## 1. MOLECULE

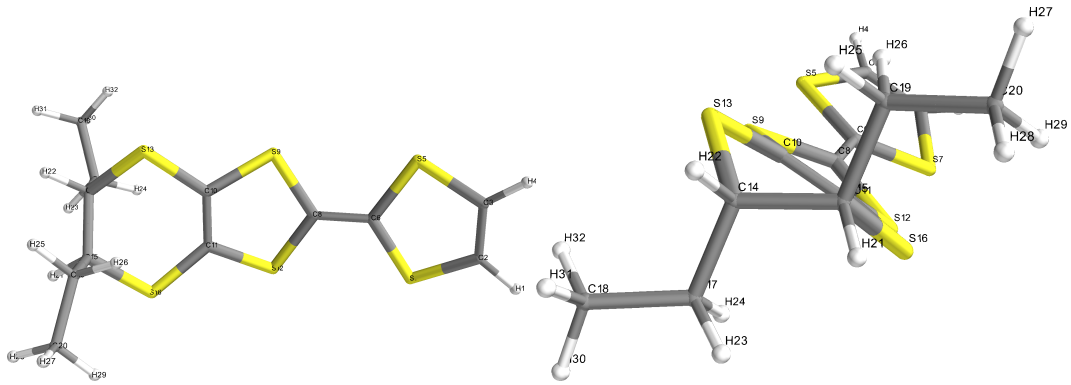


Figure 1: Chemical structure diagram with atomic numbering from two points of view.

| | |
|---|---|
| Directory name | SSdeEDTTTF_ax_ext |
| Formula | C12H14S6 |
| Charge | 0 |
| Spin multiplicity | 1 |
| Monoisotopic mass | 349.94198 Da |
| InChI | 1S/C12H14S6/c1-3-7-8(4-2)16-12-11(15-7)17-10(18-12)9-13-5-6-14-9/h5-8H,3-4H2,1-2H3/t7-,8-/m0/s1 |
| SMILES | C1=CS/C(=C/2\SC3=C(S2)S[C@H]([C@@H](S3)CC)CC)/S1 |

## 2. COMPUTATIONAL DETAILS

| | | |
|---|---|---|
| Software | Gaussian | (2009+D.01) |
| Computational method | DFT | |
| Functional | PBE1PBE | |
| Basis set name | 6-311++G(3df,2pd) | |
| Number of basis set functions | 960 | |
| 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 | 0.000009 | 0.000450 |
| RMS Force value and threshold | 0.000002 | 0.000300 |
| Max Displacement value and threshold | 0.000398 | 0.001800 |
| RMS Displacement value and threshold | 0.000108 | 0.001200 |
| | | |
| Job type: Time-dependent calculation | | |
| Number of calculated excited states and spin state | 40 | ['Singlet-A'] |
| | | |
| Job type: Frequency and thermochemical analysis | | |
| Temperature | 298.15 K | |
| Anharmonic effects | None | |
| Anharmonic effects | None | |

## 3. RESULTS

| | |
|---|---|
| Total molecular energy | -2853.67768 hartrees |
| HOMO number | 91 |
| LUMO+1 energies | -0.63 eV |
| LUMO energies | -1.01 eV |
| HOMO energies | -4.92 eV |
| HOMO-1 energies | -6.00 eV |
| | |
| Geometry optimization specific results | |
| Converged nuclear repulsion energy | 2202.67569 Hartrees |
| | |
| Frequency and Thermochemistry specific results | |

| | | |
|---|---|---|
| Enthalpy at 298.15 K | -2853.42218 Hartrees | |
| Gibbs free energy at 298.15 K | -2853.49332 Hartrees | |
| Entropy at 298.15 K | 0.00024 Hartrees | |
| Mean Mulliken atomic charge and standard deviation | -0.0000 e- | 0.4042 e- |
| Atoms with negatives charges under the standard deviation | NÂ° | Mulliken charge |
| | S 9 | -0.775 |
| | S 12 | -0.770 |
| | S 13 | -0.747 |
| | S 16 | -0.668 |
| | S 7 | -0.507 |
| | S 5 | -0.487 |
| Atoms with positives charges over the standard deviation | NÂ° | Mulliken charge |
| | C 8 | +0.460 |
| | C 6 | +0.650 |
| | C 11 | +0.836 |
| | C 10 | +0.956 |

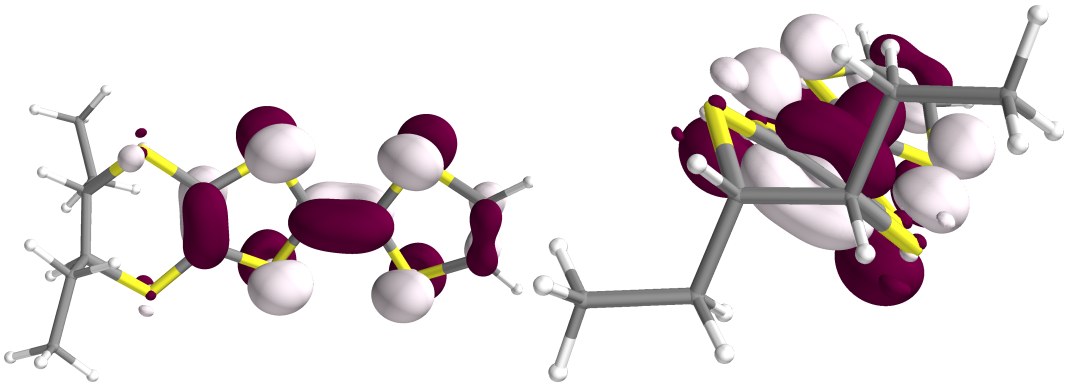

Figure 2: Representation of the HOMO from two points of view.

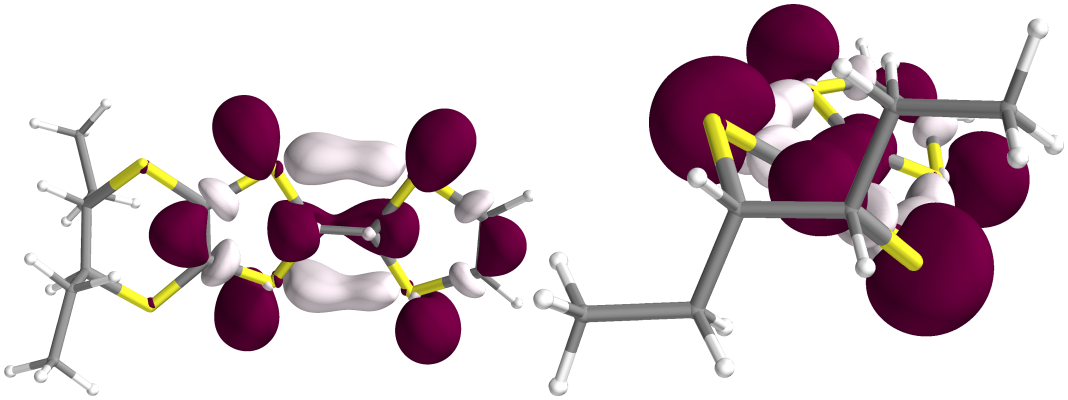

Figure 3: Representation of the LUMO from two points of view.

