Electronic Supplementary Information

Effect of substituent position on electrochemical, optical and structural properties of donor-acceptor type acridone derivatives

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1. Synthesis

Characterization techniques

^{1}H and ^{13}C NMR spectra were recorded on a Varian Mercury (500 and 125 MHz) spectrometer and referenced with respect to TMS and solvents. IR spectra were monitored on Bio-RAD FTS-165 spectrometer using KBr pellets. UV-Vis-NIR spectra were registered using a Cary 5000 (Varian) spectrometer. Mass spectra were measured by EI method on an AMD 604 mass spectrometer. All synthesized compounds studied were subject to C, H, N elemental combustion analysis.

Reagents

3-bromoaniline, 2-bromobenzoic acid, 1-bromohexane, phenoxazine, Cu powder, Cu_2O, (dibenzylideneacetone)palladium(0), $Pddba_2$, tris-*tert*-butylphosphine, *t*-Bu_3P, sodium *tert*-butoxide, *t*-BuONa, potassium carbonate, cesium carbonate, polyphosphoric acid, sodium acetate, anhydrous toluene, anhydrous THF, N-methylpyrrolidinone, NMP were purchased from Aldrich. Acridone was purchased from Acros Organics.

All glassware was oven dried, assembled hot, and cooled under a dry argon stream before use. All reactions were performed under dry argon.

N-(3-bromophenyl)anthranilic acid, 1

The synthesis was performer according to the procedure described in [1]. A mixture of 2-bromobenzoic acid (1.6 g, 8 mmol), 3-bromoaniline (1.8 g, 10.5 mmol), K_2CO_3 (1.1 g, 8 mmol), Cu powder (49.5 mg, 0.78 mmol), Cu_2O (50.5 mg, 0.35 mmol) and 3 ml of 2-ethoxyethanol was refluxed at 130 °C for 24 h under an argon atmosphere.

^{1}H NMR (500 MHz, DMSO-d_6) δ, 9.31 (s, 1H), 8.07 (dd, J=6.5, 1.5 Hz, 1H), 7.44 (t, J=2.5 Hz, 1H), 7.41 (dt, J=7.5, 1.5 Hz, 1H), 7.27 (d, J=7.5, 1H), 7.24-7.20 (m, 3H), 6.83 (dt, J=6.5, 1.5 Hz, 1H).

IR (cm^{-1}): 3333, 3058, 1671, 1587, 1564, 1518, 1449, 1428, 1331, 1275, 1237, 1154, 891, 766, 744, 509.

Compounds 2a and 2b

Compound **1** (0.93 g, 3.18 mmol) was mixed with 20 g of polyphosphoric acid and heated at 170 °C for 4.5 h under an argon atmosphere. After cooling the mixture was dispersed in 200 ml of distilled water. The resulting orange powder was filtered washed with water and dispersed in 100 ml of water. $NH_{3\ aq.}$ was slowly added to the dispersion until the pH became *ca.* 8. The powder was formed which was filtered, washed with water and dried on air and then in vacuum to give 0.78 g (2.85 mmol) of yellow powder. The crude product was alkylated with 1-bromohexane. Thus the mixture of bromoacridone (0.78 g, 2.85 mmol), cesium carbonate (1.88 g, 5.7 mmol) and 4 ml of anhydrous NMP was heated under an argon atmosphere. When oil bath reached 70 °C, 1-bromohexane was added dropwise. The mixture was heated at 100 °C for 24 h. After cooling to room temperature water was added and the

product was extracted two times with diethyl ether and two times with chloroform. The organic phase was dried over Na_2SO_4. The crude product was purified by chromatography on silica gel eluting with CH_2Cl_2/THF (from 2.5% to 10%). Two isomers were isolated giving 0.45 g of N-hexyl-1-bromoacridone (**2a**) and 0.30 g of N-hexyl-3-bromoacridone (**2b**).

2a: ^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.50 (dd, J=6.5, 1.5 Hz, 1H), 7.69 (dt, J=6.5, 1.5 Hz, 1H), 7.51 (t, J=4.2 Hz, 1H), 7.42-7.38 (m, 3H), 7.27 (dt, J=6.5, 1.5 Hz, 1H), 4.25 (t, J=8.5 Hz, 2H), 1.95-1.89 (m, 2H), 1.59-1.52 (m, 2H), 1.42-1.37 (m, 4H), 0.94 (t, J=7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ, 177.2, 144.2, 141.1, 134.0, 133.0, 128.6, 128.4, 123.7, 123.2, 121.9, 119.7, 114.5, 114.4, 47.6, 31.6, 27.1, 26.7, 22.8, 14.1.

IR (cm^{-1}): 3068, 2923, 2859, 1629, 1605, 1591, 1490, 1458, 1367, 1279, 1260, 1179, 936, 796, 668.

Anal. Calcd. for $C_{19}H_{20}BrNO$: C, 63.70; H, 5.63; N, 3.91; Br, 22.30; O, 4.46.

Found: C, 63.35; H, 5.44; N, 3.56; Br, 22.33.

2b: ^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.54 (dd, J=6.5, 1.5 Hz, 1H), 8.41 (d, J=8.5 Hz, 1H), 7.74 (dt, J=6.5, 1.5 Hz, 1H), 7.63 (d, J=1.5 Hz, 1H), 7.47 (d, J=8.5, 1H), 7.38 (dd, J=9.5, 1.5 Hz, 1H), 7.31 (dt, J=6.5, 1.5 Hz, 1H), 4.27 (t, 8 Hz, 2H), 1.94-1.89 (m, 2H), 1.63-1.54 (m, 2H), 1.47-1.40 (m, 4H), 0.96 (t, J=7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ, 177.6, 142.6, 141.8, 134.3, 129.8, 129.2, 128.1, 124.8, 122.8, 121.9, 121.3, 117.6, 114.8, 46.5, 31.6, 27.1, 26.7, 22.8, 14.1.

IR (cm^{-1}): 3069, 2931, 2854, 1633, 1606, 1591, 1486, 1459, 1429, 1288, 1254, 1177, 936, 796, 668.

Found: C, 63.78; H, 5.62; N, 3.84; Br, 22.42.

N-hexyl-2-bromoacridone, 2c

N-hexylacridone (1.4 g, 5 mmol) and sodium acetate (1.07 g) were dissolved in 20 ml of acetic acid and heated at 130 °C under an argon atmosphere. Bromine (0.31 g, 6 mmol) was dissolved in 15 ml of acetic acid and added drop wise during 2 h to the solution of acridone. Then, the reaction mixture was heated for additional 0.5 h. After cooling to room temperature the mixture was purred into 300 ml of water and extracted with chloroform. The organic phase was washed with basic solution of Na_2SO_3, then with water and dried over Na_2SO_4. The crude product was purified by chromatography on silica gel eluting with $CHCl_3$ to give 0.84 g (2.35 mmol, 47% yield) of N-hexyl-2-bromoacridone. ^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.64 (dd, J=2, 0.5 Hz, 1H), 8.52 (dd, J=7, 1 Hz, 1H), 7.75-7.71 (m, 2H), 7.46 (d, J=9 Hz, 1H), 7.34 (d, J=9 Hz, 1H), 7.28 (dt, J=7, 1 Hz, 1H), 4.28 (t, J=8 Hz, 2H), 1.92-1.86 (m, 2H), 1.58-1.52 (m, 2H), 1.43-1.39 (m, 4H), 0.94 (t, J=7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ, 176.8, 141.7, 140.6, 136.7, 134.3, 130.4, 128.2, 123.8, 122.5, 121.7, 116.8, 114.8, 114.6, 46.5, 31.6, 27.2, 26.7, 22.8, 14.1.

IR (cm^{-1}): 3068, 2923, 2859, 1629, 1605, 1591, 1490, 1458, 1367, 1279, 1260, 1179, 804, 756, 666, 541.

Anal. Calcd. for $C_{19}H_{20}BrNO$: C, 63.70; H, 5.63; N, 3.91; Br, 22.30; O, 4.46.

Found: C, 63.62; H, 5.54; N, 3.82; Br, 22.45.

***o*-A, *m*-A, *p*-A**

$Pddba_2$ (26.5 mg, 0.046 mmol) and *t*-Bu_3P (18.6 mg, 0.092 mmol) were mixed in 1 ml of dry toluene and stirred under an argon atmosphere for 0.5 h. Then bromoacridone (0.33 g, 0.92 mmol), phenoxazine (0.183 g, 1 mmol), *t*-BuONa (0.144 g, 1.5 mmol) and 5 ml of dry toluene were added to the reaction flask. The mixture was stirred and heated at 90 ºC for 20 h. Then the mixture was cooled to room temperature, washed with 50 ml of NH_4Cl solution and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4. After evaporation of the solvent the crude product was purified by chromatography on silica gel eluting with CH_2Cl_2/THF (2.5%). The product was crystallized from CH_2Cl_2/diethyl ether mixture.

