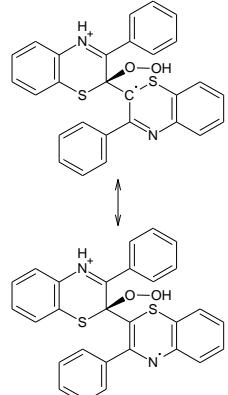
 <p> S 0.50516 2.36928 1.61360  C 0.43637 0.65430 0.93007  C 1.82757 0.40135 0.40007  N 2.26824 1.25417 -0.49940  C 2.08192 3.11264 -2.03407  C 1.63475 4.39720 -2.30233  C 0.83595 5.07029 -1.37337  C 0.46504 4.45782 -0.18145  C 0.89814 3.16012 0.09786  C 1.72017 2.50118 -0.83038  C 2.71120 -0.66949 0.83253  C 2.23114 -1.94905 1.17163  C 3.12566 -2.95426 1.51178  C 4.49630 -2.69809 1.54518  C 4.98039 -1.42571 1.23674  C 4.09858 -0.41735 0.87969  H 2.70615 2.58182 -2.74671  H 1.90893 4.87647 -3.23595  H 0.48825 6.07620 -1.58534  H -0.16869 4.97647 0.53054  H 1.17073 -2.16134 1.15078  H 2.74928 -3.94271 1.75447  H 5.18807 -3.48713 1.82383  H 6.04359 -1.21582 1.28981  H 4.48349 0.58158 0.69595  S -0.51005 0.02310 -1.77252  C -0.77680 0.46652 -0.04732  C -1.66391 -0.53422 0.74212  N -1.43697 -1.92960 0.55401  C -0.74178 -3.87416 -0.56088  C -0.21238 -4.52857 -1.64654  C 0.22722 -3.79056 -2.76211  C 0.14157 -2.39965 -2.76821  C -0.39422 -1.71771 -1.67913  C -0.87600 -2.44526 -0.53535  C -3.14524 -0.19331 0.66419  C -3.61381 0.99201 1.24120  C -4.96389 1.32063 1.15874  C -5.85187 0.47571 0.49223  C -5.38429 -0.70188 -0.08646  C -4.03472 -1.04076 0.00338  H -1.30124 1.42194 -0.10344  H -1.09241 -4.41243 0.31432 </p>	-	2133.28973	-	2132.84629	-	2132.93188	-	2133.32068	-	2132.96283	-	2134.53918	-	2134.18133	-	2134.93507	-	2134.57721	6.7
--	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

H -0.13133 -5.61079 -1.64553 H 0.64910 -4.30164 -3.62168 H 0.50259 -1.84083 -3.62718 H -2.92785 1.65400 1.76231 H -5.32157 2.23869 1.61547 H -6.90437 0.73542 0.42585 H -6.06945 -1.36457 -0.60676 H -3.67936 -1.96582 -0.43859 O 0.17378 -0.20425 2.00627 O -1.26083 -0.22390 2.08982 H 3.14344 1.01729 -0.95936											
	S -0.54243 -2.39447 -1.99763 C 0.20258 -0.96487 -1.11359 C 1.06009 -1.53578 -0.00085 N 0.47892 -2.38250 0.81235 C -1.38349 -3.57627 1.78552 C -2.57027 -4.27538 1.62499 C -3.14473 -4.39497 0.35700 C -2.54685 -3.80699 -0.75276 C -1.35862 -3.08934 -0.60526 C -0.78186 -2.98963 0.67030 C 2.45310 -1.18168 0.25362 C 2.86471 -0.96206 1.58094 C 4.20105 -0.70876 1.85863 C 5.13862 -0.69864 0.82579 C 4.73503 -0.92455 -0.49008 C 3.39717 -1.14929 -0.78657 H -0.92406 -3.47540 2.76442 H -3.04779 -4.72809 2.48722 H -4.07364 -4.94206 0.23219 H -3.00463 -3.89225 -1.73300 H 2.13501 -0.93682 2.38608 H 4.50867 -0.51376 2.88090 H 6.18475 -0.50943 1.04643 H 5.46556 -0.92412 -1.29269 H 3.09638 -1.33441 -1.81055 S -1.54027 0.20920 0.95938 C -0.82637 0.09866 -0.68888 C -0.16688 1.41104 -1.14098 N -1.15178 2.40040 -1.41339 C -3.06272 3.61050 -0.79177 C -4.10530 3.90129 0.05656	2133.27030	2132.82707	2132.91119	2133.30095	2132.94184	2134.52348	2134.16437	2134.91946	2134.56035	17.3

	C -4.33183 3.09389 1.18401 C -3.52681 1.98291 1.42966 C -2.46857 1.66457 0.58285 C -2.17807 2.51078 -0.55481 C 0.97425 2.04156 -0.33555 C 0.75522 2.61735 0.92246 C 1.79331 3.24893 1.60307 C 3.06050 3.33691 1.03062 C 3.27853 2.79250 -0.23267 C 2.24443 2.15216 -0.91128 H -1.66661 -0.03807 -1.37905 H -2.85227 4.22270 -1.66325 H -4.74878 4.75223 -0.14207 H -5.15040 3.31717 1.86085 H -3.73738 1.34502 2.28367 H -0.22545 2.59890 1.38206 H 1.60209 3.68471 2.57937 H 3.86712 3.83611 1.55976 H 4.25725 2.86411 -0.69815 H 2.42890 1.73872 -1.89557 O 1.00652 -0.27842 -2.05723 O 0.32191 0.93888 -2.41384 H 1.05370 -2.73882 1.57365							
Single-bond dimer, dioxane radical			2133.25477		2133.28083		2134.49633	2134.89450

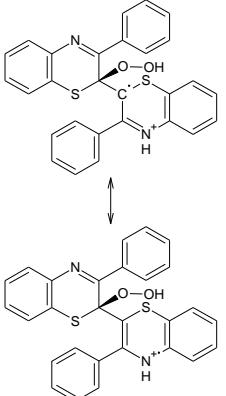
H -6.71163 0.31483 0.68122 H -4.73848 -0.75986 1.73280 H 1.24272 1.77049 -2.28350 H 2.99266 3.51724 -2.36750 H 3.24146 5.12609 -0.49288 H 1.71215 4.99121 1.46319 H -0.04211 3.24840 1.54391 S 1.98514 0.28422 1.52131 C 0.60001 -0.39494 0.84818 C 0.63114 -1.38375 -0.29494 N 1.85477 -2.06777 -0.44197 C 4.24189 -2.16242 -0.76648 C 5.51853 -1.71719 -0.45424 C 5.71203 -0.66386 0.44554 C 4.61078 -0.06126 1.03290 C 3.32112 -0.50749 0.71750 C 3.11789 -1.56496 -0.18176 C -0.50123 -2.38847 -0.35926 C -1.34904 -2.47009 -1.46294 C -2.33414 -3.45674 -1.50608 C -2.47159 -4.36077 -0.45510 C -1.61441 -4.28559 0.64357 C -0.62901 -3.30477 0.69068 H 4.10189 -2.98068 -1.46723 H 6.37380 -2.19484 -0.92207 H 6.71165 -0.31544 0.68162 H 4.73848 0.75929 1.73325 H -1.24366 -1.76984 -2.28317 H -2.99350 -3.51668 -2.36685 H -3.24133 -5.12608 -0.49259 H -1.71103 -4.99175 1.46277 H 0.04317 -3.24885 1.54314 H 1.81405 -2.85863 -1.07043 O 0.59018 -0.39897 -1.43234 O -0.59048 0.39932 -1.43224 H -1.81418 2.85903 -1.06969											
	S -1.65135 -1.47044 -1.36946 C -0.66834 -0.54348 -0.28798 C -1.41426 0.38437 0.64805 N -2.26167 -0.46918 1.46554 C -4.26281 -1.78247 1.70722 C -5.25143 -2.53557 1.11924	2133.30064	2132.85694	2132.94224	2133.32908	2132.97068	2134.54846	2134.19006	2134.94676	2134.58836	0.0

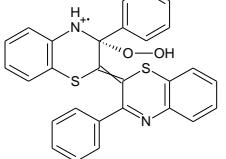
C -5.20541 -2.84741 -0.25784 C -4.13926 -2.43276 -1.02687 C -3.09940 -1.69012 -0.43907 C -3.18619 -1.29815 0.92913 C -2.18235 1.49585 -0.06033 C -1.61264 2.11577 -1.17587 C -2.26877 3.17361 -1.79664 C -3.49580 3.61995 -1.30502 C -4.06106 3.00793 -0.18860 C -3.40640 1.94706 0.43543 H -4.31564 -1.50840 2.75645 H -6.08799 -2.87842 1.71945 H -5.99949 -3.43319 -0.70802 H -4.07536 -2.70633 -2.07570 H -0.65600 1.77557 -1.56182 H -1.82242 3.64784 -2.66539 H -4.00952 4.44329 -1.79247 H -5.01443 3.35252 0.20014 H -3.85744 1.47915 1.30474 S 1.53952 -1.74213 -1.29154 C 0.69001 -0.68530 -0.23036 C 1.42662 0.06614 0.87463 N 2.40761 -0.81547 1.46972 C 4.72895 -1.46918 1.17695 C 5.73217 -2.01181 0.38609 C 5.46928 -2.40425 -0.93012 C 4.18813 -2.26342 -1.44339 C 3.17044 -1.73624 -0.64054 C 3.42976 -1.32086 0.67484 C 1.99348 1.41744 0.45892 C 2.34682 2.32870 1.46098 C 2.93184 3.54483 1.12607 C 3.17561 3.86206 -0.21177 C 2.82810 2.95707 -1.21034 C 2.23775 1.73734 -0.87660 H 4.94214 -1.15010 2.19361 H 6.73236 -2.11619 0.79506 H 6.25840 -2.81464 -1.55123 H 3.96649 -2.56865 -2.46210 H 2.14917 2.09380 2.50329 H 3.19441 4.24872 1.91030 H 3.63189 4.81265 -0.47180 H 3.01174 3.19579 -2.25367 H 1.96989 1.04572 -1.67028 H 2.73830 -0.44252 2.35363 O 0.49598 0.20398 1.95488 O -0.52735 1.08896 1.48935 H -2.30679 -0.24910 2.45407								
<b>Single-bond dimer, C2-hydroperoxylalkyl radical</b>								



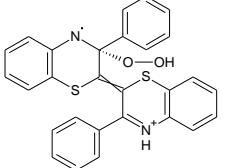
S	1.88905	0.68927	-1.47678
C	0.84202	0.32413	-0.01105
C	1.21643	-1.00930	0.64802
N	2.43944	-1.46899	0.59219
C	4.79429	-1.60906	0.16443
C	5.91976	-1.19217	-0.52655
C	5.81185	-0.18230	-1.48785
C	4.58579	0.41480	-1.75440
C	3.44362	0.00167	-1.06346
C	3.55800	-1.01470	-0.11109
C	0.25749	-1.74012	1.47535
C	-0.67731	-1.05538	2.27057
C	-1.54699	-1.77221	3.08301
C	-1.50772	-3.16639	3.10125
C	-0.58914	-3.85142	2.30535
C	0.29284	-3.14583	1.49780
H	4.86369	-2.38782	0.91884
H	6.88045	-1.64966	-0.31687
H	6.69237	0.14690	-2.03019
H	4.50890	1.20337	-2.49654
H	-0.69117	0.02824	2.28834
H	-2.25383	-1.23812	3.71000
H	-2.19600	-3.71981	3.73271
H	-0.56849	-4.93641	2.30235
H	0.96740	-3.69207	0.84341
C	-0.58335	0.30403	-0.53187
S	-0.85463	-1.09444	-1.53362
C	-2.59675	-1.19934	-1.52847
C	-3.37952	-0.13868	-1.01542
N	-2.89026	1.04302	-0.52874
C	-1.59697	1.25700	-0.30779
C	-3.19084	-2.34320	-0.27077
C	-4.57370	-2.45559	-2.08980
C	-5.37090	-1.42645	-1.56781

2133.28862 2132.84576 2132.93500 2133.32039 2132.96676 2134.53955 2134.18592 2134.93758 2134.58396 9.5

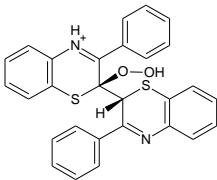
C -4.78351 -0.28932 -1.04555 C -1.30582 2.62895 0.20006 C -0.43493 3.47746 -0.49109 C -0.23111 4.78306 -0.05127 C -0.88798 5.24836 1.08787 C -1.76330 4.40772 1.77605 C -1.98154 3.10785 1.32675 H -2.57028 -3.14142 -2.46921 H -5.03376 -3.34564 -2.50725 H -6.45242 -1.51938 -1.58116 H -5.38246 0.52486 -0.64916 H 0.07221 3.12372 -1.38449 H 0.43834 5.43821 -0.60127 H -0.72390 6.26490 1.43379 H -2.28152 4.76657 2.66071 H -2.67312 2.45445 1.85069 O 0.92443 1.30382 1.00372 O 2.26140 1.32905 1.49653 H 2.57715 2.17916 1.14696 H 2.62073 -2.28021 1.18118										
 <p>S 1.14639 -2.19511 0.34012 C 0.46463 -0.87148 -0.72908 C 1.35671 0.37208 -0.85997 N 2.61394 0.39836 -0.61221 C 4.75900 -0.41169 -0.00661 C 5.61083 -1.37901 0.50526 C 5.08824 -2.59727 0.94829 C 3.72151 -2.84301 0.87199 C 2.86783 -1.86689 0.35136 C 3.37414 -0.63400 -0.09082 C 0.76339 1.60077 -1.45255 C -0.40117 1.59806 -2.23480 C -0.89430 2.78380 -2.77622 C -0.23545 3.98961 -2.54919</p>	2133.30164	2132.85838	2132.94677	2133.33090	2132.97603	2134.55554	2134.20067	2134.95405	2134.59917	0.0

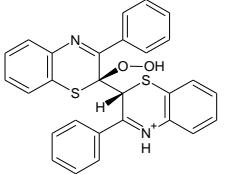
C 0.92902 4.00244 -1.77865 C 1.42214 2.82242 -1.23788 H 5.13707 0.54371 -0.35811 H 6.67797 -1.18891 0.56190 H 5.74566 -3.36126 1.35199 H 3.31698 -3.79233 1.21234 H -0.91420 0.67164 -2.46397 H -1.79183 2.75793 -3.38724 H -0.62249 4.91241 -2.97167 H 1.44973 4.93750 -1.59289 H 2.32012 2.82959 -0.62949 C -0.94700 -0.66232 -0.19543 S -2.08440 -1.74133 -0.94496 C -3.58492 -1.36760 -0.14359 C -3.68413 -0.38158 0.85159 N -2.56712 0.31189 1.26829 C -1.28882 0.20679 0.82986 C -4.72276 -2.08152 -0.53574 C -5.94344 -1.80905 0.06062 C -6.04191 -0.82134 1.05052 C -4.92335 -0.11061 1.44671 C -0.36735 1.12684 1.54467 C -0.65539 2.49927 1.52311 C 0.12744 3.38583 2.25443 C 1.19113 2.91054 3.02053 C 1.46774 1.54480 3.05741 C 0.69255 0.65075 2.32435 H -4.64302 -2.84292 -1.30555 H -6.82456 -2.36337 -0.24440 H -7.00029 -0.60988 1.51269 H -4.99460 0.65441 2.21396 H -1.47280 2.87387 0.91275 H -0.09162 4.44855 2.22063 H 1.80083 3.60372 3.59234 H 2.28467 1.16875 3.66561 H 0.89647 -0.41309 2.37412 O 0.23908 -1.37606 -2.05533 O 1.47831 -1.75016 -2.62715 H 1.49568 -2.70789 -2.45901 H -2.70608 0.95894 2.03756										
<b>Single-bond dimer, C3-hydroperoxylalkyl radical</b>										
	2133.28616	2132.84361	2132.93291	2133.31398	2132.96073	2134.53273	2134.17947	2134.93316	2134.57991	0.0

S 1.76714 -1.14799 1.01775									
C 0.92268 0.22849 0.37361									
C 1.74093 1.35385 -0.09493									
N 2.93191 1.22558 -0.59641									
C 4.85672 0.01683 -1.30787									
C 5.69761 -1.07271 -1.19427									
C 5.36801 -2.13782 -0.33673									
C 4.18190 -2.12712 0.37491									
C 3.30064 -1.04523 0.22136									
C 3.64622 0.06125 -0.58919									
C 1.24624 2.74283 0.05010									
C 0.59227 3.14304 1.22400									
C 0.19996 4.46772 1.38393									
C 0.44365 5.39775 0.37234									
C 1.09912 5.00359 -0.79497									
C 1.51020 3.68434 -0.95267									
H 5.11163 0.87007 -1.92828									
H 6.62880 -1.09812 -1.75101									
H 6.04310 -2.98153 -0.23617									
H 3.91703 -2.95899 1.02074									
H 0.39849 2.42024 2.01253									
H -0.29535 4.77527 2.29997									
H 0.12671 6.42921 0.49558									
H 1.29098 5.72578 -1.58290									
H 2.02499 3.36879 -1.85469									
S -1.29181 1.35798 -0.63958									
C -0.47380 0.17036 0.28292									
C -1.23581 -0.99290 0.92569									
N -2.63573 -0.67682 1.15624									
C -4.82280 -0.42265 0.14274									
C -5.63966 0.19522 -0.79141									
C -5.11982 1.12731 -1.70040									
C -3.77326 1.44305 -1.65891									
C -2.94511 0.82305 -0.71044									
C -3.45598 -0.11671 0.19725									
C -1.06706 -2.31037 0.17274									
C -1.23323 -3.52120 0.85531									
C -1.17417 -4.72507 0.15910									
C -0.95973 -4.73105 -1.21914									
C -0.80412 -3.52585 -1.90029									
C -0.85749 -2.31758 -1.20815									
H -5.23273 -1.14817 0.83978									
H -6.69510 -0.05701 -0.82052									
H -5.76472 1.59899 -2.43385									
H -3.35179 2.16615 -2.35123									
H -1.39845 -3.52708 1.92822									
H -1.29485 -5.66068 0.69696									
H -0.91504 -5.67194 -1.75948									
H -0.63820 -3.52113 -2.97331									
H -0.72486 -1.38740 -1.75371									