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

| E.S. | Symmetry | nm | $cm^{-1}$ | $f$ | R | $\Lambda$ | $d_{CT}$ | $q_{CT}$ | Excitation description : initial OM - ending OM (% if > 5%) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Singlet-A | 462 | 21607 | 0.003 | 0.9 | 0.58 | 18.07 | 0.66 | 91-92(97); |
| 2 | Singlet-A | 379 | 26360 | 0.016 | -11.9 | 0.63 | 60.02 | 0.59 | 91-93(93); |
| 3 | Singlet-A | 332 | 30051 | 0.062 | -0.1 | 0.50 | 127.51 | 0.53 | 90-92(46); 91-94(31); 91-100(7); |
| 4 | Singlet-A | 324 | 30774 | 0.019 | 29.2 | 0.53 | 357.40 | 0.56 | 91-94(11); 91-95(29); 91-96(49); 91-97(6); |
| 5 | Singlet-A | 321 | 31078 | 0.044 | -6.2 | 0.47 | 384.53 | 0.56 | 91-94(11); 91-95(7); 91-97(65); |
| 6 | Singlet-A | 308 | 32429 | 0.248 | 10.8 | 0.54 | 27.91 | 0.48 | 90-92(24); 91-94(40); 91-96(6); 91-97(12); |
| 9 | Singlet-A | 287 | 34763 | 0.019 | -14.7 | 0.43 | 173.83 | 0.57 | 91-95(12); 91-96(6); 91-98(19); 91-100(43); |
| 10 | Singlet-A | 281 | 35504 | 0.015 | -10.1 | 0.43 | 185.01 | 0.53 | 90-93(19); 90-97(9); 91-101(33); 91-105(17); |
| 13 | Singlet-A | 268 | 37282 | 0.024 | -51.7 | 0.41 | 133.76 | 0.54 | 90-93(28); 91-99(25); 91-102(20); 91-103(9); |
| 15 | Singlet-A | 263 | 37990 | 0.008 | 24.0 | 0.33 | 309.32 | 0.58 | 90-94(6); 91-99(24); 91-103(8); 91-104(23); 91-106(10); |
| 16 | Singlet-A | 261 | 38281 | 0.059 | 18.1 | 0.42 | 236.20 | 0.57 | 90-94(75); 91-101(9); |
| 20 | Singlet-A | 249 | 40046 | 0.019 | -17.5 | 0.34 | 328.38 | 0.59 | 91-104(8); 91-106(29); 91-107(24); 91-108(7); 91-109(7); |
| 21 | Singlet-A | 246 | 40514 | 0.019 | -42.3 | 0.44 | 194.72 | 0.49 | 90-95(31); 90-96(25); 91-107(10); |
| 24 | Singlet-A | 241 | 41413 | 0.026 | 36.7 | 0.43 | 185.84 | 0.49 | 90-95(7); 90-96(43); 91-107(11); 91-108(7); |
| 25 | Singlet-A | 237 | 42086 | 0.034 | 17.0 | 0.38 | 162.24 | 0.53 | 88-92(14); 90-95(22); 90-100(9); 91-109(13); 91-112(8); |
| 31 | Singlet-A | 225 | 44254 | 0.062 | 22.4 | 0.39 | 230.67 | 0.50 | 88-92(29); 89-93(28); 90-98(6); |
| 35 | Singlet-A | 219 | 45504 | 0.008 | 12.9 | 0.29 | 141.91 | 0.56 | 90-99(32); 90-103(14); 90-105(17); |
| 38 | Singlet-A | 215 | 46441 | 0.026 | 11.0 | 0.29 | 237.98 | 0.50 | 89-94(48); 90-102(7); 91-113(7); |
| 39 | Singlet-A | 214 | 46609 | 0.006 | -18.7 | 0.31 | 130.62 | 0.55 | 89-94(9); 90-102(46); 90-104(11); |

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

| Frequencies | Intensity | Symmetry |
|---|---|---|
| 656 | 57 | A |

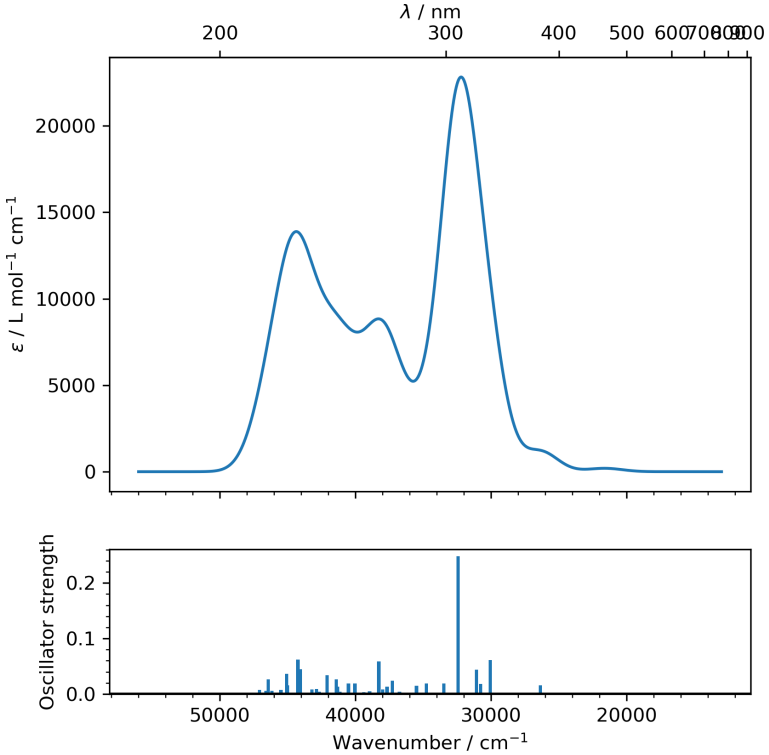


Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

| Atom | X | Y | Z |
|---|---|---|---|
| H | -6.2064 | 1.5613 | 0.0512 |
| C | -5.3760 | 0.8746 | 0.1302 |
| C | -5.3777 | -0.2406 | 0.8570 |
| H | -6.2098 | -0.5882 | 1.4522 |
| S | -3.9569 | -1.2387 | 0.8003 |

| | | | |
|---|---|---|---|
| C | -3.0080 | -0.0797 | -0.1091 |
| S | -3.9527 | 1.2224 | -0.8036 |
| C | -1.6785 | -0.1944 | -0.2796 |
| S | -0.7325 | -1.5082 | 0.3761 |
| C | 0.7859 | -0.6283 | 0.2754 |
| C | 0.7858 | 0.4984 | -0.4562 |
| S | -0.7359 | 0.9307 | -1.2278 |
| S | 2.1319 | -1.3856 | 1.0744 |
| C | 3.4968 | -0.6742 | 0.1081 |
| C | 3.4642 | 0.8573 | 0.1427 |
| S | 2.1148 | 1.5465 | -0.8645 |
| C | 3.6010 | -1.2600 | -1.2939 |
| C | 4.0007 | -2.7247 | -1.3146 |
| C | 3.4912 | 1.4418 | 1.5500 |
| C | 3.8173 | 2.9241 | 1.5888 |
| H | 4.3487 | 1.2052 | -0.4032 |
| H | 4.3721 | -0.9803 | 0.6918 |
| H | 4.3385 | -0.6656 | -1.8450 |
| H | 2.6503 | -1.1195 | -1.8128 |
| H | 4.2399 | 0.8834 | 2.1242 |
| H | 2.5320 | 1.2501 | 2.0344 |
| H | 3.8315 | 3.2888 | 2.6167 |
| H | 4.7979 | 3.1280 | 1.1510 |
| H | 3.0758 | 3.5056 | 1.0388 |
| H | 4.0638 | -3.0922 | -2.3396 |
| H | 4.9764 | -2.8782 | -0.8466 |
| H | 3.2726 | -3.3393 | -0.7834 |