***o*-A**: orange powder, 53% yield

^1H NMR (500 MHz, $CDCl_3$) δ, 8.43 (dd, J=8.5, 1.5 Hz, 1H), 7.85 (t, J=8 Hz, 1H), 7.69-7.64 (m, 2H), 7.45 (d, J=8.5 Hz, 1H), 7.21-7.17 (m, 2H), 6.69 (dd, J=8, 1.5 Hz, 2H) 6.55 (dt, J=7.5, 1.5 Hz, 2H), 6.45 (dt, J=7.5, 1.5 Hz, 2H), 5.70 (dd, J=7.5, 1.5 Hz, 2H), 4.36 (t, J=8.5 Hz, 2H), 2.04-2.01 (m, 2H), 1.63-1.56 (m, 2H), 1.51-1.44 (m, 4H), 0.98 (t, J=7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ, 175.7, 145.3, 144.4, 141.3, 138.8, 134.7, 134.6, 133.8, 128.7, 126.1, 123.8, 123.0, 121.6, 120.8, 120.6, 116.1, 115.5, 114.3, 112.4, 47.6, 31.7, 27.2, 26.7, 22.8, 14.2.

IR (cm^{-1}): 3062, 2953, 2856, 1636, 1601, 1488, 1340, 1270, 1165, 738, 676.

Anal. Calcd. for $C_{31}H_{28}N_2O_2$: C, 80.84; H, 6.13; N, 6.08; O, 6.95.

Found: C, 80.22; H, 6.23; N, 5.92.

M/z=460.1

***m*-A**: yellow powder, 92% yield

^1H NMR (500 MHz, $CDCl_3$) δ, 8.61-8.59 (m, 2H), 7.78 (dt, J=7.5, 1.5 Hz, 1H), 7.73-7.67 (m, 2H), 7.55 (d, J=8.5 Hz, 1H), 7.35 (dt, J=7.5, 1.5 Hz, 1H), 6.71 (dd, J=8, 1.5 Hz, 2H), 6.65 (dt, J=7.5, 1.5 Hz, 2H), 6.56 (dt, J=7.5, 1.5 Hz, 2H), 5.95 (dd, J=7.5, 1.5 Hz, 2H), 4.40 (t, J=8 Hz, 2H), 2.04-1.98 (m, 2H), 1.63-1.58 (m, 2H), 1.50-1.40 (m, 4H), 0.96 (t, J=7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ, 177.4, 144.2, 141.9, 141.4, 136.4, 134.5, 134.4, 132.3, 130.9, 128.3, 124.3, 123.4, 122.6, 122.0, 121.6, 118.0, 115.6, 114.8, 113.6, 46.8, 31.6, 27.4, 26.7, 22.8, 14.2.

IR (cm^{-1}): 3056, 2928, 2852, 1637, 1596, 1484, 1333, 1290, 1269, 742.

Found: C, 80.47; H, 6.27; N, 6.14.

M/z=460.1

***p*-A**: green-yellow powder, 87% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.80 (d, J=7.5 Hz, 1H), 8.62 (dd, J=8, 1.5 Hz, 1H), 7.78 (dt, J=8, 1.5 Hz, 1H), 7.53-7.51 (m, 2H), 7.35 (dt, J=7.5, 1.5 Hz, 1 H), 7.27 (dd, J=8.5, 1.5 Hz, 1H), 6.76 (dd, J=8, 1.5 Hz, 2H), 6.71 (dt, J=7.5, 1.5 Hz, 2H), 6.63 (dt, J=7.5, 1.5 Hz, 2H), 6.03 (dd, J=8, 1.5 Hz, 2H), 4.31 (t, J=8 Hz, 2H), 1.93-1.86 (m, 2H), 1.49-1.37 (m, 2H), 1.35-1.32 (m, 4H), 0.88 (t, J=7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ, 177.5, 144.4, 142.2, 143.9, 134.4, 134.0, 131.6, 128.3, 123.5, 123.0, 122.9, 122.2, 122.0, 121.9, 117.0, 115.9, 114.8, 113.6, 46.5, 31.6, 27.4, 26.6, 22.7, 14.1.

IR (cm^{-1}): 3077, 2948, 2850, 1632, 1604, 1484, 1462, 1334, 1269, 1170, 737, 678.

Found: C, 80.82; H, 6.18; N, 6.08.

M/z=460.1

2,7-bis(phenoxazine)-*N*-hexylacridone, di-*m*-A

$Pddba_2$ (60.4 mg, 0.105 mmol) and *t*-Bu_3P (42.5 mg, 0.21 mmol) were mixed in 2 ml of dry toluene and stirred under an argon atmosphere for 0.5 h. Then 2,7-dibromo-N-hexylacridone (0.545 g, 1.25 mmol), phenoxazine (0.503 g, 2.75 mmol), *t*-BuONa (0.34 g, 3.5 mmol) and 5 ml of dry toluene were added to the reaction flask. The mixture was stirred and heated at 90 ºC for 20 h. Then the mixture was cooled to room temperature, washed with 50 ml of NH_4Cl solution and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4. After evaporation of the solvent the crude product was purified by chromatography on silica gel eluting with CH_2Cl_2. The product was crystallized from CH_2Cl_2 to give 0.66 g (1.03 mmol, 82% yield) of yellow crystals.

^{1}H NMR (500 MHz, DMSO-d_6) δ, 8.63 (d, J=2.5 Hz, 2H), 7.78-7.72 (m, 4H), 6.72 (dd, J=7.5, 1.5 Hz, 4H), 6.66 (td, J=7.5, 1.5 Hz, 4H), 6.57 (td, J=7.5, 1.5 Hz, 4H), 5.94 (dd, J=7.5, 1.5 Hz, 4H), 4.45 (t, J=8 Hz, 2H), 2.09-2.06 (m, 2H), 1.67-1.61 (m, 2H), 1.52-1.42 (m, 4H), 0.97 (t, J=7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ, 176.6, 144.2, 141.5, 136.9, 134.4, 132.9, 131.1, 124.4, 123.4, 121.8, 118.2, 115.7, 113.5, 47.2, 31.7, 27.4, 26.8, 22.8, 14.2.

IR (cm^{-1}): 3056, 2928, 2852, 1637, 1596, 1484, 1333, 1290, 1269, 742.

Anal. Calcd. for $C_{43}H_{35}N_3O_3$: C, 80.48; H, 5.49; N, 6.55; O, 7.48.

Found: C, 80.72; H, 6.23; N, 6.12.

2. Electrochemical studies

Cyclic voltammograms (scan rate 50 mV/s) and differential pulse voltammograms (modulation time: 50 ms, modulation amplitude: 10 mV, step potential: 5 mV) of the synthesized compounds (concentration 10^{-3} M in 0.1 M Bu_4NBF_4/dichloromethane electrolyte) were registered using an Autolab potentiostat (EcoChemie). The measurements were performed in an inert atmosphere, using a platinum working electrode of the surface area of 3 mm^2, a platinum wire counter electrode and an Ag/0.1 M Ag^+/acetonitrile reference electrode, whose potential was verified using the ferrocene couple at the end of each set of experiment.

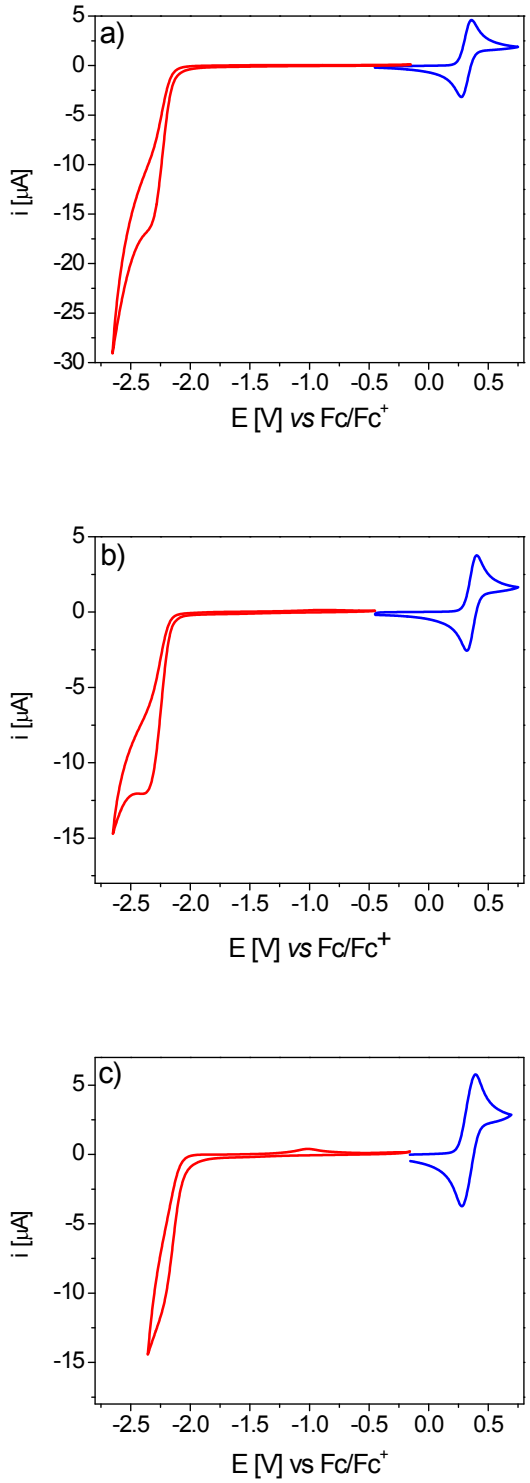


Figure S1. Cyclic voltammograms registered for: a) ***p*-A** b) ***m*-A** and c) **di-*m*-A.** Electrolyte: 0.1 M Bu_4NBF_4/CH_2Cl_2, scan rate: 50 mV/s, E *vs* Fc/Fc^+.

