Molecular Calculation Report generated by quchemreport

February 9, 2022

1 MOLECULE

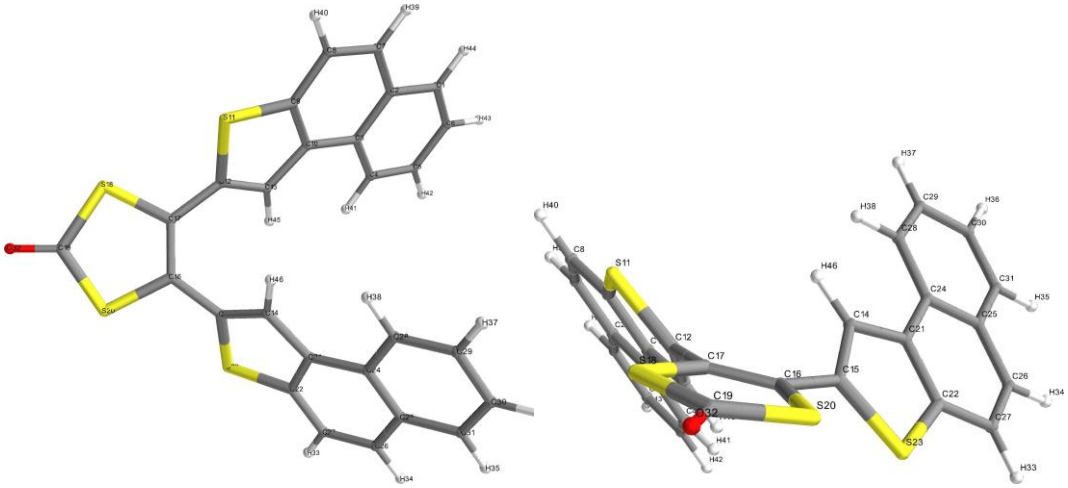

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	4
Formula	C27H14OS4
Charge	0
Spin multiplicity	1

2 COMPUTATIONAL DETAILS

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Number of basis set functions	980	
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	0.000038	0.000450
RMS Force value and threshold	0.000006	0.000300
Max Displacement value and threshold	0.001432	0.001800
RMS Displacement value and threshold	0.000288	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	20	['Singlet-A']

3 RESULTS

Total molecular energy	-2703.83854 hartrees
HOMO number	124
LUMO+1 energies	-1.50 eV
LUMO energies	-2.12 eV

HOMO energies	-5.98 eV
HOMO-1 energies	-6.51 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	3605.14873 Hartrees
Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-2703.48465 Hartrees
Gibbs free energy at 298.15 K	-2703.56855 Hartrees
Entropy at 298.15 K	0.00028 Hartrees

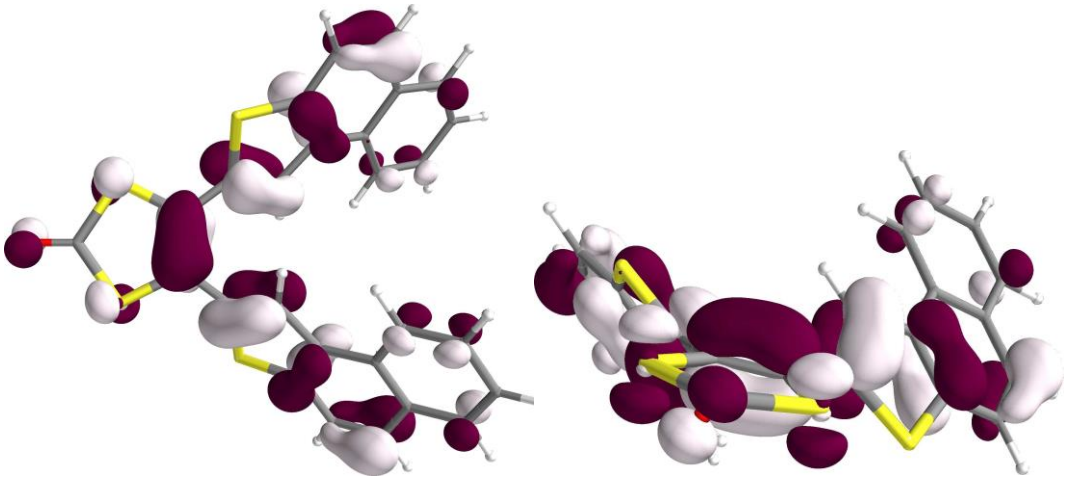

Figure 2: Representation of the HOMO from two points of view.

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

Frequencies	Intensity	Symmetry
1782	895	A
1150	61	A
870	70	A
818	77	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	393	25419	0.301	147.9	0.78	96.57	0.43	124-125(97);
2	Singlet-A	332	30063	0.040	-16.5	0.67	273.41	0.44	123-125(74); 124-126(21);
3	Singlet-A	318	31358	0.013	11.0	0.63	124.85	0.34	122-125(31); 124-127(40); 124-128(15);
4	Singlet-A	317	31541	0.316	-122.1	0.70	195.72	0.37	123-125(21); 124-126(73);
5	Singlet-A	315	31649	0.017	100.3	0.61	261.31	0.37	122-125(52); 124-127(7); 124-128(22); 124-131(6);
6	Singlet-A	310	32217	0.011	-32.3	0.59	238.26	0.46	121-125(78); 124-130(10);
7	Singlet-A	296	33674	0.011	4.8	0.62	90.89	0.47	124-127(44); 124-128(41);
8	Singlet-A	294	33922	0.009	-7.0	0.64	42.49	0.50	120-125(83); 124-128(10);
9	Singlet-A	291	34318	0.024	17.5	0.38	519.30	0.82	124-129(95);
10	Singlet-A	283	35302	0.004	14.1	0.71	72.05	0.24	121-126(12); 122-127(7); 123-126(52); 124-131(14);
11	Singlet-A	282	35373	0.000	-2.5	0.60	177.27	0.29	121-125(16); 121-127(7); 122-126(35); 124-130(28);
12	Singlet-A	280	35668	0.043	5.9	0.66	133.74	0.23	121-126(17); 123-126(39); 124-131(20);
13	Singlet-A	267	37325	0.009	-16.2	0.64	92.46	0.40	123-127(17); 124-132(66);
14	Singlet-A	267	37382	0.004	-5.2	0.64	92.75	0.41	123-127(59); 124-130(13); 124-132(13);
15	Singlet-A	259	38534	0.066	382.3	0.55	133.85	0.31	121-126(15); 122-127(10); 124-131(42);
16	Singlet-A	258	38652	0.131	-422.4	0.62	357.60	0.31	122-126(36); 123-127(7); 123-131(6); 124-130(40);
17	Singlet-A	257	38832	0.010	-12.7	0.52	421.75	0.58	123-128(76);
18	Singlet-A	256	39025	0.026	1.3	0.54	136.64	0.35	119-125(8); 120-127(6); 120-128(13); 121-126(12); 122-127(10); 122-128(12); 124-133(8);
19	Singlet-A	254	39260	0.004	2.7	0.56	404.22	0.54	120-126(88);
20	Singlet-A	254	39369	0.036	-57.0	0.60	86.48	0.37	119-125(63); 124-131(7);

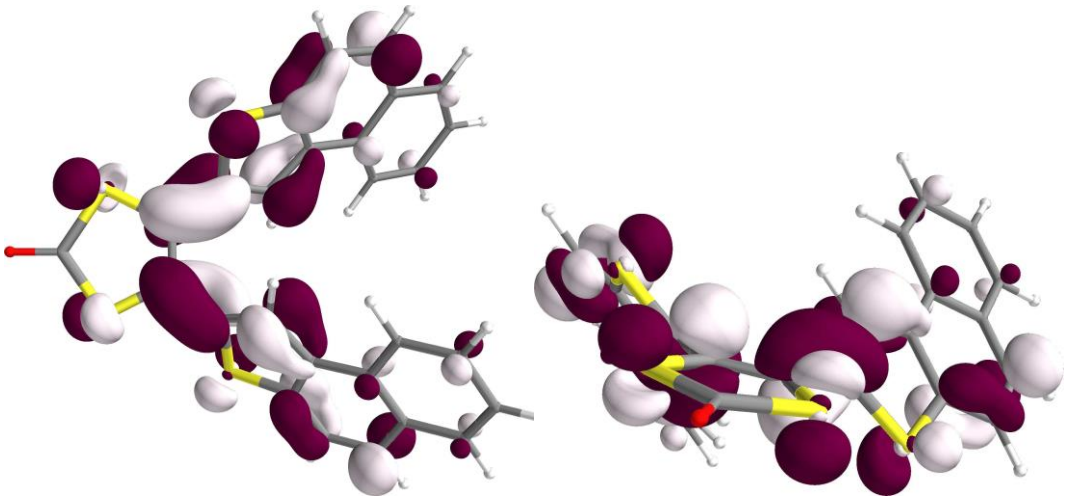

Figure 3: Representation of the LUMO from two points of view.

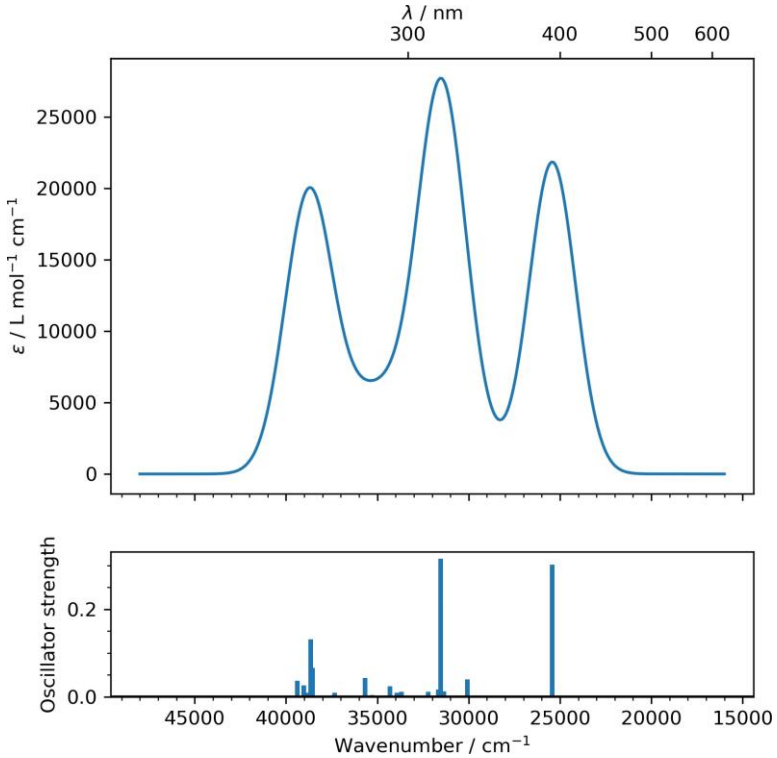

Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-3.8839	-4.2391	-0.8134
C	-2.6541	-3.8978	-0.2144
C	-1.8561	-2.8854	-0.8117
C	-2.3208	-2.2550	-1.9814
C	-3.5223	-2.6095	-2.5414
C	-4.3121	-3.6103	-1.9537
C	-2.2086	-4.5492	0.9698
C	-1.0230	-4.2291	1.5612
C	-0.2308	-3.2244	0.9739
C	-0.6136	-2.5521	-0.1876
S	1.2945	-2.6621	1.5604
C	1.4294	-1.5235	0.2473
C	0.3554	-1.5915	-0.5875
C	0.3549	1.5916	0.5875
C	1.4287	1.5238	-0.2476
C	2.5962	0.6636	-0.1362
C	2.5965	-0.6628	0.1357
S	4.1572	-1.4351	0.3144
C	5.1592	0.0011	0.0003
S	4.1565	1.4366	-0.3145
C	-0.6145	2.5519	0.1876

C	-0.2322	3.2241	-0.9741
S	1.2932	2.6622	-1.5609
C	-1.8570	2.8849	0.8119
C	-2.6553	3.8970	0.2146
C	-2.2103	4.5484	-0.9698
C	-1.0248	4.2285	-1.5615
C	-2.3214	2.2543	1.9816
C	-3.5230	2.6085	2.5418
C	-4.3131	3.6091	1.9541
C	-3.8852	4.2380	0.8138
O	6.3538	0.0014	0.0005
H	-0.6973	4.7339	-2.4628
H	-2.8400	5.3190	-1.4024
H	-4.4918	5.0120	0.3539
H	-5.2614	3.8819	2.4037
H	-3.8655	2.1113	3.4427
H	-1.7227	1.4773	2.4435
H	-2.8380	-5.3201	1.4025
H	-0.6951	-4.7347	2.4623
H	-1.7223	-1.4779	-2.4435
H	-3.8651	-2.1125	-3.4424
H	-5.2605	-3.8834	-2.4032
H	-4.4903	-5.0133	-0.3535
H	0.2744	-0.9652	-1.4661
H	0.2741	0.9651	1.4659