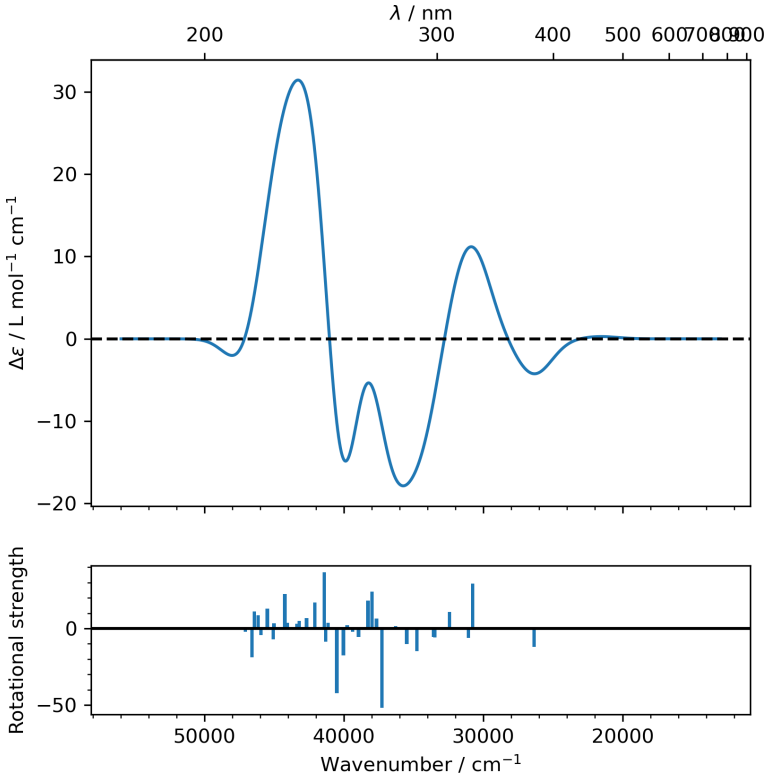


Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

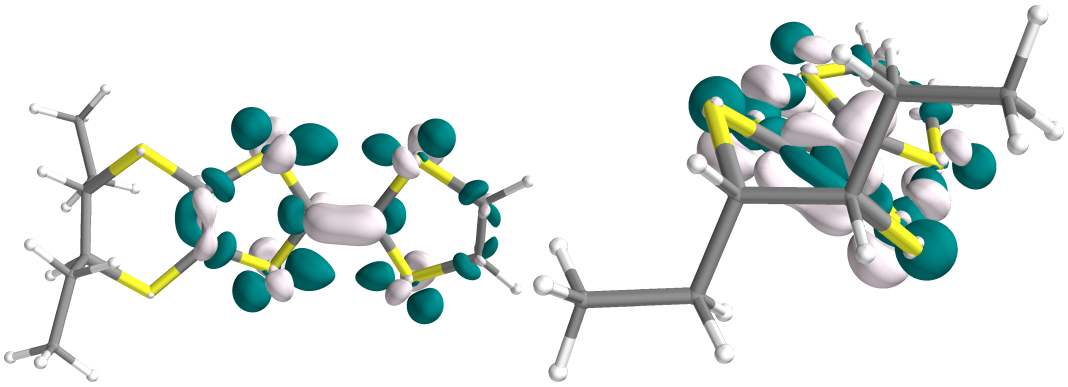

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

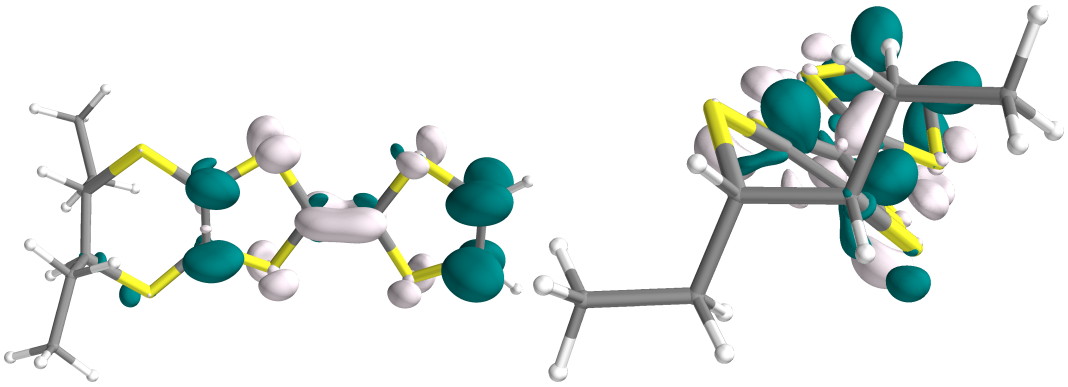

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.

## 1. MOLECULE

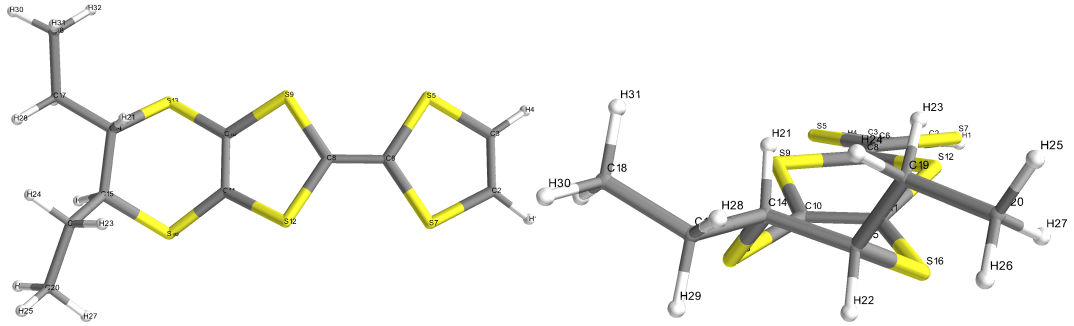


Figure 1: Chemical structure diagram with atomic numbering from two points of view.

| | |
|---|---|
| Directory name | SSdeEDTTTF_eq_ext |
| Formula | C12H14S6 |
| Charge | 0 |
| Spin multiplicity | 1 |
| Monoisotopic mass | 349.94198 Da |
| InChI | 1S/C12H14S6/c1-3-7-8(4-2)16-12-11(15-7)17-10(18-12)9-13-5-6-14-9/h5-8H,3-4H2,1-2H3/t7-,8-/m0/s1 |
| SMILES | C1=CS/C(=C/2\SC3=C(S2)S[C@H]([C@@H](S3)CC)CC)/S1 |

## 2. COMPUTATIONAL DETAILS

| | | |
|---|---|---|
| Software | Gaussian | (2009+D.01) |
| Computational method | DFT | |
| Functional | PBE1PBE | |
| Basis set name | 6-311++G(3df,2pd) | |
| Number of basis set functions | 960 | |
| 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 | 0.000029 | 0.000450 |
| RMS Force value and threshold | 0.000006 | 0.000300 |
| Max Displacement value and threshold | 0.001409 | 0.001800 |
| RMS Displacement value and threshold | 0.000440 | 0.001200 |
| | | |
| Job type: Time-dependent calculation | | |
| Number of calculated excited states and spin state | 40 | ['Singlet-A'] |
| | | |
| Job type: Frequency and thermochemical analysis | | |
| Temperature | 298.15 K | |
| Anharmonic effects | None | |
| Anharmonic effects | None | |

## 3. RESULTS

| | |
|---|---|
| Total molecular energy | -2853.67575 hartrees |
| HOMO number | 91 |
| LUMO+1 energies | -0.84 eV |
| LUMO energies | -0.96 eV |
| HOMO energies | -4.95 eV |
| HOMO-1 energies | -6.35 eV |
| | |
| Geometry optimization specific results | |
| Converged nuclear repulsion energy | 2176.13942 Hartrees |
| | |
| Frequency and Thermochemistry specific results | |
| Enthalpy at 298.15 K | -2853.42031 Hartrees |
| Gibbs free energy at 298.15 K | -2853.49181 Hartrees |

| | | |
|---|---|---|
| Entropy at 298.15 K | 0.00024 Hartrees | |
| Mean Mulliken atomic charge and standard deviation | 0.0000 e- | 0.4139 e- |
| Atoms with negatives charges under the standard deviation | NÂ° | Mulliken charge |
| | S 16 | -0.837 |
| | S 12 | -0.810 |
| | S 13 | -0.694 |
| | S 9 | -0.618 |
| | S 5 | -0.512 |
| | S 7 | -0.492 |
| Atoms with positives charges over the standard deviation | NÂ° | Mulliken charge |
| | C 8 | +0.465 |
| | C 11 | +0.571 |
| | C 6 | +0.682 |
| | C 10 | +1.231 |

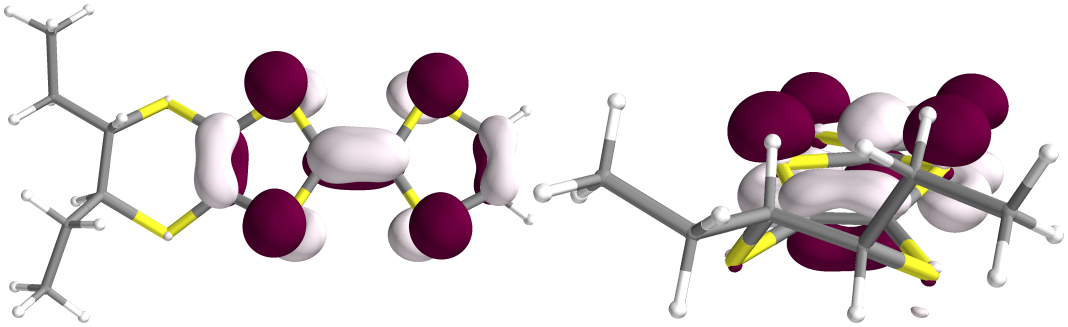

Figure 2: Representation of the HOMO from two points of view.

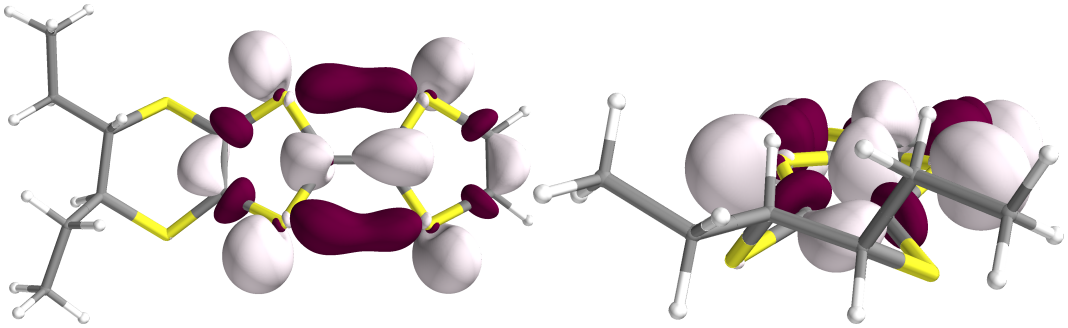

Figure 3: Representation of the LUMO from two points of view.