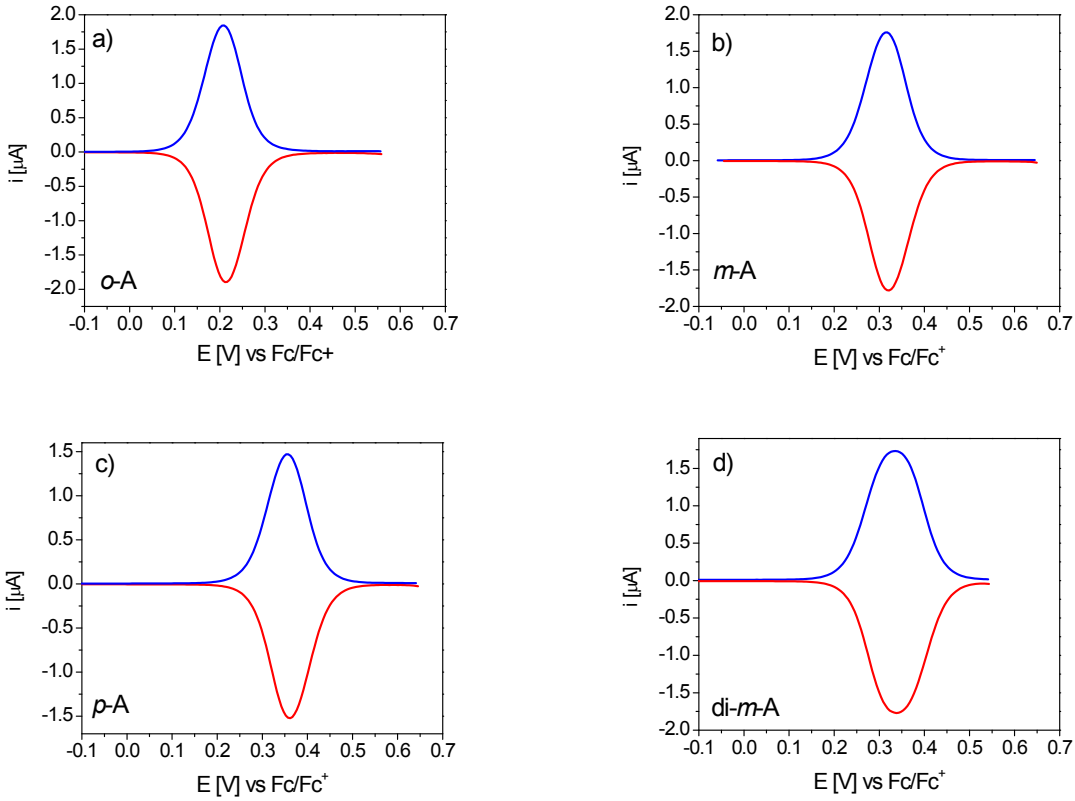


Figure S2. Differential pulse voltammograms registered at positive potentials. a) ***o*-A**, b) **p-A**, c) **m-A**, d) **di-m-A**. Electrolyte: 0.1 M Bu_4NBF_4/CH_2Cl_2, E *vs* Fc/Fc^+. Modulation time: 50 ms, modulation amplitude: 10 mV, step potential: 5 mV.

3. Theoretical background of the thermally activated delayed fluorescence and model details

In order to model the thermally activated delayed fluorescence, it is essential to calculate the intersystem crossing rates between the lowest singlet (S_1) and triplet (T_1) excited states. Transitions between these states are forbidden within non-relativistic quantum theory. They become possible only due to the presence of the spin-orbit coupling (SOC), which is typically small in comparison with other interactions present in organic molecules. Thus, intersystem crossing rates can be calculated by means of the Fermi golden rule:

$$k = \frac{2\pi}{\hbar}\left|\langle S_1 \left| \hat{H}_{SO} \right| T_1 \rangle\right|^2 \rho_{FC} \quad (1)$$

,

where $\langle S_1 \left| \hat{H}_{SO} \right| T_1 \rangle$ is the SOC matrix element between the S_1 and T_1 states, ρ_{FC} the Franck-Condon weighted density of states, and $\hbar$ reduced Planck constant. If we restrict our study to the room-temperature processes, ρ_{FC} can be described by the semi-classical Marcus theory[2,3]

$$\rho_{FC} = \frac{1}{\sqrt{4\pi\lambda k_B T}} \exp\left(\frac{-\left(\Delta E_{ST} + \lambda\right)^2}{4\lambda k_B T} \right), \quad (2)$$

where ΔE_{ST} is the energy difference between states S_1 and T_1 at their equilibrium geometries, k_B Boltzmann constant, T temperature, and λ is the Marcus reorganization energy, which is equal to the decrease of the final electronic state energy associated with the conformational change from the initial state to the final state equilibrium geometry.

Generally, the reorganization energy includes contributions from both the intramolecular deformations, λ_{int}, and from the reorientation of the solvent molecules, λ_{ext}. For intersystem crossing, the solvent reorientation is often neglected.[4] Then, λ of the $S_1 \rightarrow T_1$ process can be calculated as

$$\lambda \approx \lambda_{int} = E^{T1}(S_1) - E^{T1}(T_1), \quad (3)$$

where $E^{T1}(S_1)$ and $E^{T1}(T_1)$ are the energies of the T_1 state in the S_1 and T_1 equilibrium geometries, respectively. Reorganization energy of the reversed process $T_1 \rightarrow S_1$ is obtained by analogy.

The SOC matrix element, $\left|\langle S_1 \left| \hat{H}_{SO} \right| T_1 \rangle\right|$, is determined using the scalar relativistic zero-order regular approximation (ZORA) to the Dirac equation at the initial state equilibrium geometry.[5] In this approximation, three individual triplet substates are considered to be degenerate and the perturbative SOC Hamiltonian is taken as[6,7]

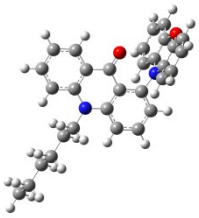
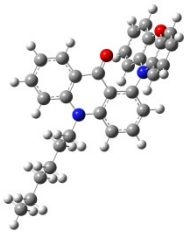
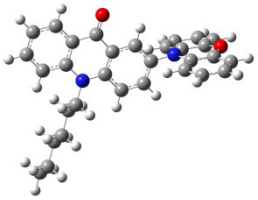
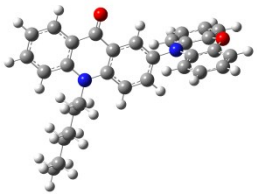
$$\hat{H}_{SO} = \frac{c^2}{\left(2c^2 - V\right)^2} \sigma \cdot (\nabla V \times p) \quad (4)$$

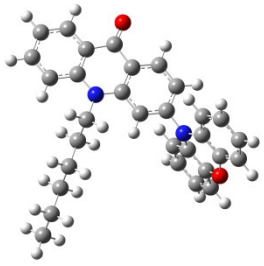
where $\boldsymbol{\sigma}$ is the Pauli matrix vector, V the Kohn-Sham potential, $\boldsymbol{p}$ moment operator, c is the speed of light. Then, the calculated SOC matrix elements between S_1 and individual T_1^m substates $\left|\langle S_1 \left| \hat{H}_{SO} \right| T_1^m \rangle\right|$ are averaged

$$\left|\langle S_1 \left| \hat{H}_{SO} \right| T_1 \rangle\right| = \sqrt{\frac{\sum_{m=0,\pm 1} \left|\langle S_1 \left| \hat{H}_{SO} \right| T_1^m \rangle\right|^2}{3}}. \quad (5)$$

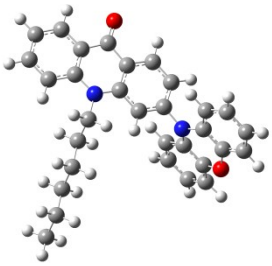
Calculations of the equilibrium geometries in the ground state and S_1 and T_1 states, intramolecular reorganization energies λ_{int}, singlet-triplet state energy differences ΔE_{ST}, and SOC matrix elements were performed using the ADF2019 program.[8] As the DFT functional was chosen PBE0 [9,10] with the GD3BJ dispersion correction and the all-electron Slater-type basis set TZP.[11] This method was shown to properly predict properties of the excited states and SOC for similar organic compounds.[12-15] Solvation effects were included by means of the COnductor-like Screening MOdel (COSMO).[16,17] Excited states were calculated by means of the perturbative SOC TD DFT calculation (pSOC-TD DFT).[18] Similar approaches were recently successfully used by several authors for modeling of the TADF in different organic emitters.[3,5,19,20]

4. Molecular conformations calculated by DFT methods

Toluene	Dichloromethane
	
***o*-A**	***o*-A**
	
***m*-A**	***m*-A**



***p*-A**



***p*-A**

Figure S3. Ground state molecular conformations of the studied acridone derivatives in toluene and dichloromethane calculated by means of the PCM-B3LYP-GD3BJ/6-311++G(d,p) method.