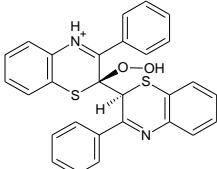
O -0.69257 -1.22649 2.22377 O -0.75568 -0.02788 2.98948 H -1.70952 0.06215 3.16522 H -3.07843 -1.44526 1.65080									
 <p>S 1.98428 -0.71521 1.38087  C 0.88663 0.31879 0.42513  C 1.45160 1.61033 0.06038  N 2.72207 1.69594 -0.27255  C 4.79877 0.80411 -1.13057  C 5.74025 -0.21609 -1.16653  C 5.52081 -1.39220 -0.44731  C 4.35913 -1.55811 0.30187  C 3.40608 -0.53980 0.34735  C 3.63898 0.63736 -0.37251  C 0.69043 2.86099 0.15561  C -0.24837 3.01681 1.18839  C -0.92042 4.22361 1.33089  C -0.67683 5.27269 0.44317  C 0.24823 5.11717 -0.58983  C 0.93708 3.91933 -0.73298  H 4.95456 1.72358 -1.68749  H 6.64246 -0.09381 -1.75628  H 6.25508 -2.19106 -0.47451  H 4.18786 -2.47779 0.85271  H -0.43337 2.20015 1.88027  H -1.63517 4.34739 2.13836  H -1.21152 6.21121 0.55367  H 0.42525 5.92570 -1.29181  H 1.62264 3.79495 -1.56728  S -1.16332 0.73167 -1.23869  C -0.38809 -0.05523 0.09728  C -1.08558 -1.24087 0.75563  N -2.51331 -1.14805 0.89425  C -4.70924 -0.56683 0.28851  C -5.60717 0.06599 -0.53902  C -5.14310 0.86522 -1.59986  C -3.77551 1.04296 -1.80718  C -2.85716 0.41377 -0.97394  C -3.29600 -0.44623 0.08514  C -0.75526 -2.58146 0.10134  C -1.24702 -3.74172 0.71251  C -0.99530 -4.98779 0.14713</p>	2133.27929	2132.83687	2132.92611	2133.30956	2132.95638	2134.52711	2134.17392	2134.92579	2134.57261

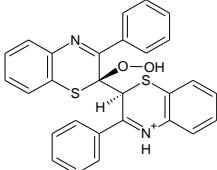
4.6

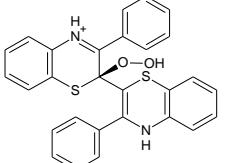
C -0.25843 -5.08565 -1.03372 C 0.22920 -3.93173 -1.64358 C -0.01674 -2.68120 -1.07898 H -5.03598 -1.20172 1.10607 H -6.67365 -0.05376 -0.37808 H -5.84925 1.36338 -2.25627 H -3.42891 1.68698 -2.61047 H -1.82281 -3.66176 1.62839 H -1.37630 -5.88339 0.62896 H -0.06457 -6.05849 -1.47608 H 0.80612 -4.00021 -2.56106 H 0.37474 -1.79341 -1.56530 O -0.58615 -1.36738 2.09713 O -1.04175 -0.24971 2.86021 H -1.96899 -0.49403 3.02853 H 3.09650 2.62863 -0.42374									
<b>Single-bond dimer, C2-hydroperoxide</b>									
 S 0.64489 -1.27858 -0.99965 C 0.17244 0.41356 -0.51420 C 1.34494 1.26506 -0.03120 N 2.57235 1.00596 -0.39021 C 4.44579 0.03458 -1.52845 C 4.99470 -0.98226 -2.29108 C 4.19975 -2.06554 -2.67971 C 2.86206 -2.13347 -2.31121 C 2.29749 -1.11377 -1.53981 C 3.09954 -0.03781 -1.15383 C 1.13819 2.48391 0.76081 C 0.14438 3.41443 0.41402 C 0.01918 4.59120 1.14266 C 0.86599 4.84630 2.22107 C 1.85121 3.92315 2.57098 C 1.99449 2.74850 1.84351 H 5.04685 0.88642 -1.22242 H 6.03713 -0.93269 -2.58590 H 4.62587 -2.86314 -3.27975 H 2.24989 -2.97548 -2.61905 H -0.49072 3.23884 -0.44753 H -0.73818 5.31524 0.85961 H 0.75736 5.76457 2.78997 H 2.50289 4.11179 3.41805 H 2.73524 2.01326 2.14636	2133.92148	2133.46528	2133.55350	2133.95502	2133.58704	2135.17929	2134.81131	2135.57731	2135.20933

C -0.93763 0.32032 0.57910 S -0.29198 -0.07124 2.22698 C -0.34378 -1.82820 2.18126 C -1.26650 -2.48607 1.34801 N -2.19032 -1.83040 0.54042 C -2.10276 -0.59441 0.20266 C 0.49303 -2.55816 3.02596 C 0.42900 -3.94910 3.03567 C -0.46655 -4.61598 2.19700 C -1.31141 -3.88712 1.36949 C -3.19762 -0.02940 -0.62132 C -3.90925 -0.88745 -1.47511 C -4.95779 -0.40720 -2.24977 C -5.32448 0.93806 -2.17760 C -4.63060 1.79719 -1.32811 C -3.56929 1.32103 -0.56196 H 1.19858 -2.03868 3.66847 H 1.08428 -4.51027 3.69493 H -0.51232 -5.70059 2.19808 H -2.02777 -4.38286 0.72098 H -3.61865 -1.93168 -1.52576 H -5.48893 -1.08213 -2.91464 H -6.14576 1.31363 -2.78094 H -4.91495 2.84279 -1.25722 H -3.06350 2.01390 0.10358 O -0.45574 1.11874 -1.57262 O 0.49400 1.31208 -2.61851 H 0.18897 0.66997 -3.28137 H -1.31886 1.33624 0.68952 H 3.25876 1.70444 -0.10774											
	S 0.67182 -2.18165 -1.69338 C 0.01553 -0.66237 -0.89995 C 1.09594 0.42235 -1.01902 N 2.31702 0.18860 -0.68444 C 4.00043 -1.15773 0.35242 C 4.59176 -2.38718 0.60368 C 3.99658 -3.55851 0.12521 C 2.79478 -3.50023 -0.57224 C 2.17947 -2.26562 -0.79814 C 2.79068 -1.07294 -0.35604 C 0.78309 1.78036 -1.53188 C -0.46693 2.40800 -1.39306	2133.92288	2133.46689	2133.55369	2133.95732	2133.58812	2135.18402	2134.81482	2135.58165	2135.21246	0.1

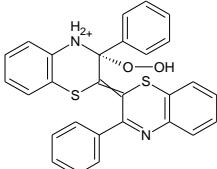
C -0.66872 3.69922 -1.87783									
C 0.36554 4.38281 -2.51199									
C 1.61008 3.76788 -2.65927									
C 1.81653 2.48274 -2.17519									
H 4.46107 -0.23295 0.68683									
H 5.52421 -2.43639 1.15729									
H 4.46330 -4.52201 0.30567									
H 2.32129 -4.41108 -0.92692									
H -1.29148 1.90337 -0.90293									
H -1.64007 4.16853 -1.75460									
H 0.20300 5.38638 -2.89366									
H 2.42005 4.28955 -3.16044									
H 2.77998 1.99826 -2.29322									
C -0.33951 -0.96576 0.60159									
S -1.47574 -2.35355 0.85871									
C -2.99837 -1.54192 0.54303									
C -3.14794 -0.17942 0.83394									
N -2.07687 0.54134 1.38518									
C -0.80287 0.23248 1.38082									
C -4.10443 -2.25835 0.08482									
C -5.32737 -1.61705 -0.08545									
C -5.46245 -0.25491 0.19326									
C -4.37288 0.46724 0.65747									
C 0.13824 1.08736 2.09502									
C 1.29428 0.53788 2.67832									
C 2.16746 1.34800 3.39154									
C 1.91689 2.71412 3.51197									
C 0.78034 3.27243 2.92421									
C -0.10820 2.46832 2.22699									
H -4.00211 -3.31455 -0.14332									
H -6.17955 -2.18428 -0.44592									
H -6.41549 0.24262 0.04965									
H -4.46203 1.52678 0.87899									
H 1.49903 -0.52610 2.62271									
H 3.04547 0.90964 3.85451									
H 2.60941 3.34621 4.05912									
H 0.59324 4.33859 2.99863									
H -0.96074 2.93391 1.74044									
O -1.21597 -0.35372 -1.49954									
O -1.07237 -0.22714 -2.91030									
H -0.96302 0.73572 -3.01697									
H 0.60067 -1.30716 1.04122									
H -2.34561 1.36027 1.92563									

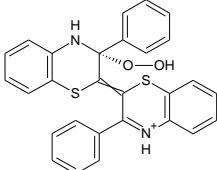
 <p> S 1.21626 -1.04251 1.58502  C -0.16693 -0.40122 0.53437  C -0.90839 -1.64595 0.05023  N -0.19537 -2.55974 -0.57202  C 1.78485 -3.52016 -1.56676  C 3.15233 -3.74253 -1.52829  C 3.93129 -3.13909 -0.53649  C 3.35331 -2.29553 0.40482  C 1.97782 -2.05153 0.37176  C 1.20038 -2.68446 -0.61055  C -2.32441 -1.90699 0.25454  C -3.28543 -0.88060 0.21454  C -4.63025 -1.18848 0.36206  C -5.03366 -2.50754 0.57341  C -4.08545 -3.52917 0.64040  C -2.73922 -3.23550 0.48018  H 1.16547 -3.98937 -2.32544  H 3.61253 -4.38839 -2.26826  H 5.00161 -3.31591 -0.50520  H 3.96507 -1.81217 1.15952  H -2.98396 0.14498 0.04608  H -5.36802 -0.39402 0.31268  H -6.08730 -2.73839 0.69805  H -4.39356 -4.55179 0.83217  H -2.00695 -4.03076 0.58869  C 0.34739 0.46851 -0.65141  S -0.89339 0.78261 -1.93754  C -1.74368 2.12707 -1.18307  C -1.06106 2.96576 -0.28013  N 0.29658 2.85823 -0.00674  C 0.97448 1.78596 -0.20144  C -3.07345 2.38599 -1.52293  C -3.74440 3.45720 -0.93970  C -3.09059 4.27303 -0.01323  C -1.75887 4.03536 0.29973  C 2.43633 1.84407 0.03048  C 3.34492 1.07894 -0.71327  C 4.71576 1.20298 -0.49792  C 5.19752 2.07701 0.47409  C 4.29974 2.83952 1.22425  C 2.93321 2.73093 0.99907  H -3.58433 1.74238 -2.23402  H -4.77939 3.64952 -1.20566 </p>	-	2133.92238	-	2133.46613	-	2133.55294	-	2133.95564	-	2133.58620	-	2135.18267	-	2134.81323	-	2135.58041	-	2135.21097	1.0
--	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

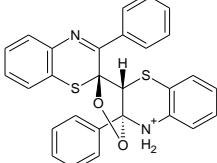
H -3.61567 5.10291 0.44960 H -1.22270 4.67608 0.99369 H 3.00227 0.40438 -1.49235 H 5.40651 0.61442 -1.09443 H 6.26621 2.16480 0.64683 H 4.66725 3.51922 1.98758 H 2.23002 3.32249 1.57624 O -0.95486 0.44403 1.30881 O -1.36083 -0.22674 2.50592 H -1.03122 0.39451 3.17609 H 1.10095 -0.13196 -1.16509 H -0.71497 -3.31355 -1.01554									
 S 1.22683 -1.01732 1.58519 C -0.17739 -0.45503 0.53314 C -0.86619 -1.72576 0.00944 N -0.18893 -2.65642 -0.56620 C 1.82813 -3.49527 -1.54944 C 3.20231 -3.68274 -1.52825 C 3.97315 -3.08489 -0.52640 C 3.37344 -2.26807 0.42592 C 1.99410 -2.04538 0.38411 C 1.19851 -2.68337 -0.59211 C -2.31859 -1.95959 0.20240 C -3.28606 -0.94145 0.18754 C -4.63445 -1.24740 0.36256 C -5.03876 -2.56635 0.55708 C -4.08501 -3.58519 0.57471 C -2.73950 -3.28536 0.40060 H 1.20603 -3.98101 -2.29528 H 3.67453 -4.30934 -2.27846 H 5.04662 -3.24435 -0.49388 H 3.97445 -1.78458 1.19047 H -2.99859 0.08952 0.02083 H -5.36909 -0.44797 0.34036 H -6.09005 -2.79963 0.69772 H -4.39001 -4.61534 0.73342 H -1.99298 -4.07249 0.42328 C 0.33064 0.43291 -0.64749 S -0.89342 0.79358 -1.94209 C -1.76338 2.10428 -1.16087 C -1.11057 2.94821 -0.25262 N 0.25660 2.76911 0.01324	2133.92422	2133.46797	2133.55456	2133.95684	2133.58718	2135.18428	2134.81461	2135.58224	2135.21257

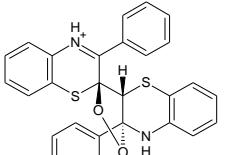
C 0.99106 1.70623 -0.19041 C -3.09073 2.37453 -1.49814 C -3.74890 3.45765 -0.92340 C -3.09498 4.28087 -0.00458 C -1.77118 4.03150 0.32864 C 2.42650 1.78952 0.04944 C 3.32350 1.08205 -0.76851 C 4.69259 1.22069 -0.57846 C 5.18062 2.03580 0.44149 C 4.29502 2.72454 1.27291 C 2.92705 2.61296 1.07588 H -3.60533 1.73336 -2.20727 H -4.78195 3.65514 -1.19118 H -3.61466 5.11805 0.44873 H -1.24765 4.66708 1.03689 H 2.96513 0.46131 -1.58274 H 5.37897 0.68896 -1.22935 H 6.25130 2.13022 0.59424 H 4.67172 3.34136 2.08229 H 2.25189 3.11945 1.75978 O -0.98289 0.40404 1.29843 O -1.36577 -0.21236 2.52243 H -2.23966 -0.58212 2.29740 H 1.07981 -0.17293 -1.16391 H 0.74506 3.60751 0.31972									
 S 2.10731 0.78907 -1.35608 C 0.88732 0.36617 -0.04755 C 1.13614 -1.02477 0.54432 N 2.34392 -1.52516 0.60073 C 4.72646 -1.73643 0.42523 C 5.93835 -1.32453 -0.10519 C 5.97681 -0.25115 -0.99990 C 4.81007 0.41354 -1.35828 C 3.58238 0.00619 -0.83003 C 3.55124 -1.07369 0.05618 C 0.07293 -1.76860 1.21994 C 0.07098 -3.17415 1.16627 C -0.90057 -3.89674 1.84495 C -1.87512 -3.22973 2.58883 C -1.87977 -1.83676 2.64392 C -0.91861 -1.10200 1.95889 H 4.68232 -2.56553 1.12611	2133.92388	2133.46724	2133.55477	2133.95699	2133.58788	2135.18208	2134.81297	2135.58059	2135.21148

H 6.85174 -1.83619 0.17814 H 6.92431 0.07464 -1.41714 H 4.84581 1.25188 -2.04714 H 0.79356 -3.70283 0.54982 H -0.90516 -4.98026 1.78241 H -2.63320 -3.79665 3.12067 H -2.63212 -1.31644 3.22830 H -0.90924 -0.02113 2.03288 C -0.44779 0.44067 -0.73530 S -0.71302 -0.92399 -1.84998 C -2.41554 -1.23033 -1.46063 C -3.23182 -0.11825 -1.22285 N -2.66010 1.15921 -1.15826 C -1.40634 1.39722 -0.62135 C -2.95465 -2.51476 -1.47540 C -4.32652 -2.69184 -1.30258 C -5.14615 -1.58345 -1.09014 C -4.60351 -0.30210 -1.03343 C -1.27445 2.71557 0.04759 C -0.31325 3.63688 -0.38326 C -0.22960 4.89122 0.21410 C -1.10211 5.23490 1.24685 C -2.06834 4.32425 1.67361 C -2.16255 3.07279 1.06988 H -2.30404 -3.36746 -1.64608 H -4.75092 -3.69023 -1.33838 H -6.21554 -1.71425 -0.95503 H -5.24099 0.55711 -0.84163 H 0.36012 3.37319 -1.19343 H 0.51455 5.60314 -0.13070 H -1.03330 6.21309 1.71388 H -2.75014 4.58736 2.47689 H -2.91369 2.36290 1.40705 O 0.89235 1.27336 1.03812 O 2.17877 1.25177 1.65247 H 2.55455 2.09316 1.34371 H -3.31154 1.92775 -1.07881 H 2.43267 -2.37485 1.15534								
	n.d.							
Single-bond dimer, C3-hydroperoxide								