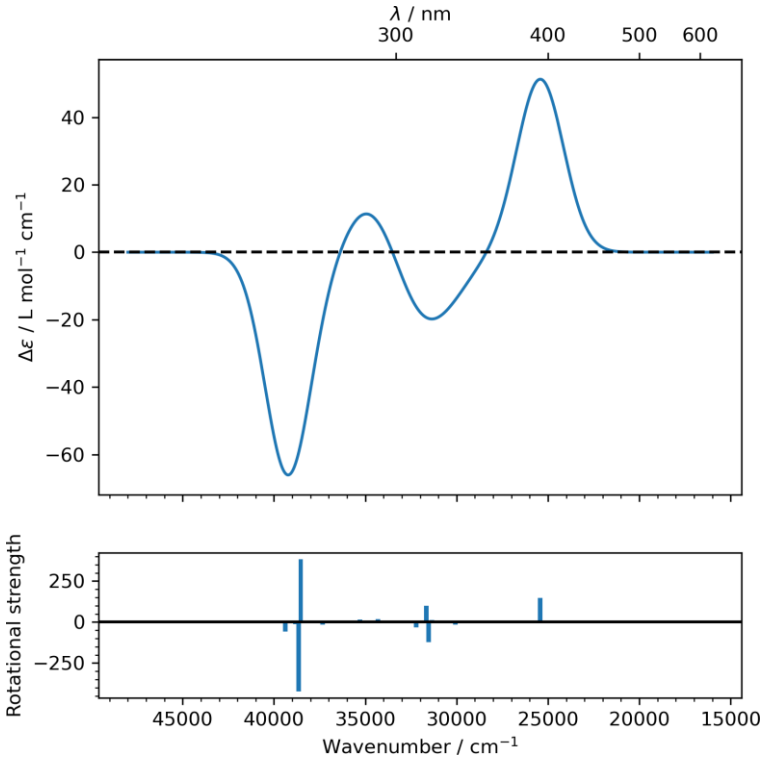

Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

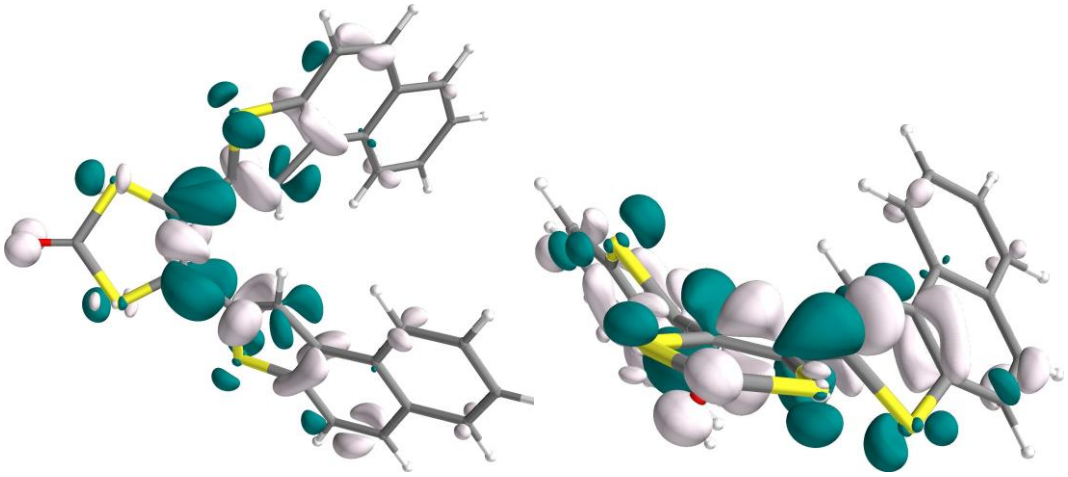

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

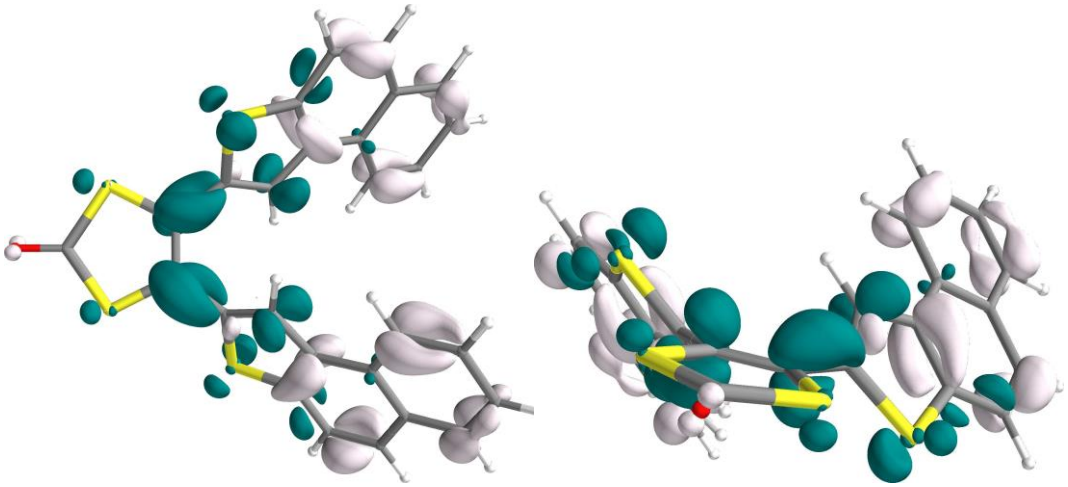

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.

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1 MOLECULE

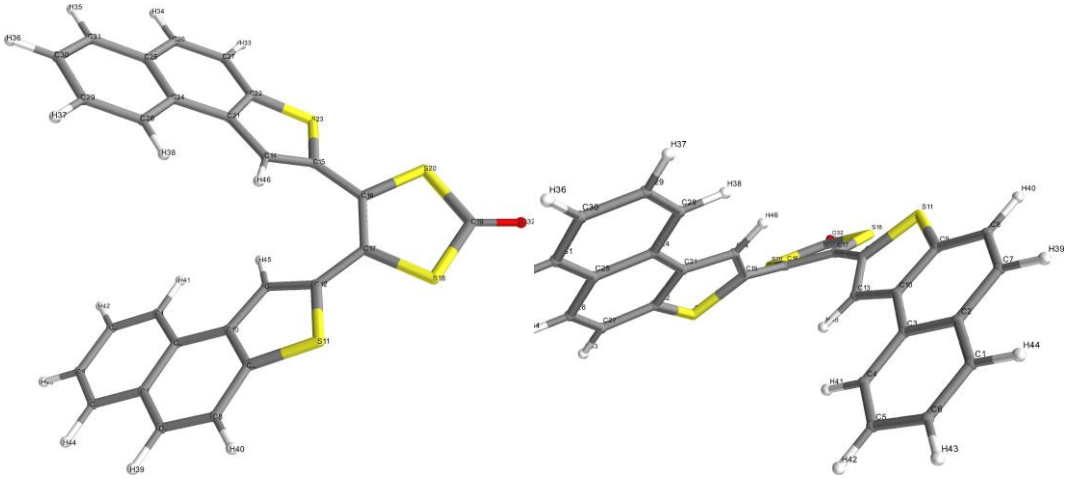

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	4-cat
Formula	C27H14OS4+
Charge	1
Spin multiplicity	2

2 COMPUTATIONAL DETAILS

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Number of basis set functions	980	
Closed shell calculation	False	
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	0.000004	0.000450
RMS Force value and threshold	0.000001	0.000300
Max Displacement value and threshold	0.000315	0.001800
RMS Displacement value and threshold	0.000063	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	20	['2.019-A' '2.042-A' '2.043-A' '2.048-A' '2.062-A' '2.085-A' '2.105-A' '2.134-A' '2.178-A' '2.206-A' '2.309-A' '2.348-A' '2.408-A' '2.427-A' '3.137-A' '3.143-A' '3.173-A' '3.179-A' '3.197-A' '3.258-A']

3 RESULTS

Total molecular energy	-2703.58821 hartrees	
Unrestricted calculation	Alpha spin MO	Beta spin MO
HOMO number	124	123
LUMO+1 energies	-4.62 eV	-5.62 eV
LUMO energies	-5.91 eV	-7.66 eV
HOMO energies	-9.00 eV	-9.27 eV
HOMO-1 energies	-9.57 eV	-9.78 eV
Geometry optimization specific results		
Converged nuclear repulsion energy	3613.73041 Hartrees	
Frequency and Thermochemistry specific results		
Enthalpy at 298.15 K	-2703.23427 Hartrees	
Gibbs free energy at 298.15 K	-2703.31765 Hartrees	
Entropy at 298.15 K	0.00028 Hartrees	

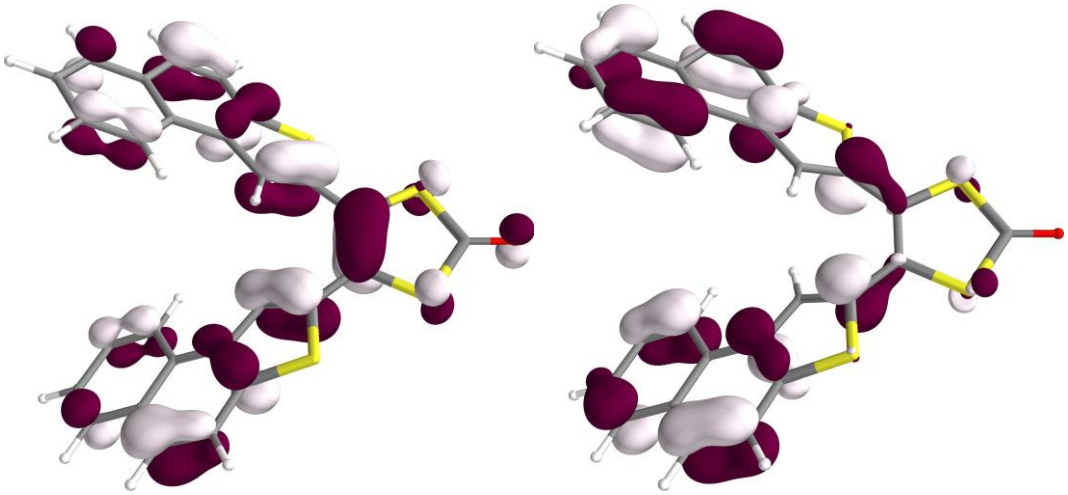

Figure 2: Representation of the HOMO of spin alpha (left) and spin beta (right).

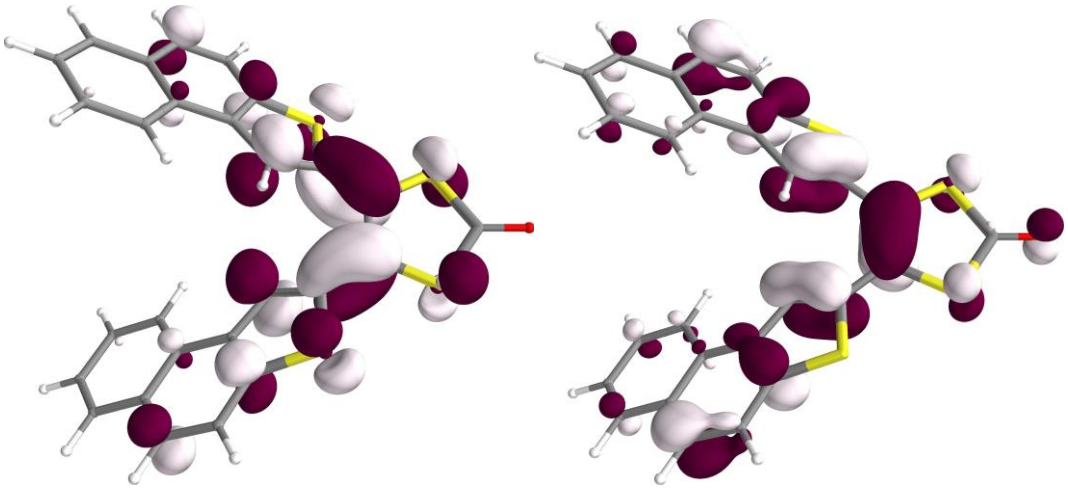

Figure 3: Representation of the LUMO of spin alpha (left) and spin beta (right).

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

Frequencies	Intensity	Symmetry
1829	944	A
1626	195	A
1618	532	A
1592	64	A
1564	100	A
1558	315	A
1516	374	A
1481	50	A
1469	95	A
1406	519	A
1405	330	A
1378	1152	A
1280	138	A
1228	495	A
1181	82	A
1158	273	A
857	111	A
834	60	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	2.019-A	1228	8140	0.129	71.5	0.63	364.62	0.63	123b-124b (96)
2	2.043-A	992	10077	0.004	33.1	0.62	349.96	0.59	121b-124b (26) 122b-124b (71)
3	2.048-A	916	10906	0.001	26.4	0.54	383.61	0.65	120b-124b (96)
4	2.042-A	829	12048	0.114	-121.4	0.64	269.57	0.58	121b-124b (70) 122b-124b (25)
5	2.105-A	613	16295	0.159	218.0	0.70	269.88	0.46	124a-125a (77) 119b-124b (8)
6	2.206-A	544	18368	0.003	13.0	0.69	223.53	0.48	118b-124b (87)
7	2.062-A	540	18512	0.054	-46.1	0.66	343.29	0.53	124a-125a (8) 119b-124b (87)
8	3.197-A	508	19677	0.008	-0.3	0.67	158.24	0.35	123a-125a (22) 124a-126a (8) 118b-124b (8) 123b-125b (43)
9	2.085-A	473	21118	0.002	4.4	0.38	576.98	0.79	117b-124b (95)
10	3.258-A	435	22957	0.003	-1.1	0.61	73.40	0.30	120a-125a (18) 123a-126a (9) 124a-128a (7) 121b-125b (19) 122b-125b (6) 123b-126b (10)
11	2.408-A	426	23462	0.009	8.7	0.59	195.87	0.60	122a-125a (15) 116b-124b (75)
12	3.179-A	422	23695	0.009	-2.8	0.56	332.06	0.56	122a-125a (48) 116b-124b (14) 122b-125b (18)
13	2.348-A	414	24098	0.000	-0.7	0.64	23.96	0.46	121a-125a (10) 123a-125a (6) 115b-124b (73)
14	3.137-A	409	24393	0.002	5.5	0.53	338.55	0.59	121a-125a (49) 115b-124b (19) 120b-125b (15)
15	2.178-A	400	24943	0.199	-136.4	0.64	370.59	0.49	123a-125a (56) 123b-125b (28)
16	3.173-A	385	25920	0.048	-25.0	0.64	69.14	0.26	123a-128a (10) 124a-126a (19) 123b-125b (12) 123b-128b (13)
17	2.427-A	383	26086	0.019	-12.5	0.62	320.18	0.44	114b-124b (73)
18	3.143-A	376	26588	0.008	-1.5	0.64	33.15	0.29	120a-125a (17) 114b-124b (18) 121b-125b (6) 122b-125b (8) 123b-126b (6)
19	2.134-A	364	27405	0.022	7.3	0.54	471.94	0.59	122a-125a (24) 121b-125b (12) 122b-125b (53)
20	2.309-A	356	28060	0.002	4.9	0.61	93.20	0.39	121a-125a (14) 113b-124b (24) 120b-125b (38)

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	3.8726	4.2403	-0.8894
C	2.6162	3.9399	-0.3292
C	1.9060	2.8002	-0.7897
C	2.4773	2.0022	-1.7893
C	3.7076	2.3204	-2.3214
C	4.4105	3.4439	-1.8706
C	2.0579	4.7634	0.6855
C	0.8358	4.5054	1.2516
C	0.1273	3.3887	0.8008
C	0.6278	2.5258	-0.1954
S	-1.4285	2.8887	1.3643
C	-1.4192	1.5168	0.2925

C	-0.2602	1.4787	-0.4706
C	-0.2606	-1.4787	0.4706
C	-1.4195	-1.5165	-0.2925
C	-2.5621	-0.6687	-0.1924
C	-2.5619	0.6692	0.1924
S	-4.1113	1.4017	0.4812
C	-5.1134	0.0006	-0.0000
S	-4.1117	-1.4008	-0.4812
C	0.6273	-2.5259	0.1954
C	0.1265	-3.3888	-0.8007
S	-1.4292	-2.8885	-1.3642
C	1.9054	-2.8006	0.7896
C	2.6154	-3.9404	0.3292
C	2.0568	-4.7639	-0.6854
C	0.8348	-4.5058	-1.2515
C	2.4769	-2.0026	1.7892
C	3.7071	-2.3211	2.3212
C	4.4098	-3.4447	1.8705
C	3.8717	-4.2411	0.8894
O	-6.2978	0.0007	-0.0000
H	0.4281	-5.1550	-2.0175
H	2.6224	-5.6300	-1.0133
H	4.4090	-5.1143	0.5345
H	5.3762	-3.6850	2.2981
H	4.1340	-1.6967	3.0980
H	1.9499	-1.1283	2.1541
H	2.6237	5.6293	1.0135
H	0.4294	5.1547	2.0178
H	1.9500	1.1279	-2.1542
H	4.1343	1.6959	-3.0982
H	5.3769	3.6840	-2.2982
H	4.4101	5.1134	-0.5345
H	-0.1055	0.7328	-1.2377
H	-0.1056	-0.7327	1.2376

