Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Dimerization reactions with oxidized brominated thiophenes

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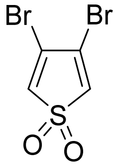
A- Experimental Procedure

General information. 3,4-dibromothiophene S,S-dioxide was prepared by the procedure of Lu.[1] 2,5-dibromothiophene, 2,3,4,5-tetrabromothiophene S,S-dioxides are synthesized following the procedure of V. G. Nenajdenko.[2] Reagents and chemicals from commercial sources were used without further purification. Solvents were dried and purified using standard techniques. Microwave-assisted reactions were performed in the cavity of a Biotage Initiator+ system in sealed reactors. Flexible plates ALUGRAM® Xtra SIL G UV254 from MACHEREY-NAGEL were used for TLC. Compounds were detected by UV irradiation (Bio block Scientific). NMR spectra were recorded with a Bruker AVANCE III 300 (^{1}H, 300 MHz and ^{13}C, 75MHz) or a Bruker AVANCE DRX500 (^{1}H, 500 MHz; ^{13}C, 125 MHz). Chemical shifts are given in ppm relative to the deuterated solvent and coupling constants J in Hz. Matrix-Assisted Laser Desorption/Ionization was performed on MALDI-TOF MS BIFLEX III Bruker Daltonics spectrometer. High-resolution mass spectrometry (HRMS) was performed with a JEOL JMS700 B/E or a JEOL Spiral-TOF JMS3000.

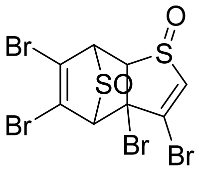
❖ Synthesis of 1-SO$_2$



Formula: $C_4H_2Br_2O_2S$
MW= 271.8142g/mol

To a 100 ml three-neck round-bottom flask fitted with a dropping funnel and a thermometer, 1.6 ml (35eq) of 30% H_2O_2 was added dropwise to the mixture of trifluoroacetic anhydride (4.23 ml,15eq) and sulfuric acid (0.25ml) and stirred in a NaCl-ice bath (-15 to -20 °C) so that the temperature was kept below 0°C. The solution was stirred for another 15 min, and 0.5 g (2.1 mmol) of 3,4-dibromothiophene in 5 ml of dichloromethane was added all at once. The reaction mixture was allowed to warm to room temperature with stirring for 3 h. Then the solution was transferred to a 250 ml erlenmeyer flask in a NaCl-ice bath, and 150 ml of saturated sodium carbonate solution were slowly added to bring the pH up to around 7. The solution was extracted with dichloromethane. The organic phases were combined and dried over $MgSO_4$. Solvents were removed on a rotary evaporator, to give a white-pale yellow powder with a yield of 76%. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 6.83 (s, 1H).

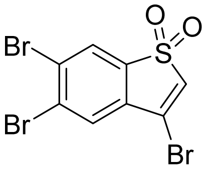
❖ Synthesis of 1-CySO



Formula: $C_8H_4Br_4O_2S_2$
MW: 511.6386g/mol

To a 100 ml three-neck round-bottom flask fitted with a dropping funnel and a thermometer, 0.38 ml (8eq) of 30% H_2O_2 was added dropwise to the mixture of trifluoroacetic anhydride (4.23 ml,15eq) and sulfuric acid (0.25ml) and stirred in a NaCl-ice bath (-15 to -20 °C) so that the temperature was kept below 0°C. The solution was stirred for another 15 min, and 0.5 g (2.1 mmol) of 3,4-dibromothiophene in 5 ml of dichloromethane was added all at once. The reaction mixture was allowed to warm to room temperature with stirring for 3 h. Then the solution was transferred to a 250 ml erlenmeyer flask in a NaCl-ice bath, and 150 ml of saturated sodium carbonate solution was slowly added to bring the pH up to around 7. The solution was extracted with dichloromethane. The organic solutions were combined and dried over $MgSO_4$. Solvents were removed on a rotary evaporator, and the remaining brown-orange solid was washed with 20 ml of ethanol (three times). A gray precipitate was obtained in 42 % yield. **^{1}H NMR** (300 MHz, DMSO-*d*$_6$) δ 7.43 (s, 1H), 5.52 (d, *J* = 3.7 Hz, 1H), 5.04 (dd, *J* = 2.1, 0.5 Hz, 1H), 4.74 (dd, *J* = 3.7, 2.1 Hz, 1H). **^{13}C NMR** (75 MHz, DMSO-*d*$_6$) δ 138.1, 131.4, 121.7, 117.2, 79.9, 72.6, 70.6, 70.4. **HRMS** (EI) m/z: Calc for $C_8H_4Br_4O_2S$ (M+),511.6386; Found 367.7499 (extrusion of SO_2, HBr upon measurement). **IR**: 1148 , 1123, 1052, 1028 cm^{-1} .

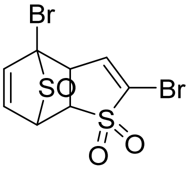
❖ Synthesis of 1-BtSO$_2$



Formula: $C_8H_3Br_3O_2S$
MW= 399.7404

Into a round bottom flask charged stirring bar, 3g of 3,4-dibromothiophene S,S-dioxyde **1-SO$_2$** were dissolved in 40 ml of acetic acid and heated at 170°C for 2 days. Purification using column chromatography with (PE/DCM;1/1) as eluent gave a white powder with 82% (1.8g) yield. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.94 (s, 1H), 7.78 (s, 1H), 6.99 (s, 1H). **^{13}C NMR** (75 MHz, Chloroform-*d*) δ 136.59, 131.26, 131.10, 130.73, 129.55, 128.96, 127.60, 125.84. **HRMS** (EI) m/z: Calc for $C_8H_3Br_3O_2S$ (M+), 399.7404; Found: 399.7402. **Mp**= 200-203°C. IR: 1306 cm^{-1}.

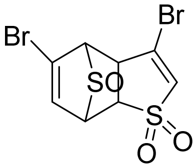
❖ Synthesis of 2-Cymix



Formula: $C_8H_6Br_2O_3S_2$
MW=374.0610 g/mol

To a round bottom flask charged with 0.3g of 2-bromothiophene in 5ml of DCM, 1.58g (3.5eq) of m-CPBA dissolved in 15ml of DCM was added dropwise while stirring the mixture at 0°C. This mixture was allowed to come back to room temperature and was stirred for 17h. The reaction medium is diluted with DCM (15ml) and then washed with 1M $NaHCO_3$ solution, and 1M $NaHSO_3$ solution. The organic phase was dried over $MgSO_4$. The solvent was removed on a rotary evaporator, and purified with SiO_2 column chromatography using PE/DCM (6/4) as eluent to give a pale-yellow color powder with a 70% yield. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 6.73 (dd, *J* = 3.1, 0.7 Hz, 1H), 6.39 (ddd, *J* = 7.0, 5.0, 0.6 Hz, 1H), 6.21 (ddd, *J* = 7.0, 1.6, 0.6 Hz, 1H), 4.67 – 4.60 (m, 1H), 4.31 (dd, *J* = 8.4, 3.0 Hz, 1H), 4.25 (t, *J* = 4.5 Hz, 1H). **^{13}C NMR** (75 MHz, Chloroform-*d*) δ 132.30, 131.55, 128.44, 124.90, 62.09, 61.54, 54.04. **HRMS** (EI) m/z: Calc for $C_8H_6Br_2O_3S_2$ (M+): 371.8125; Found: 371.8122. Mp= 166-168°C. **IR**: 1307, 1133, 1115.80, 1092 cm^{-1}.

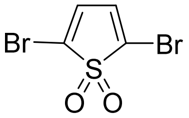
❖ Synthesis of **3-Cymix**



Formula: $C_8H_6Br_2O_3S_2$
MW=374.0610 g/mol

This compound was synthesized using the same procedure than 2-bromothiophene but using 3-bromothiophene. A pale-yellow powder was obtained and isolated with a 70% yield. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 6.77 (dd, *J* = 1.7, 0.6 Hz, 1H), 6.58 (dd, *J* = 4.8, 1.7 Hz, 1H), 4.72 (ddd, *J* = 8.0, 3.9, 1.7 Hz, 1H), 4.56 (ddt, *J* = 8.0, 3.9, 0.5 Hz, 1H), 4.33 (ddd, *J* = 5.1, 3.9, 1.5 Hz, 1H), 4.27 (dt, *J* = 3.9, 1.6 Hz, 1H). **^{13}C NMR** (125 MHz, DMSO-*d*$_6$) δ 135.50, 133.61, 129.62, 115.32, 70.54, 64.81, 64.29, 54.72. **HRMS** (EI) m/z: Calc for $C_8H_6 Br_2O_3 S_2$ (M+): 371.8125; Found: 371.8119. **Mp**= 112-114°C. **IR**: 1298, 1284, 1216, 11249, 1086 cm^{-1}.

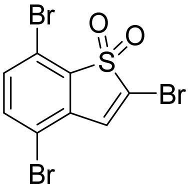
❖ Synthesis of **4-SO$_2$**



Formula: $C_4H_2Br_2O_2S$
MW= 271.8142g/mol

To a 100 ml three-neck round-bottom flask fitted with a dropping funnel and a thermometer, 1.6 ml (35eq) of 30% H_2O_2 was added to the mixture of trifluoroacetic anhydride (4.23 ml,15eq) and sulfuric acid (0.25ml) and stirred in a NaCl-ice bath (-15 to -20 °C) so that the temperature was kept below 0°C. The solution was stirred for another 15 min, and 0.5 g (2.1 mmol) of 2,5-dibromothiophene in 5 ml of acetonitrile was added all at once. The reaction mixture was allowed to warm to room temperature with stirring for 3 h. Then the solution was transferred to a 250 ml erlenmeyer flask in a NaCl-ice bath, and 150 ml of saturated sodium carbonate solution was slowly added to bring the pH up to around 7. The solution was extracted with dichloromethane. The organic phases were combined and dried over $MgSO_4$. Solvents were removed on a rotary evaporator, to give a white-pale yellow powder with a yield of 69%. **^{1}H NMR** (300 MHz, Chloroform-*d*) 6.87 (s, 1H).

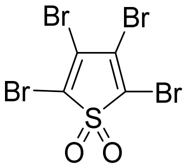
❖ Synthesis of **4-BtSO$_2$**



Formula: $C_8H_3Br_3O_2S$
MW= 399.7404

Into a round bottom flask charged with stirring bar, 0.45g of 2,5-dibromothiophene was dissolved in 20 ml of acetic acid and heated at 170°C for 2 days and followed by TLC. Purification using column chromatography with (PE/DCM;1/1) as eluent gave a white powder (260 mg, 77%). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.6 Hz, 1H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.37 (s, 1H). **^{13}C NMR** (76 MHz, Chloroform-*d*) δ 138.11, 136.64, 134.89, 133.97, 128.28, 125.15, 118.15, 116.14. **HRMS** (EI) m/z: Calc for $C_8H_3 Br_3O_2S$ (M+),399.7404; Found :399.7402. **Mp**= 175-177°C. **IR**: 1315, 1149.59 cm^{-1}.

Synthesis of 5-SO_2



Formula: $C_4Br_4O_2S$
MW= 427.6353g/mol

To a 100 ml three-neck round-bottom flask fitted with a dropping funnel and a thermometer, 2ml (35eq) of 30% H_2O_2 were added dropwise to a mixture of trifluoroacetic anhydride (5.2ml,15eq) and sulfuric acid (1ml) and stirred in a NaCl-ice bath (-15 to -20 °C) so that the temperature was kept below 0°C. The solution was stirred for another 15 min, and 1 g (2.5mmol) of 2,3,4,5-tetrabromothiophene in 5 ml of dichloromethane was added all at once. The reaction mixture was allowed to warm to room temperature with stirring for 3 h. Then the solution was transferred to a 250 ml erlenmeyer flask in a NaCl-ice bath, and 150 ml of saturated sodium carbonate solution was slowly added to bring the pH up to around 7. The solution was extracted with dichloromethane. The organic phases were combined and dried over $MgSO_4$. Solvents were removed on a rotary evaporator, to give a gray-brown powder with a yield of 80%. **HRMS** (EI) m/z: Calc for $C_4Br_4O_2S$ (M+): 427.6353; Found: 427.6345. **^{13}C NMR** (76 MHz, Chloroform-*d*) δ 128.55, 120.49. Mp=198-200°C

