Supporting Information

Table of contents

Computational details

All calculations were carried out using density functional theory (DFT)[1] and its time-dependent variant (TD-DFT)[2] within the Gaussian 16 software package[3]. The B3LYP-D3(BJ) hybrid functional[4] was applied alongside the 6-311++G(d,p) triple-ζ basis set[5] for geometry optimization, frequency evaluation and absorption spectra calculation. Notably, the "D3(BJ)"[6] term refers to the inclusion of Grimme's dispersion correction, which enhances the accuracy of long-range interaction modeling. B3LYP has well-known limitations in accurately describing charge-transfer (CT) excited states. Nevertheless, for this initial screening, we prioritized methodological consistency with previous studies. Benchmarking against related donor core systems[7] showed that B3LYP reproduces key experimental properties, including LUMO energies and absorption maxima, supporting its use in the present work. Following these computations, analytical frequency calculations confirmed the nature of each stationary point as a minimum, with all frequencies showing positive values. It is also important to mention that, for each compound, several isomers were explored by evaluating different orientations of the indane-derived acceptor groups. Variations in substituents on these acceptor units can lead to steric hindrance or attractive and repulsive interactions with the central donor motifs, allowing us to identify the energetically most favorable configuration. The maximum absorption wavelengths were calculated using TDDFT, based on the ground-state geometry and considering forty singlet excited states. Charge Transfer Matrice (CTM) and InterFragment Charge Transfer (IFCT) values were generated with Multiwfn 3.6 package.[8] The structural geometries of the minimum energy configurations shown below were visualized with the Chemcraft[9] software. Molecular orbitals are represented using an isovalue of 0.04 electrons/bohr.

[1] a) P. Hohenberg, W. Kohn, *Phys. Rev.,* **1964**, 136, B864–B871; b) W. Kohn, L. J. Sham, *Phys. Rev*. **1965**, 140, A1133–A1138.

[2] E. Runge, E. K. U. Gross, *Phys. Rev. Lett*. **1984**, 52, 997.

[3] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, R. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssel, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliar, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, *Gaussian 16, Revision C.01*, Gaussian Inc., Wallingford, CT, **2016**.

[4] A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648–5652

[5] a) R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys.* **1980**, *72*, 650–654; b) T. Clark, J. Chandrasekhar, G. W. Spitznagel, P. V. R. Schleyer, *J. Comput. Chem.* **1983**, 4, 294–301.

[6] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, 32, 1456–1465.

[7] J. Garo, T. Nicolini, J. M. Sotiropoulos and J.-M. Raimundo, *Chem. Eur. J*., 2024, **30**, e202402461.

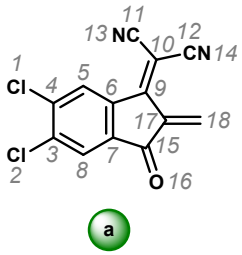
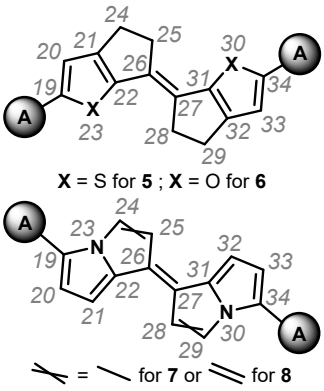
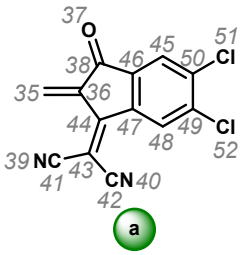
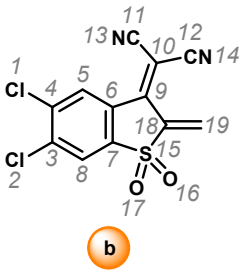
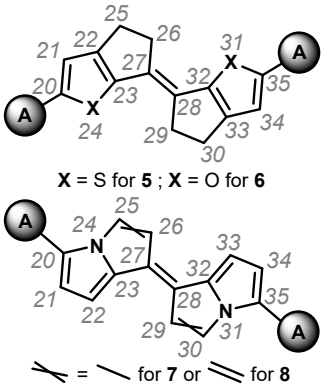
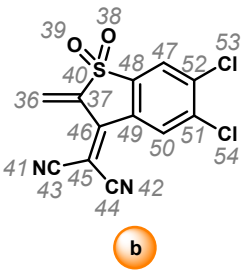
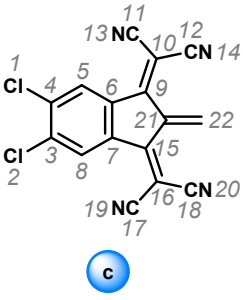
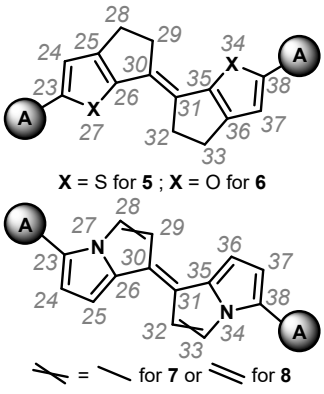
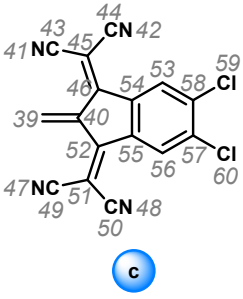
[8] a) T. Lu, F. Chen, *J. Comput. Chem.* **2012**, *33*, 580–592; b) T. Lu, *J. Chem. Phys.* **2024**, 161, 082503.

Methodologies

- Charge Transfer Matrix (CTM) and InterFragment Charge Transfer (IFCT)

First, before calculations, it is highly recommended to prepare the input file by manually adjusting the atomic indices continuously along the molecular backbone in a perfectly symmetric manner (**Table S1**). This approach greatly simplifies the interpretation of the matrices. It is to note that since hydrogen atoms do not participate in charge transfer, this indexing method allows them to be excluded at the end of the atom list.

Table S1. Atom indexation depending on donor and acceptor moieties.

Acceptor on the left (A)	Donor	(A) Acceptor on the right
		
		
		

[9] G. A. Zhurko, “Chemcraft.”, can be found under http://www.chemcraftprog.com/, **2005** (accessed: 1 Apr 2024).

We then performed a second TDDFT calculation based on the ground state geometry, using the same level of theory as described above (td=(singlets,nstates=40) B3LYP-D3(BJ)/6-311++G(d,p)), but with the addition of the keyword iop(9/40=4) and ensuring the .chk file is generated. This file was then converted to .fchk format to be read by Multiwfn. Since the maximum absorption wavelength (λ_{max}) corresponds to the transitions from the ground state (S_0) to the first excited state (S_1), we chose to compute the CTM and IFCT corresponding for this transition.

Steps in Multiwfn for CTM:

- **18** // Electron exciton analysis
- **8** // Calculate interfragment Charge Transfer amount via IFCT method
- *Enter the input path of the Gaussian output file, e.g "*****.out**" if in the current folder*
- **1** // To study S0 $\rightarrow$ S1 excitation
- **-1** // Export atom-atom CTM to atmCTmat.txt in current folder
- **2** // Plot atom/fragment transition matrix of various kinds as heat map
- *Enter "**atmCTmat.txt**"*
- **3** // Export transition density matrix to tmat.txt in current folder

The tmat.txt file was then used to plot the CTM heat map in Origin. Alternatively, rather than exporting the tmat.txt file, it is possible to save the heat map directly as a graphical file (.png), in which case various parameters can be adjusted in the final menu.

In charge transfer matrices (CTMs) of size $N \times N$, the atoms are arranged in ascending order: in row ***i*** from bottom to top and in column ***j*** from left to right (**Figure S1**).

The CTMs assume that charge transfer occurs from atom N_j (hole) to atom N_i (electron), effectively associating the (electron,hole) pair with the (N_i,N_j) pair. For example, the element (**1**,**2**) in the matrix represents charge transfer from atom **2** to atom **1**. The associated density value indicates the intensity of the transfer.

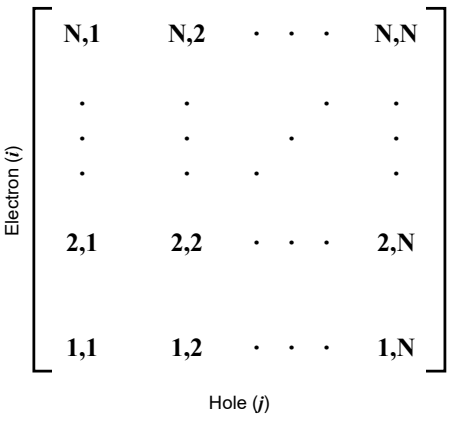


Figure S1. CTM principle.

Steps in Multiwfn for IFCT:

- **18** // Electron exciton analysis
- **8** // Calculate interfragment Charge Transfer amount via IFCT method
- *Enter the input path of the Gaussian output file, e.g "*****.out**" if in the current folder*
- **1** // To study $S_0 \rightarrow S_1$ excitation
- **3** // Define 3 fragments (below is the example of compound **6a**)
- *Enter the atomic indices of fragment 1 (Acceptor on the left), e.g "**1-18**" for **a***
- *Enter the atomic indices of fragment 2 (Donor), e.g "**19-34**" for **6***
- *Enter the atomic indices of fragment 3 (Acceptor on the right), e.g "**35-52**" for **a***
- **Results**: In our case we only focused on "Variation of population number" for each fragment. For **6a** the values are:

  Variation of population number of fragment 1: 0.13776
  Variation of population number of fragment 2: -0.27552
  Variation of population number of fragment 3: 0.13776

More specifically, this variation of population number yields a negative value when a fragment donates more electrons than it receives, and a positive value when it receives more electrons than it donates. In our case, all compounds exhibit negative values for the central moieties (fragment 2) and positive values for the terminal ones (fragment 1 and 3), confirming their roles as electron donors and electron acceptors, respectively. Due to the molecular symmetry, the variation of population number values for the terminal moieties are identical, and their sum matches the absolute one of the central moieties to get the global zero value.

Thus, being sufficiently representative of the charge transfer occurring within the different compounds, the IFCT section of the article focuses solely on presenting the absolute value of the central moiety, *e.g.* |-0.27552| for **6a**.

- Reorganization energies

Reorganization energy[10] is divided into two contributions: internal reorganization energy and external reorganization energy. Internal reorganization is associated with changes in the internal geometry, while external reorganization, which we neglect here, is related to polarization effects on the external environment. More specifically, the inner intramolecular

[10] a) S. Ahmed, I. Irshad, S. Nazir, S. Naz, M. A. Asghar, S. M. Alshehri, S. Bullo, M. L. Sanyang, *Sci. Rep.* **2023**, 13, 15064; b) T. Hassan, I. Sajid, M. Ramzan Saeed Ashraf Janjua, Z. Shafiq, M. Yasir Mehboob, N. Sultan, *Comput. Theor. Chem.* **2023**, 1224, 114128.

reorganization energy comprises two parts that result from geometric relaxation when transitioning from the geometry of the neutral molecule to that of charged radical species, and vice versa. Thus, by analyzing the geometries of the radical anion and cation, we can obtain insights into the electron and hole mobilities, respectively. As we are studying NFAs designed to exhibit good electron transport properties, we focused on calculating the reorganization energy specific to electron transport (λ_e) using the following equation:

$$\lambda_e = \lambda_{e1} + \lambda_{e2} = \left[E^0(G^-) - E^0(G^0)\right] + \left[E^-(G^0) - E^-(G^-)\right]$$

Where $E^0(G^0)$ and $E^-(G^-)$ are the ground-state electronic energies of the neutral molecule, and the radical anion (**Figure S2**). $E^0(G^-)$ is the energy of the neutral molecule at the radical anion geometry. $E^-(G^0)$ is the energy of the radical anion at the geometry of the neutral molecule. See **Table S5** for λ_{e1} and λ_{e2} values.