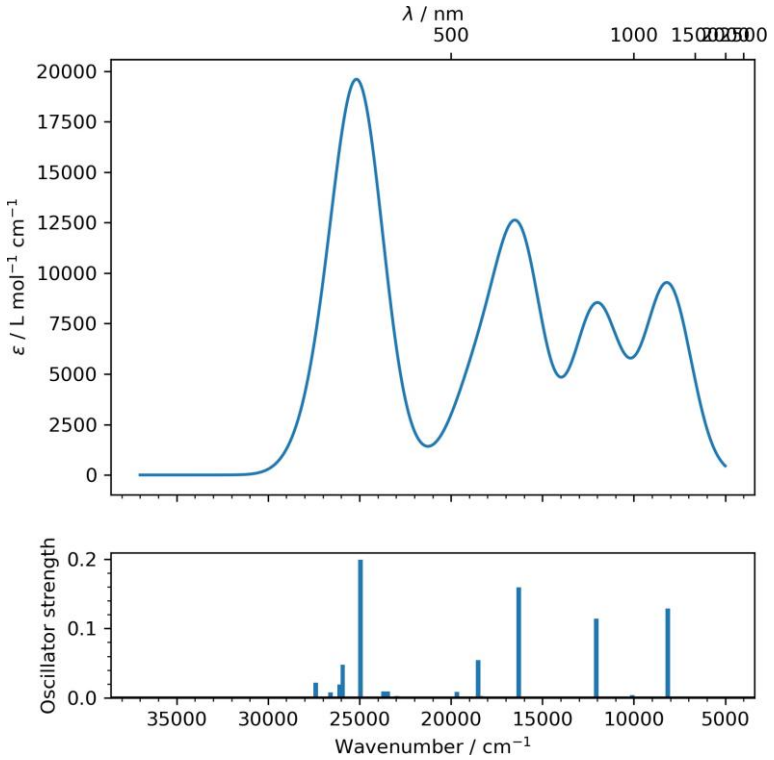

Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

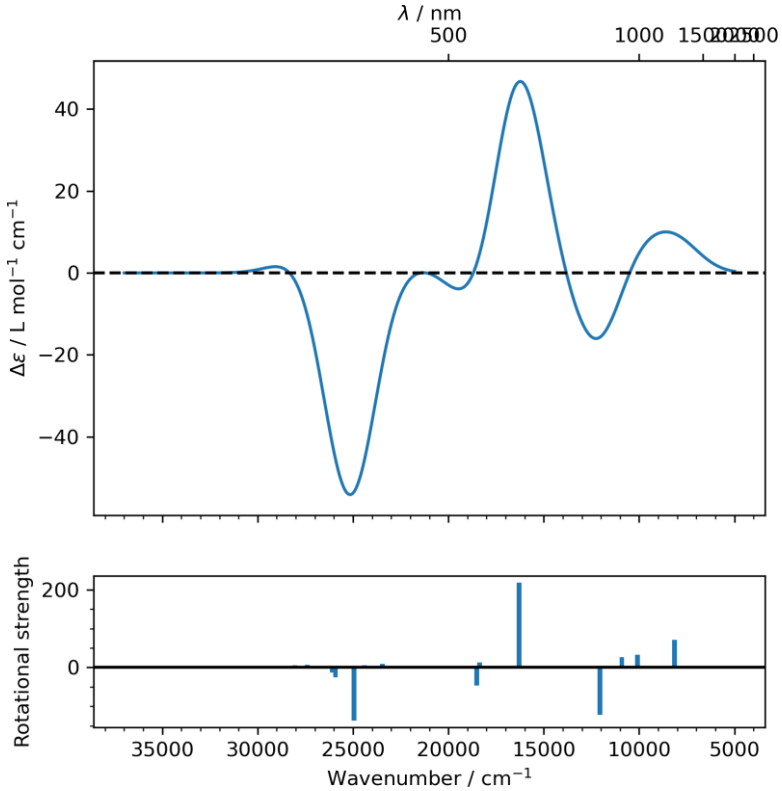

Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

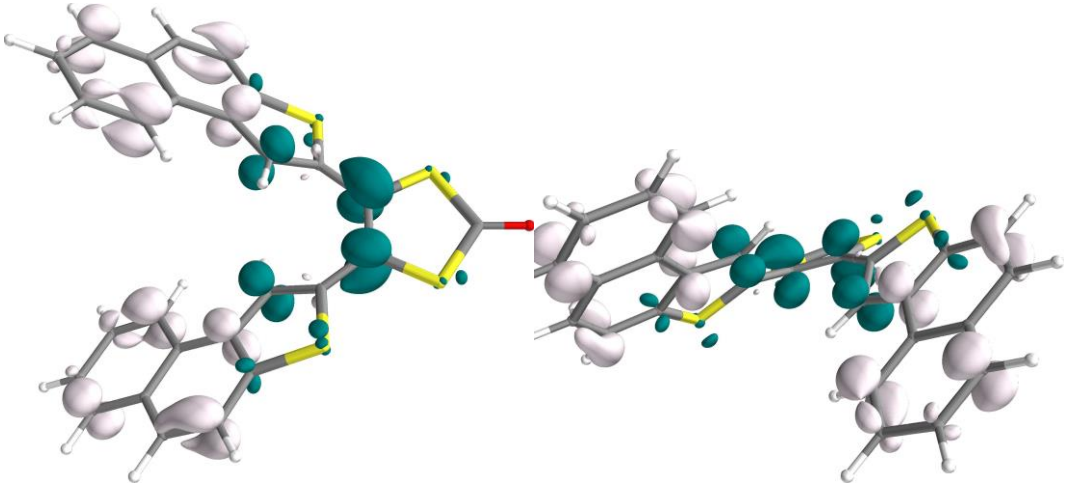

Figure 6: Representation of the Electron Density Difference (ES1-GS) from two points of view.

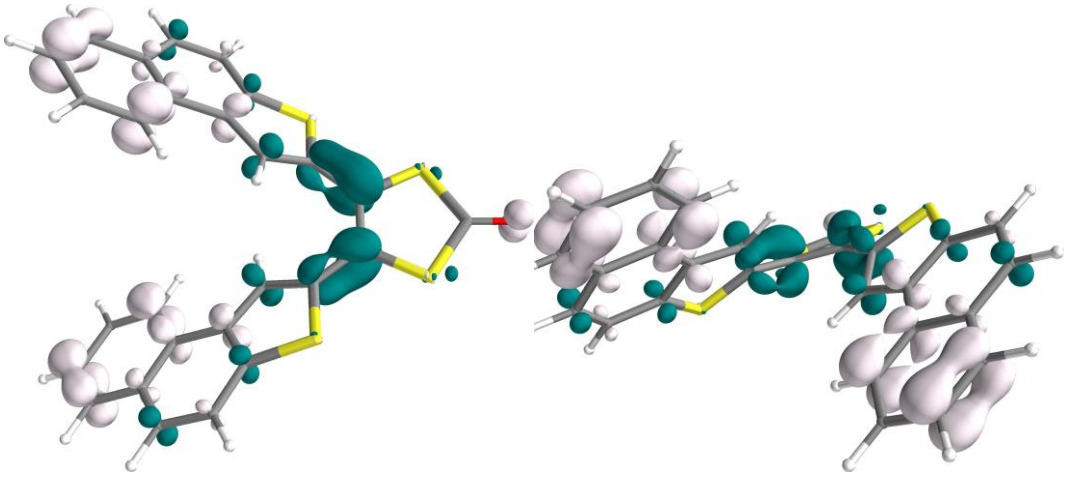

Figure 7: Representation of the Electron Density Difference (ES2-GS) from two points of view.

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1 MOLECULE

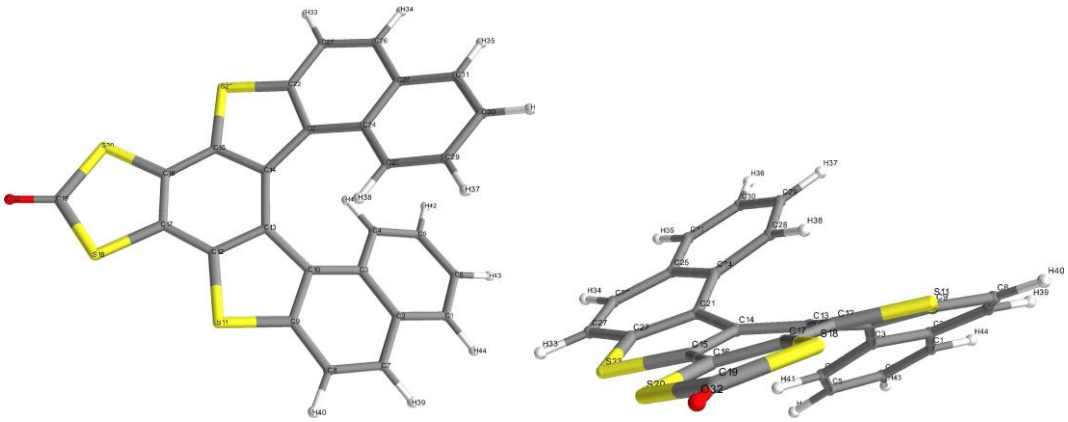

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-dTH-M
Formula	C27H12OS4
Charge	0
Spin multiplicity	1

2 COMPUTATIONAL DETAILS

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Number of basis set functions	968	
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	0.000083	0.000450
RMS Force value and threshold	0.000010	0.000300
Max Displacement value and threshold	0.001429	0.001800
RMS Displacement value and threshold	0.000365	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	40	['Singlet-A']

3 RESULTS

Total molecular energy	-2702.65945 hartrees
HOMO number	123
LUMO+1 energies	-1.46 eV
LUMO energies	-2.22 eV
HOMO energies	-5.98 eV
HOMO-1 energies	-6.29 eV

Geometry optimization specific results

Converged nuclear repulsion energy	3746.02588 Hartrees
Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-2702.32747 Hartrees
Gibbs free energy at 298.15 K	-2702.40424 Hartrees
Entropy at 298.15 K	0.00026 Hartrees

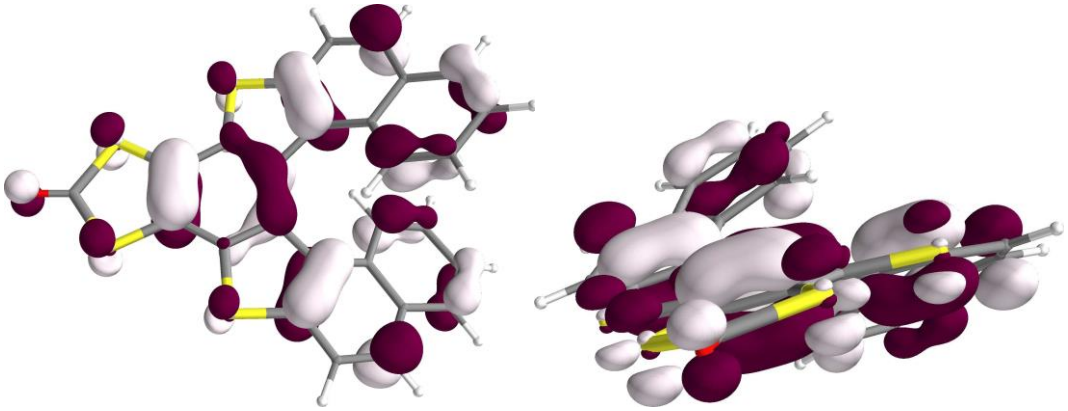

Figure 2: Representation of the HOMO from two points of view.

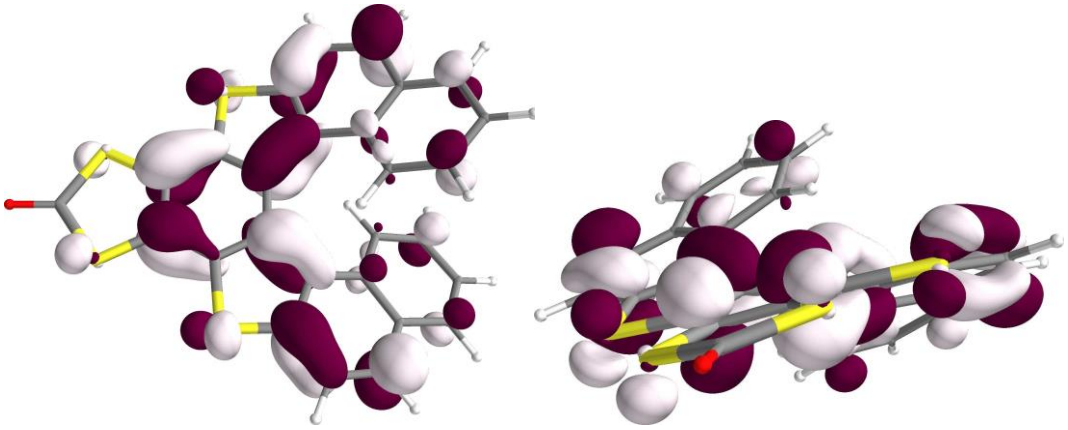

Figure 3: Representation of the LUMO from two points of view.

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

Frequencies	Intensity	Symmetry
1794	932	A
1367	94	A
820	78	A

Table. First five calculated mono-electronic excitations and those with f > 0.1 or R > 10.