Table S1. Cartesian coordinates of **o-A, m-A,** and **p-A.**

Cartesian coordinates calculated by means of the B3LYP-GD3BJ/6-311++G(d,p) method in vacuum (in Angstroms):

```
   63 atoms
derivative ortho
O     -1.895054     1.452573    -0.197365
N      2.016576     0.392392    -0.798272
C     -0.723318     1.105388    -0.285785
C      0.360816     2.100782    -0.326012
C      0.035605     3.449447    -0.117809
C      1.006739     4.430590    -0.141600
C      2.336231     4.060577    -0.376976
C      2.683416     2.737664    -0.588661
C      1.696745     1.728670    -0.573320
C      1.078085    -0.614200    -0.596574
C      1.477119    -1.968938    -0.645892
C      0.562741    -2.983808    -0.452807
C     -0.778138    -2.693992    -0.193614
C     -1.191914    -1.377367    -0.134824
C     -0.284905    -0.306936    -0.337341
H     -1.006777     3.681018     0.060560
H      0.747623     5.468777     0.024464
H      3.114961     4.814656    -0.387427
H      3.723613     2.495227    -0.744019
H      2.509948    -2.232054    -0.810313
H      0.897570    -4.013778    -0.488489
H     -1.506641    -3.476282    -0.026571
C      3.377502     0.046385    -1.224369
H      3.747122     0.859593    -1.848536
H      3.318037    -0.819324    -1.883641
C      4.338710    -0.219646    -0.064123
H      3.944425    -1.031406     0.555384
H      4.376265     0.663199     0.581709
C      5.744789    -0.570953    -0.551647
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H      5.696528    -1.453490    -1.202405
H      6.129602     0.245311    -1.176273
C      6.727012    -0.838929     0.590399
H      6.342328    -1.655155     1.214624
H      6.775418     0.043635     1.240402
C      8.136938    -1.191158     0.110484
H      8.086518    -2.073218    -0.538929
H      8.519357    -0.374684    -0.513537
C      9.110233    -1.456365     1.260424
H     10.108253    -1.705017     0.890614
H      8.767812    -2.289606     1.881669
H      9.203550    -0.578715     1.907328
N     -2.571811    -1.143334     0.152531
O     -5.140299    -0.105663     0.639039
C     -4.208702    -0.176834     1.653053
C     -4.599073     0.265642     2.904737
C     -3.712886     0.196309     3.981513
C     -2.438263    -0.319013     3.784218
C     -2.046932    -0.761917     2.519909
C     -2.924139    -0.694592     1.437677
C     -3.449029    -0.890031    -0.917895
C     -3.104497    -1.144706    -2.244757
C     -4.010148    -0.896465    -3.277226
C     -5.271008    -0.387091    -2.995011
C     -5.622996    -0.123202    -1.669920
C     -4.723374    -0.372950    -0.648761
H     -5.599526     0.664638     3.018010
H     -4.023945     0.543370     4.959035
H     -1.738187    -0.381412     4.608674
H     -1.052487    -1.161356     2.371151
H     -2.121507    -1.535818    -2.470756
H     -3.718457    -1.103027    -4.299965
H     -5.979066    -0.190576    -3.790482
H     -6.592997     0.282644    -1.410435


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   63 atoms
derivative meta
O      0.091512    -3.811650    -1.110452
N      2.508630    -0.899691     0.496122
C      0.820477    -2.927885    -0.669306
C      2.281271    -3.071133    -0.589472
C      2.873568    -4.239095    -1.092655
C      4.241911    -4.419147    -1.060725
C      5.043282    -3.405773    -0.521277
C      4.485751    -2.244474    -0.015566
C      3.087036    -2.054974    -0.027635
C      1.149226    -0.653369     0.349599
C      0.578512     0.578707     0.745586
C     -0.776845     0.802250     0.608656
C     -1.620041    -0.180951     0.071720
C     -1.078114    -1.382164    -0.331209
C      0.295868    -1.633645    -0.205637
H      2.208759    -4.987056    -1.506350
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H      4.690645    -5.323224    -1.452872
H      6.121084    -3.520300    -0.501767
H      5.145306    -1.481483     0.368753
H      1.192179     1.373306     1.141329
H     -1.200697     1.752659     0.910601
H     -1.699900    -2.159907    -0.756141
C      3.350666     0.079961     1.191608
H      4.143312    -0.461968     1.706514
H      2.754784     0.538060     1.980685
C      3.937490     1.148534     0.267939
H      3.122076     1.670332    -0.243316
H      4.526792     0.662600    -0.516184
C      4.804456     2.152901     1.028102
H      4.207445     2.626996     1.817669
H      5.616569     1.621048     1.540114
C      5.399731     3.236215     0.126512
H      4.587526     3.767559    -0.385117
H      5.997333     2.762545    -0.662339
C      6.267773     4.246001     0.880981
H      5.668926     4.717572     1.669179
H      7.078653     3.713165     1.391742
C      6.857028     5.324727    -0.029541
H      7.471431     6.031775     0.533672
H      6.066441     5.893722    -0.528188
H      7.486518     4.882250    -0.807636
N     -3.020241     0.071458    -0.063962
O     -5.712442     0.856975    -0.204810
C     -5.191543     0.356233     0.972181
C     -6.050600     0.243318     2.051253
C     -5.595794    -0.299727     3.254416
C     -4.275077    -0.717509     3.358977
C     -3.407442    -0.592718     2.273071
C     -3.852898    -0.055023     1.064222
C     -3.476822     0.836211    -1.154317
C     -2.646914     1.210272    -2.212769
C     -3.149048     1.951924    -3.283005
C     -4.483672     2.336619    -3.306141
C     -5.321408     1.971721    -2.250484
C     -4.824155     1.227008    -1.195345
H     -7.073735     0.576810     1.929413
H     -6.273534    -0.393926     4.093612
H     -3.907524    -1.145728     4.283605
H     -2.381572    -0.924502     2.357503
H     -1.608479     0.908390    -2.202011
H     -2.486750     2.222487    -4.096382
H     -4.878880     2.912239    -4.133746
H     -6.368029     2.249524    -2.233820

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   63 atoms
derivative para
O     -2.998980    -4.018788     1.280931
N     -2.448455    -0.384721    -0.563349
C     -2.838320    -2.914369     0.768464
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C	-3.961933	-2.066918	0.342867
C	-5.270932	-2.507796	0.589023
C	-6.363494	-1.742294	0.233923
C	-6.147795	-0.499643	-0.374185
C	-4.867939	-0.040823	-0.631730
C	-3.742977	-0.821965	-0.290428
C	-1.346790	-1.083786	-0.087153
C	-0.040068	-0.572033	-0.233240
C	1.049189	-1.273174	0.249291
C	0.894515	-2.510898	0.886724
C	-0.378827	-3.022864	1.031211
C	-1.504279	-2.329368	0.562019
H	-5.381427	-3.471022	1.071268
H	-7.370176	-2.089964	0.429463
H	-6.991732	0.124787	-0.644390
H	-4.750053	0.933733	-1.080413
H	0.152271	0.384680	-0.692449
H	1.764662	-3.035904	1.259181
H	-0.556045	-3.972647	1.520118
C	-2.238176	0.854066	-1.321103
H	-3.053368	0.956970	-2.035941
H	-1.339140	0.730734	-1.924959
C	-2.128054	2.097418	-0.437028
H	-1.331931	1.946055	0.298967
H	-3.054187	2.216449	0.134658
C	-1.846342	3.360530	-1.251190
H	-0.927041	3.220317	-1.833958
H	-2.650068	3.512867	-1.982874
C	-1.705932	4.613068	-0.383895
H	-0.901320	4.458009	0.345496
H	-2.623979	4.754400	0.200245
C	-1.419189	5.881734	-1.190336
H	-0.502369	5.737278	-1.773992
H	-2.224010	6.035370	-1.919106
C	-1.277027	7.126911	-0.313239
H	-1.072272	8.017487	-0.912955
H	-0.457827	7.011735	0.402999
H	-2.191835	7.312678	0.257956
N	2.344306	-0.684259	0.113201
O	4.914473	0.416745	-0.081174
C	4.100731	0.730598	0.989511
C	4.598746	1.612944	1.932151
C	3.809220	1.996650	3.017982
C	2.527975	1.475917	3.148842
C	2.030798	0.578337	2.202749
C	2.807056	0.199523	1.105865
C	3.263392	-1.208436	-0.813813
C	2.943528	-2.242281	-1.695524
C	3.886320	-2.712357	-2.610863
C	5.160075	-2.159705	-2.654237