NMR Spectra of synthesized compounds

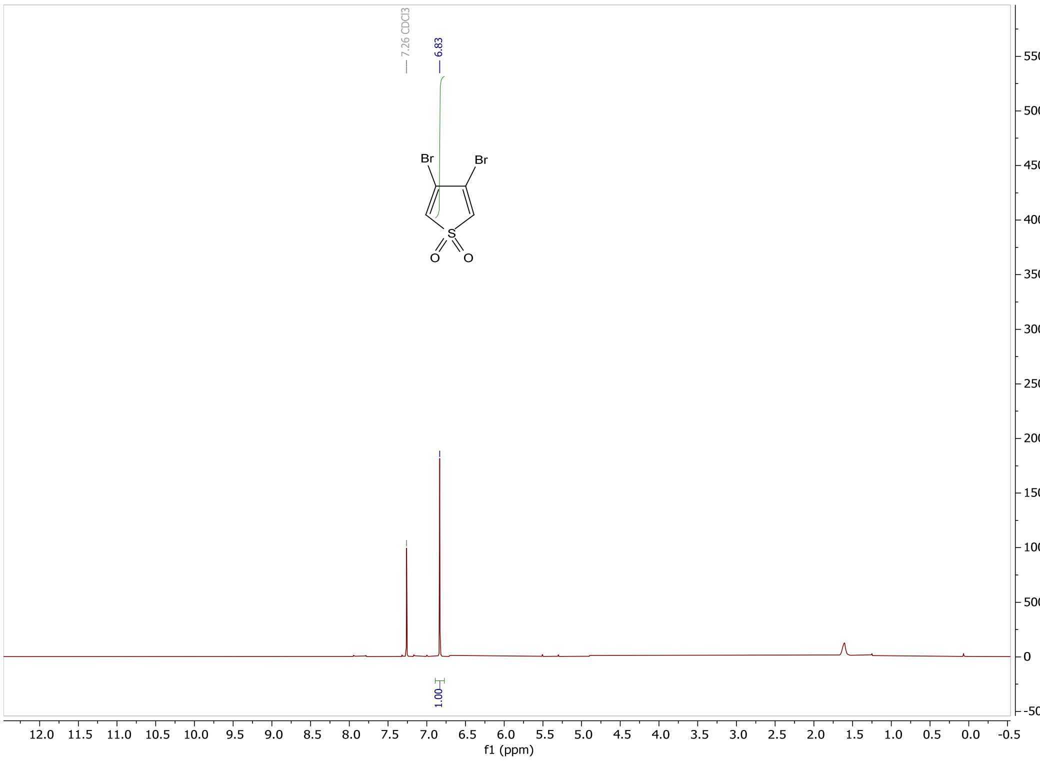


*Figure S 1 : ^{1}H NMR spectrum of **1-SO$_2$***

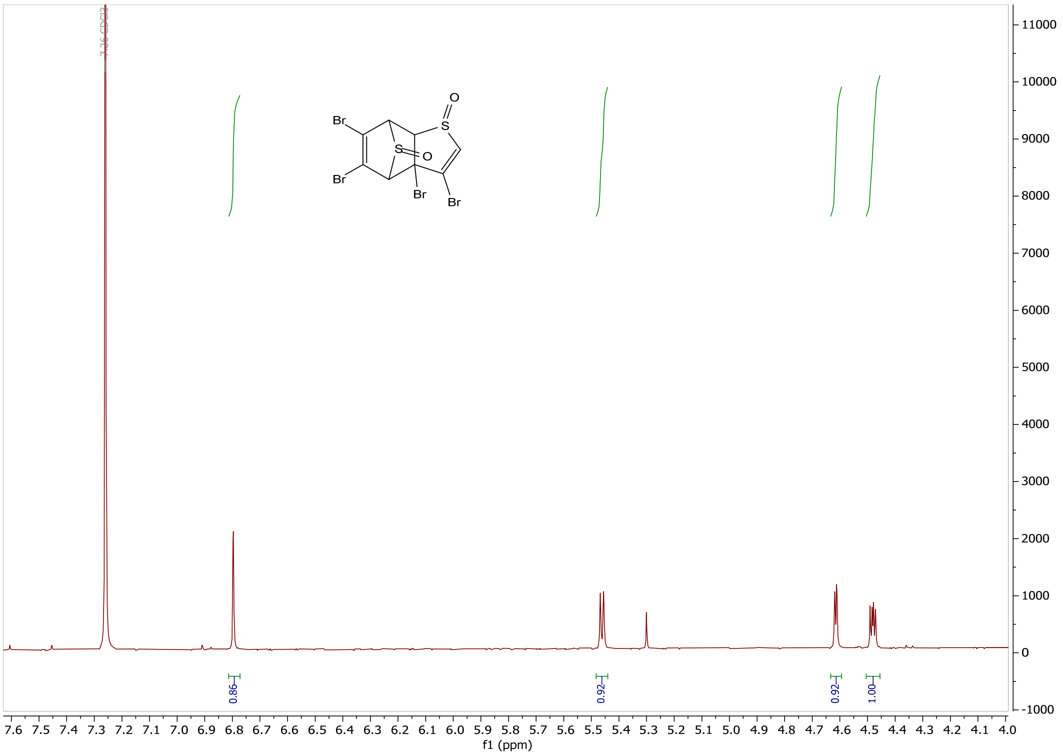


*Figure S 2 : ^{1}H NMR spectrum of **1-CySO***

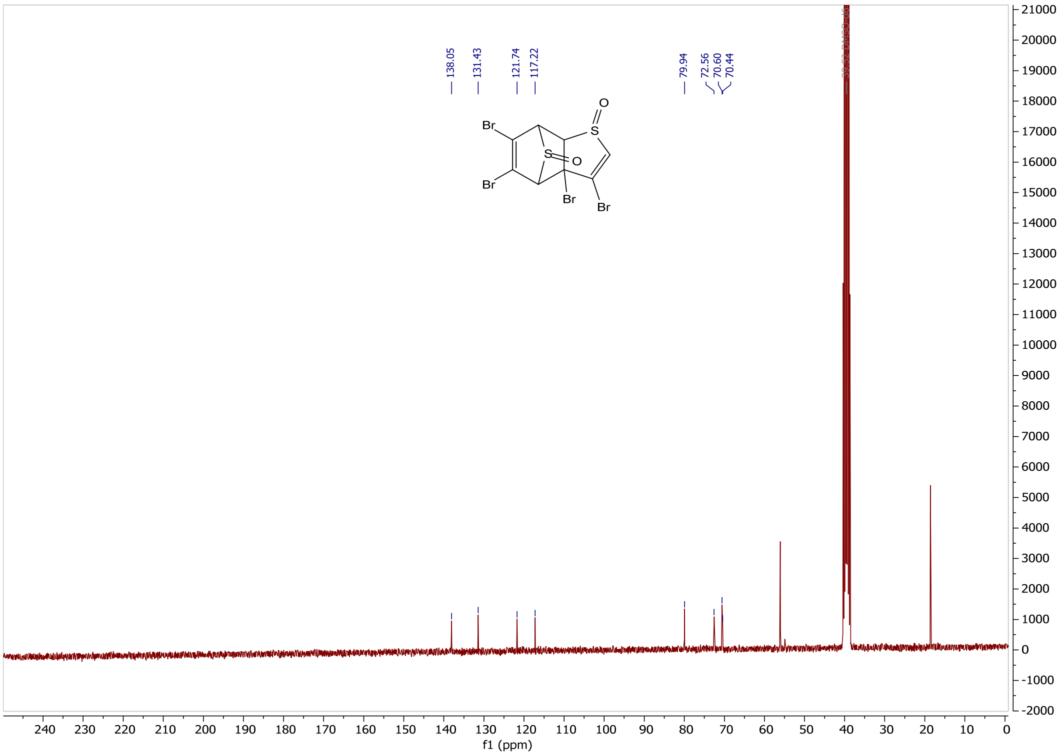


Figure S 3: ^{13}C NMR spectrum of ***1-CySO***

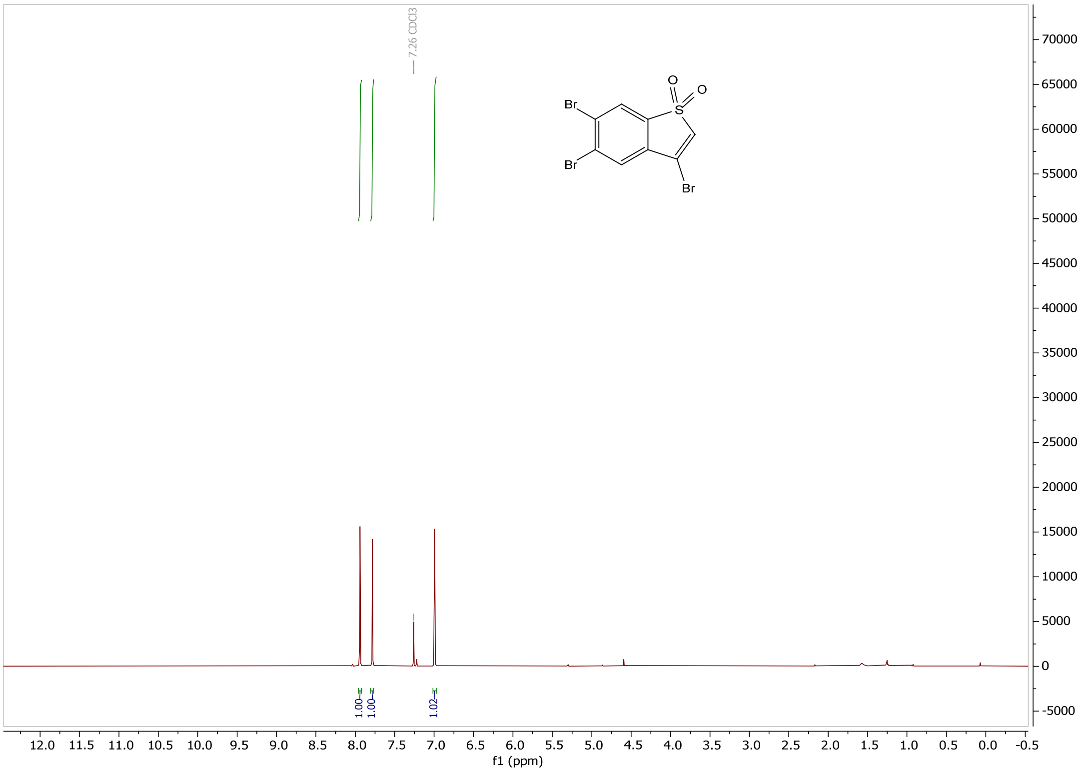


*Figure S 4: ^{1}H NMR spectrum of **1-BtSO$_2$***

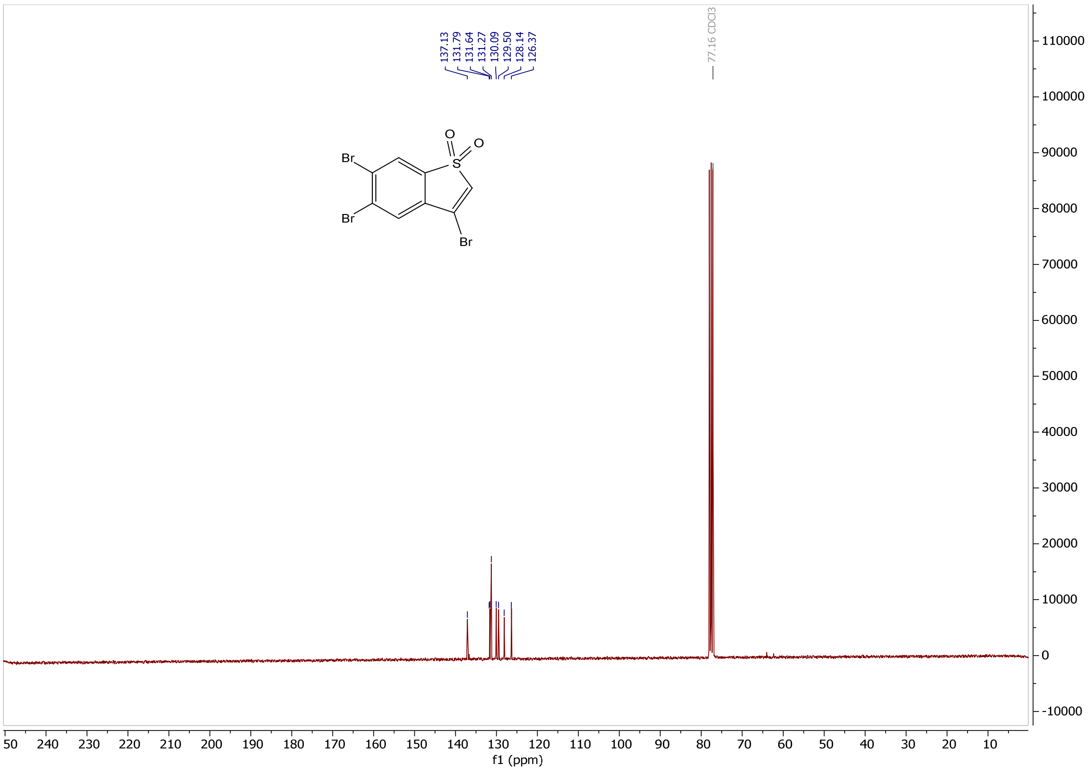


*Figure S 5: ^{13}C NMR spectrum of **1-BtSO$_2$***

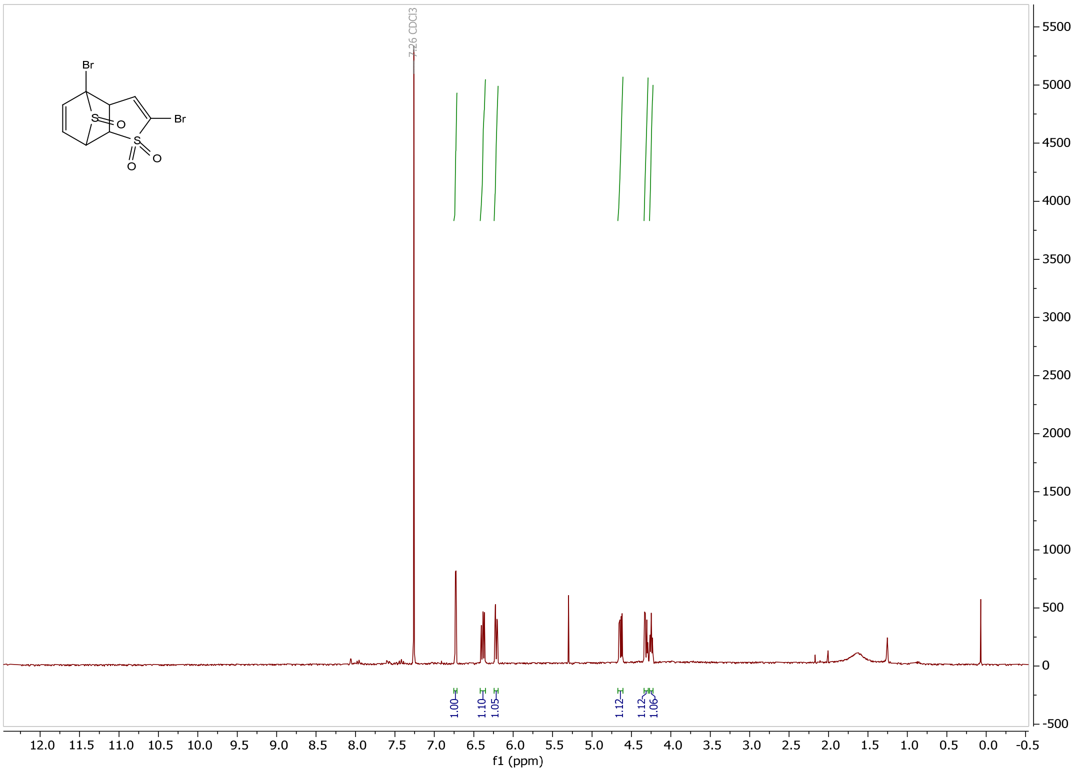


*Figure S 6: ^{1}H NMR spectrum of **2-Cymix***

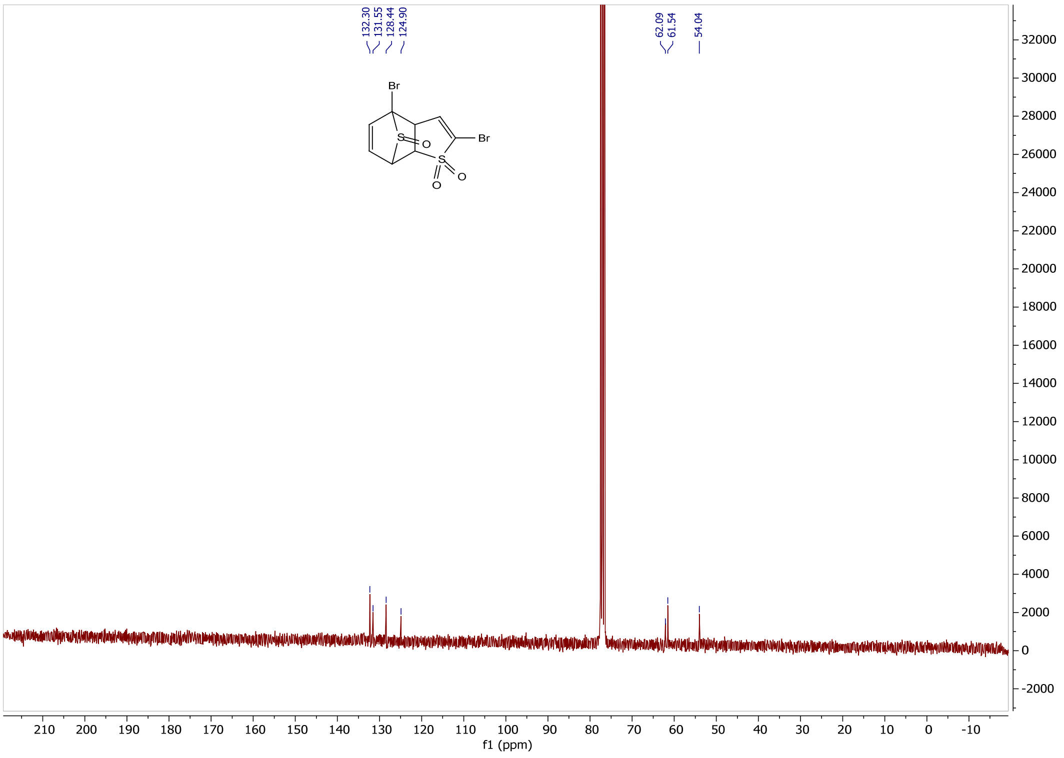


*Figure S 7: ^{13}C NMR spectrum of **2-Cymix***

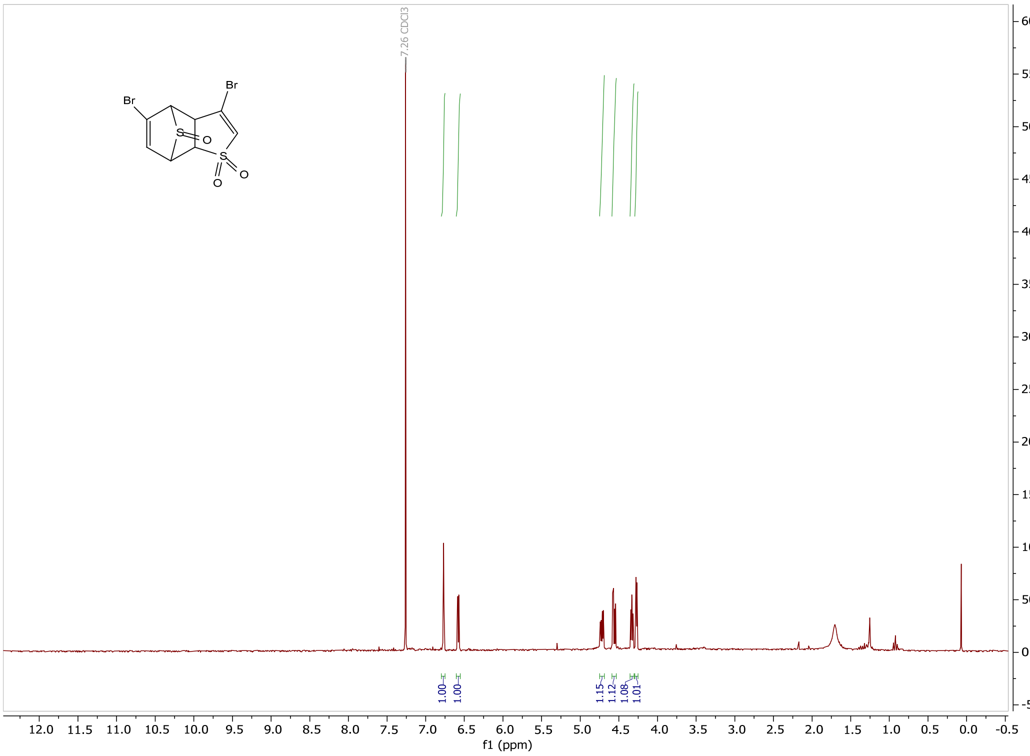


*Figure S 8: ^{1}H NMR spectrum of **3-Cymix***

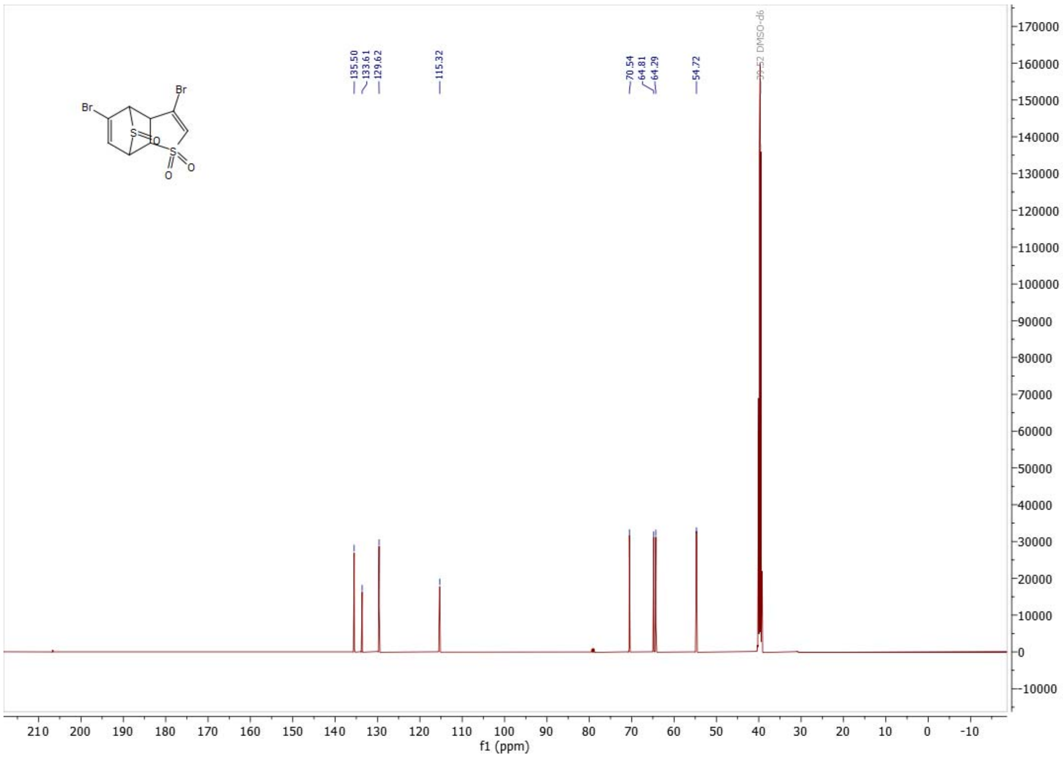


*Figure S 9: ^{13}C NMR spectrum of **3-Cymix***

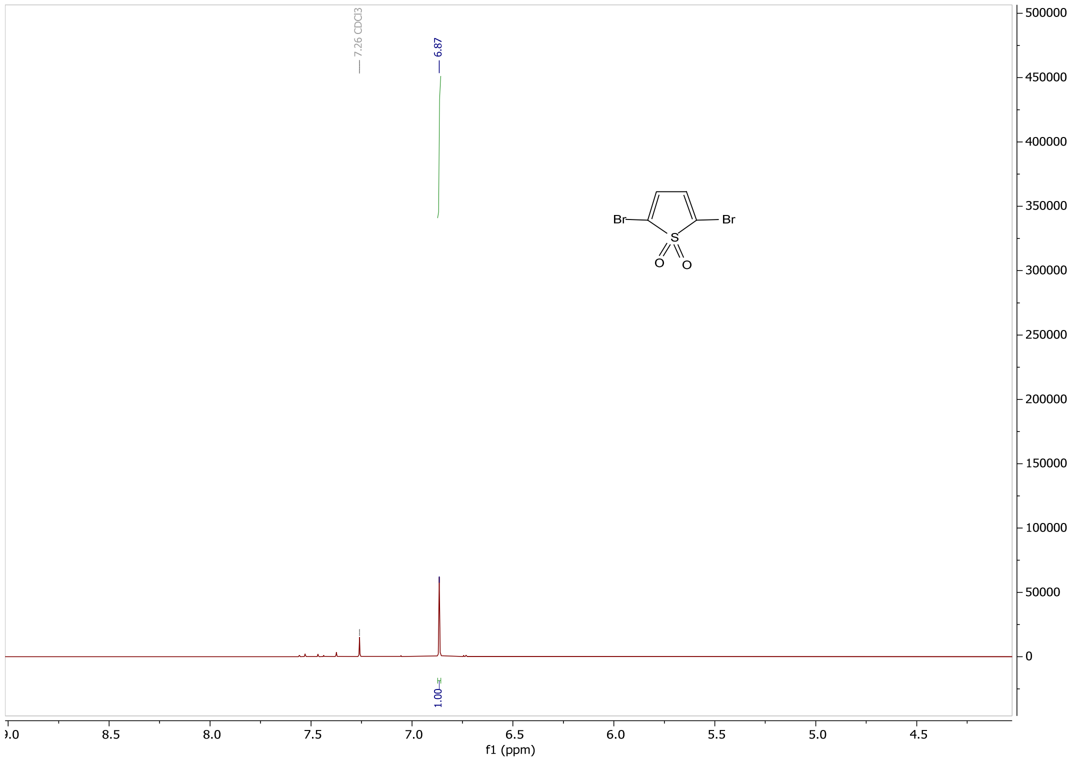


*Figure S 10 : ^{1}H NMR spectrum of **4-SO$_2$***

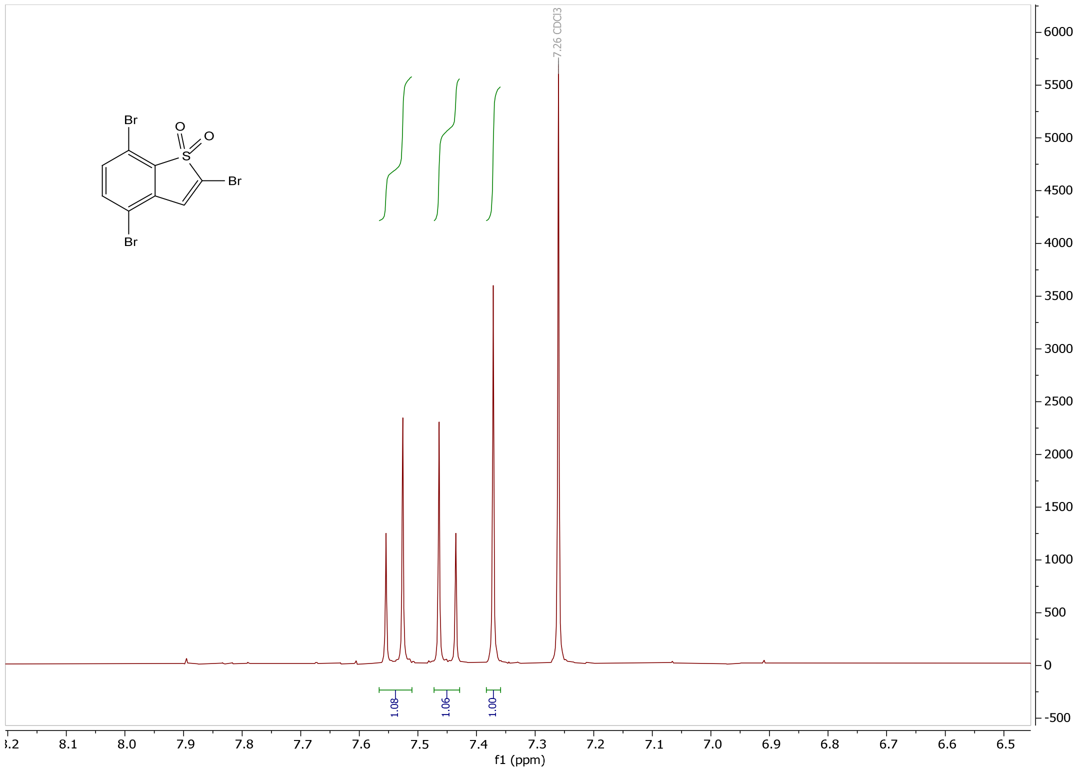


*Figure S 11: ^{1}H NMR spectrum of **4-BtSO$_2$***

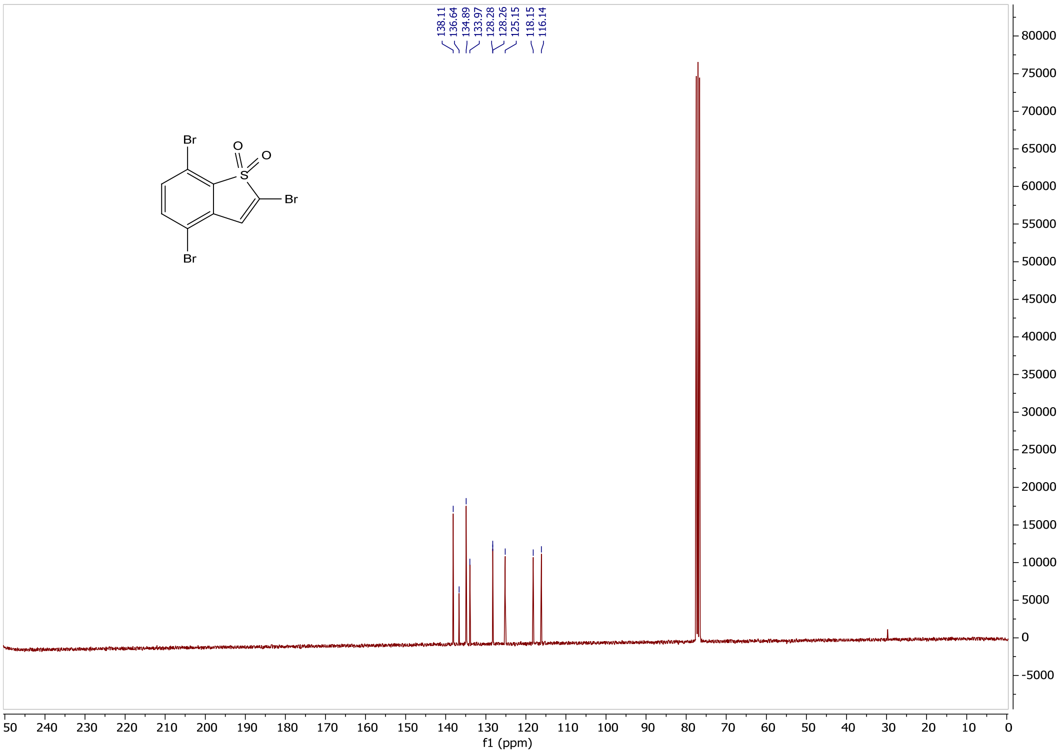


Figure S 12: ^{13}C NMR spectrum of ***4-BtSO$_2$***

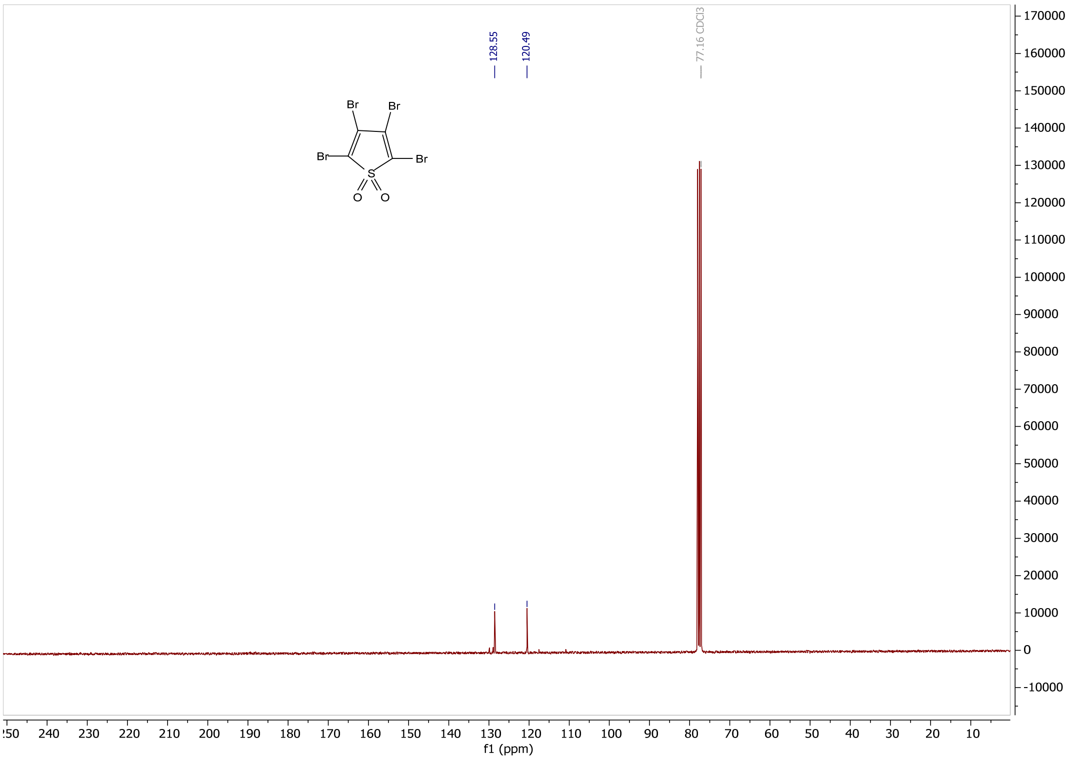


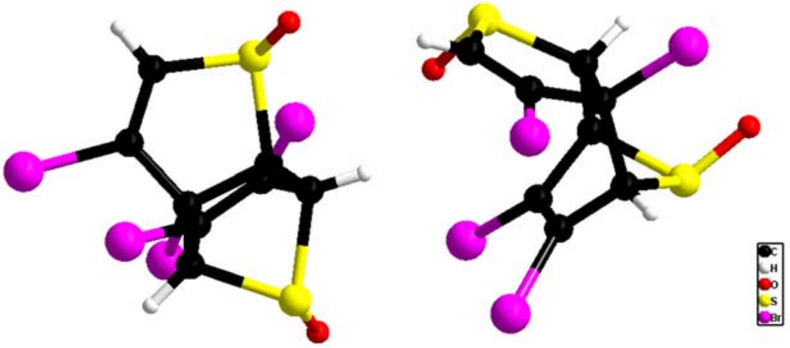
Figure S 13: ^{13}C NMR spectrum of ***5-SO$_2$***

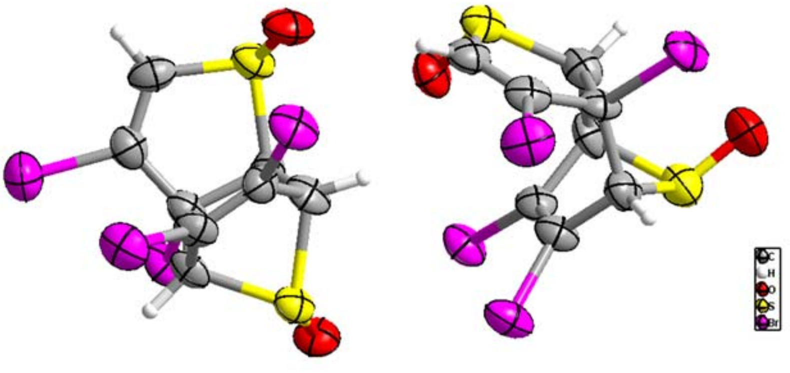
X-ray structures

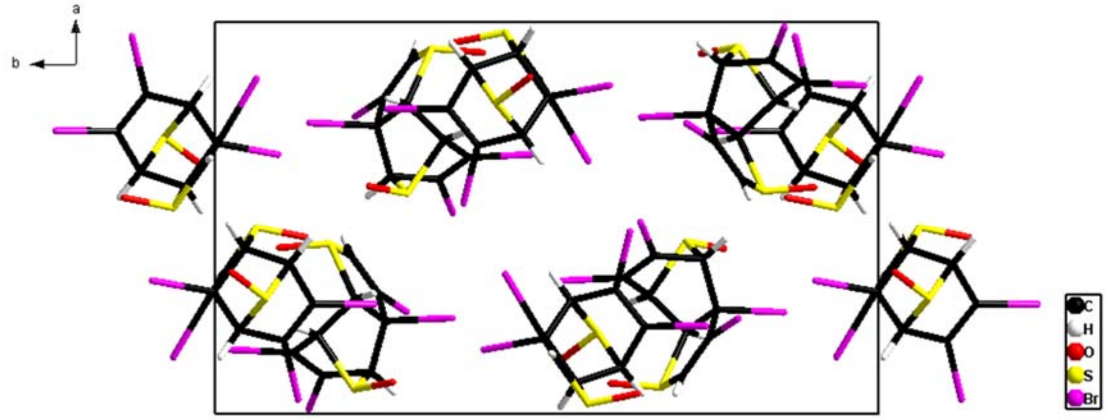
X-ray single-crystal diffraction data were collected at 293K on a BRUKER-NONIUS KappaCCD diffractometer equipped with a graphite monochromator utilizing MoKα radiation(λ = 0.71073Å). The structures were solved by direct methods using SIR92 (Altomare et al.,1993) and the two refinements were performed on F^2 by full matrix least-squares techniques using SHELX-97 package (G.M. Sheldrick, 1998). All non-H atoms were refined anisotropically and the H atoms were included in the calculation without refinement. Absorption was corrected by Sadabs program (Sheldrick, Bruker, 2000).

X-ray structure of **1-CySO**

Colorless plate (0.150 x 0.092 x 0.021 mm); C8 H4 Br4 O2 S2; Monoclinic, P 21/n; a = 11.4291(6) Å b = 19.1658(7) Å c = 11.4923(7) Å . Volume 2495.0(2) Å ^{3} ; Z 8 Calculated density 2.747 g/cm^3; Absorption coefficient 18.748 mm^{-1}; F(000)1920; Theta range for data collection from 4.516 to 78.446 deg. Limiting indices -13<=h<=14, -23<=k<=20, -14<=l<=12; Reflections collected / unique 14452 / 4919 [R(int) = 0.0940]; Completeness to theta = 68.000 98.0 %; Max. and min. transmission 1.00000 and 0.68195; Refinement method Full-matrix least-squares on F^2; Data / restraints / parameters 4919 / 0 / 290; Goodness-of-fit on F^2 1.070; Final R indices [I>2sigma(I)] R1 = 0.0692, wR2 = 0.1875 [3211 Fo]; R indices (all data) R1 = 0.1024, wR2 = 0.2105; Extinction coefficient 0.00074(10); Largest diff. peak and hole 1.018 and -1.323 e. Å $^{-3}$.

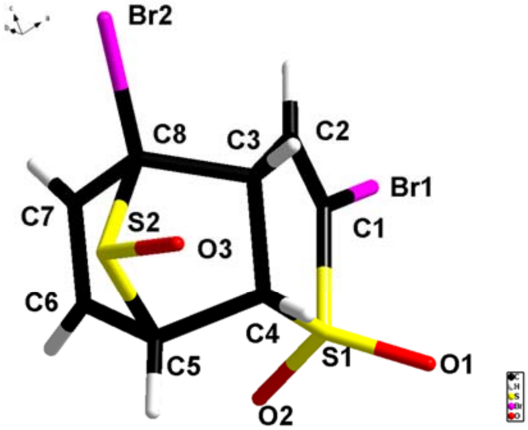


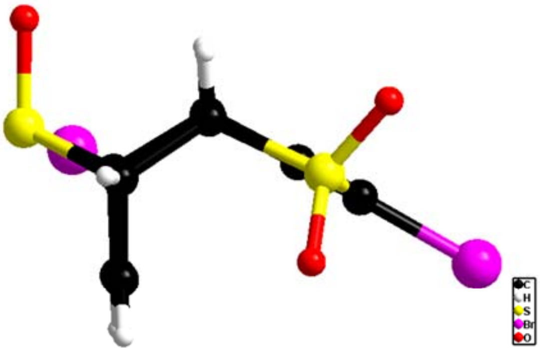


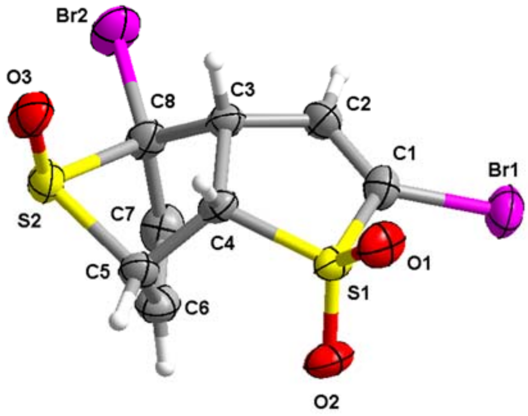


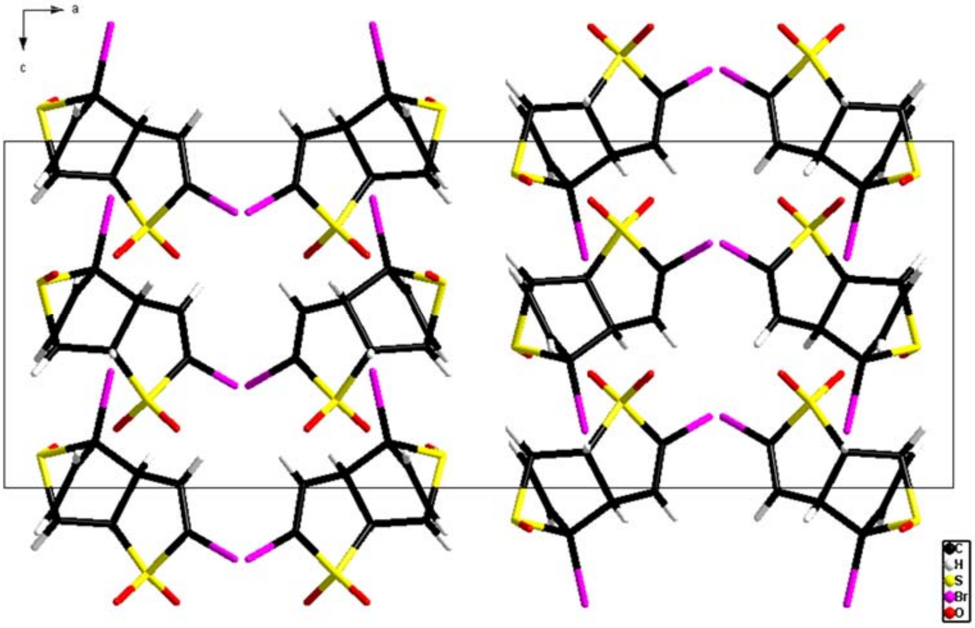
X-ray structure of **2-Cymix**

Colorless plate (0.237 x 0.151 x 0.038 mm); Orthorhombic, P b c n; a = 25.0891(6) Å b = 9.7366(2) Å c = 9.1903(2) Å. Volume 2245.03(9) Å ^{3}; Z 8; Calculated density 2.213 mg/cm^3; Absorption coefficient 12.534 mm^{-1}; F(000) 1440; Theta range for data collection from 3.523 to 76.203 deg.; Limiting indices -30<=h<=31, -10<=k<=12, -9<=l<=11 ; Reflections collected / unique 6496 / 2255 [R(int) = 0.0305]; Completeness to theta = 70.000 98.0 %; Max. and min. transmission 1.00000 and 0.35601; Refinement method Full-matrix least-squares on F^2; Data / restraints / parameters 2255 / 0 / 136 Goodness-of-fit on F^2 1.040; Final R indices [I>2sigma(I)] R1 = 0.0307, wR2 = 0.0782 [2063 Fo]; R indices (all data) R1 = 0.0340, wR2 = 0.0807; Largest diff. peak and hole 0.556 and -0.450 e.Å^{-3}.



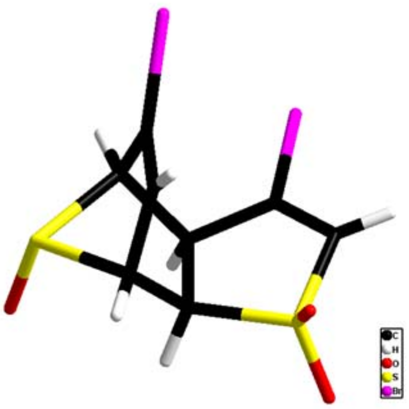


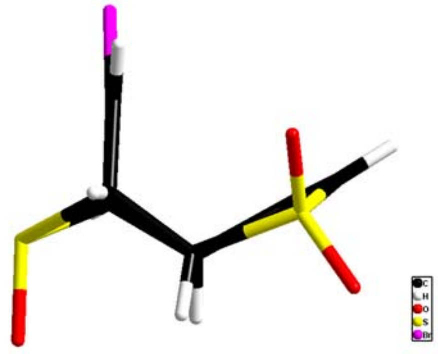


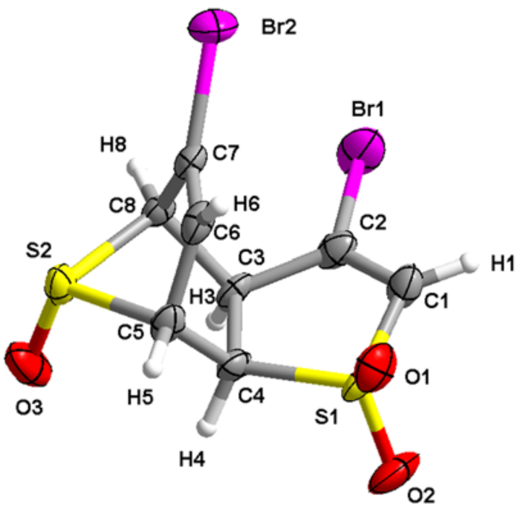


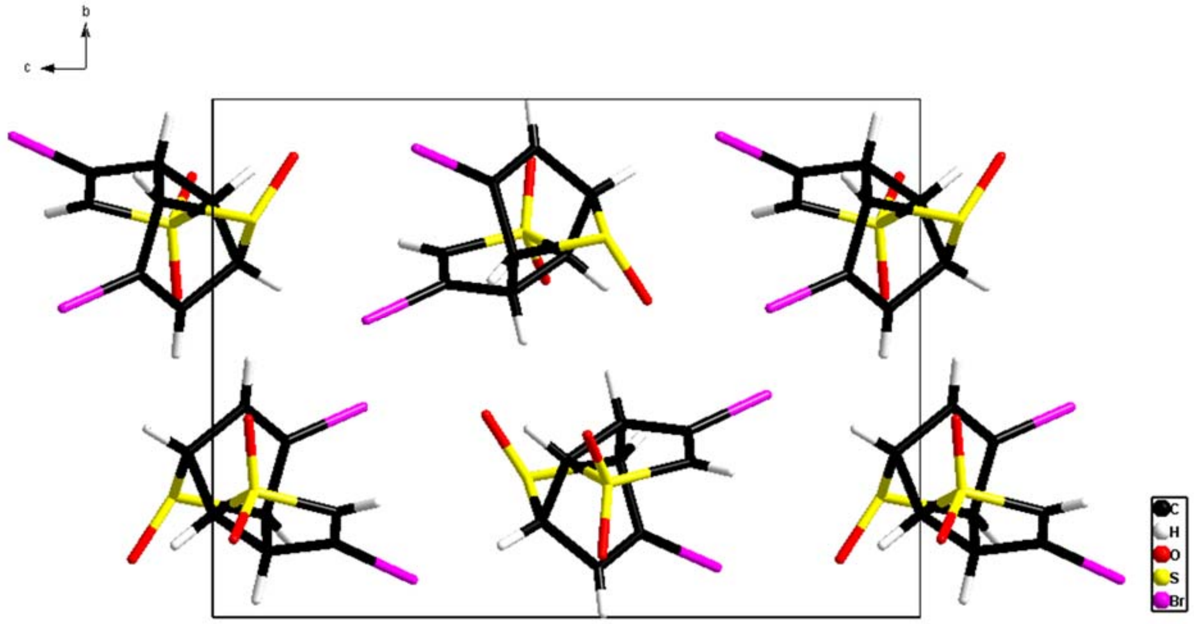
X-ray structure of **3-Cymix**

Colorless prism (0.313 x 0.298 x 0.157 mm); Monoclinic, P 21/n; Unit cell dimensions a = 7.8922(6) Å b = 10.1295(7) Å c= 14.0460(10) A; Volume 1107.29(14) $Å^3$; Z 4; Calculated density 2.244 g/cm^3; Absorption coefficient 12.707 mm^{-1};F(000) 720; Theta range for data collection from 5.410 to 76.168 deg; Limiting indices -9<=h<=9, -11<=k<=12, -17<=l<=16; Reflections collected / unique 4877 / 2246 [R(int) = 0.0443]; Completeness to theta = 74.000 98.2 %; Max. and min. transmission 1.00000 and 0.44962; Refinement method Full-matrix least-squares on F^2;Data / restraints / parameters 2246 / 0 / 136; Goodness-of-fit on F^2 1.058; Final R indices [I>2sigma(I)] R1 = 0.0452, wR2 = 0.1210 [2043 Fo]; R indices (all data) R1 = 0.0489, wR2 = 0.1261;Largest diff. peak and hole 0.686 and -1.274 e. $Å^{-3}$.






Br2
Br1
H8
C7
H6
C8
C6
C2
S2
C3
H1
H3
C1
C5
O1
O3
H5
C4
S1
H4
O2


b
c
C
H
O
S
Br

B- Theoretical Calculations

Computational details.

All calculated compounds have been optimized in gas phase by a DFT method with the B3LYP[1] hybrid functional since it is very reliable for geometry and thermochemistry and the 6–311G(2d,p) basis set. The Gaussian 09 software (revision D.01) has been used.[2] Normal modes frequencies have then been calculated to control the geometry as a minimum. The molecular orbitals pictures have been automatically generated by a homemade Python program, quchemreport, based on cclib.[34]

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[1] A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.

[2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian~09 Revision D.01*.

[3] N. M. O'boyle, A. L. Tenderholt and K. M. Langner, *J. Comput. Chem.*, 2008, **29**, 839–845.

[4] T. Cauchy and B. Da Mota, quchemreport. A python program for control quality and automatic generation of quantum chemistry results 2020.

1- 3,4-Dibromothiophene 1

a.Description

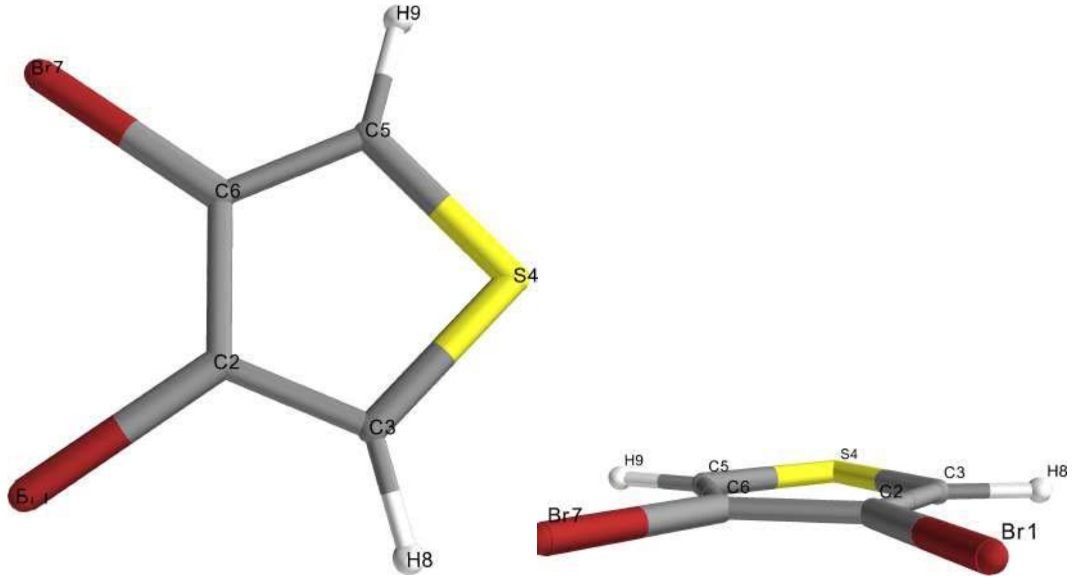

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1
Formula	C4H2Br2S
Charge	0
Spin multiplicity	1
Monoisotopic mass	239.82440 Da
InChI	1S/C4H2Br2S/c5-3-1-7-2-4(3)6/h1-2H
SMILES	Brc1cscc1Br

b. Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	233	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000153	0.000450
RMS Force value and threshold	0.000046	0.000300
Max Displacement value and threshold	0.000543	0.001800
RMS Displacement value and threshold	0.000240	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	

Anharmonic effects	None	
Anharmonic effects	None	

Job type: Time-dependent calculation

Number of calculated excited states and spin state	15	['Singlet-A']

c. Results

Total molecular energy	-5700.14795 hartrees
HOMO number	56
LUMO+1 energies	-0.92 eV
LUMO energies	-1.14 eV
HOMO energies	-6.91 eV
HOMO-1 energies	-6.95 eV

CDFT indices: Electron Affinity	-0.0010 hartrees
CDFT indices: Ionisation Potential	0.0119 hartrees
CDFT indices: Electronegativity	0.0054 hartrees
CDFT indices: Hardness	0.0129 hartrees
CDFT indices: Electrophilicity	0.0011
CDFT indices: Electron-flow	0.4202 e-

Geometry optimization specific results	
Converged nuclear repulsion energy	842.69185 Hartrees

Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-5700.09353 Hartrees
Gibbs free energy at 298.15 K	-5700.13530 Hartrees
Entropy at 298.15 K	0.00014 Hartrees

Mean Mulliken atomic charge and standard deviation	-0.0000 e-	0.0930 e-
Atoms with negatives charges under the standard deviation	NÂ°	Mulliken charge
	C 2	-0.116
	C 6	-0.116
Atoms with positives charges over the standard deviation	NÂ°	Mulliken charge
	H 8	+0.095
	H 9	+0.095
	S 4	+0.138

Table. Selection of the most important condensed Fukui functions based on Mulliken charges.

Atom	atomic dual descriptor (f+ - f-)	atomic electrophilicity f+	atomic nucleophilicity f-
Br 1	-0.06	0.18	0.24
Br 7	-0.06	0.18	0.24
S 4	0.10	0.26	0.16

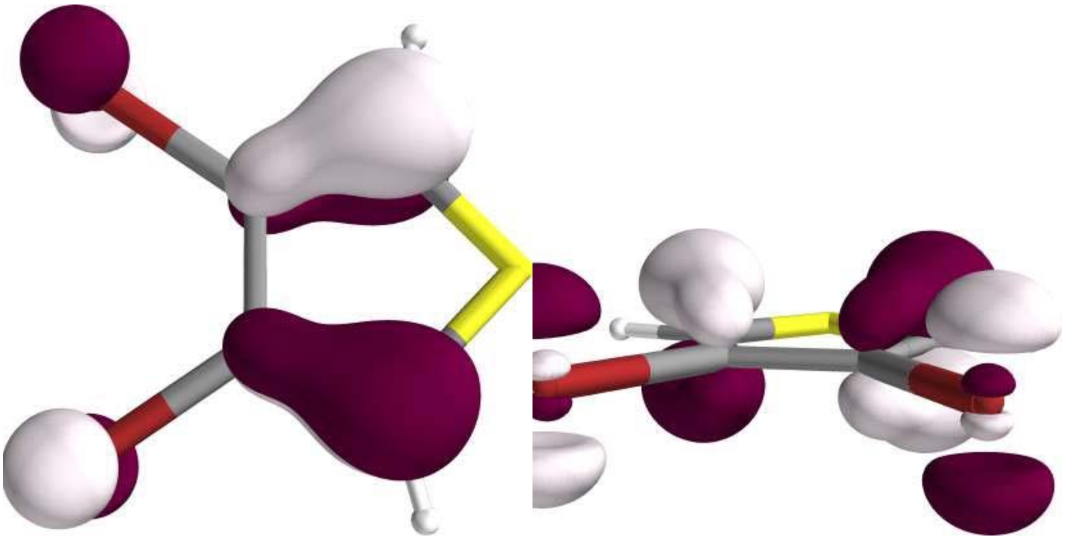

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
919	52	A
797	58	A

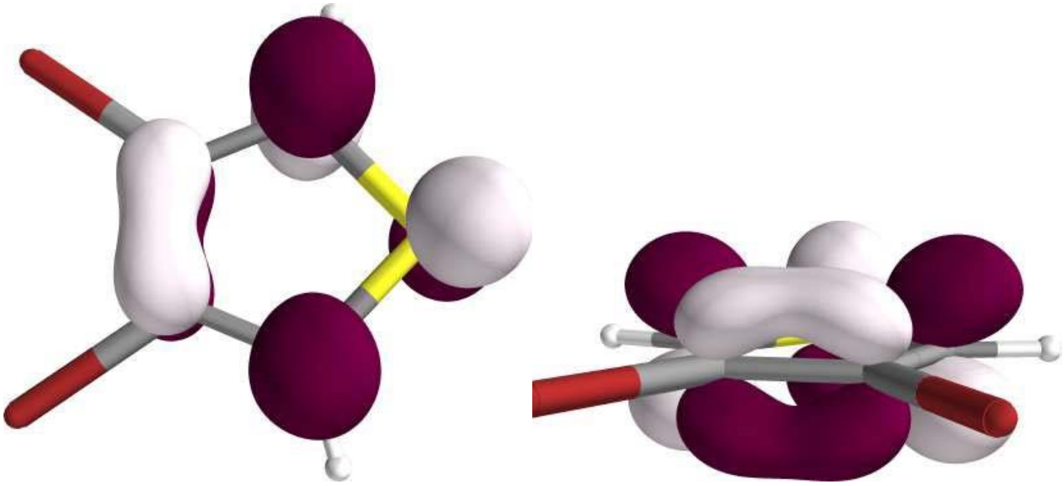

Figure 3: Representation of the LUMO from two points of view.

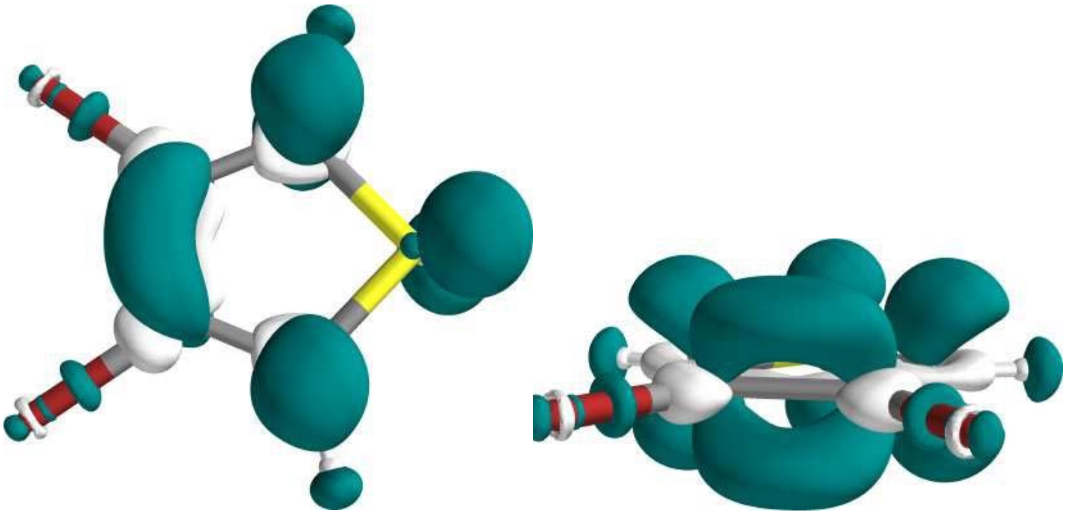

Figure 4: Representation of the F+ function from two points of view. The Blue color indicate the most electrophilic regions.

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	*f*	R	Λ	d$_{CT}$	q$_{CT}$	Excitation description : initial OM - end-ing OM (% if 5%)
1	Singlet-A	253	39401	0.000	0.0	0.49	139.81	0.73	56-58(96);
2	Singlet-A	250	39985	0.000	0.0	0.60	127.62	0.65	55-58(96);
3	Singlet-A	237	42144	0.107	0.0	0.65	175.57	0.52	55-57(91); 56-60(6);
4	Singlet-A	231	43177	0.000	0.0	0.53	86.91	0.70	56-59(96);
5	Singlet-A	230	43330	0.000	0.0	0.55	118.72	0.67	55-59(95);
6	Singlet-A	228	43738	0.017	0.0	0.75	196.69	0.39	56-57(96);
7	Singlet-A	207	48181	0.000	0.0	0.22	281.60	0.93	54-57(99);
8	Singlet-A	206	48523	0.001	0.0	0.55	111.95	0.69	54-58(96);
9	Singlet-A	195	51216	0.002	0.0	0.31	280.92	0.87	53-57(98);
10	Singlet-A	194	51442	0.003	0.0	0.55	158.40	0.68	53-58(71); 54-59(24);
11	Singlet-A	185	53990	0.003	0.0	0.49	19.71	0.70	56-61(93);
12	Singlet-A	184	54101	0.000	0.0	0.55	23.97	0.65	51-59(6); 52-58(13); 55-61(78);
13	Singlet-A	184	54252	0.001	0.0	0.49	251.82	0.73	53-58(26); 54-59(67);
14	Singlet-A	179	55811	0.107	0.0	0.65	37.78	0.55	55-60(89);
15	Singlet-A	178	56141	0.000	0.0	0.58	31.54	0.63	52-58(83); 55-61(14);

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
Br	1.0984	1.7867	0.0000
C	-0.4651	0.7138	0.0000
C	-1.7179	1.2402	0.0000
S	-2.9183	-0.0000	-0.0000
C	-1.7179	-1.2402	0.0000
C	-0.4651	-0.7138	0.0000
Br	1.0984	-1.7867	0.0000
H	-1.9980	2.2798	0.0000
H	-1.9980	-2.2798	0.0000

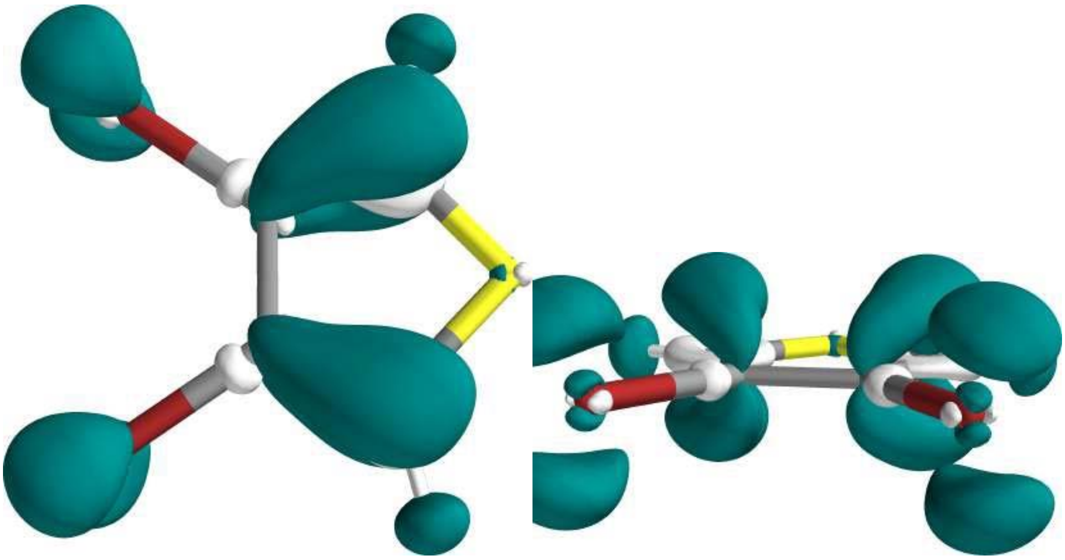

Figure 5: Representation of the F- function from two points of view. The Blue color indicate the most nucleophilic regions.

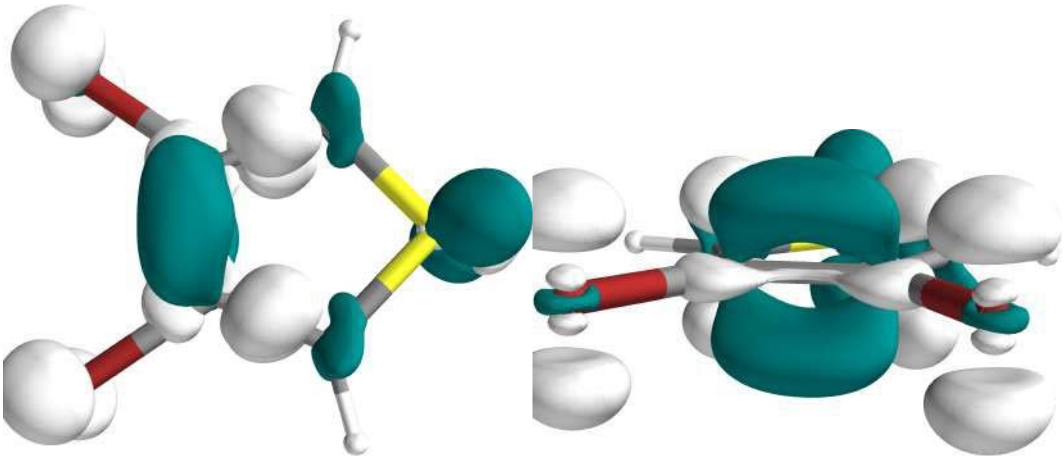

Figure 6: Representation of the Dual descriptor from two points of view. Electrophilic and nucleophilic regions correspond to blue and white surfaces.