E.S.	Symmetry	nm	cm^{-1}	*f*	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	399	25046	0.173	-77.2	0.78	18.80	0.41	123-124(96);
2	Singlet-A	370	26960	0.129	80.6	0.73	18.82	0.45	122-124(87);
3	Singlet-A	332	30100	0.019	11.7	0.71	189.54	0.46	121-124(79); 123-125(16);
4	Singlet-A	330	30275	0.010	-15.7	0.46	420.22	0.73	123-126(89);
5	Singlet-A	320	31187	0.117	-42.0	0.75	181.00	0.35	121-124(14); 123-125(80);
6	Singlet-A	314	31837	0.023	-165.9	0.61	13.53	0.37	119-124(12); 120-124(40); 122-125(30); 123-129(8);
9	Singlet-A	296	33680	0.004	-14.2	0.59	105.75	0.46	119-124(70); 122-125(23);
10	Singlet-A	294	33988	0.167	139.6	0.63	366.79	0.50	123-127(78);
11	Singlet-A	287	34768	0.112	107.5	0.62	348.22	0.32	118-124(11); 120-125(10); 123-128(44); 123-131(8);
12	Singlet-A	280	35708	0.007	16.3	0.64	321.32	0.33	118-124(27); 123-128(38); 123-131(21);
13	Singlet-A	278	35879	0.032	-106.6	0.65	113.57	0.35	121-125(18); 122-127(44); 123-129(17); 123-130(15);
14	Singlet-A	278	35969	0.007	-18.3	0.64	193.71	0.30	121-125(39); 123-129(35);
15	Singlet-A	273	36505	0.071	-412.4	0.65	112.66	0.39	122-127(9); 122-128(8); 123-129(7); 123-130(62);
17	Singlet-A	269	37116	0.010	17.9	0.42	517.36	0.60	118-124(12); 121-126(66);
18	Singlet-A	264	37745	0.088	-42.4	0.58	253.40	0.37	121-125(14); 122-128(51); 123-130(6);
19	Singlet-A	263	37914	0.013	-12.7	0.61	179.61	0.27	118-124(27); 121-126(15); 122-129(17); 122-130(9); 123-131(17);
20	Singlet-A	257	38843	0.188	-22.8	0.61	231.00	0.40	118-124(7); 120-125(15); 122-129(62);
21	Singlet-A	257	38857	0.009	-88.2	0.50	483.60	0.57	121-127(58); 121-128(20);
23	Singlet-A	254	39363	0.043	31.1	0.57	278.13	0.34	119-125(10); 122-130(55); 123-131(20);
24	Singlet-A	251	39695	0.002	19.2	0.61	67.98	0.26	119-125(12); 120-125(30); 121-129(23); 123-131(15);
25	Singlet-A	250	39866	0.020	-41.7	0.47	346.31	0.47	120-126(33); 122-131(31); 122-132(15);
26	Singlet-A	250	39879	0.047	108.3	0.56	258.35	0.40	119-125(60); 122-130(12);
27	Singlet-A	247	40440	0.028	21.9	0.39	191.86	0.64	123-132(75);
28	Singlet-A	246	40622	0.015	25.6	0.57	366.64	0.40	120-126(10); 121-127(17); 121-128(10); 121-131(9); 122-131(35);
29	Singlet-A	243	41098	0.005	-39.9	0.55	454.45	0.41	117-124(9); 120-126(8); 121-127(7); 121-128(37); 122-131(20);
30	Singlet-A	242	41239	0.018	18.4	0.55	27.43	0.43	117-124(70); 119-126(7);
34	Singlet-A	236	42336	0.006	-49.4	0.54	118.47	0.28	116-124(7); 118-125(33); 121-128(17); 121-131(23);
37	Singlet-A	233	42790	0.002	-29.8	0.27	602.14	0.78	116-124(85);
38	Singlet-A	233	42868	0.248	42.3	0.47	518.05	0.39	115-124(8); 118-126(21); 119-127(13); 120-127(25); 121-130(6);
39	Singlet-A	231	43236	0.160	-0.5	0.57	400.45	0.40	115-124(8); 118-126(16); 119-127(53);
40	Singlet-A	229	43638	0.097	59.5	0.50	44.38	0.43	115-124(54); 118-126(8); 121-129(6);

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-4.1226	2.7302	-1.1722
C	-2.8415	2.7798	-0.5842
C	-1.9833	1.6468	-0.6821
C	-2.4112	0.5628	-1.4746
C	-3.6479	0.5594	-2.0676
C	-4.5278	1.6381	-1.8923
C	-2.3839	3.9707	0.0361
C	-1.0976	4.0860	0.4693
C	-0.2571	2.9628	0.3817
C	-0.6925	1.7136	-0.0593
S	1.4412	3.0087	0.7301
C	1.5912	1.3299	0.3229
C	0.3528	0.7117	0.0600
C	0.3528	-0.7117	-0.0596
C	1.5912	-1.3300	-0.3226
C	2.8097	-0.6609	-0.2056
C	2.8097	0.6607	0.2057
S	4.3601	1.4126	0.4619
C	5.3494	-0.0001	-0.0002
S	4.3600	-1.4127	-0.4620
C	-0.6926	-1.7136	0.0596
C	-0.2573	-2.9628	-0.3815
S	1.4411	-3.0088	-0.7297
C	-1.9835	-1.6468	0.6821

C	-2.8417	-2.7797	0.5841
C	-2.3842	-3.9706	-0.0363
C	-1.0977	-4.0859	-0.4692
C	-2.4114	-0.5628	1.4747
C	-3.6482	-0.5592	2.0674
C	-4.5281	-1.6379	1.8919
C	-4.1229	-2.7300	1.1718
O	6.5413	-0.0000	-0.0003
H	-0.7212	-5.0215	-0.8668
H	-3.0610	-4.8160	-0.1040
H	-4.7742	-3.5921	1.0664
H	-5.5113	-1.6173	2.3489
H	-3.9447	0.2849	2.6804
H	-1.7436	0.2711	1.6410
H	-3.0606	4.8162	0.1036
H	-0.7210	5.0215	0.8668
H	-1.7435	-0.2711	-1.6408
H	-3.9444	-0.2847	-2.6806
H	-5.5109	1.6175	-2.3493
H	-4.7739	3.5924	-1.0668

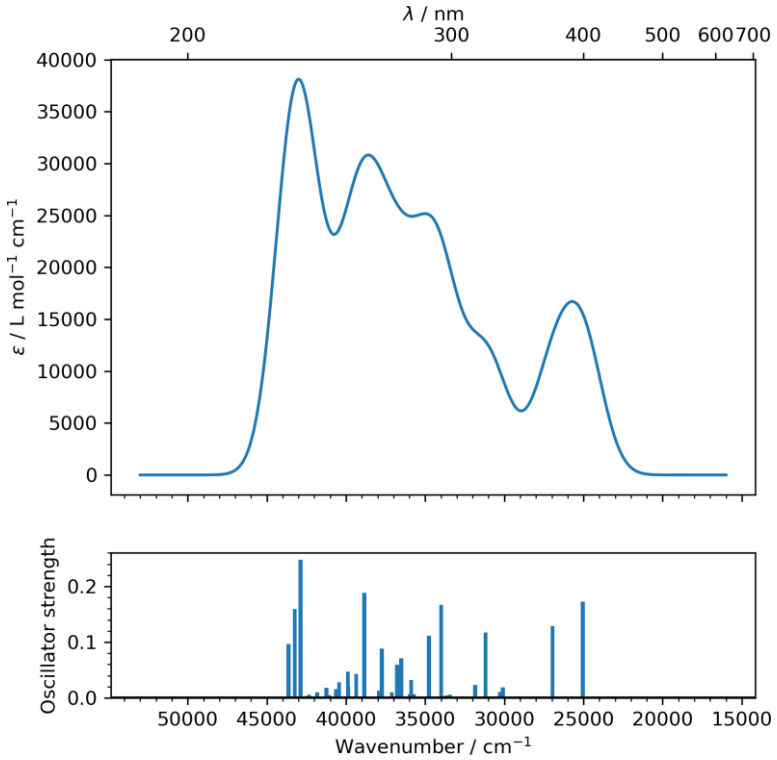

Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

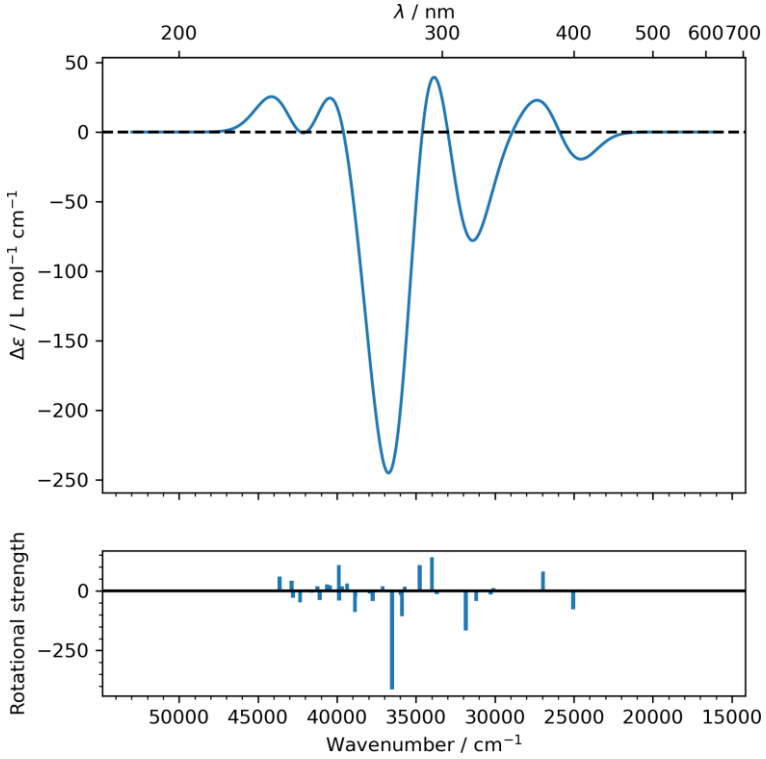

Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

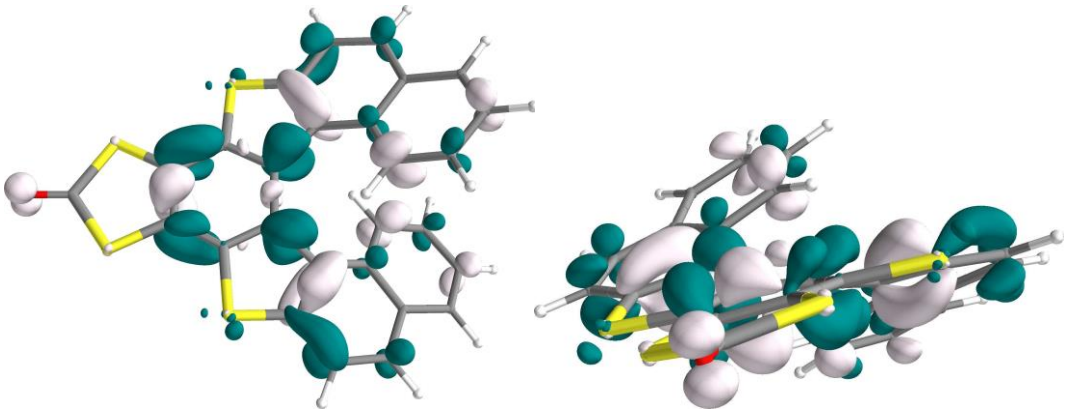

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

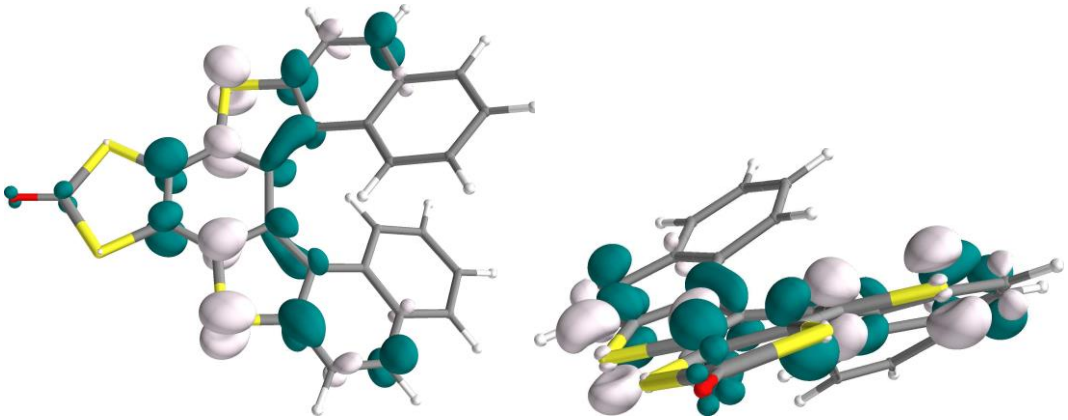

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.

1 Supplementary theoretical results generated by quchemreport

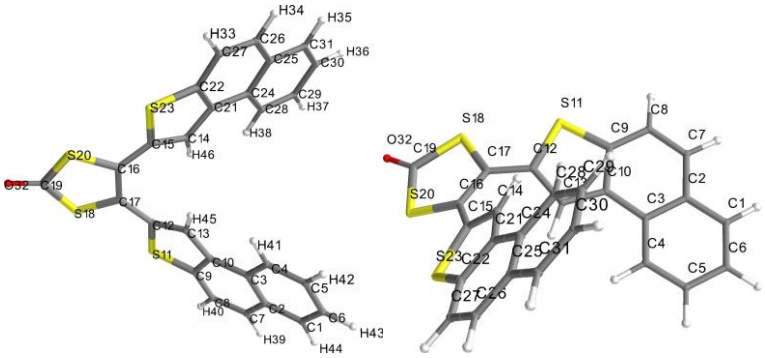

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Compound name and Formula	4_dicat	C27H14OS4++
Charge and Multiplicity	2	1
Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Solvent	Gas	
Total molecular energy	-2703.22557 hartrees	
HOMO number	123	
LUMO+1 energies	-9.25 eV	
LUMO energies	-10.67 eV	
HOMO energies	-12.34 eV	
HOMO-1 energies	-12.82 eV	
Sum of electronic and zero-point energy	-2702.89729 Hartrees	
Sum of electronic and thermal energies at 298.15 K	-2702.87224 Hartrees	
Enthalpy at 298.15 K	-2702.87129 Hartrees	
Gibbs free energy at 298.15 K	-2702.95471 Hartrees	
Entropy at 298.15 K	0.00028 Hartrees	

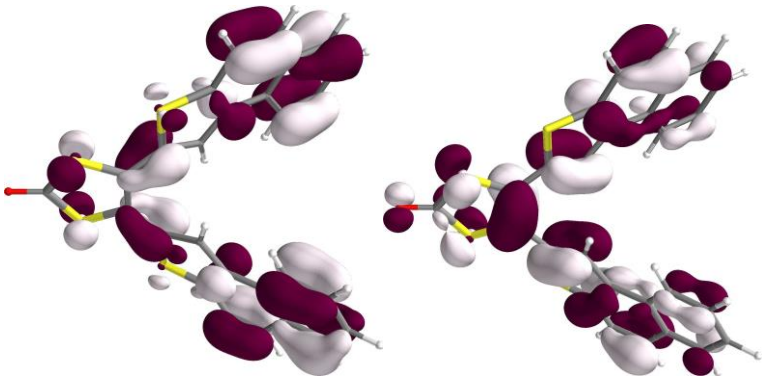

Figure 2: Representation of the Frontier Molecular Orbitals HOMO (left) and LUMO (right).