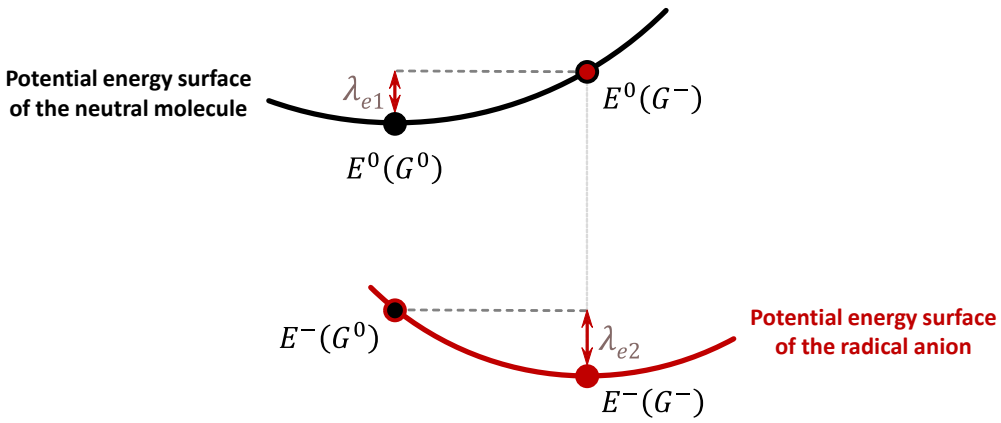


Figure S2. Details of the methodology for calculating reorganization energy relative to electron transport.

- Radar plots of studied compounds similarity to Y6

To ensure a comprehensive comparative study, the same computational methodologies were applied to the reference compound Y6 in order to compute its six key electronic and photophysical properties (**Table S2**).

Table S2. Computed values of key electronic and photophysical properties for Y6.

Electronic properties			Photophysical properties		
λ_e (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	f (a.u)	λ_{max} (nm)	IFCT (a.u)
0.1508	-6.07	-4.01	2.12	667	0.3551

Based on these calculated values, we established a scale to quantify the similarity between the calculated properties of the studied NFAs and those of Y6. This similarity is expressed through a score ranging from 0 to 100, where 0 corresponds to the most distant value from Y6,

and 100 represents the exact computed value of Y6 (**Table S3**). The score is calculated using the following formula:

$$Score = \left(1 - \frac{|\Delta_{rel}|}{|\Delta_{rel}|^{max}}\right) * 100 = \left(1 - \frac{|X_{NFA} - X_{Y6}|}{|X_{NFA} - X_{Y6}|^{max}}\right) * 100$$

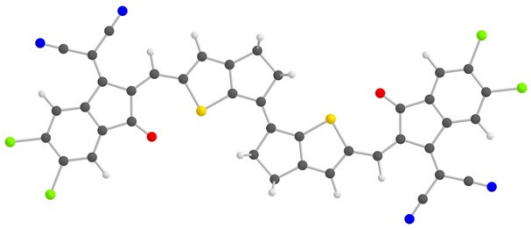
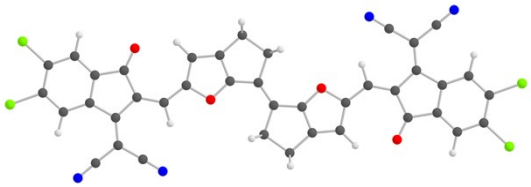
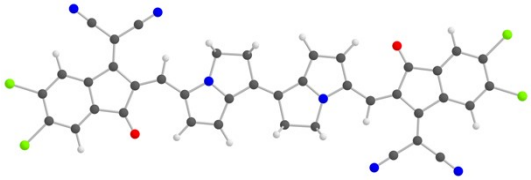
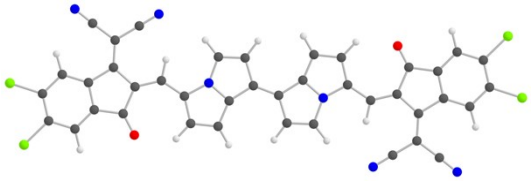
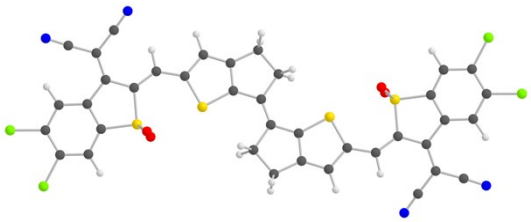
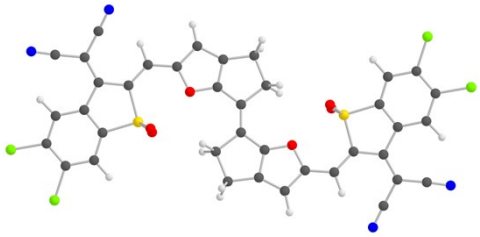
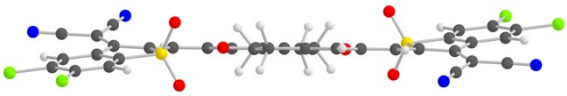
with $|\Delta_{rel}|$ representing the absolute relative difference between the calculated value for a studied NFA (X_{NFA}) and that of Y6 (X_{Y6}), and $|\Delta_{rel}|^{max}$ denoting the largest absolute relative difference within the series, the similarity score for each parameter is determined accordingly.

Subsequently, the Global Similarity Score (GSS) is calculated as the average of the three individual scores, normalized to the highest average score set to 100.

Table S3. Detailed calculations of similarity scores and corresponding Global Similarity Score (GSS).

	Y6	**5a**	**6a**	**7a**	**8a**	**5b**	**6b**	**7b**	**8b**	**5c**	**6c**	**7c**	**8c**
λ_e (eV)	0.1508	0.2544	0.2681	0.1903	0.3179	0.2701	0.2472	0.1901	0.2770	0.5443	0.4543	0.4881	0.5120
$\|\Delta_{rel}\|$ (eV)	0	0.1036	0.1173	0.0395	0.1671	0.1193	0.0964	0.0393	0.1262	0.3935	0.3035	0.3373	0.3612
Score	100	74	70	90	58	70	76	90	68	0	23	14	8
E_{HOMO} (eV)	-6.07	-6.10	-6.09	-6.08	-6.29	-6.21	-6.13	-6.18	-6.41	-6.33	-6.31	-6.22	-6.44
$\|\Delta_{rel}\|$ (eV)	0	0.03	0.02	0.01	0.22	0.14	0.06	0.11	0.34	0.26	0.24	0.15	0.37
Score	100	91	94	96	40	62	83	70	8	29	35	59	0
E_{LUMO} (eV)	-4.01	-4.17	-4.20	-3.93	-4.45	-4.36	-4.39	-4.20	-4.65	-4.56	-4.57	-4.25	-4.71
$\|\Delta_{rel}\|$ (eV)	0	0.16	0.19	0.08	0.44	0.35	0.38	0.19	0.64	0.55	0.56	0.24	0.70
Score	100	78	73	88	37	50	46	73	9	22	20	66	0
f (a.u)	2.12	2.24	2.29	2.17	2.34	3.13	1.70	2.13	2.25	1.48	1.21	1.76	2.06
$\|\Delta_{rel}\|$ (a.u)	0	0.12	0.18	0.06	0.22	0.01	0.42	0.01	0.13	0.64	0.90	0.35	0.06
Score	100	86	80	94	76	99	54	99	85	29	0	61	93
λ_{max} (nm)	667	679	686	628	691	704	734	662	710	778	785	707	746
$\|\Delta_{rel}\|$ (nm)	0	12	19	39	24	37	67	5	43	111	118	40	79
Score	100	90	84	67	80	69	43	96	64	6	0	66	33
IFCT (a.u)	0.3551	0.2707	0.2755	0.3375	0.0447	0.3251	0.3141	0.3607	0.1099	0.2353	0.2067	0.2987	0.0538
$\|\Delta_{rel}\|$ (a.u)	0	0.0844	0.0796	0.0176	0.3104	0.0300	0.0410	0.0056	0.2452	0.1198	0.1484	0.0564	0.3013
Score	100	73	74	94	0	90	87	98	21	61	52	82	3
Mean Score	-	82	79	88	48	73	65	88	42	25	22	58	23
GSS	-	93	90	100	55	83	73	99	47.8	28	25	66	26

Table S4. Top and front view of optimized structures of all compounds.

	Top view	Front view
5a		
6a		
7a		
8a		
5b		
6b		

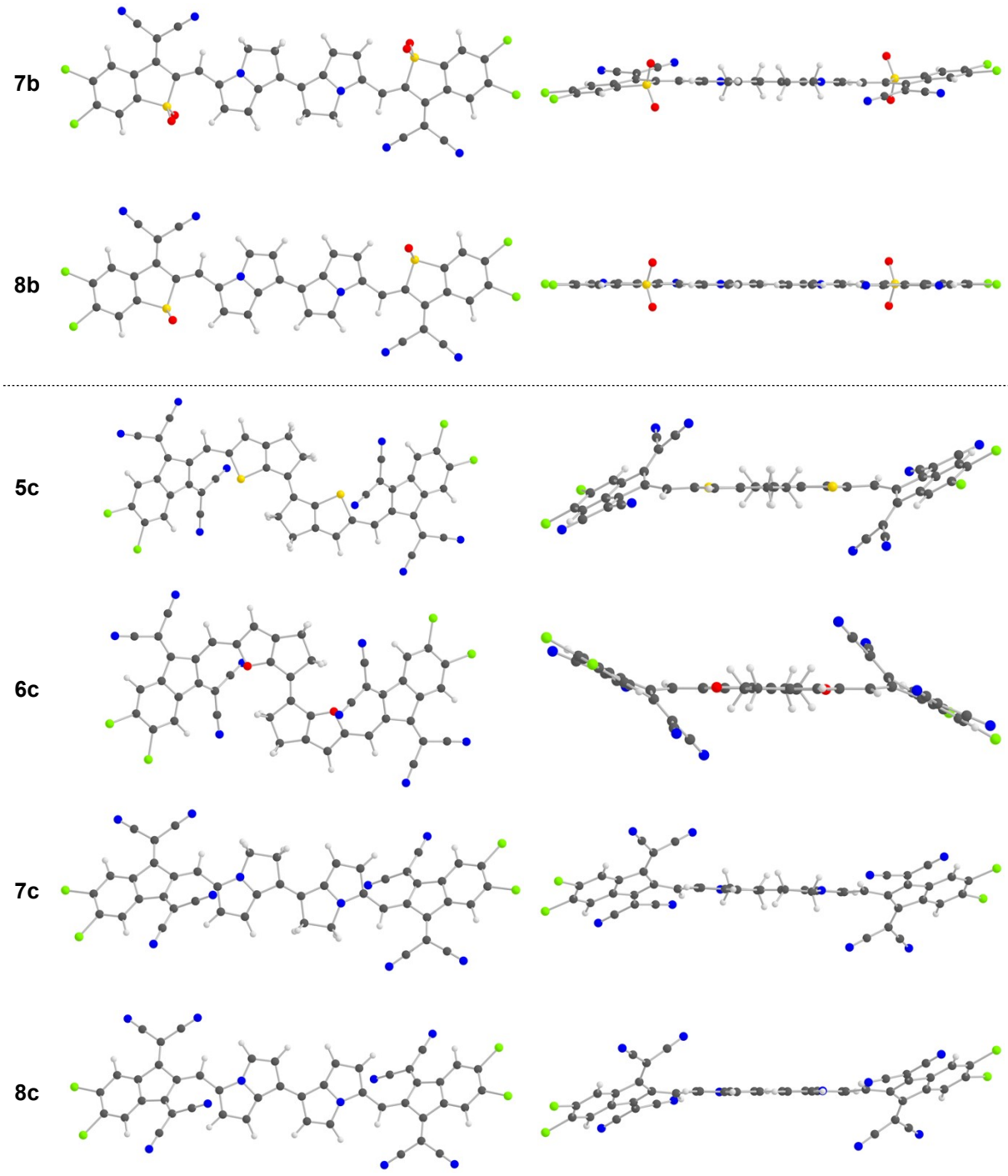
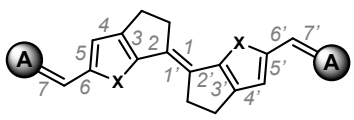
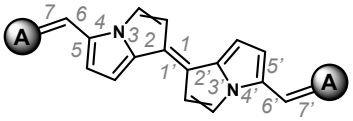


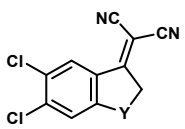
Table S5. Details of calculated[a] bond lengths, mean and BLA values obtained for all compounds. Bonds are numbered *1* through *7* according to the scheme below (due to the symmetrical nature of the molecules, *1'*, *2'*, … are used to indicate identical bonds).