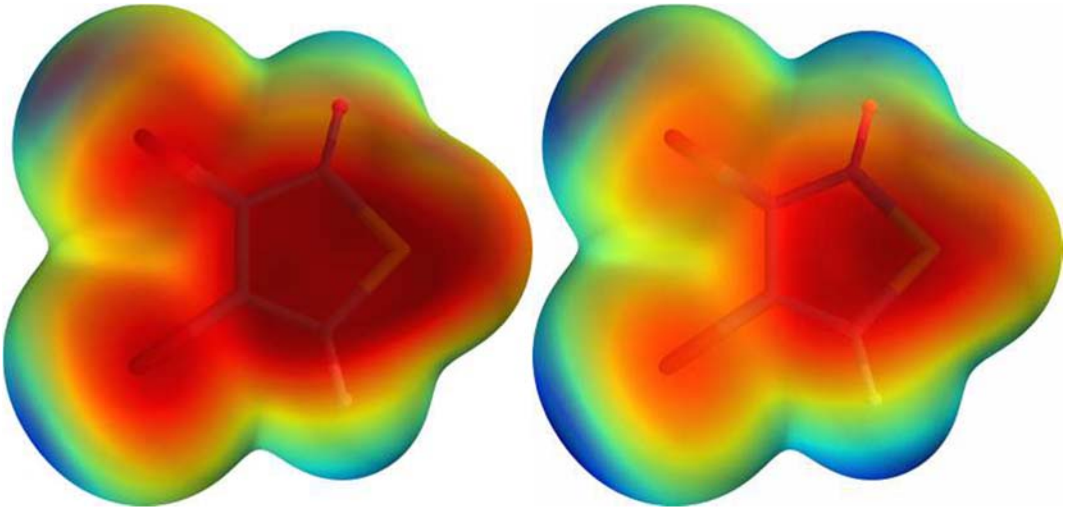

Figure 7: Representations of the Molecular Electrostatic Potential mapped on the electron density (cutoff value of

0.002 e-/bohr3). On the left, red, blue and green regions correspond to negative values < -0.06 a.u., positive values >

0.08 a.u. and neutral values respectively. On the right, the scale is set automatically to highlight the minimum values in red and the maximum values in blues.

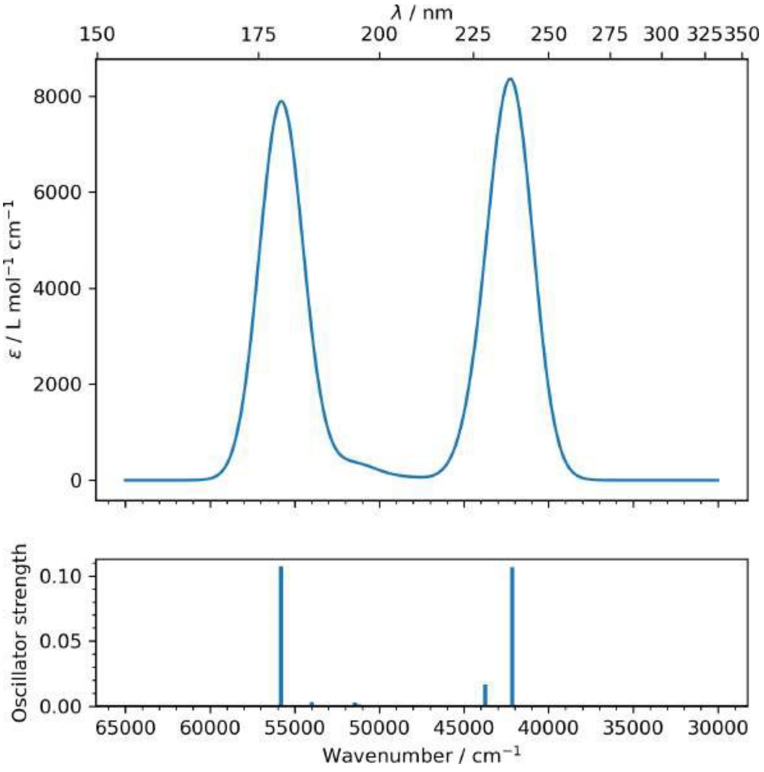

Figure 8: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

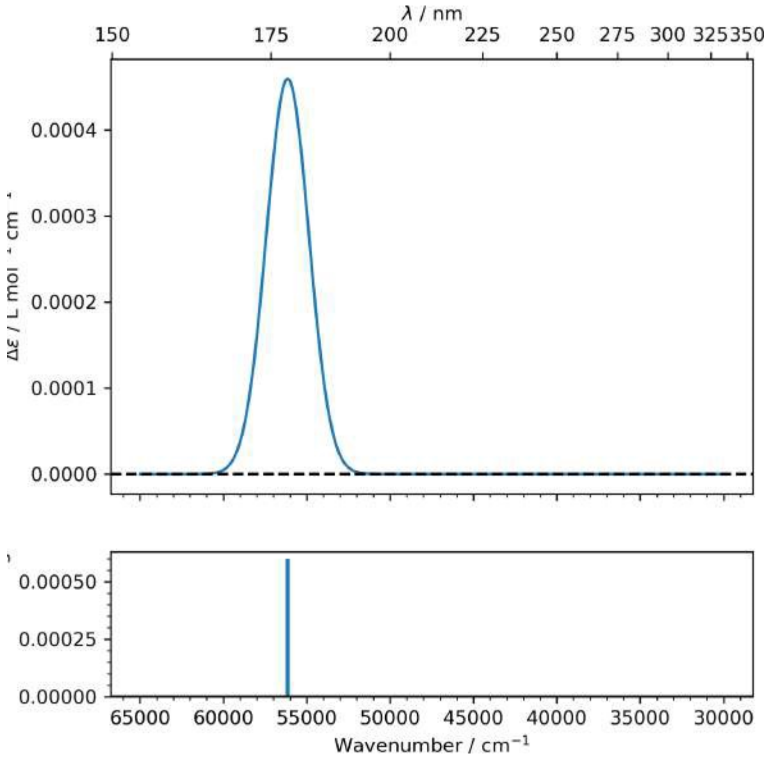

Figure 9: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

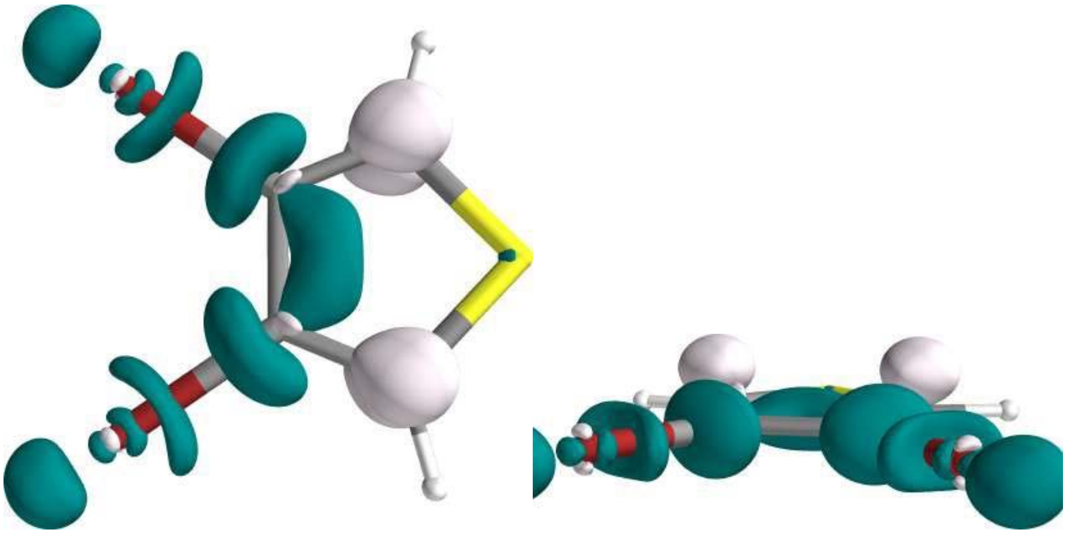

Figure 10: Representation of the Electron Density Difference (S1-S0) from two points of view.

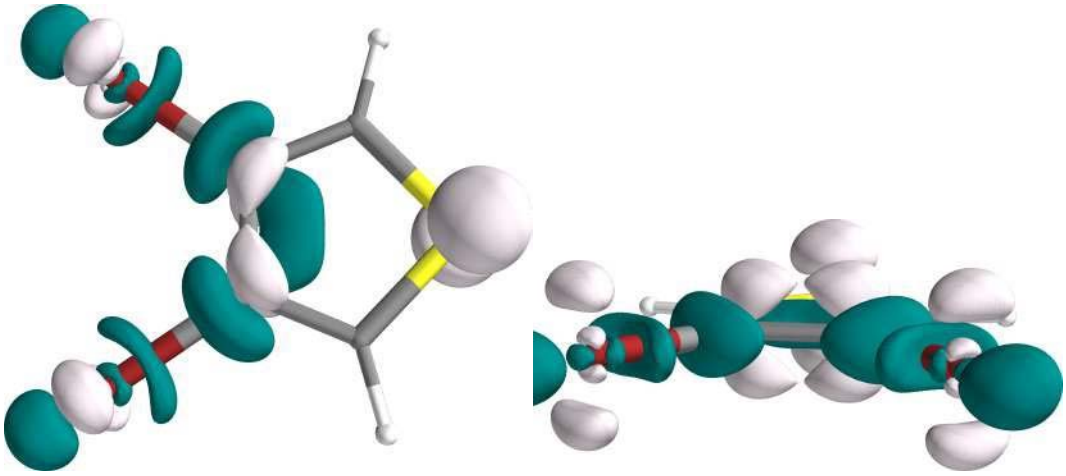

Figure 11: Representation of the Electron Density Difference (S2-S0) from two points of view.

2- 3,4-dibromothiophene sulfoxide 1-SO

a. Description

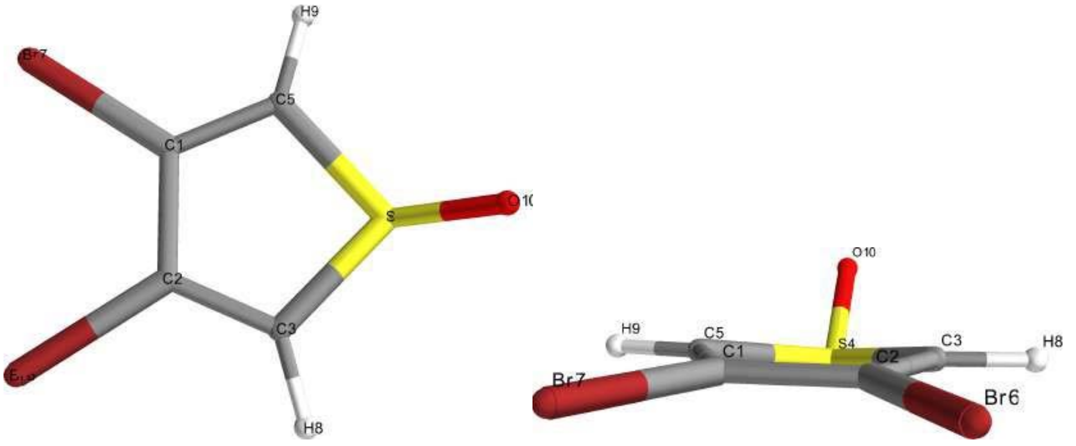

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-SO
Formula	C4H2Br2OS
Charge	0
Spin multiplicity	1
Monoisotopic mass	255.81931 Da
InChI	1S/C4H2Br2OS/c5-3-1-8(7)2-4(3)6/h1-2H
SMILES	c1(c(cs(=O)c1)Br)Br

b. Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	256	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization		
Max Force value and threshold	0.000104	0.000450
RMS Force value and threshold	0.000033	0.000300
Max Displacement value and threshold	0.001386	0.001800
RMS Displacement value and threshold	0.000477	0.001200

Job type: Frequency and thermochemical analysis	
Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

Job type: Time-dependent calculation		
Number of calculated excited states and spin state	15	['Singlet-A']

c. Results

Total molecular energy	-5775.32020 hartrees
HOMO number	60
LUMO+1 energies	-1.35 eV
LUMO energies	-2.67 eV
HOMO energies	-6.97 eV
HOMO-1 energies	-7.28 eV

CDFT indices: Electron Affinity	0.0011 hartrees

CDFT indices: Ionisation Potential	0.0121 hartrees
CDFT indices: Electronegativity	0.0066 hartrees
CDFT indices: Hardness	0.0111 hartrees
CDFT indices: Electrophilicity	0.0020
CDFT indices: Electron-flow	0.5977 e-

Geometry optimization specific results	
Converged nuclear repulsion energy	974.68476 Hartrees

Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-5775.26175 Hartrees
Gibbs free energy at 298.15 K	-5775.30658 Hartrees
Entropy at 298.15 K	0.00015 Hartrees

Mean Mulliken atomic charge and standard deviation	0.0000 e-	0.2971 e-
Atoms with negatives charges under the standard deviation	NÂ°	Mulliken charge
	O 10	-0.621
Atoms with positives charges over the standard deviation	NÂ°	Mulliken charge
	S 4	+0.659

Table. Selection of the most important condensed Fukui functions based on Mulliken charges.

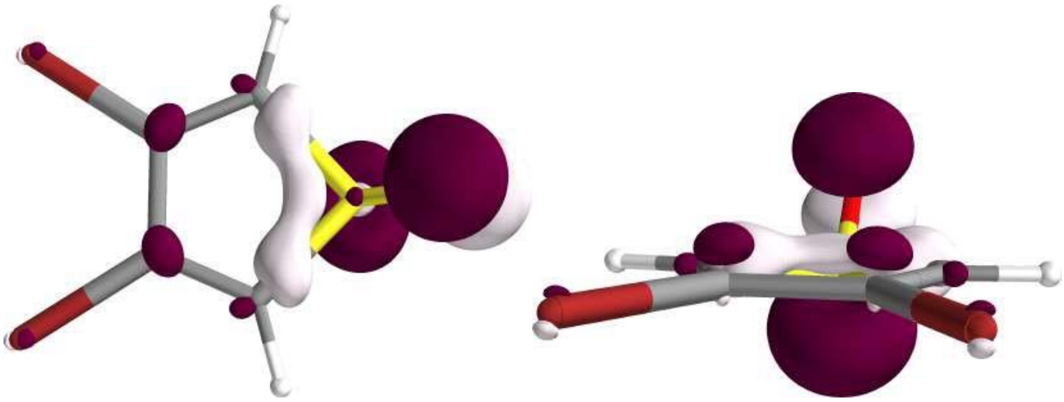

Figure 2: Representation of the HOMO from two points of view.

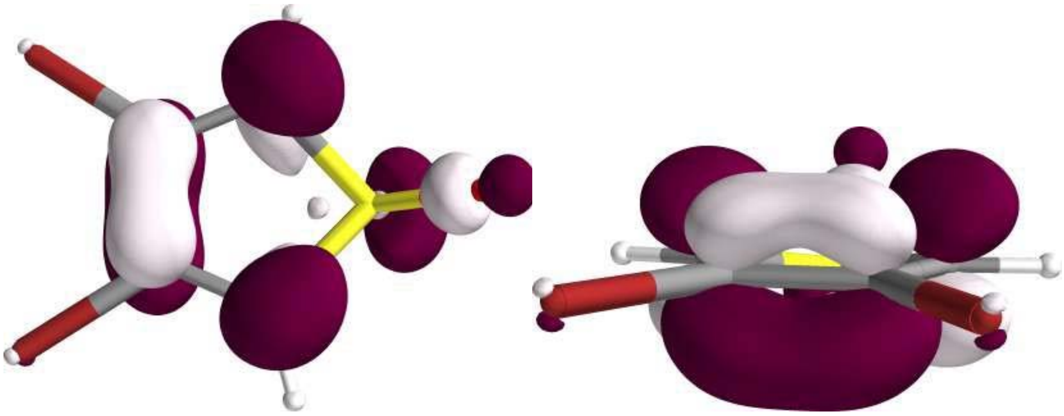

Figure 3: Representation of the LUMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1267	123	A
1108	95	A
1055	112	A
894	78	A
815	52	A

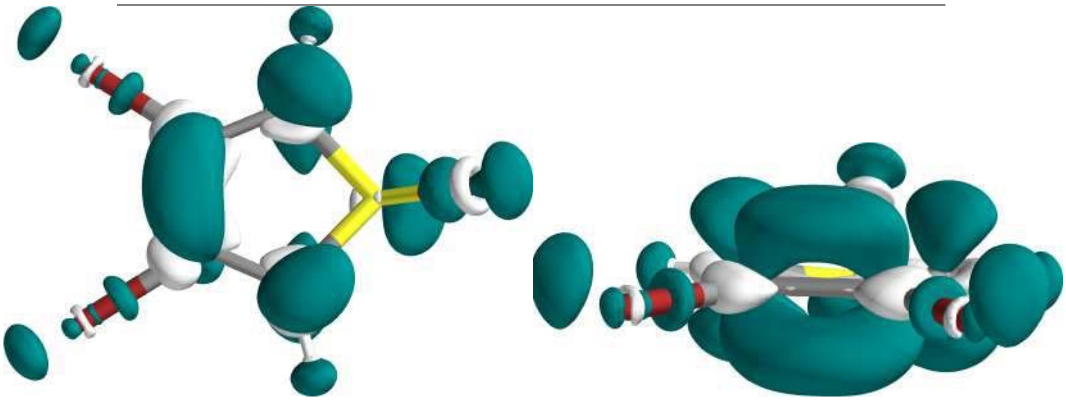

Figure 4: Representation of the F+ function from two points of view. The Blue color indicate the most electrophilic regions.

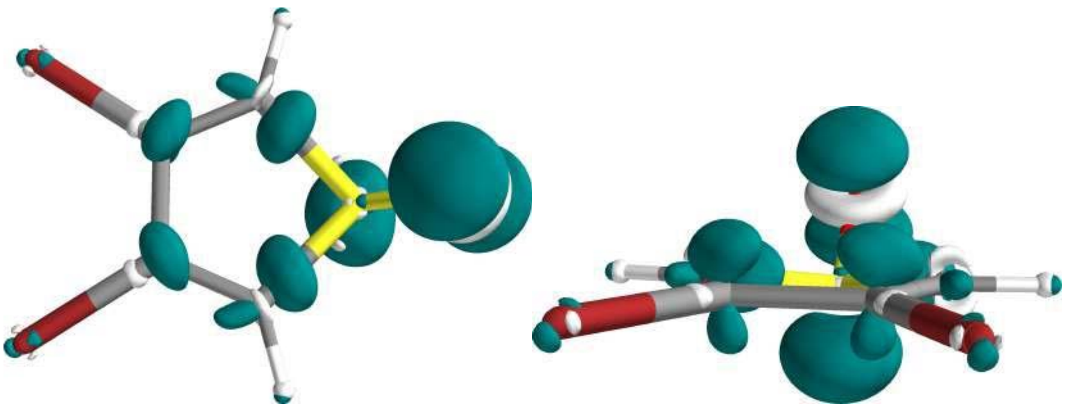

Figure 5: Representation of the F- function from two points of view. The Blue color indicate the most nucleophilic regions.

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	f	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - end-ing OM (% if > 5%)
1	Singlet-A	379	26341	0.012	-0.0	0.54	194.25	0.70	60-61(97);
2	Singlet-A	324	30825	0.000	-0.1	0.74	120.04	0.49	59-61(91);
3	Singlet-A	270	36939	0.001	-0.0	0.44	132.20	0.71	58-61(88);
4	Singlet-A	258	38679	0.000	-0.0	0.52	199.66	0.58	57-61(41); 60-62(56);
5	Singlet-A	254	39236	0.001	-0.0	0.51	169.40	0.69	59-62(95);
6	Singlet-A	247	40451	0.000	0.1	0.44	37.99	0.76	56-61(91);
7	Singlet-A	241	41459	0.152	0.1	0.53	95.41	0.52	57-61(49); 60-62(37);
8	Singlet-A	231	43190	0.003	-0.0	0.33	278.48	0.86	55-61(98);
9	Singlet-A	230	43435	0.035	-0.3	0.54	296.38	0.61	60-63(86);
10	Singlet-A	221	45233	0.015	0.0	0.63	34.84	0.59	57-62(6); 59-63(84);
11	Singlet-A	211	47322	0.000	0.0	0.54	101.03	0.65	58-62(88);
12	Singlet-A	205	48552	0.015	0.3	0.58	39.42	0.62	57-62(84); 59-63(7);
13	Singlet-A	205	48746	0.079	-0.4	0.62	229.53	0.58	54-61(85);
14	Singlet-A	199	50020	0.004	0.0	0.39	342.82	0.77	60-64(95);
15	Singlet-A	192	51863	0.001	-0.3	0.55	60.50	0.60	55-62(45); 58-63(42); 59-64(6);

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-0.2173	-0.7361	-0.0036
C	-0.2173	0.7358	-0.0043
C	-1.4389	1.2693	-0.0528
S	-2.6749	-0.0004	-0.3538
C	-1.4389	-1.2697	-0.0511
Br	1.3798	1.7595	0.0232
Br	1.3795	-1.7595	0.0230
H	-1.7227	2.3085	-0.0831
H	-1.7222	-2.3090	-0.0818
O	-3.8075	0.0012	0.6096

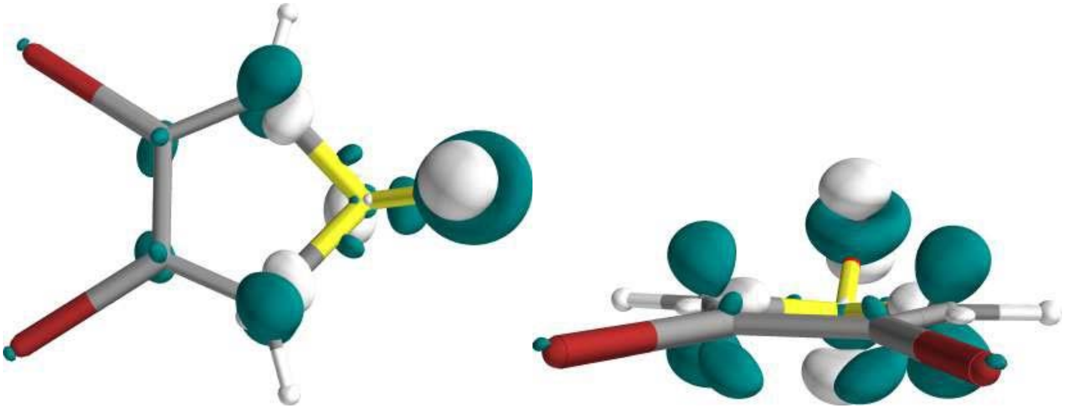

Figure 6: Representation of the Dual descriptor from two points of view. Electrophilic and nucleophilic regions correspond to blue and white surfaces.

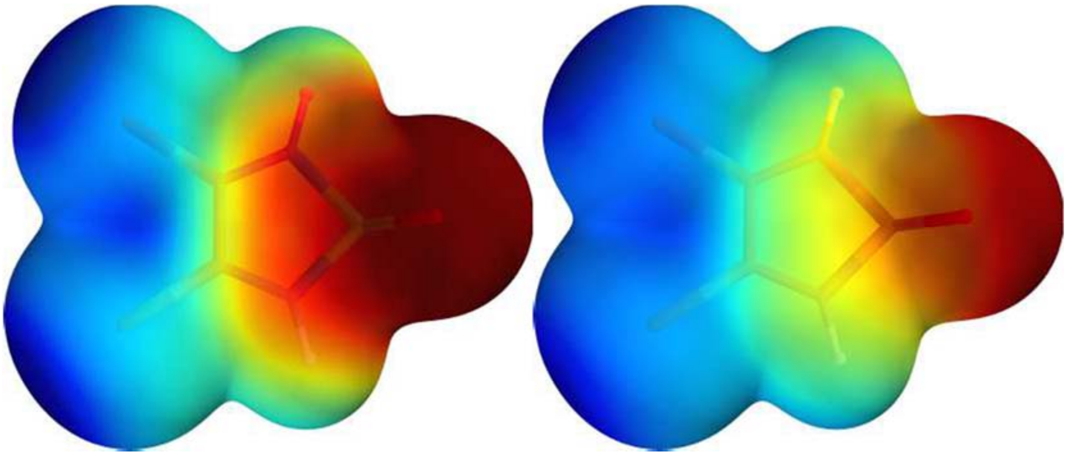

Figure 7: Representations of the Molecular Electrostatic Potential mapped on the electron density (cutoff value of

0.002 e-/bohr3). On the left, red, blue and green regions correspond to negative values < -0.06 a.u., positive values >

0.08 a.u. and neutral values respectively. On the right, the scale is set automatically to highlight the minimum values in red and the maximum values in blues.

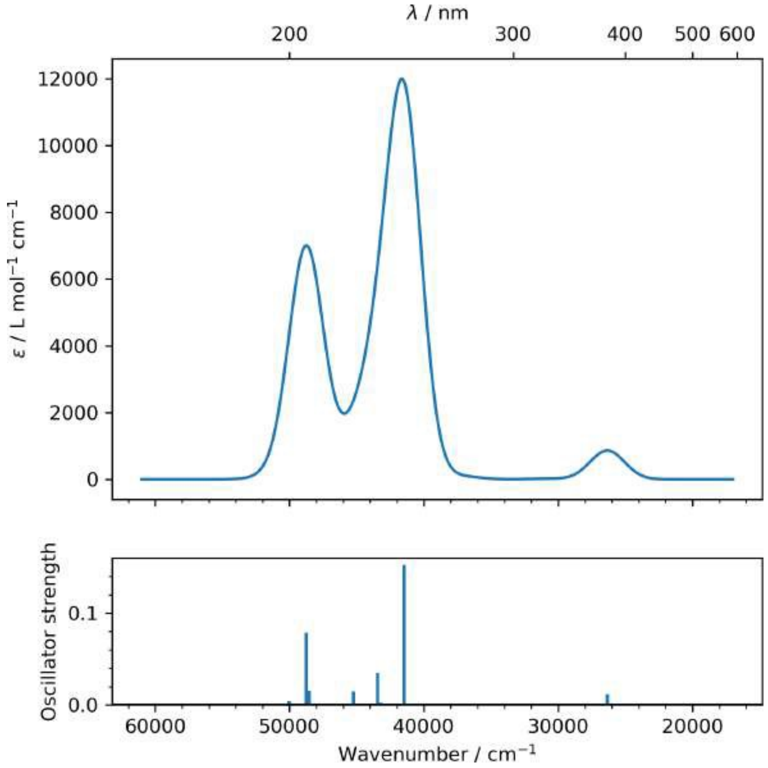

Figure 8: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

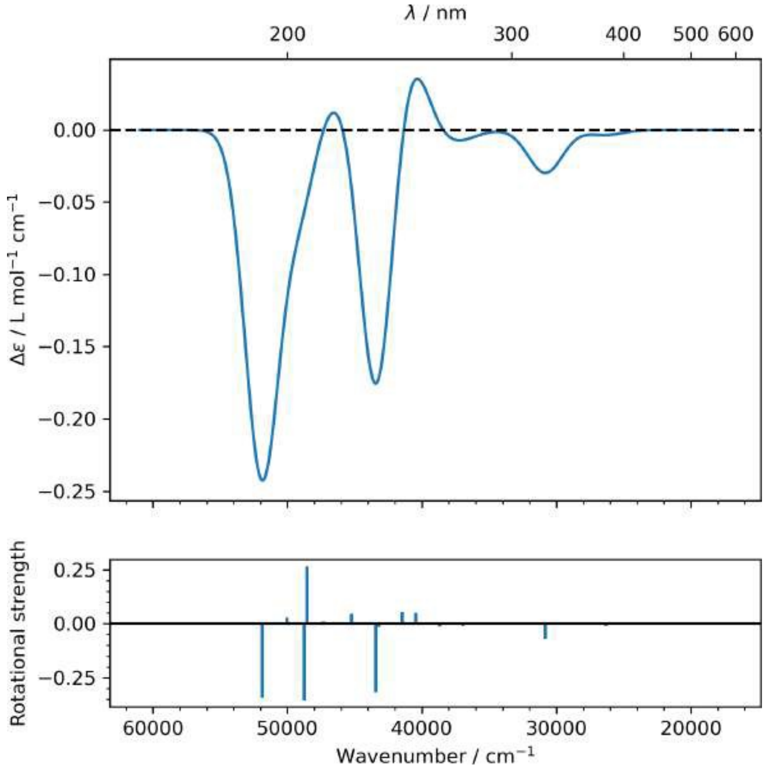

Figure 9: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

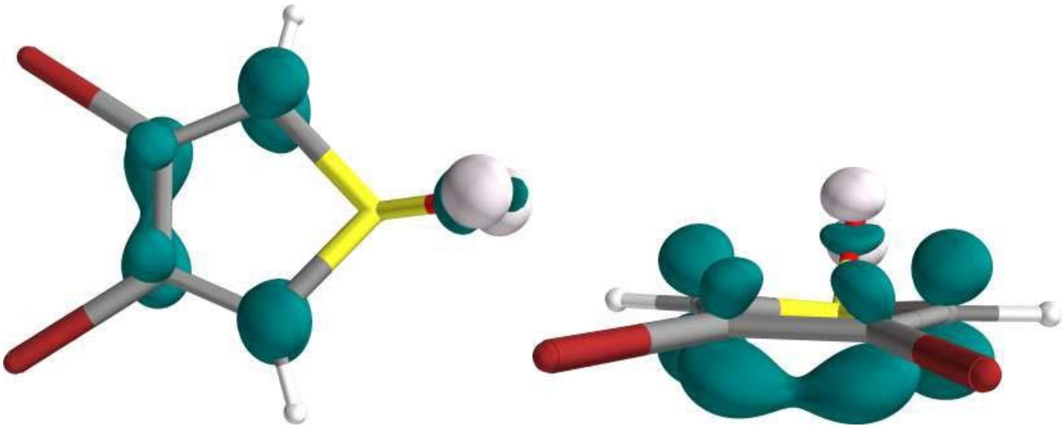

Figure 10: Representation of the Electron Density Difference (S1-S0) from two points of view.

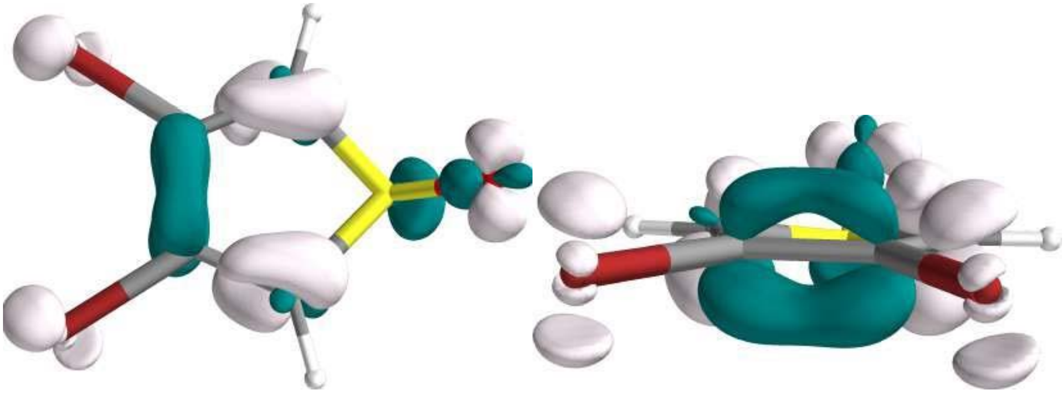

Figure 11: Representation of the Electron Density Difference (S2-S0) from two points of view.

3- 3,4-dibromothiophene sulfone 1-SO2

a. Description

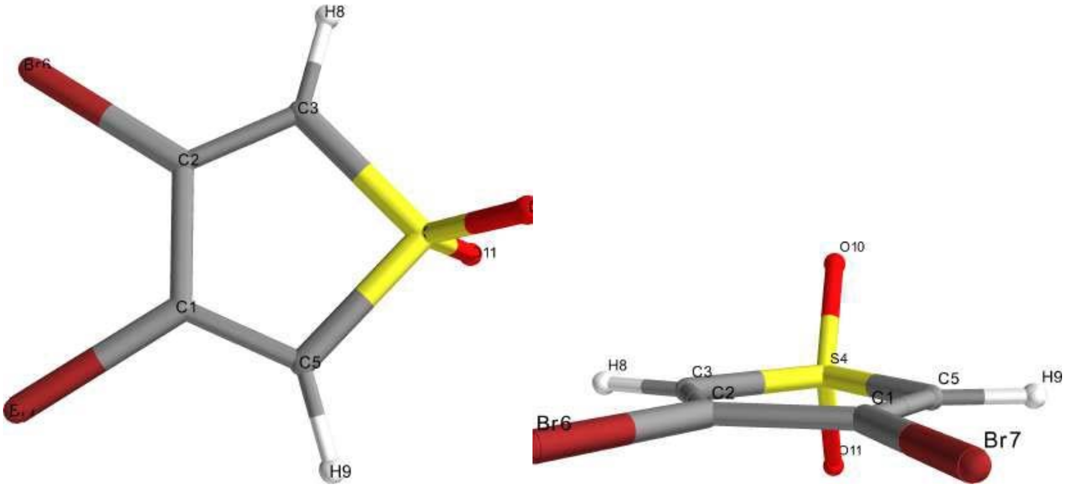

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-SO2
Formula	C4H2Br2O2S
Charge	0
Spin multiplicity	1
Monoisotopic mass	271.81422 Da
InChI	1S/C4H2Br2O2S/c5-3-1-9(7,8)2-4(3)6/h1-2H
SMILES	C1(=CS(=O)(=O)C=C1Br)Br

b. Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	279	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000081	0.000450
RMS Force value and threshold	0.000017	0.000300
Max Displacement value and threshold	0.000355	0.001800
RMS Displacement value and threshold	0.000084	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	
Job type: Time-dependent calculation		
Number of calculated excited states and spin state	15	['Singlet-A']

c. Results

Total molecular energy	-5850.55860 hartrees
HOMO number	64
LUMO+1 energies	-1.68 eV
LUMO energies	-3.01 eV
HOMO energies	-7.50 eV
HOMO-1 energies	-8.36 eV

CDFT indices: Electron Affinity	0.0015 hartrees
CDFT indices: Ionisation Potential	0.0127 hartrees
CDFT indices: Electronegativity	0.0071 hartrees
CDFT indices: Hardness	0.0111 hartrees
CDFT indices: Electrophilicity	0.0023
CDFT indices: Electron-flow	0.6379 e-

Geometry optimization specific results	
Converged nuclear repulsion energy	1136.05341 Hartrees

Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-5850.49421 Hartrees
Gibbs free energy at 298.15 K	-5850.54054 Hartrees
Entropy at 298.15 K	0.00016 Hartrees

Mean Mulliken atomic charge and standard deviation	0.0000 e-	0.4076 e-
Atoms with negatives charges under the standard deviation	NÂ°	Mulliken charge
	O 10	-0.561
	O 11	-0.561
Atoms with positives charges over the standard deviation	NÂ°	Mulliken charge
	S 4	+1.064

Table. Selection of the most important condensed Fukui functions based on Mulliken charges.

Atom	atomic dual descriptor (f+ - f-)	atomic electrophilicity f+	atomic nucleophilicity f-
Br 7	-0.05	0.19	0.24
Br 6	-0.05	0.19	0.24
S 4	0.05	0.06	0.02

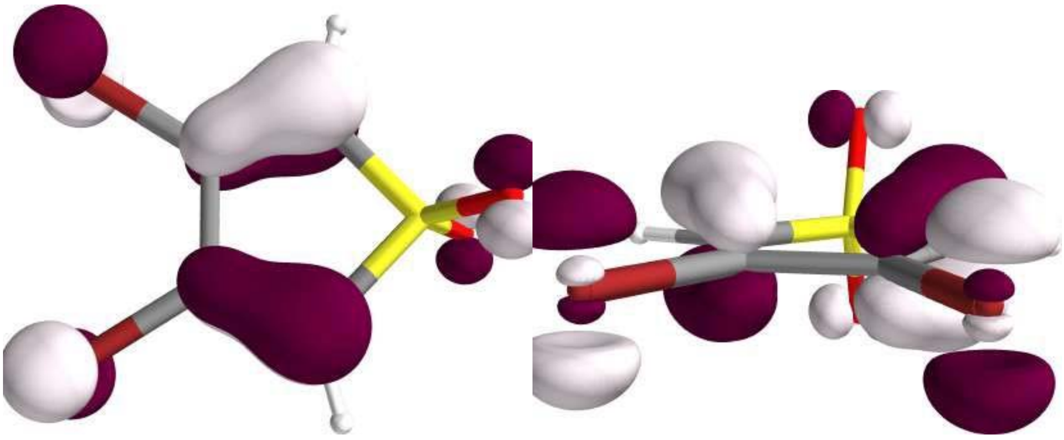

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1587	51	A
1326	166	A
1253	164	A
1143	101	A
1031	77	A
929	107	A
806	53	A
484	66	A

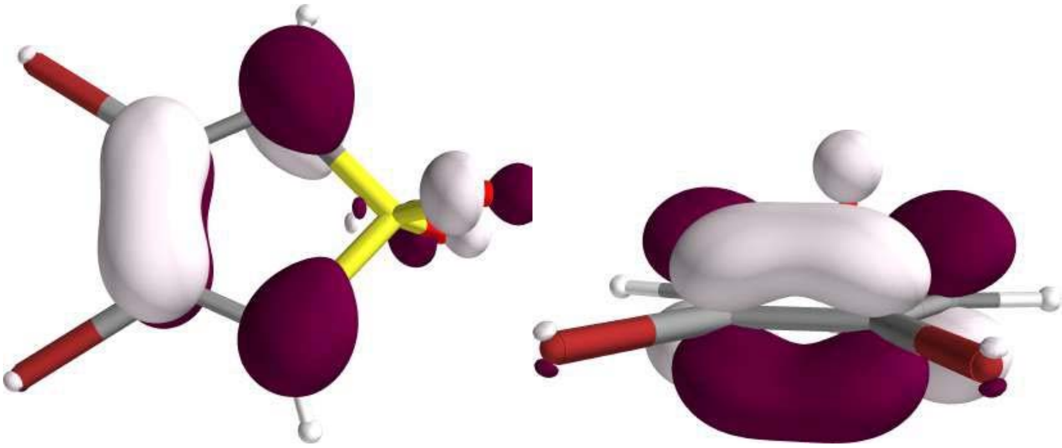

Figure 3: Representation of the LUMO from two points of view.

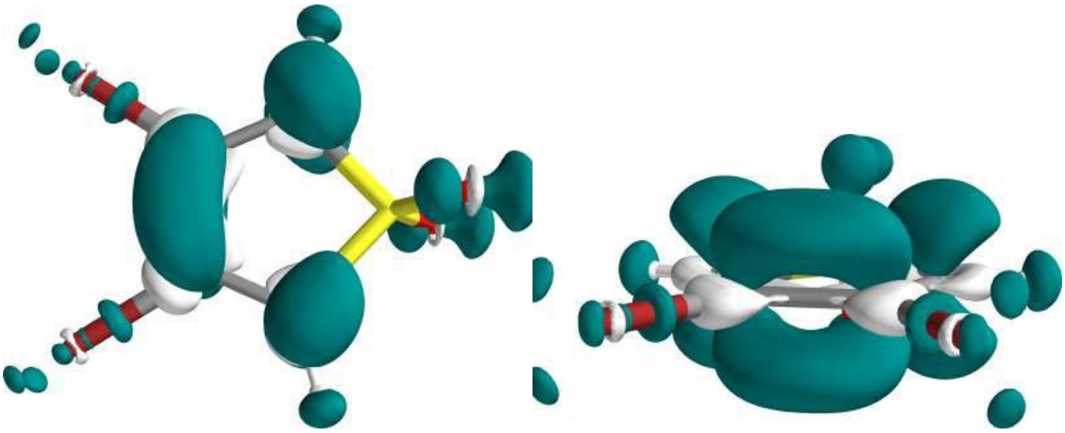

Figure 4: Representation of the F+ function from two points of view. The Blue color indicate the most electrophilic regions.