C	5.488802	-1.122676	-1.779054
C	4.549384	-0.650149	-0.879649
H	5.603570	1.993898	1.797806
H	4.200727	2.691804	3.750013
H	1.905431	1.757095	3.989538
H	1.035968	0.169037	2.314129
H	1.953309	-2.676172	-1.666661

H	3.613533	-3.513987	-3.286310
H	5.896212	-2.522725	-3.360402
H	6.468251	-0.660710	-1.788173

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Cartesian coordinates calculated by means of the PCM-B3LYP-GD3BJ/6-311++G(d,p) method in toluene (in Angstroms):

63 atoms
derivative ortho

O	1.875206	1.493905	0.004223
N	-2.030645	0.471775	0.728444
C	0.703475	1.150026	0.143601
C	-0.385533	2.136135	0.090462
C	-0.072040	3.462669	-0.246835
C	-1.050229	4.433843	-0.315279
C	-2.377721	4.077519	-0.043285
C	-2.714198	2.779178	0.295280
C	-1.719462	1.780108	0.375808
C	-1.084573	-0.540355	0.631717
C	-1.475256	-1.886788	0.814443
C	-0.553993	-2.909001	0.730984
C	0.788697	-2.636533	0.456570
C	1.193495	-1.330700	0.267339
C	0.278213	-0.249857	0.347862
H	0.967043	3.687718	-0.449559
H	-0.799466	5.453286	-0.580478
H	-3.162188	4.822977	-0.104325
H	-3.752095	2.544939	0.475265
H	-2.507503	-2.138649	0.997334
H	-0.882201	-3.932434	0.867317
H	1.522625	-3.427777	0.379726
C	-3.390141	0.160000	1.193111
H	-3.762217	1.029033	1.734106
H	-3.320991	-0.633888	1.935719
C	-4.351767	-0.227957	0.068991
H	-3.959884	-1.101963	-0.460701
H	-4.392559	0.581000	-0.667024
C	-5.756061	-0.524883	0.596643
H	-5.703711	-1.327917	1.342698
H	-6.141085	0.356783	1.124347
C	-6.739087	-0.923306	-0.505860
H	-6.353962	-1.805227	-1.032859
H	-6.790928	-0.120578	-1.251936
C	-8.147032	-1.220997	0.014920
H	-8.092669	-2.022553	0.761136
H	-8.529946	-0.338757	0.541454
C	-9.122471	-1.619036	-1.094287
H	-10.119019	-1.825860	-0.695419
H	-8.778821	-2.517447	-1.616276
H	-9.219259	-0.821530	-1.837441
N	2.577485	-1.119255	-0.022729
O	5.187225	-0.244868	-0.585864
C	4.263376	-0.397182	-1.601135
C	4.684312	-0.117611	-2.889405

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C      3.808087    -0.282789    -3.964726
C      2.512872    -0.726107    -3.727050
C      2.090497    -1.002119    -2.425527
C      2.958074    -0.840060    -1.344840
C      3.440140    -0.753398     1.023472
C      3.063144    -0.818396     2.365053
C      3.958552    -0.463995     3.375616
C      5.241391    -0.035420     3.057532
C      5.626218     0.039238     1.716804
C      4.737075    -0.317477     0.718304
H      5.700094     0.229219    -3.034927
H      4.142484    -0.064259    -4.971265
H      1.819724    -0.859870    -4.548873
H      1.079725    -1.343426    -2.246141
H      2.063700    -1.145434     2.618589
H      3.641445    -0.524213     4.409822
H      5.941061     0.242989     3.835758
H      6.614942     0.375419     1.429365

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   63 atoms
derivative meta
O     -0.086686    -3.794507     1.156804
N     -2.508415    -0.908059    -0.495989
C     -0.819522    -2.916189     0.698727
C     -2.276248    -3.066954     0.613581
C     -2.869265    -4.232749     1.125221
C     -4.236301    -4.416515     1.089298
C     -5.038671    -3.409236     0.536820
C     -4.482475    -2.252106     0.022185
C     -3.083574    -2.058312     0.037513
C     -1.151749    -0.658390    -0.350620
C     -0.582497     0.569587    -0.763911
C      0.770992     0.798820    -0.626970
C      1.615189    -0.174870    -0.072421
C      1.076809    -1.371032     0.346551
C     -0.296937    -1.629592     0.221025
H     -2.208126    -4.977423     1.549914
H     -4.684503    -5.317935     1.487993
H     -6.115958    -3.526670     0.514458
H     -5.142633    -1.495191    -0.372261
H     -1.196487     1.356114    -1.174062
H      1.191748     1.746044    -0.942700
H      1.702477    -2.137979     0.784444
C     -3.354001     0.067766    -1.198196
H     -4.146802    -0.478177    -1.707312
H     -2.760139     0.519127    -1.991859
C     -3.936947     1.141124    -0.278504
H     -3.120256     1.665112     0.228420
H     -4.527389     0.660733     0.508111
C     -4.802454     2.142279    -1.044458
H     -4.203609     2.612421    -1.834688
H     -5.614060     1.607843    -1.553954
C     -5.397386     3.229240    -0.147239
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H     -4.585053     3.761758     0.362954
H     -5.996954     2.758949     0.642107
C     -6.263200     4.236991    -0.906880
H     -5.662484     4.704990    -1.695781
H     -7.074056     3.702883    -1.416299
C     -6.852419     5.319843    -0.001086
H     -7.465517     6.025539    -0.567722
H     -6.061233     5.889370     0.496242
H     -7.483012     4.880279     0.777898
N      3.015352     0.082156     0.063535
O      5.712384     0.848469     0.209862
C      5.195238     0.331706    -0.963291
C      6.060873     0.193683    -2.034327
C      5.609729    -0.367937    -3.230962
C      4.286137    -0.777966    -3.336279
C      3.412234    -0.627204    -2.258288
C      3.853886    -0.071181    -1.055906
C      3.468567     0.865463     1.140996
C      2.633013     1.267314     2.185244
C      3.132218     2.027869     3.243968
C      4.469607     2.404391     3.269886
C      5.313242     2.011622     2.228311
C      4.818342     1.248089     1.185404
H      7.086063     0.521476    -1.913317
H      6.292199    -0.481944    -4.063848
H      3.920972    -1.219700    -4.255499
H      2.384254    -0.951947    -2.344209
H      1.592352     0.973310     2.172607
H      2.465195     2.320058     4.045941
H      4.862439     2.994719     4.088208
H      6.361837     2.282558     2.215686

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   63 atoms
derivative para
O     -2.849062    -4.103809     1.242845
N     -2.435147    -0.416826    -0.536673
C     -2.729145    -2.981491     0.747676
C     -3.882495    -2.166925     0.348810
C     -5.176289    -2.654882     0.595305
C     -6.295373    -1.920253     0.261031
C     -6.124943    -0.659943    -0.327735
C     -4.863553    -0.154770    -0.585650
C     -3.710013    -0.903363    -0.263989
C     -1.308598    -1.087810    -0.084759
C     -0.020089    -0.528109    -0.229952
C      1.094755    -1.207058     0.220327
C      0.989485    -2.465455     0.828438
C     -0.264051    -3.019769     0.979142
C     -1.418524    -2.352110     0.539678
H     -5.255975    -3.629060     1.060738
H     -7.288655    -2.304175     0.457034
H     -6.990953    -0.059734    -0.581939
H     -4.781461     0.829816    -1.019510
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H	0.134387	0.445430	-0.667430
H	1.881044	-2.972776	1.173727
H	-0.399572	-3.986222	1.447517
C	-2.275962	0.842392	-1.277872
H	-3.094391	0.919394	-1.991802
H	-1.372832	0.765085	-1.882185
C	-2.220656	2.075796	-0.376008
H	-1.403421	1.961309	0.343365
H	-3.141630	2.134809	0.212794
C	-2.028517	3.362748	-1.178879
H	-1.112855	3.284187	-1.778246
H	-2.853307	3.473964	-1.894049
C	-1.949896	4.610981	-0.297901
H	-1.124500	4.497711	0.415860
H	-2.864906	4.688701	0.302644
C	-1.755934	5.903929	-1.093317
H	-0.841638	5.823323	-1.693028
H	-2.581079	6.015034	-1.806888
C	-1.677030	7.145803	-0.203489
H	-1.537691	8.054107	-0.795609
H	-0.840638	7.073344	0.498509
H	-2.592436	7.267289	0.383957
N	2.373781	-0.581399	0.074559
O	4.947278	0.507918	-0.108194
C	4.191547	0.694810	1.034338
C	4.747217	1.449963	2.052343
C	4.010975	1.712331	3.210010
C	2.724798	1.200534	3.332837
C	2.170798	0.429168	2.309714
C	2.895013	0.169435	1.144587
C	3.251877	-1.023953	-0.931366
C	2.887696	-1.970326	-1.891072
C	3.789566	-2.358662	-2.883247
C	5.066972	-1.813023	-2.925132
C	5.441598	-0.866739	-1.968452
C	4.541803	-0.474458	-0.992897