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%). a and b represent alpha or beta spinorbitals
1	Singlet-A	878	11380	0.000	9.4	0.66	200.96	0.54	121-124(65); 122-124(33);
2	Singlet-A	845	11824	0.078	-175.6	0.61	294.63	0.60	120-124(74); 123-124(25);
3	Singlet-A	828	12070	0.295	751.4	0.74	309.60	0.52	120-124(24); 123-124(78);
4	Singlet-A	688	14532	0.147	-178.2	0.70	253.68	0.51	121-124(30); 122-124(60); 123-125(9);
5	Singlet-A	478	20914	0.161	-297.2	0.68	230.22	0.47	118-124(33); 123-125(59);
6	Singlet-A	471	21193	0.040	-37.2	0.75	145.28	0.42	119-124(94);
7	Singlet-A	459	21755	0.021	-23.8	0.41	477.87	0.77	117-124(90);
8	Singlet-A	439	22739	0.282	-58.9	0.69	14.71	0.42	117-124(7); 118-124(58); 123-125(25);
9	Singlet-A	426	23423	0.015	10.9	0.63	286.06	0.64	122-125(97);
10	Singlet-A	417	23931	0.012	61.5	0.62	195.75	0.59	116-124(23); 121-125(72);
11	Singlet-A	411	24287	0.000	-4.7	0.57	353.57	0.66	120-125(97);
12	Singlet-A	405	24642	0.074	-37.1	0.62	80.45	0.56	116-124(71); 121-125(21);
13	Singlet-A	394	25343	0.021	16.4	0.55	40.71	0.65	115-124(95);
14	Singlet-A	338	29558	0.093	-68.0	0.70	116.77	0.48	114-124(93);
15	Singlet-A	314	31829	0.040	6.3	0.68	10.03	0.53	118-125(94);
16	Singlet-A	311	32054	0.067	-0.8	0.71	247.79	0.40	113-124(36); 119-125(58);
17	Singlet-A	308	32395	0.117	52.5	0.67	245.38	0.34	113-124(53); 119-125(33);
18	Singlet-A	302	33009	0.007	9.3	0.36	372.60	0.77	117-125(87);
19	Singlet-A	300	33239	0.000	-0.2	0.33	389.23	0.78	112-124(92);
20	Singlet-A	300	33308	0.000	0.7	0.34	372.98	0.78	111-124(86);

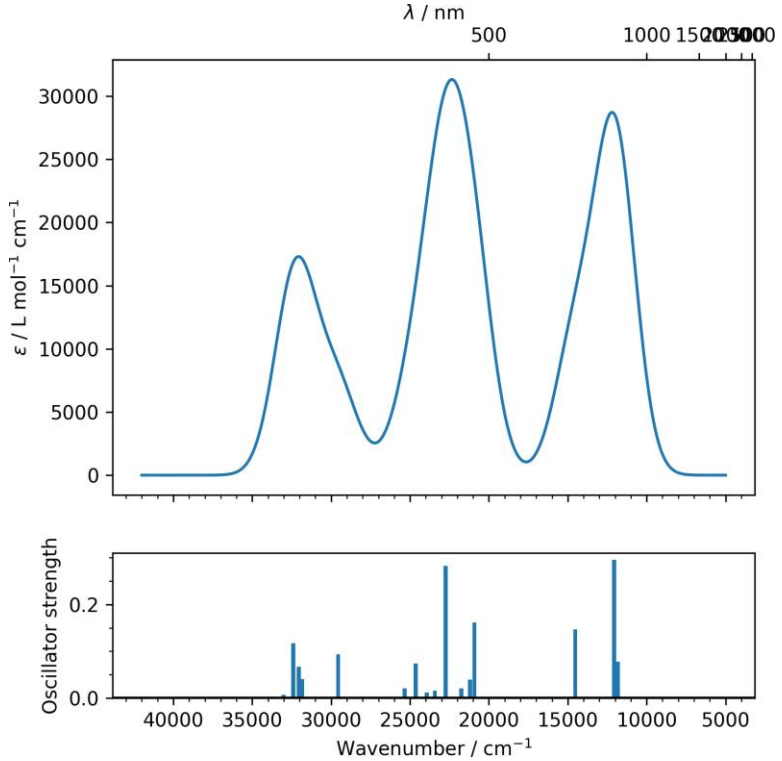

Figure 3: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-4.4614	3.7939	-0.9549
C	-4.0778	2.5860	-0.3409
C	-2.9124	1.9068	-0.7900
C	-2.1750	2.4578	-1.8346
C	-2.5759	3.6461	-2.4267
C	-3.7172	4.3178	-1.9881
C	-4.8516	2.0455	0.7118
C	-4.5390	0.8552	1.3436
C	-3.4111	0.1766	0.9148
C	-2.5676	0.6707	-0.1275
S	-2.8682	-1.3426	1.5321
C	-1.5028	-1.3344	0.4467

C	-1.5058	-0.1772	-0.3686
C	1.5007	-0.2207	0.3757
C	1.4591	-1.3752	-0.4428
C	0.6019	-2.4704	-0.3271
C	-0.6764	-2.4531	0.3316
S	-1.2643	-3.9811	0.8887
C	-0.0739	-4.9975	-0.0019
S	1.1460	-4.0130	-0.8883
C	2.5856	0.5965	0.1305
C	3.4073	0.0812	-0.9191
S	2.8171	-1.4197	-1.5367
C	2.9714	1.8202	0.7941
C	4.1522	2.4666	0.3369
C	4.9019	1.9075	-0.7235
C	4.5506	0.7283	-1.3554
C	2.2599	2.3890	1.8471
C	2.7008	3.5630	2.4395
C	3.8571	4.2026	1.9928
C	4.5762	3.6608	0.9510
O	-0.0909	-6.1729	-0.0041
H	5.1652	0.3220	-2.1496
H	5.8022	2.4238	-1.0432
H	5.4788	4.1459	0.5949
H	4.1888	5.1183	2.4677
H	2.1401	3.9857	3.2657
H	1.3601	1.9157	2.2237
H	-5.7396	2.5861	1.0259
H	-5.1713	0.4648	2.1319
H	-1.2860	1.9597	-2.2047
H	-1.9956	4.0552	-3.2461
H	-4.0175	5.2444	-2.4626
H	-5.3527	4.3039	-0.6051
H	-0.7840	-0.0383	-1.1617
H	0.7879	-0.0628	1.1734

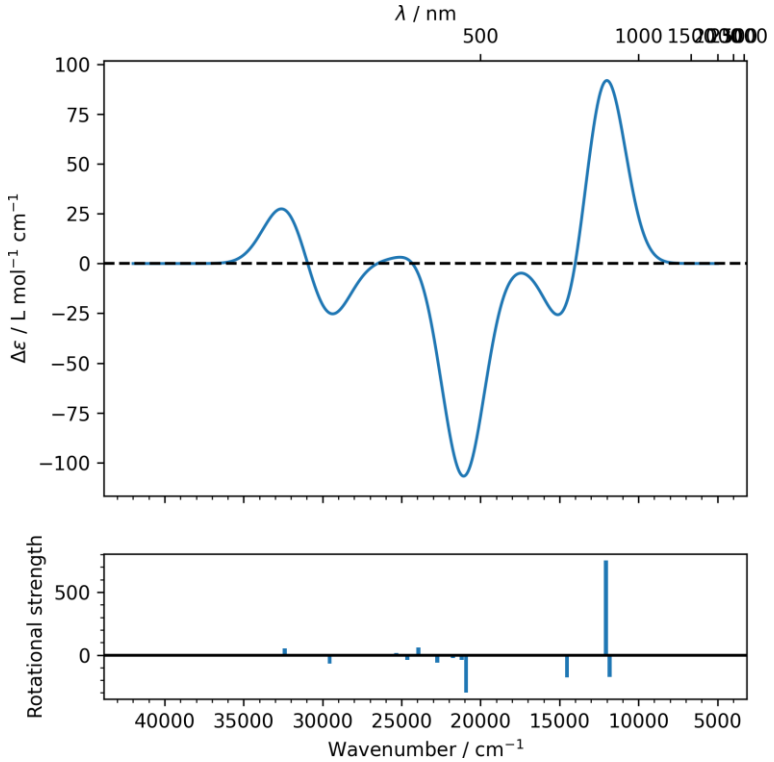

Figure 4: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

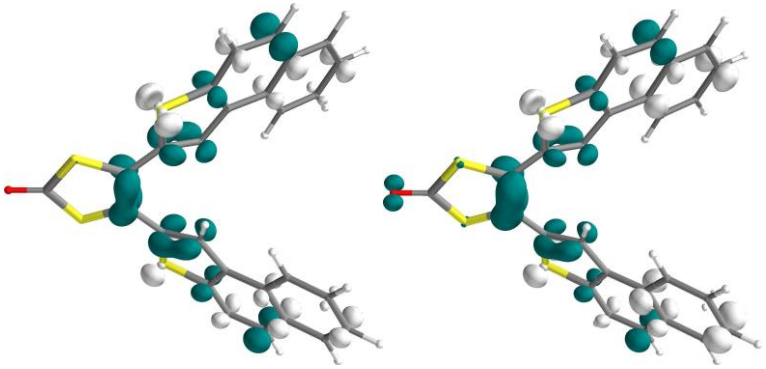

Figure 5: Representation of the Electron Density Difference (S1-S0 left) and (S2-S0 right). The excited electron and the hole regions are indicated by respectively blue and white surfaces.

1 Supplementary theoretical results generated by quchemreport

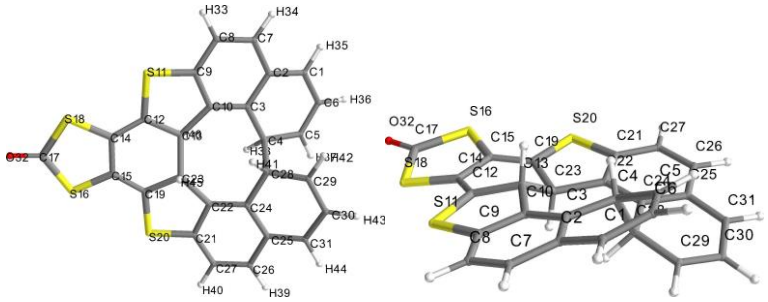

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Compound name and Formula	4"_dicat	C27H14OS4++
Charge and Multiplicity	2	1
Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Solvent	Gas	
Total molecular energy	-2703.17178 hartrees	
HOMO number	123	
LUMO+1 energies	-9.81 eV	
LUMO energies	-9.99 eV	
HOMO energies	-11.65 eV	
HOMO-1 energies	-12.60 eV	
Sum of electronic and zero-point energy	-2702.84013 Hartrees	
Sum of electronic and thermal energies at 298.15 K	-2702.81702 Hartrees	
Enthalpy at 298.15 K	-2702.81607 Hartrees	
Gibbs free energy at 298.15 K	-2702.89166 Hartrees	
Entropy at 298.15 K	0.00025 Hartrees	

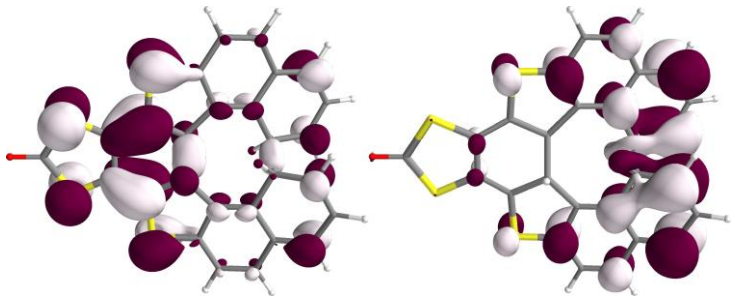

Figure 2: Representation of the Frontier Molecular Orbitals HOMO (left) and LUMO (right).

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%). a and b represent alpha or beta spinorbitals
1	Singlet-A	1089	9181	0.027	218.5	0.62	513.61	0.70	123-124(100);
2	Singlet-A	841	11882	0.094	-40.6	0.73	529.16	0.58	122-124(11); 123-125(88);
3	Singlet-A	547	18278	0.021	99.2	0.62	646.32	0.61	122-125(95);
4	Singlet-A	546	18302	0.336	-196.3	0.55	618.23	0.73	122-124(87); 123-125(11);
5	Singlet-A	432	23118	0.005	159.1	0.62	523.98	0.54	120-124(64); 123-126(28);
6	Singlet-A	420	23770	0.000	-0.7	0.12	829.63	0.97	121-124(99);
7	Singlet-A	415	24060	0.038	-59.2	0.61	489.95	0.61	119-124(79); 120-125(17);
8	Singlet-A	410	24351	0.011	-22.7	0.66	467.37	0.43	119-125(37); 120-124(22); 123-126(31);
9	Singlet-A	402	24865	0.000	-0.1	0.13	765.91	0.95	121-125(98);
10	Singlet-A	388	25744	0.018	53.3	0.60	340.34	0.44	117-125(6); 118-124(35); 119-125(21); 120-124(10); 123-126(20);
11	Singlet-A	385	25915	0.146	-169.2	0.61	528.99	0.55	118-125(10); 119-124(14); 120-125(70);
12	Singlet-A	377	26521	0.177	98.9	0.59	289.81	0.47	117-125(6); 118-124(41); 119-125(34); 123-126(13);
13	Singlet-A	374	26700	0.016	-11.2	0.52	150.62	0.69	117-124(60); 118-125(34);
14	Singlet-A	347	28813	0.070	-95.3	0.51	231.43	0.55	117-124(27); 118-125(45); 123-127(16);
15	Singlet-A	346	28860	0.013	14.0	0.47	448.46	0.59	117-124(9); 118-125(9); 123-127(76);
16	Singlet-A	343	29076	0.002	-6.2	0.48	82.97	0.74	117-125(84); 118-124(14);
17	Singlet-A	338	29569	0.000	-1.3	0.57	76.74	0.63	123-129(64); 123-131(27);
18	Singlet-A	331	30122	0.021	-24.7	0.61	178.22	0.58	123-128(92);
19	Singlet-A	315	31662	0.004	-5.5	0.56	3.40	0.61	123-129(24); 123-131(62);
20	Singlet-A	315	31695	0.024	-15.5	0.55	506.87	0.53	116-124(52); 123-130(42);