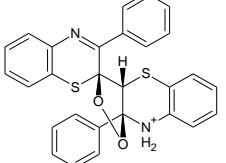
 <p> S 0.94811 -1.71063 1.42228  C 0.94733 -0.19613 0.51293  C 2.25630 0.08118 -0.14176  N 2.89474 -0.82435 -0.80098  C 3.01966 -2.98763 -1.81927  C 2.76895 -4.35147 -1.80741  C 2.00169 -4.91138 -0.78064  C 1.45788 -4.09997 0.20888  C 1.67754 -2.72043 0.17506  C 2.48615 -2.14802 -0.82753  C 2.88907 1.40950 0.01544  C 2.68311 2.16612 1.17821  C 3.33175 3.38759 1.34493  C 4.17716 3.87298 0.34929  C 4.38328 3.12511 -0.81281  C 3.75235 1.89789 -0.97619  H 3.64334 -2.53763 -2.58613  H 3.18418 -4.98510 -2.58500  H 1.81755 -5.98109 -0.75580  H 0.84372 -4.53078 0.99468  H 2.02907 1.79285 1.96208  H 3.17516 3.95912 2.25501  H 4.67492 4.83002 0.47594  H 5.03824 3.50203 -1.59304  H 3.90966 1.30926 -1.87442  S -0.06066 2.17596 -0.39075  C -0.13876 0.60580 0.45090  C -1.42008 0.22620 1.18708  N -2.39207 1.42696 1.13064  C -4.08198 1.86353 -0.63317  C -4.35072 2.30617 -1.92666  C -3.30906 2.70404 -2.76448  C -1.98504 2.65069 -2.33301  C -1.70663 2.21454 -1.03883  C -2.76233 1.84682 -0.21099  C -2.14965 -0.99125 0.65691  C -3.04316 -1.67493 1.48906  C -3.76248 -2.75706 0.98954  C -3.60331 -3.15228 -0.33789  C -2.72139 -2.46279 -1.16817  C -1.99375 -1.38364 -0.67446  H -4.88582 1.55147 0.02719  H -5.37652 2.33695 -2.27793 </p>	-	2133.90833	-	2133.45183	-	2133.53970	-	2133.94297	-	2133.57434	-	2135.17180	-	2134.80317	-	2135.57092	-	2135.20229	6.4
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

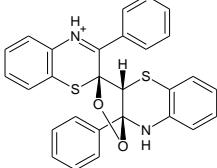
H -3.52649 3.04571 -3.77145 H -1.17367 2.93806 -2.99380 H -3.16819 -1.37959 2.52620 H -4.44656 -3.29154 1.64136 H -4.16619 -3.99652 -0.72465 H -2.59426 -2.76517 -2.20300 H -1.30024 -0.85852 -1.32401 H -3.22119 1.16914 1.67465 O -1.19888 0.01072 2.55147 O -0.56433 1.19747 3.06177 H -0.96778 1.24129 3.94459 H -1.92461 2.19403 1.63993									
 S 1.57107 -1.20517 1.41997 C 0.91761 0.19016 0.52687 C 1.95480 1.05798 -0.02157 N 3.01385 0.51131 -0.57827 C 4.23245 -1.28113 -1.64351 C 4.57381 -2.62491 -1.70578 C 3.98573 -3.53577 -0.82515 C 3.04761 -3.11190 0.11106 C 2.69077 -1.76425 0.17960 C 3.29440 -0.85740 -0.70037 C 1.89686 2.51481 0.06129 C 1.37669 3.10799 1.22438 C 1.38011 4.49081 1.35178 C 1.87405 5.28771 0.31865 C 2.37549 4.70248 -0.84591 C 2.39811 3.32084 -0.97556 H 4.68299 -0.56002 -2.31942 H 5.29807 -2.96180 -2.43970 H 4.25367 -4.58652 -0.87171 H 2.58673 -3.82408 0.78840 H 0.99386 2.48314 2.02638 H 0.99442 4.94784 2.25737 H 1.86299 6.36893 0.41727 H 2.74168 5.32470 -1.65611 H 2.75456 2.87542 -1.90049 S -1.03630 1.85027 -0.41416 C -0.42033 0.42661 0.40855 C -1.41147 -0.52670 1.09118 N -2.76914 0.02153 1.13752 C -4.68966 0.13926 -0.37535	2133.92514	2133.46843	2133.55589	2133.95743	2133.58817	2135.18240	2134.81314	2135.58174	2135.21248

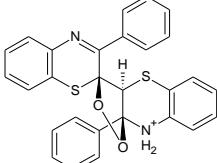
C -5.27096 0.66726 -1.52413 C -4.54175 1.50829 -2.36606 C -3.22393 1.82750 -2.05037 C -2.65349 1.32098 -0.88267 C -3.37533 0.47492 -0.03829 C -1.39881 -1.92684 0.49048 C -1.75237 -3.03089 1.27353 C -1.83964 -4.29500 0.69556 C -1.58922 -4.46607 -0.66586 C -1.25198 -3.36435 -1.44946 C -1.15761 -2.09830 -0.87489 H -5.25444 -0.52757 0.27106 H -6.29629 0.40749 -1.76934 H -4.99190 1.90755 -3.26926 H -2.64074 2.47387 -2.69998 H -1.94743 -2.90783 2.33420 H -2.10319 -5.14864 1.31323 H -1.65860 -5.45319 -1.11339 H -1.05883 -3.48660 -2.51116 H -0.88605 -1.24906 -1.49601 H -3.35897 -0.65092 1.62026 O -1.03695 -0.67198 2.45810 O -1.03327 0.61387 3.07544 H -1.95123 0.91302 2.92030 H 3.73937 1.14309 -0.90577										
<b>Single-bond dimer, dioxolane</b>										
	S -1.69362 -1.64736 -0.73646 C -1.12437 -0.13311 0.10596 C -2.15390 0.98468 -0.10907 N -3.41376 0.77343 0.00563 C -5.27731 -0.52624 0.73788 C -5.91814 -1.74090 0.93500 C -5.26411 -2.93456 0.61625 C -3.96315 -2.91176 0.12485 C -3.30788 -1.69048 -0.04517 C -3.96438 -0.47996 0.24584 C -1.70448 2.36296 -0.42801 C -2.19035 2.98572 -1.58349 C -1.81402 4.29161 -1.88663 C -0.96169 4.99069 -1.03246 C -0.48817 4.38139 0.12922 C -0.85212 3.07106 0.43035	2133.91789	2133.46025	2133.54566	2133.95136	2133.57913	2135.17601	2134.80378	2135.57288	2135.20065

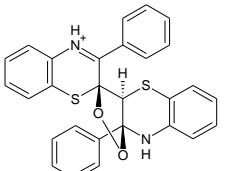
H -5.77346 0.41449 0.95698 H -6.93146 -1.76148 1.32367 H -5.76573 -3.88711 0.75686 H -3.45016 -3.83865 -0.11461 H -2.85819 2.43811 -2.24187 H -2.18858 4.76372 -2.79009 H -0.67141 6.01037 -1.26805 H 0.16025 4.92770 0.80773 H -0.50508 2.61656 1.35513 S 0.76947 -0.28165 -1.99221 C 0.35028 0.13648 -0.26109 C 1.10141 -0.63471 0.84650 N 1.65038 -1.95397 0.28561 C 3.93964 -2.36795 -0.55644 C 4.89348 -2.18006 -1.55279 C 4.59295 -1.39770 -2.66762 C 3.34926 -0.78540 -2.79656 C 2.38117 -0.97374 -1.80826 C 2.69583 -1.77710 -0.71477 C 2.20566 0.11987 1.54606 C 2.99112 1.05459 0.86455 C 4.02515 1.70919 1.52852 C 4.27899 1.43516 2.87107 C 3.49489 0.50566 3.55255 C 2.45968 -0.15207 2.89443 H 0.54843 1.19904 -0.12026 H 4.15853 -2.97195 0.31970 H 5.87013 -2.64094 -1.45291 H 5.34035 -1.24742 -3.44006 H 3.12897 -0.15793 -3.65407 H 2.80912 1.28479 -0.18138 H 4.62803 2.43686 0.99442 H 5.08325 1.95043 3.38756 H 3.68210 0.29589 4.60104 H 1.83870 -0.85996 3.43438 O -1.04063 -0.26790 1.51639 O 0.10613 -1.09692 1.74087 H 2.00277 -2.51141 1.07093 H 0.84710 -2.47444 -0.10309											
	S 1.56336 -1.41965 0.44661 C 0.81208 0.10073 -0.18755 C 1.74435 1.26788 0.10932	2133.93467	2133.47780	2133.56471	2133.96709	2133.59713	2135.18854	2134.81858	2135.58530	2135.21534	2.0

N 3.02639 1.12648 -0.12283									
C 5.03845 0.10007 -0.96186									
C 5.76450 -1.04361 -1.24916									
C 5.19449 -2.30481 -1.04306									
C 3.89788 -2.42835 -0.56001									
C 3.15192 -1.28199 -0.27348									
C 3.73476 -0.02555 -0.47094									
C 1.30772 2.58211 0.58756									
C 0.29353 3.28946 -0.07784									
C -0.06020 4.55961 0.35795									
C 0.57390 5.12284 1.46640									
C 1.57854 4.42208 2.13170									
C 1.95740 3.15862 1.69093									
H 5.46722 1.08597 -1.11546									
H 6.77490 -0.95669 -1.63368									
H 5.76461 -3.19993 -1.27001									
H 3.45689 -3.40873 -0.41071									
H -0.18004 2.86649 -0.95809									
H -0.83049 5.11169 -0.17092									
H 0.28350 6.11048 1.81120									
H 2.06717 4.85597 2.99813									
H 2.72476 2.60438 2.22411									
S -1.12274 -0.61965 1.85540									
C -0.64194 0.23958 0.35543									
C -1.48346 -0.09562 -0.89544									
N -1.58735 -1.50738 -1.10060									
C -2.02028 -3.79795 -0.51851									
C -2.11534 -4.82273 0.41193									
C -1.88230 -4.57170 1.76595									
C -1.55208 -3.28333 2.16760									
C -1.46625 -2.24326 1.23711									
C -1.69861 -2.48783 -0.12589									
C -2.81316 0.64351 -0.95598									
C -3.92546 0.06305 -0.33880									
C -5.15330 0.72037 -0.34251									
C -5.28615 1.95470 -0.97645									
C -4.18346 2.52914 -1.60551									
C -2.94909 1.88185 -1.59189									
H -0.82337 1.28874 0.59239									
H -2.19659 -3.99972 -1.57213									
H -2.37011 -5.82342 0.07584									
H -1.95118 -5.36873 2.49914									
H -1.35928 -3.07181 3.21622									
H -3.83944 -0.90626 0.14278									
H -6.00804 0.26136 0.14542									
H -6.24587 2.46296 -0.98572									
H -4.27999 3.48448 -2.11293									
H -2.10395 2.33651 -2.09688									
O 0.66863 0.02115 -1.60704									
O -0.66654 0.45925 -1.92444									

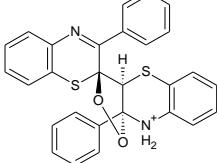
H -1.98751 -1.74797 -1.99790 H 3.58616 1.97295 -0.03921										
 S -1.60971 -1.24340 -0.71006 C -0.96462 0.11479 0.30551 C -1.78970 1.40017 0.12298 N -3.04943 1.42205 -0.10938 C -5.23153 0.47436 -0.22208 C -6.09347 -0.59353 -0.42212 C -5.57630 -1.86191 -0.70400 C -4.20192 -2.06128 -0.76702 C -3.33497 -0.98647 -0.55237 C -3.84069 0.29570 -0.28487 C -1.10515 2.71194 0.28089 C -0.40674 3.04345 1.45087 C 0.18444 4.29843 1.58031 C 0.09199 5.22802 0.54516 C -0.60642 4.90463 -0.61784 C -1.20694 3.65519 -0.74838 H -5.60676 1.47163 -0.01269 H -7.16688 -0.44207 -0.36693 H -6.24569 -2.70057 -0.86934 H -3.79840 -3.04794 -0.97601 H -0.35675 2.33544 2.27387 H 0.71081 4.55139 2.49594 H 0.55755 6.20390 0.64738 H -0.68519 5.62635 -1.42557 H -1.75532 3.40024 -1.65037 S 1.22115 0.21291 -1.57625 C 0.53081 0.24990 0.07063 C 1.11149 -0.80898 1.02136 N 2.47463 -0.25089 1.39964 C 4.68247 0.41430 0.63097 C 5.58710 0.85211 -0.32597 C 5.14769 1.09443 -1.62685 C 3.81371 0.91014 -1.96106 C 2.88087 0.47366 -1.01020 C 3.34709 0.22279 0.28828 C 1.24018 -2.27199 0.63594 C 0.40787 -3.19747 1.27685 C 0.49799 -4.55260 0.97513 C 1.42160 -5.00219 0.03404 C 2.26111 -4.08826 -0.59801	2133.90068	2133.44291	2133.52768	2133.93597	2133.56297	2135.16116	2134.78816	2135.55787	2135.18487	21.1

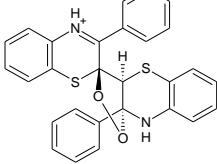
C 2.17576 -2.73019 -0.30142 H 0.80359 1.22106 0.49744 H 5.01422 0.21906 1.64704 H 6.62647 1.00022 -0.05439 H 5.84468 1.43546 -2.38536 H 3.47455 1.10952 -2.97325 H -0.31143 -2.85721 2.01245 H -0.15653 -5.25620 1.48026 H 1.49152 -6.05995 -0.20146 H 2.99042 -4.42711 -1.32718 H 2.85327 -2.05212 -0.80612 O -0.98668 -0.10942 1.72615 O 0.30252 -0.65631 2.16070 H 2.30437 0.51910 2.06047 H 2.98271 -0.96939 1.92770									
 S -1.52438 -1.10262 -0.93183 C -0.83624 0.12856 0.21349 C -1.59891 1.43913 0.13583 N -2.89675 1.42710 -0.03100 C -5.13549 0.55468 -0.15304 C -5.99943 -0.49101 -0.43145 C -5.49074 -1.72915 -0.83856 C -4.12146 -1.92863 -0.95913 C -3.23921 -0.88154 -0.67961 C -3.75679 0.35534 -0.28408 C -0.97074 2.74791 0.33229 C -0.12462 2.98493 1.42945 C 0.40296 4.25472 1.62541 C 0.11159 5.28470 0.72964 C -0.72286 5.05044 -0.36199 C -1.27375 3.78934 -0.55978 H -5.51577 1.52028 0.16855 H -7.06944 -0.34565 -0.33048 H -6.16857 -2.54836 -1.05546 H -3.72932 -2.89311 -1.26601 H 0.08325 2.19623 2.14664 H 1.04007 4.44146 2.48393 H 0.53702 6.27156 0.88387 H -0.94247 5.84750 -1.06492 H -1.90138 3.60173 -1.42663 S 1.35319 0.08557 -1.66302 C 0.66564 0.22783 -0.01594	2133.92271	2133.46534	2133.54978	2133.95448	2133.58155	2135.17638	2134.80346	2135.57325	2135.20033

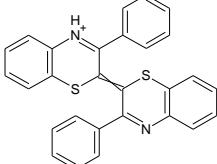
C 1.22062 -0.78289 1.00375 N 2.56961 -0.40718 1.26733 C 4.77517 0.22525 0.57419 C 5.70245 0.64718 -0.36685 C 5.30142 0.91485 -1.67687 C 3.96596 0.75571 -2.02086 C 3.02458 0.31420 -1.08385 C 3.42411 0.03830 0.24101 C 1.05099 -2.27767 0.76377 C 0.18597 -3.04206 1.55322 C 0.07827 -4.41676 1.35497 C 0.83014 -5.04551 0.36445 C 1.70799 -4.29277 -0.41387 C 1.82572 -2.91974 -0.21032 H 0.98754 1.19864 0.36719 H 5.08780 0.02841 1.59658 H 6.73964 0.77512 -0.07229 H 6.01660 1.25373 -2.41935 H 3.63524 0.97265 -3.03312 H -0.40600 -2.56388 2.32498 H -0.59714 -4.99576 1.97822 H 0.74253 -6.11681 0.20786 H 2.31289 -4.77406 -1.17680 H 2.53570 -2.35762 -0.80743 O -0.92560 -0.28380 1.59083 O 0.41828 -0.35713 2.13089 H 3.03368 -1.01574 1.93037 H -3.35440 2.33243 0.06214										
	S -1.33190 -1.34508 -1.67771 C -0.00762 -0.53385 -0.68553 C 1.03296 -1.60572 -0.35149 N 0.65671 -2.70475 0.19392 C -0.98627 -4.05004 1.30143 C -2.27626 -4.54893 1.41061 C -3.27797 -4.09218 0.54883 C -2.99458 -3.11227 -0.39655 C -1.70423 -2.58370 -0.48706 C -0.67504 -3.06513 0.35070 C 2.48220 -1.39748 -0.57302 C 3.37115 -1.92662 0.37596 C 4.74453 -1.80330 0.20336 C 5.25300 -1.16284 -0.92775	2133.92161	2133.46413	2133.54815	2133.95572	2133.58226	2135.18415	2134.81069	2135.58100	2135.20754