X = S for **5** ; **X** = O for **6**



= for **7** or = for **8**

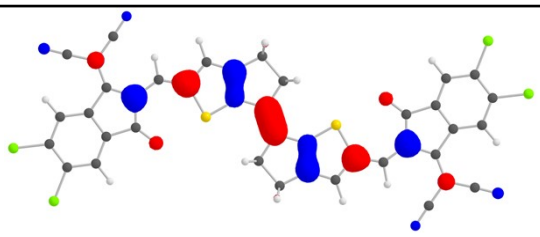
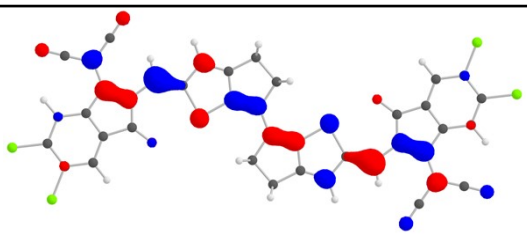
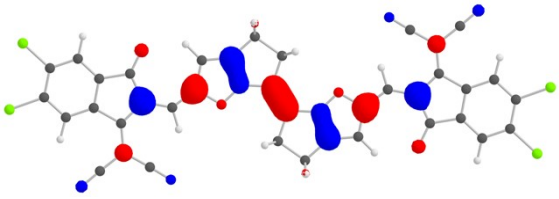
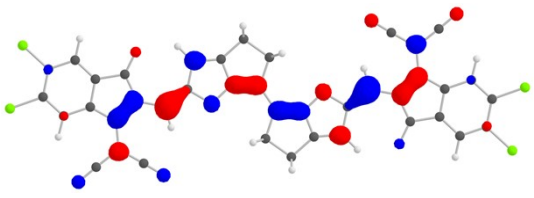
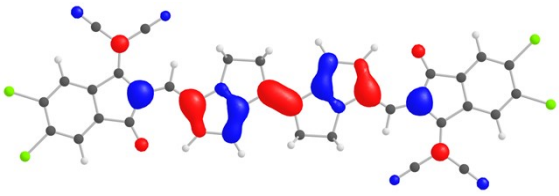
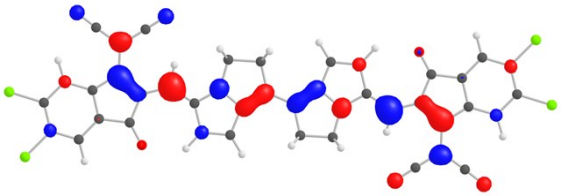


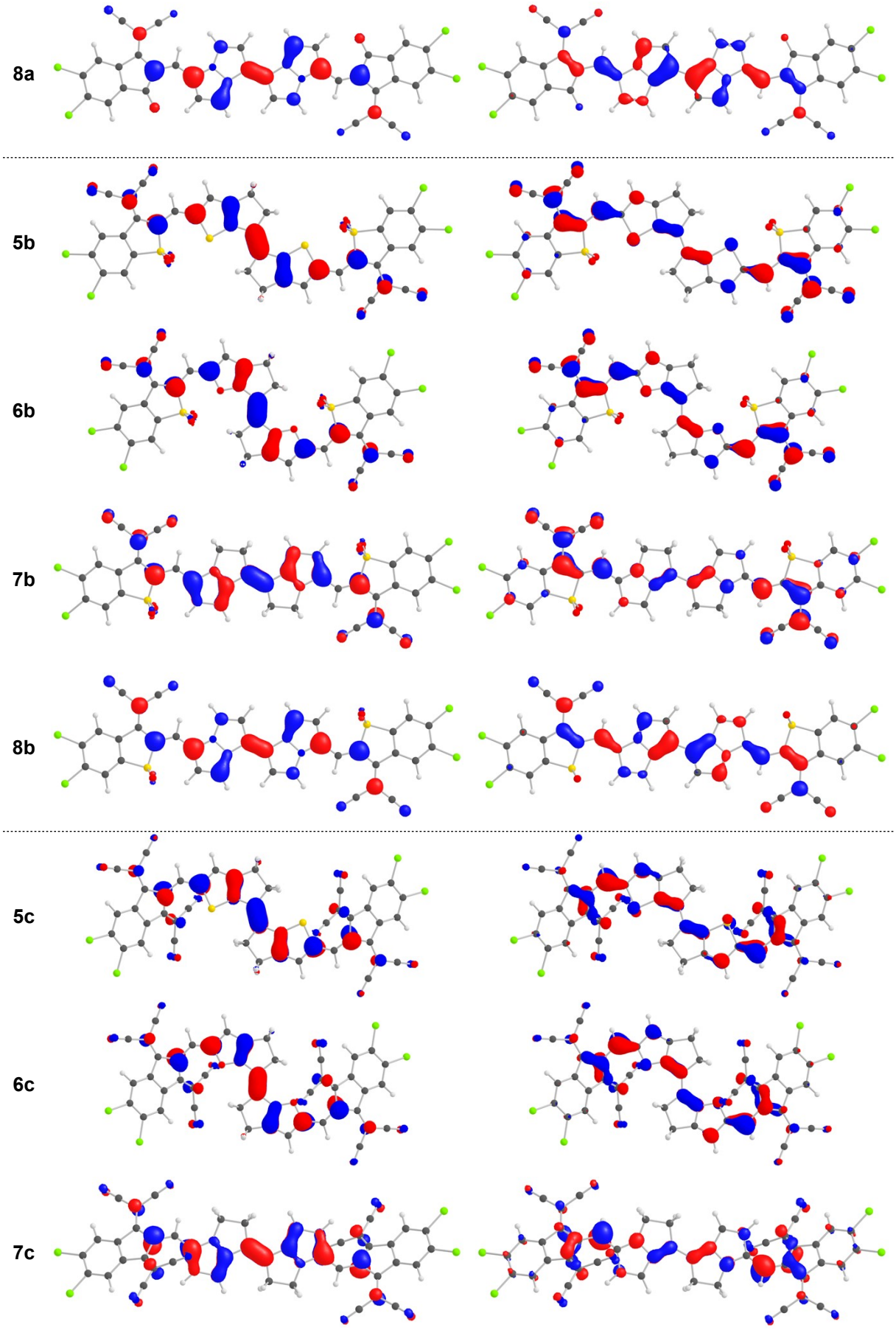
Y = C=O for **a**
= SO_2 for **b**
= $C=C(CN)_2$ for **c**

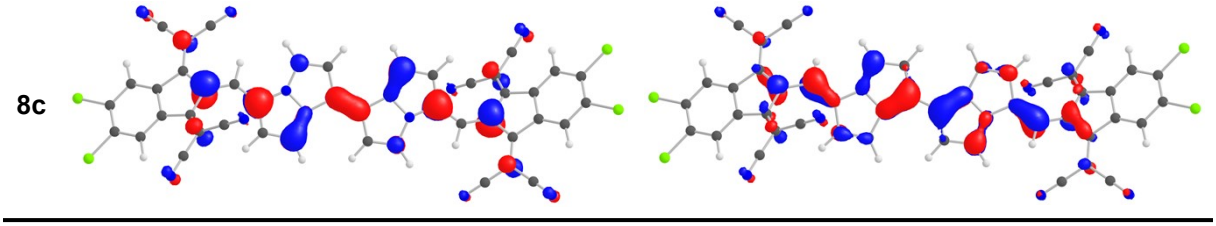
	Bond number[b](bond type[c])									
	1(d)	2/2'(s)	3/3'(d)	4/4'(s)	5/5'(d)	6/6'(s)	7/7'(d)	$\bar{l}_{s}$[d]	$\bar{l}_{d}$[e]	BLA
5a	1.363	1.429	1.397	1.388	1.410	1.414	1.376	1.410	1.386	0.024
6a	1.361	1.417	1.384	1.398	1.404	1.405	1.377	1.407	1.381	0.026
7a	1.354	1.433	1.413	1.390	1.424	1.406	1.379	1.410	1.392	0.018
8a	1.375	1.448	1.406	1.398	1.417	1.406	1.377	1.417	1.394	0.023
5b	1.363	1.427	1.396	1.390	1.407	1.415	1.369	1.411	1.384	0.027
6b	1.363	1.410	1.386	1.400	1.405	1.400	1.373	1.403	1.382	0.021
7b	1.354	1.432	1.413	1.389	1.423	1.407	1.371	1.409	1.390	0.019
8b	1.375	1.447	1.406	1.397	1.416	1.406	1.371	1.417	1.392	0.025
5c	1.364	1.424	1.394	1.393	1.402	1.415	1.377	1.411	1.384	0.027
6c	1.364	1.410	1.384	1.399	1.404	1.400	1.381	1.403	1.383	0.020
7c	1.354	1.431	1.413	1.389	1.421	1.406	1.381	1.408	1.393	0.015
8c	1.376	1.446	1.406	1.396	1.415	1.405	1.378	1.416	1.394	0.022

[a] B3LYP-D3(BJ)/6-311++G(d,p) level of theory. [b] Based on the figure above. [c] **s** or **d** for single or double bond, respectively. [d] Average length of single bonds. [e] Average length of double bonds.

Table S6. FMOs of all compounds at the B3LYP-D3(BJ)/6-311++G(d,p) level of theory (contour value: 0.04 electrons/bohr^3).

	HOMO	LUMO
5a		
6a		
7a		


8a
5b
6b
7b
8b
5c
6c
7c



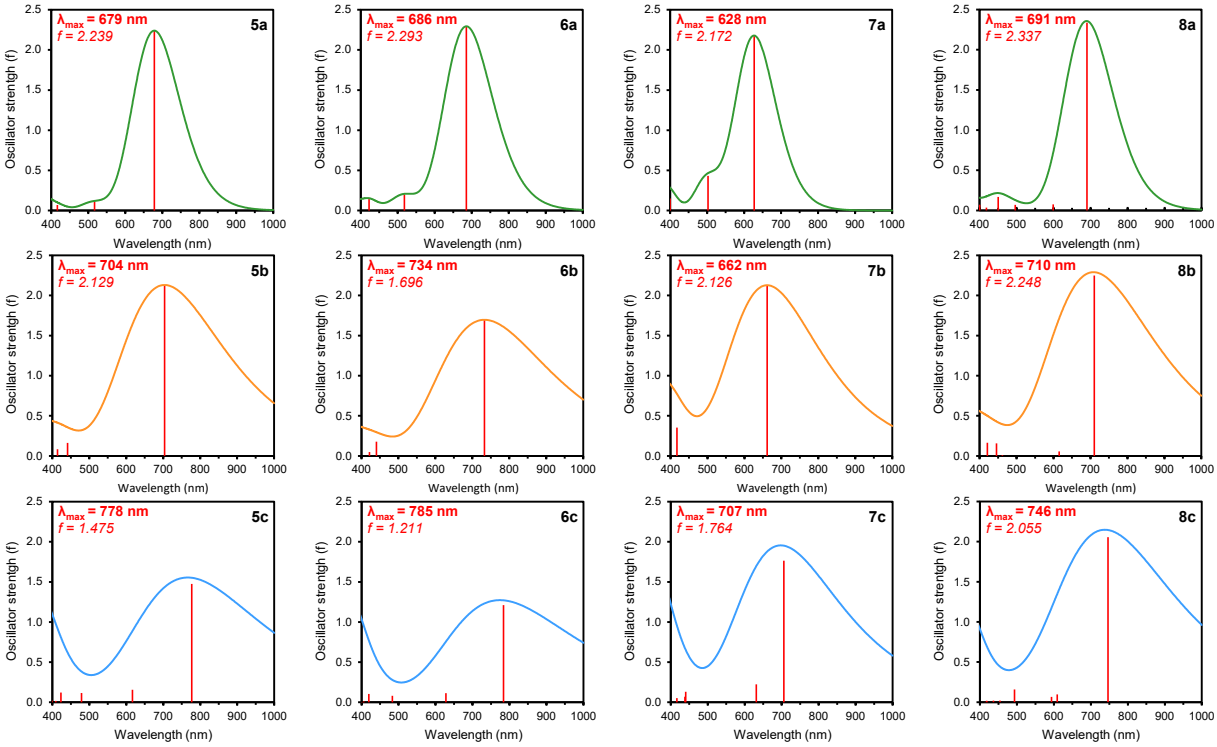


Figure S3. Computational absorption spectra with excited-state vertical transitions depicted in red for all compounds at the B3LYP-D3(BJ)/6-311++G(d,p) level of theory. Maximum absorption wavelengths (λ_{max}) and corresponding oscillator strengths (**f**) are displayed on the top left of each spectrum.