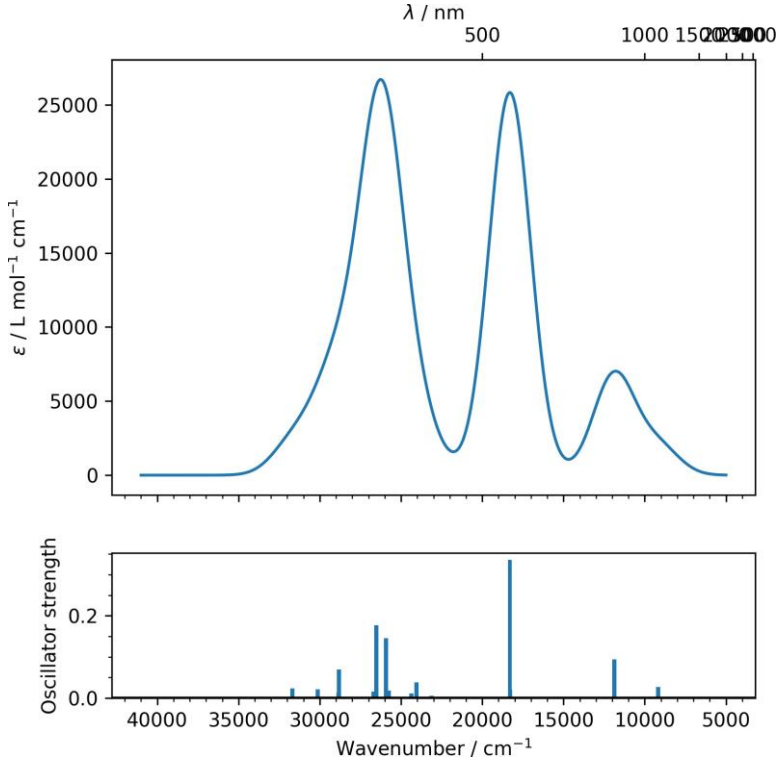

Figure 3: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	4.1380	-2.9321	0.7479
C	2.8177	-2.9545	0.3167
C	2.0433	-1.7512	0.3420
C	2.7291	-0.4598	0.6478
C	4.1166	-0.5815	1.1815
C	4.7716	-1.7615	1.2283
C	2.2171	-4.1835	-0.0612
C	0.8864	-4.2379	-0.3419
C	0.1345	-3.0574	-0.2311
C	0.6942	-1.7924	0.0827

S	-1.5594	-3.0574	-0.4097
C	-1.6816	-1.3656	-0.0882
C	-0.3630	-0.7098	0.3201
C	-2.8614	-0.7105	-0.1327
C	-2.8614	0.7105	0.1326
S	-4.4039	1.4440	0.4369
C	-5.3939	0.0000	-0.0002
S	-4.4039	-1.4440	-0.4370
C	-1.6816	1.3657	0.0882
S	-1.5594	3.0574	0.4099
C	0.1345	3.0574	0.2314
C	0.6941	1.7925	-0.0827
C	-0.3630	0.7098	-0.3200
C	2.0432	1.7513	-0.3421
C	2.8178	2.9545	-0.3166
C	2.2171	4.1834	0.0615
C	0.8865	4.2379	0.3423
C	2.7288	0.4599	-0.6484
C	4.1162	0.5816	-1.1823
C	4.7715	1.7614	-1.2284
C	4.1381	2.9320	-0.7476
O	-6.5706	0.0000	-0.0001
H	0.4050	-5.1716	-0.6089
H	2.8246	-5.0815	-0.0945
H	4.6946	-3.8651	0.7482
H	5.7807	-1.8224	1.6189
H	4.5885	0.3244	1.5477
H	2.1382	0.0722	1.4076
H	2.8246	5.0815	0.0948
H	0.4052	5.1715	0.6095
H	2.1376	-0.0720	-1.4079
H	4.5878	-0.3243	-1.5491
H	5.7806	1.8223	-1.6189
H	4.6949	3.8649	-0.7476
H	-0.4062	0.5616	-1.4150
H	-0.4064	-0.5619	1.4151

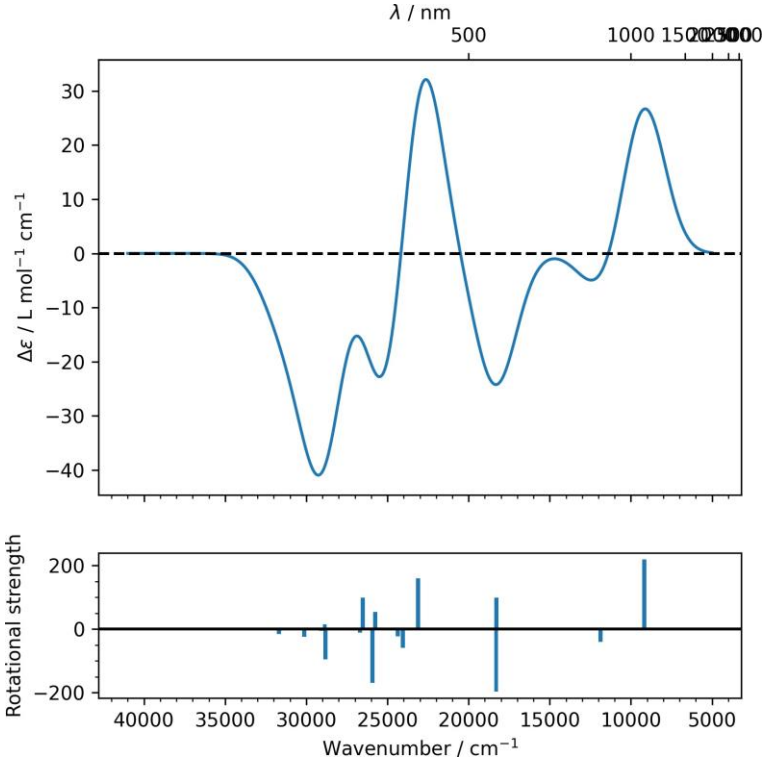

Figure 4: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

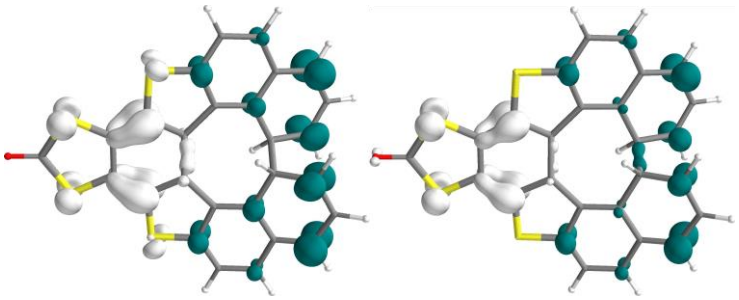

Figure 5: Representation of the Electron Density Difference (S1-S0 left) and (S2-S0 right). The excited electron and the hole regions are indicated by respectively blue and white surfaces.

Molecular Calculation Report generated by quchemreport

March 30, 2022

1 MOLECULE

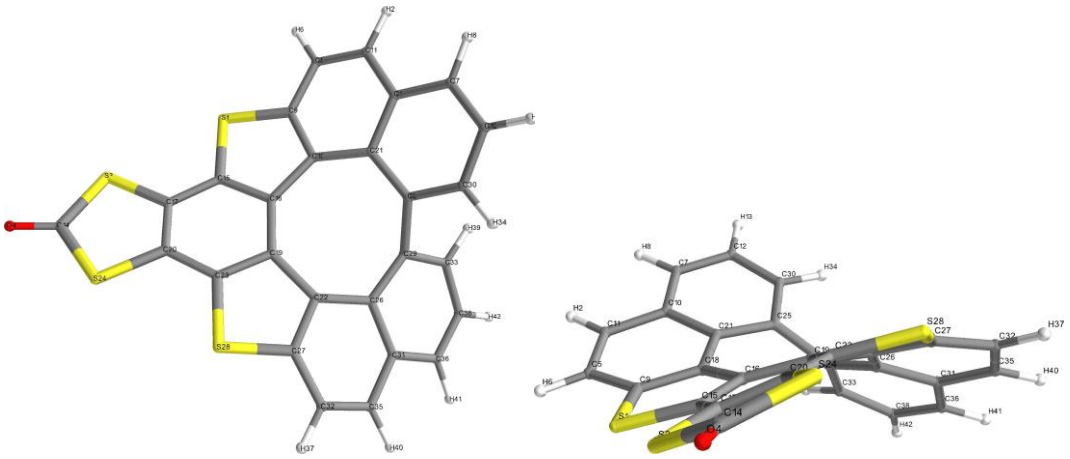

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-dTQC-M
Formula	C27H10OS4
Charge	0
Spin multiplicity	1

2 COMPUTATIONAL DETAILS

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Number of basis set functions	956	
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	0.000036	0.000450
RMS Force value and threshold	0.000004	0.000300
Max Displacement value and threshold	0.000215	0.001800
RMS Displacement value and threshold	0.000051	0.001200
Job type: Frequency and thermochemical analysis		
Temperature	298.15 K	
Anharmonic effects	None	
Anharmonic effects	None	

3 RESULTS

Total molecular energy	-2701.44291 hartrees
HOMO number	122
LUMO+1 energies	-1.64 eV
LUMO energies	-2.13 eV
HOMO energies	-5.99 eV
HOMO-1 energies	-6.31 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	3696.05192 Hartrees

Frequency and Thermochemistry specific results

Enthalpy at 298.15 K	-2701.13375 Hartrees
Gibbs free energy at 298.15 K	-2701.20720 Hartrees
Entropy at 298.15 K	0.00025 Hartrees

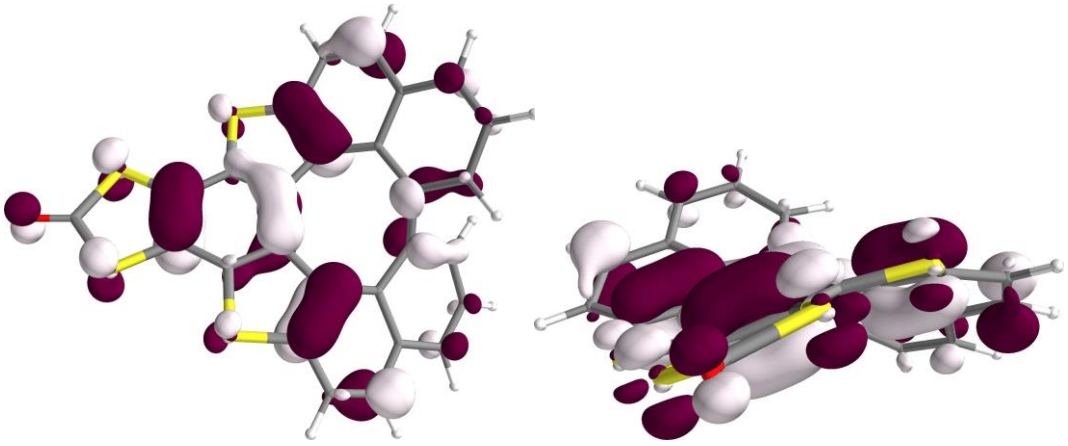

Figure 2: Representation of the HOMO from two points of view.

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

Frequencies	Intensity	Symmetry
1795	918	A
1366	72	A
846	51	A

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
S	1.4554	-2.9145	-0.9829
H	-2.5211	-5.1501	0.5467
S	4.2899	-1.3445	-0.6349
O	6.4712	-0.0000	0.0001
C	-0.8725	-4.2072	-0.4075
H	-0.3959	-5.1261	-0.7288
C	-3.8157	-3.0541	1.4758
H	-4.1765	-4.0246	1.8007
C	-0.2193	-2.9731	-0.5757
C	-2.6454	-2.9998	0.6962
C	-2.0365	-4.2148	0.2880
C	-4.4790	-1.9069	1.8118
H	-5.3590	-1.9330	2.4445
C	5.2794	0.0000	0.0000
C	1.5185	-1.2560	-0.5067
C	0.2602	-0.6886	-0.2048
C	2.7421	-0.6222	-0.2923
C	-0.7617	-1.7342	-0.2300
C	0.2602	0.6886	0.2047
C	2.7421	0.6223	0.2923
C	-2.1008	-1.7418	0.2896
C	-0.7618	1.7342	0.2300
C	1.5185	1.2560	0.5066
S	4.2899	1.3445	0.6348
C	-2.9409	-0.6111	0.4275
C	-2.1008	1.7418	-0.2896
C	-0.2193	2.9731	0.5757
S	1.4554	2.9145	0.9829
C	-2.9410	0.6111	-0.4275
C	-4.0676	-0.7054	1.2297
C	-2.6454	2.9998	-0.6962
C	-0.8726	4.2072	0.4075
C	-4.0677	0.7053	-1.2297
H	-4.6832	0.1791	1.3511
C	-2.0366	4.2148	-0.2880
C	-3.8157	3.0540	-1.4758
H	-0.3960	5.1261	0.7288
C	-4.4791	1.9069	-1.8118
H	-4.6832	-0.1791	-1.3510
H	-2.5212	5.1501	-0.5467
H	-4.1765	4.0246	-1.8006
H	-5.3590	1.9329	-2.4445

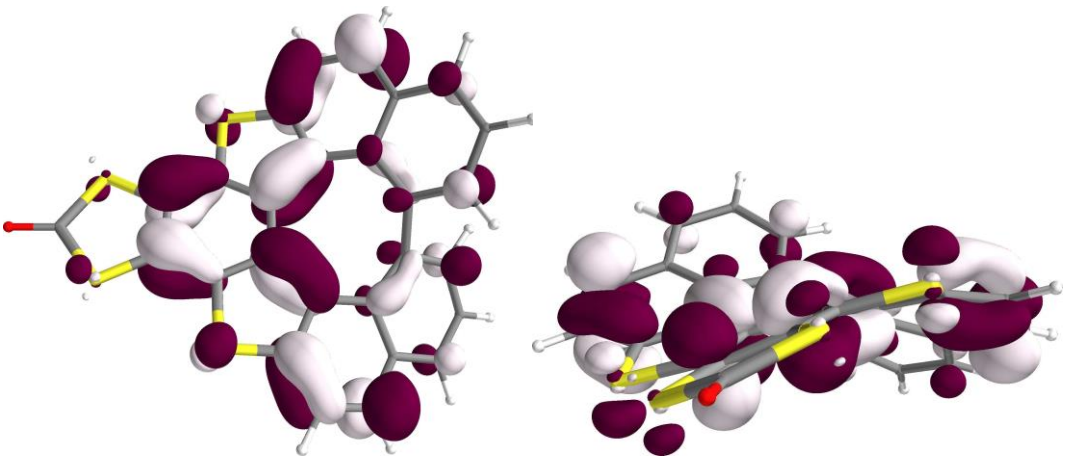

Figure 3: Representation of the LUMO from two points of view.