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

| E.S. | Symmetry | nm | $cm^{-1}$ | $f$ | R | $\Lambda$ | $d_{CT}$ | $q_{CT}$ | Excitation description : initial OM - ending OM (% if > 5%) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Singlet-A | 450 | 22178 | 0.005 | -0.5 | 0.58 | 12.02 | 0.64 | 91-92(96); |
| 2 | Singlet-A | 391 | 25543 | 0.025 | -3.0 | 0.60 | 295.99 | 0.61 | 91-93(94); |
| 3 | Singlet-A | 338 | 29567 | 0.001 | -5.0 | 0.59 | 248.70 | 0.64 | 91-95(92); |
| 4 | Singlet-A | 322 | 30970 | 0.227 | 11.2 | 0.61 | 107.58 | 0.45 | 90-92(12); 91-94(70); |
| 5 | Singlet-A | 302 | 33066 | 0.012 | -1.8 | 0.44 | 68.34 | 0.59 | 91-98(17); 91-100(68); |
| 6 | Singlet-A | 301 | 33205 | 0.108 | -3.0 | 0.41 | 347.13 | 0.55 | 90-92(11); 91-94(17); 91-96(17); 91-98(7); 91-99(11); 91-101(7); 91-102(15); |
| 13 | Singlet-A | 265 | 37595 | 0.029 | -15.8 | 0.56 | 268.79 | 0.45 | 90-93(62); 91-101(14); |
| 17 | Singlet-A | 248 | 40174 | 0.086 | -25.5 | 0.48 | 316.41 | 0.54 | 89-93(53); 90-94(22); |
| 23 | Singlet-A | 236 | 42199 | 0.021 | 12.8 | 0.47 | 192.11 | 0.47 | 90-95(41); 91-109(17); 91-110(16); |
| 25 | Singlet-A | 232 | 42949 | 0.008 | -12.0 | 0.33 | 267.36 | 0.57 | 91-106(15); 91-107(6); 91-110(7); 91-111(46); |
| 29 | Singlet-A | 224 | 44542 | 0.005 | 29.0 | 0.47 | 29.54 | 0.47 | 87-92(6); 88-93(48); 91-113(12); |
| 31 | Singlet-A | 222 | 44867 | 0.004 | 15.2 | 0.31 | 127.68 | 0.53 | 90-96(10); 90-97(15); 90-99(9); 90-100(10); 91-112(13); 91-113(9); |
| 32 | Singlet-A | 221 | 45147 | 0.003 | -24.3 | 0.36 | 126.93 | 0.50 | 87-92(14); 90-95(6); 90-96(22); 90-98(8); 90-100(20); |
| 40 | Singlet-A | 210 | 47570 | 0.018 | 13.3 | 0.30 | 292.46 | 0.52 | 90-98(6); 90-99(6); 91-115(6); 91-117(27); 91-119(14); |

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

| Frequencies | Intensity | Symmetry |
|---|---|---|
| 656 | 57 | A |

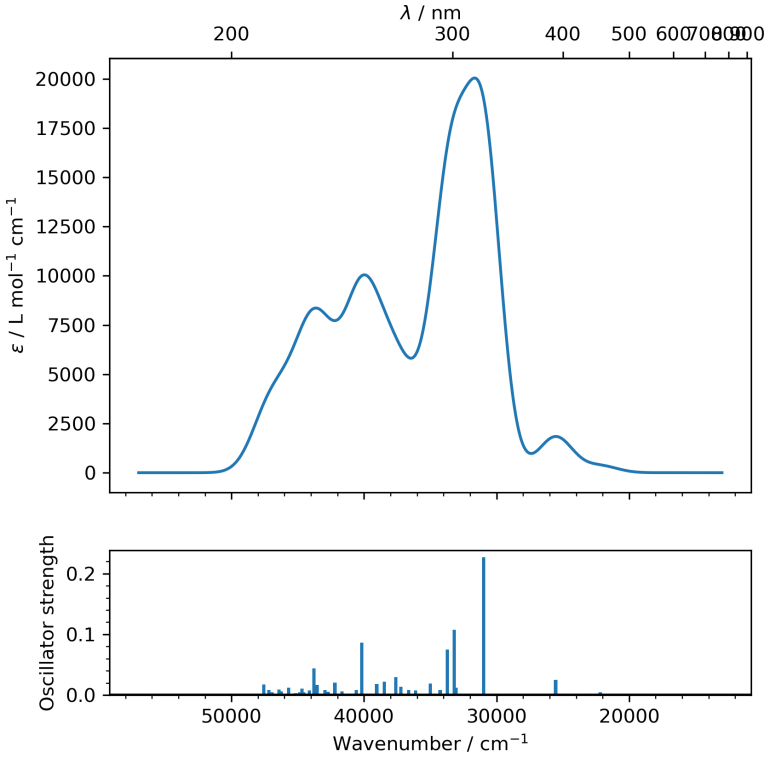


Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

| Atom | X | Y | Z |
|---|---|---|---|
| H | -6.4393 | 1.3092 | -0.2847 |
| C | -5.5744 | 0.6824 | -0.1217 |
| C | -5.5864 | -0.6485 | -0.1343 |
| H | -6.4624 | -1.2565 | -0.3088 |
| S | -4.0932 | -1.4686 | 0.2062 |
| C | -3.1244 | -0.0083 | 0.1982 |
| S | -4.0668 | 1.4688 | 0.2342 |
| C | -1.7791 | -0.0210 | 0.1935 |
| S | -0.8298 | -1.4943 | 0.2015 |
| C | 0.5880 | -0.7086 | -0.4579 |
| C | 0.6049 | 0.6366 | -0.4399 |
| S | -0.8032 | 1.4351 | 0.2274 |
| S | 1.9951 | -1.6108 | -0.9016 |
| C | 3.1978 | -0.7163 | 0.1503 |
| C | 3.4094 | 0.7442 | -0.2439 |
| S | 1.9450 | 1.5808 | -0.9921 |
| C | 4.5124 | -1.4954 | 0.1134 |
| C | 4.4679 | -2.8207 | 0.8551 |
| C | 3.9278 | 1.5605 | 0.9396 |
| C | 4.4501 | 2.9337 | 0.5564 |
| H | 2.7749 | -0.7492 | 1.1583 |
| H | 4.1347 | 0.7791 | -1.0634 |
| H | 3.1217 | 1.6516 | 1.6734 |
| H | 4.7294 | 0.9948 | 1.4268 |
| H | 4.8110 | 3.4708 | 1.4345 |
| H | 5.2796 | 2.8564 | -0.1507 |
| H | 3.6684 | 3.5389 | 0.0943 |
| H | 5.2952 | -0.8644 | 0.5439 |
| H | 4.7948 | -1.6530 | -0.9329 |
| H | 5.4326 | -3.3268 | 0.7988 |
| H | 4.2311 | -2.6699 | 1.9106 |
| H | 3.7129 | -3.4882 | 0.4383 |