C 4.37756 -0.64840 -1.88239 C 2.99995 -0.75717 -1.70739 H -0.18689 -4.41546 1.93913 H -2.50184 -5.30553 2.15572 H -4.28526 -4.49074 0.62099 H -3.77596 -2.73962 -1.05245 H 2.96765 -2.42306 1.25266 H 5.41953 -2.20562 0.95321 H 6.32630 -1.06806 -1.06502 H 4.76574 -0.16205 -2.77241 H 2.33732 -0.36642 -2.47121 S 0.51934 0.38470 1.97491 C -0.60180 0.19985 0.54274 C -1.04313 1.53112 -0.11927 N -0.39110 2.73176 0.61534 C 1.83268 3.71585 0.12598 C 3.21664 3.63975 0.27390 C 3.79318 2.56705 0.95291 C 3.00463 1.54164 1.47246 C 1.62054 1.60899 1.33259 C 1.06407 2.70664 0.68061 C -2.52961 1.80205 -0.15902 C -3.13403 2.25161 -1.33574 C -4.49629 2.54112 -1.34322 C -5.25368 2.39121 -0.18314 C -4.64808 1.94786 0.99165 C -3.28803 1.65276 1.00688 H -1.46150 -0.33947 0.94356 H 1.37104 4.54902 -0.39583 H 3.84181 4.42219 -0.14283 H 4.87159 2.51638 1.06488 H 3.45789 0.69071 1.96958 H -2.55108 2.36138 -2.24395 H -4.96467 2.88201 -2.26130 H -6.31581 2.61626 -0.19442 H -5.23324 1.82393 1.89736 H -2.83523 1.29751 1.92988 O 0.53089 0.52107 -1.43668 O -0.51420 1.52108 -1.41134 H -0.77757 2.75199 1.56976 H -0.72040 3.58503 0.15250																
 S -1.32623 -1.55316 -1.65445	2133.93805	-	2133.48105	-	2133.56612	-	2133.96917	2133.59723	2135.19382	-	2134.82189	-	2135.59045	-	2135.21852	0.0

C -0.06110 -0.55241 -0.74866									
C 1.04243 -1.50940 -0.34802									
N 0.66831 -2.58026 0.30684									
C -0.87093 -3.94063 1.58093									
C -2.13842 -4.48191 1.73740									
C -3.16490 -4.12553 0.85908									
C -2.93614 -3.21619 -0.16810									
C -1.66817 -2.65494 -0.33330									
C -0.64009 -3.03298 0.54472									
C 2.46415 -1.30921 -0.60569									
C 3.39718 -1.72159 0.36580									
C 4.75676 -1.59757 0.12266									
C 5.20462 -1.07743 -1.09250									
C 4.28678 -0.67110 -2.05992									
C 2.92191 -0.77150 -1.82139									
H -0.06292 -4.21259 2.25357									
H -2.32682 -5.18228 2.54391									
H -4.15607 -4.54989 0.98254									
H -3.73941 -2.93024 -0.83935									
H 3.06549 -2.08446 1.33499									
H 5.46721 -1.89573 0.88679									
H 6.26959 -0.98433 -1.28208									
H 4.63323 -0.27377 -3.00850									
H 2.22076 -0.47041 -2.58949									
S 0.40007 0.42927 1.88928									
C -0.66667 0.26266 0.42725									
C -1.02542 1.61702 -0.27072									
N -0.31537 2.73468 0.26746									
C 1.92485 3.70339 0.12870									
C 3.26391 3.67050 0.51048									
C 3.75735 2.61399 1.27598									
C 2.90238 1.58364 1.66335									
C 1.55717 1.62853 1.30384									
C 1.05623 2.68747 0.53541									
C -2.51749 1.91857 -0.26205									
C -3.35027 1.54475 -1.32049									
C -4.71643 1.81596 -1.26229									
C -5.26295 2.44860 -0.14747									
C -4.43463 2.81647 0.91188									
C -3.06715 2.55785 0.85439									
H -1.57153 -0.21707 0.80304									
H 1.54448 4.52392 -0.47439									
H 3.92663 4.47192 0.19761									
H 4.80304 2.58590 1.56588									
H 3.27344 0.75343 2.25698									
H -2.93593 1.04684 -2.18946									
H -5.35330 1.53012 -2.09437									
H -6.32837 2.65538 -0.10476									
H -4.85062 3.30933 1.78571									
H -2.42169 2.85024 1.67670									

O 0.41946 0.43153 -1.61533 O -0.66949 1.36169 -1.65937 H -0.60858 3.59642 -0.17769 H 1.41000 -3.20903 0.60489										
 <p>S 1.65041 1.90071 -1.98451  C 0.30801 1.04339 -1.08383  C -0.12460 1.93444 0.08458  N 0.74975 2.40308 0.89958  C 2.96949 2.53299 1.78408  C 4.34554 2.59189 1.61847  C 4.90019 2.47022 0.34111  C 4.07949 2.25781 -0.76189  C 2.69647 2.16127 -0.59195  C 2.12191 2.31966 0.68631  C -1.55117 2.23750 0.35108  C -2.01930 2.12573 1.66741  C -3.32810 2.47748 1.98160  C -4.17828 2.96535 0.98914  C -3.71418 3.09197 -0.31966  C -2.41181 2.72117 -0.64338  H 2.51544 2.65654 2.76279  H 4.98792 2.74898 2.47933  H 5.97545 2.53029 0.20358  H 4.51073 2.14447 -1.75225  H -1.34922 1.75640 2.43768  H -3.68293 2.37359 3.00291  H -5.19804 3.24737 1.23501  H -4.36732 3.48308 -1.09430  H -2.06221 2.83646 -1.66383  S 1.21852 -0.85618 0.95254  C 0.68170 -0.40644 -0.69885  C -0.54185 -1.19045 -1.19629  N -0.01631 -2.55127 -1.56188  C 0.88028 -4.62479 -0.66548  C 1.59912 -5.37351 0.25527  C 2.19689 -4.73456 1.34108  C 2.07958 -3.36120 1.49768  C 1.36021 -2.58223 0.57966  C 0.76345 -3.24819 -0.50047  C -1.83021 -1.31661 -0.40395  C -1.89989 -1.96780 0.83514  C -3.12448 -2.11248 1.48260</p>	2133.89451	2133.43671	2133.52046	2133.93049	2133.55644	2135.16075	2134.78670	2135.55783	2135.18378	21.8

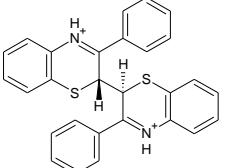
C -4.29030 -1.61504 0.90695 C -4.22762 -0.97477 -0.32833 C -3.00816 -0.82709 -0.98148 H 1.50441 -0.67537 -1.37098 H 0.40860 -5.11011 -1.51537 H 1.68878 -6.44608 0.12331 H 2.76147 -5.30704 2.06976 H 2.55049 -2.86907 2.34345 H -1.01866 -2.37594 1.31151 H -3.15956 -2.61997 2.44165 H -5.24260 -1.72940 1.41624 H -5.12939 -0.58484 -0.79029 H -2.97432 -0.32770 -1.94189 O -0.75133 0.85486 -2.02544 O -0.73696 -0.52798 -2.43384 H 0.56421 -2.44889 -2.40583 H -0.80803 -3.14729 -1.83038									
 S -0.57343 -2.34359 -2.00941 C 0.21125 -0.94321 -1.11223 C 1.05533 -1.54371 -0.00407 N 0.46236 -2.39408 0.79622 C -1.40327 -3.59323 1.75372 C -2.59756 -4.27793 1.58616 C -3.18080 -4.36524 0.31962 C -2.58371 -3.75979 -0.78125 C -1.38826 -3.05614 -0.62580 C -0.80351 -2.98833 0.64763 C 2.45240 -1.21131 0.25975 C 2.86005 -1.00063 1.58949 C 4.19911 -0.77012 1.87461 C 5.14220 -0.77426 0.84685 C 4.74187 -0.99100 -0.47156 C 3.40199 -1.19268 -0.77543 H -0.93689 -3.51734 2.73159 H -3.07387 -4.74452 2.44165 H -4.11554 -4.90092 0.18899 H -3.04782 -3.82058 -1.76035 H 2.12636 -0.96479 2.39067 H 4.50449 -0.58192 2.89884 H 6.19019 -0.60314 1.07335 H 5.47656 -1.00136 -1.27033 H 3.10261 -1.36994 -1.80130	2133.91502	2133.45798	2133.54199	2133.94649	2133.57346	2135.17377	2134.80075	2135.57067	2135.19764

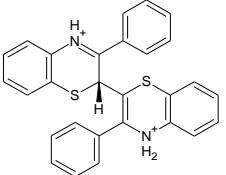
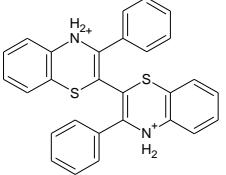
S -1.49421 0.23434 0.98136 C -0.79439 0.14007 -0.66962 C -0.10571 1.43942 -1.12912 N -1.14532 2.38544 -1.37668 C -3.08003 3.61883 -0.67907 C -4.17148 3.84336 0.14640 C -4.45472 2.96197 1.19129 C -3.63207 1.86169 1.38924 C -2.51713 1.63526 0.57343 C -2.22570 2.52162 -0.48496 C 1.05628 2.03137 -0.33860 C 0.83174 2.61864 0.91410 C 1.87274 3.23739 1.60220 C 3.14794 3.29751 1.04327 C 3.37243 2.73772 -0.21238 C 2.33584 2.10768 -0.89772 H -1.63878 0.02712 -1.35721 H -2.86757 4.30127 -1.49825 H -4.80618 4.70587 -0.03277 H -5.31081 3.12302 1.83841 H -3.84539 1.15982 2.19114 H -0.15779 2.61519 1.35642 H 1.67944 3.68400 2.57327 H 3.95743 3.78599 1.57812 H 4.35863 2.78747 -0.66484 H 2.52517 1.67929 -1.87507 O 1.03046 -0.27208 -2.04911 O 0.35110 0.94988 -2.40962 H -0.79917 3.27691 -1.71044 H 1.03229 -2.76517 1.55418										
<b>Double-bond dimers</b>										
 S -1.30306 2.41219 -0.91938 C -0.57651 0.84003 -0.48839 C -1.36681 -0.31109 -0.82649 N -2.68895 -0.23152 -0.77386 C -4.75303 0.59928 0.17334 C -5.51996 1.66300 0.63387 C -4.98551 2.95141 0.65872 C -3.68195 3.18359 0.22605 C -2.90963 2.12318 -0.24393 C -3.44996 0.83347 -0.26628 C -0.80041 -1.55367 -1.35954	1982.50999	1982.08785	1982.17029	1982.53709	1982.19739	1983.66106	1983.32136	1984.01083	1983.67113	0.0

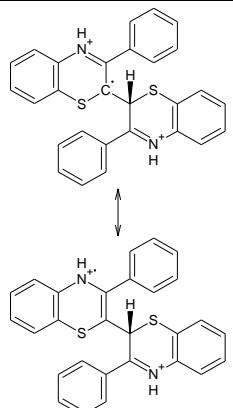
C 0.32511 -1.50023 -2.19675									
C 0.81712 -2.66540 -2.77241									
C 0.19679 -3.88816 -2.51757									
C -0.92063 -3.94746 -1.68290									
C -1.42105 -2.78838 -1.10629									
H -5.15618 -0.40916 0.15568									
H -6.53368 1.48392 0.97623									
H -5.58267 3.78229 1.02049									
H -3.26478 4.18531 0.24771									
H 0.78829 -0.54533 -2.42333									
H 1.67960 -2.61662 -3.42954									
H 0.58507 -4.79697 -2.96739									
H -1.39209 -4.90121 -1.46830									
H -2.25633 -2.85368 -0.41417									
S 1.58853 2.31970 -0.06906									
C 0.72193 0.81244 -0.00992									
C 1.38285 -0.33622 0.63789									
N 2.66601 -0.47385 0.74512									
C 4.94800 0.11957 0.40676									
C 5.93217 1.06796 0.19036									
C 5.57966 2.40632 -0.02945									
C 4.24503 2.78579 -0.06471									
C 3.25111 1.81696 0.10785									
C 3.58718 0.47641 0.37526									
C 0.57060 -1.37106 1.33382									
C -0.57327 -1.03113 2.06890									
C -1.25887 -2.00488 2.79135									
C -0.81635 -3.32671 2.78279									
C 0.32881 -3.66799 2.06146									
C 1.02342 -2.69617 1.35013									
H 5.19509 -0.91552 0.62173									
H 6.97814 0.77909 0.21235									
H 6.35057 3.15548 -0.18007									
H 3.97303 3.82068 -0.25165									
H -0.91658 -0.00141 2.10423									
H -2.13597 -1.72558 3.36775									
H -1.35722 -4.08635 3.33961									
H 0.67969 -4.69585 2.05082									
H 1.91578 -2.95609 0.78978									
H -3.21186 -1.02089 -1.13904									

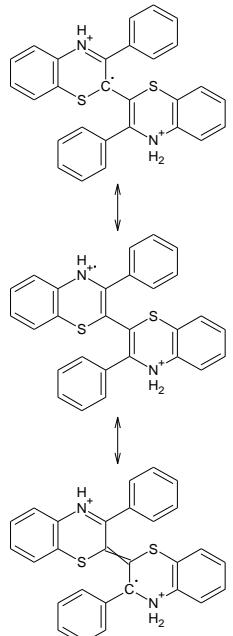
**Table S6.** Diprotonated forms in methanol. For each chemical species, values are reported for the most stable conformer / geometric isomer identified.  $G_{RRHO,calc}$  [M062X / 6-311++G(2d,2p) / SMD] =  $G_{el}$  [M062X / 6-311++G(2d,2p) / SMD // PBE0 / 6-31+G(d,p) / PCM] -  $G_{el}$  [PBE0 / 6-31+G(d,p) / PCM] +  $G_{RRHO}$  [PBE0 / 6-31+G(d,p) / PCM]; and likewise for  $G_{RRHO,calc}$  [PBE0 / 6-31+G(d,p) / SMD] and for  $G_{RRHO,calc}$  [M062X / 6-31+G(d,p) / SMD].

Species	PBE0 / 6-31+G(d,p) / PCM			PBE0 / 6-31+G(d,p) / SMD		M062X / 6-31+G(d,p) / SMD		M062X / 6-311++G(2d,2p) / SMD		
	$G_{el}$ / Ha	$H_{RRHO}$ / Ha	$G_{RRHO}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$G_{el}$ / Ha	$G_{RRHO,calc}$ / Ha	$\Delta G_{RRHO,calc}$ / kcal mol <sup>-1</sup>
Cartesian coordinates / Å										
Single-bond dimer										
S 1.48772 0.74668 -2.37006 C 0.46346 0.63469 -0.88292 C 1.35000 0.69047 0.32880 N 2.40712 -0.08488 0.35642 C 3.80887 -1.90788 -0.38000 C 4.36660 -2.64977 -1.41071 C 4.02550 -2.37217 -2.73673 C 3.12090 -1.35970 -3.03861 C 2.54937 -0.60594 -2.01218 C 2.90324 -0.88836 -0.68357 C 1.03019 1.51832 1.48196 C 1.42333 1.12345 2.77675 C 1.13518 1.92775 3.86768 C 0.46346 3.13905 3.68720 C 0.06991 3.53886 2.41108 C 0.33912 2.73227 1.31326 H -0.16877 1.52365 -0.90681 H 4.06809 -2.11260 0.65465 H 5.06726 -3.44509 -1.18063 H 4.46191 -2.95350 -3.54244 H 2.85206 -1.15125 -4.06916 H 1.90030 0.16213 2.94668 H 1.42239 1.60472 4.86290 H 0.24265 3.76775 4.54421 H -0.44422 4.48336 2.26730 H 0.05372 3.08158 0.32670 S -1.48772 -0.74668 -2.37006 C -0.46346 -0.63469 -0.88292 C -1.35000 -0.69047 0.32880 N -2.40712 0.08488 0.35642 C -3.80887 1.90788 -0.38000	1984.16444	1983.70324	1983.78656	1984.21051	1983.83263	1985.32719	1984.94930	1985.67717	1985.29929	0.0