H	5.752366	1.831527	1.921408
H	4.446356	2.309167	4.001607
H	2.141882	1.392009	4.225527
H	1.171330	0.028998	2.413105
H	1.895539	-2.400018	-1.862347
H	3.482751	-3.092046	-3.618991
H	5.771357	-2.112858	-3.690853
H	6.426584	-0.416368	-1.972435

****

Cartesian coordinates calculated by means of the PCM-B3LYP-GD3BJ/6-311++G(d,p) method in dichloromethane (in Angstroms):

63 atoms
derivative ortho

O	-1.865097	1.525283	0.037713
N	2.038595	0.521877	-0.734693
C	-0.690198	1.182031	-0.114146
C	0.400955	2.158020	-0.010968

C	0.096240	3.468841	0.394924
C	1.079806	4.428685	0.514333
C	2.406391	4.078373	0.224071
C	2.734899	2.798310	-0.181938
C	1.734125	1.809609	-0.314528
C	1.087699	-0.487270	-0.690959
C	1.470024	-1.824278	-0.949979
C	0.545548	-2.844931	-0.913324
C	-0.794232	-2.582169	-0.610537
C	-1.191421	-1.287554	-0.350665
C	-0.273179	-0.205239	-0.385252
H	-0.940257	3.692820	0.610805
H	0.835655	5.434350	0.832914
H	3.195390	4.814521	0.324462
H	3.771212	2.568264	-0.374572
H	2.498808	-2.070929	-1.156279
H	0.867777	-3.860717	-1.107288
H	-1.528466	-3.375679	-0.566103
C	3.402417	0.224210	-1.203762
H	3.785285	1.117394	-1.694407
H	3.334360	-0.528022	-1.987871
C	4.347147	-0.229167	-0.090312
H	3.939700	-1.122799	0.392792
H	4.392390	0.544059	0.682987
C	5.752056	-0.519142	-0.619984
H	5.695358	-1.287169	-1.401392
H	6.151972	0.381209	-1.102616
C	6.719069	-0.979677	0.472360
H	6.318941	-1.881088	0.953227
H	6.772677	-0.212715	1.255106
C	8.128748	-1.268831	-0.048582
H	8.072653	-2.033461	-0.832460
H	8.526840	-0.366799	-0.528237
C	9.088188	-1.730752	1.049946
H	10.086804	-1.929434	0.651647
H	8.728719	-2.649289	1.524303
H	9.185188	-0.970617	1.831429
N	-2.571672	-1.089328	-0.028694
O	-5.201213	-0.347202	0.615727
C	-4.253842	-0.509882	1.609939
C	-4.663650	-0.309791	2.916646
C	-3.763695	-0.496376	3.969498
C	-2.457153	-0.879117	3.689421
C	-2.046139	-1.073292	2.369260
C	-2.937431	-0.890562	1.310504
C	-3.457313	-0.691155	-1.040795
C	-3.095423	-0.660138	-2.388434
C	-4.015379	-0.274832	-3.365532
C	-5.307856	0.091243	-3.008417
C	-5.678038	0.070783	-1.660937
C	-4.764758	-0.318288	-0.696586
H	-5.689293	-0.010995	3.096421
H	-4.089083	-0.342121	4.990729
H	-1.745792	-1.028870	4.492677
H	-1.026790	-1.367740	2.158626
H	-2.089231	-0.937508	-2.672500
H	-3.709499	-0.261674	-4.404757

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H     -6.026265     0.392682    -3.760492
H     -6.674683     0.353865    -1.344546

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   63 atoms
derivative meta
O      0.076044    -3.782701    -1.174401
N      2.507145    -0.912677     0.499722
C      0.814180    -2.906695    -0.708034
C      2.267203    -3.063901    -0.622954
C      2.859435    -4.228984    -1.141208
C      4.225293    -4.416214    -1.104683
C      5.030108    -3.413588    -0.544187
C      4.476667    -2.258963    -0.023027
C      3.077647    -2.060581    -0.039137
C      1.152926    -0.659217     0.356150
C      0.586942     0.568038     0.778181
C     -0.764800     0.802938     0.641759
C     -1.611780    -0.165007     0.079327
C     -1.078252    -1.359572    -0.347143
C      0.295251    -1.624845    -0.223092
H      2.200283    -4.971376    -1.572587
H      4.672157    -5.315941    -1.508587
H      6.106891    -3.533925    -0.521211
H      5.138401    -1.507103     0.377682
H      1.202717     1.349268     1.195075
H     -1.181263     1.749711     0.964141
H     -1.708739    -2.119080    -0.790548
C      3.357981     0.060790     1.203896
H      4.149929    -0.488628     1.709488
H      2.766817     0.510728     1.999658
C      3.939532     1.133297     0.283086
H      3.122321     1.663141    -0.216794
H      4.524738     0.652801    -0.507322
C      4.813462     2.127673     1.048180
H      4.220600     2.595873     1.843700
H      5.626648     1.587285     1.548269
C      5.405154     3.216207     0.150854
H      4.590604     3.754228    -0.350012
H      5.997441     2.747059    -0.644680
C      6.280402     4.217246     0.908523
H      5.687160     4.683570     1.704034
H      7.093414     3.677651     1.408602
C      6.866378     5.302477     0.003268
H      7.486522     6.003437     0.568447
H      6.072841     5.876806    -0.484960
H      7.489145     4.863861    -0.782664
N     -3.011836     0.095203    -0.057887
O     -5.717164     0.817355    -0.228247
C     -5.201503     0.315078     0.953223
C     -6.073203     0.168759     2.018372
C     -5.622246    -0.382551     3.220489
C     -4.293124    -0.772935     3.336247
C     -3.413400    -0.612836     2.263896
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C     -3.854767    -0.067458     1.056161
C     -3.463679     0.881226    -1.133217
C     -2.622559     1.305794    -2.164341
C     -3.122022     2.068421    -3.221911
C     -4.465045     2.425050    -3.259698
C     -5.314355     2.009891    -2.230787
C     -4.818640     1.243913    -1.189918
H     -7.102535     0.481006     1.890631
H     -6.308745    -0.503007     4.049113
H     -3.927614    -1.204961     4.259922
H     -2.380972    -0.920233     2.359656
H     -1.577136     1.029840    -2.142226
H     -2.450299     2.379201    -4.012879
H     -4.857722     3.017414    -4.076591
H     -6.366909     2.265763    -2.228663

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   63 atoms
derivative para
O     -2.840711    -4.097119     1.275716
N     -2.434234    -0.423888    -0.539208
C     -2.722655    -2.975800     0.767029
C     -3.876363    -2.171690     0.358649
C     -5.171247    -2.660925     0.605320
C     -6.290792    -1.932715     0.261401
C     -6.121921    -0.676010    -0.338341
C     -4.861952    -0.169775    -0.597217
C     -3.706325    -0.912237    -0.265640
C     -1.307993    -1.088320    -0.082091
C     -0.020066    -0.526902    -0.233269
C      1.094908    -1.198636     0.224153
C      0.993484    -2.451854     0.845451
C     -0.257685    -3.007814     1.001126
C     -1.415306    -2.347636     0.554783
H     -5.253552    -3.630636     1.079235
H     -7.283699    -2.317349     0.457720
H     -6.988764    -0.080581    -0.600121
H     -4.781985     0.810811    -1.039878
H      0.131039     0.442064    -0.681524
H      1.885998    -2.953681     1.196109
H     -0.386450    -3.969874     1.479824
C     -2.277739     0.834780    -1.286194
H     -3.095216     0.906289    -2.000967
H     -1.374286     0.757255    -1.889065
C     -2.227485     2.068961    -0.385729
H     -1.413609     1.956108     0.337722
H     -3.152120     2.129812     0.197010
C     -2.030948     3.354011    -1.190458
H     -1.110917     3.274247    -1.782597
H     -2.851641     3.462694    -1.910255
C     -1.959362     4.603155    -0.310253
H     -1.138830     4.491203     0.409452
H     -2.879184     4.681302     0.282799
C     -1.760065     5.895184    -1.105795
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H	-0.841074	5.814261	-1.698306
H	-2.580186	6.004846	-1.825279
C	-1.688595	7.138239	-0.216776
H	-1.545428	8.046173	-0.808831
H	-0.857332	7.066597	0.491585
H	-2.608723	7.259179	0.363508
N	2.374382	-0.573890	0.073259
O	4.964200	0.485884	-0.099041
C	4.195005	0.701886	1.030317
C	4.746944	1.469843	2.041054
C	4.000070	1.760768	3.185494
C	2.706676	1.264784	3.301615
C	2.156501	0.481119	2.285486
C	2.891613	0.191889	1.133813
C	3.253588	-1.029218	-0.924927
C	2.883958	-1.975498	-1.883189
C	3.787022	-2.379702	-2.868252
C	5.071533	-1.849610	-2.905347
C	5.451516	-0.902720	-1.950763
C	4.550537	-0.495535	-0.982087
H	5.757579	1.839177	1.916564
H	4.432620	2.367410	3.971143
H	2.114561	1.479341	4.182913