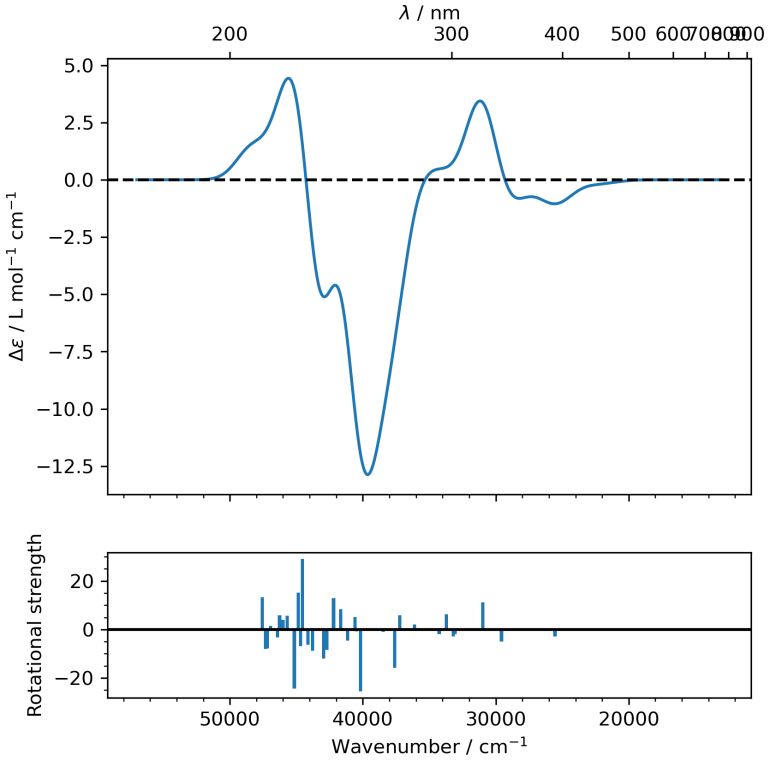


Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

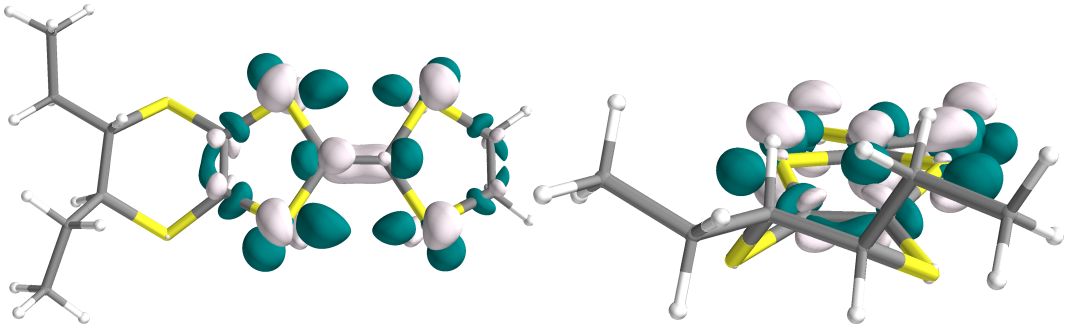

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

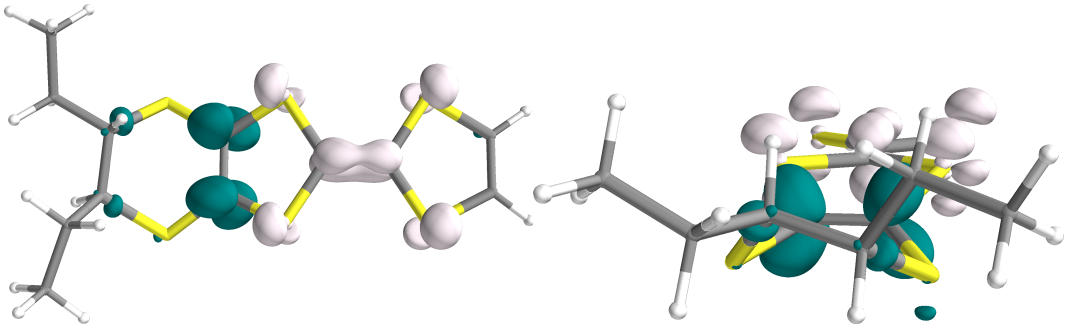

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.

## 1. MOLECULE

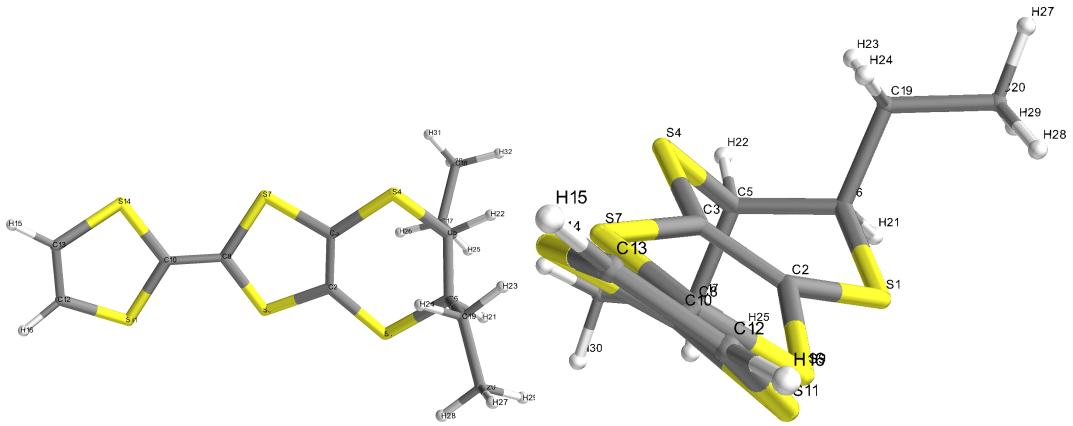


Figure 1: Chemical structure diagram with atomic numbering from two points of view.

| | |
|---|---|
| Directory name | RRdeEDTTTF_ax_ext |
| Formula | C12H14S6 |
| Charge | 0 |
| Spin multiplicity | 1 |
| Monoisotopic mass | 349.94198 Da |
| InChI | 1S/C12H14S6/c1-3-7-8(4-2)16-12-11(15-7)17-10(18-12)9-13-5-6-14-9/h5-8H,3-4H2,1-2H3/t7-,8-/m1/s1 |
| SMILES | S1C2=C(S[C@@H]([C@H]1CC)CC)S/C(=C\1/SC=CS1)/S2 |

## 2. COMPUTATIONAL DETAILS

| | | |
|---|---|---|
| Software | Gaussian | (2009+D.01) |
| Computational method | DFT | |
| Functional | PBE1PBE | |
| Basis set name | 6-311++G(3df,2pd) | |
| Number of basis set functions | 960 | |
| 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 | 0.000012 | 0.000450 |
| RMS Force value and threshold | 0.000002 | 0.000300 |
| Max Displacement value and threshold | 0.001142 | 0.001800 |
| RMS Displacement value and threshold | 0.000302 | 0.001200 |
| | | |
| Job type: Time-dependent calculation | | |
| Number of calculated excited states and spin state | 40 | ['Singlet-A'] |

## 3. RESULTS

| | |
|---|---|
| Total molecular energy | -2853.67768 hartrees |
| HOMO number | 91 |
| LUMO+1 energies | -0.63 eV |
| LUMO energies | -1.01 eV |
| HOMO energies | -4.92 eV |
| HOMO-1 energies | -6.00 eV |

| | | |
|---|---|---|
| Geometry optimization specific results | | |
| Converged nuclear repulsion energy | 2202.67308 Hartrees | |
| | | |
| Mean Mulliken atomic charge and standard deviation | 0.0000 e- | 0.4042 e- |
| Atoms with negatives charges under the standard deviation | NÂ° | Mulliken charge |
| | S 7 | -0.775 |
| | S 9 | -0.770 |

| | | |
|---|---|---|
| | S 4 | -0.747 |
| | S 1 | -0.668 |
| | S 11 | -0.507 |
| | S 14 | -0.487 |
| Atoms with positives charges over the standard deviation | NÂ° | Mulliken charge |
| | C 8 | +0.460 |
| | C 10 | +0.650 |
| | C 2 | +0.836 |
| | C 3 | +0.956 |

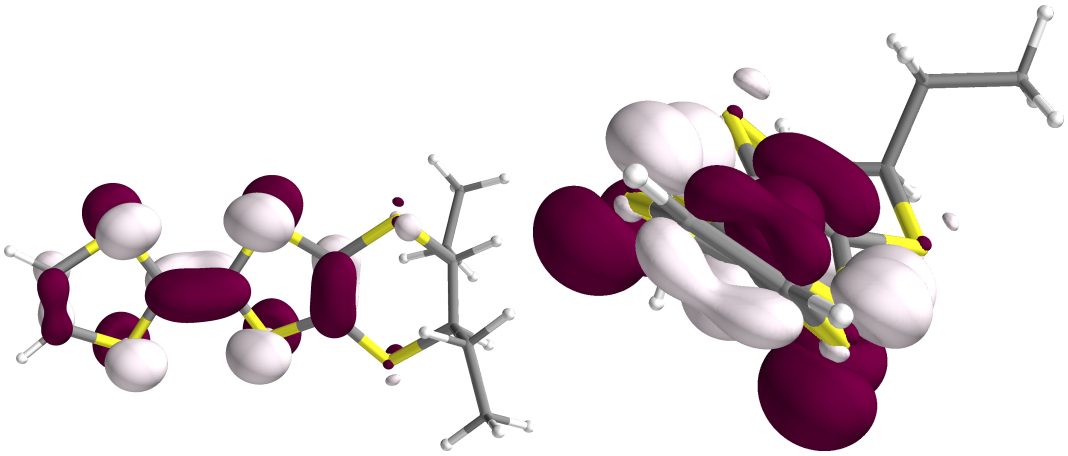

Figure 2: Representation of the HOMO from two points of view.

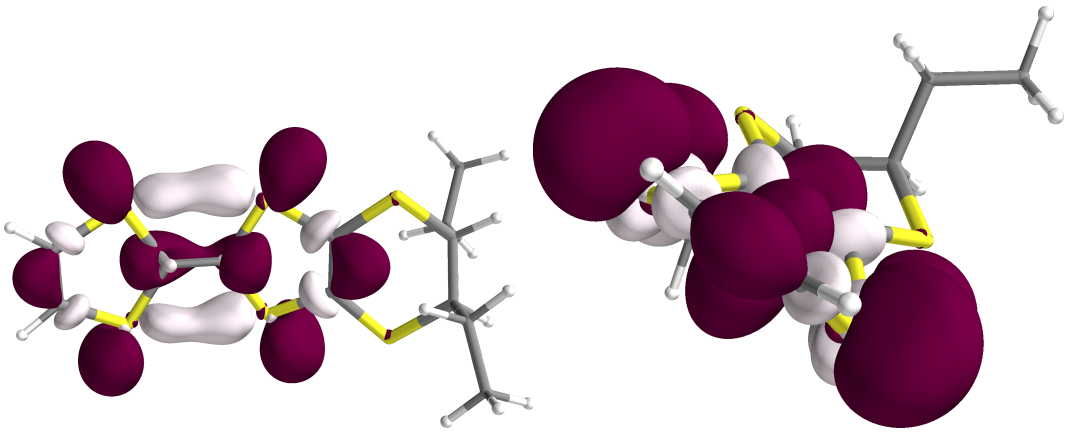

Figure 3: Representation of the LUMO from two points of view.