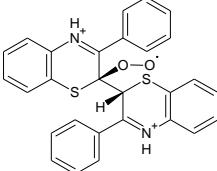
C -4.36660 2.64977 -1.41071 C -4.02550 2.37217 -2.73673 C -3.12090 1.35970 -3.03861 C -2.54937 0.60594 -2.01218 C -2.90324 0.88836 -0.68357 C -1.03019 -1.51832 1.48196 C -1.42333 -1.12345 2.77675 C -1.13518 -1.92775 3.86768 C -0.46346 -3.13905 3.68720 C -0.06991 -3.53886 2.41108 C -0.33912 -2.73227 1.31326 H 0.16877 -1.52365 -0.90681 H -4.06809 2.11260 0.65465 H -5.06726 3.44509 -1.18063 H -4.46191 2.95350 -3.54244 H -2.85206 1.15125 -4.06916 H -1.90030 -0.16213 2.94668 H -1.42239 -1.60472 4.86290 H -0.24265 -3.76775 4.54421 H 0.44422 -4.48336 2.26730 H -0.05372 -3.08158 0.32670 H 2.98748 -0.04771 1.19062 H -2.98748 0.04771 1.19062										
 S 1.06336 1.00452 1.87155 C -0.18875 0.45585 0.67580 C -0.96179 1.64932 0.18016 N -0.28073 2.69143 -0.22335 C 1.69503 3.90670 -0.88759 C 3.03510 4.21156 -0.69982 C 3.77682 3.53208 0.26928 C 3.18944 2.53453 1.04051 C 1.84434 2.20793 0.85484 C 1.10356 2.91012 -0.10817 C -2.41394 1.66177 0.10169 C -3.06608 2.40354 -0.90374 C -4.45047 2.44108 -0.95146 C -5.20362 1.75837 0.00685 C -4.56701 1.02237 1.00430 C -3.18016 0.95659 1.04650 H -0.86228 -0.17830 1.25443 H 1.10265 4.43330 -1.63033 H 3.50042 4.98146 -1.30561	1984.16481	1983.70346	1983.78586	1984.20846	1983.82950	1985.32702	1984.94806	1985.67748	1985.29853	0.5

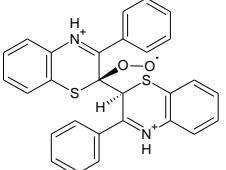
H 4.82353 3.77470 0.42144 H 3.77158 2.00335 1.78721 H -2.50007 2.90198 -1.68613 H -4.94491 2.99440 -1.74308 H -6.28793 1.79559 -0.03058 H -5.15013 0.49518 1.75214 H -2.70661 0.39824 1.84718 S -0.83243 -0.83208 -1.75953 C 0.40057 -0.36484 -0.50453 C 1.02523 -1.66333 -0.06588 N 0.21144 -2.56895 0.43736 C -1.93033 -3.46160 1.11964 C -3.28907 -3.60956 0.88707 C -3.90062 -2.91643 -0.16126 C -3.16409 -2.05368 -0.96514 C -1.79794 -1.88365 -0.73440 C -1.18471 -2.60902 0.30058 C 2.43602 -1.96250 -0.20493 C 2.87277 -3.30258 -0.27103 C 4.22354 -3.59251 -0.37525 C 5.15937 -2.55677 -0.42345 C 4.73853 -1.22755 -0.38280 C 3.38760 -0.92839 -0.28390 H 1.13606 0.22675 -1.05231 H -1.44050 -4.00364 1.92313 H -3.87259 -4.26970 1.51972 H -4.96337 -3.03730 -0.34466 H -3.64652 -1.50040 -1.76465 H 2.16059 -4.12208 -0.29680 H 4.54794 -4.62587 -0.43841 H 6.21682 -2.78726 -0.50874 H 5.46413 -0.42223 -0.42911 H 3.08464 0.11134 -0.24307 H 0.63284 -3.38690 0.86850 H -0.81228 3.48454 -0.57396								
	n.d.							
	n.d.							

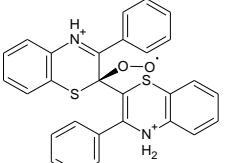
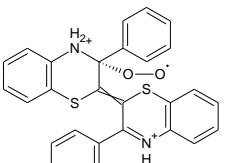
Single-bond dimer, radical										
 <p>S -1.09722 1.34996 0.45623      C 0.19334 0.47089 -0.28420      C 1.44536 1.02230 -0.51726      N 1.75842 2.27662 -0.12580      C 1.49425 4.43431 0.89117      C 0.69992 5.35586 1.54827      C -0.63126 5.05073 1.86637      C -1.16770 3.81990 1.52573      C -0.37228 2.87975 0.86217      C 0.96352 3.18555 0.54214      C 2.54943 0.29189 -1.18373      C 2.43057 -0.11833 -2.51759      C 3.49369 -0.76976 -3.13615      C 4.67162 -1.01440 -2.43094      C 4.79234 -0.60112 -1.10499      C 3.73701 0.05598 -0.47875      H 2.52514 4.66612 0.64104      H 1.11387 6.32174 1.81726      H -1.24788 5.77919 2.38174      H -2.19784 3.58026 1.77007      H 1.52402 0.09497 -3.07698      H 3.40245 -1.07876 -4.17267      H 5.49748 -1.52517 -2.91667      H 5.70757 -0.79226 -0.55351      H 3.82709 0.36426 0.55935      S -1.06542 -1.16084 -2.22147      C -0.11008 -0.95698 -0.67472      C -0.73308 -1.74951 0.44849      N -2.03604 -1.80034 0.55368      C -4.30209 -1.05773 0.20551      C -5.27801 -0.51848 -0.62072      C -4.95682 -0.14006 -1.92609      C -3.66090 -0.29064 -2.40920</p>	-	1983.54274	1983.09441	1983.17911	1983.58334	1983.21971	1984.69628	1984.33264	1985.04719	1984.68356

C -2.66992 -0.83557 -1.59112 C -3.00445 -1.21707 -0.28415 C 0.09714 -2.39131 1.45613 C 1.33898 -2.95332 1.10838 C 2.10821 -3.58822 2.07396 C 1.66519 -3.64964 3.39483 C 0.44240 -3.07899 3.75274 C -0.34295 -2.45865 2.79325 H 0.84895 -1.42369 -0.90738 H -4.53640 -1.34650 1.22622 H -6.28753 -0.39034 -0.24556 H -5.71962 0.28256 -2.57199 H -3.41344 0.00910 -3.42254 H 1.68815 -2.94751 0.08123 H 3.05417 -4.03911 1.79278 H 2.27578 -4.13722 4.14842 H 0.10729 -3.10553 4.78435 H -1.26660 -1.97660 3.10060 H 2.69284 2.59134 -0.36771 H -2.41065 -2.35107 1.32345										
 S -1.12157 -2.25883 0.00683 C -0.66618 -0.64844 -0.44761 C -1.58804 0.35991 -0.71276 N -2.91082 0.16928 -0.52535 C -4.94964 -0.92981 0.09675	1983.52436	1983.07529	1983.15901	1983.56676	1983.20140	1984.68444	1984.31908	1985.03644	1984.67109	7.8

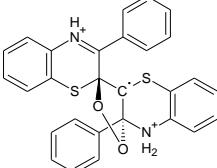
C -5.61461 -2.06462 0.52413 C -4.90783 -3.24642 0.78739 C -3.53300 -3.29064 0.62332 C -2.84886 -2.14748 0.19461 C -3.55920 -0.96207 -0.07072 C -1.22294 1.69795 -1.22101 C -0.40292 1.83431 -2.34878 C -0.11878 3.10038 -2.84797 C -0.64514 4.23451 -2.22785 C -1.46379 4.10145 -1.10817 C -1.75783 2.83767 -0.60498 H -5.49320 -0.01289 -0.11043 H -6.69112 -2.03572 0.65410 H -5.43589 -4.13300 1.12163 H -2.98290 -4.20408 0.82659 H -0.01240 0.95458 -2.85129 H 0.50619 3.20068 -3.72991 H -0.41894 5.22119 -2.62061 H -1.87025 4.98110 -0.61904 H -2.37503 2.74330 0.28476 S 1.63901 -1.58152 -1.61889 C 0.78674 -0.45416 -0.54843 C 1.46278 0.48760 0.14526 N 2.88266 0.65228 -0.24873 C 4.81873 -0.61317 0.68049 C 5.52523 -1.81159 0.74537 C 5.06252 -2.93985 0.06760 C 3.87920 -2.89938 -0.66525 C 3.16239 -1.70482 -0.73280 C 3.65903 -0.58499 -0.07673 C 1.00382 1.33137 1.25129 C 0.22713 0.77823 2.28119 C -0.20503 1.57596 3.33432 C 0.14062 2.92670 3.37922 C 0.92160 3.48040 2.36542 C 1.35168 2.69073 1.30451 H 5.17412 0.27451 1.19491 H 6.44148 -1.85937 1.32384 H 5.61931 -3.86958 0.12386 H 3.50647 -3.78722 -1.16542 H -0.01167 -0.28059 2.27108 H -0.79828 1.13720 4.13057 H -0.19310 3.54553 4.20657 H 1.18902 4.53200 2.39322 H 1.92327 3.15394 0.50319 H 3.30638 1.40630 0.30045 H -3.50736 0.94430 -0.79661 H 2.93583 0.94424 -1.23692									
<b>Single-bond dimer, C2-peroxy radical</b>									

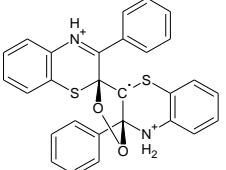
 <p>S 0.45579 -1.68125 -0.16188      C 0.36761 0.08940 -0.45534      C 1.74584 0.71766 -0.27039      N 2.75248 0.11455 -0.85111      C 3.87395 -1.43643 -2.31602      C 3.94667 -2.69421 -2.89121      C 2.94557 -3.63847 -2.64299      C 1.86062 -3.32921 -1.83045      C 1.77167 -2.06104 -1.25674      C 2.78508 -1.12515 -1.49515      C 2.05013 1.91543 0.51129      C 1.37575 3.13166 0.30808      C 1.74111 4.25052 1.04494      C 2.76242 4.16761 1.99246      C 3.44031 2.96540 2.19074      C 3.09700 1.84334 1.44811      H 4.64536 -0.69422 -2.49878      H 4.78421 -2.94265 -3.53371      H 3.00515 -4.62270 -3.09581      H 1.08059 -4.06181 -1.65100      H 0.62513 3.22441 -0.46959      H 1.23379 5.19354 0.86957      H 3.03322 5.04399 2.57305      H 4.23299 2.89791 2.92872      H 3.60137 0.89822 1.62847      S -0.46728 0.80003 2.18916      C -0.75838 0.74117 0.39990      C -2.12992 0.18844 0.07951      N -2.62034 -0.78707 0.79833      C -2.56014 -2.66854 2.30580      C -2.03589 -3.28939 3.43091      C -1.01376 -2.67376 4.15595      C -0.50342 -1.44210 3.75638      C -1.02150 -0.80864 2.62759      C -2.05174 -1.42976 1.91139      C -2.90652 0.70642 -1.03662      C -3.70952 -0.16853 -1.79420      C -4.45982 0.31995 -2.85313      C -4.43196 1.68095 -3.16139      C -3.64149 2.55407 -2.41422      C -2.87026 2.07334 -1.36520      H -0.76958 1.79022 0.09854</p>	-	2133.70062	-	2133.33065	-	2133.74493	-	2133.37495	-	2134.95844	-	2134.58847	-	2135.35570	-	2134.98572	0.5
--	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

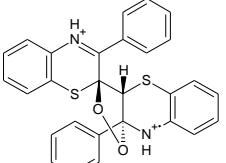
H -3.35003 -3.13926 1.72799 H -2.42360 -4.25366 3.74099 H -0.60379 -3.15893 5.03578 H 0.29614 -0.96955 4.31798 H -3.70190 -1.23714 -1.59922 H -5.05630 -0.36384 -3.44789 H -5.02271 2.06019 -3.98934 H -3.62699 3.61367 -2.64674 H -2.28993 2.77712 -0.77775 O -0.00522 0.24622 -1.87979 O 0.18813 1.47431 -2.28232 H -3.55631 -1.10337 0.55082 H 3.64222 0.60977 -0.81207									
 S 1.15006 -1.03758 1.58687 C -0.17830 -0.43824 0.48298 C -0.90855 -1.68987 0.01151 N -0.17646 -2.58714 -0.61309 C 1.85220 -3.48894 -1.57613 C 3.22584 -3.66125 -1.50729 C 3.96396 -3.02764 -0.50348 C 3.33881 -2.20239 0.42459 C 1.95721 -2.01131 0.36217 C 1.22155 -2.67234 -0.63331 C -2.30366 -1.99042 0.27594 C -2.64673 -3.32708 0.57183 C -3.96984 -3.67322 0.79822 C -4.96669 -2.69914 0.72633 C -4.63624 -1.37355 0.44107 C -3.31467 -1.01130 0.22856 H 1.26591 -3.98073 -2.34621 H 3.72379 -4.29274 -2.23498 H 5.03890 -3.16623 -0.45134 H 3.91794 -1.69713 1.19067 H -1.87254 -4.08098 0.68172 H -4.22202 -4.69905 1.04552 H -6.00258 -2.97173 0.90327 H -5.41259 -0.61776 0.38359 H -3.07931 0.01886 -0.00466 S -0.94338 0.78495 -1.97046 C 0.31300 0.45154 -0.70297 C 0.95747 1.72839 -0.22880 N 0.20502 2.77745 -0.01804	2133.70225	2133.24444	2133.33259	2133.74530	2133.37564	2134.95889	2134.58923	2135.35612	2134.98646

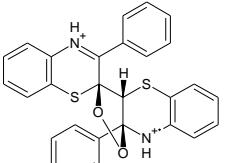
C -1.83349 4.01865 0.30656 C -3.16574 4.24490 -0.00846 C -3.82178 3.40494 -0.90982 C -3.15669 2.32734 -1.48808 C -1.82079 2.08221 -1.16970 C -1.16549 2.94133 -0.27767 C 2.38587 1.80980 0.03389 C 2.86823 2.61527 1.08435 C 4.23225 2.72087 1.30651 C 5.13128 2.04447 0.47902 C 4.66184 1.24803 -0.56443 C 3.29681 1.11455 -0.78115 H 1.07035 -0.13423 -1.23063 H -1.31021 4.66658 1.00358 H -3.69074 5.07759 0.44665 H -4.86171 3.58459 -1.16237 H -3.67235 1.67558 -2.18664 H 2.18171 3.11009 1.76530 H 4.59574 3.32250 2.13298 H 6.19903 2.13483 0.65264 H 5.35948 0.72920 -1.21352 H 2.95410 0.51755 -1.61974 O -1.08145 0.36590 1.27026 O -0.76845 0.42661 2.53624 H 0.68189 3.61917 0.29991 H -0.67826 -3.35981 -1.04569																		
	n.d.																	
<b>Single-bond dimer, C3-peroxy radical</b>																		
									0.0									
S -0.96547 1.68992 1.48735 C -0.94642 0.16157 0.59295 C -2.23631 -0.16623 -0.02936 N -2.88591 0.79658 -0.64214 C -3.10648 2.94767 -1.72020 C -2.81181 4.30274 -1.75451 C -1.94440 4.85568 -0.80949 C -1.35703 4.05789 0.16715	-	2133.68733	-	2133.22926	-	2133.31674	-	2133.73224	2133.36165	-	2134.94842	-	2134.57783	-	2135.34718	-	2134.97659	0.0

C -1.63890 2.69264 0.20490 C -2.51940 2.14616 -0.73857 C -2.83413 -1.49269 0.03774 C -2.70432 -2.24249 1.22043 C -3.31859 -3.48375 1.31875 C -4.04043 -3.99399 0.23966 C -4.16044 -3.25785 -0.94125 C -3.57003 -2.00682 -1.04511 H -3.78163 2.50739 -2.44792 H -3.25979 4.92945 -2.51799 H -1.71622 5.91622 -0.83668 H -0.67615 4.48924 0.89395 H -2.15812 -1.83820 2.06736 H -3.23422 -4.05308 2.23858 H -4.50795 -4.97083 0.31569 H -4.70759 -3.66511 -1.78514 H -3.63304 -1.46049 -1.98230 S 0.11775 -2.23987 -0.21772 C 0.15526 -0.63088 0.52087 C 1.45466 -0.15552 1.16252 N 2.46433 -1.29284 1.19316 C 4.12366 -1.81777 -0.57608 C 4.37391 -2.34669 -1.84089 C 3.32552 -2.82986 -2.62228 C 2.00998 -2.78478 -2.16302 C 1.75342 -2.26701 -0.89629 C 2.81427 -1.80591 -0.12684 C 2.08460 1.06899 0.55383 C 1.87993 1.36562 -0.79668 C 2.52827 2.45551 -1.36948 C 3.37832 3.24764 -0.60029 C 3.58491 2.94801 0.74563 C 2.94543 1.85761 1.32687 H 4.93232 -1.43888 0.04114 H 5.39183 -2.37612 -2.21390 H 3.52908 -3.23619 -3.60766 H 1.19333 -3.14345 -2.78062 H 1.21696 0.75724 -1.40433 H 2.36579 2.68386 -2.41798 H 3.87985 4.09956 -1.04916 H 4.24294 3.56493 1.34919 H 3.10640 1.64374 2.37922 H 3.30636 -0.95343 1.67269 H -3.79197 0.55517 -1.03727 O 1.22122 0.12529 2.58386 O 0.95546 -0.95682 3.26600 H 2.06204 -2.03871 1.78742									
<b>Single-bond dimer, dioxolane radical</b>									