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	*f*	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	321	31070	0.002	-0.0	0.79	100.72	0.43	64-65(98);
2	Singlet-A	286	34855	0.000	0.0	0.42	123.77	0.81	62-65(96);
3	Singlet-A	262	38079	0.000	-0.0	0.52	163.34	0.71	64-66(98);
4	Singlet-A	261	38288	0.130	-0.0	0.66	77.47	0.64	63-65(94);
5	Singlet-A	245	40760	0.000	0.0	0.48	10.28	0.76	61-65(95);
6	Singlet-A	237	42124	0.001	-0.0	0.35	251.30	0.85	60-65(99);
7	Singlet-A	224	44483	0.002	-0.0	0.55	94.90	0.72	59-65(97);
8	Singlet-A	224	44517	0.002	0.0	0.49	15.36	0.73	58-65(91); 62-66(6);
9	Singlet-A	220	45344	0.000	-0.0	0.55	167.11	0.67	63-66(81); 64-67(16);
10	Singlet-A	215	46394	0.010	0.0	0.55	85.32	0.63	62-66(88);
11	Singlet-A	210	47484	0.004	0.0	0.50	247.05	0.65	57-65(85); 64-67(10);
12	Singlet-A	204	48781	0.001	0.0	0.54	225.03	0.62	57-65(11); 63-66(15); 64-67(72);
13	Singlet-A	199	50075	0.057	-0.0	0.68	84.21	0.55	56-65(92);
14	Singlet-A	193	51801	0.002	-0.0	0.58	58.23	0.64	60-66(85); 62-67(11);
15	Singlet-A	189	52810	0.024	0.0	0.55	245.49	0.67	61-66(93);

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-0.0330	0.7460	-0.0001
C	-0.0331	-0.7462	0.0001
C	-1.2438	-1.2896	0.0001
S	-2.4871	0.0002	-0.0000
C	-1.2435	1.2898	-0.0002
Br	1.5647	-1.7522	-0.0000
Br	1.5654	1.7519	0.0000
H	-1.5305	-2.3284	0.0001
H	-1.5301	2.3287	0.0001
O	-3.2111	0.0003	1.2524
O	-3.2113	0.0004	-1.2523

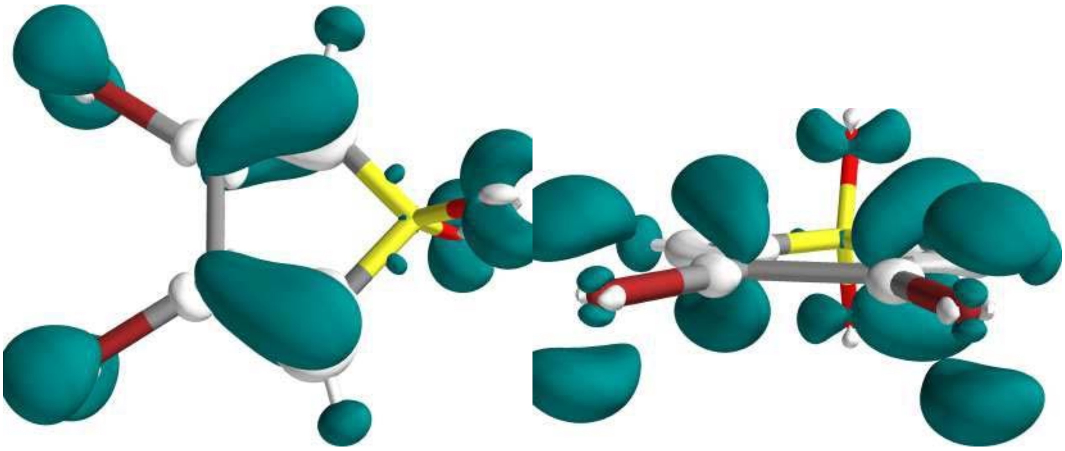

Figure 5: Representation of the F- function from two points of view. The Blue color indicate the most nucleophilic regions.

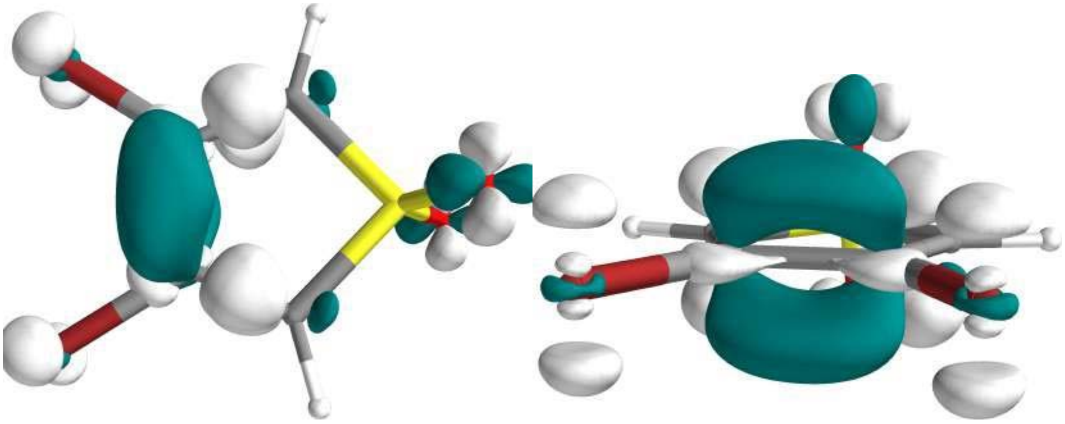

Figure 6: Representation of the Dual descriptor from two points of view. Electrophilic and nucleophilic regions correspond to blue and white surfaces.

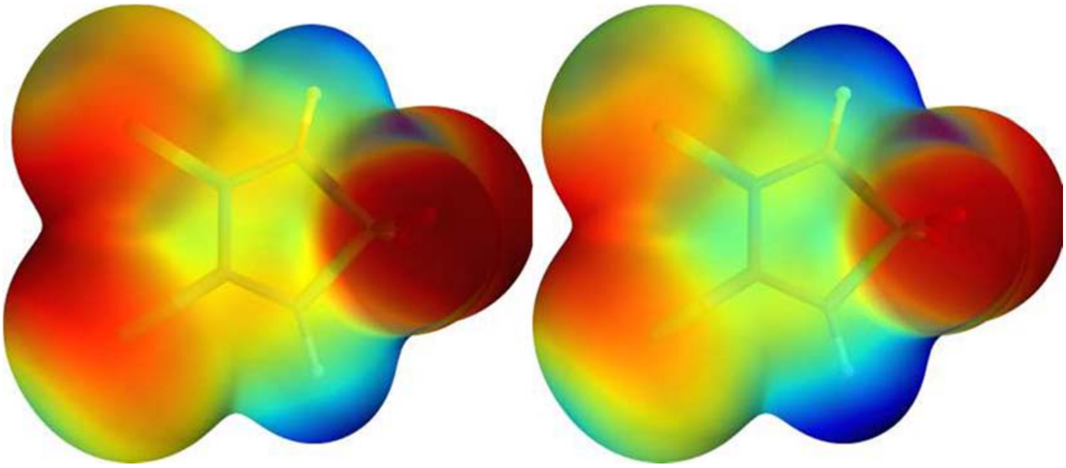

Figure 7: Representations of the Molecular Electrostatic Potential mapped on the electron density (cutoff value of

0.002 e-/bohr3). On the left, red, blue and green regions correspond to negative values < -0.06 a.u., positive values >

0.08 a.u. and neutral values respectively. On the right, the scale is set automatically to highlight the minimum values in red and the maximum values in blues.

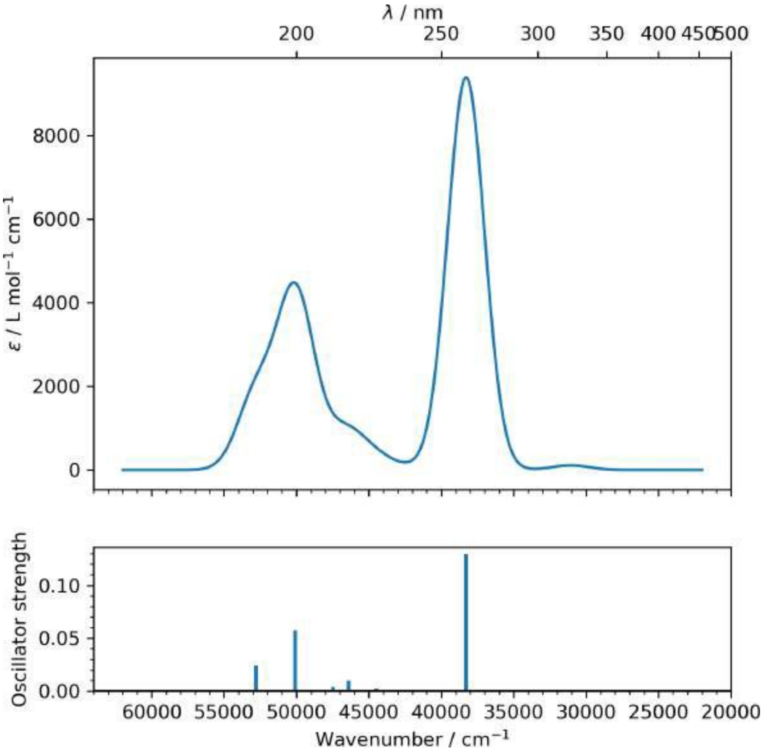

Figure 8: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

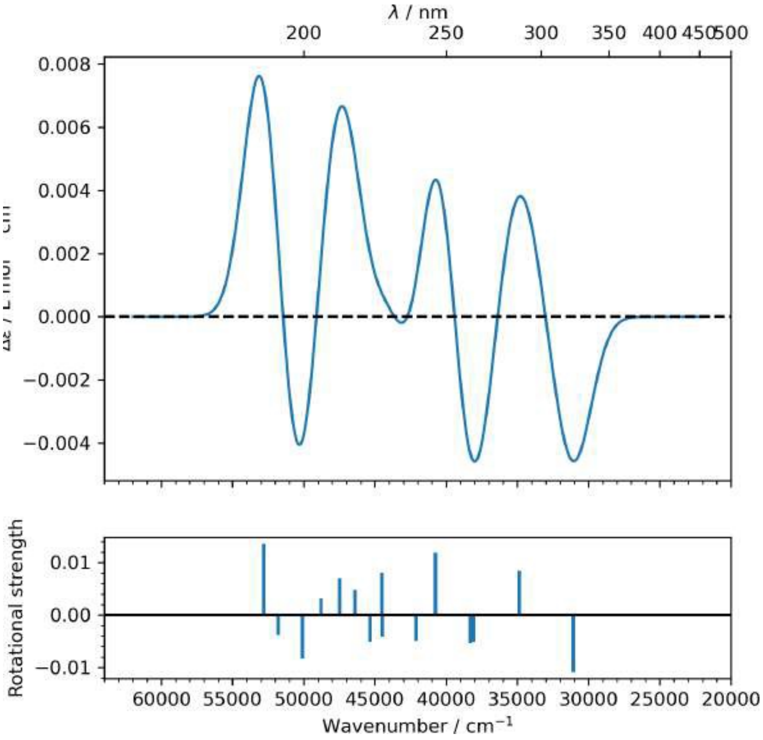

Figure 9: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

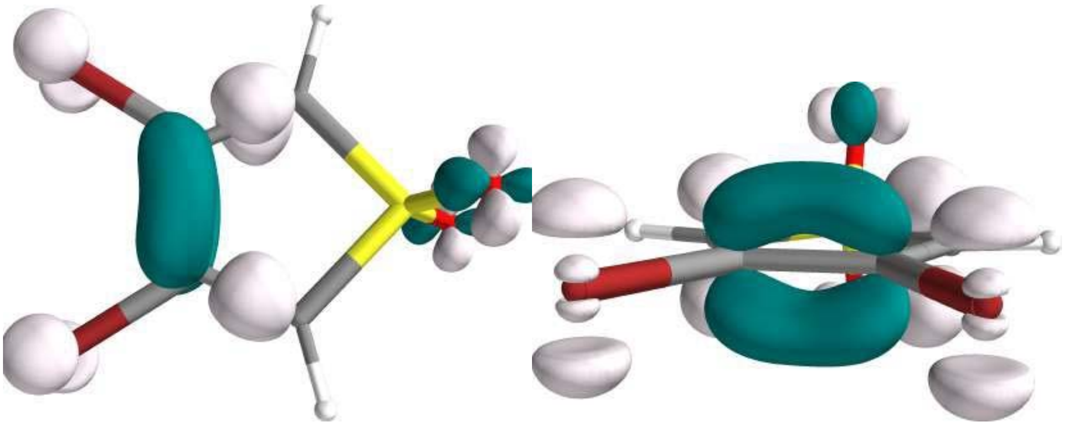

Figure 10: Representation of the Electron Density Difference (S1-S0) from two points of view.

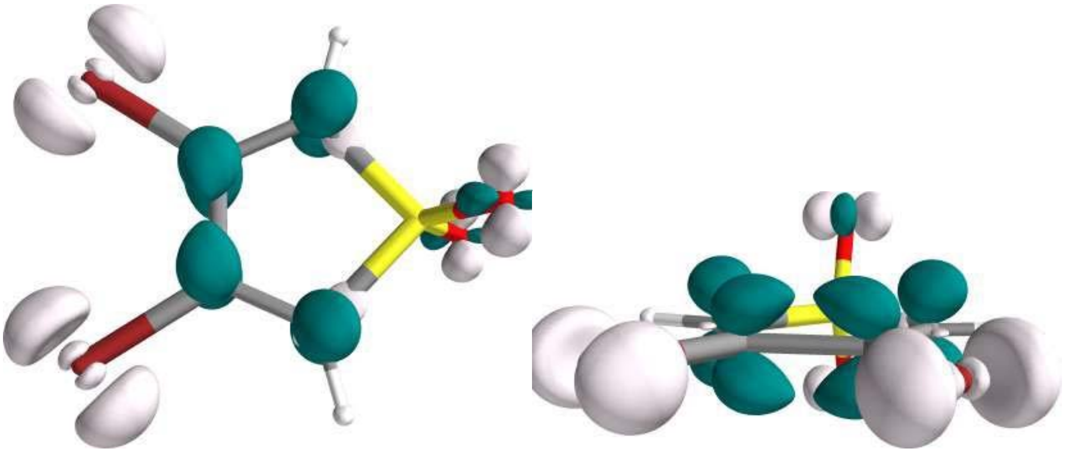

Figure 11: Representation of the Electron Density Difference (S2-S0) from two points of view.

4- Cycloadduct sulfoxide 1-CySO

a- Description

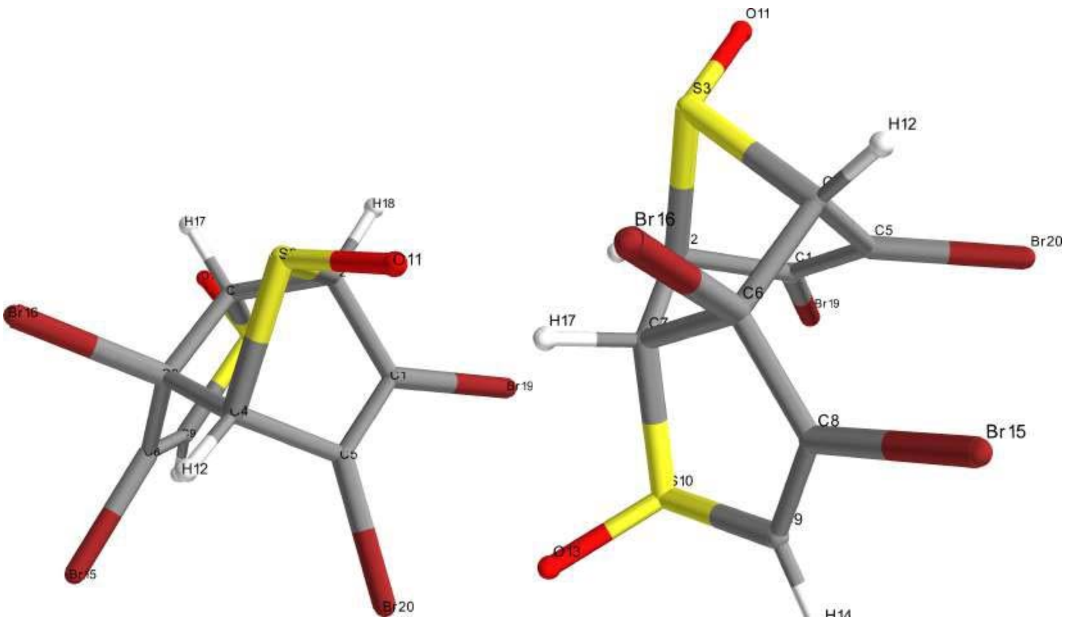

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-CySO
Formula	C8H4Br4O2S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	512	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000234	0.000450
RMS Force value and threshold	0.000032	0.000300
Max Displacement value and threshold	0.000732	0.001800
RMS Displacement value and threshold	0.000207	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-11550.68070 hartrees
HOMO number	120
LUMO+1 energies	-1.99 eV
LUMO energies	-2.65 eV
HOMO energies	-7.01 eV
HOMO-1 energies	-7.15 eV

Geometry optimization specific results

Converged nuclear repulsion energy	3626.70487 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-11550.55883 Hartrees
Gibbs free energy at 298.15 K	-11550.62387 Hartrees
Entropy at 298.15 K	0.00022 Hartrees

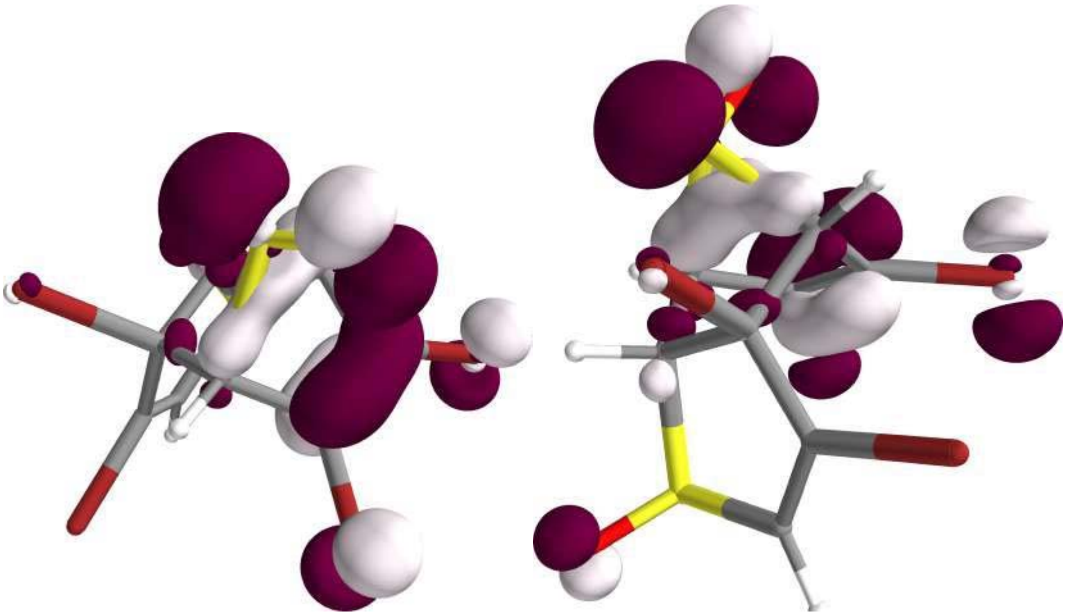

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1621	58	A
1160	98	A
1140	91	A
1097	60	A
1095	97	A
856	53	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-1.7734	-0.4679	0.1689
C	-1.0008	-1.7278	0.4586
S	-0.3669	-1.3669	2.2328
C	0.1952	0.1883	1.2481
C	-1.1008	0.6004	0.6009
C	1.1155	-0.4764	0.1936
C	0.3306	-1.7170	-0.3074
C	1.4660	0.3532	-0.9999
C	1.0803	-0.0848	-2.1896
S	0.1007	-1.5995	-2.1859
O	-1.5007	-1.0112	3.1112
H	0.6779	0.9305	1.8733
O	0.8652	-2.7114	-2.8134
H	1.2573	0.3991	-3.1387
Br	2.3802	2.0072	-0.7642
Br	2.8383	-1.0230	1.1060
H	0.8919	-2.6423	-0.2049
H	-1.5611	-2.6556	0.4047
Br	-3.4377	-0.5008	-0.7096
Br	-1.6036	2.4082	0.4505

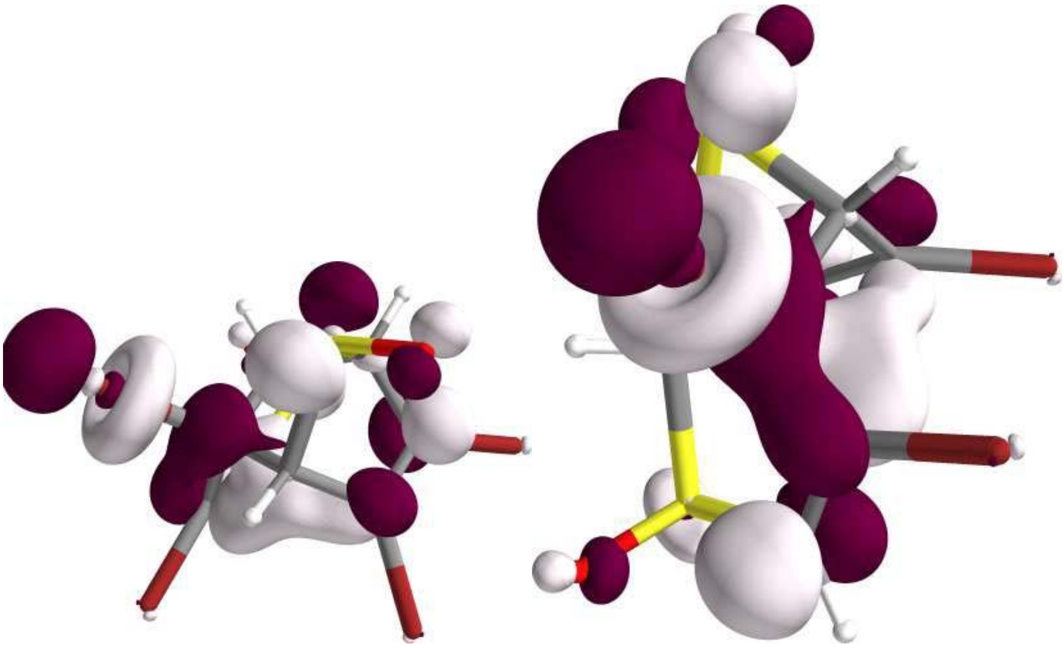

Figure 3: Representation of the LUMO from two points of view.

5- Cycloadduct 1-Cymix

a- Description

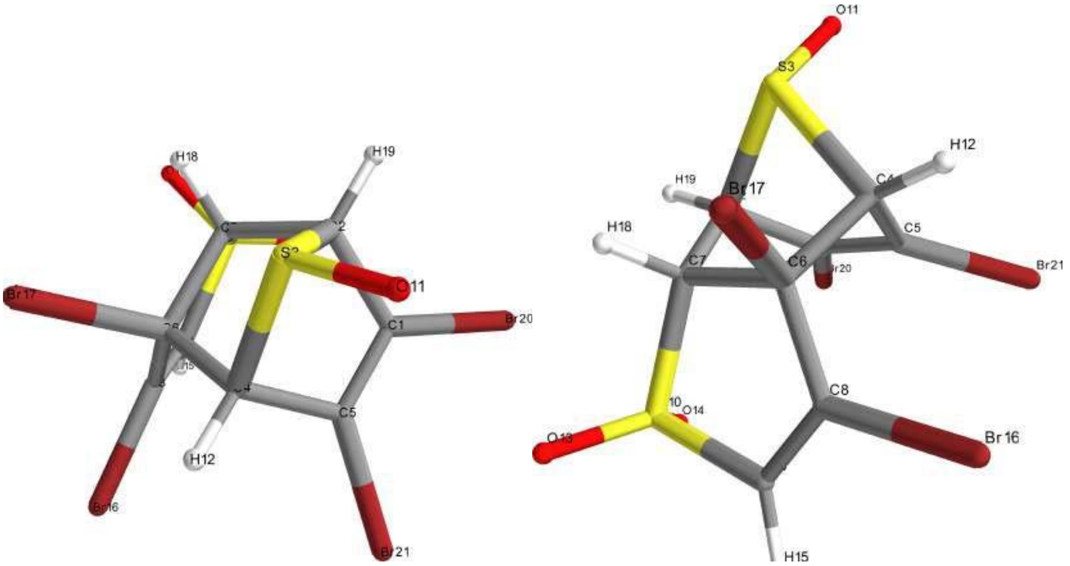

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-Cymix
Formula	C8H4Br4O3S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	535	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000127	0.000450
RMS Force value and threshold	0.000016	0.000300
Max Displacement value and threshold	0.001595	0.001800
RMS Displacement value and threshold	0.000354	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-11625.92075 hartrees
HOMO number	124
LUMO+1 energies	-2.08 eV
LUMO energies	-2.79 eV
HOMO energies	-6.99 eV
HOMO-1 energies	-7.72 eV

Geometry optimization specific results	
Converged nuclear repulsion energy	3907.02077 Hartrees

Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-11625.79284 Hartrees
Gibbs free energy at 298.15 K	-11625.85884 Hartrees
Entropy at 298.15 K	0.00022 Hartrees

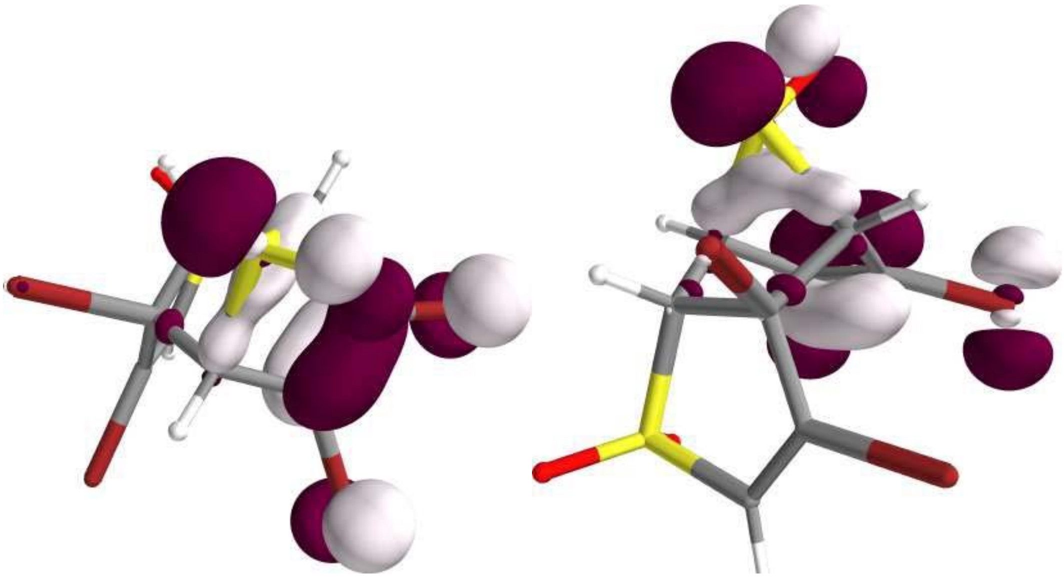

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1637	50	A
1338	130	A
1256	80	A
1160	111	A
1147	189	A
878	61	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-1.7443	-0.3831	0.2962
C	-0.9620	-1.5287	0.8800
S	-0.3646	-0.7484	2.5403
C	0.1974	0.5415	1.2229
C	-1.0938	0.7672	0.4832
C	1.1484	-0.3297	0.3680
C	0.4187	-1.7020	0.2261
C	1.4592	0.1943	-1.0083
C	1.1575	-0.5685	-2.0471
S	0.4367	-2.1210	-1.5729
O	-1.5141	-0.2065	3.2916
H	0.6567	1.4177	1.6655
O	1.3903	-3.1878	-1.7879
O	-0.9075	-2.2315	-2.0963
H	1.3093	-0.3570	-3.0945
Br	2.2418	1.9113	-1.1984
Br	2.8927	-0.5529	1.3488
H	0.9796	-2.5091	0.6895
H	-1.5106	-2.4519	1.0338
Br	-3.4324	-0.6217	-0.4883
Br	-1.6399	2.4882	-0.0495

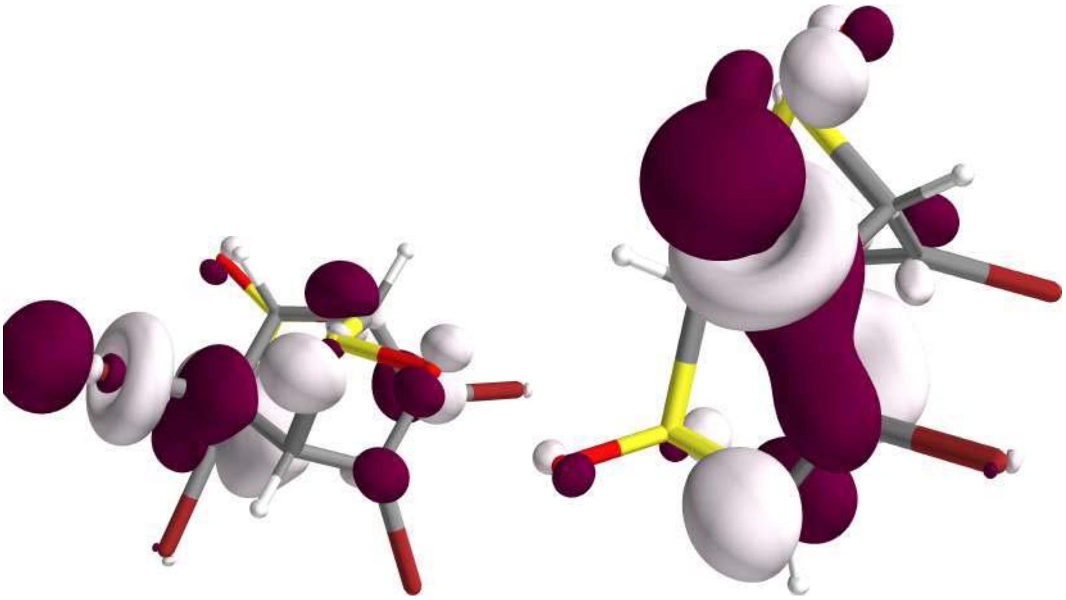

Figure 3: Representation of the LUMO from two points of view.

6- Cycloadduct 1-Cy

a- Description

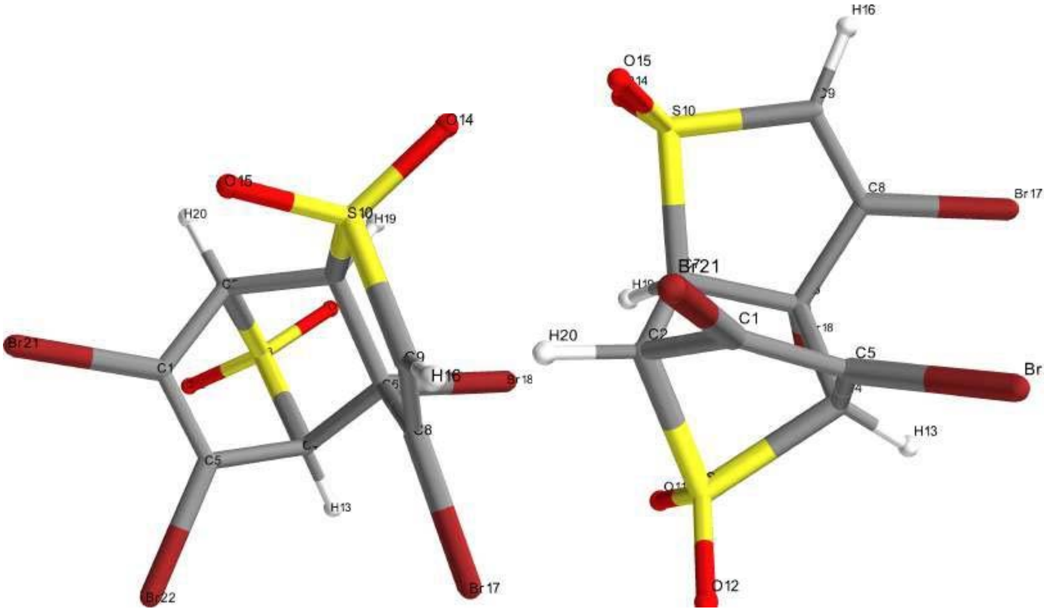

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-Cy
Formula	C8H4Br4O4S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	558	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000070	0.000450
RMS Force value and threshold	0.000011	0.000300
Max Displacement value and threshold	0.001046	0.001800
RMS Displacement value and threshold	0.000202	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-11701.15995 hartrees
HOMO number	128
LUMO+1 energies	-1.83 eV
LUMO energies	-2.68 eV
HOMO energies	-7.50 eV
HOMO-1 energies	-8.22 eV

Geometry optimization specific results

Converged nuclear repulsion energy	4192.70369 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-11701.02631 Hartrees
Gibbs free energy at 298.15 K	-11701.09353 Hartrees
Entropy at 298.15 K	0.00023 Hartrees

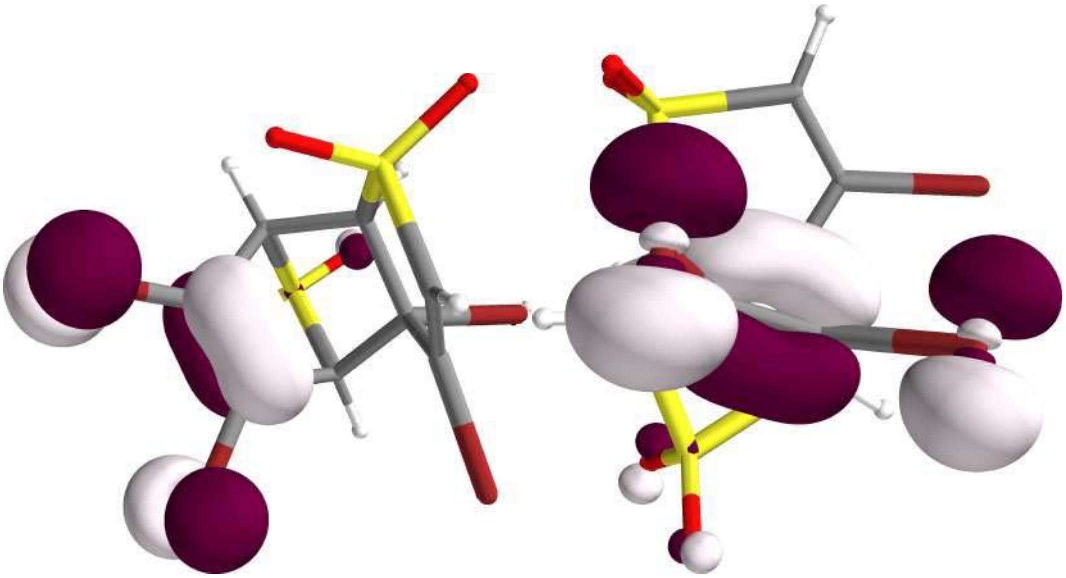

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1639	52	A
1350	139	A
1337	125	A
1253	90	A
1175	182	A
1145	179	A
882	71	A
539	55	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	1.6890	-0.4547	-0.0549
C	0.8982	-1.6654	-0.4326
S	0.4449	-1.1460	-2.2109
C	-0.1720	0.3803	-1.2244
C	1.1059	0.6684	-0.5029
C	-1.1705	-0.2834	-0.2403
C	-0.5268	-1.6556	0.1459
C	-1.3995	0.4967	1.0330
C	-1.1749	-0.1090	2.1879
S	-0.6069	-1.7770	1.9853
O	-0.6098	-1.9793	-2.7399
O	1.5862	-0.8097	-3.0261
H	-0.5799	1.1773	-1.8340
O	-1.6567	-2.7040	2.3445
O	0.7201	-1.9271	2.5441
H	-1.3090	0.2857	3.1833
Br	-2.0045	2.2911	0.9313
Br	-2.9607	-0.5133	-1.1007
H	-1.1062	-2.4956	-0.2257
H	1.4119	-2.6186	-0.3727
Br	3.3865	-0.6008	0.7315
Br	1.8176	2.4091	-0.4361

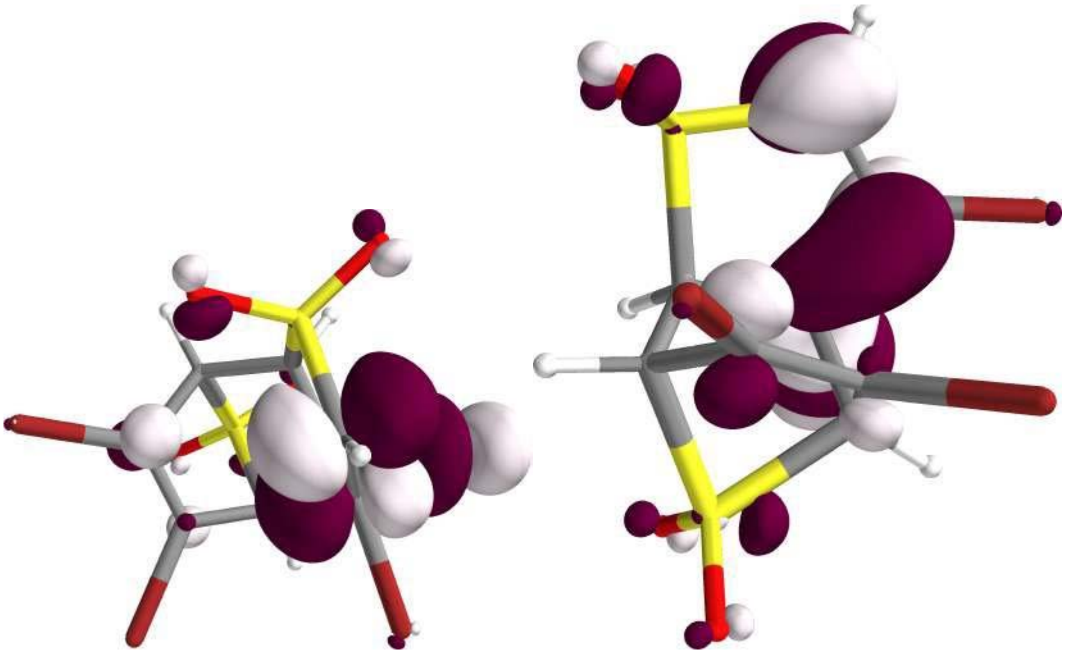

Figure 3: Representation of the LUMO from two points of view.