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

| E.S. | Symmetry | nm | $cm^{-1}$ | $f$ | R | $\Lambda$ | $d_{CT}$ | $q_{CT}$ | Excitation description : initial OM - ending OM (% if > 5%) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Singlet-A | 462 | 21605 | 0.003 | -0.9 | 0.58 | 18.10 | 0.66 | 91-92(97); |
| 2 | Singlet-A | 379 | 26360 | 0.016 | 11.9 | 0.63 | 60.00 | 0.59 | 91-93(93); |
| 3 | Singlet-A | 332 | 30051 | 0.061 | 0.1 | 0.50 | 127.70 | 0.53 | 90-92(46); 91-94(31); 91-100(7); |
| 4 | Singlet-A | 324 | 30774 | 0.019 | -29.2 | 0.53 | 356.00 | 0.56 | 91-94(11); 91-95(29); 91-96(49); 91-97(6); |
| 5 | Singlet-A | 321 | 31077 | 0.044 | 6.1 | 0.47 | 384.23 | 0.56 | 91-94(11); 91-95(7); 91-97(65); |
| 6 | Singlet-A | 308 | 32429 | 0.248 | -10.7 | 0.54 | 27.31 | 0.48 | 90-92(24); 91-94(40); 91-96(7); 91-97(12); |
| 9 | Singlet-A | 287 | 34762 | 0.019 | 14.7 | 0.43 | 172.72 | 0.57 | 91-95(12); 91-96(6); 91-98(19); 91-100(43); |
| 10 | Singlet-A | 281 | 35504 | 0.015 | 10.1 | 0.43 | 184.73 | 0.53 | 90-93(19); 90-97(9); 91-101(33); 91-105(17); |
| 13 | Singlet-A | 268 | 37282 | 0.024 | 51.7 | 0.41 | 132.70 | 0.54 | 90-93(28); 91-99(25); 91-102(20); 91-103(9); |
| 15 | Singlet-A | 263 | 37989 | 0.008 | -24.0 | 0.33 | 308.51 | 0.58 | 90-94(6); 91-99(24); 91-103(8); 91-104(23); 91-106(10); |
| 16 | Singlet-A | 261 | 38282 | 0.059 | -18.1 | 0.42 | 236.69 | 0.57 | 90-94(75); 91-101(9); |
| 20 | Singlet-A | 249 | 40045 | 0.019 | 17.5 | 0.34 | 327.49 | 0.59 | 91-104(8); 91-106(29); 91-107(24); 91-108(7); 91-109(7); |
| 21 | Singlet-A | 246 | 40515 | 0.019 | 42.3 | 0.44 | 193.32 | 0.49 | 90-95(31); 90-96(25); 91-107(10); |
| 24 | Singlet-A | 241 | 41413 | 0.026 | -36.7 | 0.43 | 183.66 | 0.49 | 90-95(7); 90-96(44); 91-107(11); 91-108(7); |
| 25 | Singlet-A | 237 | 42085 | 0.034 | -17.0 | 0.38 | 161.39 | 0.53 | 88-92(14); 90-95(22); 90-100(9); 91-109(13); 91-112(8); |
| 31 | Singlet-A | 225 | 44254 | 0.062 | -22.5 | 0.39 | 231.81 | 0.50 | 88-92(29); 89-93(28); 90-98(6); |
| 35 | Singlet-A | 219 | 45504 | 0.008 | -12.9 | 0.29 | 140.54 | 0.56 | 90-99(32); 90-103(14); 90-105(17); |
| 38 | Singlet-A | 215 | 46442 | 0.026 | -11.1 | 0.29 | 239.16 | 0.50 | 89-94(48); 90-102(7); 91-113(6); |
| 39 | Singlet-A | 214 | 46609 | 0.006 | 18.9 | 0.31 | 132.54 | 0.55 | 89-94(9); 90-102(46); 90-104(11); |

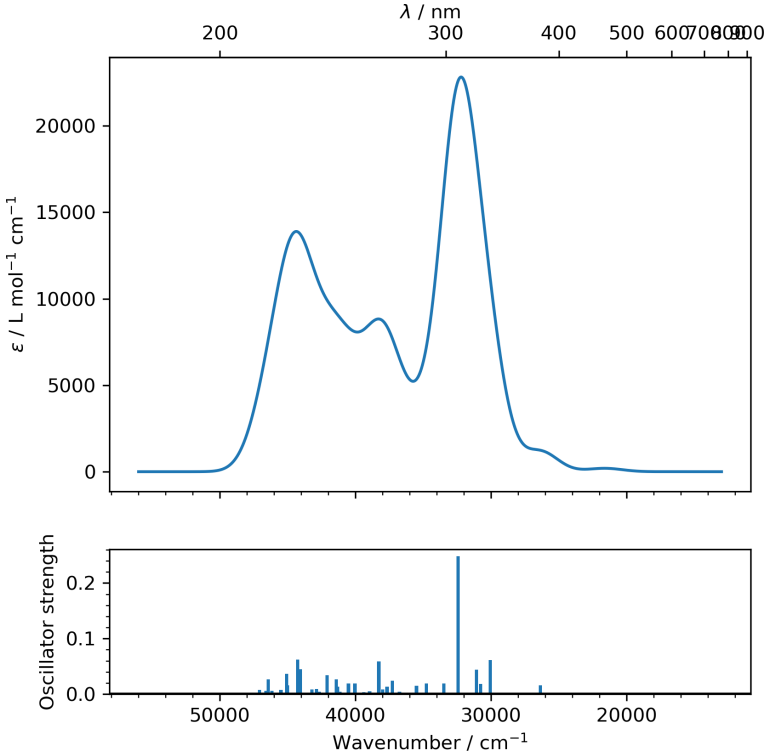


Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

| Atom | X | Y | Z |
|---|---|---|---|
| S | -2.1149 | 1.5465 | -0.8644 |
| C | -0.7859 | 0.4985 | -0.4560 |
| C | -0.7858 | -0.6283 | 0.2756 |
| S | -2.1319 | -1.3856 | 1.0744 |
| C | -3.4967 | -0.6744 | 0.1079 |
| C | -3.4643 | 0.8572 | 0.1425 |
| S | 0.7325 | -1.5081 | 0.3763 |
| C | 1.6785 | -0.1943 | -0.2794 |
| S | 0.7358 | 0.9309 | -1.2276 |

| | | | |
|---|---|---|---|
| C | 3.0080 | -0.0796 | -0.1091 |
| S | 3.9526 | 1.2226 | -0.8035 |
| C | 5.3760 | 0.8747 | 0.1301 |
| C | 5.3779 | -0.2406 | 0.8568 |
| S | 3.9570 | -1.2387 | 0.8002 |
| H | 6.2100 | -0.5884 | 1.4519 |
| H | 6.2064 | 1.5614 | 0.0510 |
| C | -3.6006 | -1.2602 | -1.2941 |
| C | -4.0001 | -2.7249 | -1.3149 |
| C | -3.4917 | 1.4416 | 1.5499 |
| C | -3.8179 | 2.9240 | 1.5886 |
| H | -4.3488 | 1.2049 | -0.4035 |
| H | -4.3721 | -0.9806 | 0.6915 |
| H | -4.2404 | 0.8832 | 2.1239 |
| H | -2.5325 | 1.2500 | 2.0344 |
| H | -4.3382 | -0.6658 | -1.8453 |
| H | -2.6499 | -1.1194 | -1.8129 |
| H | -3.8323 | 3.2886 | 2.6165 |
| H | -3.0763 | 3.5055 | 1.0388 |
| H | -4.7984 | 3.1278 | 1.1506 |
| H | -4.0630 | -3.0924 | -2.3399 |
| H | -3.2720 | -3.3394 | -0.7836 |
| H | -4.9758 | -2.8786 | -0.8470 |