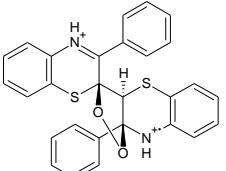
 <p> S -1.85693 -1.63894 -0.85811  C -1.09092 -0.25120 0.07779  C -1.96091 0.97550 -0.12790  N -3.25007 0.83817 0.07771  C -5.28278 -0.24713 0.77854  C -6.04899 -1.39628 0.88485  C -5.52988 -2.62638 0.46829  C -4.24050 -2.71679 -0.04214  C -3.45446 -1.56743 -0.14711  C -3.98834 -0.33572 0.25770  C -1.44761 2.27520 -0.52018  C -2.17562 3.04860 -1.44437  C -1.72089 4.31120 -1.79786  C -0.55335 4.81754 -1.22549  C 0.16740 4.05796 -0.30218  C -0.26597 2.78649 0.04517  H -5.67248 0.71479 1.09774  H -7.05252 -1.33659 1.29176  H -6.13225 -3.52506 0.55225  H -3.83681 -3.67479 -0.35313  H -3.06055 2.64080 -1.92498  H -2.27087 4.89559 -2.52808  H -0.20142 5.80660 -1.50224  H 1.06697 4.46003 0.15240  H 0.28162 2.21734 0.78836  S 0.94490 -0.16852 -1.88505  C 0.35877 -0.20084 -0.28129  C 1.09645 -0.79272 0.88222  N 1.80773 -2.06946 0.41550  C 4.03772 -2.46579 -0.53695  C 4.97517 -2.28021 -1.54894  C 4.67137 -1.46496 -2.63717  C 3.44012 -0.82323 -2.71814  C 2.48811 -1.01074 -1.71317  C 2.80408 -1.84081 -0.63644  C 2.06391 0.08957 1.63667  C 2.21528 -0.10570 3.01402  C 3.12561 0.66970 3.72604  C 3.88423 1.63834 3.07052  C 3.72972 1.83564 1.69955  C 2.81997 1.06566 0.98016  H 4.26357 -3.09941 0.31611 </p>	-	2133.69785	-	2133.32524	-	2133.74320	-	2133.37059	-	2134.95769	-	2134.58508	-	2135.35533	-	2134.98272	12.4
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	------

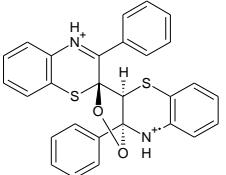
H 5.94045 -2.76937 -1.47966 H 5.40167 -1.31345 -3.42505 H 3.21659 -0.17025 -3.55615 H 1.61465 -0.84825 3.53014 H 3.23585 0.51928 4.79534 H 4.59104 2.24424 3.62927 H 4.31238 2.59411 1.18638 H 2.70228 1.24326 -0.08435 O -1.05767 -0.45697 1.48338 O 0.06088 -1.31743 1.70364 H 1.08434 -2.73394 0.10608 H -3.79479 1.69893 0.07226 H 2.26723 -2.50314 1.22439										
 <p>S 1.17957 -1.70590 1.63896 C 1.04495 -0.05574 0.78791 C 2.35068 0.10407 0.05033 N 2.63016 -0.84367 -0.81925 C 2.20322 -2.84367 -2.10643 C 1.70531 -4.13520 -2.17452 C 1.03957 -4.68863 -1.07685 C 0.85299 -3.95101 0.08688 C 1.34043 -2.64520 0.16797 C 2.02577 -2.10534 -0.93279 C 3.30646 1.17679 0.25310 C 4.68035 0.86817 0.16449 C 5.62931 1.86893 0.30429 C 5.22526 3.18652 0.52434 C 3.86881 3.50024 0.61838 C 2.90970 2.50559 0.49669 H 2.72784 -2.40287 -2.94867 H 1.83699 -4.71374 -3.08242 H 0.65091 -5.70030 -1.13240 H 0.32193 -4.37897 0.93087 H 5.00570 -0.16117 0.04517 H 6.68413 1.61963 0.25636 H 5.96980 3.96919 0.63252 H 3.55640 4.52553 0.78646 H 1.86276 2.76719 0.56103 S -0.37088 0.22364 -1.67997 C -0.22209 0.09703 0.01448 C -1.21116 0.63828 0.99287 N -1.65907 2.03655 0.48387</p>	2133.69566	2133.23678	2133.32141	2133.74228	2133.36803	2134.95648	2134.58223	2135.35432	2134.98007	14.0

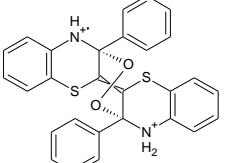
C -3.52099 2.71456 -0.97264 C -4.17970 2.67429 -2.19837 C -3.67756 1.88805 -3.23294 C -2.52404 1.13337 -3.04941 C -1.85015 1.17523 -1.82647 C -2.36006 1.97582 -0.80196 C -2.44527 -0.16262 1.32893 C -2.77320 -1.30784 0.60311 C -3.91378 -2.03360 0.93886 C -4.71757 -1.62348 1.99987 C -4.38147 -0.48523 2.73290 C -3.24762 0.24841 2.40035 H -3.90650 3.32391 -0.16057 H -5.08575 3.25376 -2.33712 H -4.19088 1.84994 -4.18797 H -2.14562 0.50772 -3.85165 H -2.14502 -1.64132 -0.21697 H -4.16959 -2.92181 0.36991 H -5.60496 -2.19242 2.26000 H -4.99909 -0.16858 3.56727 H -2.98760 1.12105 2.99499 O 0.92075 0.92537 1.79518 O -0.46883 0.82141 2.17559 H -2.27697 2.45587 1.18723 H 3.43221 -0.67849 -1.42374 H -0.83761 2.65083 0.42708										
 S 1.76083 -1.25084 0.70944 C 0.80983 0.07590 -0.06050 C 1.60008 1.37513 0.09008 N 2.86433 1.35405 -0.25312 C 4.89160 0.45787 -1.20679 C 5.72138 -0.62760 -1.43664 C 5.33601 -1.90614 -1.02146 C 4.11470 -2.11103 -0.38968 C 3.26536 -1.02692 -0.16586 C 3.66674 0.25324 -0.56443 C 1.06939 2.64665 0.57885 C 1.78262 3.33140 1.57841 C 1.32221 4.55974 2.03732 C 0.16947 5.12222 1.49127 C -0.52997 4.45511 0.48438 C -0.09305 3.21706 0.03312	2133.72169	2133.26445	2133.35065	2133.76427	2133.39322	2134.97674	2134.60570	2135.37329	2135.00224	0.1

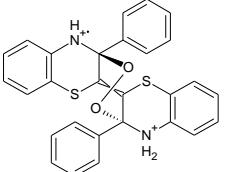
H 5.17975 1.45667 -1.52168 H 6.67148 -0.47992 -1.93833 H 5.98895 -2.75388 -1.20171 H 3.81401 -3.10693 -0.08056 H 2.66730 2.88328 2.02166 H 1.86276 5.07424 2.82508 H -0.18571 6.08339 1.84975 H -1.41584 4.90183 0.04484 H -0.62155 2.72551 -0.77720 S -1.05010 -0.90218 1.92175 C -0.65457 0.11088 0.48334 C -1.48096 -0.16012 -0.79131 N -1.68384 -1.58443 -1.03640 C -1.83408 -3.93198 -0.71998 C -1.81400 -5.01128 0.11632 C -1.55486 -4.83914 1.49978 C -1.30455 -3.58065 2.02607 C -1.30585 -2.45823 1.19825 C -1.59638 -2.62230 -0.20143 C -2.80134 0.57932 -0.89841 C -3.85576 0.21032 -0.05699 C -5.07016 0.88433 -0.13262 C -5.24256 1.91610 -1.05498 C -4.19761 2.26952 -1.90552 C -2.97576 1.60386 -1.83314 H -0.89141 1.12132 0.82045 H -2.03310 -4.04368 -1.78130 H -1.99598 -6.00502 -0.27755 H -1.53930 -5.70370 2.15467 H -1.09267 -3.46429 3.08388 H -3.74172 -0.59931 0.65770 H -5.88297 0.59806 0.52731 H -6.19274 2.43800 -1.11492 H -4.32916 3.06403 -2.63344 H -2.17384 1.88042 -2.50934 O 0.65766 -0.22496 -1.44928 O -0.62325 0.31997 -1.80391 H 3.33454 2.25727 -0.26643 H -1.96086 -1.78592 -1.99462										
 S 1.50691 -1.15570 0.87474 C 0.85186 0.12143 -0.22984 C 1.64780 1.41243 -0.14686	2133.70430	2133.24672	2133.33212	2133.74689	2133.37471	2134.95953	2134.58735	2135.35612	2134.98394	11.6

N 2.94097 1.36732 0.04008									
C 5.15991 0.45333 0.19715									
C 5.99812 -0.61303 0.47485									
C 5.45922 -1.84852 0.84900									
C 4.08422 -2.02614 0.93773									
C 3.22965 -0.95737 0.65957									
C 3.77536 0.27741 0.29713									
C 1.04487 2.73265 -0.34175									
C 0.22881 2.99669 -1.45587									
C -0.28049 4.27499 -1.64313									
C 0.00051 5.28671 -0.72338									
C 0.80596 5.02572 0.38373									
C 1.33760 3.75545 0.57508									
H 5.56422 1.41610 -0.10214									
H 7.07234 -0.48594 0.39807									
H 6.11750 -2.68358 1.06520									
H 3.66917 -2.98859 1.21926									
H 0.03628 2.22603 -2.19635									
H -0.89178 4.48374 -2.51515									
H -0.40918 6.28090 -0.87235									
H 1.01846 5.80928 1.10369									
H 1.94235 3.54654 1.45303									
S -1.33886 0.18152 1.66287									
C -0.64563 0.26306 0.01109									
C -1.22363 -0.74717 -0.98925									
N -2.59983 -0.35321 -1.20361									
C -4.79001 0.30291 -0.57915									
C -5.68917 0.69114 0.37263									
C -5.26762 0.90741 1.70845									
C -3.93981 0.74841 2.06647									
C -2.98450 0.37154 1.11888									
C -3.41772 0.11116 -0.24064									
C -1.12650 -2.24778 -0.75815									
C -0.30973 -3.02247 -1.58888									
C -0.22535 -4.39865 -1.39862									
C -0.95569 -5.01406 -0.38431									
C -1.78742 -4.24839 0.43145									
C -1.88100 -2.87325 0.24169									
H -0.93799 1.23990 -0.38439									
H -5.10071 0.12558 -1.60394									
H -6.73089 0.83192 0.10651									
H -5.98891 1.21653 2.45726									
H -3.62612 0.93648 3.08817									
H 0.26416 -2.55291 -2.37893									
H 0.41387 -4.98889 -2.04796									
H -0.88772 -6.08772 -0.23695									
H -2.37426 -4.72043 1.21316									
H -2.55492 -2.30880 0.87648									
O 0.88778 -0.26298 -1.62771									
O -0.47028 -0.34043 -2.12946									

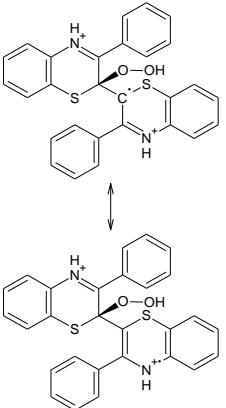
H 3.41938 2.26391 -0.03932 H -3.02952 -0.65846 -2.07341										
 <p> S -1.02168 -2.12676 -1.63486  C -0.02026 -0.76106 -0.91790  C 1.29981 -1.35394 -0.47120  N 1.21824 -2.39456 0.31919  C 0.09710 -3.92351 1.81605  C -0.99518 -4.72858 2.10308  C -2.10293 -4.73602 1.25191  C -2.13498 -3.92805 0.11984  C -1.04817 -3.10452 -0.17659  C 0.06757 -3.11776 0.67571  C 2.61242 -0.81436 -0.80225  C 3.62356 -0.83690 0.18005  C 4.89453 -0.37075 -0.11910  C 5.18105 0.10328 -1.39999  C 4.18848 0.11968 -2.37951  C 2.90502 -0.32201 -2.08769  H 0.96688 -3.91038 2.46608  H -0.98306 -5.35242 2.99017  H -2.95584 -5.36765 1.47784  H -3.00251 -3.92700 -0.53193  H 3.40703 -1.16613 1.19255  H 5.65934 -0.36896 0.65054  H 6.17835 0.46342 -1.63291  H 4.41364 0.47671 -3.37910  H 2.15229 -0.32444 -2.86605  S -0.04966 0.30009 1.79767  C -0.82412 0.02836 0.19004  C -1.25012 1.29895 -0.58649  N -0.38546 2.44792 -0.36832  C 1.47243 3.77387 0.29191  C 2.50127 4.00437 1.15989  C 2.77158 3.09096 2.21185  C 2.00812 1.94595 2.37385  C 0.95577 1.67530 1.49789  C 0.66204 2.60895 0.44361  C -2.70965 1.67371 -0.43297  C -3.68377 0.93012 -1.10782  C -5.02813 1.24707 -0.94222  C -5.40518 2.29393 -0.10086  C -4.43331 3.02672 0.57598 </p>	2133.72133	2133.26362	2133.35026	2133.76319	2133.39212	2134.97707	2134.60601	2135.37348	2135.00242	0.0

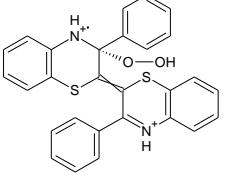
C -3.08379 2.72089 0.41077 H -1.72559 -0.53609 0.43473 H 1.25430 4.45980 -0.52036 H 3.11911 4.88806 1.04437 H 3.59415 3.28485 2.89200 H 2.22877 1.25038 3.17695 H -3.39719 0.11247 -1.76171 H -5.78188 0.67366 -1.47285 H -6.45584 2.53650 0.02657 H -4.72049 3.84015 1.23482 H -2.33415 3.29668 0.94481 O 0.18489 0.19576 -1.92087 O -1.05616 0.90992 -1.94246 H 2.09878 -2.78576 0.64730 H -0.56074 3.19599 -1.03514										
	S -0.45036 -2.37990 -2.00733 C 0.25081 -0.94049 -1.11667 C 1.14314 -1.48233 -0.01352 N 0.59765 -2.35461 0.79755 C -1.21173 -3.62502 1.77546 C -2.37568 -4.36139 1.61736 C -2.95949 -4.48486 0.35391 C -2.39382 -3.86483 -0.75523 C -1.22876 -3.11015 -0.61005 C -0.64196 -3.00441 0.66119 C 2.52575 -1.08368 0.22276 C 2.95153 -0.87429 1.54809 C 4.28257 -0.58100 1.80875 C 5.20224 -0.52063 0.76151 C 4.78575 -0.73751 -0.55183 C 3.45206 -1.00249 -0.83176 H -0.74460 -3.52321 2.75061 H -2.82818 -4.84114 2.47835 H -3.87075 -5.06132 0.23211 H -2.85836 -3.95517 -1.73175 H 2.23575 -0.88692 2.36587 H 4.60018 -0.39384 2.82933 H 6.24478 -0.30001 0.96925 H 5.50309 -0.70036 -1.36528 H 3.14520 -1.18592 -1.85430 S -1.62784 0.10772 0.92016 C -0.81781 0.08726 -0.68465	2133.69680	2133.23934	2133.32534	2133.73885	2133.36739	2134.95665	2134.58520	2135.35326	2134.98180

C -0.16032 1.41475 -1.08320 N -1.24036 2.35605 -1.28391 C -3.22943 3.52116 -0.72515 C -4.31408 3.69827 0.08572 C -4.56791 2.79651 1.14974 C -3.73770 1.71269 1.37211 C -2.62635 1.48622 0.55390 C -2.33949 2.42824 -0.51006 C 0.95418 2.05835 -0.27025 C 0.72509 2.54633 1.02280 C 1.74289 3.19067 1.71850 C 2.99286 3.37150 1.12793 C 3.21762 2.90846 -0.16590 C 2.20465 2.25835 -0.86494 H -1.62319 -0.04883 -1.41563 H -3.02008 4.20779 -1.53954 H -4.98390 4.53419 -0.08304 H -5.43215 2.94680 1.78780 H -3.95551 1.01611 2.17539 H -0.24156 2.44614 1.50244 H 1.55204 3.56024 2.72119 H 3.78373 3.87976 1.67141 H 4.18371 3.05320 -0.63946 H 2.38921 1.90969 -1.87402 O 1.01972 -0.20473 -2.05802 O 0.29990 1.00433 -2.37059 H 1.19190 -2.69625 1.55106 H -1.03771 3.15276 -1.88278											
<b>Single-bond dimer, dioxane radical</b>											
 S -1.50857 -0.47385 -1.86598 C -0.47297 0.07425 -0.57228 C -1.09572 0.18613 0.80263 N -2.22601 1.09188 0.72661 C -4.40982 1.71288 -0.00870 C -5.44210 1.53601 -0.88777 C -5.30689 0.66123 -1.99745 C -4.11827 0.00231 -2.23531 C -3.03009 0.18588 -1.37038 C -3.19237 1.00389 0.19778 C -1.46399 -1.16423 1.40392 C -2.44343 -1.22654 2.40084 C -2.73352 -2.43949 3.01688		2133.69369	2133.23512	2133.32059	2133.73956	2133.36646	2134.95833	2134.58523	2135.35649	2134.98339	6.3