Table S7. Calculated[a] λ_{max} and details of excited-state vertical transitions for all compounds.

	λ_{max} (nm)	Transitions (f[b] ≥ 0.2)	λ (nm)	f	MO contributions[c]
5a	679	$S_0 \rightarrow S_1$	679	2.239	H[d]→L[e] (71%)
6a	686	$S_0 \rightarrow S_1$	686	2.293	H→L (71%)
		$S_0 \rightarrow S_3$	519	0.201	H→L+2 (69%)
7a	628	$S_0 \rightarrow S_1$	628	2.172	H→L (70%)
		$S_0 \rightarrow S_3$	503	0.432	H→L+2 (69%)
8a	691	$S_0 \rightarrow S_1$	691	2.337	H→L (70%)
5b	704	$S_0 \rightarrow S_1$	704	2.129	H→L (71%)
6b	734	$S_0 \rightarrow S_1$	734	1.696	H→L (71%)
7b	662	$S_0 \rightarrow S_1$	662	2.126	H→L (71%)
		$S_0 \rightarrow S_4$	418	0.354	H-1→L (66%)
					H→L+1 (25%)
8b	711	$S_0 \rightarrow S_1$	711	2.248	H→L (71%)
5c	778	$S_0 \rightarrow S_1$	778	1.475	H→L (70%)

6c	785	$S_0 \rightarrow S_1$	785	1.211	H→L (71%)
7c	707	$S_0 \rightarrow S_1$	707	1.764	H→L (69%)
		$S_0 \rightarrow S_3$	632	0.224	H→L+2 (68%)
8c	747	$S_0 \rightarrow S_1$	747	2.055	H→L (70%)

[a] B3LYP-D3(BJ)/6-311++G(d,p) level of theory. [b] Oscillator strength. [c] Major contributions (≥25%). [d] HOMO. [e] LUMO.

Table S8. Details of the calculation of the reorganization energy relative to electron transport (λ_e in eV) for all compounds at B3LYP-D3(BJ)/6-311++G(d,p) level of theory.

	Electron transport		
	λ_{e1}	λ_{e2}	λ_e
5a	0.1324	0.1220	0.2544
6a	0.1401	0.1281	0.2681
7a	0.0995	0.0908	0.1903
8a	0.1608	0.1571	0.3179
5b	0.1437	0.1264	0.2701
6b	0.1262	0.1210	0.2472
7b	0.1024	0.0878	0.1901
8b	0.1418	0.1352	0.2770
5c	0.2876	0.2566	0.5443
6c	0.2332	0.2211	0.4543
7c	0.2758	0.2124	0.4881
8c	0.2690	0.2430	0.5120

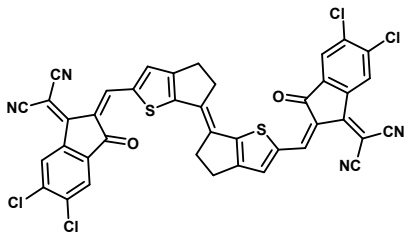
Cartesian coordinates of optimized structures

At B3LYP-D3(BJ)/6-311++G(d,p) level of theory, E and G correspond to the zero-point and the Gibbs free energies.

5a

E = -4540.790388 Hartree

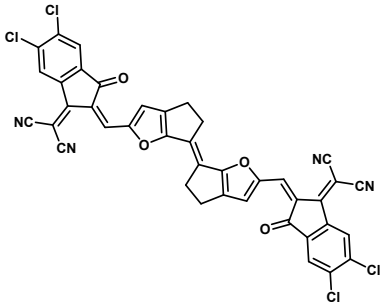
G = -4540.877235 Hartree



C	-8.741410000	0.339340000	-0.000035000	S	-3.126291000	0.176604000	0.000012000	C	8.403791000	-2.850079000	-0.000162000
C	-10.121856000	0.153473000	0.000040000	C	-1.620533000	1.027858000	0.000037000	C	9.796918000	-3.143566000	-0.000255000
C	-10.625872000	-1.148966000	0.000069000	C	-0.246694000	0.635271000	0.000013000	N	10.920681000	-3.416565000	-0.000334000
Cl	-12.351939000	-1.357176000	0.000148000	C	0.246694000	-0.635254000	0.000054000	C	7.589902000	-4.018377000	-0.000215000
C	-9.768764000	-2.262789000	0.000035000	C	1.620534000	-1.027839000	0.000040000	N	6.951978000	-4.983511000	-0.000260000
Cl	-10.397730000	-3.883116000	0.000073000	S	3.126293000	-0.176584000	0.000064000	C	5.398961000	-1.950545000	0.000083000
C	-8.387957000	-2.076959000	-0.000020000	C	4.004300000	-1.718053000	0.000093000	H	-7.713220000	-2.923034000	-0.000035000
C	-7.900905000	-0.784400000	-0.000050000	C	3.105461000	-2.803953000	0.000170000	H	3.461990000	-3.826236000	0.000217000
C	-6.487624000	-0.345325000	-0.000074000	C	1.772856000	-2.416099000	0.000110000	H	-1.236418000	-1.951634000	-0.876143000
O	-5.511559000	-1.076642000	-0.000097000	C	0.433061000	-3.099855000	0.000160000	H	0.307679000	-3.738360000	-0.877912000

C	-6.506296000	1.133026000	-0.000100000	C	-0.583308000	-1.916409000	0.000144000	H	0.307726000	-3.738324000	0.878262000
C	-7.905015000	1.565220000	-0.000089000	C	8.741418000	-0.339346000	-0.000003000	H	1.236440000	1.951636000	0.876200000
C	-8.403830000	2.850072000	-0.000119000	C	10.121867000	-0.153491000	-0.000070000	H	-0.307730000	3.738366000	-0.878132000
C	-9.796966000	3.143515000	-0.000097000	C	10.625894000	1.148944000	-0.000009000	H	-0.307669000	3.738354000	0.878043000
N	-10.920735000	3.416489000	-0.000084000	Cl	12.351963000	1.357140000	-0.000082000	H	-3.461989000	3.826256000	-0.000139000
C	-7.589983000	4.018399000	-0.000156000	C	9.768796000	2.262774000	0.000111000	H	1.236334000	1.951576000	-0.876423000
N	-6.952109000	4.983567000	-0.000184000	Cl	10.397779000	3.883095000	0.000185000	H	-1.236354000	-1.951545000	0.876480000
C	-5.398960000	1.950564000	-0.000160000	C	8.387987000	2.076958000	0.000171000	H	5.597979000	-3.013814000	0.000096000
C	0.583310000	1.916426000	-0.000072000	C	7.900924000	0.784402000	0.000115000	H	10.822637000	-0.972972000	-0.000160000
C	-0.433059000	3.099873000	-0.000046000	C	6.487638000	0.345341000	0.000136000	H	7.713257000	2.923038000	0.000256000
C	-1.772854000	2.416118000	-0.000009000	O	5.511578000	1.076665000	0.000220000	H	-5.597977000	3.013832000	-0.000234000
C	-3.105459000	2.803972000	-0.000090000	C	6.506296000	-1.133009000	0.000041000	H	-10.822631000	0.972949000	0.000065000
C	-4.004299000	1.718073000	-0.000098000	C	7.905006000	-1.565218000	-0.000046000				

6a

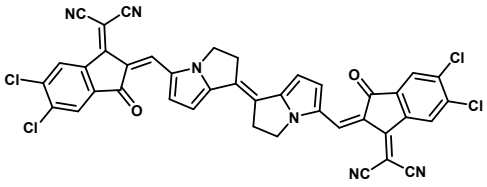


E = -4540.790388
Hartree

G = -4540.877235
Hartree

C	8.810358000	-0.439191000	-0.000098000	O	2.769604000	-0.283158000	-0.000122000	C	-7.398065000	2.541287000	0.000371000
C	10.130672000	-0.883075000	0.000126000	C	1.799723000	0.638674000	-0.000266000	C	-8.519138000	3.419055000	0.000348000
C	11.158670000	0.062212000	0.000168000	C	0.384622000	0.561177000	-0.000064000	N	-9.406058000	4.161218000	0.000342000
Cl	12.798866000	-0.514470000	0.000449000	C	-0.384647000	-0.561199000	0.000278000	C	-6.154825000	3.235152000	0.000548000
C	10.882403000	1.440207000	0.000004000	C	-1.799748000	-0.638694000	0.000478000	N	-5.163081000	3.830916000	0.000691000
Cl	12.162910000	2.615369000	0.000062000	O	-2.769629000	0.283141000	0.000361000	C	-5.100478000	0.420183000	0.000393000
C	9.561642000	1.883824000	-0.000191000	C	-3.982536000	-0.430291000	0.000487000	H	-4.463507000	-2.562858000	0.000870000
C	8.553365000	0.939719000	-0.000241000	C	-3.699715000	-1.805594000	0.000708000	H	0.723635000	-2.209858000	0.874447000
C	7.091456000	1.176431000	-0.000364000	C	-2.306655000	-1.926543000	0.000697000	H	-1.214260000	-3.571343000	0.878758000
O	6.553001000	2.270255000	-0.000492000	C	-1.183993000	-2.921916000	0.000734000	H	-1.214546000	-3.571787000	-0.876945000
C	6.453418000	-0.163353000	-0.000253000	C	0.098832000	-2.014740000	0.000344000	H	-0.723689000	2.209827000	-0.874216000
C	7.518127000	-1.167964000	-0.000181000	C	-8.810370000	0.439203000	0.000055000	H	1.214527000	3.571797000	0.877092000
C	7.398108000	-2.541290000	-0.000268000	C	-10.130689000	0.883085000	-0.000259000	H	1.214224000	3.571288000	-0.878611000
C	8.519227000	-3.418999000	-0.000236000	C	-11.158686000	-0.062203000	-0.000406000	H	4.463483000	2.562845000	-0.000676000
N	9.406235000	-4.161056000	-0.000215000	Cl	-12.798882000	0.514479000	-0.000799000	H	-0.723218000	2.210011000	0.874248000
C	6.154898000	-3.235206000	-0.000399000	C	-10.882422000	-1.440197000	-0.000261000	H	0.723219000	-2.210028000	-0.874018000
N	5.163184000	-3.831020000	-0.000498000	Cl	-12.162932000	-2.615356000	-0.000452000	H	-4.792667000	1.457306000	0.000341000
C	5.100459000	-0.420196000	-0.000195000	C	-9.561662000	-1.883816000	0.000018000	H	-10.397101000	1.927831000	-0.000386000
C	-0.098858000	2.014717000	-0.000132000	C	-8.553383000	-0.939711000	0.000177000	H	-9.329833000	-2.940886000	0.000102000
C	1.183966000	2.921894000	-0.000563000	C	-7.091476000	-1.176432000	0.000382000	H	4.792650000	-1.457317000	-0.000058000
C	2.306630000	1.926523000	-0.000505000	O	-6.553019000	-2.270255000	0.000508000	H	9.329813000	2.940894000	-0.000296000
C	3.699690000	1.805582000	-0.000513000	C	-6.453435000	0.163347000	0.000342000	H	10.397078000	-1.927824000	0.000263000
C	3.982515000	0.430278000	-0.000275000	C	-7.518131000	1.167966000	0.000237000				