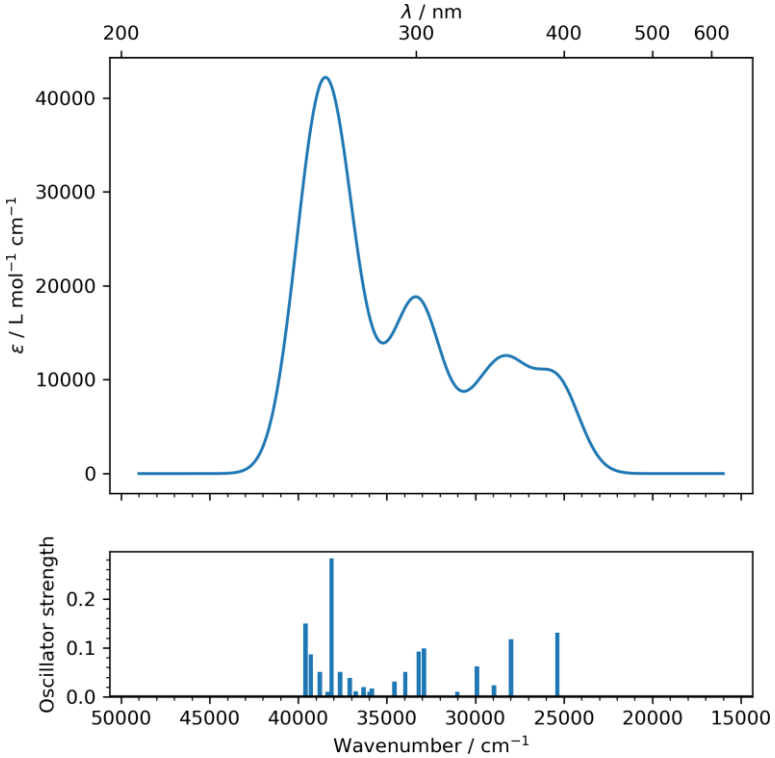

Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

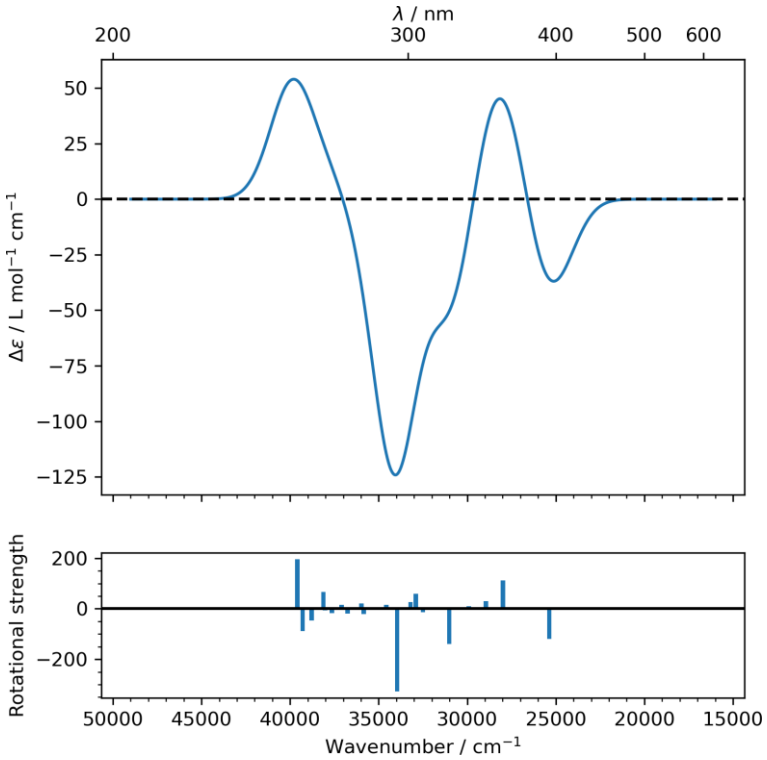

Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

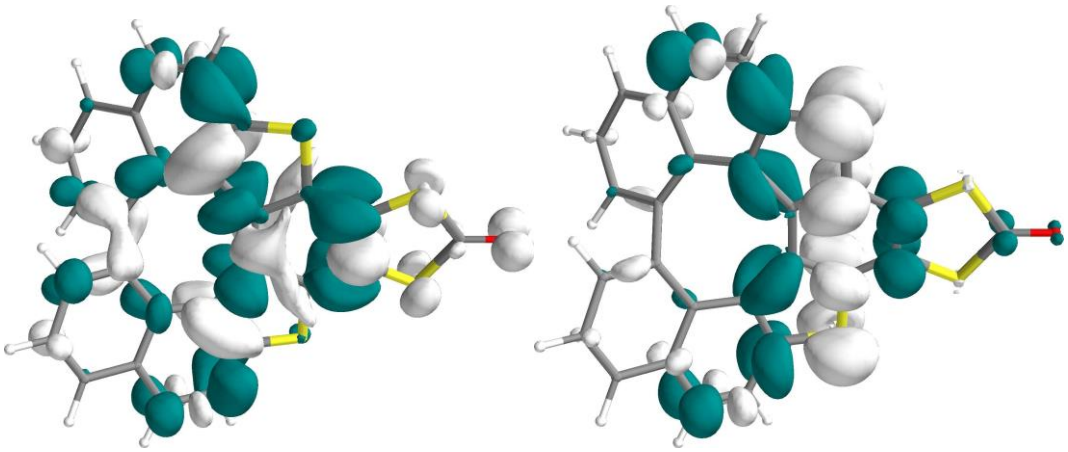

Figure 6: Representation of the Electron Density Difference (S1-S0 left) and (S2-S0 right). The excited electron and the hole regions are indicated by respectively blue and white surfaces.

Molecular Calculation Report generated by quchemreport

February 9, 2022

1 MOLECULE

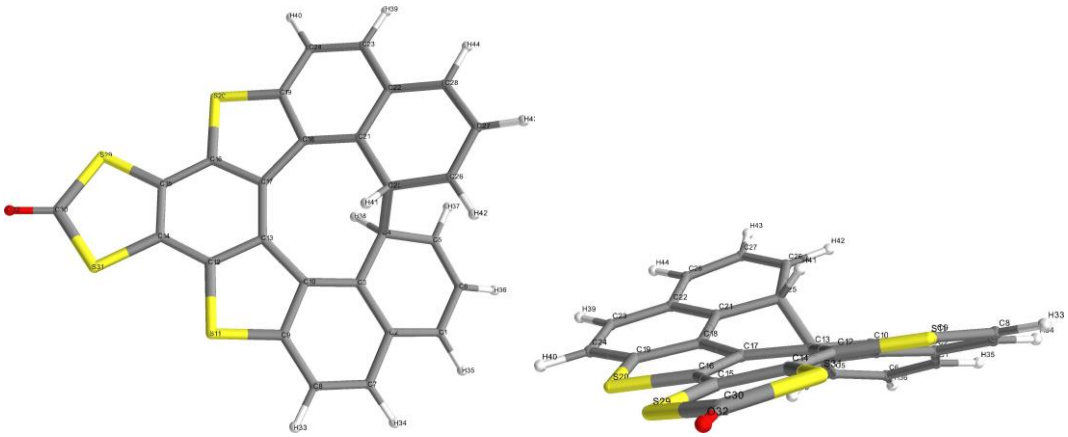

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	1-dTH'-dicat-M
Formula	C27H12OS4++
Charge	2
Spin multiplicity	1

2 COMPUTATIONAL DETAILS

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Number of basis set functions	968	
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	0.000016	0.000450
RMS Force value and threshold	0.000002	0.000300
Max Displacement value and threshold	0.000768	0.001800
RMS Displacement value and threshold	0.000170	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	40	['Singlet-A']

3 RESULTS

Total molecular energy	-2702.02257 hartrees
HOMO number	122
LUMO+1 energies	-9.90 eV
LUMO energies	-10.18 eV
HOMO energies	-12.23 eV
HOMO-1 energies	-12.56 eV

Geometry optimization specific results

Converged nuclear repulsion energy	3763.11718 Hartrees

Frequency and Thermochemistry specific results	
Enthalpy at 298.15 K	-2701.68948 Hartrees
Gibbs free energy at 298.15 K	-2701.76405 Hartrees
Entropy at 298.15 K	0.00025 Hartrees

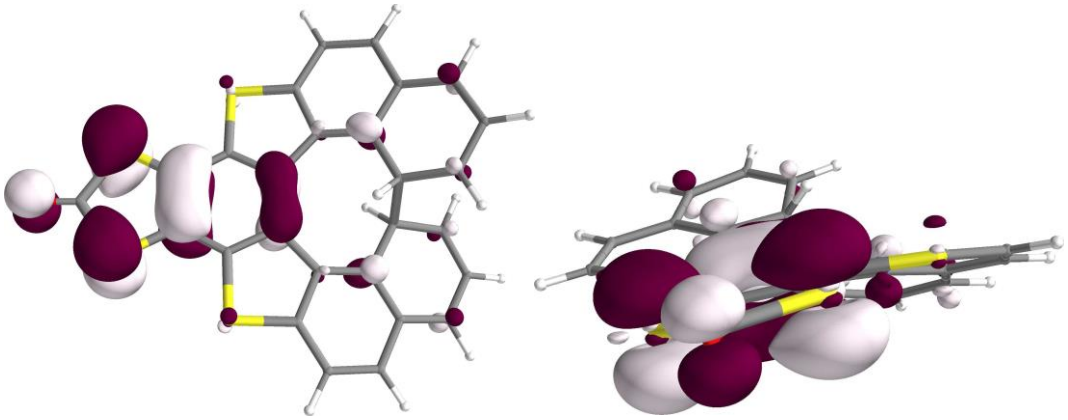

Figure 2: Representation of the HOMO from two points of view.

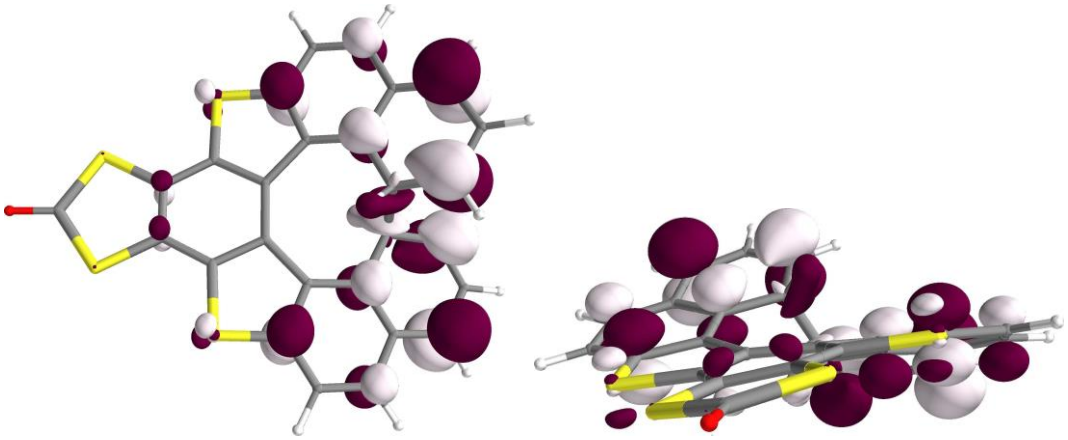

Figure 3: Representation of the LUMO from two points of view.

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

Frequencies	Intensity	Symmetry
1869	901	A
1670	78	A
1668	77	A
1615	167	A
1584	91	A
1580	87	A
1526	130	A
1517	133	A
1502	176	A
1466	68	A
1378	80	A
1355	62	A
1283	88	A
1210	311	A
1161	52	A
859	65	A

Table. First five calculated mono-electronic excitations and those with f > 0.1 or R > 10.

E.S.	Symmetry	nm	cm^{-1}	*f*	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	771	12957	0.076	49.0	0.56	647.45	0.72	122-123(91);
2	Singlet-A	732	13659	0.006	-17.4	0.52	593.39	0.69	121-123(51); 122-124(46);
3	Singlet-A	688	14515	0.023	-153.9	0.52	603.73	0.70	121-123(47); 122-124(52);
4	Singlet-A	600	16646	0.069	42.2	0.53	503.42	0.70	121-124(90);
5	Singlet-A	464	21518	0.046	74.9	0.54	500.18	0.63	117-123(8); 118-123(64); 120-123(22);
6	Singlet-A	459	21781	0.009	-132.0	0.57	507.58	0.66	119-123(94);
7	Singlet-A	454	21990	0.006	14.6	0.26	785.39	0.81	118-123(19); 120-123(77);
8	Singlet-A	423	23619	0.015	-202.0	0.61	416.41	0.56	118-124(81); 120-124(7);
11	Singlet-A	394	25333	0.005	-27.2	0.47	405.24	0.67	117-124(88);
12	Singlet-A	389	25653	0.195	238.5	0.57	535.12	0.58	117-123(14); 118-123(8); 119-124(67); 121-125(6);
14	Singlet-A	345	28924	0.195	-3.6	0.60	523.90	0.44	115-123(8); 116-123(46); 122-125(35);
15	Singlet-A	332	30054	0.203	173.4	0.65	291.34	0.43	116-124(9); 121-125(71); 122-127(6);
16	Singlet-A	328	30455	0.065	56.8	0.52	421.54	0.62	116-124(81); 121-125(7);
17	Singlet-A	317	31447	0.022	-43.5	0.62	316.40	0.56	115-123(87); 116-123(6);
19	Singlet-A	297	33668	0.086	91.3	0.62	374.79	0.56	115-124(85);
20	Singlet-A	295	33830	0.015	23.1	0.66	246.52	0.50	114-123(85); 122-127(8);
22	Singlet-A	287	34832	0.200	67.6	0.57	461.30	0.54	121-126(8); 122-127(64); 122-128(9);
23	Singlet-A	280	35702	0.007	-51.3	0.66	258.79	0.42	114-124(55); 121-127(31);
26	Singlet-A	273	36601	0.031	-27.8	0.45	496.77	0.56	113-123(13); 121-129(15); 122-128(53);
29	Singlet-A	270	37027	0.002	-20.1	0.65	171.80	0.37	114-124(28); 118-125(28); 121-127(24);
30	Singlet-A	267	37412	0.002	-18.9	0.64	85.13	0.38	111-123(6); 118-125(46); 121-127(29); 121-128(9);
31	Singlet-A	263	38019	0.164	-89.9	0.53	338.37	0.38	113-123(13); 119-125(18); 121-126(18); 121-129(19); 122-127(7);
33	Singlet-A	258	38615	0.026	-43.5	0.60	344.11	0.38	111-123(8); 117-125(28); 118-125(12); 121-128(37);
36	Singlet-A	254	39313	0.007	-14.8	0.56	385.49	0.53	111-123(20); 113-124(57);
37	Singlet-A	252	39585	0.218	-2.9	0.58	276.23	0.57	122-130(85);
38	Singlet-A	247	40344	0.118	13.5	0.63	289.88	0.36	111-123(25); 117-125(35); 118-126(7); 121-128(9);
40	Singlet-A	242	41183	0.003	37.1	0.35	414.56	0.75	120-127(41); 120-130(10); 120-131(41);