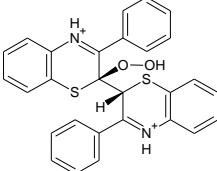
C -2.05051 -3.59692 2.64327 C -1.07301 -3.53659 1.65317 C -0.77893 -2.32424 1.03347 H -4.51466 2.35259 0.86172 H -6.38009 2.05633 -0.72716 H -6.13996 0.52543 -2.67856 H -4.00582 -0.63034 -3.10985 H -2.98396 -0.33677 2.70903 H -3.49459 -2.47884 3.78999 H -2.28121 -4.54303 3.12352 H -0.53700 -4.43278 1.35658 H -0.01245 -2.29651 0.26544 S 1.71302 -0.04808 -2.24853 C 0.83928 0.29700 -0.74849 C 1.65344 0.75502 0.43537 N 2.99725 0.01351 0.42523 C 3.67117 -2.36533 0.44470 C 3.81362 -3.57375 -0.23378 C 3.35026 -3.70233 -1.54140 C 2.71535 -2.63918 -2.18116 C 2.57197 -1.42562 -1.51379 C 3.06448 -1.30737 -0.21326 C 1.93521 2.24087 0.51426 C 2.48417 2.74819 1.69819 C 2.78055 4.10304 1.79862 C 2.52712 4.95579 0.72411 C 1.97022 4.45251 -0.44905 C 1.67135 3.09614 -0.55694 H 4.03935 -2.25341 1.46015 H 4.28906 -4.41172 0.26426 H 3.46428 -4.64531 -0.06623 H 2.32340 -2.75151 -3.18665 H 2.65874 2.09665 2.55015 H 3.20240 4.49293 2.71956 H 2.75773 6.01365 0.80518 H 1.76141 5.11410 -1.28374 H 1.22697 2.72260 -1.47333 H 3.32753 -0.04555 1.39681 O 1.04854 0.26562 1.62669 O -0.20903 0.91531 1.66737 H -2.36522 1.71620 1.51663 H 3.65859 0.64358 -0.04799																			
	-	2133.70596	-	2133.24733	-	2133.33164	-	2133.75110	-	2133.37679	-	2134.96969	-	2134.59537	-	2135.36782	-	2134.99350	0.0

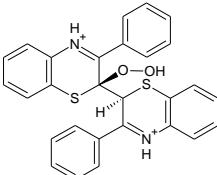
S -1.77636 -1.31075 -1.45934									
C -0.75023 -0.46843 -0.32302									
C -1.46065 0.47968 0.61363									
N -2.36345 -0.33411 1.42249									
C -4.27825 -1.73171 1.73121									
C -5.24606 -2.52608 1.17947									
C -5.21306 -2.85652 -0.19954									
C -4.18308 -2.41630 -1.00519									
C -3.15713 -1.62974 -0.46135									
C -3.23586 -1.21712 0.91353									
C -2.16882 1.63243 -0.08633									
C -1.53119 2.26015 -1.16108									
C -2.13129 3.34835 -1.78451									
C -3.36761 3.81516 -1.33735									
C -3.99935 3.19394 -0.26260									
C -3.40256 2.10287 0.36619									
H -4.31471 -1.44111 2.77619									
H -6.05698 -2.89366 1.79899									
H -5.99228 -3.48238 -0.62082									
H -4.13777 -2.71078 -2.04878									
H -0.56840 1.90174 -1.51370									
H -1.63469 3.82876 -2.62175									
H -3.83735 4.66245 -1.82777									
H -4.95993 3.55539 0.09078									
H -3.90932 1.63220 1.20228									
S 1.37755 -1.86365 -1.27001									
C 0.57789 -0.70347 -0.23869									
C 1.32633 0.00274 0.87871									
N 2.26269 -1.01306 1.51607									
C 4.65825 -1.42146 1.10035									
C 5.67711 -1.83455 0.24635									
C 5.37734 -2.22849 -1.05605									
C 4.06587 -2.20743 -1.52158									
C 3.03582 -1.80650 -0.66957									
C 3.35458 -1.42727 0.63152									
C 2.08580 1.25414 0.50942									
C 2.50117 2.10653 1.53912									
C 3.22360 3.25491 1.23533									
C 3.52989 3.55880 -0.09150									
C 3.10943 2.71407 -1.11584									
C 2.38673 1.56091 -0.81852									
H 4.87920 -1.10639 2.11611									
H 6.70190 -1.84045 0.60078									
H 6.17174 -2.54392 -1.72434									
H 3.84049 -2.49692 -2.54299									
H 2.24264 1.89189 2.57250									
H 3.53990 3.91669 2.03536									
H 4.09146 4.45801 -0.32585									
H 3.33948 2.95010 -2.14992									
H 2.06239 0.91395 -1.62822									

H 2.65266 -0.58710 2.36540 O 0.42324 0.19911 1.95488 O -0.54954 1.13380 1.47470 H -2.43350 -0.08414 2.40496 H 1.71178 -1.82461 1.83129													
<b>Single-bond dimer, C2-hydroperoxylalkyl radical</b>													
 <p>S -1.15520 -2.09766 -0.59066 C -0.48420 -0.88824 0.60781 C -1.33645 0.35888 0.80659 N -2.62769 0.30117 0.60328 C -4.82230 -0.50169 0.07815 C -5.65635 -1.46835 -0.45789 C -5.11010 -2.63088 -1.00950 C -3.73488 -2.83199 -1.02158 C -2.88605 -1.86329 -0.48243 C -3.43678 -0.69886 0.05844 C -0.79537 1.57527 1.40375 C 0.29489 1.53046 2.29180 C 0.75205 2.69919 2.88569 C 0.13985 3.92007 2.60243 C -0.93683 3.97426 1.71652 C -1.40280 2.81321 1.11840 H -5.23290 0.40479 0.51434 H -6.73037 -1.31923 -0.44542 H -5.76114 -3.39089 -1.42906 H -3.31724 -3.74030 -1.44457 H 0.75138 0.58549 2.56038 H 1.58211 2.65324 3.58316 H 0.50435 4.83028 3.06854 H -1.40174 4.92476 1.47626 H -2.19725 2.88536 0.37988 C 0.95589 -0.67133 0.15558</p>	2133.72927	-	2133.27153	-	2133.35890	-	2133.77068	2133.40031	2134.98871	2134.61834	2135.38753	2135.01716	0.0

S 2.01639 -1.84559 0.87392 C 3.56140 -1.46923 0.17155 C 3.74087 -0.41779 -0.74436 N 2.67068 0.34744 -1.15541 C 1.37086 0.25851 -0.78636 C 4.65336 -2.25372 0.56046 C 5.90767 -1.98644 0.03775 C 6.08631 -0.93562 -0.87396 C 5.01447 -0.15485 -1.26547 C 0.51477 1.26286 -1.46658 C 0.86946 2.61622 -1.35504 C 0.14672 3.58277 -2.04424 C -0.92354 3.20951 -2.85757 C -1.26519 1.86490 -2.98551 C -0.54934 0.88901 -2.29621 H 4.51210 -3.06445 1.26843 H 6.75394 -2.59456 0.33857 H 7.07174 -0.73090 -1.27850 H 5.14818 0.65821 -1.97222 H 1.68870 2.91470 -0.70644 H 0.41706 4.62893 -1.94118 H -1.48548 3.96632 -3.39638 H -2.08256 1.56717 -3.63478 H -0.79601 -0.15768 -2.43221 O -0.34226 -1.45522 1.91320 O -1.61726 -1.85765 2.38305 H -1.56148 -2.82555 2.30436 H 2.86931 1.04577 -1.86508 H -3.14687 1.11618 0.92544										
<b>Single-bond dimer, C3-hydroperoxylalkyl radical</b>										
 S 1.94682 -0.27484 1.34971 C 0.68278 0.51164 0.39888 C 1.00860 1.89021 0.01729 N 2.22591 2.16409 -0.39315 C 4.42758 1.63656 -1.23788 C 5.54743 0.81912 -1.21689 C 5.56287 -0.32767 -0.41817 C 4.45711 -0.67206 0.35159 C 3.31894 0.13514 0.32704 C 3.31755 1.29142 -0.46340 C 0.05748 2.99363 0.14931	2133.71053	2133.25395	2133.34462	2133.75264	2133.38673	2134.96576	2134.59985	2135.36526	2134.99935	0.0

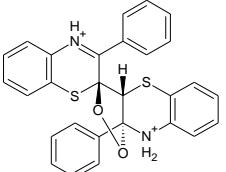
C -0.81375 3.01227 1.25238 C -1.66909 4.08972 1.43350 C -1.68094 5.13784 0.51186 C -0.82762 5.11479 -0.59240 C 0.04788 4.05244 -0.77401 H 4.40348 2.53360 -1.84926 H 6.41086 1.07646 -1.82070 H 6.44121 -0.96467 -0.40050 H 4.46911 -1.56896 0.96259 H -0.80249 2.19799 1.97088 H -2.32825 4.11236 2.29523 H -2.36080 5.97269 0.65134 H -0.85110 5.92094 -1.31836 H 0.67846 4.02388 -1.65869 S -1.62553 0.70390 -0.95091 C -0.50901 -0.10187 0.10883 C -0.78167 -1.49066 0.68144 N -2.14101 -1.96723 0.48373 C -4.44725 -2.09616 -0.09800 C -5.52457 -1.56391 -0.75084 C -5.41089 -0.33953 -1.45857 C -4.21090 0.33964 -1.49845 C -3.09369 -0.17882 -0.82680 C -3.19753 -1.41565 -0.12098 C 0.15510 -2.56635 0.13382 C 0.53849 -3.64154 0.94164 C 1.32134 -4.66019 0.40498 C 1.71506 -4.61557 -0.93177 C 1.32025 -3.54855 -1.73742 C 0.53745 -2.52602 -1.20959 H -4.52427 -3.03349 0.44338 H -6.47677 -2.08282 -0.72801 H -6.27618 0.07003 -1.96822 H -4.12644 1.27852 -2.03632 H 0.24517 -3.67917 1.98567 H 1.62620 -5.48872 1.03689 H 2.32628 -5.41195 -1.34550 H 1.62004 -3.50961 -2.78008 H 0.23579 -1.70139 -1.84909 O -0.55708 -1.44233 2.08263 O -1.39979 -0.42858 2.62831 H -2.02702 -0.95328 3.15253 H 2.42578 3.13925 -0.60389 H -2.28302 -2.88662 0.89351									
<b>Single-bond dimer, C2-hydroperoxide</b>									

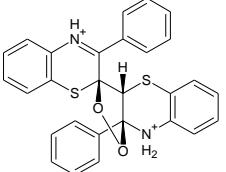
 <p>S 0.59730 -2.38348 -1.20966      C 0.13189 -0.66476 -0.75050      C 1.39285 0.16598 -0.96514      N 2.49652 -0.24687 -0.37369      C 3.83107 -1.62230 1.09795      C 4.11817 -2.87003 1.62846      C 3.32085 -3.97133 1.30218      C 2.22487 -3.83075 0.45844      C 1.91917 -2.57797 -0.07707      C 2.73624 -1.48287 0.23905      C 1.45509 1.38551 -1.75007      C 0.37921 2.29233 -1.80145      C 0.51636 3.49016 -2.48749      C 1.70577 3.78811 -3.15283      C 2.76814 2.88266 -3.13362      C 2.65008 1.69123 -2.43516      H 4.44158 -0.75806 1.34329      H 4.96379 -2.98686 2.29742      H 3.54738 -4.94694 1.71983      H 1.59913 -4.68475 0.22061      H -0.55338 2.07424 -1.29804      H -0.31020 4.19273 -2.50642      H 1.80118 4.72192 -3.69827      H 3.68297 3.10003 -3.67487      H 3.46500 0.97349 -2.47090      C -0.41711 -0.58378 0.72837      S -1.56984 -1.90708 1.17257      C -2.99436 -1.34276 0.32016      C -3.20789 0.03155 0.14363      N -2.30341 0.94459 0.69459      C -1.08110 0.71095 1.13037      C -3.96249 -2.24470 -0.12157      C -5.11168 -1.77251 -0.74732      C -5.30514 -0.40210 -0.94268      C -4.35602 0.50475 -0.49598      C -0.44244 1.68352 1.99996      C 0.95501 1.69808 2.16644      C 1.56055 2.65302 2.96980      C 0.78277 3.59762 3.63785      C -0.60787 3.57657 3.50975      C -1.21830 2.62908 2.70469      H -3.80842 -3.31039 0.01426</p>	-	2134.34771	-	2133.96824	-	2134.39581	-	2134.01634	-	2135.61306	-	2135.23359	-	2136.01115	-	2135.63168	1.1
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	-----

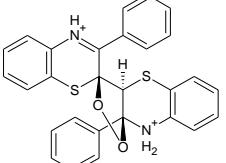
H -5.85667 -2.48063 -1.09541 H -6.19842 -0.04186 -1.44142 H -4.49688 1.57237 -0.63697 H 1.58534 0.97611 1.66280 H 2.63991 2.65670 3.07742 H 1.25689 4.33900 4.27334 H -1.21772 4.28897 4.05517 H -2.30329 2.60143 2.67691 O -0.93100 -0.26081 -1.55154 O -0.59405 -0.43003 -2.92973 H -1.33402 -0.98619 -3.22697 H 0.43019 -0.75502 1.39572 H 3.29464 0.38306 -0.42046 H -2.68205 1.87059 0.87290									
 S 1.21893 -1.03079 1.58143 C -0.16606 -0.41619 0.52683 C -0.88599 -1.67355 0.04158 N -0.15254 -2.56777 -0.58715 C 1.85176 -3.47996 -1.58220 C 3.22402 -3.66889 -1.54055 C 3.98682 -3.04947 -0.54618 C 3.38756 -2.22248 0.39679 C 2.00688 -2.01350 0.36090 C 1.24531 -2.66129 -0.62460 C -2.29129 -1.96531 0.25993 C -3.27780 -0.96159 0.24085 C -4.61308 -1.30259 0.39666 C -4.98257 -2.63334 0.59657 C -4.00977 -3.63306 0.64487 C -2.67298 -3.30630 0.47632 H 1.24621 -3.96153 -2.34405 H 3.70113 -4.30176 -2.28091 H 5.06088 -3.20079 -0.51344 H 3.98588 -1.72847 1.15536 H -3.00568 0.07370 0.08471 H -5.36990 -0.52563 0.36318 H -6.02921 -2.89040 0.72800 H -4.29185 -4.66435 0.82950 H -1.92143 -4.08479 0.57288 C 0.32770 0.45904 -0.67242 S -0.92083 0.78264 -1.95127 C -1.79814 2.09197 -1.17180	2134.35192	2133.88156	2133.96934	2134.39741	2134.01483	2135.61800	2135.23542	2136.01606	2135.63348

C -1.14130 2.96298 -0.29276 N 0.22917 2.80038 -0.03265 C 0.97398 1.74194 -0.21648 C -3.13375 2.33502 -1.49303 C -3.79692 3.42232 -0.93086 C -3.13890 4.27479 -0.04286 C -1.80664 4.05063 0.27465 C 2.40326 1.82594 0.04674 C 3.31587 1.11988 -0.75643 C 4.68054 1.25696 -0.53906 C 5.14814 2.06905 0.49316 C 4.24724 2.75657 1.30904 C 2.88342 2.64698 1.08549 H -3.65096 1.67301 -2.18069 H -4.83676 3.59993 -1.18543 H -3.66204 5.11548 0.39963 H -1.28133 4.70855 0.96079 H 2.97454 0.50789 -1.58471 H 5.37957 0.72866 -1.17903 H 6.21560 2.16257 0.66704 H 4.60882 3.37087 2.12703 H 2.19483 3.15166 1.75716 O -0.96528 0.43529 1.28184 O -1.34991 -0.20796 2.49837 H -1.04718 0.44742 3.14920 H 1.08597 -0.13207 -1.19203 H -0.65592 -3.33214 -1.03204 H 0.71069 3.64646 0.26533										
	n.d.									
<b>Single-bond dimer, C3-hydroperoxide</b>										
 S 1.17817 -1.58495 1.42435 C 0.96023 -0.06767 0.52885 C 2.19962 0.44617 -0.06677 N 3.01410 -0.40040 -0.65213 C 3.63643 -2.49573 -1.67836 C 3.57904 -3.88137 -1.69573	2134.33888	2133.86790	2133.95589	2134.38555	2134.00256	2135.60808	2135.22509	2136.00750	2135.62451	0.0

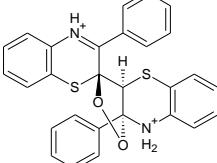
C 2.77933 -4.55948 -0.77258									
C 2.02514 -3.85861 0.16285									
C 2.06763 -2.46407 0.18418									
C 2.88110 -1.79246 -0.73723									
C 2.58513 1.84976 0.01374									
C 2.29073 2.57087 1.18502									
C 2.71235 3.88845 1.30563									
C 3.40241 4.50093 0.25969									
C 3.68381 3.79260 -0.91089									
C 3.28847 2.46892 -1.03539									
H 4.25772 -1.95591 -2.38670									
H 4.15903 -4.43349 -2.42725									
H 2.73633 -5.64375 -0.78465									
H 1.39938 -4.38938 0.87333									
H 1.76343 2.09050 2.00428									
H 2.50123 4.43817 2.21708									
H 3.71806 5.53550 0.35290									
H 4.20451 4.27698 -1.73044									
H 3.47765 1.93990 -1.96570									
S -0.41855 2.13292 -0.36926									
C -0.23507 0.57210 0.44892									
C -1.44375 -0.03782 1.16809									
N -2.57899 1.00579 1.20325									
C -4.37335 1.28695 -0.48649									
C -4.74043 1.72766 -1.75647									
C -3.78789 2.27806 -2.61287									
C -2.45408 2.38666 -2.22330									
C -2.08203 1.95688 -0.95149									
C -3.04955 1.42913 -0.10502									
C -1.97765 -1.31697 0.56127									
C -2.75258 -2.17658 1.34857									
C -3.29438 -3.32681 0.78278									
C -3.07573 -3.61686 -0.56330									
C -2.31164 -2.75450 -1.34707									
C -1.76068 -1.60478 -0.78846									
H -5.10563 0.85299 0.18766									
H -5.77309 1.63518 -2.07510									
H -4.08066 2.61506 -3.60201									
H -1.71010 2.79580 -2.89888									
H -2.92125 -1.96563 2.40009									
H -3.88645 -3.99714 1.39783									
H -3.50088 -4.51502 -1.00092									
H -2.13979 -2.97474 -2.39590									
H -1.15999 -0.94467 -1.40689									
H -3.34312 0.59439 1.74874									
O -1.15656 -0.29680 2.50929									
O -0.70547 0.94402 3.08297									
H -1.07228 0.86383 3.97973									
H 3.87887 -0.01571 -1.02458									
H -2.22226 1.80565 1.75092									