7- 2-bromothiophene

a. Description

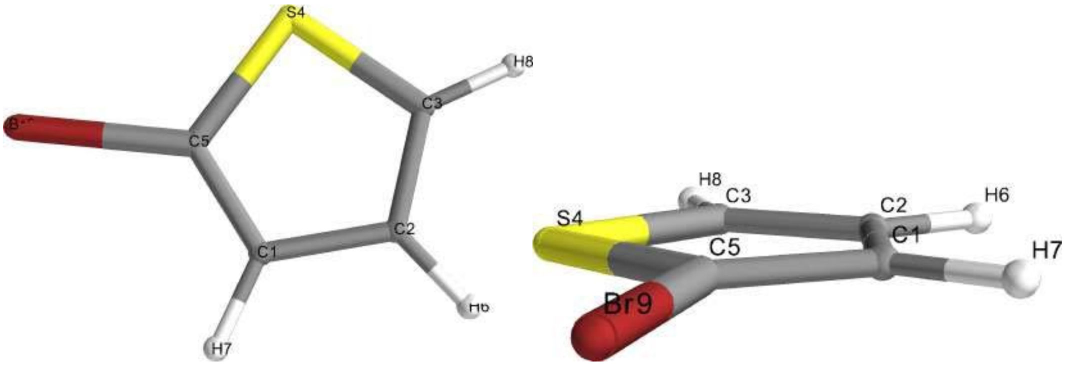

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	2
Formula	C4H3BrS
Charge	0
Spin multiplicity	1
Monoisotopic mass	161.91388 Da
InChI	1S/C4H3BrS/c5-4-2-1-3-6-4/h1-3H
SMILES	c1ccsc1Br

b. Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	190	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization		
Max Force value and threshold	0.000375	0.000450
RMS Force value and threshold	0.000143	0.000300
Max Displacement value and threshold	0.001759	0.001800
RMS Displacement value and threshold	0.000573	0.001200

Job type: Frequency and thermochemical analysis	
Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

Job type: Time-dependent calculation		
Number of calculated excited states and spin state	15	['Singlet-A']

c. Results

Total molecular energy	-3126.61034 hartrees	
HOMO number	39	
LUMO+1 energies	-0.48 eV	
LUMO energies	-0.84 eV	
HOMO energies	-6.50 eV	
HOMO-1 energies	-7.27 eV	
CDFT indices: Electron Affinity	-0.0016 hartrees	
CDFT indices: Ionisation Potential	0.0116 hartrees	
CDFT indices: Electronegativity	0.0050 hartrees	
CDFT indices: Hardness	0.0131 hartrees	
CDFT indices: Electrophilicity	0.0010	
CDFT indices: Electron-flow	0.3815 e-	
Geometry optimization specific results		
Converged nuclear repulsion energy	448.65937 Hartrees	
Frequency and Thermochemistry specific results		
Enthalpy at 298.15 K	-3126.54734 Hartrees	
Gibbs free energy at 298.15 K	-3126.58449 Hartrees	
Entropy at 298.15 K	0.00012 Hartrees	
Mean Mulliken atomic charge and standard deviation	0.0000 e-	0.0825 e-
Atoms with negatives charges under the standard deviation	NÂ°	Mulliken charge
	C 1	-0.105
	C 2	-0.092
	C 3	-0.087
Atoms with positives charges over the standard deviation	NÂ°	Mulliken charge
	S 4	+0.114

Table. Selection of the most important condensed Fukui functions based on Mulliken charges.

Atom	atomic dual descriptor (f+ - f-)	atomic electrophilicity f+	atomic nucleophilicity f-
Br 9	-0.11	0.22	0.32
S 4	0.11	0.28	0.17

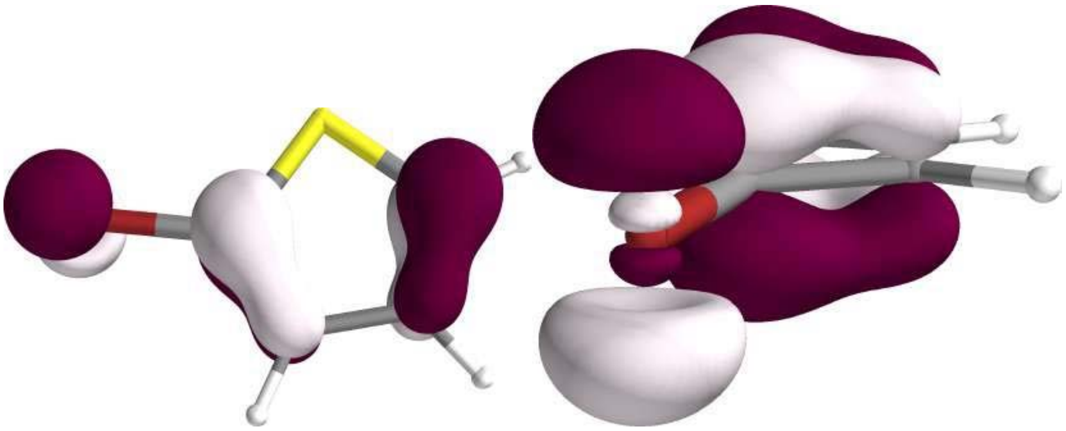

Figure 2: Representation of the HOMO from two points of view.

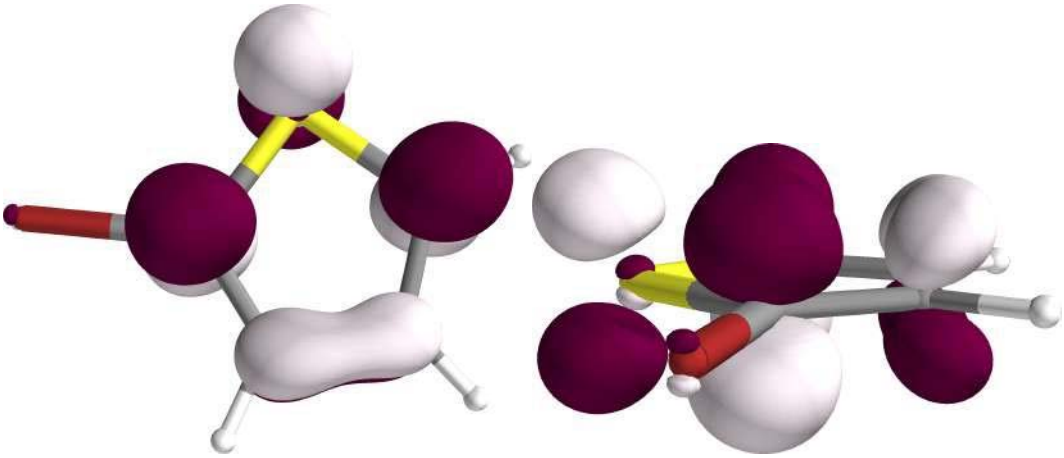

Figure 3: Representation of the LUMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
694	70	A

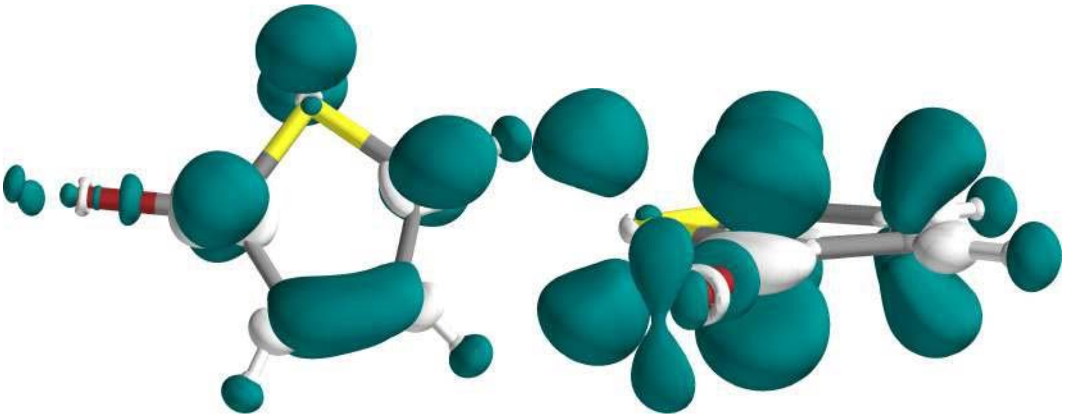

Figure 4: Representation of the F+ function from two points of view. The Blue color indicate the most electrophilic regions.

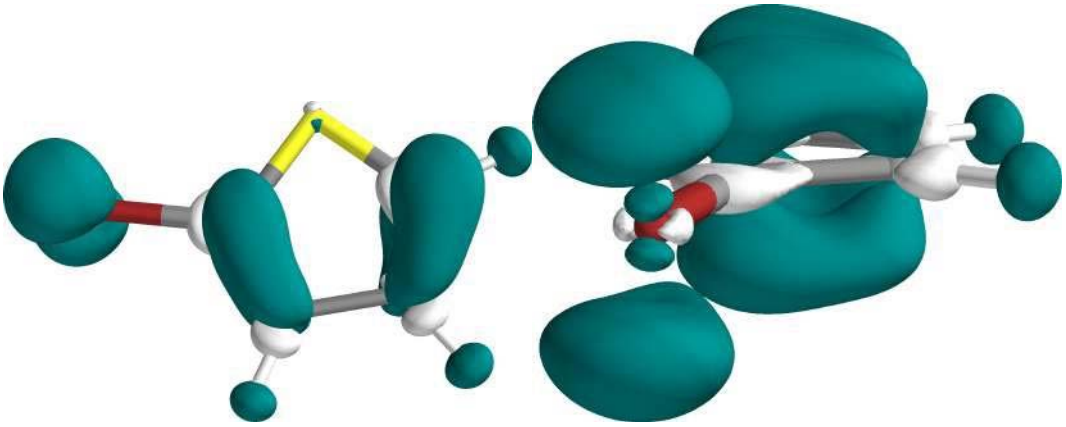

Figure 5: Representation of the F- function from two points of view. The Blue color indicate the most nucleophilic regions.

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	f	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	253	39517	0.000	0.0	0.53	214.47	0.70	39-41(99);
2	Singlet-A	234	42556	0.145	-0.0	0.77	141.77	0.40	39-40(96);
3	Singlet-A	223	44698	0.000	0.0	0.43	173.50	0.76	39-42(97);
4	Singlet-A	216	46176	0.000	0.0	0.30	237.84	0.85	38-41(95);
5	Singlet-A	213	46823	0.067	-0.0	0.69	45.30	0.39	38-40(81); 39-43(16);
6	Singlet-A	201	49671	0.000	-0.0	0.43	120.10	0.77	38-42(96);
7	Singlet-A	194	51352	0.000	0.0	0.27	298.49	0.89	37-40(98);
8	Singlet-A	190	52606	0.005	0.0	0.58	98.89	0.66	37-41(97);
9	Singlet-A	178	56136	0.001	-0.0	0.34	159.12	0.80	39-44(97);
10	Singlet-A	173	57504	0.000	0.0	0.57	40.26	0.66	36-41(95);
11	Singlet-A	173	57651	0.033	-0.0	0.61	263.64	0.54	36-40(74); 39-43(15);
12	Singlet-A	168	59369	0.182	0.0	0.67	239.83	0.40	36-40(17); 38-40(8); 39-43(56);
13	Singlet-A	166	60089	0.005	-0.0	0.40	223.28	0.75	39-45(94);
14	Singlet-A	165	60525	0.010	0.0	0.36	322.90	0.78	37-42(88);
15	Singlet-A	161	62011	0.002	0.0	0.47	147.15	0.55	35-40(45); 38-44(51);

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-0.8587	1.3596	0.0000
C	-2.2631	1.1220	0.0000
C	-2.5811	-0.2015	0.0000
S	-1.1673	-1.1995	0.0000
C	-0.1458	0.2011	0.0000
H	-3.0025	1.9111	-0.0000
H	-0.4014	2.3384	0.0000
H	-3.5584	-0.6567	0.0000
Br	1.7352	0.0203	0.0000

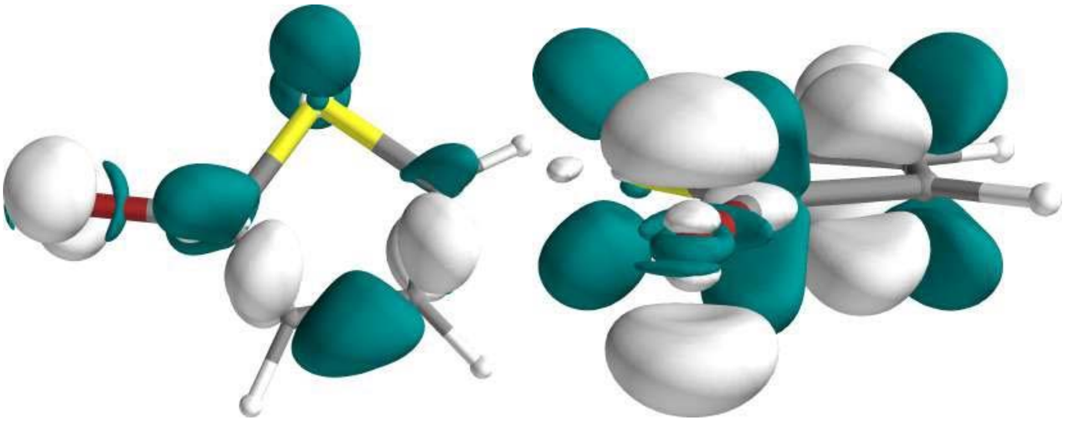

Figure 6: Representation of the Dual descriptor from two points of view. Electrophilic and nucleophilic regions correspond to blue and white surfaces.

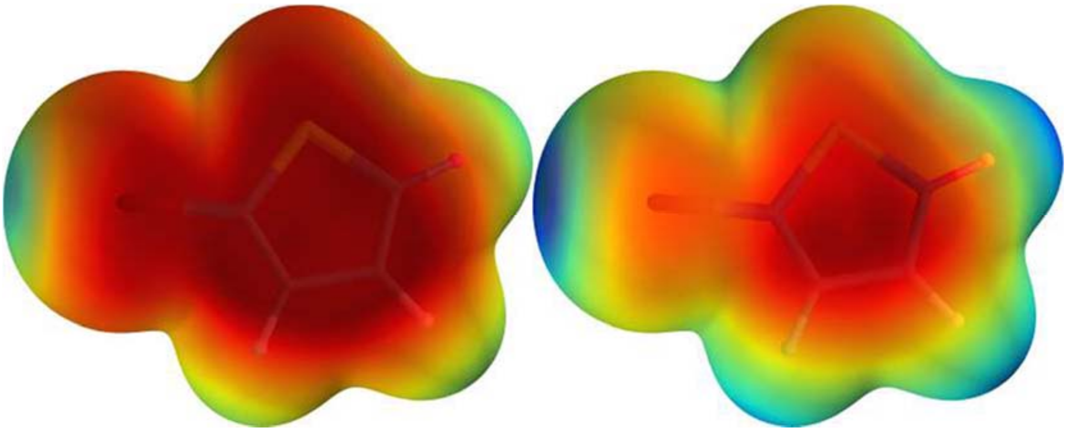

Figure 7: Representations of the Molecular Electrostatic Potential mapped on the electron density (cutoff value of

0.002 e-/bohr3). On the left, red, blue and green regions correspond to negative values < -0.06 a.u., positive values >

0.08 a.u. and neutral values respectively. On the right, the scale is set automatically to highlight the minimum values in red and the maximum values in blues.

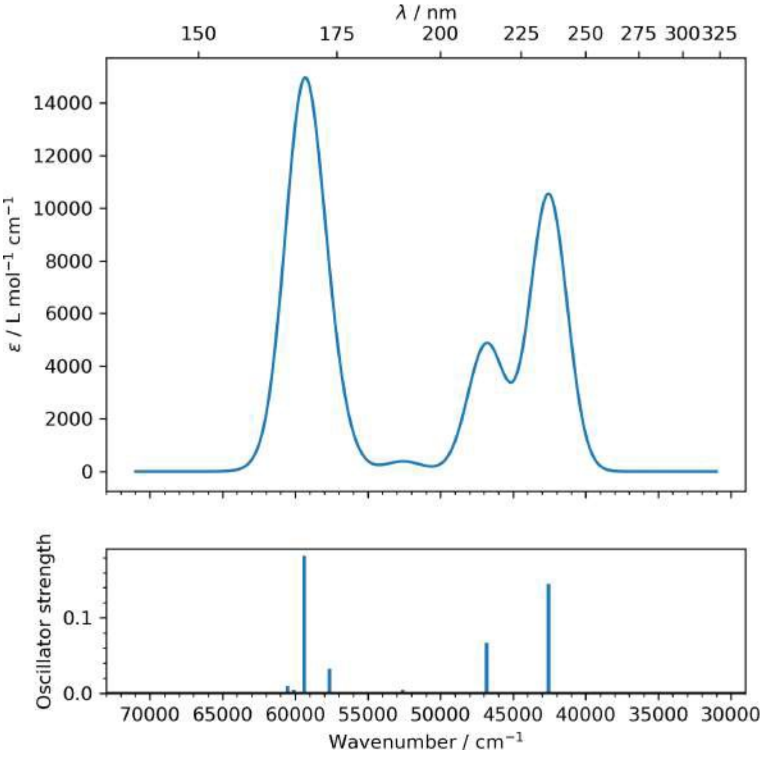

Figure 8: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

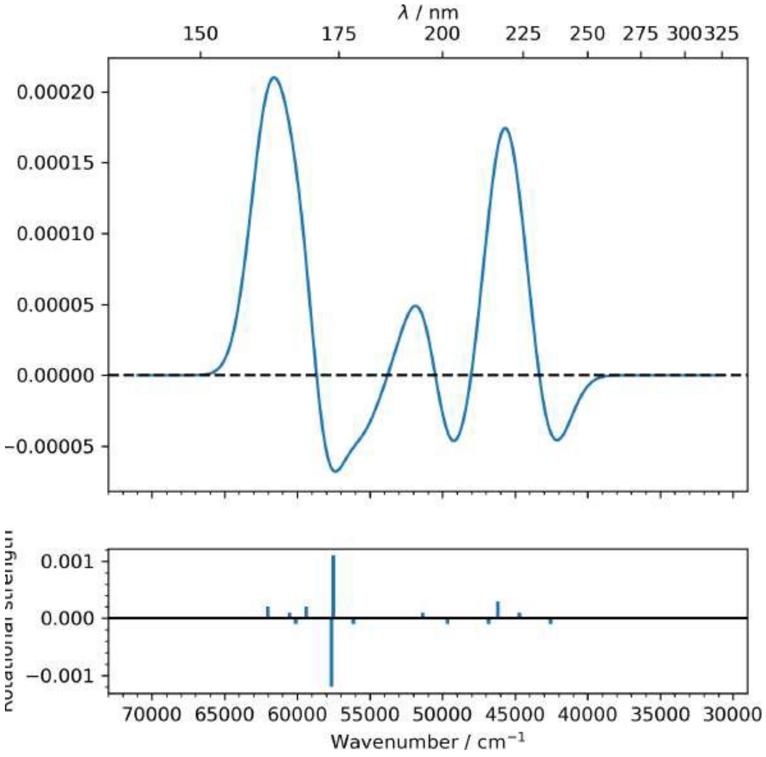

Figure 9: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

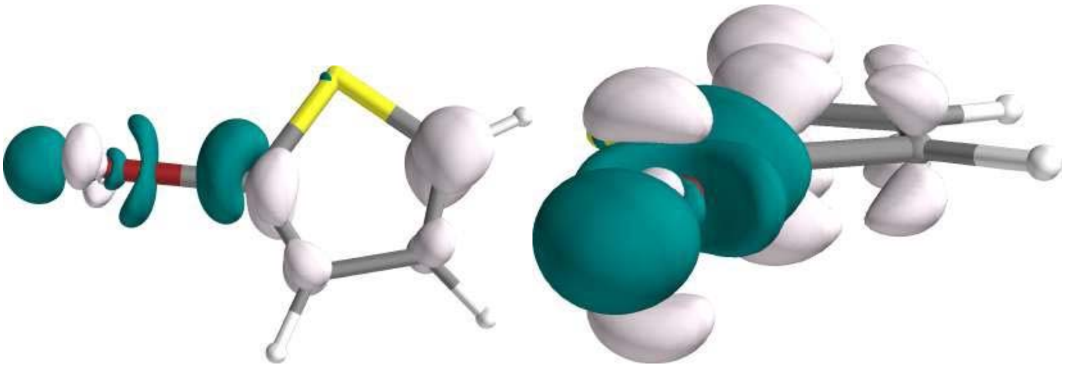

Figure 10: Representation of the Electron Density Difference (S1-S0) from two points of view.

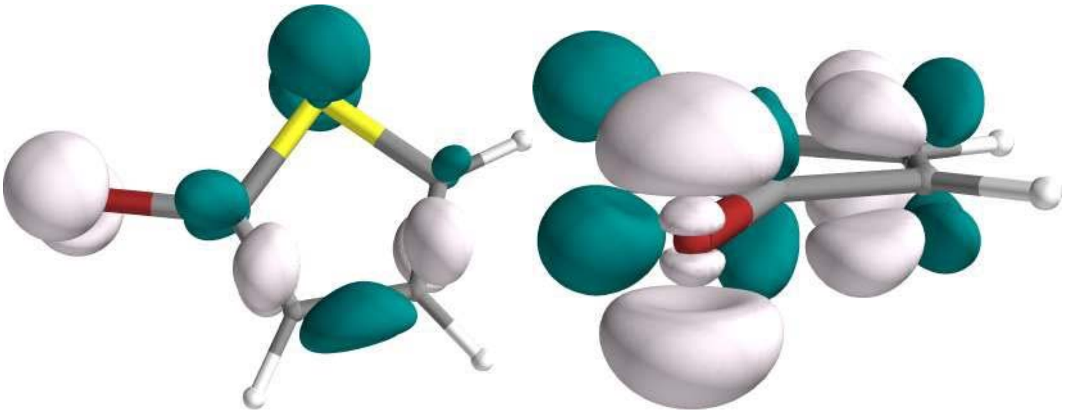

Figure 11: Representation of the Electron Density Difference (S2-S0) from two points of view.

8- 2-bromothiophene sulfoxide 2-SO

a. Description

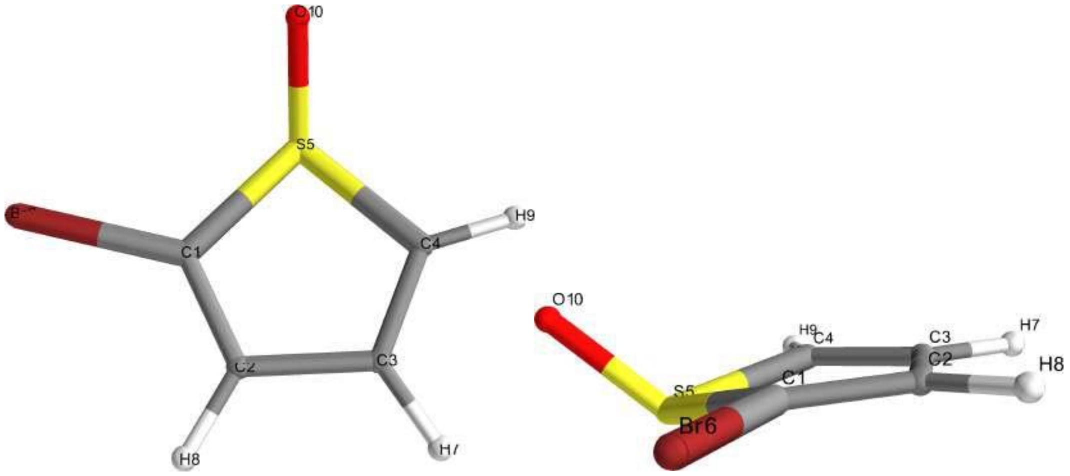

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	2-SO
Formula	C4H3BrOS
Charge	0
Spin multiplicity	1
Monoisotopic mass	177.90880 Da
InChI	1S/C4H3BrOS/c5-4-2-1-3-7(4)6/h1-3H/t7-/m0/s1
SMILES	c1(cccs1=O)Br

b. Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	213	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization		
Max Force value and threshold	0.000149	0.000450
RMS Force value and threshold	0.000039	0.000300
Max Displacement value and threshold	0.000625	0.001800
RMS Displacement value and threshold	0.000262	0.001200

Job type: Frequency and thermochemical analysis	
Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

Job type: Time-dependent calculation		
Number of calculated excited states and spin state	15	['Singlet-A']

c. Results

Total molecular energy	-3201.78226 hartrees
HOMO number	43
LUMO+1 energies	-0.69 eV
LUMO energies	-2.38 eV
HOMO energies	-6.75 eV
HOMO-1 energies	-6.96 eV

CDFT indices: Electron Affinity	0.0005 hartrees
CDFT indices: Ionisation Potential	0.0120 hartrees
CDFT indices: Electronegativity	0.0063 hartrees
CDFT indices: Hardness	0.0115 hartrees
CDFT indices: Electrophilicity	0.0017
CDFT indices: Electron-flow	0.5447 e-

Geometry optimization specific results	
Converged nuclear repulsion energy	564.64445 Hartrees

Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-3201.71508 Hartrees
Gibbs free energy at 298.15 K	-3201.75537 Hartrees
Entropy at 298.15 K	0.00014 Hartrees

Mean Mulliken atomic charge and standard deviation	-0.0000 e-	0.2923 e-
Atoms with negatives charges under the standard deviation	NÂ°	Mulliken charge
	O 10	-0.625
Atoms with positives charges over the standard deviation	NÂ°	Mulliken charge
	S 5	+0.642

Table. Selection of the most important condensed Fukui functions based on Mulliken charges.

Atom	atomic dual descriptor (f+ - f-)	atomic electrophilicity f+	atomic nucleophilicity f-
O 10	-0.12	0.08	0.20
Br 6	-0.06	0.21	0.27

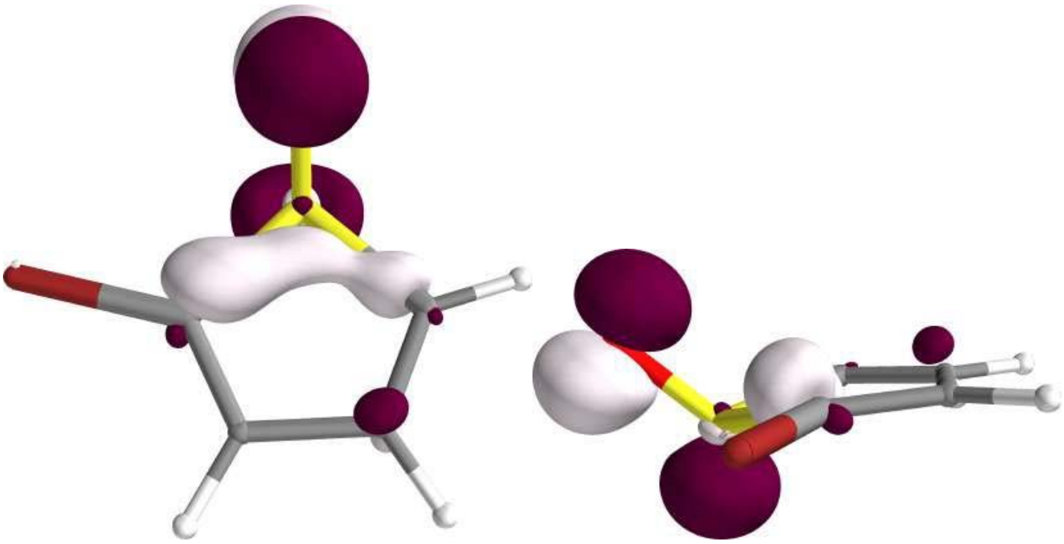

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1114	52	A
1095	86	A
702	60	A

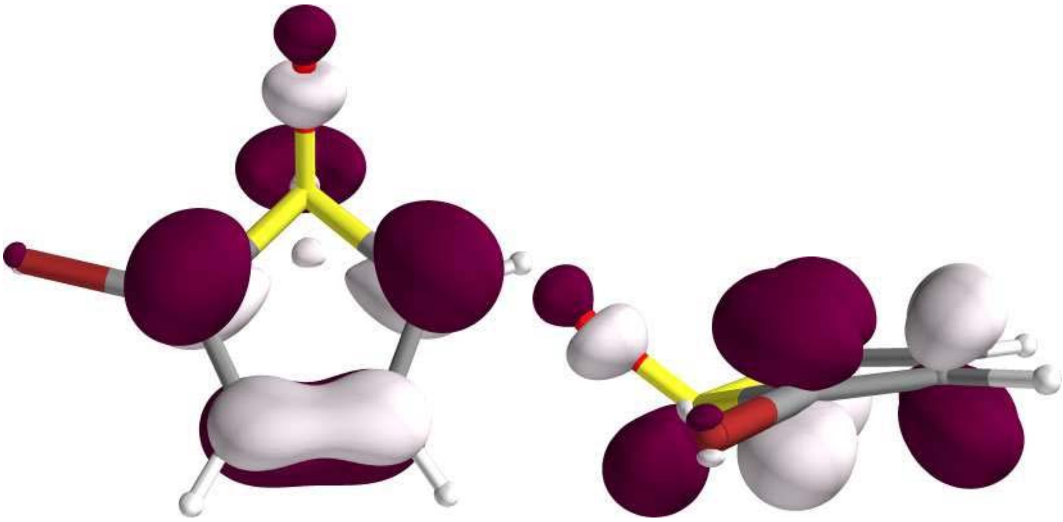

Figure 3: Representation of the LUMO from two points of view.

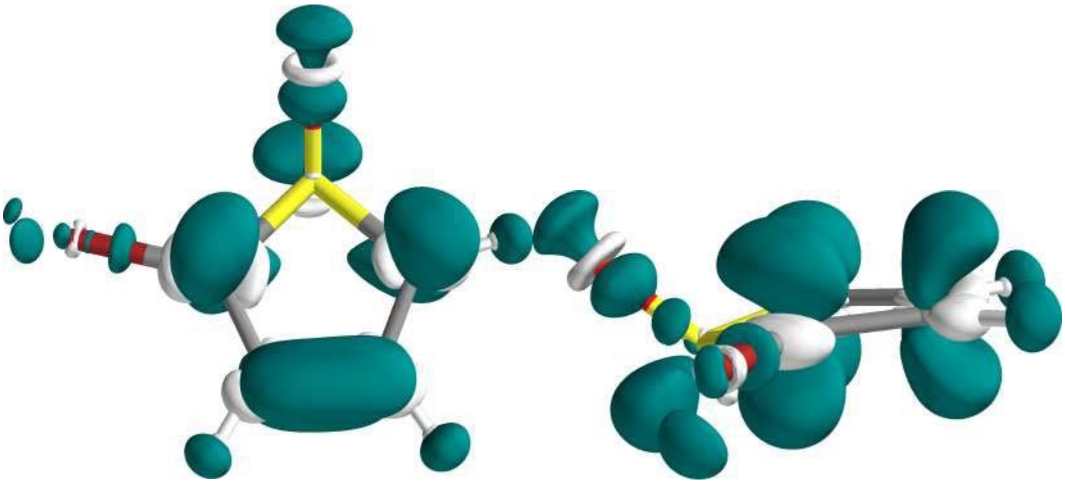

Figure 4: Representation of the F+ function from two points of view. The Blue color indicate the most electrophilic regions.

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	f	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - end-ing OM (% if > 5%)
1	Singlet-A	372	26813	0.011	7.0	0.55	212.13	0.68	43-44(96);
2	Singlet-A	323	30872	0.039	-14.2	0.72	117.23	0.47	41-44(6); 42-44(89);
3	Singlet-A	269	37132	0.030	13.6	0.49	195.64	0.71	41-44(89);
4	Singlet-A	243	41072	0.014	11.4	0.41	275.67	0.76	42-45(14); 43-45(82);
5	Singlet-A	239	41777	0.001	3.9	0.51	221.17	0.69	42-45(83); 43-45(14);
6	Singlet-A	233	42806	0.003	-10.9	0.37	271.77	0.82	40-44(95);
7	Singlet-A	218	45858	0.038	5.1	0.54	190.18	0.56	39-44(8); 43-46(77);
8	Singlet-A	212	46980	0.004	-2.4	0.66	137.66	0.44	39-44(35); 42-46(47); 43-46(11);
9	Singlet-A	199	50095	0.028	0.7	0.63	139.50	0.40	38-44(8); 39-44(43); 42-46(33);
10	Singlet-A	194	51381	0.033	5.7	0.51	213.99	0.62	41-45(82);
11	Singlet-A	183	54540	0.032	10.7	0.63	200.83	0.43	38-44(66); 41-46(11); 42-48(7);
12	Singlet-A	181	54948	0.005	-0.2	0.55	82.45	0.65	40-45(86);
13	Singlet-A	179	55615	0.017	-16.2	0.41	340.38	0.65	41-46(15); 43-47(60); 43-48(7); 43-49(6);
14	Singlet-A	177	56265	0.001	-12.7	0.50	148.15	0.61	41-46(9); 43-48(82);
15	Singlet-A	175	57118	0.014	-12.9	0.50	195.46	0.51	41-46(42); 42-48(10); 43-49(28);

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	0.0266	0.4433	0.0296
C	-0.5456	1.6487	0.1316
C	-2.0042	1.5830	0.1138
C	-2.5006	0.3448	-0.0019
S	-1.2032	-0.8390	-0.3690
Br	1.8538	0.0144	-0.0047
H	-2.6141	2.4763	0.1738
H	0.0008	2.5795	0.2065
H	-3.5300	0.0280	-0.0637
O	-1.1684	-2.0351	0.5141

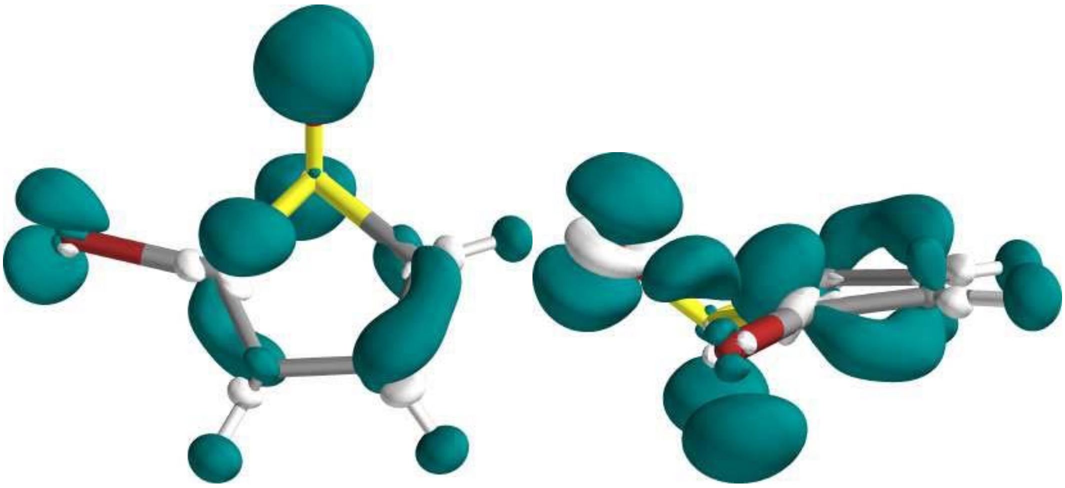

Figure 5: Representation of the F- function from two points of view. The Blue color indicate the most nucleophilic regions.

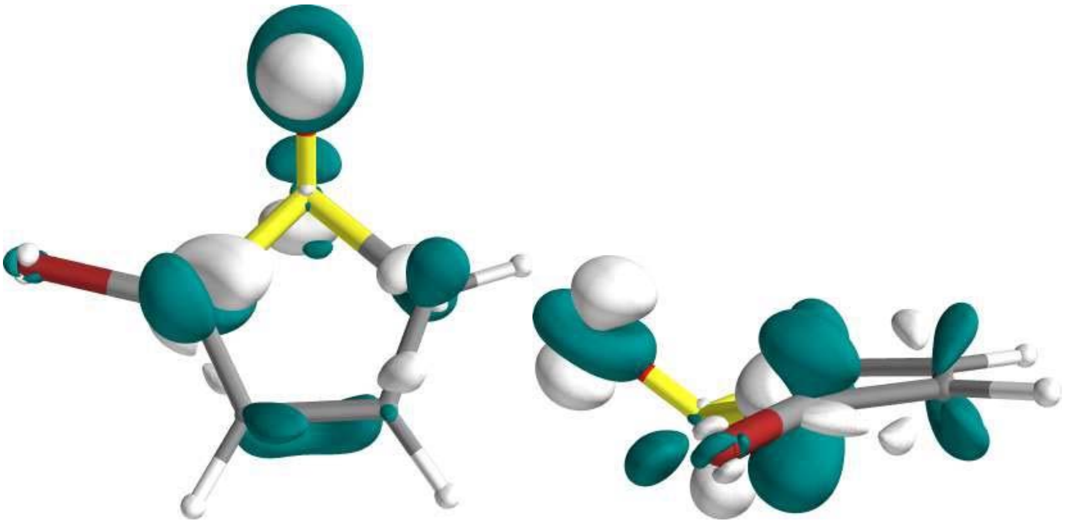

Figure 6: Representation of the Dual descriptor from two points of view. Electrophilic and nucleophilic regions correspond to blue and white surfaces.

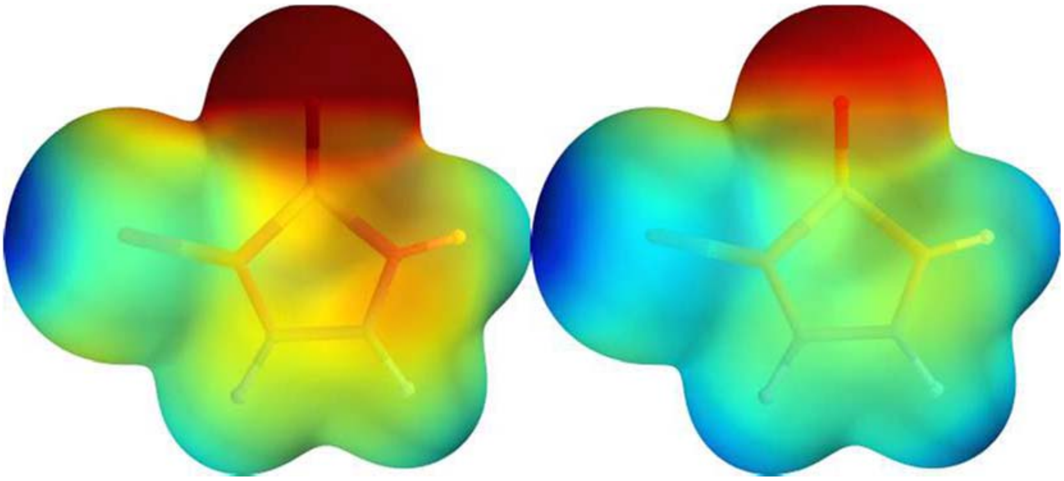

Figure 7: Representations of the Molecular Electrostatic Potential mapped on the electron density (cutoff value of

0.002 e-/bohr3). On the left, red, blue and green regions correspond to negative values < -0.06 a.u., positive values >

0.08 a.u. and neutral values respectively. On the right, the scale is set automatically to highlight the minimum values in red and the maximum values in blues.