H	1.150605	0.096091	2.383406
H	1.886186	-2.392262	-1.859800
H	3.475213	-3.112360	-3.602611
H	5.776927	-2.161187	-3.665413
H	6.442197	-0.464733	-1.952277

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Cartesian coordinates calculated by means of the COSMO-(TD)PBE0-GD3BJ/TZP method in toluene (in Angstroms):

63 atoms
derivative ortho, ground state

O	1.863722	1.488745	-0.120787
N	-2.029721	0.544976	0.665443
C	0.693489	1.153418	0.026537
C	-0.397590	2.104834	-0.186142
C	-0.090490	3.364557	-0.709050
C	-1.070685	4.302934	-0.927757
C	-2.392939	3.979396	-0.618283
C	-2.722681	2.747121	-0.098506
C	-1.725391	1.782864	0.133917
C	-1.082604	-0.457060	0.719824
C	-1.466692	-1.759742	1.092504
C	-0.545337	-2.774973	1.156123
C	0.791023	-2.541329	0.842684
C	1.190085	-1.278354	0.473362
C	0.274118	-0.203884	0.406043
H	0.950199	3.563746	-0.932809
H	-0.825296	5.274523	-1.338427
H	-3.182524	4.700899	-0.794396
H	-3.761184	2.531063	0.104326
H	-2.499491	-1.985945	1.308685

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H        -0.869509   -3.769640    1.437444
H         1.526523   -3.334707    0.873346
C        -3.382030    0.292546    1.148238
H        -3.767325    1.226404    1.555915
H        -3.317765   -0.386279    1.997922
C        -4.321803   -0.255319    0.087143
H        -3.915612   -1.189322   -0.313127
H        -4.362509    0.442956   -0.754360
C        -5.718664   -0.489742    0.635378
H        -5.666659   -1.185044    1.481917
H        -6.114282    0.450142    1.038887
C        -6.682176   -1.035152   -0.404798
H        -6.286875   -1.975571   -0.807001
H        -6.732193   -0.340177   -1.251463
C        -8.083141   -1.269510    0.136028
H        -8.030280   -1.963653    0.982011
H        -8.474830   -0.328800    0.538466
C        -9.038533   -1.813653   -0.912173
H       -10.037101   -1.973768   -0.500535
H        -8.683918   -2.769215   -1.307837
H        -9.131885   -1.122634   -1.754258
N         2.563959   -1.109874    0.146725
O         5.165142   -0.339129   -0.543155
C         4.225780   -0.585941   -1.515554
C         4.627677   -0.457930   -2.828056
C         3.738983   -0.734324   -3.862302
C         2.449026   -1.133338   -3.559791
C         2.044964   -1.254086   -2.235260
C         2.924722   -0.980190   -1.195086
C         3.430856   -0.613939    1.122260
C         3.065668   -0.498237    2.457648
C         3.967132   -0.023535    3.403502
C         5.244660    0.349147    3.024471
C         5.617181    0.245554    1.688020
C         4.722893   -0.232557    0.754086
H         5.645505   -0.143282   -3.025765
H         4.061522   -0.635979   -4.891510
H         1.743324   -1.354453   -4.351624
H         1.034194   -1.564904   -2.004010
H         2.065377   -0.782962    2.757555
H         3.657651    0.054245    4.438880
H         5.952687    0.721732    3.754458
H         6.606738    0.532623    1.352748


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  63 atoms
derivative ortho, singlet excited state S1
O         1.780626    1.587651   -0.286075
N        -2.071222    0.558550    0.744471
C         0.594476    1.242432   -0.004300
C        -0.500750    2.190403   -0.107045
C        -0.245593    3.485643   -0.569169
C        -1.258995    4.418643   -0.701551
C        -2.558786    4.056845   -0.377262
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C	-2.838641	2.774593	0.086324
C	-1.818572	1.832920	0.244055
C	-1.102582	-0.434279	0.734114
C	-1.416065	-1.748115	1.069842
C	-0.433660	-2.751522	1.116298
C	0.873071	-2.442985	0.802879
C	1.186954	-1.142425	0.441347
C	0.238577	-0.087023	0.383186
H	0.781985	3.720406	-0.817454
H	-1.040248	5.417908	-1.061111
H	-3.370971	4.766331	-0.487262
H	-3.865559	2.522295	0.308790
H	-2.435593	-2.025869	1.292203
H	-0.708673	-3.762292	1.389311
H	1.654426	-3.194141	0.823461
C	-3.405783	0.245872	1.218268
H	-3.818351	1.145055	1.677776
H	-3.320591	-0.481379	2.026811
C	-4.332561	-0.265478	0.127345
H	-3.910097	-1.177443	-0.306327
H	-4.366075	0.469873	-0.682755
C	-5.736571	-0.532602	0.638053
H	-5.699978	-1.275248	1.444362
H	-6.140536	0.383084	1.087086
C	-6.680805	-1.014750	-0.449925
H	-6.282150	-1.934572	-0.894480
H	-6.706701	-0.274070	-1.258246
C	-8.095772	-1.266841	0.043387
H	-8.069541	-2.009376	0.848609
H	-8.488881	-0.347043	0.490447
C	-9.030256	-1.738905	-1.057419
H	-10.040590	-1.912058	-0.680976
H	-8.674296	-2.673246	-1.499979
H	-9.095501	-0.998771	-1.859621
N	2.553757	-0.870507	0.091481
O	5.173291	-0.256975	-0.608292
C	4.286948	-0.658628	-1.548871
C	4.736490	-0.746851	-2.854814
C	3.858824	-1.146541	-3.841730
C	2.531953	-1.456615	-3.525160
C	2.081771	-1.370429	-2.229568
C	2.957765	-0.972223	-1.212899
C	3.445138	-0.471893	1.051583
C	3.077006	-0.344546	2.395906
C	4.005778	0.063268	3.323296
C	5.317905	0.357233	2.937715
C	5.698878	0.243781	1.616431
C	4.766396	-0.166069	0.679415
H	5.766899	-0.495181	-3.069409
H	4.202034	-1.216238	-4.866048
H	1.849990	-1.763207	-4.307684
H	1.057690	-1.596971	-1.970234
H	2.057004	-0.565115	2.675769
H	3.715486	0.162197	4.361231
H	6.040555	0.679488	3.676547
H	6.704356	0.470246	1.286543

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  63 atoms
derivative ortho, triplet excited state T1

O	1.777438	1.593991	-0.269417
N	-2.077430	0.562760	0.741568
C	0.587332	1.252258	0.003397
C	-0.507739	2.197176	-0.110263
C	-0.254801	3.491507	-0.576325
C	-1.271031	4.420045	-0.716869
C	-2.571062	4.054671	-0.397384
C	-2.848481	2.773364	0.070079
C	-1.826157	1.835915	0.236551
C	-1.105945	-0.426996	0.739642
C	-1.412323	-1.740960	1.081347
C	-0.422752	-2.736845	1.134834
C	0.882877	-2.423209	0.822026
C	1.190089	-1.122249	0.454145
C	0.233741	-0.075933	0.391597
H	0.772814	3.730103	-0.820841
H	-1.054259	5.418689	-1.079259
H	-3.385250	4.760739	-0.514102
H	-3.875501	2.518085	0.288721
H	-2.430475	-2.024183	1.303388
H	-0.691793	-3.747959	1.412667
H	1.667551	-3.170714	0.846663
C	-3.412248	0.248603	1.213658
H	-3.828431	1.148742	1.668046
H	-3.326686	-0.474787	2.025625
C	-4.335509	-0.270557	0.123354
H	-3.912786	-1.186500	-0.301581
H	-4.365575	0.458401	-0.692602
C	-5.741571	-0.531641	0.631791
H	-5.708509	-1.266531	1.445304
H	-6.145953	0.388733	1.070749
C	-6.682968	-1.022986	-0.454565
H	-6.285210	-1.948551	-0.887844
H	-6.703957	-0.290905	-1.270811
C	-8.100453	-1.265869	0.036249
H	-8.079233	-1.999418	0.849799
H	-8.492690	-0.340090	0.471577
C	-9.032228	-1.747583	-1.062684
H	-10.044408	-1.913703	-0.688022
H	-8.677358	-2.687796	-1.493537
H	-9.092507	-1.016254	-1.873301
N	2.552574	-0.843415	0.097193
O	5.179443	-0.263482	-0.610449
C	4.284549	-0.654587	-1.548473
C	4.728629	-0.748001	-2.855751
C	3.843903	-1.138856	-3.840465
C	2.515306	-1.434854	-3.519883
C	2.070286	-1.342383	-2.222525
C	2.953358	-0.952822	-1.209156
C	3.456757	-0.469556	1.057356
C	3.097312	-0.349171	2.404283

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C         4.036450    0.036504    3.331302
C         5.350118    0.315176    2.941484
C         5.722237    0.208374    1.616767
C         4.779665   -0.179547    0.680666
H         5.761298   -0.508419   -3.073505
H         4.183703   -1.212824   -4.865636
H         1.827609   -1.735389   -4.299770
H         1.044596   -1.557986   -1.959934
H         2.075520   -0.557469    2.687349
H         3.752550    0.129698    4.371554
H         6.081422    0.620295    3.679115
H         6.729235    0.423452    1.283772


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  63 atoms
derivative meta, ground state
O        -0.088293   -3.833180    1.132686
N        -2.502794   -0.943642   -0.482991