7a



E = -3855.070205
Hartree

G = -3855.157510
Hartree

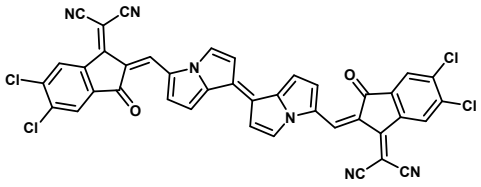
C	3.787879000	-1.619207000	0.004954000	H	-5.086276000	-1.589697000	0.001799000	C	7.218588000	-1.162372000	0.000865000
C	4.119952000	-0.234354000	0.003213000	C	-6.639278000	-0.202772000	0.001456000	C	7.743496000	1.161101000	0.000780000
C	1.865456000	-0.440401000	0.004503000	C	-7.218596000	1.162382000	0.000716000	C	8.691163000	-0.986289000	-0.001206000
C	0.620964000	0.269120000	0.004181000	C	-7.743482000	-1.161095000	0.000712000	O	6.638687000	-2.234128000	0.001662000
C	0.952573000	1.757466000	0.004170000	C	-8.691170000	0.986285000	-0.001226000	C	9.005423000	0.380446000	-0.001399000
H	0.529726000	2.251268000	-0.873602000	O	-6.638707000	2.234144000	0.001417000	C	7.683594000	2.541222000	0.002279000
C	2.502762000	1.844828000	0.000138000	C	-9.005416000	-0.380451000	-0.001356000	C	9.659231000	-1.970944000	-0.002766000
C	-0.620956000	-0.269089000	0.004276000	C	-7.683583000	-2.541214000	0.002090000	C	10.342758000	0.769678000	-0.003319000
C	-1.865447000	0.440430000	0.004372000	C	-9.659248000	1.970930000	-0.002799000	C	6.470154000	3.285006000	0.005369000
C	-0.952567000	-1.757436000	0.004715000	C	-10.342744000	-0.769700000	-0.003200000	C	8.839414000	3.371819000	0.001183000
C	-2.502750000	-1.844801000	0.000585000	C	-6.470147000	-3.285009000	0.004887000	C	10.997613000	-1.582181000	-0.004726000
C	-3.787872000	1.619233000	0.004404000	C	-8.839410000	-3.371802000	0.001085000	H	9.383707000	-3.017504000	-0.002480000
C	-4.119943000	0.234380000	0.003075000	C	-10.997627000	1.582151000	-0.004638000	C	11.330926000	-0.217399000	-0.005020000
C	2.403568000	-1.746382000	0.005765000	H	-9.383737000	3.017493000	-0.002607000	H	10.652180000	1.802528000	-0.003605000
C	-2.403560000	1.746410000	0.005226000	C	-11.330925000	0.217364000	-0.004851000	N	5.494436000	3.907890000	0.007950000
H	1.844856000	-2.667093000	0.007339000	H	-10.652152000	-1.802555000	-0.003456000	N	9.755151000	4.078376000	0.000313000
H	-1.844847000	2.667122000	0.006515000	N	-5.494433000	-3.907902000	0.007193000	Cl	12.228323000	-2.809890000	-0.006724000
H	2.898219000	2.355647000	0.879202000	N	-9.755170000	-4.078330000	0.000295000	Cl	12.994054000	0.291212000	-0.007480000
H	-0.534690000	-2.249308000	0.886005000	Cl	-12.228351000	2.809846000	-0.006644000	H	0.534630000	2.249638000	0.885255000
H	-2.893508000	-2.350202000	-0.883766000	Cl	-12.994047000	-0.291266000	-0.007211000	H	2.893564000	2.350044000	-0.884298000

N	2.901826000	0.435709000	0.003181000	H	4.523614000	-2.403491000	0.005591000	H	-0.529648000	-2.251535000	-0.872850000
N	-2.901819000	-0.435682000	0.003315000	C	5.299955000	0.530800000	0.002072000	H	-2.898256000	-2.355436000	0.879735000
H	-4.523604000	2.403519000	0.004816000	H	5.086290000	1.589721000	0.001449000				
C	-5.299947000	-0.530778000	0.002118000	C	6.639285000	0.202787000	0.001581000				

8a

E = -3852.654834 Hartree

G = -3852.737983 Hartree

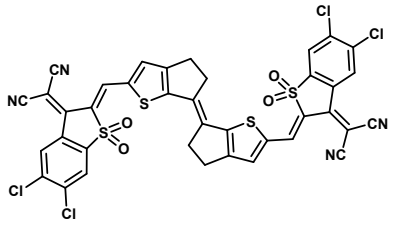


C	9.015507000	-0.387891000	-0.000060000	C	3.821919000	1.669738000	-0.000037000	C	-6.652247000	0.178863000	0.000167000
C	10.347607000	-0.795250000	-0.000061000	C	2.431358000	1.813155000	0.000038000	C	-7.744807000	1.152466000	-0.000002000
C	11.348844000	0.178164000	-0.000040000	C	1.871604000	0.523915000	-0.000023000	C	-7.664005000	2.530986000	-0.000039000
Cl	13.004411000	-0.352311000	-0.000054000	C	0.643386000	-0.242713000	0.000093000	C	-8.806990000	3.379104000	-0.000223000
C	11.033868000	1.547965000	0.000034000	C	-0.643365000	0.242557000	0.000198000	N	-9.712792000	4.098139000	-0.000380000
Cl	12.280854000	2.758093000	0.000155000	C	-1.871585000	-0.524071000	0.000351000	C	-6.437116000	3.252854000	0.000132000
C	9.701076000	1.954815000	0.000072000	C	-2.431349000	-1.813306000	0.000547000	N	-5.444303000	3.847740000	0.000263000
C	8.719487000	0.983338000	-0.000034000	C	-3.821911000	-1.669876000	0.000402000	C	-5.310808000	0.490001000	0.000045000
C	7.250183000	1.179968000	-0.000174000	C	-4.141152000	-0.289410000	0.000286000	H	0.411685000	-2.496626000	0.000157000
O	6.682071000	2.257193000	-0.000027000	N	-2.904226000	0.372400000	0.000200000	H	1.894575000	2.747280000	0.000041000
C	6.652259000	-0.178914000	-0.000092000	C	-2.418793000	1.690880000	-0.000005000	H	-1.894573000	-2.747436000	0.000585000
C	7.744848000	-1.152471000	-0.000134000	C	-1.065086000	1.641112000	-0.000032000	H	3.086158000	-2.539544000	-0.000126000
C	7.664060000	-2.530992000	-0.000255000	C	-9.015489000	0.387928000	-0.000099000	H	-0.411657000	2.496472000	-0.000368000
C	8.807054000	-3.379106000	-0.000293000	C	-10.347572000	0.795344000	-0.000238000	H	-3.086134000	2.539388000	-0.000315000
N	9.712871000	-4.098123000	-0.000318000	C	-11.348852000	-0.178026000	-0.000236000	H	-4.562452000	-2.449250000	0.000477000
C	6.437178000	-3.252863000	-0.000288000	Cl	-13.004395000	0.352521000	-0.000392000	H	-5.085061000	1.545201000	-0.000297000
N	5.444365000	-3.847752000	-0.000347000	C	-11.033934000	-1.547840000	-0.000072000	H	-9.440051000	-3.004993000	0.000216000
C	5.310838000	-0.490109000	0.000039000	Cl	-12.280971000	-2.757915000	-0.000033000	H	-10.642668000	1.832414000	-0.000346000
C	1.065114000	-1.641267000	0.000344000	C	-9.701159000	-1.954747000	0.000092000	H	4.562449000	2.449122000	-0.000167000
C	2.418820000	-1.691035000	0.000157000	C	-8.719528000	-0.983313000	0.000077000	H	5.085139000	-1.545320000	0.000166000
N	2.904249000	-0.372550000	0.000018000	C	-7.250231000	-1.179996000	0.000327000	H	9.439925000	3.005051000	0.000189000
C	4.141169000	0.289273000	0.000003000	O	-6.682162000	-2.257245000	0.000469000	H	10.642751000	-1.832306000	-0.000110000

5b

E = -5411.319996 Hartree

G = -5411.412748 Hartree



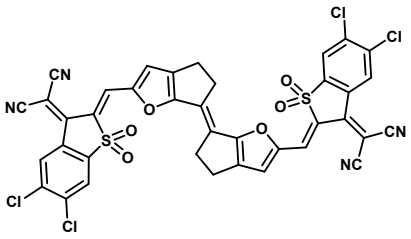
C	-3.977717000	1.738527000	-0.278438000	H	1.285898000	2.081578000	0.364349000	C	7.853049000	-1.543762000	-0.064941000
C	-3.076728000	2.783361000	-0.556442000	S	3.113035000	-0.231399000	-0.045566000	C	8.064551000	0.860936000	-0.078245000
S	-3.113062000	0.231409000	0.045219000	C	-5.374167000	1.963103000	-0.234825000	C	8.745067000	-0.358228000	-0.001854000
H	-3.424630000	3.786491000	-0.767075000	H	-5.604302000	3.001998000	-0.431844000	C	8.310086000	-2.841645000	-0.223648000
C	-1.603558000	1.031706000	-0.190421000	C	-6.457238000	1.159930000	0.001186000	C	8.681261000	2.093505000	-0.049915000
C	-0.237282000	0.623275000	-0.140048000	C	-8.745082000	0.358102000	0.002041000	C	10.136395000	-0.305486000	0.127929000
C	-1.746735000	2.383712000	-0.509208000	C	-8.064436000	-0.860926000	0.079280000	C	7.450577000	-3.961203000	-0.405562000
C	0.604736000	1.855354000	-0.460685000	C	-10.136384000	0.305086000	-0.127934000	C	9.684485000	-3.204499000	-0.264510000
H	1.228300000	1.676856000	-1.341075000	C	-8.680953000	-2.093600000	0.051445000	C	10.068422000	2.128593000	0.070806000
C	-0.399855000	3.024572000	-0.704691000	C	-10.786547000	-0.926244000	-0.164257000	H	8.111924000	3.011342000	-0.112927000
H	-0.294925000	3.441116000	-1.709491000	H	-10.738418000	1.194632000	-0.211588000	C	10.786731000	0.925732000	0.164871000
H	-0.240226000	3.845116000	-0.000836000	C	-10.068090000	-2.128952000	-0.069454000	H	10.738305000	-1.195181000	0.210924000
C	0.237252000	-0.623139000	0.140126000	H	-8.111487000	-3.011320000	0.115006000	N	6.781837000	-4.893231000	-0.557152000
C	1.603527000	-1.031594000	0.190443000	Cl	-10.867564000	-3.667424000	-0.108748000	N	10.787819000	-3.550250000	-0.301528000
C	-0.604769000	-1.855229000	0.460710000	Cl	-12.515329000	-0.935548000	-0.336020000	Cl	10.868115000	3.666933000	0.110830000
C	1.746708000	-2.383531000	0.509473000	C	-7.853209000	1.543838000	0.064155000	Cl	12.515529000	0.934707000	0.336463000
C	0.399846000	-3.024273000	0.705460000	C	-8.310537000	2.841783000	0.221557000	S	6.306837000	0.627794000	-0.191551000