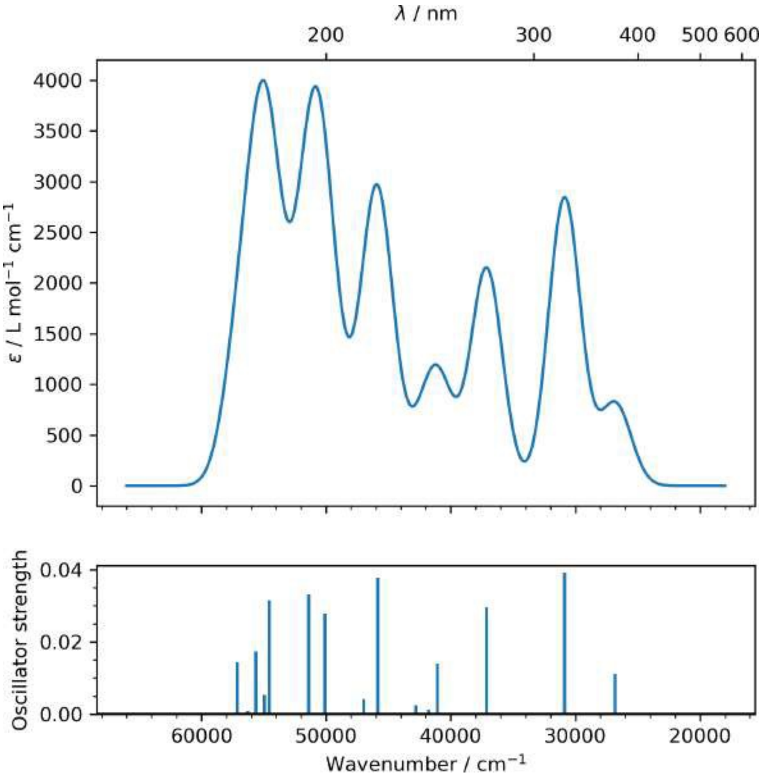

Figure 8: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

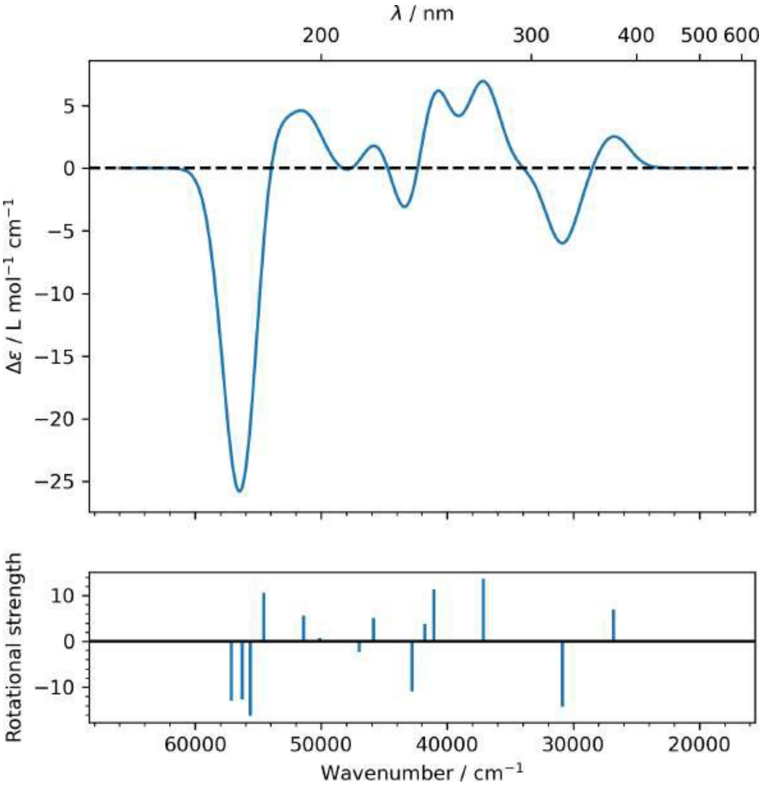

Figure 9: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

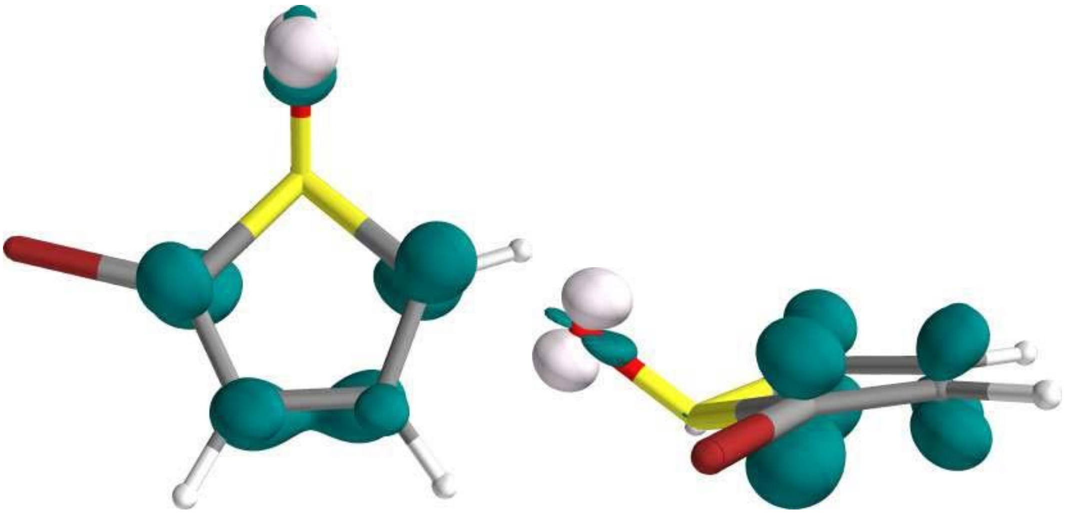

Figure 10: Representation of the Electron Density Difference (S1-S0) from two points of view.

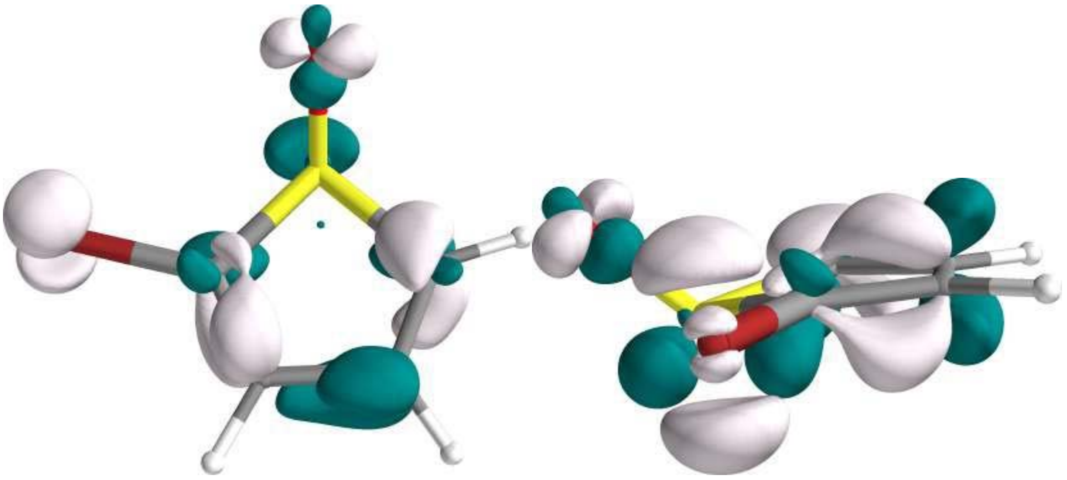

Figure 11: Representation of the Electron Density Difference (S2-S0) from two points of view.

9- 2-bromothiophene sulfone 2-SO2

a.Description

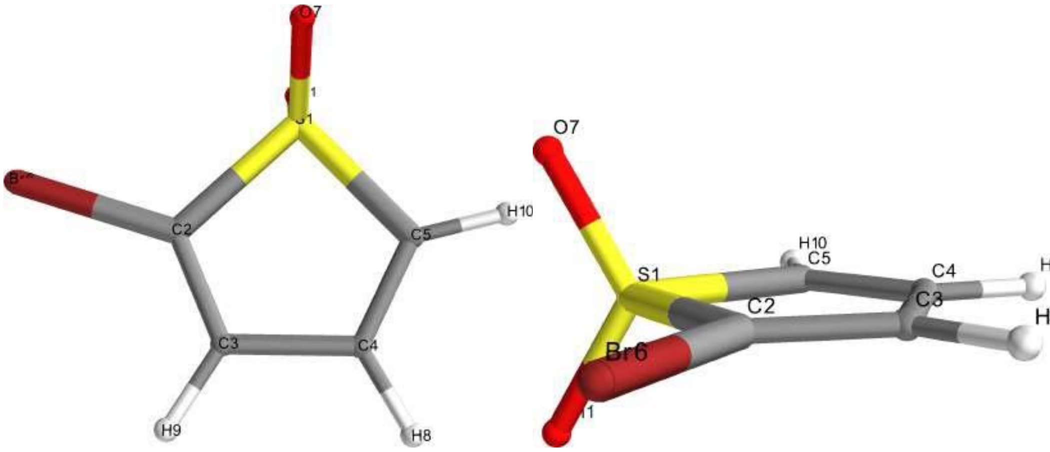

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	2-SO2
Formula	C4H3BrO2S
Charge	0
Spin multiplicity	1
Monoisotopic mass	193.90371 Da
InChI	1S/C4H3BrO2S/c5-4-2-1-3-8(4,6)7/h1-3H
SMILES	S1(=O)(=O)C(=CC=C1)Br

b. Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	236	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization		
Max Force value and threshold	0.000200	0.000450
RMS Force value and threshold	0.000037	0.000300
Max Displacement value and threshold	0.001677	0.001800
RMS Displacement value and threshold	0.000427	0.001200

Job type: Frequency and thermochemical analysis	
Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

Job type: Time-dependent calculation		
Number of calculated excited states and spin state	15	['Singlet-A']

c. Results

Total molecular energy	-3277.02314 hartrees	
HOMO number	47	
LUMO+1 energies	-0.92 eV	
LUMO energies	-2.72 eV	
HOMO energies	-7.25 eV	
HOMO-1 energies	-8.30 eV	
CDFT indices: Electron Affinity	0.0010 hartrees	
CDFT indices: Ionisation Potential	0.0125 hartrees	
CDFT indices: Electronegativity	0.0068 hartrees	
CDFT indices: Hardness	0.0116 hartrees	
CDFT indices: Electrophilicity	0.0020	
CDFT indices: Electron-flow	0.5844 e-	
Geometry optimization specific results		
Converged nuclear repulsion energy	706.02614 Hartrees	
Frequency and Thermochemistry specific results		
Enthalpy at 298.15 K	-3276.94987 Hartrees	
Gibbs free energy at 298.15 K	-3276.99167 Hartrees	
Entropy at 298.15 K	0.00014 Hartrees	
Mean Mulliken atomic charge and standard deviation	-0.0000 e-	0.4063 e-
Atoms with negatives charges under the standard deviation	NÂ°	Mulliken charge
	O 11	-0.564
	O 7	-0.564
Atoms with positives charges over the standard deviation	NÂ°	Mulliken charge
	S 1	+1.060

Table. Selection of the most important condensed Fukui functions based on Mulliken charges.

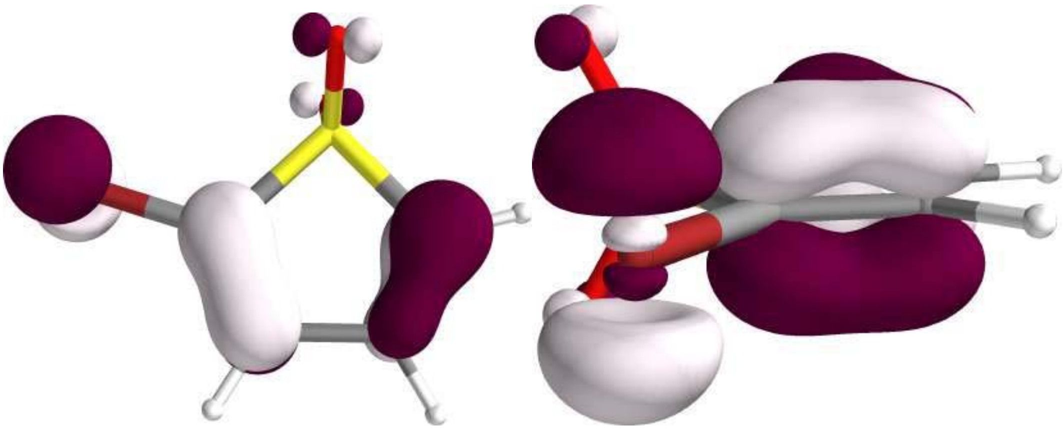

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1333	167	A
1150	134	A
697	65	A

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	f	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	315	31658	0.070	0.1	0.79	142.13	0.43	47-48(97);
2	Singlet-A	279	35838	0.000	-0.1	0.47	204.73	0.76	46-48(96);
3	Singlet-A	238	41907	0.000	0.1	0.52	197.43	0.68	47-49(95);
4	Singlet-A	236	42254	0.047	0.0	0.59	213.14	0.65	45-48(90);
5	Singlet-A	233	42888	0.001	-0.4	0.44	201.10	0.75	43-48(92);
6	Singlet-A	230	43473	0.036	0.3	0.50	219.23	0.75	44-48(91);
7	Singlet-A	206	48435	0.004	-0.0	0.50	210.65	0.74	42-48(96);
8	Singlet-A	197	50531	0.014	0.0	0.60	155.45	0.55	41-48(39); 46-49(53);
9	Singlet-A	194	51329	0.028	0.1	0.62	164.20	0.55	41-48(50); 46-49(40);
10	Singlet-A	181	55039	0.001	0.0	0.32	236.22	0.81	44-49(11); 45-49(78); 47-51(7);
11	Singlet-A	178	55909	0.000	-0.3	0.40	133.27	0.69	44-49(11); 45-49(15); 47-51(70);
12	Singlet-A	176	56553	0.016	0.2	0.77	187.91	0.38	40-48(42); 47-50(50);
13	Singlet-A	175	56892	0.001	0.3	0.45	148.86	0.69	44-49(72); 47-51(20);
14	Singlet-A	175	57067	0.026	-0.4	0.52	154.29	0.67	43-49(92);
15	Singlet-A	165	60510	0.001	0.1	0.41	211.53	0.70	47-52(67); 47-53(24);

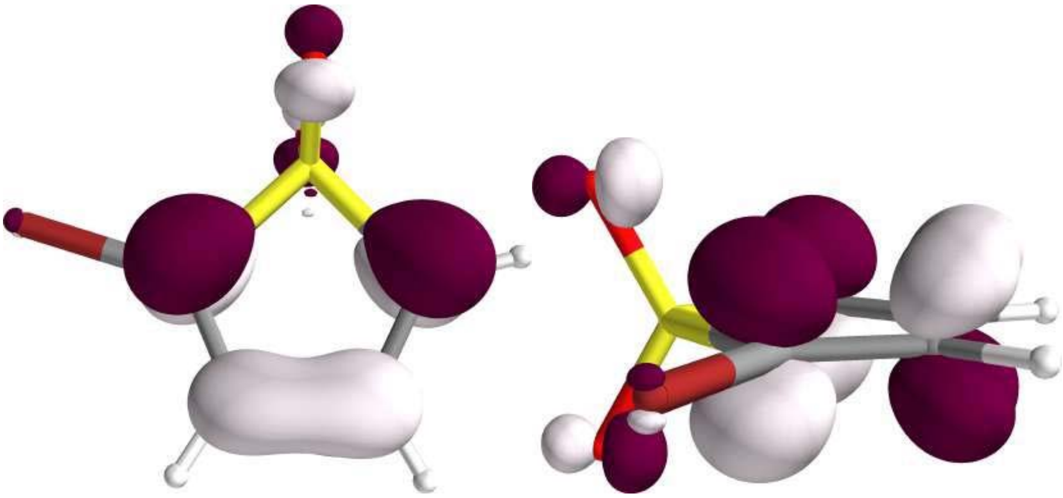

Figure 3: Representation of the LUMO from two points of view.

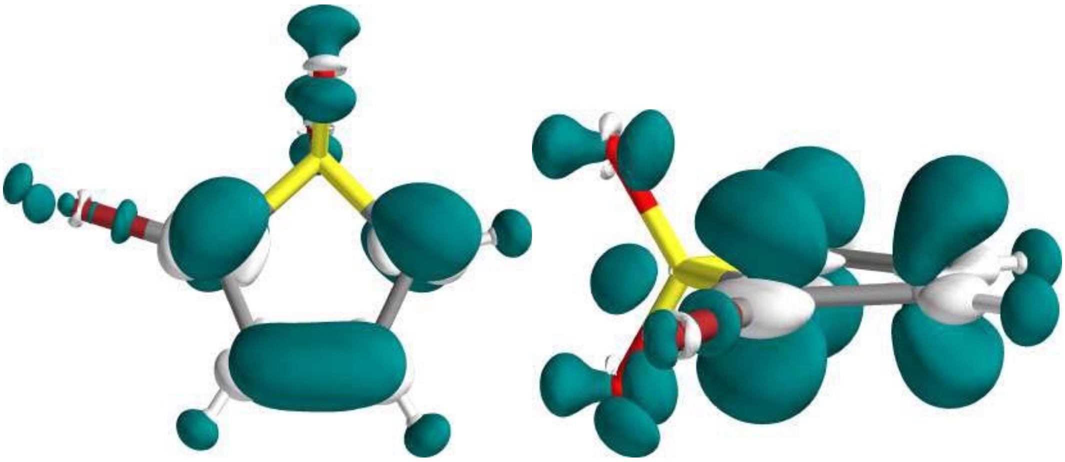

Figure 4: Representation of the F+ function from two points of view. The Blue color indicate the most electrophilic regions.

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	-1.1563	-0.6883	0.0002
C	0.1831	0.5467	-0.0011
C	-0.3277	1.7734	-0.0001
C	-1.8067	1.7961	0.0004
C	-2.3953	0.6039	0.0013
Br	1.9639	-0.0150	-0.0003
O	-1.1619	-1.4088	1.2536
H	-2.3483	2.7331	-0.0005
H	0.2619	2.6793	0.0008
H	-3.4422	0.3457	-0.0002
O	-1.1665	-1.4088	-1.2533

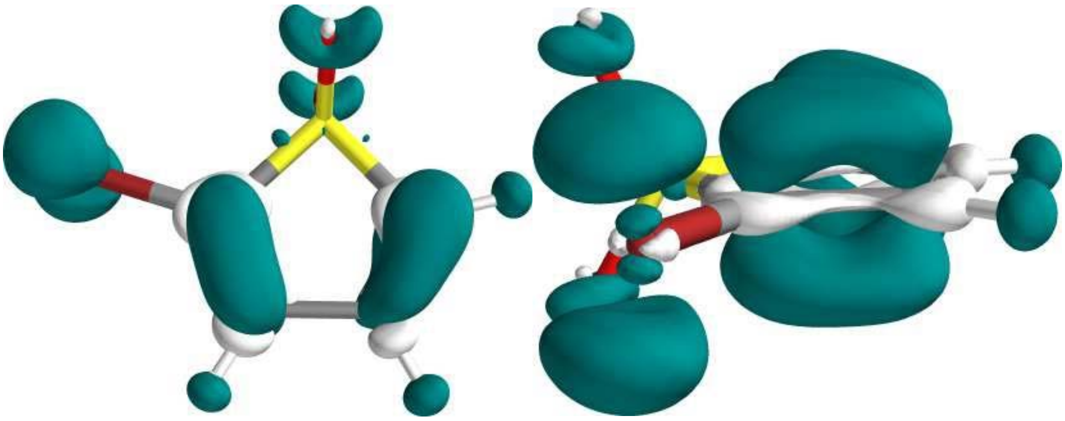

Figure 5: Representation of the F- function from two points of view. The Blue color indicate the most nucleophilic regions.

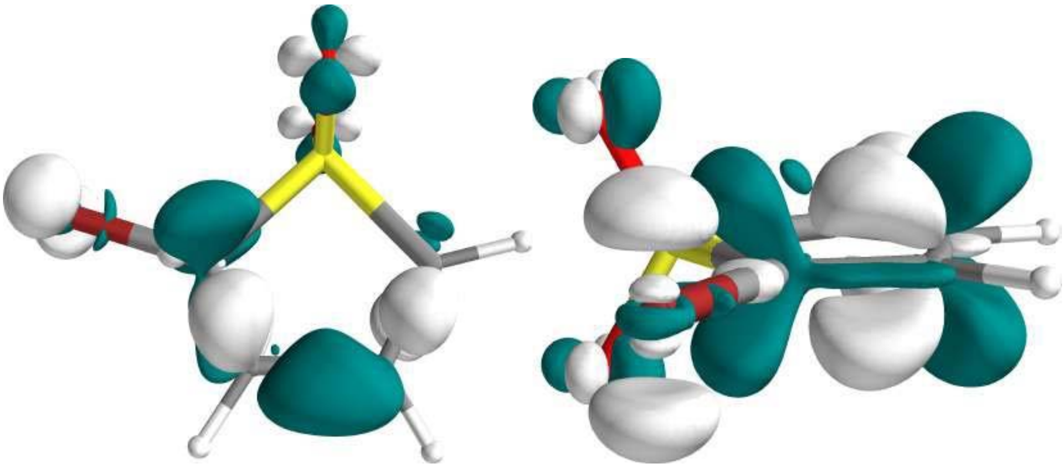

Figure 6: Representation of the Dual descriptor from two points of view. Electrophilic and nucleophilic regions correspond to blue and white surfaces.

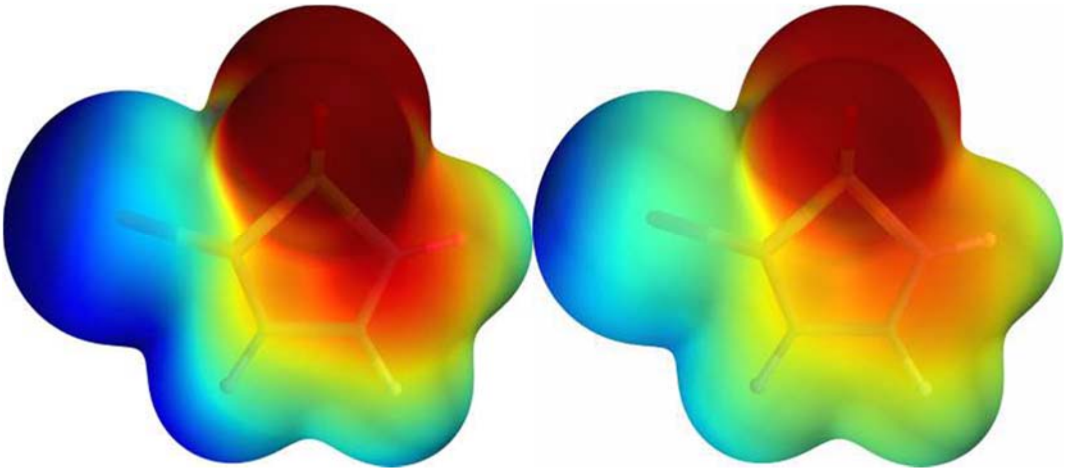

Figure 7: Representations of the Molecular Electrostatic Potential mapped on the electron density (cutoff value of

0.002 e-/bohr3). On the left, red, blue and green regions correspond to negative values < -0.06 a.u., positive values >

0.08 a.u. and neutral values respectively. On the right, the scale is set automatically to highlight the minimum values in red and the maximum values in blues.

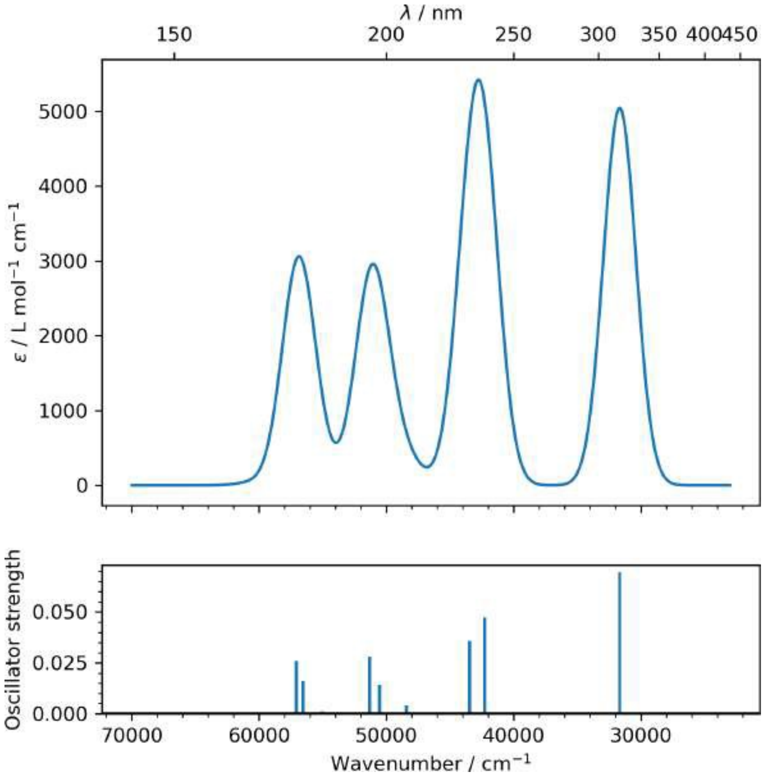

Figure 8: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

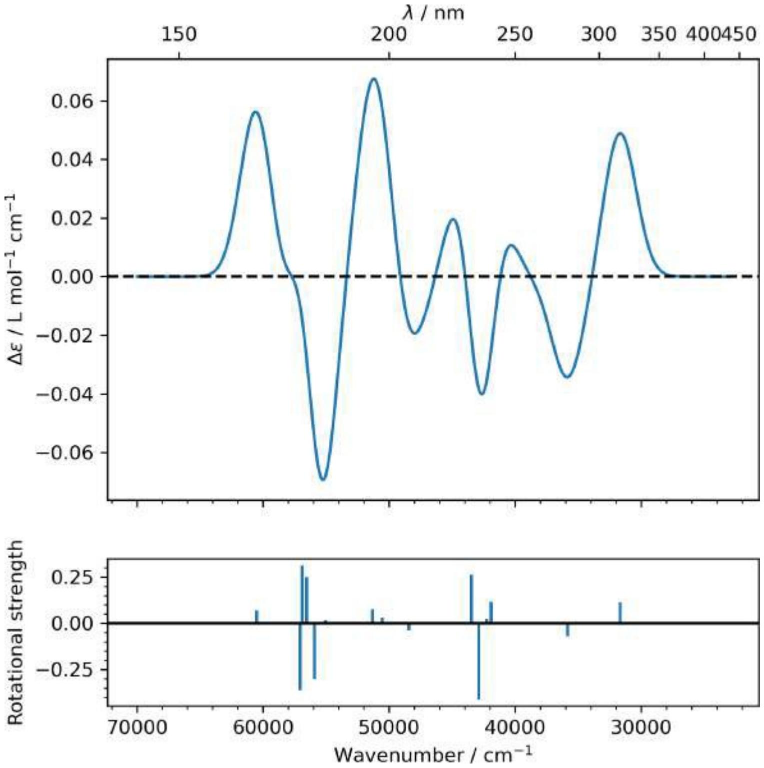

Figure 9: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

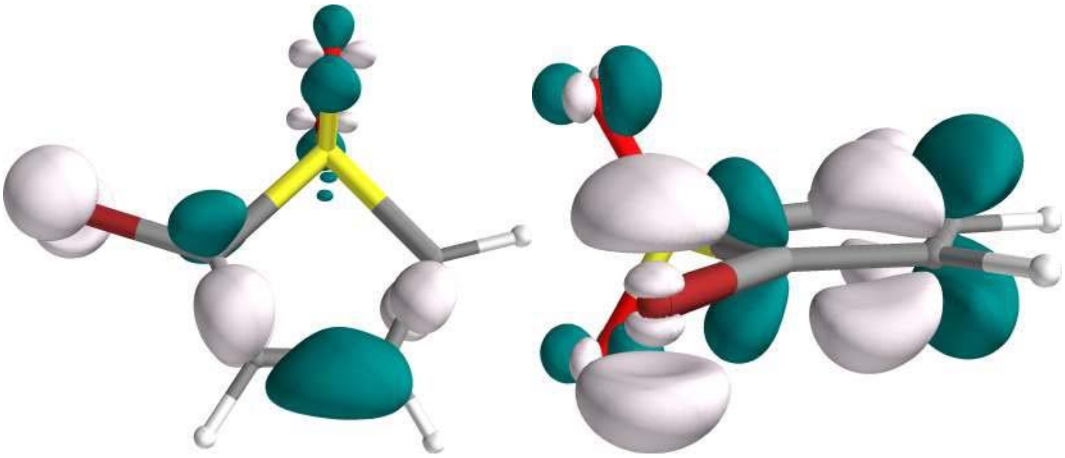

Figure 10: Representation of the Electron Density Difference (S1-S0) from two points of view.

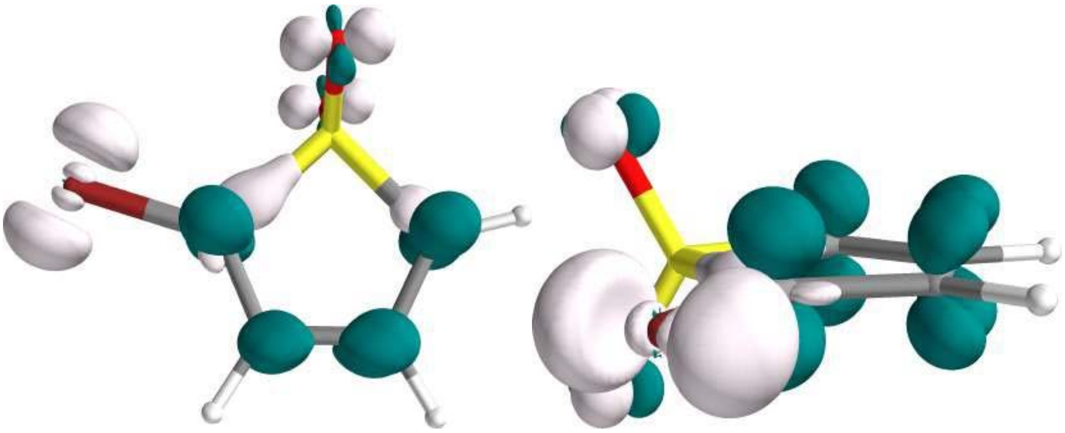

Figure 11: Representation of the Electron Density Difference (S2-S0) from two points of view.

10- Cycloadduct 2-CySO

a- Description

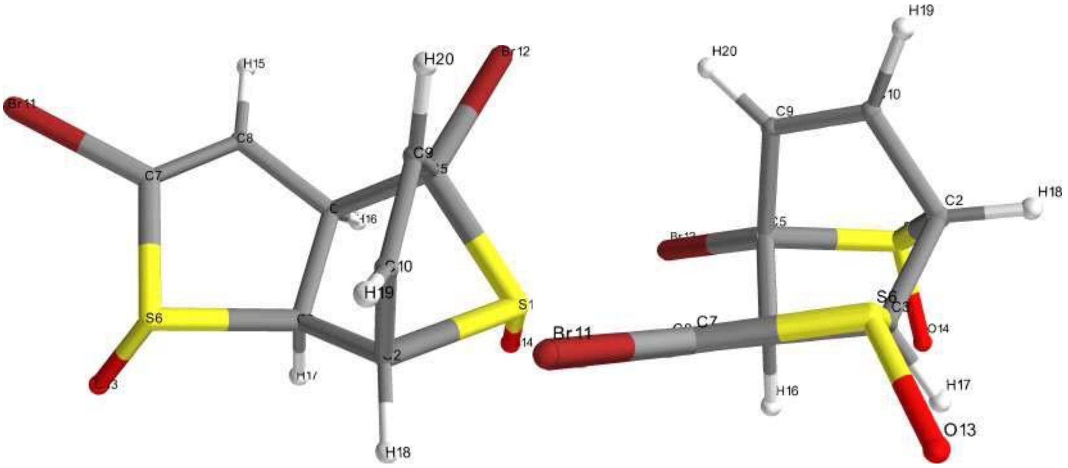

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	2-CySO
Formula	C8H6Br2O2S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	426	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000100	0.000450
RMS Force value and threshold	0.000021	0.000300
Max Displacement value and threshold	0.001761	0.001800
RMS Displacement value and threshold	0.000407	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-6403.61982 hartrees
HOMO number	86
LUMO+1 energies	-1.44 eV
LUMO energies	-1.90 eV
HOMO energies	-6.84 eV
HOMO-1 energies	-7.15 eV

Geometry optimization specific results

Converged nuclear repulsion energy	1981.64527 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-6403.48045 Hartrees
Gibbs free energy at 298.15 K	-6403.53669 Hartrees
Entropy at 298.15 K	0.00019 Hartrees

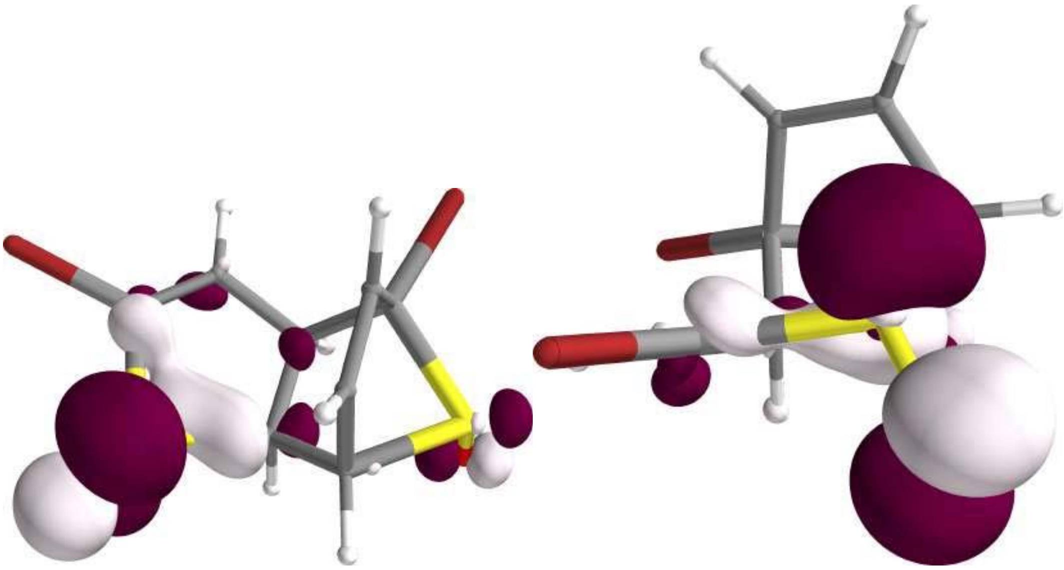

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1141	57	A
1124	71	A
1086	117	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	-2.6405	1.3811	0.0672
C	-0.9476	2.0292	0.6841
C	-0.0065	1.5065	-0.4096
C	-0.4374	0.0529	-0.7306
C	-1.5982	-0.2337	0.2595
S	1.8010	1.5484	0.1177
C	1.8776	-0.2543	-0.1948
C	0.7540	-0.8412	-0.5801
C	-1.2217	-0.0639	1.6900
C	-0.8677	1.2048	1.9292
Br	3.5491	-1.0980	0.0788
Br	-2.5979	-1.8515	-0.1558
O	2.5544	2.2763	-0.9406
O	-2.8280	1.7100	-1.3660
H	0.6766	-1.9038	-0.7788
H	-0.8544	-0.0105	-1.7388
H	-0.0191	2.1415	-1.2944
H	-0.9505	3.1077	0.8119
H	-0.5738	1.6027	2.8909
H	-1.2613	-0.8677	2.4109

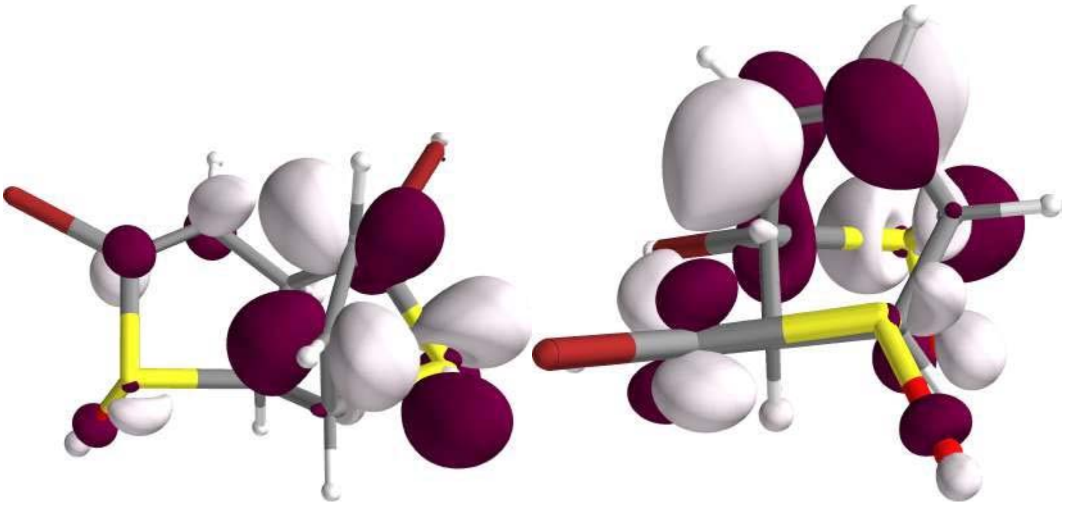

Figure 3: Representation of the LUMO from two points of view.

11- Cycloadduct 2-Cymix

a. Description

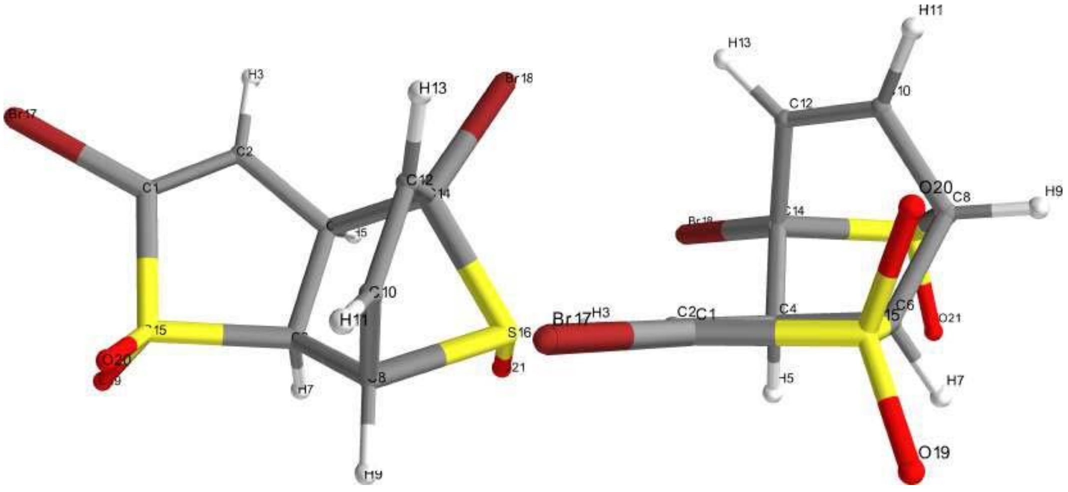

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	2-Cymix
Formula	C8H6Br2O3S2
Charge	0
Spin multiplicity	1
Monoisotopic mass	371.81251 Da
InChI	1S/C8H6Br2O3S2/c9-6-3-4-7(15(6,12)13)5-1-2-8(4,10)14(5)11/h1-5,7H/t4-,5+,7+,8-,14-/m1/s1
SMILES	C1(=C[C@@H]2[C@@H]([C@@H]3C=C[C@]2([S@@]3=O)Br)S1(=O)=O)Br

b. Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	449	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization

Max Force value and threshold	0.000103	0.000450
RMS Force value and threshold	0.000016	0.000300
Max Displacement value and threshold	0.001400	0.001800
RMS Displacement value and threshold	0.000237	0.001200

c. Results

Total molecular energy	-6478.86581 hartrees
HOMO number	90
LUMO+1 energies	-1.41 eV
LUMO energies	-1.90 eV
HOMO energies	-7.24 eV
HOMO-1 energies	-7.85 eV

Geometry optimization specific results		
Converged nuclear repulsion energy	2201.37154 Hartrees	
Mean Mulliken atomic charge and standard deviation	-0.0000 e-	0.3681 e-
Atoms with negatives charges under the standard deviation	NÂ°	Mulliken charge
	O 21	-0.616
	O 20	-0.585
	O 19	-0.561
Atoms with positives charges over the standard deviation	NÂ°	Mulliken charge
	S 16	+0.709
	S 15	+1.068

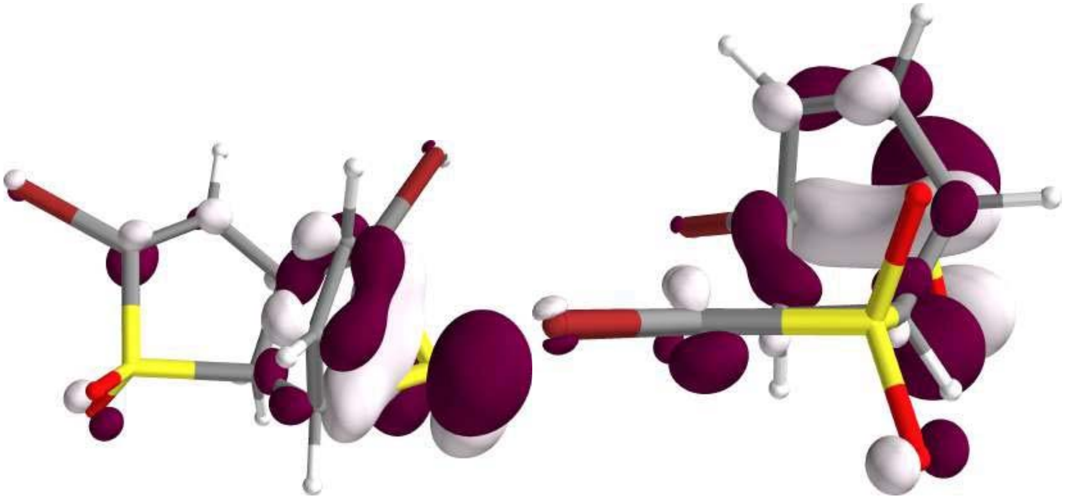

Figure 2: Representation of the HOMO from two points of view.