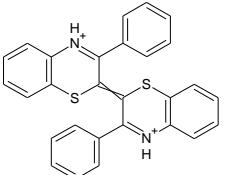
Single-bond dimer, dioxolane										
 <p>S 1.68455 -1.71512 0.69880      C 1.05639 -0.19962 -0.05308      C 2.07432 0.92433 0.11676      N 3.32902 0.65626 -0.14310      C 5.21557 -0.60267 -0.95587      C 5.83409 -1.82409 -1.16656      C 5.17520 -3.01081 -0.83034      C 3.89370 -2.98468 -0.29193      C 3.25677 -1.76046 -0.08646      C 3.92717 -0.57703 -0.41267      C 1.76031 2.29347 0.52487      C 2.52563 2.88301 1.54592      C 2.28313 4.19999 1.91735      C 1.29990 4.94048 1.26254      C 0.54945 4.36316 0.23713      C 0.76499 3.04117 -0.12829      H 5.71657 0.32733 -1.20866      H 6.83139 -1.85471 -1.59146      H 5.66167 -3.96639 -0.99675      H 3.38315 -3.90839 -0.03915      H 3.27326 2.29721 2.07306      H 2.86039 4.64535 2.72098      H 1.11678 5.97086 1.55107      H -0.20258 4.94575 -0.28488      H 0.20459 2.61343 -0.95390      S -0.94635 -0.85221 1.90524      C -0.38336 0.11413 0.46652      C -1.20904 0.00800 -0.82085      N -1.58888 -1.46111 -1.06340      C -3.61535 -2.74978 -0.54329      C -4.49027 -3.29995 0.38552      C -4.27060 -3.09503 1.74769      C -3.19195 -2.33696 2.18693      C -2.29604 -1.78840 1.26272      C -2.52592 -2.01757 -0.09078      C -2.41460 0.89024 -0.97415      C -3.05170 1.45021 0.13582      C -4.17568 2.25099 -0.04698      C -4.66131 2.49498 -1.32985      C -4.02431 1.93654 -2.43744      C -2.90335 1.13194 -2.26436</p>										

H -0.42027 1.15727 0.78510 H -3.77326 -2.89504 -1.60823 H -5.34132 -3.87933 0.04505 H -4.95372 -3.51640 2.47804 H -3.04386 -2.16134 3.24796 H -2.68975 1.26626 1.14321 H -4.66989 2.68336 0.81704 H -5.53714 3.12165 -1.46752 H -4.39645 2.12882 -3.43857 H -2.40591 0.71223 -3.13431 O 0.87502 -0.44906 -1.45929 O -0.28396 0.32988 -1.82235 H -1.99538 -1.51857 -2.00356 H -0.71862 -2.01328 -1.10319 H 3.96087 1.45520 -0.13861									
 S -1.42897 -1.23672 -0.86505 C -0.89541 0.08728 0.25135 C -1.79181 1.30834 0.14569 N -3.07493 1.15677 -0.05048 C -5.20922 0.06166 -0.21363 C -5.95314 -1.07268 -0.48984 C -5.30967 -2.26141 -0.85059 C -3.92407 -2.32478 -0.92884 C -3.16315 -1.18698 -0.65158 C -3.81417 -0.00023 -0.30124 C -1.29824 2.67708 0.31685 C -0.55662 3.03831 1.45463 C -0.14522 4.35531 1.61334 C -0.45113 5.30963 0.64174 C -1.18665 4.95259 -0.48697 C -1.62090 3.64173 -0.65078 H -5.69464 0.98952 0.07450 H -7.03484 -1.03506 -0.42263 H -5.89444 -3.14990 -1.06531 H -3.42939 -3.25153 -1.20143 H -0.35150 2.31093 2.23451 H 0.40834 4.63873 2.50265 H -0.11727 6.33485 0.76794 H -1.42038 5.69267 -1.24534 H -2.17249 3.35840 -1.54279 S 1.27475 0.29984 -1.62210 C 0.59030 0.35442 0.03016	2134.32683	2133.85473	2133.94015	2134.37537	2133.98869	2135.59397	2135.20729	2135.99130	2135.60461

C 1.21868 -0.62566 1.03363 N 2.56732 -0.04712 1.36879 C 4.77960 0.49016 0.52488 C 5.67649 0.86089 -0.46682 C 5.21616 1.06895 -1.76616 C 3.87037 0.91401 -2.06638 C 2.94600 0.54172 -1.08063 C 3.43305 0.32758 0.21504 C 1.31882 -2.11086 0.75202 C 0.61306 -2.98782 1.58487 C 0.68740 -4.36151 1.37948 C 1.46860 -4.87564 0.34676 C 2.18457 -4.00830 -0.47447 C 2.11512 -2.63168 -0.27677 H 0.78894 1.35657 0.42342 H 5.12420 0.33008 1.54277 H 6.72548 0.98599 -0.22244 H 5.90637 1.35881 -2.55150 H 3.51673 1.08416 -3.07888 H 0.00331 -2.59879 2.39166 H 0.13203 -5.02890 2.03103 H 1.52464 -5.94812 0.18660 H 2.80442 -4.39821 -1.27565 H 2.69233 -1.98814 -0.92844 O -0.93500 -0.29714 1.64808 O 0.41592 -0.34539 2.16589 H 2.41675 0.78013 1.96271 H 3.07587 -0.72546 1.94853 H -3.62398 2.01357 0.00825										
 S -1.29834 -1.35137 -1.69444 C -0.00902 -0.50928 -0.68195 C 1.05210 -1.53904 -0.35156 N 0.61617 -2.64130 0.20492 C -1.00785 -4.04535 1.31599 C -2.30132 -4.53883 1.39993 C -3.29335 -4.05385 0.54416 C -3.00447 -3.06369 -0.38896 C -1.70938 -2.55133 -0.48021 C -0.71565 -3.05709 0.37320 C 2.48245 -1.36806 -0.56477 C 3.37866 -1.90565 0.38127 C 4.74620 -1.80497 0.17791	2134.34680	2133.87518	2133.95956	2134.39334	2134.00610	2135.61557	2135.22833	2136.01288	2135.62564	0.0

C 5.23781 -1.18590 -0.97273									
C 4.35664 -0.65667 -1.91473									
C 2.98454 -0.73211 -1.71428									
H -0.22740 -4.41523 1.97407									
H -2.53698 -5.30220 2.13341									
H -4.30487 -4.44081 0.61203									
H -3.78095 -2.67816 -1.04156									
H 3.01276 -2.34517 1.30534									
H 5.42927 -2.19939 0.92297									
H 6.30922 -1.11214 -1.13140									
H 4.73782 -0.18361 -2.81376									
H 2.31295 -0.33822 -2.46706									
S 0.52823 0.39055 1.97758									
C -0.60565 0.21426 0.55516									
C -1.04809 1.54483 -0.10928									
N -0.40157 2.74360 0.62401									
C 1.81763 3.73926 0.13894									
C 3.20211 3.66964 0.28570									
C 3.78531 2.59841 0.96056									
C 3.00285 1.56653 1.47681									
C 1.61893 1.62676 1.33550									
C 1.05469 2.72403 0.68969									
C -2.53568 1.80268 -0.16250									
C -3.13461 2.23628 -1.34814									
C -4.49897 2.51425 -1.36668									
C -5.26250 2.36834 -0.21025									
C -4.66185 1.94002 0.97260									
C -3.29988 1.65625 1.00018									
H -1.46662 -0.32386 0.95441									
H 1.35144 4.57228 -0.37893									
H 3.82244 4.45743 -0.12788									
H 4.86372 2.55445 1.07397									
H 3.46160 0.72145 1.97894									
H -2.54754 2.34463 -2.25382									
H -4.96381 2.84355 -2.29062									
H -6.32615 2.58502 -0.23054									
H -5.25207 1.81935 1.87531									
H -2.85228 1.31335 1.93031									
O 0.53618 0.54639 -1.42231									
O -0.51270 1.52977 -1.40310									
H -0.79177 2.76795 1.57716									
H -0.73258 3.59618 0.15976									
H 1.32353 -3.32754 0.45913									

 <p>S 0.82942 2.38937 -1.98269      C -0.08827 1.05839 -1.12227      C -0.86482 1.69034 0.02132      N -0.18256 2.44851 0.84128      C 1.80322 3.41737 1.81753      C 3.06120 3.97890 1.65888      C 3.64218 4.04577 0.39014      C 2.97897 3.54117 -0.72381      C 1.71784 2.96287 -0.57776      C 1.13648 2.91450 0.69826      C -2.28305 1.47353 0.28604      C -2.69408 1.23926 1.61134      C -4.04471 1.11161 1.90447      C -4.99416 1.24102 0.89090      C -4.59044 1.48260 -0.42227      C -3.24187 1.58414 -0.73610      H 1.33765 3.35923 2.79707      H 3.58921 4.36585 2.52354      H 4.62675 4.48516 0.26724      H 3.43982 3.58515 -1.70516      H -1.95861 1.10620 2.40010      H -4.35461 0.90553 2.92378      H -6.05054 1.14948 1.12414      H -5.32969 1.59355 -1.20897      H -2.94301 1.78881 -1.75696      S 1.54625 -0.34118 0.88135      C 0.80023 -0.14831 -0.73901      C -0.08106 -1.32729 -1.18252      N 0.88085 -2.42000 -1.55868      C 2.46196 -4.04070 -0.66854      C 3.42927 -4.46760 0.23018      C 3.81453 -3.62907 1.27506      C 3.23893 -2.37456 1.41550      C 2.25930 -1.92291 0.52067      C 1.88506 -2.78350 -0.51983      C -1.21540 -1.87452 -0.33890      C -2.50237 -1.87335 -0.89165      C -3.57006 -2.42117 -0.18807      C -3.36767 -2.98106 1.07113      C -2.08907 -2.99316 1.62196      C -1.01475 -2.44582 0.92544      H 1.62646 -0.10373 -1.45754</p>	-	2133.84791	-	2133.93232	-	2134.36763	-	2133.98030	-	2135.59218	-	2135.20485	-	2135.98953	-	2135.60220	14.7
---	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	---	------------	------

H 2.15918 -4.68456 -1.48945 H 3.87698 -5.44796 0.11114 H 4.57034 -3.94997 1.98430 H 3.54595 -1.72410 2.22897 H -2.67290 -1.44655 -1.87282 H -4.56146 -2.40817 -0.62996 H -4.20157 -3.40940 1.61905 H -1.91729 -3.43297 2.59940 H -0.03499 -2.48501 1.38223 O -0.99114 0.50686 -2.07259 O -0.53042 -0.80901 -2.42345 H 1.36416 -2.13615 -2.42333 H 0.33870 -3.25903 -1.79731 H -0.70146 2.84475 1.62347									
<b>Double-bond dimers</b>									
 S 1.46649 -0.10793 -2.40504 C 0.69413 0.00107 -0.82824 C 1.52053 0.29110 0.32227 N 2.80079 -0.03008 0.32226 C 4.81332 -1.16368 -0.36316 C 5.58899 -1.71872 -1.36915 C 5.10409 -1.77253 -2.67877 C 3.84015 -1.28282 -2.98727 C 3.04843 -0.73573 -1.97716 C 3.54262 -0.67146 -0.67104 C 1.04838 1.07519 1.46985 C 0.20282 2.17794 1.26261 C -0.16382 2.97811 2.33800 C 0.29766 2.68434 3.62060 C 1.13805 1.58972 3.82998 C 1.52053 0.78970 2.76193 H 5.17941 -1.10935 0.65787 H 6.57424 -2.10672 -1.13481 H 5.71204 -2.20501 -3.46650 H 3.46406 -1.33362 -4.00403 H -0.12809 2.43605 0.26179 H -0.80237 3.83942 2.17042 H 0.00308 3.30850 4.45857 H 1.48459 1.35013 4.83005 H 2.13476 -0.08789 2.94692 S -1.46649 0.10793 -2.40504 C -0.69413 -0.00107 -0.82824	1982.93615	1982.49979	1982.58217	1982.97583	1982.62186	1984.09187	1983.73789	1984.44227	1984.08829

C -1.52053 -0.29110 0.32227									
N -2.80079 0.03008 0.32226									
C -4.81332 1.16368 -0.36316									
C -5.58899 1.71872 -1.36915									
C -5.10409 1.77253 -2.67877									
C -3.84015 1.28282 -2.98727									
C -3.04843 0.73573 -1.97716									
C -3.54262 0.67146 -0.67104									
C -1.04838 -1.07519 1.46985									
C -0.20282 -2.17794 1.26261									
C 0.16382 -2.97811 2.33800									
C -0.29766 -2.68434 3.62060									
C -1.13805 -1.58972 3.82998									
C -1.52053 -0.78970 2.76193									
H -5.17941 1.10935 0.65787									
H -6.57424 2.10672 -1.13481									
H -5.71204 2.20501 -3.46650									
H -3.46406 1.33362 -4.00403									
H 0.12809 -2.43605 0.26179									
H 0.80237 -3.83942 2.17042									
H -0.00308 -3.30850 4.45857									
H -1.48459 -1.35013 4.83005									
H -2.13476 0.08789 2.94692									
H -3.33823 -0.29419 1.12187									
H 3.33823 0.29419 1.12187									

**Table S7.**  $pK_a$  values computed in methanol at different theory levels for all bibenzothiazine derivatives examined. For each chemical species and for each protonation state, the  $G_{RRHO,calc}$  value (see Tables S4-S6) of the most stable stereoisomer identified was used in the calculation.

	PBE0 / 6-31+G(d,p) / SMD		M062X / 6-31+G(d,p) / SMD		M062X / 6-311++G(2d,2p) / SMD	
	$pK_{a1}$	$pK_{a2}$	$pK_{a1}$	$pK_{a2}$	$pK_{a1}$	$pK_{a2}$
Single-bond dimer	4.3	3.2	3.6	2.3	3.6	2.4
Single-bond dimer, radical	6.6	1.6	6.6	0.3	6.6	0.4
Single-bond dimer, C2-peroxyl radical	3.7	1.9	3.0	1.2	3.0	1.3
Single-bond dimer, C3-peroxyl radical	4.2	-2.0	3.4	-2.4	3.5	-2.3
Single-bond dimer, dioxolane radical	4.9	2.0	4.8	0.7	4.9	0.8
Single-bond dimer, dioxane radical	4.7	-1.0	4.2	-1.1	4.4	-1.2
Single-bond dimer, C2-hydroperoxylalkyl radical	5.4	2.4	5.4	1.5	5.6	1.6
Single-bond dimer, C3-hydroperoxylalkyl radical	5.0	2.7	4.8	2.1	5.2	1.9
Single-bond dimer, C2-hydroperoxide	3.8	3.1	3.5	2.2	3.5	2.2
Single-bond dimer, C3-hydroperoxide	4.3	0.6	3.7	0.3	3.8	0.3
Single-bond dimer, dioxolane	3.1	-0.4	2.7	-0.9	2.8	-0.7
Double-bond dimers	4.6	2.4	4.2	1.3	4.3	1.4

**Table S8.**  $pK_a$  values computed in methanol at different theory levels for some reference nitrogen bases and corresponding experimental values. For each chemical species and for each protonation state, the  $G_{RRHO,calc}$  value of the most stable stereoisomer identified was used in the calculation. At each theory level, a linear fitting with respect to the experimental values was used to correct the raw  $pK_a$  values.

	PBE0 / 6-31+G(d,p) / SMD	M062X / 6-31+G(d,p) / SMD	M062X / 6-311++G(2d,2p) / SMD	Experimental <sup>a</sup>
<b>pyridine</b>	5.87	5.90	5.85	5.44
<b>aniline</b>	4.23	4.42	4.30	6.05
<b>2-chloroaniline</b>	2.95	2.88	2.81	3.71
<b>4-chloroaniline</b>	3.77	3.87	3.76	4.95
<b>2-nitroaniline</b>	0.73	0.39	0.51	0.20
<b>4-nitroaniline</b>	1.30	1.46	1.46	1.55
<b>4-chloro-2-nitroaniline</b>	0.69	0.73	0.86	-0.67
<b>2-methylpyridine</b>	6.39	6.42	6.43	6.18
<b>quinoline</b>	5.84	5.73	5.74	5.16
<b>2-methylquinoline</b>	6.86	6.83	6.90	6.06

[a] Rived, F.; Rosés, M.; Bosch, E. *Anal. Chim. Acta* **1998**, 374, 309-324.