H	-1.228867000	-1.676621000	1.340692000	C	-7.451304000	3.961844000	0.401646000	O	5.816707000	0.979391000	-1.527156000
C	3.977687000	-1.738447000	0.278437000	N	-6.782784000	4.894264000	0.551802000	O	5.642108000	1.224712000	0.970427000
C	3.076704000	-2.783224000	0.556588000	C	-9.685003000	3.204351000	0.262782000	S	-6.306720000	-0.627464000	0.192241000
H	0.240125000	-3.845392000	0.002307000	N	-10.788364000	3.549983000	0.300123000	O	-5.816286000	-0.977972000	1.528048000
H	0.295038000	-3.439987000	1.710624000	C	5.374150000	-1.962995000	0.234492000	O	-5.642108000	-1.225173000	-0.969381000
H	3.424571000	-3.786354000	0.767283000	H	5.604387000	-3.001939000	0.431174000				
H	-1.285426000	-2.081735000	-0.364673000	C	6.457126000	-1.159736000	-0.001596000				

6b

E = -4765.339487 Hartree

G = -4765.428032 Hartree

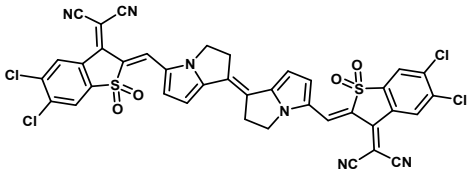


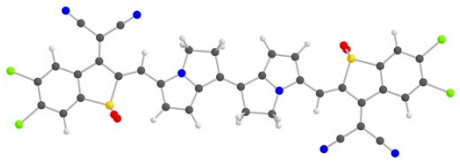
C	-3.076988000	2.469749000	-0.370266000	C	-4.472975000	2.550225000	-0.311993000	C	7.509959000	-0.370670000	0.016315000
C	-2.112185000	3.457613000	-0.630776000	H	-4.841568000	3.553695000	-0.471383000	C	7.501390000	-2.888609000	-0.225897000
H	-2.341227000	4.490556000	-0.843291000	C	-5.395201000	1.558295000	-0.087470000	C	7.024348000	2.031455000	0.027056000
C	-1.137005000	1.497777000	-0.246986000	C	-7.509963000	0.370727000	-0.016340000	C	8.876474000	-0.080850000	0.085017000
C	-0.002107000	0.668996000	-0.129812000	C	-6.627649000	-0.711689000	0.001786000	C	6.846417000	-4.141715000	-0.380874000
C	-0.867335000	2.823091000	-0.548473000	C	-8.876485000	0.080964000	-0.085164000	C	8.914350000	-3.005867000	-0.332656000
C	1.198319000	1.588991000	-0.356050000	C	-7.024459000	-2.031418000	-0.026921000	C	8.388784000	2.304709000	0.083982000
H	1.827778000	1.224817000	-1.170341000	C	-9.307052000	-1.243283000	-0.119092000	H	6.303278000	2.837793000	0.012049000
C	0.617684000	3.018138000	-0.663245000	H	-9.625835000	0.854068000	-0.121119000	C	9.306985000	1.243414000	0.118953000
H	0.905122000	3.357318000	-1.661449000	C	-8.388902000	-2.304615000	-0.083965000	H	9.625865000	-0.853920000	0.120851000
H	0.988037000	3.761788000	0.046210000	H	-6.303429000	-2.837789000	-0.011810000	N	6.345621000	-5.176767000	-0.510943000
C	0.002185000	-0.669163000	0.129844000	Cl	-8.912374000	-3.958166000	-0.121332000	N	10.057776000	-3.156568000	-0.424390000
C	1.137092000	-1.497929000	0.246984000	Cl	-11.015127000	-1.548577000	-0.211726000	Cl	8.912188000	3.958280000	0.121403000
C	-1.198219000	-1.589172000	0.356138000	C	-6.831296000	1.690221000	0.032063000	Cl	11.015057000	1.548777000	0.211427000
C	0.867462000	-2.823244000	0.548520000	C	-7.501346000	2.888657000	0.225790000	O	-2.450920000	1.263977000	-0.128834000
C	-0.617547000	-3.018288000	0.663425000	C	-6.846394000	4.141786000	0.380652000	O	2.450984000	-1.264100000	0.128780000
H	-1.827687000	-1.224954000	1.170400000	N	-6.345642000	5.176869000	0.510639000	S	-4.926234000	-0.194043000	0.033650000
C	3.077095000	-2.469857000	0.370268000	C	-8.914297000	3.005894000	0.332679000	O	-4.329316000	-0.509051000	1.335374000
C	2.112324000	-3.457746000	0.630822000	N	-10.057711000	3.156611000	0.424534000	O	-4.258607000	-0.673289000	-1.180220000
H	-0.987978000	-3.762024000	-0.045898000	C	4.473075000	-2.550291000	0.311976000	S	4.926205000	0.193999000	-0.033520000
H	-0.904881000	-3.357346000	1.661702000	H	4.841712000	-3.553751000	0.471337000	O	4.329242000	0.509152000	-1.335184000
H	2.341398000	-4.490680000	0.843349000	C	5.395243000	-1.558313000	0.087429000	O	4.258564000	0.673055000	1.180429000
H	-1.841906000	-1.599799000	-0.526804000	C	6.831332000	-1.690184000	-0.032144000				
H	1.842001000	1.599542000	0.526896000	C	6.627597000	0.711711000	-0.001667000				

7b

E = -4725.603480 Hartree

G = -4725.694812 Hartree





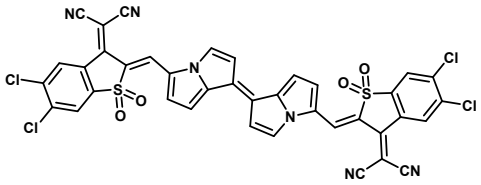
C	-3.821500000	-1.479508000	0.409953000	H	5.081448000	-1.713107000	0.098524000	C	-9.029567000	0.437065000	0.018307000
C	-4.118148000	-0.112264000	0.149460000	C	6.614872000	-0.334116000	-0.151864000	C	-7.714216000	2.595119000	0.202165000
C	-1.873247000	-0.379735000	0.130983000	C	7.762944000	-1.209116000	-0.117676000	C	-9.881449000	-1.863949000	0.037108000
C	-0.614521000	0.282819000	-0.030028000	C	8.853417000	0.947758000	-0.098305000	C	-10.337924000	0.903627000	-0.144552000
C	-0.911473000	1.757525000	-0.280585000	C	9.029535000	-0.437476000	-0.019941000	C	-6.507174000	3.326462000	0.374728000
H	-0.486409000	2.376774000	0.512862000	C	7.713481000	-2.594887000	-0.206346000	C	-8.853053000	3.443904000	0.155197000
C	-2.459479000	1.877333000	-0.309055000	C	9.881992000	1.863339000	-0.036274000	C	-11.178921000	-1.382183000	-0.118949000
C	0.614570000	-0.281583000	0.034753000	C	10.337828000	-0.904587000	0.141833000	H	-9.694394000	-2.927512000	0.103922000
C	1.873314000	0.380969000	-0.126088000	C	6.506123000	-3.325569000	-0.379539000	C	-11.397086000	0.001498000	-0.212557000
C	0.911431000	-1.756283000	0.285466000	C	8.852123000	-3.444049000	-0.161476000	H	-10.566383000	1.953117000	-0.227042000
C	2.459456000	-1.876978000	0.309745000	C	11.179405000	1.381038000	0.118654000	N	-5.534705000	3.940027000	0.510582000
C	3.821572000	1.480693000	-0.405205000	H	9.695185000	2.927032000	-0.101687000	N	-9.745002000	4.180307000	0.120909000
C	4.118154000	0.113140000	-0.146276000	C	11.397253000	-0.002814000	0.210480000	Cl	-12.490376000	-2.514220000	-0.199326000
C	-2.442317000	-1.645388000	0.396957000	H	10.566026000	-1.954238000	0.223017000	Cl	-13.001333000	0.635585000	-0.421191000
C	2.442428000	1.646793000	-0.391154000	N	5.533406000	-3.938608000	-0.515984000	H	-0.474355000	2.092326000	-1.223545000
H	-1.908090000	-2.565202000	0.564177000	N	9.743928000	-4.180704000	-0.128938000	H	-2.846626000	2.573776000	0.435868000

H	1.908254000	2.566887000	-0.556994000	Cl	12.491186000	2.512637000	0.199925000	H	0.476862000	-2.089806000	1.230087000
H	-2.833692000	2.182085000	-1.288336000	Cl	13.001415000	-0.637565000	0.417747000	H	2.844311000	-2.571287000	-0.438375000
H	0.483653000	-2.376117000	-0.506026000	H	-4.549908000	-2.249055000	0.597021000	S	-7.139392000	-1.384333000	0.268783000
H	2.836023000	-2.185049000	1.287057000	C	-5.287000000	0.665591000	0.064549000	O	-6.869997000	-1.934673000	1.601148000
N	-2.889174000	0.509729000	-0.009724000	H	-5.081525000	1.713589000	-0.097707000	O	-6.690447000	-2.152819000	-0.895609000
N	2.889190000	-0.508759000	0.013315000	C	-6.614967000	0.334514000	0.152200000	S	7.139646000	1.384667000	-0.267531000
H	4.549991000	2.250368000	-0.591701000	C	-7.763231000	1.209178000	0.115762000	O	6.691547000	2.152559000	0.897583000
C	5.286936000	-0.665012000	-0.063123000	C	-8.853128000	-0.948030000	0.098422000	O	6.869685000	1.935888000	-1.599406000

8b

E = -4723.186678 Hartree

G = -4723.276508 Hartree

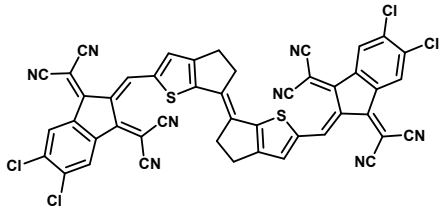


C	3.861005000	-1.574922000	-0.000269000	C	-7.769645000	-1.198413000	0.000256000	C	9.051759000	0.445129000	0.000038000
C	4.143122000	-0.187084000	-0.000268000	C	-8.892956000	0.944429000	0.000329000	C	7.698706000	2.586148000	0.000105000
C	1.882952000	-0.478641000	-0.000473000	C	-9.051757000	-0.445116000	0.000119000	C	9.937251000	-1.844234000	-0.000307000
C	0.637515000	0.257943000	-0.000411000	C	-7.698725000	-2.586135000	0.000602000	C	10.362941000	0.933451000	0.000387000
C	1.024866000	1.666725000	-0.000298000	C	-9.937265000	1.844240000	0.000243000	C	6.476016000	3.311417000	0.000125000
C	2.376587000	1.749681000	-0.000324000	C	-10.362936000	-0.933450000	-0.000244000	C	8.826209000	3.451619000	0.000153000
C	-0.637505000	-0.257971000	-0.000511000	C	-6.476052000	-3.311432000	0.000774000	C	11.235576000	-1.340789000	-0.000026000
C	-1.882941000	0.478616000	-0.000390000	C	-8.826241000	-3.451587000	0.000941000	H	9.761679000	-2.911847000	-0.000519000
C	-1.024860000	-1.666750000	-0.000656000	C	-11.235587000	1.340785000	-0.000075000	C	11.438506000	0.048693000	0.000331000
C	-2.376581000	-1.749703000	-0.000651000	H	-9.761699000	2.911855000	0.000393000	H	10.583124000	1.987671000	0.000708000
C	-3.860983000	1.574911000	-0.000051000	C	-11.438507000	-0.048700000	-0.000334000	N	5.487168000	3.913614000	0.000142000
C	-4.143111000	0.187077000	-0.000249000	H	-10.583109000	-1.987672000	-0.000462000	N	9.704204000	4.205186000	0.000197000
C	2.475702000	-1.753698000	-0.000336000	N	-5.487184000	-3.913596000	0.000879000	Cl	12.566499000	-2.451433000	-0.000044000
C	-2.475679000	1.753676000	-0.000046000	N	-9.704287000	-4.205095000	0.001245000	Cl	13.044332000	0.711000000	0.000761000
H	1.965013000	-2.702159000	-0.000395000	Cl	-12.566517000	2.451421000	-0.000186000	H	0.350598000	2.505729000	-0.000292000
H	-1.964987000	2.702136000	0.000256000	Cl	-13.044329000	-0.711021000	-0.000776000	H	3.024060000	2.613302000	-0.000319000
N	2.893162000	0.442881000	-0.000432000	H	4.596266000	-2.359827000	-0.000248000	H	-0.350594000	-2.505756000	-0.000848000
N	-2.893155000	-0.442903000	-0.000516000	C	5.298173000	0.614544000	-0.000150000	H	-3.024051000	-2.613326000	-0.000773000
H	-4.596260000	2.359802000	0.000008000	H	5.070136000	1.668684000	-0.000092000	S	7.181163000	-1.412834000	-0.000268000
C	-5.298167000	-0.614544000	-0.000222000	C	6.633019000	0.303491000	-0.000093000	O	6.827124000	-2.078812000	-1.256736000
H	-5.070134000	-1.668684000	-0.000541000	C	7.769645000	1.198427000	0.000039000	O	6.827379000	-2.078941000	1.256196000
C	-6.633010000	-0.303483000	0.000127000	C	8.892944000	-0.944418000	-0.000331000	S	-7.181135000	1.412851000	0.000501000