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	1.7921	-0.4359	-0.2574
C	0.6220	-0.9834	-0.5446
H	0.4757	-2.0526	-0.6355
C	-0.5379	-0.0462	-0.7530
H	-0.9481	-0.1608	-1.7582
C	-0.0748	1.4162	-0.5322
H	-0.1845	2.0107	-1.4364
C	-0.9178	1.9938	0.6125
H	-0.8575	3.0723	0.7191
C	-0.8384	1.1902	1.8696
H	-0.4693	1.5919	2.8019
C	-1.2772	-0.0585	1.6766
H	-1.3356	-0.8424	2.4178
C	-1.6990	-0.2419	0.2603
S	1.7363	1.3627	-0.2014
S	-2.6599	1.4192	0.0569
Br	3.4335	-1.2947	0.0684
Br	-2.7829	-1.8165	-0.1005
O	2.4462	1.9056	-1.3392
O	2.0390	1.8362	1.1342
O	-2.8715	1.7281	-1.3780

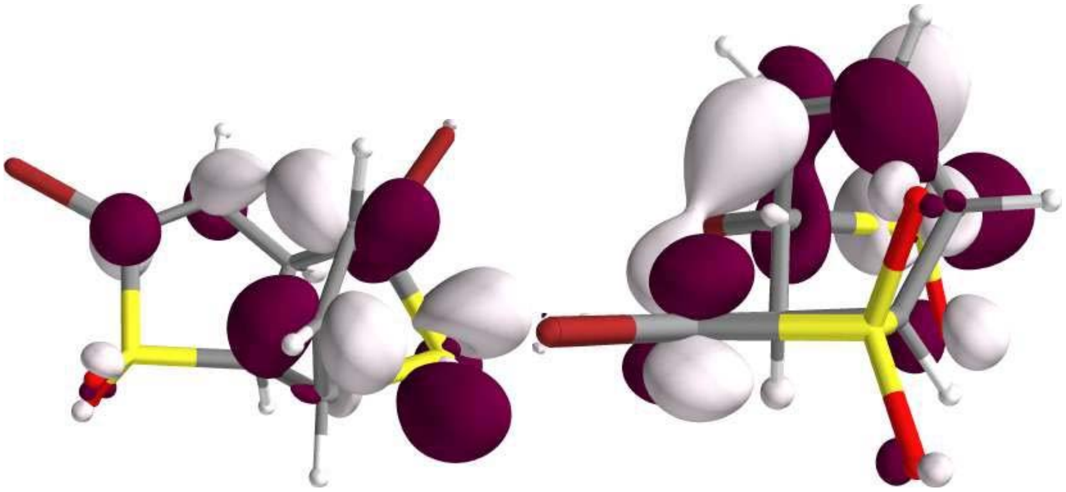

Figure 3: Representation of the LUMO from two points of view.

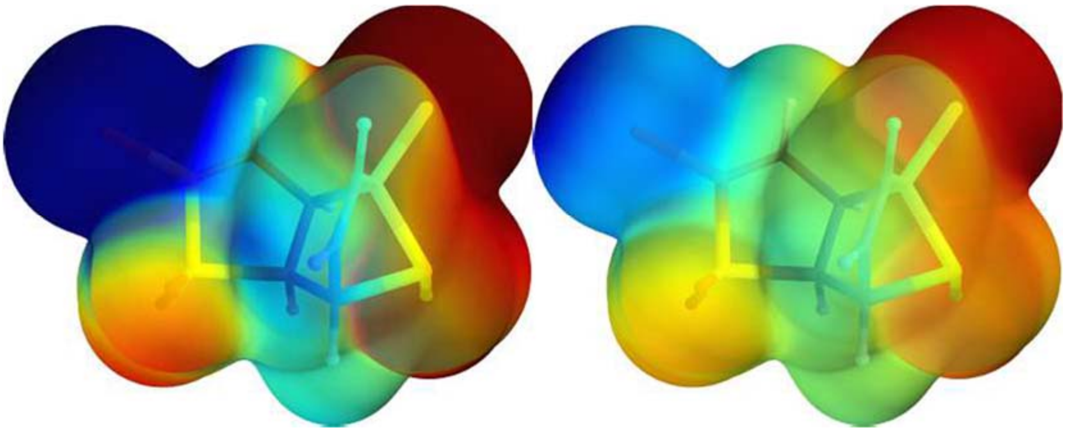

Figure 4: Representations of the Molecular Electrostatic Potential mapped on the electron density (cutoff value of

0.002 e-/bohr3). On the left, red, blue and green regions correspond to negative values < -0.06 a.u., positive values >

0.08 a.u. and neutral values respectively. On the right, the scale is set automatically to highlight the minimum values in red and the maximum values in blues.

12- Cycloadduct 2-Cy

a- Description

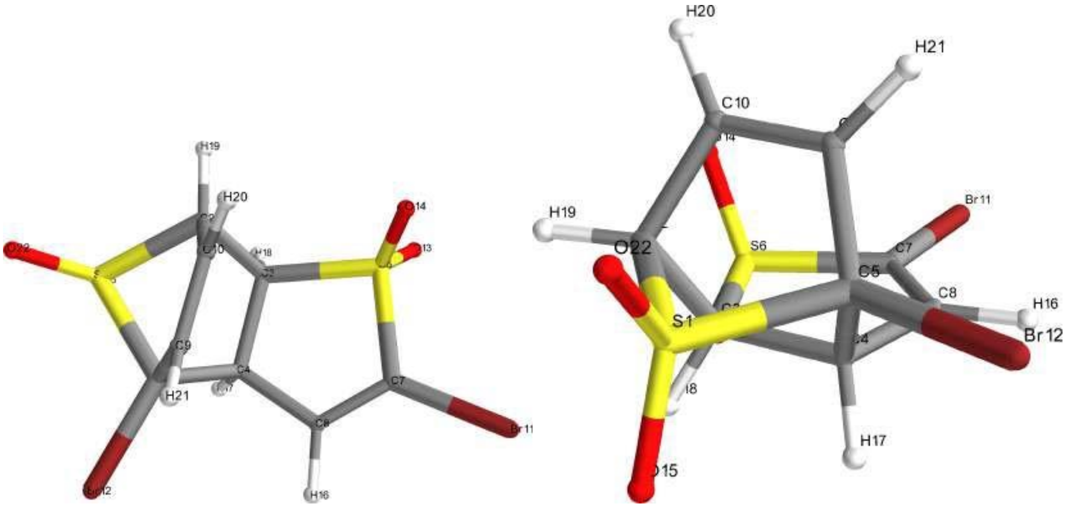

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	2-Cy
Formula	C8H6Br2O4S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	472	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000060	0.000450
RMS Force value and threshold	0.000010	0.000300
Max Displacement value and threshold	0.001217	0.001800
RMS Displacement value and threshold	0.000250	0.001200

c- Results

Total molecular energy	-6554.09647 hartrees
HOMO number	94
LUMO+1 energies	-1.54 eV
LUMO energies	-1.81 eV
HOMO energies	-7.91 eV
HOMO-1 energies	-8.19 eV

Geometry optimization specific results	
Converged nuclear repulsion energy	2411.77097 Hartrees

Table. Converged cartesian atomic coordinates in Angstrom

Atom	X	Y	Z
S	2.5299	-1.2080	-0.1339
C	0.8826	-1.9170	0.5029
C	-0.0121	-1.3402	-0.6098
C	0.3672	0.1621	-0.7937
C	1.5427	0.4097	0.1982
S	-1.8172	-1.3920	-0.2241
C	-1.9693	0.4006	-0.2210
C	-0.8392	1.0211	-0.5159
C	1.1249	0.1470	1.5999
C	0.7614	-1.1303	1.7642
Br	-3.6504	1.1553	0.1471
Br	2.5327	2.0404	-0.1232
O	-2.5227	-1.9356	-1.3634
O	-2.0577	-1.9253	1.1004
O	2.6933	-1.4411	-1.5544
H	-0.7552	2.0987	-0.5792
H	0.7286	0.3374	-1.8079
H	0.0910	-1.8982	-1.5366
H	0.8793	-2.9990	0.5843
H	0.4501	-1.5774	2.6960
H	1.1693	0.9005	2.3721
O	3.6375	-1.4017	0.7689

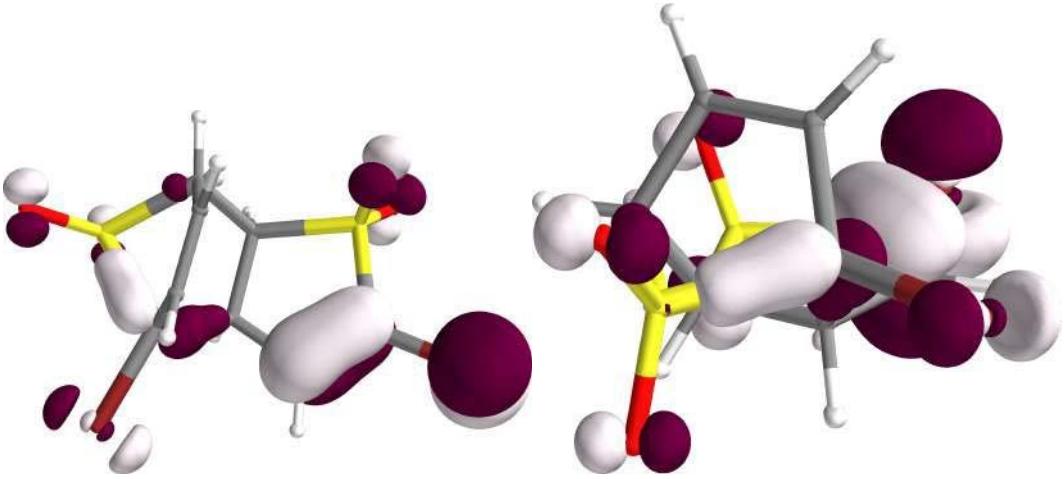

Figure 2: Representation of the HOMO from two points of view.

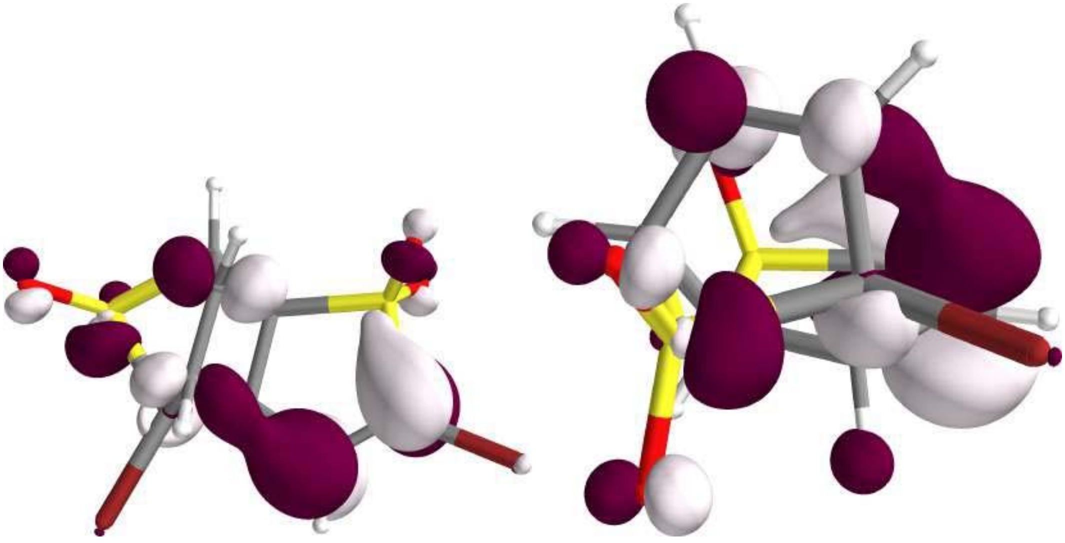

Figure 3: Representation of the LUMO from two points of view.

13- 3-bromothiophene 3

a- Description

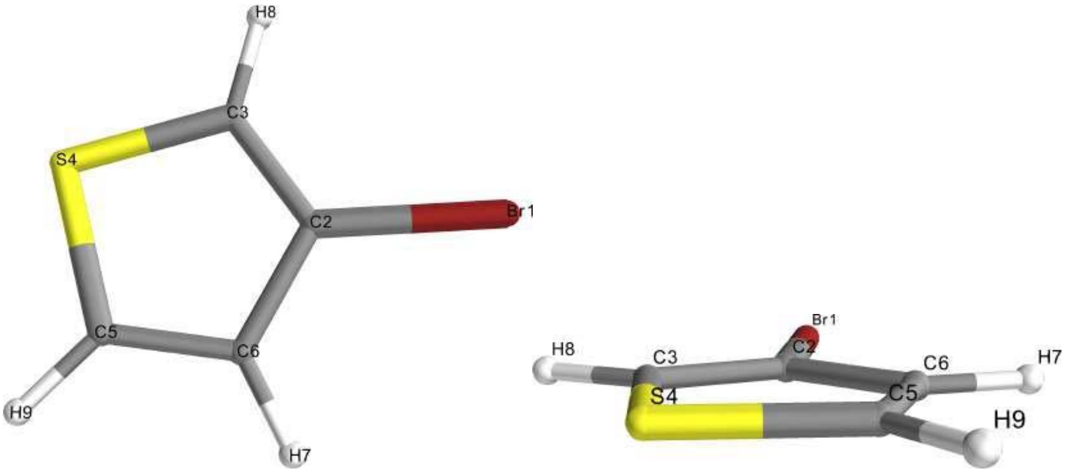

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	3
Formula	C4H3BrS
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	190	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization		
Max Force value and threshold	0.000149	0.000450
RMS Force value and threshold	0.000043	0.000300
Max Displacement value and threshold	0.000711	0.001800
RMS Displacement value and threshold	0.000210	0.001200

Job type: Frequency and thermochemical analysis	
Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

Job type: Time-dependent calculation	
Number of calculated excited states and spin state	15['Singlet-A']

c- Results

Total molecular energy	-3126.61469 hartrees
HOMO number	39
LUMO+1 energies	-0.49 eV
LUMO energies	-0.86 eV
HOMO energies	-6.67 eV
HOMO-1 energies	-7.16 eV

Geometry optimization specific results

Converged nuclear repulsion energy	437.62442 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-3126.55174 Hartrees
Gibbs free energy at 298.15 K	-3126.58884 Hartrees
Entropy at 298.15 K	0.00012 Hartrees

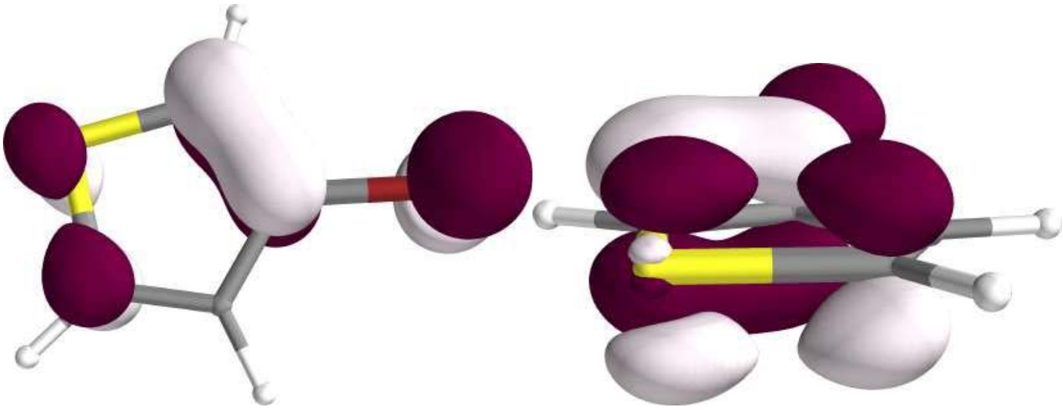

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in avenumbers

Frequencies	Intensity	Symmetry
780	72	A

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	f	R	Λ	d$_{CT}$	q$_{CT}$	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	246	40604	0.000	0.0	0.59	64.90	0.67	39-41(99);
2	Singlet-A	231	43243	0.078	-0.0	0.78	223.46	0.41	38-40(6); 39-40(86);
3	Singlet-A	222	45044	0.000	-0.0	0.40	182.77	0.80	38-41(98);
4	Singlet-A	211	47310	0.064	-0.0	0.80	63.68	0.36	38-40(82); 39-40(8);
5	Singlet-A	208	48037	0.001	0.0	0.48	172.46	0.73	39-42(97);
6	Singlet-A	197	50648	0.001	0.0	0.25	332.82	0.91	37-40(98);
7	Singlet-A	194	51325	0.002	-0.0	0.48	119.59	0.72	38-42(96);
8	Singlet-A	193	51743	0.002	-0.0	0.52	219.07	0.72	37-41(95);
9	Singlet-A	175	56870	0.153	-0.0	0.61	202.50	0.43	36-40(37); 39-43(51);
10	Singlet-A	173	57715	0.001	-0.0	0.56	56.08	0.62	36-41(92);
11	Singlet-A	172	57876	0.072	-0.0	0.59	222.13	0.45	36-40(53); 38-43(12); 39-43(28);
12	Singlet-A	170	58553	0.001	0.0	0.39	227.37	0.76	39-44(85); 39-45(7);
13	Singlet-A	162	61440	0.006	0.0	0.42	241.08	0.69	39-44(7); 39-45(85);
14	Singlet-A	161	61819	0.002	0.0	0.46	124.30	0.57	35-40(25); 38-44(69);
15	Singlet-A	160	62238	0.118	-0.0	0.43	321.71	0.64	37-42(64); 38-43(18);

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
Br	-1.8732	-0.0499	-0.0000
C	0.0286	0.0585	0.0000
C	0.8356	-1.0348	0.0000
S	2.4969	-0.5590	-0.0000
C	2.0732	1.1171	0.0000
C	0.7247	1.2981	0.0000
H	0.2374	2.2619	-0.0000
H	0.5565	-2.0747	0.0000
H	2.8459	1.8687	0.0000

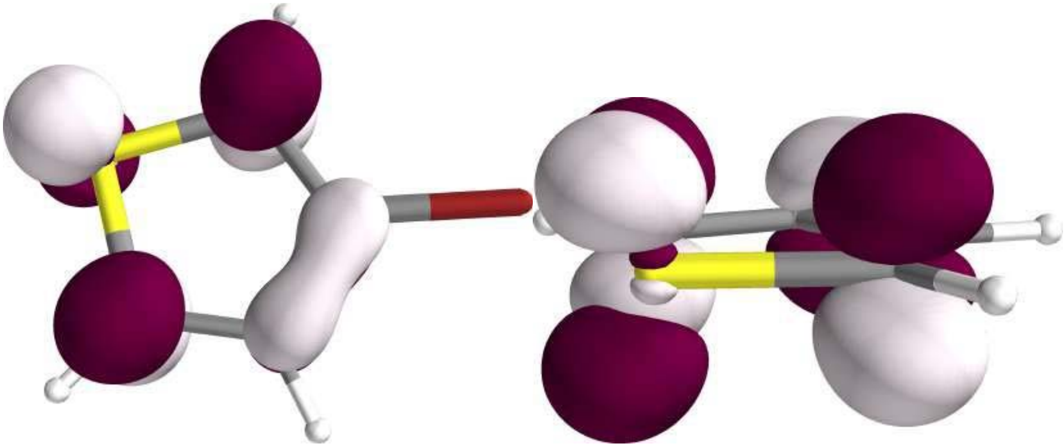

Figure 3: Representation of the LUMO from two points of view.

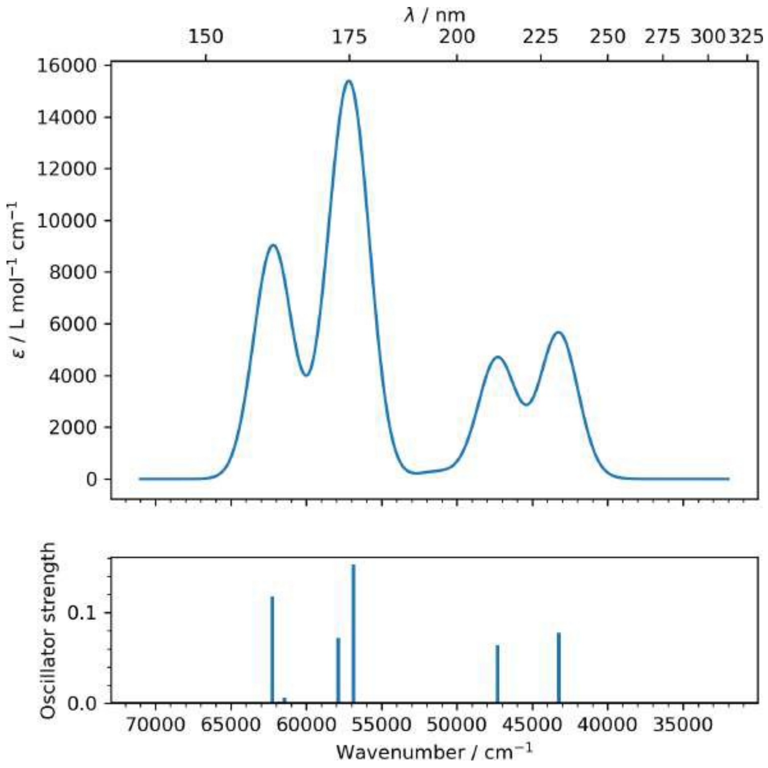

Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

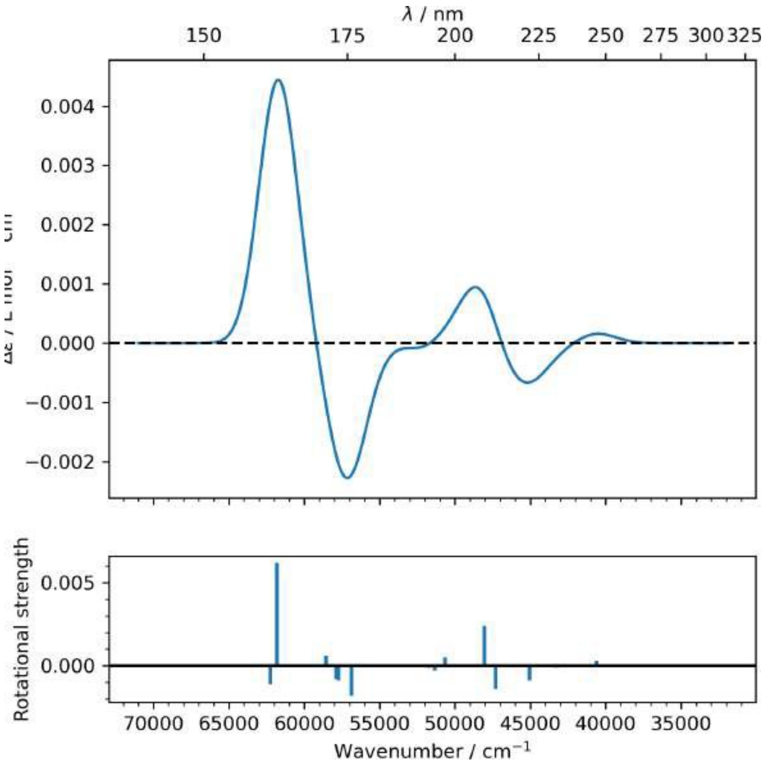

Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

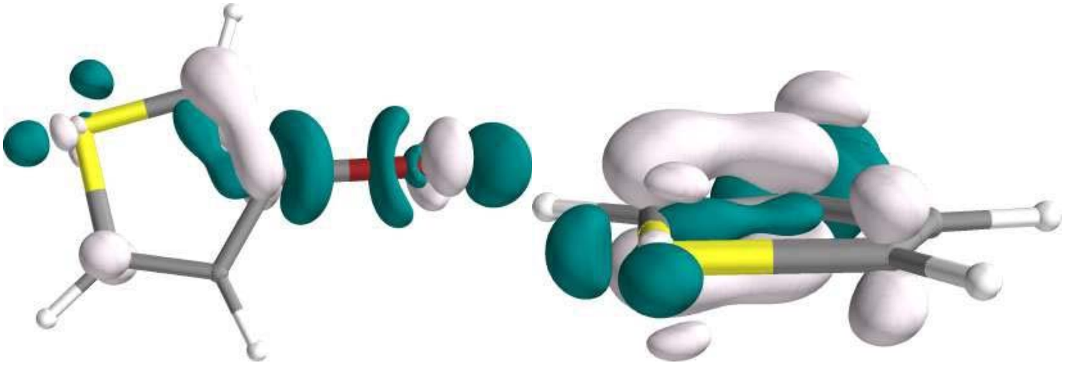

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

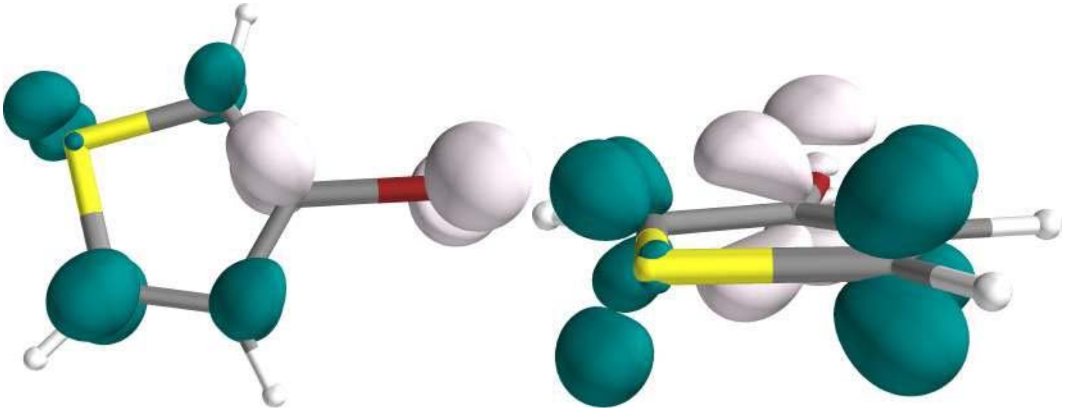

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.

14- 3-bromothiophene sulfoxyde 3-SO

a- Description

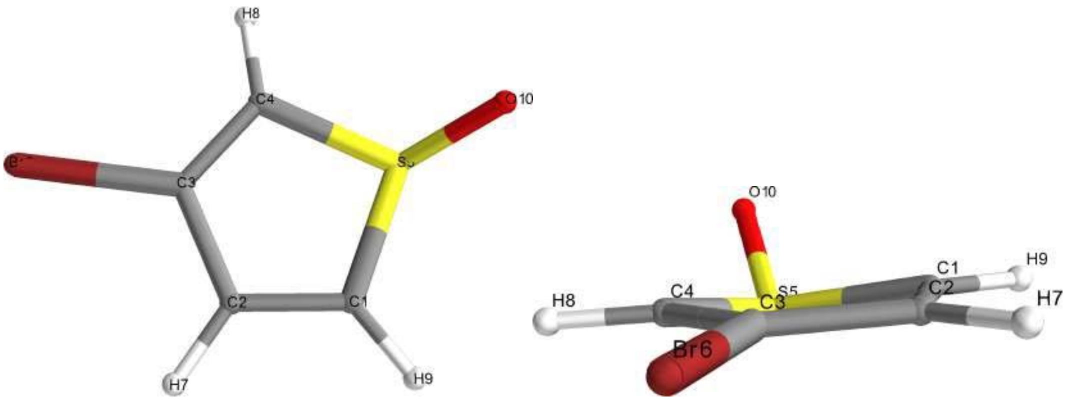

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	3-SO
Formula	C4H3BrOS
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	213	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization

Max Force value and threshold	0.000191	0.000450
RMS Force value and threshold	0.000045	0.000300
Max Displacement value and threshold	0.001031	0.001800
RMS Displacement value and threshold	0.000348	0.001200

Job type: Frequency and thermochemical analysis

Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

Job type: Time-dependent calculation

Number of calculated excited states and spin state	15	['Singlet-A']

c- Results

Total molecular energy	-3201.78642 hartrees
HOMO number	43
LUMO+1 energies	-0.85 eV
LUMO energies	-2.44 eV
HOMO energies	-6.75 eV
HOMO-1 energies	-7.26 eV

Geometry optimization specific results

Converged nuclear repulsion energy	541.86637 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-3201.71938 Hartrees
Gibbs free energy at 298.15 K	-3201.75952 Hartrees
Entropy at 298.15 K	0.00013 Hartrees

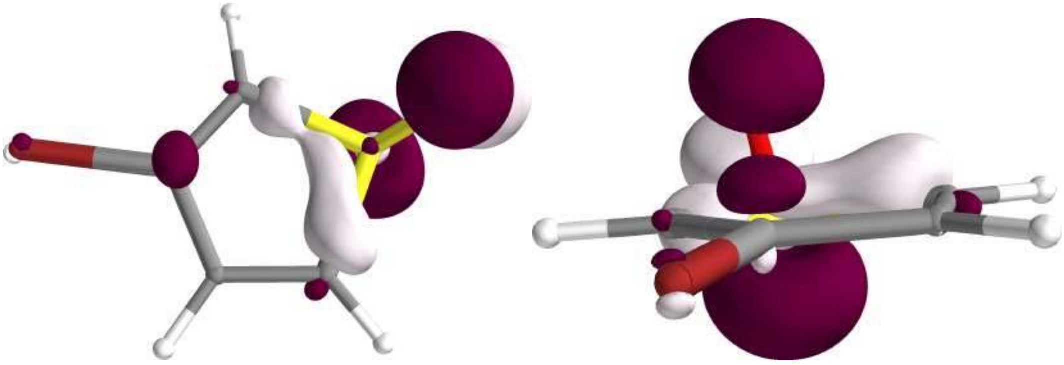

Figure 2: Representation of the HOMO from two points of view.

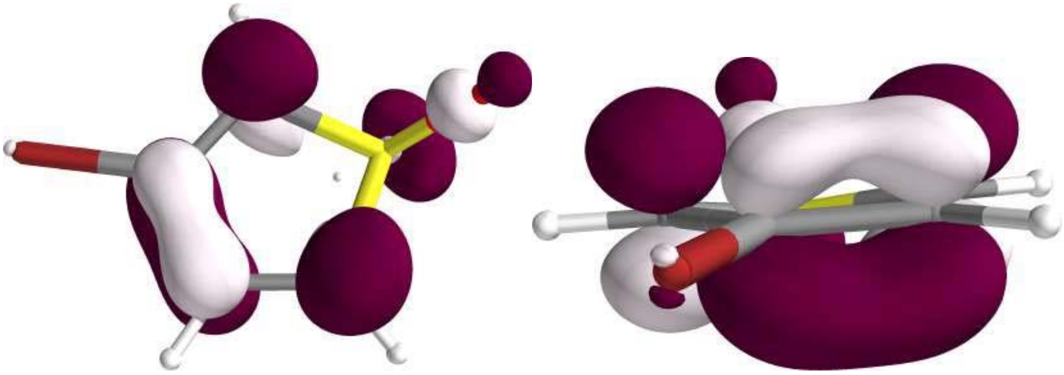

Figure 3: Representation of the LUMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in

	wavenumbers	
Frequencies	Intensity	Symmetry
1112	54	A
1092	72	A
1037	58	A
874	55	A
796	58	A

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm^{-1}	*f*	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	377	26524	0.014	0.2	0.55	195.31	0.68	43-44(96);
2	Singlet-A	312	32033	0.006	-10.8	0.73	96.97	0.48	41-44(8); 42-44(88);
3	Singlet-A	258	38610	0.013	1.8	0.51	107.03	0.67	41-44(86); 42-44(7);
4	Singlet-A	245	40685	0.016	-21.8	0.46	391.46	0.66	39-44(6); 42-45(7); 43-45(80);
5	Singlet-A	236	42229	0.003	8.5	0.43	296.49	0.76	39-44(16); 40-44(80);
6	Singlet-A	232	43085	0.001	-3.7	0.52	214.91	0.62	39-44(9); 42-45(82);
7	Singlet-A	222	44892	0.110	-6.4	0.54	52.08	0.49	39-44(50); 40-44(12); 43-45(12); 43-46(8);
8	Singlet-A	212	47122	0.050	-8.9	0.52	209.08	0.61	39-44(8); 43-46(83);
9	Singlet-A	196	50954	0.017	2.8	0.57	177.09	0.50	41-45(37); 42-46(46);
10	Singlet-A	192	51963	0.047	-2.8	0.55	131.48	0.50	39-45(6); 40-45(24); 41-45(31); 42-46(25);
11	Singlet-A	187	53245	0.030	4.2	0.53	15.22	0.60	40-45(72); 41-45(12);
12	Singlet-A	182	54843	0.006	-10.6	0.47	186.06	0.63	39-45(17); 43-47(64);
13	Singlet-A	180	55419	0.005	-1.3	0.50	170.04	0.54	38-44(11); 39-45(49); 41-45(6); 43-47(18);
14	Singlet-A	176	56566	0.019	-10.0	0.54	113.58	0.49	38-44(31); 41-46(10); 43-48(38);
15	Singlet-A	175	57073	0.024	46.5	0.49	141.04	0.49	38-44(10); 39-45(11); 41-46(16); 43-48(43);

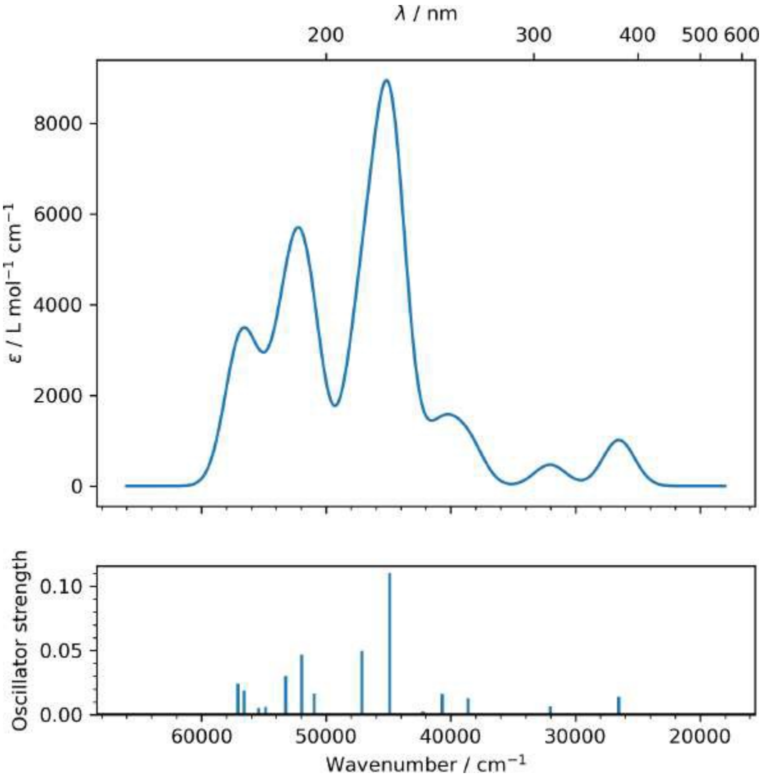

Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-1.6035	1.4144	0.0362
C	-0.2672	1.4257	0.0776
C	0.3081	0.0848	0.0158
C	-0.5790	-0.9082	-0.0797
S	-2.2183	-0.2260	-0.3542
Br	2.1985	-0.1474	0.0271
H	0.3498	2.3131	0.1256
H	-0.4159	-1.9694	-0.1688
H	-2.2882	2.2483	0.0411
O	-3.2814	-0.7397	0.5527

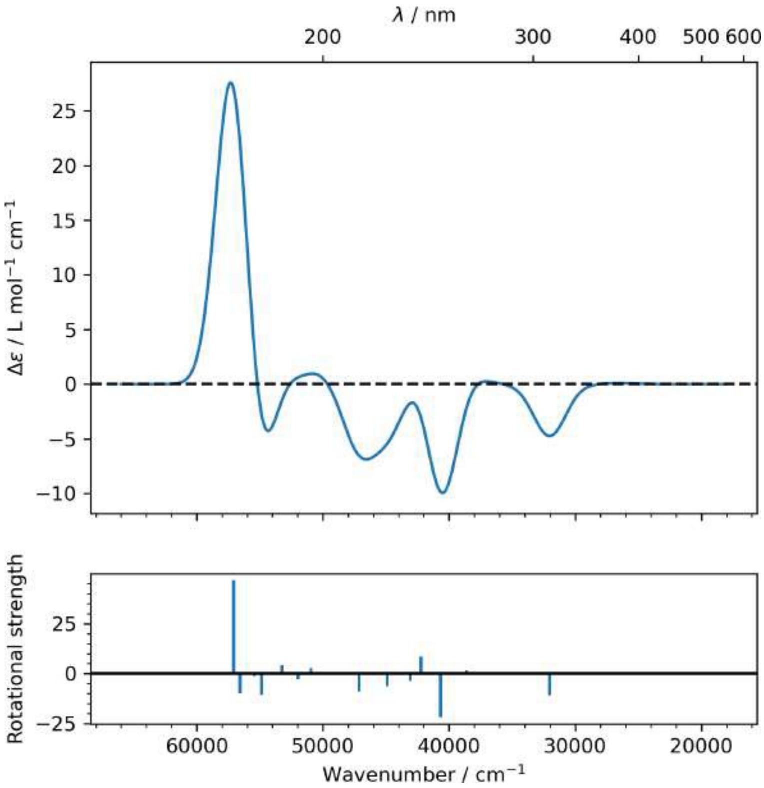

Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

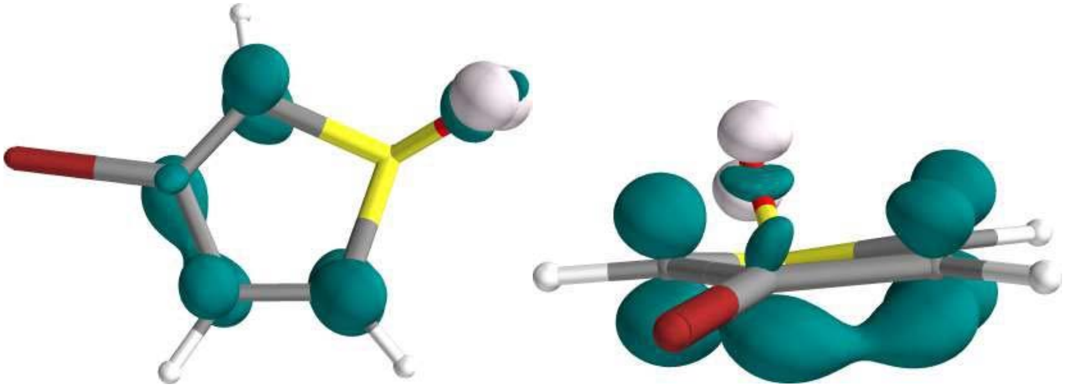

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

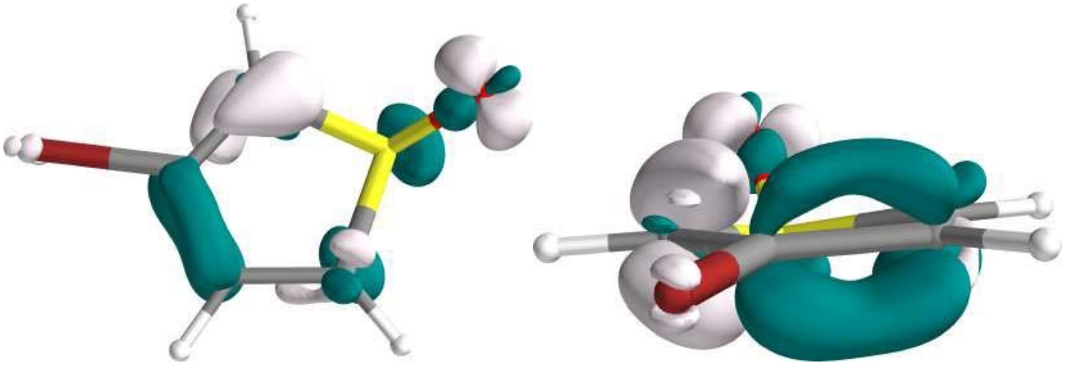

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.