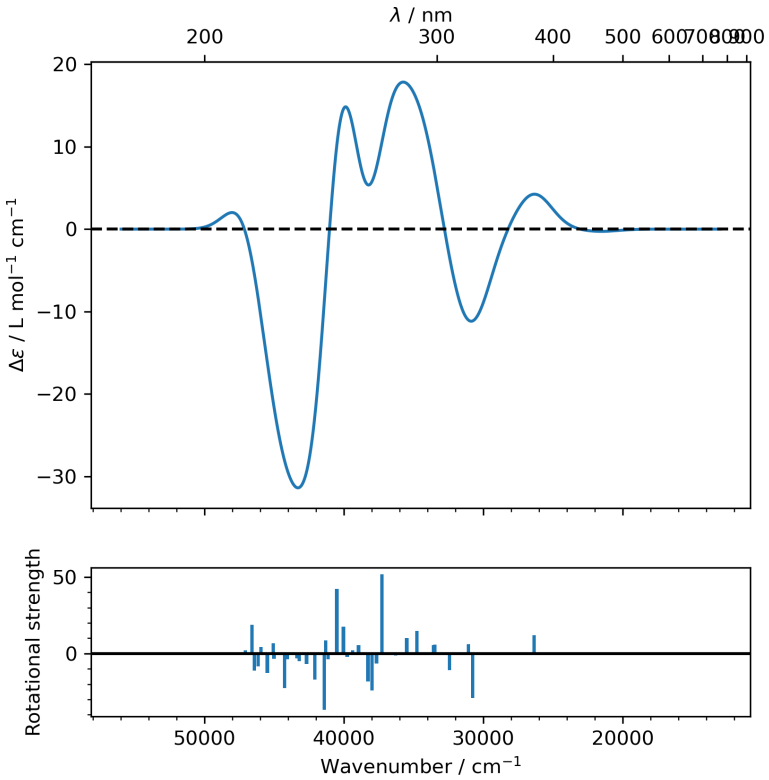


Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

## 1. MOLECULE

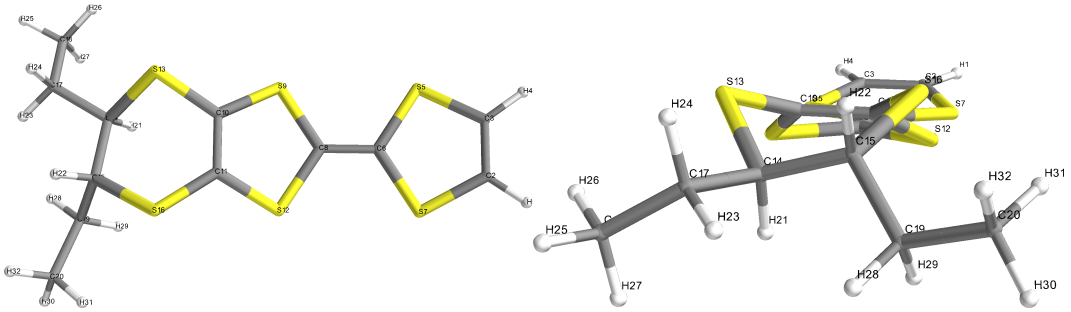

Figure 1: Chemical structure diagram with atomic numbering from two points of view.

| | |
|---|---|
| Directory name | RRdeEDTTTF_eq_ext |
| Formula | C12H14S6 |
| Charge | 0 |
| Spin multiplicity | 1 |
| Monoisotopic mass | 349.94198 Da |
| InChI | 1S/C12H14S6/c1-3-7-8(4-2)16-12-11(15-7)17-10(18-12)9-13-5-6-14-9/h5-8H,3-4H2,1-2H3/t7-,8-/m1/s1 |
| SMILES | C1=CS/C(=C/2\SC3=C(S2)S[C@@H]([C@H](S3)CC)CC)/S1 |

## 2. COMPUTATIONAL DETAILS

| | | |
|---|---|---|
| Software | Gaussian | (2009+D.01) |
| Computational method | DFT | |
| Functional | PBE1PBE | |
| Basis set name | 6-311++G(3df,2pd) | |
| Number of basis set functions | 960 | |
| 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 | 0.000138 | 0.000450 |
| RMS Force value and threshold | 0.000013 | 0.000300 |
| Max Displacement value and threshold | 0.000819 | 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 | -2853.67575 hartrees |
| HOMO number | 91 |
| LUMO+1 energies | -0.84 eV |
| LUMO energies | -0.96 eV |
| HOMO energies | -4.95 eV |
| HOMO-1 energies | -6.35 eV |
| | |
| Geometry optimization specific results | |
| Converged nuclear repulsion energy | 2176.13999 Hartrees |
| | |
| Frequency and Thermochemistry specific results | |
| Enthalpy at 298.15 K | -2853.42030 Hartrees |
| Gibbs free energy at 298.15 K | -2853.49182 Hartrees |

| | | |
|---|---|---|
| Entropy at 298.15 K | 0.00024 Hartrees | |
| Mean Mulliken atomic charge and standard deviation | 0.0000 e- | 0.4139 e- |
| Atoms with negatives charges under the standard deviation | NÂ° | Mulliken charge |
| | S 16 | -0.836 |
| | S 12 | -0.810 |
| | S 13 | -0.694 |
| | S 9 | -0.618 |
| | S 5 | -0.512 |
| | S 7 | -0.492 |
| Atoms with positives charges over the standard deviation | NÂ° | Mulliken charge |
| | C 8 | +0.466 |
| | C 11 | +0.571 |
| | C 6 | +0.682 |
| | C 10 | +1.231 |

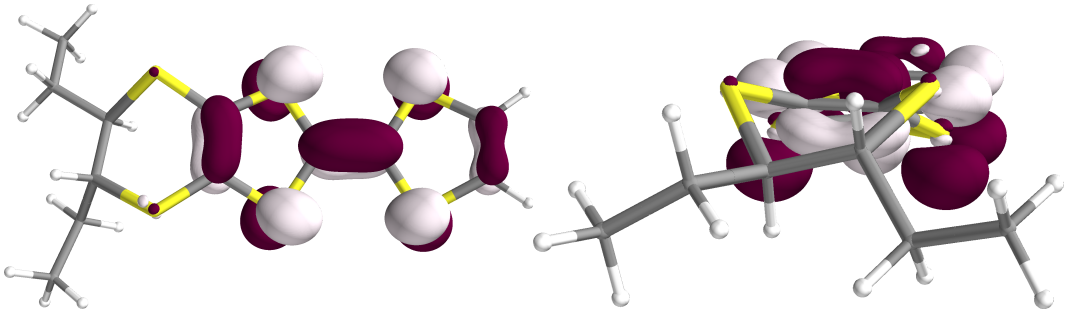

Figure 2: Representation of the HOMO from two points of view.

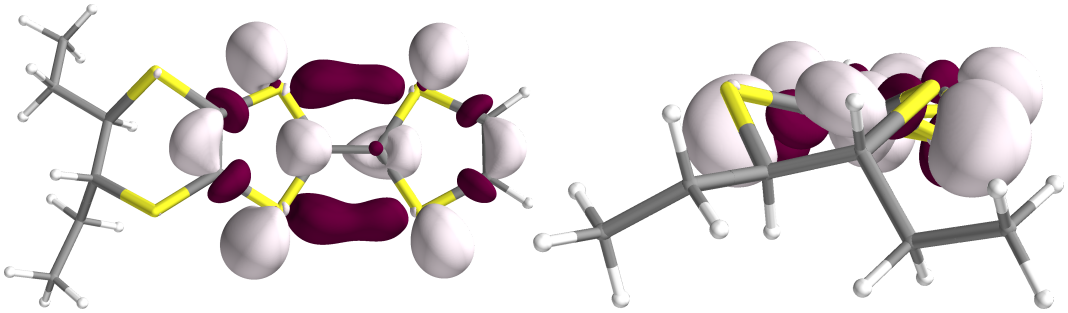

Figure 3: Representation of the LUMO from two points of view.

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

| Frequencies | Intensity | Symmetry |
|---|---|---|
| 656 | 57 | 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 | $\Lambda$ | $d_{CT}$ | $q_{CT}$ | Excitation description : initial OM - ending OM (% if > 5%) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Singlet-A | 450 | 22176 | 0.005 | 0.5 | 0.58 | 11.94 | 0.64 | 91-92(96); |
| 2 | Singlet-A | 391 | 25544 | 0.025 | 2.9 | 0.60 | 296.16 | 0.61 | 91-93(94); |
| 3 | Singlet-A | 338 | 29569 | 0.001 | 5.0 | 0.59 | 248.80 | 0.64 | 91-95(92); |
| 4 | Singlet-A | 322 | 30971 | 0.227 | -11.2 | 0.61 | 107.76 | 0.45 | 90-92(12); 91-94(70); |
| 5 | Singlet-A | 302 | 33063 | 0.012 | 2.0 | 0.44 | 65.66 | 0.59 | 91-98(17); 91-100(68); |
| 6 | Singlet-A | 301 | 33201 | 0.108 | 2.8 | 0.41 | 347.04 | 0.55 | 90-92(11); 91-94(17); 91-96(17); 91-98(8); 91-99(11); 91-101(7); 91-102(15); |
| 13 | Singlet-A | 265 | 37595 | 0.029 | 15.8 | 0.56 | 268.08 | 0.45 | 90-93(62); 91-101(14); |
| 17 | Singlet-A | 248 | 40176 | 0.086 | 25.4 | 0.48 | 315.93 | 0.54 | 89-93(53); 90-94(22); |
| 23 | Singlet-A | 236 | 42200 | 0.021 | -12.8 | 0.47 | 194.29 | 0.47 | 88-93(6); 90-95(41); 91-109(17); 91-110(16); |
| 25 | Singlet-A | 232 | 42949 | 0.008 | 12.1 | 0.33 | 267.43 | 0.57 | 91-106(15); 91-107(6); 91-110(7); 91-111(46); |
| 29 | Singlet-A | 224 | 44542 | 0.005 | -29.4 | 0.47 | 29.42 | 0.47 | 87-92(6); 88-93(47); 91-113(12); |
| 31 | Singlet-A | 222 | 44863 | 0.004 | -15.3 | 0.31 | 127.65 | 0.53 | 90-96(11); 90-97(15); 90-99(9); 90-100(10); 91-112(13); 91-113(9); |
| 32 | Singlet-A | 221 | 45146 | 0.003 | 24.3 | 0.36 | 125.31 | 0.50 | 87-92(14); 90-95(6); 90-96(22); 90-98(8); 90-100(20); |
| 40 | Singlet-A | 210 | 47568 | 0.018 | -13.4 | 0.29 | 289.57 | 0.51 | 90-98(6); 90-99(6); 91-115(7); 91-117(27); 91-119(14); |