5c

E = -4837.927107 Hartree

G = -4838.023630 Hartree



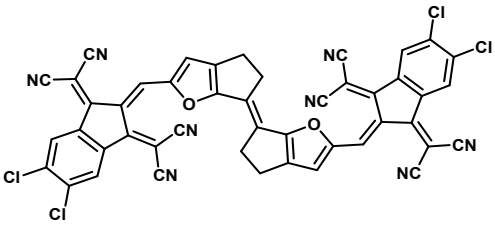
C	-3.822894000	-2.054347000	0.388775000	C	-5.212714000	-2.321906000	0.403219000	C	8.281825000	0.433510000	0.137911000
C	-2.839712000	-3.052379000	0.429738000	H	-5.430329000	-3.356343000	0.168213000	C	8.191424000	2.964884000	0.301036000
S	-3.092606000	-0.459380000	0.166949000	C	-6.292040000	-1.480253000	0.555869000	C	7.853518000	-1.889459000	-0.466567000
H	-3.099469000	-4.097230000	0.540437000	C	-8.281804000	-0.433347000	-0.137791000	C	9.478506000	0.072354000	0.747011000
C	-1.511655000	-1.162257000	0.181556000	C	-7.470264000	0.554703000	0.472082000	C	7.533469000	4.205092000	0.066570000
C	-0.186123000	-0.651932000	0.074456000	C	-9.478507000	-0.072021000	-0.746745000	C	9.496005000	3.097702000	0.854134000
C	-1.544838000	-2.547400000	0.336193000	C	-7.853490000	1.889447000	0.467350000	C	9.043936000	-2.247788000	0.164823000
C	0.755135000	-1.850081000	0.169306000	C	-9.853503000	1.271141000	-0.764396000	H	7.253718000	-2.660710000	-0.925070000
H	1.443321000	-1.732142000	1.010622000	H	-10.128351000	-0.794788000	-1.214587000	C	9.853507000	-1.270802000	0.765045000
C	-0.149857000	-3.108400000	0.351081000	C	-9.043918000	2.247958000	-0.163915000	H	10.128339000	0.795256000	1.214660000
H	0.061914000	-3.622969000	1.291575000	H	-7.253682000	2.660565000	0.926067000	N	7.004486000	5.217478000	-0.114280000
H	0.001693000	-3.833832000	-0.451939000	Cl	-9.492697000	3.924297000	-0.189302000	N	10.552043000	3.228189000	1.306498000
C	0.186127000	0.651850000	-0.075129000	Cl	-11.340272000	1.701016000	-1.550421000	Cl	9.492689000	-3.924126000	0.190741000
C	1.511660000	1.162179000	-0.182214000	C	-6.306905000	-0.108969000	1.069336000	Cl	11.340228000	-1.700460000	1.551276000
C	-0.755131000	1.849999000	-0.169974000	C	-7.632487000	-1.746995000	0.009793000	C	-5.538923000	0.373662000	2.103654000
C	1.544841000	2.547319000	-0.336881000	C	-8.191350000	-2.964674000	-0.301699000	C	5.538886000	-0.374132000	-2.103269000
C	0.149855000	3.108308000	-0.351844000	C	-7.533323000	-4.204921000	-0.067655000	C	5.608096000	-1.726064000	-2.539788000

H	-1.443375000	1.732034000	-1.011237000	N	-7.004253000	-5.217323000	0.112851000	N	5.635854000	-2.829306000	-2.885346000
C	3.822900000	2.054275000	-0.389312000	C	-9.495930000	-3.097367000	-0.854830000	C	4.670962000	0.456162000	-2.866153000
C	2.839716000	3.052300000	-0.430392000	N	-10.551968000	-3.227731000	-1.307229000	N	3.980894000	1.120312000	-3.513275000
H	-0.001721000	3.833819000	0.451099000	C	5.212717000	2.321861000	-0.403645000	C	-4.671113000	-0.456850000	2.866427000
H	-0.061897000	3.622780000	-1.292395000	H	5.430275000	3.356345000	-0.168801000	N	-3.981136000	-1.121157000	3.513486000
H	3.099480000	4.097148000	-0.541104000	C	6.292072000	1.480216000	-0.556074000	C	-5.608193000	1.725465000	2.540553000
H	-1.367585000	1.928087000	0.732908000	C	6.306942000	0.108786000	-1.069148000	N	-5.636018000	2.828621000	2.886381000
H	1.367652000	-1.928133000	-0.733535000	C	7.632524000	1.747120000	-0.010067000	C	8.281825000	0.433510000	0.137911000
S	3.092610000	0.459303000	-0.167565000	C	7.470305000	-0.554713000	-0.471706000				

6c

E = -4191.946513 Hartree

G = -4192.040534 Hartree

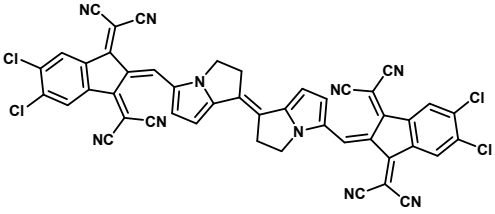


C	-3.080609000	-2.514696000	0.126393000	C	-5.425633000	-1.655999000	0.479988000	C	6.612039000	-1.863406000	-0.445529000
C	-2.111917000	-3.519477000	-0.024131000	C	-7.347549000	-0.405128000	-0.051084000	C	8.551628000	-0.075833000	0.552894000
H	-2.332506000	-4.575652000	-0.045530000	C	-6.377152000	0.494837000	0.451902000	C	7.012972000	4.235176000	-0.047954000
C	-1.148893000	-1.516976000	-0.025553000	C	-8.551581000	0.076329000	-0.552541000	C	8.906860000	2.927930000	0.581354000
C	-0.014640000	-0.679682000	-0.054223000	C	-6.611804000	1.863445000	0.446311000	C	7.812441000	-2.341738000	0.078879000
C	-0.875263000	-2.871454000	-0.110179000	C	-8.778459000	1.452444000	-0.571230000	H	5.891055000	-2.572033000	-0.822772000
C	1.177986000	-1.622745000	-0.216161000	H	-9.318542000	-0.577415000	-0.937085000	C	8.778614000	-1.451924000	0.571998000
H	1.895770000	-1.480536000	0.593880000	C	-7.812192000	2.342032000	-0.077900000	H	9.318510000	0.578091000	0.937290000
C	0.605345000	-3.085249000	-0.228078000	H	-5.890751000	2.571909000	0.823727000	N	6.585730000	5.298268000	-0.205485000
H	0.994443000	-3.671798000	0.607365000	Cl	-8.074471000	4.057868000	-0.105610000	N	10.009611000	2.948318000	0.928409000
H	0.879848000	-3.611749000	-1.144878000	Cl	-10.279127000	2.031903000	-1.223632000	Cl	8.074830000	-4.057546000	0.107179000
C	0.014444000	0.679367000	0.053368000	C	-5.235908000	-0.283041000	0.949715000	Cl	10.279247000	-2.031080000	1.224741000
C	1.148687000	1.516683000	0.024841000	C	-6.831936000	-1.779091000	0.066817000	C	-4.309527000	0.147731000	1.871661000
C	-1.178203000	1.622410000	0.215271000	C	-7.548429000	-2.932135000	-0.158240000	C	4.309693000	-0.148246000	-1.871498000
C	0.875047000	2.871138000	0.109643000	C	-7.013267000	-4.234995000	0.046671000	C	4.188471000	-1.511996000	-2.256934000
C	-0.605570000	3.084911000	0.227476000	N	-6.586151000	-5.298200000	0.203795000	N	4.044359000	-2.620644000	-2.554807000
H	-1.895858000	1.480312000	-0.594907000	C	-8.906983000	-2.927355000	-0.582232000	C	3.448584000	0.740278000	-2.574238000
C	3.080408000	2.514431000	-0.126796000	N	-10.009708000	-2.947558000	-0.929387000	N	2.758976000	1.445026000	-3.177500000
C	2.111716000	3.519183000	0.023801000	C	4.471446000	2.626334000	-0.244418000	C	-3.448484000	-0.741023000	2.574183000
H	-0.880138000	3.611251000	1.144349000	H	4.818003000	3.626756000	-0.022433000	N	-2.758904000	-1.445947000	3.177275000
H	-0.994615000	3.671604000	-0.607892000	C	5.425557000	1.655921000	-0.480220000	C	-4.188211000	1.511365000	2.257460000
H	2.332300000	4.575355000	0.045396000	C	5.235998000	0.282813000	-0.949632000	N	-4.043958000	2.619915000	2.555636000
H	-1.705746000	1.404116000	1.145314000	C	6.831871000	1.779262000	-0.067105000	O	-2.465615000	-1.272607000	0.100878000
H	1.705379000	-1.404589000	-1.146324000	C	6.377288000	-0.494815000	-0.451549000	O	2.465430000	1.272337000	-0.101513000
C	-4.471619000	-2.626546000	0.244167000	C	7.347590000	0.405378000	0.051215000				
H	-4.818266000	-3.626958000	0.022290000	C	7.548273000	2.932448000	0.157458000				