15- 3-bromothiophene sulfone 3-SO2

a- Descrption

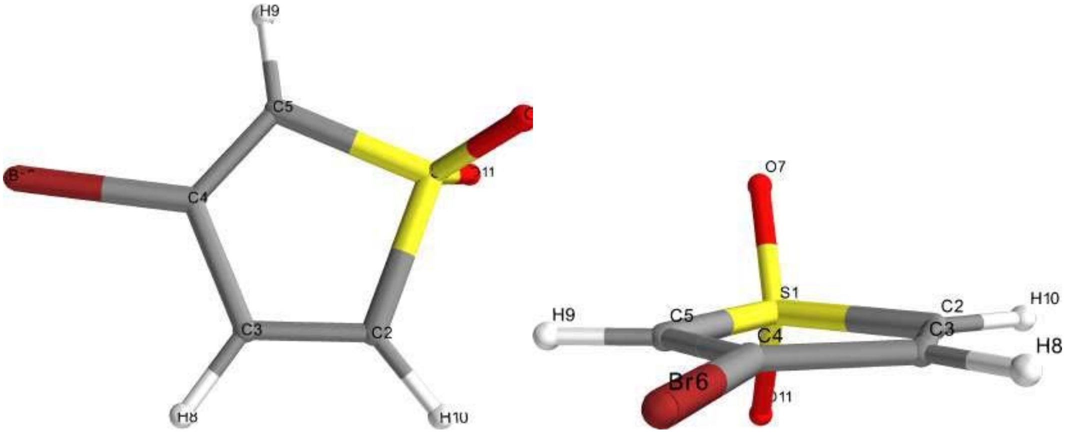

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	3-SO2
Formula	C4H3BrO2S
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	236	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000056	0.000450
RMS Force value and threshold	0.000013	0.000300
Max Displacement value and threshold	0.000414	0.001800
RMS Displacement value and threshold	0.000108	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-3277.02656 hartrees
HOMO number	47
LUMO+1 energies	-1.10 eV
LUMO energies	-2.82 eV
HOMO energies	-7.50 eV
HOMO-1 energies	-8.53 eV

Geometry optimization specific results	
Converged nuclear repulsion energy	672.89356 Hartrees

Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-3276.95356 Hartrees
Gibbs free energy at 298.15 K	-3276.99525 Hartrees
Entropy at 298.15 K	0.00014 Hartrees

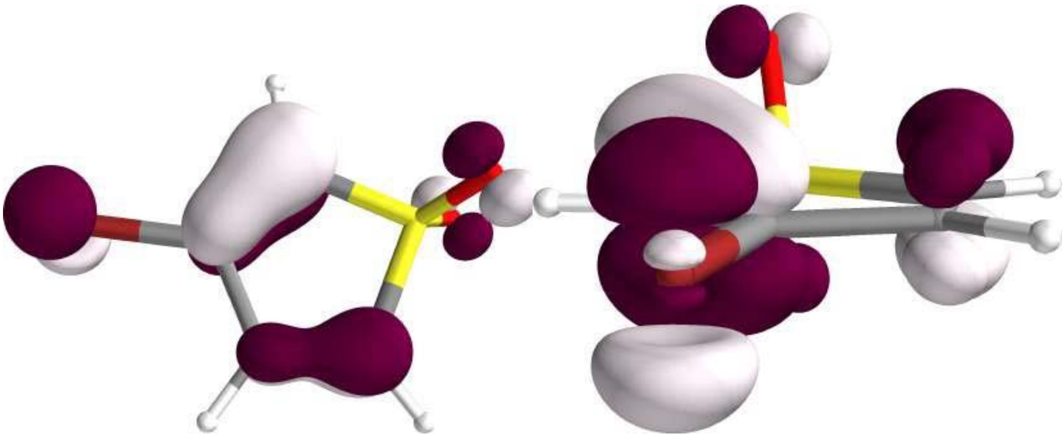

Figure 2: Representation of the HOMO from two points of view.

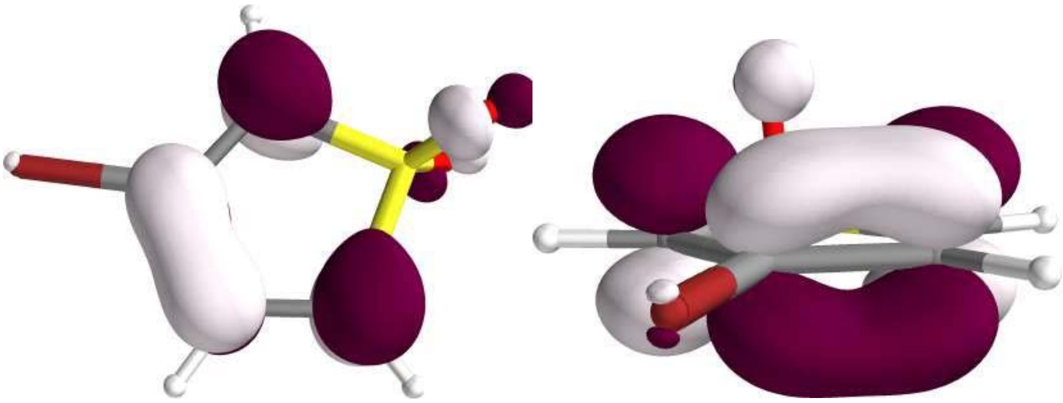

Figure 3: Representation of the LUMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1324	174	A
1198	100	A
1142	88	A
1009	51	A
908	70	A
783	61	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	-2.0136	-0.1826	-0.0000
C	-1.3614	1.4906	0.0004
C	-0.0346	1.4589	0.0003
C	0.5262	0.0877	-0.0002
C	-0.3630	-0.8955	-0.0004
Br	2.4056	-0.1495	-0.0000
O	-2.6830	-0.4628	1.2524
H	0.6079	2.3281	0.0003
H	-0.2272	-1.9641	-0.0006
H	-2.0312	2.3362	0.0004
O	-2.6835	-0.4617	-1.2524

16- Cycloadduct 3-CySO

a- Description

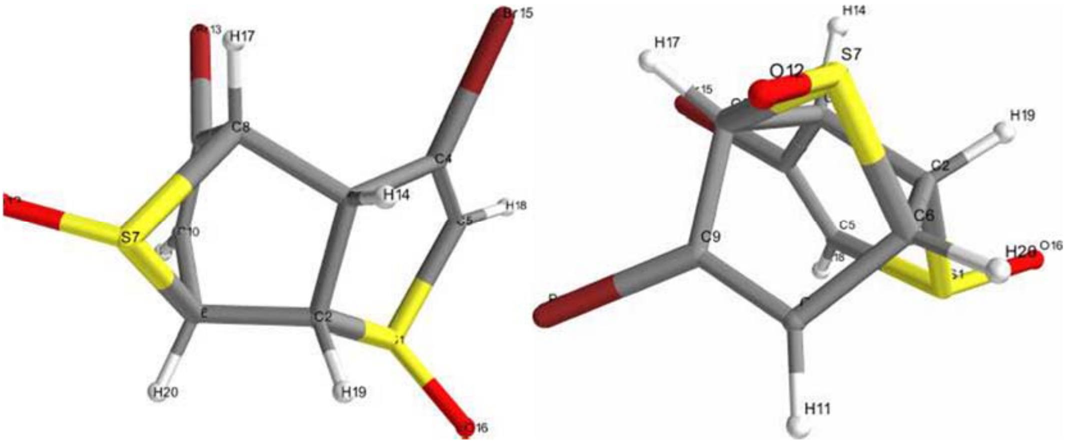

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	3-CySO
Formula	C8H6Br2O2S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	426	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000041	0.000450
RMS Force value and threshold	0.000007	0.000300
Max Displacement value and threshold	0.000582	0.001800
RMS Displacement value and threshold	0.000133	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-6403.61565 hartrees
HOMO number	86
LUMO+1 energies	-1.53 eV
LUMO energies	-1.92 eV
HOMO energies	-6.79 eV
HOMO-1 energies	-7.04 eV

Geometry optimization specific results

Converged nuclear repulsion energy	2005.28079 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-6403.47612 Hartrees
Gibbs free energy at 298.15 K	-6403.53225 Hartrees
Entropy at 298.15 K	0.00019 Hartrees

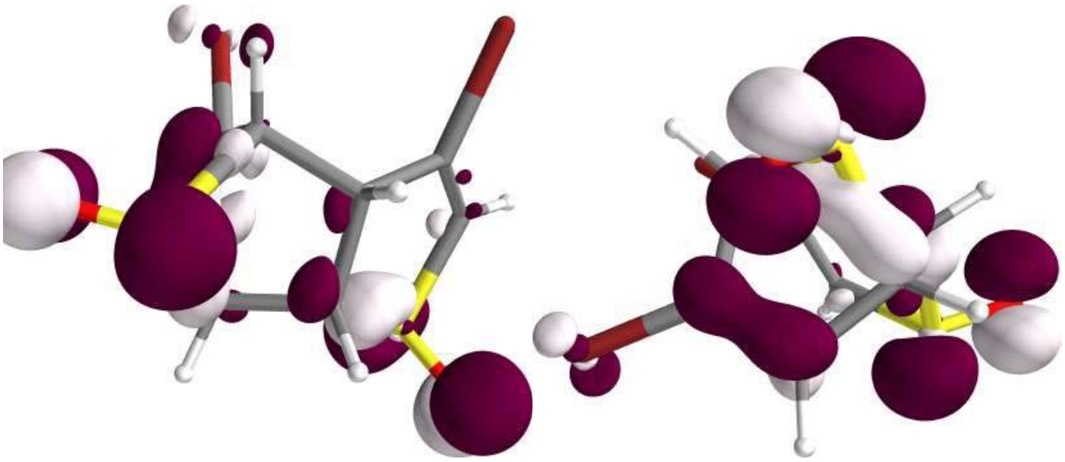

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1644	93	A
1152	142	A
1084	168	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	-1.1700	2.1776	-1.3175
C	-0.1125	1.9987	0.2392
C	-0.4752	0.6743	0.9710
C	-1.6023	0.0502	0.2077
C	-2.0283	0.6393	-0.8962
C	1.3920	1.9289	-0.0737
S	2.0040	1.2502	1.6067
C	0.8542	-0.1440	0.9995
C	1.3633	-0.3678	-0.3926
C	1.6677	0.7751	-1.0023
H	2.0274	0.8885	-2.0138
O	3.4237	0.8414	1.5277
Br	1.4704	-2.1007	-1.1494
H	-0.7905	0.8516	2.0024
Br	-2.3581	-1.5664	0.8924
O	-2.0927	3.3289	-1.0955
H	0.8505	-1.0006	1.6653
H	-2.8272	0.3106	-1.5437
H	-0.3946	2.8845	0.8073
H	1.8588	2.8772	-0.3241

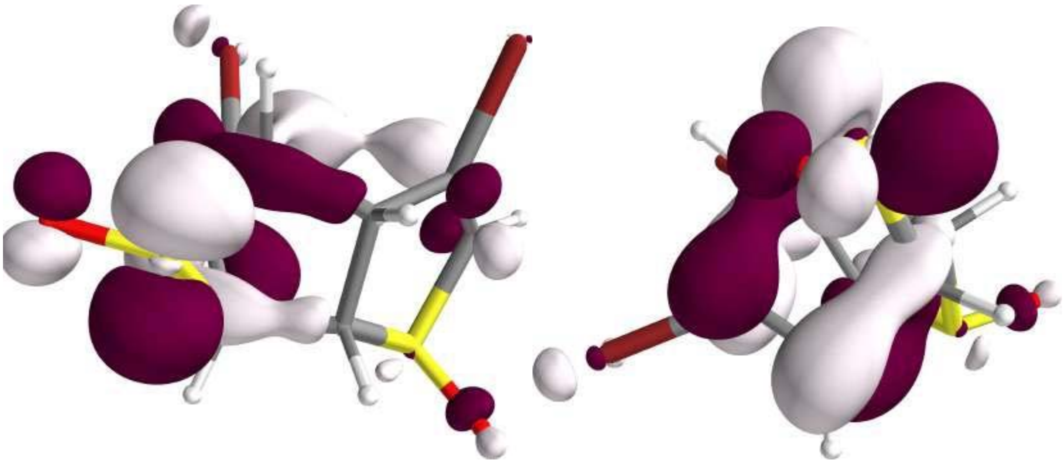

Figure 3: Representation of the LUMO from two points of view.

17- Cycloadduct 3-Cymix

a-Description

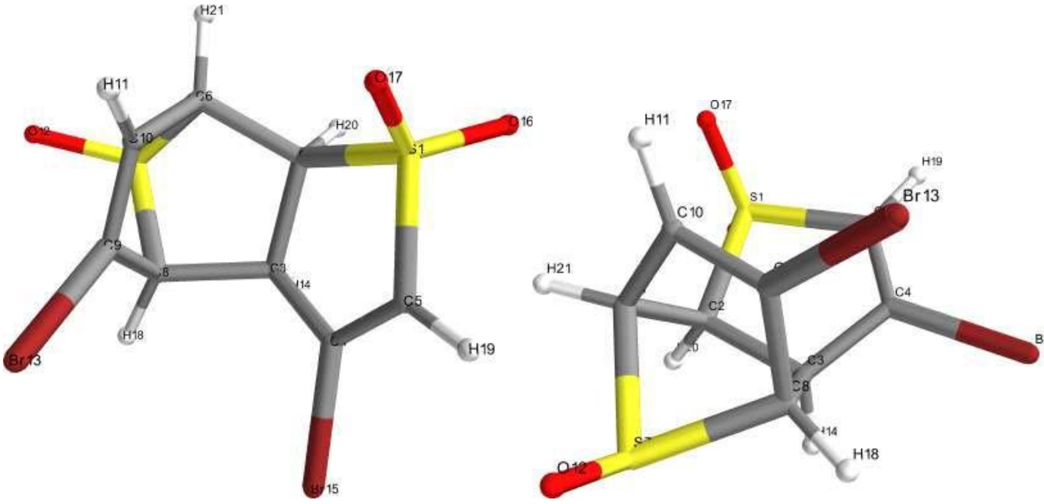

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	3-Cymix
Formula	C8H6Br2O3S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	449	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization		
Max Force value and threshold	0.000129	0.000450
RMS Force value and threshold	0.000017	0.000300
Max Displacement value and threshold	0.000755	0.001800
RMS Displacement value and threshold	0.000161	0.001200

Job type: Frequency and thermochemical analysis	
Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

c- Results

Total molecular energy	-6478.86009 hartrees
HOMO number	90
LUMO+1 energies	-1.59 eV
LUMO energies	-1.95 eV
HOMO energies	-6.96 eV
HOMO-1 energies	-7.69 eV

Geometry optimization specific results

Converged nuclear repulsion energy	2222.36871 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-6478.71438 Hartrees
Gibbs free energy at 298.15 K	-6478.77161 Hartrees
Entropy at 298.15 K	0.00019 Hartrees

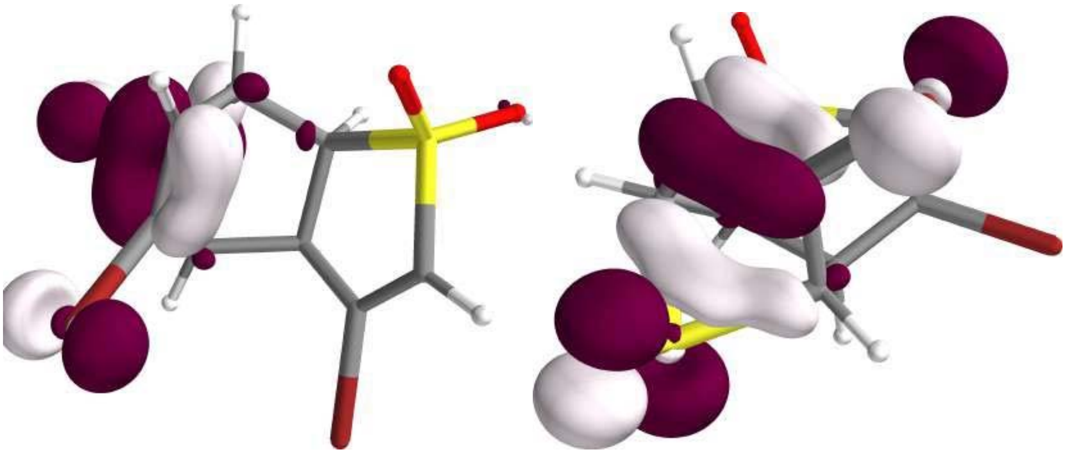

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1653	69	A
1329	68	A
1322	99	A
1237	64	A
1155	152	A
1130	100	A
1125	90	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	-2.1834	-1.3326	0.8232
C	-0.9640	-1.6348	-0.5292
C	-0.5952	-0.2376	-1.1211
C	-1.3260	0.8146	-0.3291
C	-2.1144	0.4385	0.6625
C	0.3593	-2.2822	-0.0853
S	1.3517	-1.9214	-1.6877
C	0.9611	-0.1681	-1.0440
C	1.4140	-0.2699	0.3820
C	1.0758	-1.4326	0.9297
H	1.2317	-1.7358	1.9526
O	2.7839	-2.2402	-1.5068
Br	2.2869	1.1670	1.2551
H	-0.9031	-0.1661	-2.1664
Br	-1.1006	2.6310	-0.8435
O	-3.4832	-1.8022	0.3864
O	-1.6631	-1.7566	2.1078
H	1.4149	0.6068	-1.6526
H	-2.7147	1.0506	1.3176
H	-1.5073	-2.2516	-1.2425
H	0.2989	-3.3452	0.1267

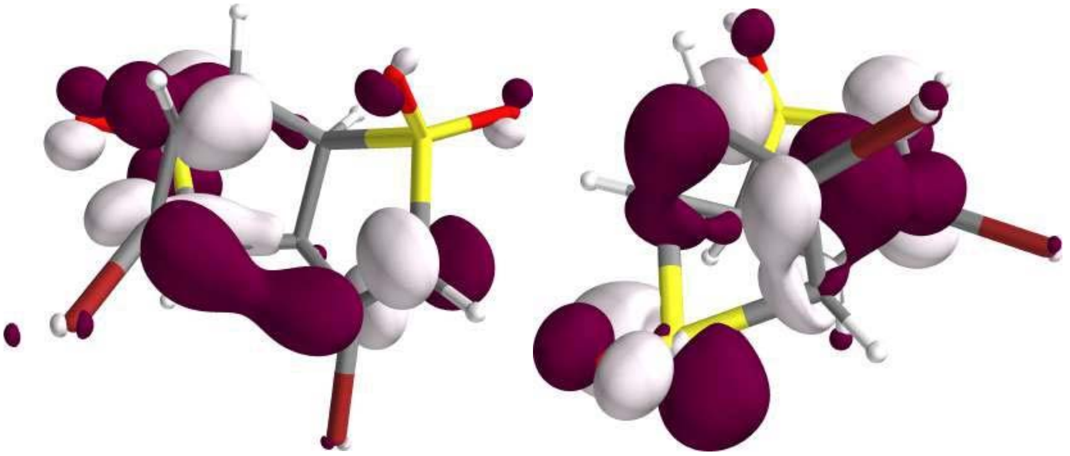

Figure 3: Representation of the LUMO from two points of view.

18- Cycloadduct 3-Cy

a- Description

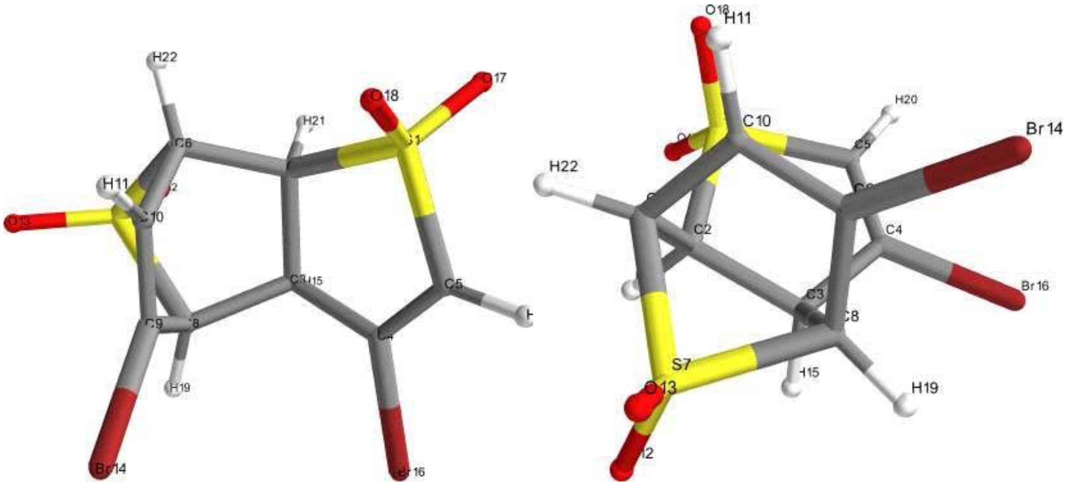

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	3-Cy
Formula	C8H6Br2O4S2
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	472	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000108	0.000450
RMS Force value and threshold	0.000020	0.000300
Max Displacement value and threshold	0.001683	0.001800
RMS Displacement value and threshold	0.000355	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-6554.10540 hartrees
HOMO number	94
LUMO+1 energies	-1.54 eV
LUMO energies	-1.86 eV
HOMO energies	-7.64 eV
HOMO-1 energies	-8.07 eV

Geometry optimization specific results

Converged nuclear repulsion energy	2430.79511 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-6553.95379 Hartrees
Gibbs free energy at 298.15 K	-6554.01243 Hartrees
Entropy at 298.15 K	0.00020 Hartrees

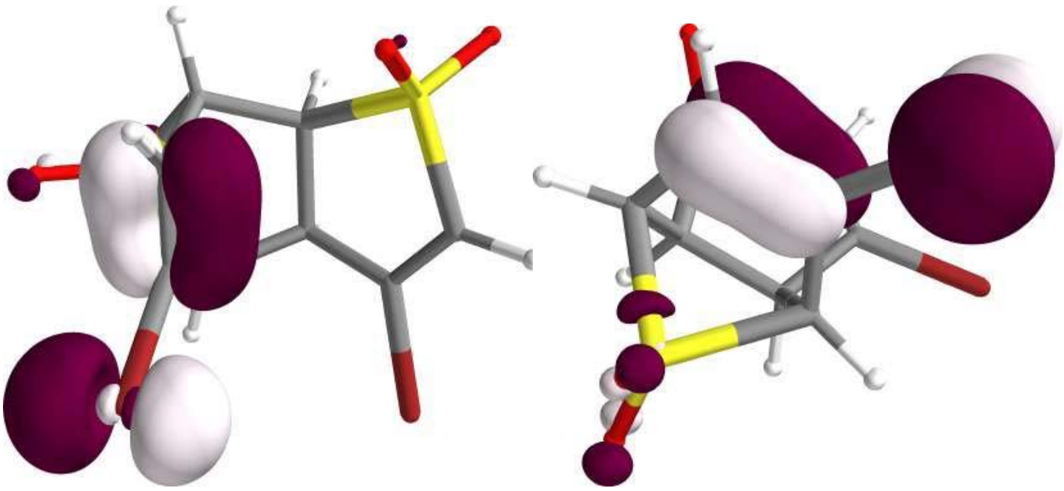

Figure 2: Representation of the HOMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1654	67	A
1339	162	A
1325	145	A
1233	70	A
1179	101	A
1172	88	A
1131	143	A
1101	78	A
550	51	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	-1.7786	-1.7742	1.0410
C	-0.4407	-1.8172	-0.2310
C	-0.5024	-0.4522	-0.9922
C	-1.5836	0.3860	-0.3614
C	-2.2777	-0.1130	0.6462
C	0.9776	-1.9515	0.3467
S	1.9201	-1.4242	-1.2188
C	0.9280	0.1572	-0.8851
C	1.2973	0.3525	0.5437
C	1.3233	-0.7942	1.2288
H	1.5979	-0.9111	2.2649
O	1.4246	-2.1087	-2.3974
O	3.3400	-1.2649	-1.0163
Br	1.7521	2.0563	1.2293
H	-0.7339	-0.6155	-2.0453
Br	-1.9157	2.1063	-1.1000
O	-2.8228	-2.6956	0.6425
O	-1.2329	-1.8436	2.3822
H	1.1440	0.9635	-1.5770
H	-3.0936	0.3356	1.1915
H	-0.6948	-2.6519	-0.8792
H	1.2421	-2.9403	0.7072

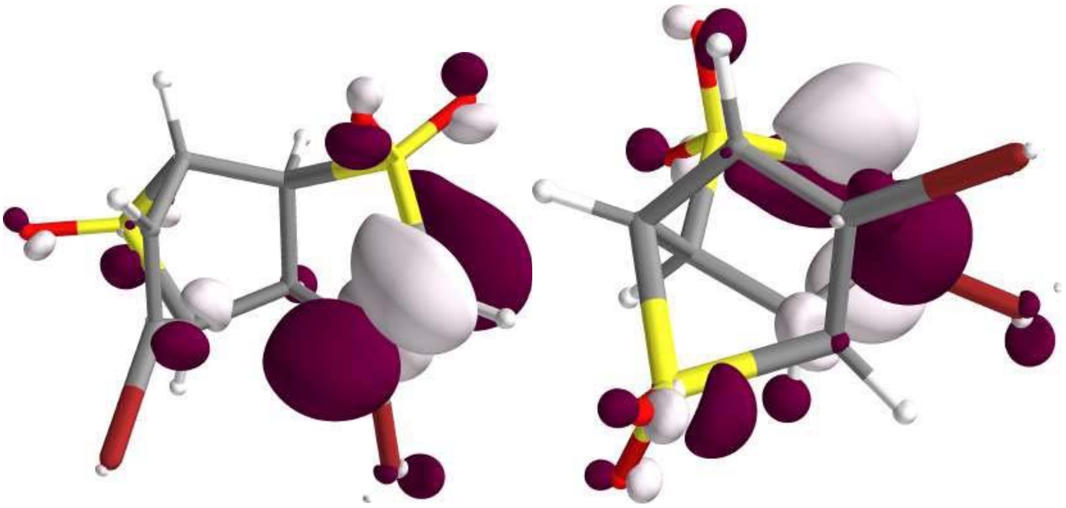

Figure 3: Representation of the LUMO from two points of view.

19- 2,5-dibromothiophene 4

a- Description

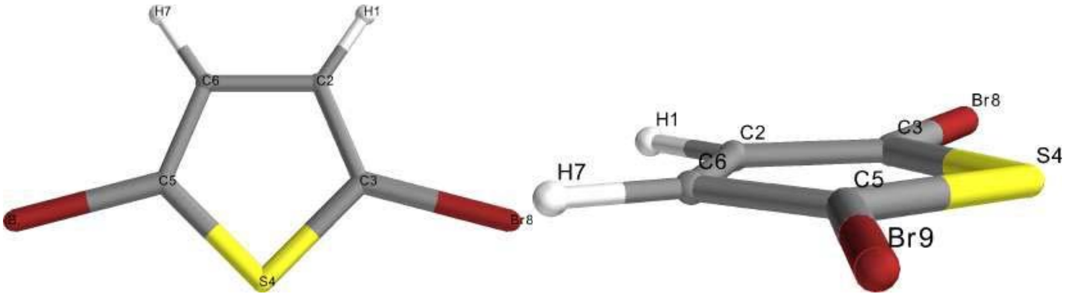

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	4
Formula	C4H2Br2S
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	233	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Geometry optimization		
Max Force value and threshold	0.000135	0.000450
RMS Force value and threshold	0.000031	0.000300
Max Displacement value and threshold	0.000581	0.001800
RMS Displacement value and threshold	0.000141	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

c- Results

Total molecular energy	-5700.14275 hartrees
HOMO number	56
LUMO+1 energies	-1.08 eV
LUMO energies	-1.19 eV
HOMO energies	-6.49 eV
HOMO-1 energies	-7.58 eV

Geometry optimization specific results

Converged nuclear repulsion energy	794.18300 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-5700.08819 Hartrees
Gibbs free energy at 298.15 K	-5700.13025 Hartrees
Entropy at 298.15 K	0.00014 Hartrees

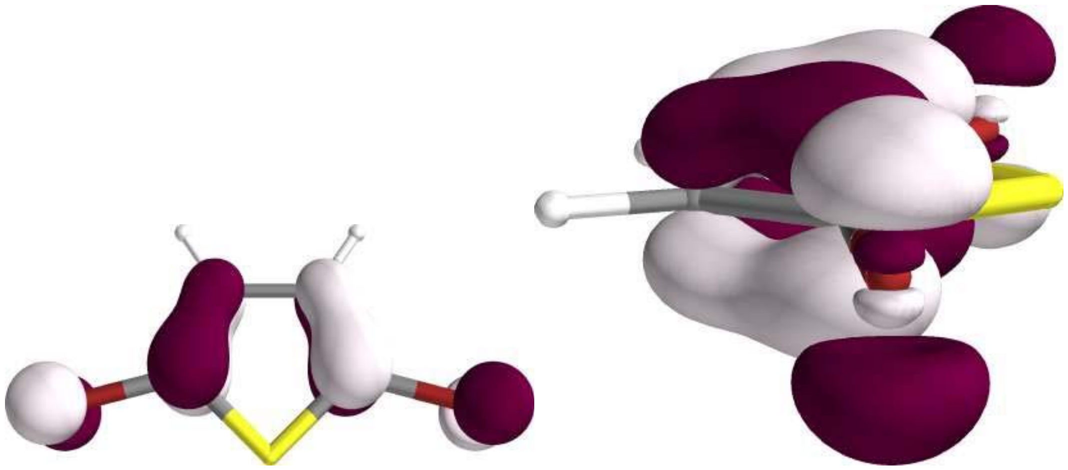

Figure 2: Representation of the HOMO from two points of view.

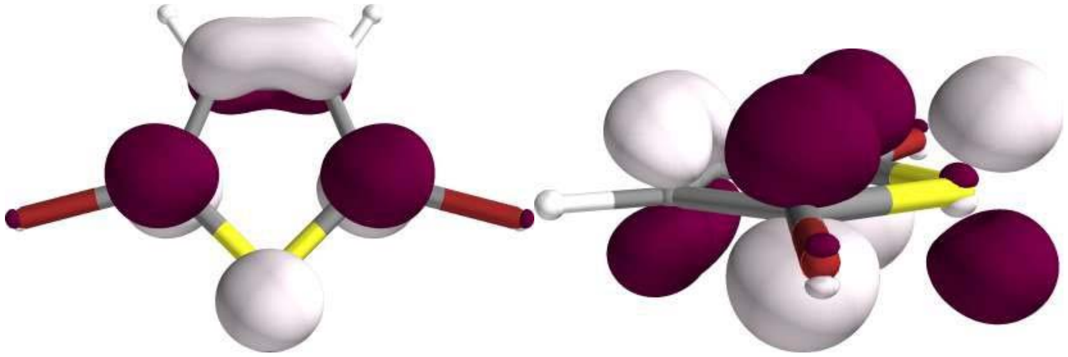

Figure 3: Representation of the LUMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
978	87	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
H	-1.3179	-2.4553	0.0000
C	-0.7126	-1.5604	0.0000
C	-1.2303	-0.3038	0.0000
S	0.0000	0.9222	0.0000
C	1.2303	-0.3038	0.0000
C	0.7126	-1.5604	0.0000
H	1.3179	-2.4553	0.0000
Br	-3.0567	0.1790	-0.0000
Br	3.0567	0.1790	-0.0000

20- 2,5-dibromothiophene sulfoxide 4-SO

a- Description

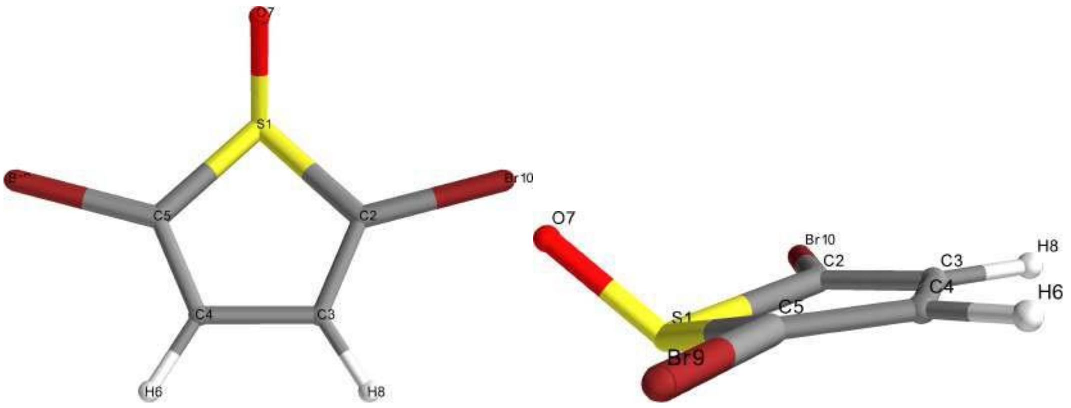

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	4-SO
Formula	C4H2Br2OS
Charge	0
Spin multiplicity	1

b- Computational details

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-311G(2d,p)	
Number of basis set functions	256	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	

Job type: Geometry optimization		
Max Force value and threshold	0.000211	0.000450
RMS Force value and threshold	0.000063	0.000300
Max Displacement value and threshold	0.001361	0.001800
RMS Displacement value and threshold	0.000400	0.001200

Job type: Frequency and thermochemical analysis	
Temperature	298.15 K
Anharmonic effects	None
Anharmonic effects	None

c- Results

Total molecular energy	-5775.31615 hartrees
HOMO number	60
LUMO+1 energies	-1.19 eV
LUMO energies	-2.60 eV
HOMO energies	-6.86 eV
HOMO-1 energies	-7.04 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	946.71174 Hartrees
Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-5775.25730 Hartrees
Gibbs free energy at 298.15 K	-5775.30266 Hartrees
Entropy at 298.15 K	0.00015 Hartrees

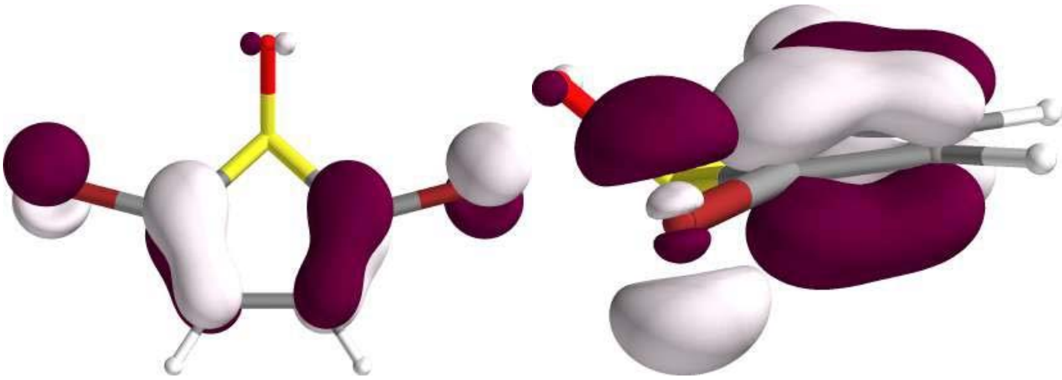

Figure 2: Representation of the HOMO from two points of view.

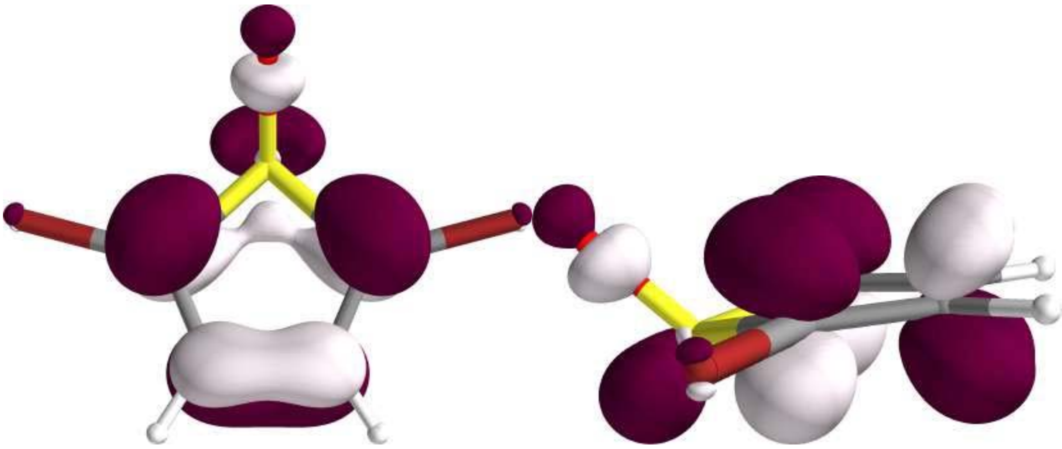

Figure 3: Representation of the LUMO from two points of view.

Table. Most intense (> 50 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1113	117	A
961	63	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	0.0001	-0.8066	-0.3589
C	-1.2643	0.4540	0.0286
C	-0.7306	1.6743	0.1448
C	0.7307	1.6743	0.1449
C	1.2645	0.4541	0.0285
H	1.3076	2.5862	0.2281
O	0.0003	-1.9636	0.5676
H	-1.3075	2.5861	0.2279
Br	3.0772	-0.0300	-0.0191
Br	-3.0773	-0.0300	-0.0191