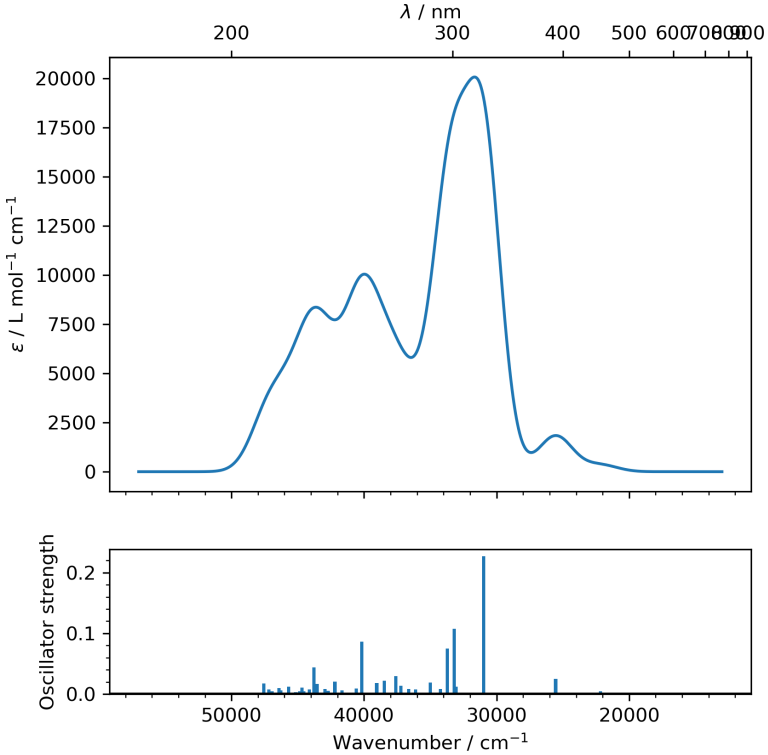


Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm-1)

Table. Converged cartesian atomic coordinates in Angstroms

| Atom | X | Y | Z |
|---|---|---|---|
| H | -6.4394 | 1.3087 | 0.2858 |
| C | -5.5746 | 0.6819 | 0.1224 |
| C | -5.5863 | -0.6490 | 0.1342 |
| H | -6.4620 | -1.2569 | 0.3086 |
| S | -4.0930 | -1.4688 | -0.2064 |
| C | -3.1245 | -0.0084 | -0.1983 |
| S | -4.0670 | 1.4685 | -0.2332 |
| C | -1.7791 | -0.0211 | -0.1941 |
| S | -0.8296 | -1.4942 | -0.2026 |
| C | 0.5881 | -0.7086 | 0.4572 |
| C | 0.6047 | 0.6366 | 0.4397 |
| S | -0.8034 | 1.4352 | -0.2273 |
| S | 1.9950 | -1.6110 | 0.9010 |
| C | 3.1981 | -0.7162 | -0.1502 |

| | | | |
|---|---|---|---|
| C | 3.4092 | 0.7444 | 0.2439 |
| S | 1.9448 | 1.5808 | 0.9924 |
| C | 4.5131 | -1.4948 | -0.1124 |
| C | 4.4696 | -2.8205 | -0.8534 |
| C | 3.9269 | 1.5608 | -0.9399 |
| C | 4.4488 | 2.9342 | -0.5571 |
| H | 2.7759 | -0.7493 | -1.1584 |
| H | 4.1347 | 0.7798 | 1.0631 |
| H | 5.2957 | -0.8635 | -0.5427 |
| H | 4.7950 | -1.6517 | 0.9341 |
| H | 5.4348 | -3.3257 | -0.7969 |
| H | 3.7153 | -3.4885 | -0.4363 |
| H | 4.2326 | -2.6704 | -1.9090 |
| H | 4.7286 | 0.9953 | -1.4272 |
| H | 3.1206 | 1.6514 | -1.6735 |
| H | 4.8092 | 3.4714 | -1.4353 |
| H | 3.6669 | 3.5391 | -0.0948 |
| H | 5.2786 | 2.8573 | 0.1498 |

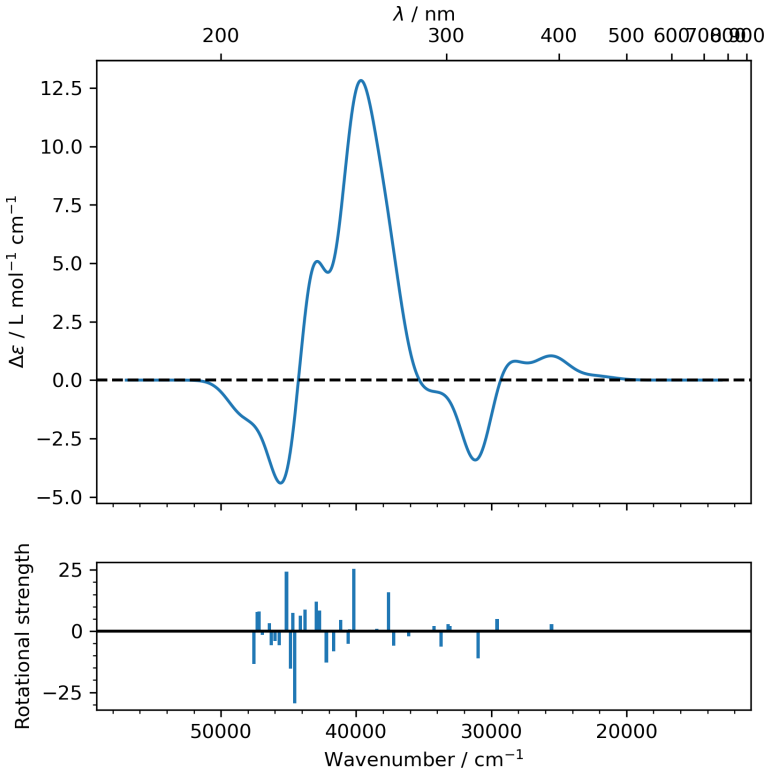


Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm-1)

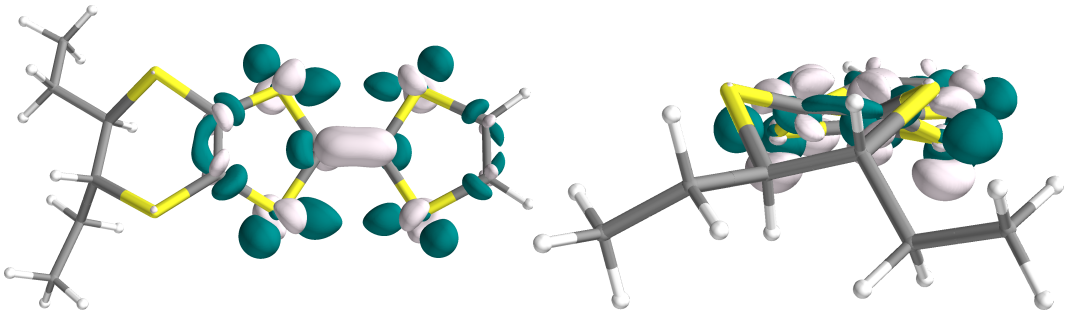

Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

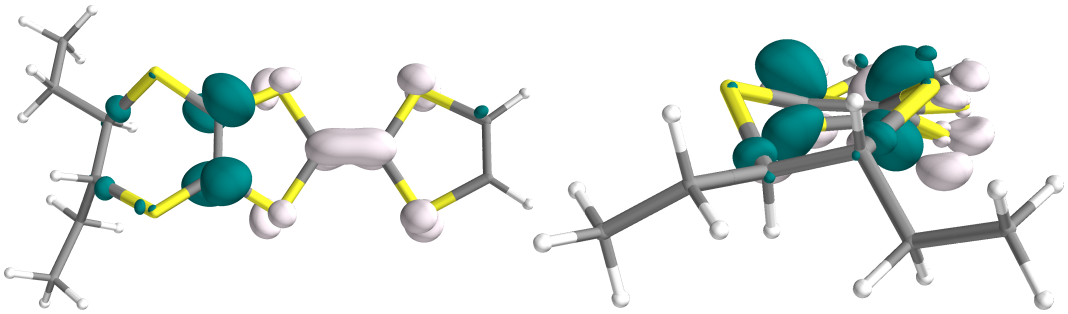

Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.