7c

E = -4152.208236 Hartree

G = -4152.304323 Hartree

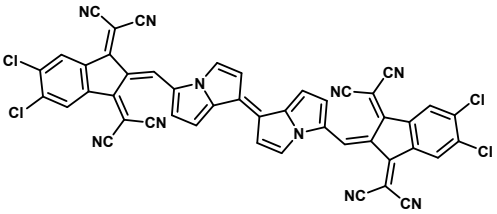


C	3.927888000	1.124065000	0.482708000	C	5.240578000	-0.916218000	-0.457803000	C	-5.240641000	0.916429000	0.458165000
C	4.112925000	-0.137045000	-0.146360000	H	5.011690000	-1.967549000	-0.566340000	H	-5.011741000	1.967761000	0.566651000
C	1.898635000	0.219530000	0.123204000	C	6.574637000	-0.569073000	-0.542769000	C	-6.574726000	0.569289000	0.542845000
C	0.591319000	-0.298104000	-0.141047000	C	7.161607000	0.763812000	-0.661971000	C	-7.161600000	-0.763603000	0.662285000
C	0.773194000	-1.659950000	-0.803242000	C	7.679012000	-1.515628000	-0.345006000	C	-7.679103000	1.515703000	0.344505000
H	0.243396000	-1.711797000	-1.756237000	C	8.543322000	0.665052000	-0.175443000	C	-8.543224000	-0.665099000	0.175462000
C	2.302926000	-1.826510000	-1.008344000	C	6.616971000	1.839579000	-1.328970000	C	-6.616983000	-1.839128000	1.329691000
H	2.587890000	-1.800015000	-2.061568000	C	8.863410000	-0.705043000	-0.014665000	C	-8.863379000	0.704927000	0.014206000
H	2.694093000	-2.745012000	-0.568572000	C	7.647866000	-2.890903000	-0.444362000	C	-7.648035000	2.891042000	0.443169000
C	-0.591392000	0.298084000	0.141920000	C	9.488363000	1.648236000	0.086302000	C	-9.488154000	-1.648428000	-0.086162000
C	-1.898707000	-0.219563000	-0.122296000	C	5.409631000	1.746848000	-2.074189000	C	-7.270146000	-3.099815000	1.415475000
C	-0.773242000	1.659921000	0.804143000	C	7.270220000	3.100238000	-1.414473000	C	-5.409799000	-1.746109000	2.075122000
C	-2.303010000	1.826750000	1.008793000	C	10.135766000	-1.078580000	0.402887000	C	-10.135713000	1.078252000	-0.403623000
H	-0.243744000	1.711550000	1.757322000	C	6.486629000	-3.618905000	-0.826443000	C	-6.486909000	3.619290000	0.825109000
C	-3.927973000	-1.123990000	-0.481979000	C	8.785101000	-3.711786000	-0.206127000	C	-8.785243000	3.711770000	0.204305000
C	-4.112994000	0.137180000	0.146988000	C	10.756453000	1.267948000	0.525368000	C	-10.756218000	-1.268358000	-0.525494000

H	-2.693948000	2.745105000	0.568502000	H	9.271343000	2.699129000	-0.027603000	H	-9.271065000	-2.699275000	0.028027000
H	-2.588251000	1.800775000	2.061952000	N	4.443013000	1.676889000	-2.704503000	N	-7.779749000	-4.136235000	1.476474000
H	-0.374416000	2.451498000	0.164668000	N	7.779851000	4.136663000	-1.475160000	N	-4.443319000	-1.675903000	2.705620000
H	0.374735000	-2.451534000	-0.163539000	C	11.078931000	-0.088566000	0.678578000	C	-11.078788000	0.088096000	-0.679109000
N	2.842505000	-0.651101000	-0.322411000	H	10.421478000	-2.110952000	0.528914000	H	-10.421487000	2.110567000	-0.529970000
N	-2.842568000	0.651131000	0.323212000	N	5.540901000	-4.212777000	-1.129532000	N	-5.541272000	4.213318000	1.128176000
C	-2.568179000	-1.342351000	-0.659442000	N	9.693284000	-4.402038000	-0.015847000	N	-9.693405000	4.401903000	0.013477000
C	2.568082000	1.342303000	0.660393000	Cl	11.915543000	2.511346000	0.876870000	Cl	-11.915128000	-2.511954000	-0.876907000
H	2.110013000	2.203432000	1.116368000	Cl	12.654298000	-0.579327000	1.219207000	Cl	-12.654143000	0.578596000	-1.220008000
H	-2.110116000	-2.203505000	-1.115379000	H	4.724998000	1.778738000	0.795317000	H	-4.725094000	-1.778639000	-0.794614000

8c

E = -4149.790447 Hartree

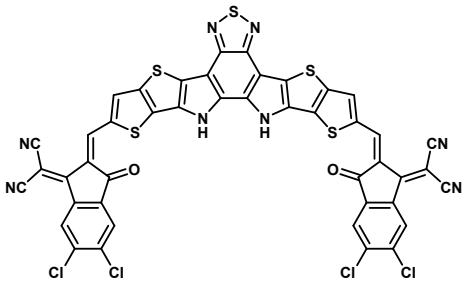


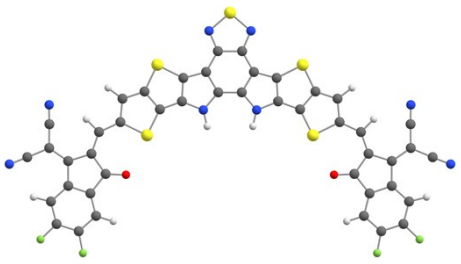
G = -4149.883662 Hartree

C	3.936480000	1.334052000	0.281181000	C	7.259464000	0.841038000	-0.690744000	C	-6.602721000	0.463315000	0.612847000
C	4.136730000	0.037418000	-0.249503000	C	7.659758000	-1.468246000	-0.425044000	C	-7.259165000	-0.840755000	0.691313000
C	1.904849000	0.375551000	0.057383000	C	8.617976000	0.661761000	-0.162630000	C	-7.660007000	1.468298000	0.424478000
C	0.621340000	-0.260634000	-0.138885000	C	6.788716000	1.955253000	-1.347219000	C	-8.617822000	-0.662023000	0.163387000
C	0.925708000	-1.575745000	-0.698067000	C	8.867996000	-0.726221000	-0.032134000	C	-6.788060000	-1.954470000	1.348359000
H	0.204259000	-2.327680000	-0.967497000	C	7.569282000	-2.832389000	-0.597795000	C	-8.868153000	0.725833000	0.032170000
C	2.268286000	-1.699212000	-0.823861000	C	9.599268000	1.590326000	0.158318000	C	-7.569793000	2.832507000	0.596792000
H	2.865664000	-2.515922000	-1.198636000	C	5.606188000	1.938257000	-2.136104000	C	-9.598973000	-1.590960000	-0.156942000
C	-0.621446000	0.261488000	0.137169000	C	7.507490000	3.183165000	-1.382663000	C	-7.506702000	-3.182434000	1.384887000
C	-1.904943000	-0.374785000	-0.058890000	C	10.106578000	-1.173081000	0.414088000	C	-5.605301000	-1.936787000	2.136875000
C	-0.925824000	1.576736000	0.696028000	C	6.387263000	-3.480947000	-1.054606000	C	-10.106883000	1.172216000	-0.414125000
C	-2.268400000	1.700220000	0.821807000	C	8.661189000	-3.715655000	-0.369825000	C	-6.387813000	3.481419000	1.053211000
H	-0.204379000	2.328756000	0.965233000	C	10.832539000	1.136689000	0.626024000	C	-8.661947000	3.715464000	0.368815000
C	-3.936514000	-1.333732000	-0.281406000	H	9.436333000	2.653324000	0.069089000	C	-10.832395000	-1.137821000	-0.624737000
C	-4.136771000	-0.036813000	0.248546000	N	4.660536000	1.935173000	-2.800766000	H	-9.435819000	-2.653875000	-0.067140000
H	-2.865799000	2.517078000	1.196237000	N	8.071633000	4.192295000	-1.402321000	N	-8.070728000	-4.191610000	1.405462000
N	2.859387000	-0.513565000	-0.357624000	C	11.085601000	-0.238089000	0.749309000	N	-4.659481000	-1.933087000	2.801291000
N	-2.859500000	0.514468000	0.355836000	H	10.337749000	-2.221506000	0.518555000	C	-11.085765000	0.236845000	-0.748705000
C	-2.569910000	-1.539874000	-0.479444000	N	5.420189000	-4.003407000	-1.415571000	H	-10.338266000	2.220542000	-0.519112000
C	2.569861000	1.540245000	0.478978000	N	9.533274000	-4.452962000	-0.188521000	N	-5.420744000	4.004077000	1.413896000
H	2.117733000	2.432717000	0.878047000	Cl	12.036558000	2.311600000	1.051033000	N	-9.534281000	4.452467000	0.187477000
H	-2.117777000	-2.432536000	-0.878081000	Cl	12.616505000	-0.818604000	1.325689000	Cl	-12.036253000	-2.313203000	-1.048887000
C	5.259895000	-0.760816000	-0.525063000	H	4.720913000	2.031717000	0.521120000	Cl	-12.616863000	0.816734000	-1.325190000
H	5.012342000	-1.810496000	-0.591775000	C	-5.259987000	0.761412000	0.523966000	H	-4.720926000	-2.031635000	-0.520721000
C	6.602753000	-0.462948000	-0.613228000	H	-5.012613000	1.811188000	0.589755000				

Y6

E = -4661.952370 Hartree





G = -4662.044590 Hartree

F	-11.374313000	6.169131000	-0.000424000	C	-2.884877000	-2.081887000	0.000173000	N	13.243053000	1.667705000	0.000435000
F	-8.826620000	6.989477000	-0.000742000	N	-1.601371000	-1.567484000	0.000173000	C	10.837723000	-0.718613000	0.001514000
C	-9.077041000	5.674277000	-0.000507000	C	-0.706716000	-2.621434000	0.000034000	C	12.163745000	1.252497000	0.000614000
C	-10.407337000	5.243327000	-0.000294000	C	-1.434193000	-3.838506000	-0.000302000	C	10.849524000	0.705185000	0.000839000
C	-10.746707000	3.899100000	0.000024000	C	-0.726761000	-5.081996000	-0.000587000	C	9.711442000	1.482013000	0.000432000
C	-9.707333000	2.965878000	0.000120000	N	-1.257565000	-6.295318000	-0.000923000	C	8.038672000	4.759750000	-0.000693000
C	-8.377668000	3.416145000	-0.000112000	S	-0.000017000	-7.372635000	-0.001108000	C	8.377678000	3.416175000	-0.000343000
C	-8.038647000	4.759716000	-0.000408000	N	1.257542000	-6.295328000	-0.000764000	C	9.707343000	2.965900000	-0.000026000
C	-9.711444000	1.482002000	0.000367000	C	0.726745000	-5.081999000	-0.000495000	C	10.746728000	3.899117000	-0.000067000
C	-10.849543000	0.705209000	0.000630000	C	1.434193000	-3.838519000	-0.000186000	C	10.407365000	5.243350000	-0.000434000
C	-12.163744000	1.252573000	0.000837000	C	0.706718000	-2.621431000	0.000047000	C	9.077068000	5.674304000	-0.000743000
C	-10.837792000	-0.718596000	0.000743000	N	1.601384000	-1.567487000	0.000372000	F	8.826655000	6.989506000	-0.001039000
N	-13.243014000	1.667880000	0.001025000	C	2.884883000	-2.081896000	0.000163000	F	11.374341000	6.169150000	-0.000540000
N	-10.853219000	-1.875335000	0.000830000	C	2.801308000	-3.483613000	-0.000111000	H	-7.318518000	-2.891070000	-0.000231000
C	-7.463202000	2.253659000	-0.000026000	S	4.362010000	-4.265660000	-0.000285000	H	-8.624563000	-1.019352000	0.000410000

O	-6.243984000	2.304211000	-0.000181000	S	4.980645000	-0.054892000	0.000406000	H	-11.793316000	3.635766000	0.000162000
C	-8.314033000	1.046340000	0.000276000	C	4.206530000	-1.604993000	0.000257000	H	-7.006348000	5.085749000	-0.000553000
C	-7.861352000	-0.252737000	0.000361000	C	5.128639000	-2.672622000	0.000057000	H	-1.370538000	-0.588303000	0.001134000
C	-6.578055000	-0.845250000	0.000339000	C	6.451724000	-2.243771000	0.000091000	H	1.370543000	-0.588306000	-0.000216000
C	-6.451718000	-2.243758000	-0.000019000	C	6.578056000	-0.845255000	0.000276000	H	7.318530000	-2.891076000	0.000010000
C	-5.128634000	-2.672595000	-0.000095000	C	7.861352000	-0.252725000	0.000394000	H	8.624563000	-1.019335000	0.000509000
C	-4.206527000	-1.604969000	0.000221000	C	8.314023000	1.046366000	0.000361000	H	7.006377000	5.085795000	-0.000884000
S	-4.980645000	-0.054852000	0.000636000	O	6.243986000	2.304265000	-0.000339000	H	11.793332000	3.635777000	0.000134000
S	-4.362009000	-4.265638000	-0.000552000	C	7.463202000	2.253706000	-0.000096000				
C	-2.801311000	-3.483592000	-0.000220000	N	10.853112000	-1.875348000	0.002053000				