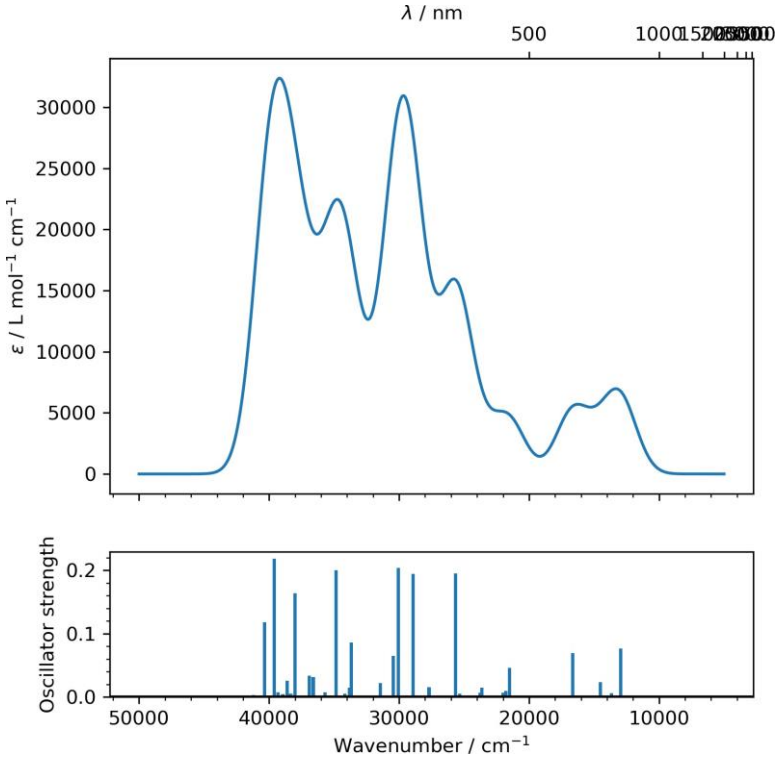

Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z

C	-4.0662	2.9190	-0.9279
C	-2.7718	2.9539	-0.4236
C	-2.0204	1.7437	-0.3488
C	-2.6868	0.4645	-0.6660
C	-4.0418	0.5551	-1.2530
C	-4.6903	1.7328	-1.3817
C	-2.1913	4.1973	-0.0509
C	-0.8845	4.2478	0.3198
C	-0.1392	3.0573	0.3100
C	-0.6852	1.7678	0.0335
S	1.5387	3.0362	0.5554
C	1.6000	1.3240	0.2691
C	0.3356	0.7130	0.0863
C	2.8262	0.6759	0.1670
C	2.8262	-0.6759	-0.1671
C	1.5999	-1.3240	-0.2690
C	0.3356	-0.7130	-0.0862
C	-0.6853	-1.7678	-0.0332
C	-0.1392	-3.0573	-0.3095
S	1.5387	-3.0362	-0.5550
C	-2.0206	-1.7437	0.3487
C	-2.7719	-2.9539	0.4238
C	-2.1913	-4.1974	0.0515
C	-0.8845	-4.2479	-0.3191
C	-2.6870	-0.4644	0.6656
C	-4.0423	-0.5550	1.2521
C	-4.6907	-1.7327	1.3810
C	-4.0664	-2.9190	0.9278
S	4.3572	-1.4535	-0.3722
C	5.3591	-0.0000	-0.0002
S	4.3573	1.4534	0.3719
O	6.5365	-0.0000	-0.0002
H	-0.4078	5.1866	0.5773
H	-2.7904	5.0998	-0.0998
H	-4.6158	3.8543	-0.9946
H	-5.6812	1.7818	-1.8177
H	-4.5059	-0.3687	-1.5851
H	-2.0567	-0.0788	-1.3811
H	-2.7903	-5.0999	0.1006
H	-0.4077	-5.1867	-0.5763
H	-2.0573	0.0788	1.3810
H	-4.5066	0.3689	1.5837
H	-5.6818	-1.7815	1.8167
H	-4.6159	-3.8543	0.9946

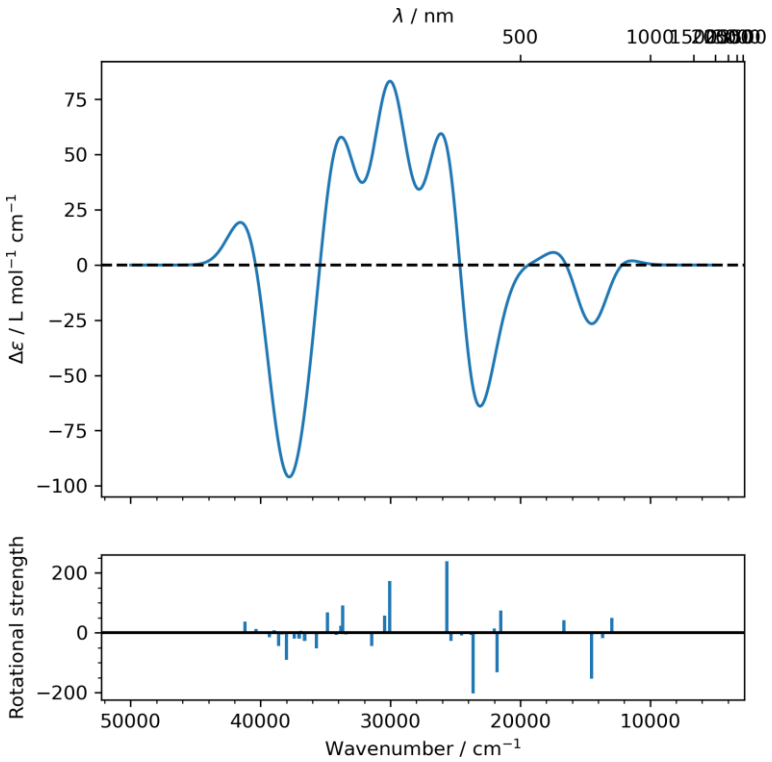

Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

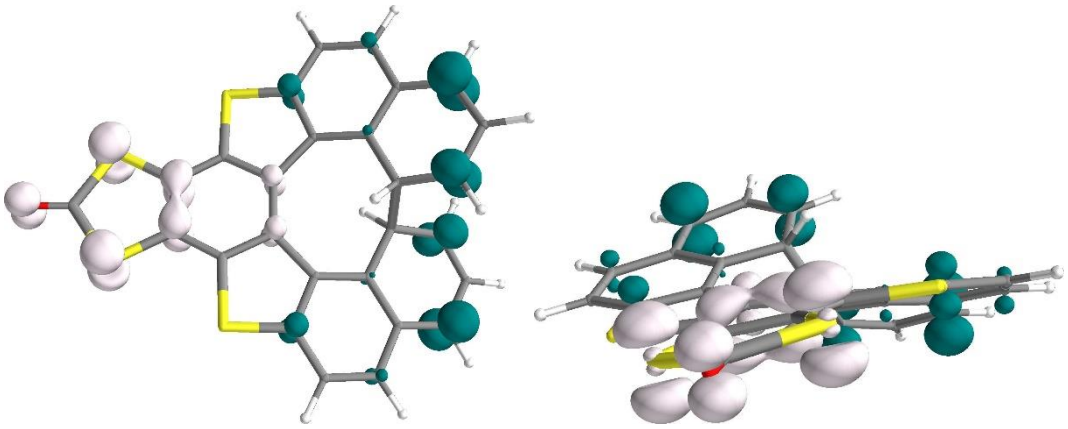

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

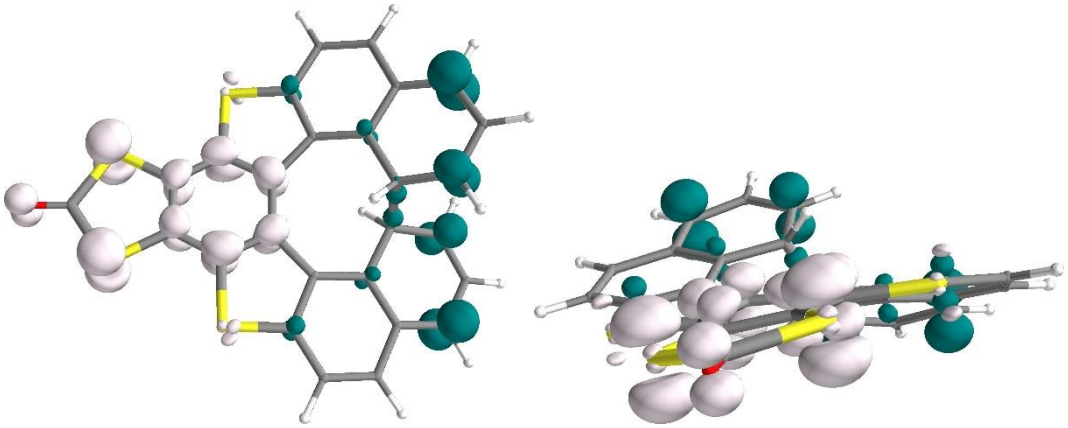

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.

Molecular Calculation Report generated by quchemreport

May 31, 2022

1 MOLECULE

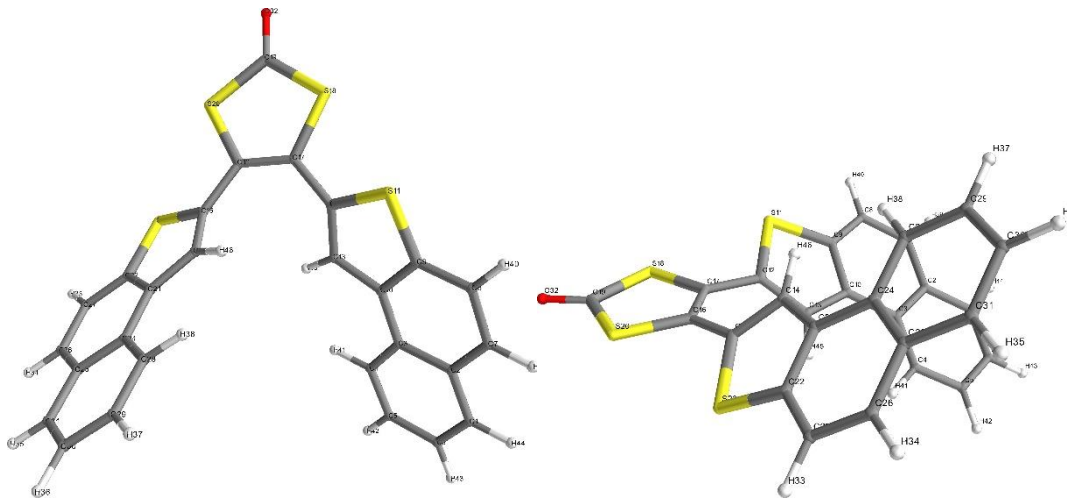

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	4-dicat-triplet
Formula	C27H14OS4++
Charge	2
Spin multiplicity	3

2 COMPUTATIONAL DETAILS

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	PBE1PBE	
Basis set name	6-311+G(2d,p)	
Number of basis set functions	980	
Closed shell calculation	False	
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	0.000018	0.000450
RMS Force value and threshold	0.000003	0.000300
Max Displacement value and threshold	0.001744	0.001800
RMS Displacement value and threshold	0.000348	0.001200

3 RESULTS

Total molecular energy	-2703.21414 hartrees	
Unrestricted calculation	Alpha spin MO	Beta spin MO
HOMO number	124	122
LUMO+1 energies	-7.90 eV	-10.40 eV
LUMO energies	-8.62 eV	-11.07 eV
HOMO energies	-12.01 eV	-12.35 eV
HOMO-1 energies	-12.71 eV	-12.82 eV
Geometry optimization specific results		
Converged nuclear repulsion energy	3574.36874 Hartrees	

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-4.8007	3.6641	-0.7941
C	-4.2978	2.5001	-0.1790
C	-3.1686	1.8436	-0.7414
C	-2.5943	2.3731	-1.8958
C	-3.1128	3.5233	-2.4890
C	-4.2125	4.1701	-1.9407
C	-4.9210	1.9832	0.9760
C	-4.4758	0.8209	1.5967
C	-3.3863	0.1673	1.0527
C	-2.6950	0.6497	-0.0952
S	-2.7093	-1.3120	1.6433
C	-1.5164	-1.2983	0.3846
C	-1.6304	-0.1895	-0.4423
C	1.6304	-0.1896	0.4424
C	1.5162	-1.2984	-0.3845
C	0.6538	-2.4444	-0.2166
C	-0.6540	-2.4444	0.2166
S	-1.3991	-3.9857	0.4943
C	-0.0001	-4.9988	0.0000
S	1.3988	-3.9858	-0.4943
C	2.6950	0.6495	0.0952
C	3.3861	0.1672	-1.0529
S	2.7090	-1.3121	-1.6434
C	3.1688	1.8433	0.7415
C	4.2982	2.4996	0.1792
C	4.9213	1.9826	-0.9759
C	4.4757	0.8207	-1.5969
C	2.5944	2.3731	1.8957
C	3.1131	3.5232	2.4889
C	4.2130	4.1697	1.9408
C	4.8013	3.6635	0.7943
O	-0.0001	-6.1780	0.0001
H	4.9852	0.4380	-2.4738
H	5.7834	2.5016	-1.3824
H	5.6635	4.1584	0.3598
H	4.6121	5.0613	2.4095
H	2.6531	3.9101	3.3912
H	1.7414	1.8864	2.3550
H	-5.7829	2.5024	1.3827
H	-4.9854	0.4382	2.4736
H	-1.7416	1.8861	-2.3553
H	-2.6530	3.9100	-3.3915
H	-4.6115	5.0618	-2.4094
H	0.9949	-0.0536	1.3075

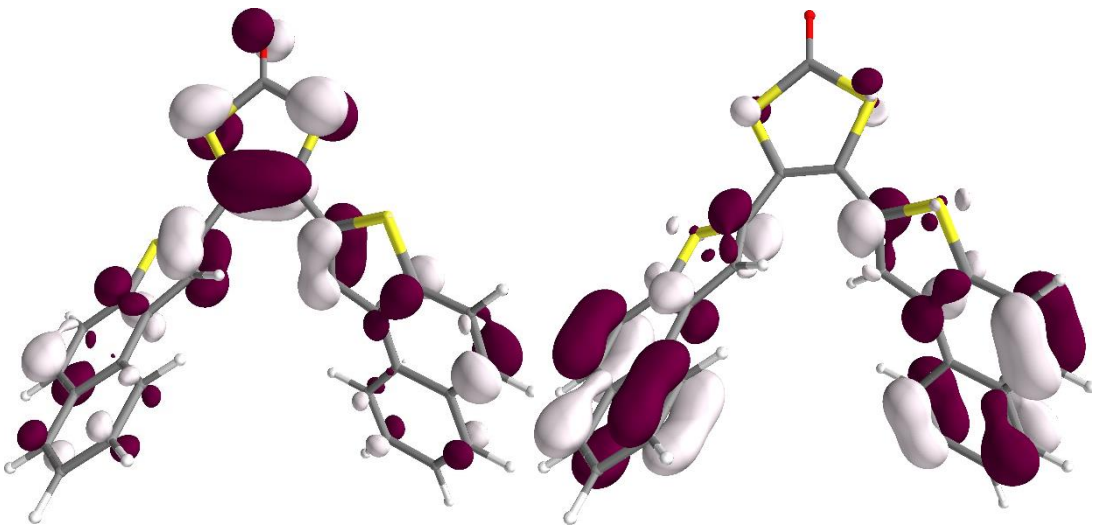

Figure 2: Representation of the two SOMO of spin alpha.