C        -0.820591   -2.951779    0.686638
C        -2.270212   -3.100076    0.603225
C        -2.859982   -4.264480    1.104766
C        -4.221569   -4.446709    1.068852
C        -5.019921   -3.437900    0.526382
C        -4.466126   -2.282045    0.021880
C        -3.072852   -2.090739    0.037721
C        -1.155136   -0.697499   -0.338347
C        -0.590930    0.529560   -0.741283
C         0.756271    0.758318   -0.604584
C         1.600607   -0.215545   -0.061203
C         1.065885   -1.411321    0.346557
C        -0.302177   -1.667349    0.221663
H        -2.196877   -5.011509    1.523628
H        -4.670323   -5.350574    1.461803
H        -6.097494   -3.553562    0.503708
H        -5.126380   -1.520418   -0.365944
H        -1.207636    1.319066   -1.143947
H         1.173545    1.709742   -0.913499
H         1.691515   -2.183218    0.777254
C        -3.341654    0.030338   -1.171276
H        -4.136289   -0.511866   -1.682040
H        -2.748910    0.481990   -1.966120
C        -3.914647    1.094635   -0.252467
H        -3.094869    1.612190    0.255798
H        -4.504691    0.613617    0.533889
C        -4.770427    2.096033   -1.007482
H        -4.174258    2.557968   -1.803679
H        -5.591806    1.570242   -1.508918
C        -5.340423    3.183707   -0.112803
H        -4.517649    3.708763    0.386952
H        -5.935723    2.722579    0.684223
C        -6.197281    4.190952   -0.861697
H        -5.601356    4.645594   -1.660753
H        -7.020371    3.664600   -1.357499
C        -6.755793    5.278511    0.040052
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H        -7.366767    5.989284   -0.520028
H        -5.950948    5.838984    0.523245
H        -7.380262    4.851559    0.829431
N         2.993836    0.038972    0.077878
O         5.665568    0.827510    0.226011
C         5.140681    0.377348   -0.962966
C         5.987683    0.310535   -2.048725
C         5.528830   -0.195354   -3.260597
C         4.215352   -0.618238   -3.367238
C         3.359246   -0.535558   -2.274995
C         3.809519   -0.038142   -1.057311
C         3.427924    0.843037    1.138697
C         2.586450    1.249136    2.168228
C         3.070468    2.025962    3.214629
C         4.397905    2.416717    3.240736
C         5.246804    2.022034    2.211807
C         4.767690    1.238893    1.183244
H         7.010494    0.646249   -1.925902
H         6.200466   -0.256713   -4.107963
H         3.842759   -1.019008   -4.302276
H         2.334404   -0.872084   -2.362335
H         1.548605    0.942815    2.155037
H         2.396692    2.320808    4.010129
H         4.780617    3.022412    4.052870
H         6.292806    2.304407    2.200395

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  63 atoms
derivative meta, singlet excited state S1
O         0.033432   -3.569731    1.079084
N        -2.445165   -0.722994   -0.564191
C        -0.730020   -2.681090    0.605843
C        -2.169036   -2.863283    0.545987
C        -2.741572   -4.030960    1.061849
C        -4.110100   -4.233704    1.044954
C        -4.933610   -3.252187    0.511257
C        -4.388812   -2.081705   -0.010088
C        -3.007114   -1.875364   -0.014986
C        -1.098429   -0.433459   -0.417433
C        -0.568562    0.794255   -0.812381
C         0.808806    1.060677   -0.706448
C         1.623512    0.075918   -0.183017
C         1.141794   -1.141021    0.242383
C        -0.240493   -1.422973    0.141621
H        -2.061364   -4.765831    1.474828
H        -4.534294   -5.145618    1.450322
H        -6.009674   -3.383234    0.500000
H        -5.062968   -1.331546   -0.398136
H        -1.206709    1.576304   -1.195862
H         1.217781    2.012651   -1.018419
H         1.788554   -1.902862    0.656565
C        -3.310034    0.220868   -1.243872
H        -4.084132   -0.345755   -1.763828
H        -2.731744    0.711946   -2.027893
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C        -3.940228    1.245212   -0.314019
H        -3.151708    1.845670    0.150964
H        -4.442864    0.717482    0.502636
C        -4.931847    2.143445   -1.030019
H        -4.423917    2.687448   -1.835686
H        -5.694646    1.523354   -1.517012
C        -5.613877    3.133441   -0.101557
H        -4.856237    3.767346    0.374707
H        -6.103699    2.583978    0.711398
C        -6.638932    4.011040   -0.799998
H        -6.148533    4.565703   -1.607685
H        -7.388258    3.372475   -1.280836
C        -7.327151    4.982163    0.143902
H        -8.060823    5.599676   -0.378386
H        -6.602293    5.651528    0.615206
H        -7.849059    4.447675    0.942385
N         3.040150    0.332448   -0.064228
O         5.763101    0.829503    0.162930
C         5.266646    0.232331   -0.944977
C         6.162039   -0.112099   -1.943121
C         5.688170   -0.723332   -3.084837
C         4.321476   -0.990340   -3.232585
C         3.427597   -0.648892   -2.246946
C         3.888530   -0.027778   -1.078496
C         3.536699    0.918140    1.071194
C         2.709720    1.278384    2.143409
C         3.259134    1.864547    3.257708
C         4.636078    2.107444    3.334956
C         5.467481    1.758257    2.291696
C         4.920287    1.164550    1.167010
H         7.212265    0.105450   -1.799886
H         6.380673   -0.999371   -3.869578
H         3.963338   -1.473899   -4.131921
H         2.371104   -0.853700   -2.343026
H         1.650227    1.079592    2.070458
H         2.618618    2.138594    4.085698
H         5.054573    2.569798    4.219629
H         6.535324    1.929996    2.323915


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  63 atoms
derivative meta, triplet excited state T1
O         0.045011   -3.697666    0.575884
N        -2.449279   -0.685250   -0.707497
C        -0.725616   -2.763422    0.213113
C        -2.161598   -2.948420    0.124920
C        -2.728257   -4.173398    0.490108
C        -4.096272   -4.378809    0.439191
C        -4.925888   -3.345789    0.027507
C        -4.386133   -2.116438   -0.342187
C        -3.006593   -1.905888   -0.312988
C        -1.110849   -0.408729   -0.527518
C        -0.589445    0.866472   -0.761067
C         0.778236    1.128812   -0.610388
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C	1.616528	0.091571	-0.227650
C	1.133747	-1.181851	0.026405
C	-0.242079	-1.456656	-0.098181
H	-2.046451	-4.950160	0.813413
H	-4.515697	-5.336969	0.725009
H	-6.000513	-3.481877	-0.005584
H	-5.062415	-1.327301	-0.637310
H	-1.231119	1.681483	-1.059620
H	1.174915	2.116270	-0.804089
H	1.781577	-1.986239	0.346932
C	-3.321643	0.333151	-1.264021
H	-4.093610	-0.168493	-1.847907
H	-2.746306	0.919871	-1.980240
C	-3.949969	1.230512	-0.209916
H	-3.159183	1.761619	0.329151
H	-4.459211	0.605937	0.530295
C	-4.931641	2.220825	-0.809729
H	-4.416495	2.852642	-1.543285
H	-5.701964	1.674413	-1.367604
C	-5.599467	3.099050	0.234334
H	-4.832283	3.656990	0.784509
H	-6.099427	2.461929	0.973651
C	-6.608327	4.073267	-0.350643
H	-6.107359	4.712654	-1.085865
H	-7.369069	3.511722	-0.904086
C	-7.278293	4.935517	0.705377
H	-7.999082	5.626216	0.262869
H	-6.540919	5.528358	1.253391
H	-7.811472	4.318536	1.433749
N	3.010345	0.342198	-0.074340
O	5.741468	0.852930	0.215087
C	5.299733	-0.045538	-0.700871
C	6.257688	-0.673772	-1.477514
C	5.860216	-1.561720	-2.457129
C	4.502682	-1.802957	-2.673593
C	3.546713	-1.179078	-1.903310
C	3.930314	-0.306206	-0.878168
C	3.457834	1.225567	0.891586
C	2.591459	1.839521	1.803627
C	3.084351	2.717518	2.743121
C	4.450773	2.995800	2.809151
C	5.326414	2.367787	1.946413
C	4.834357	1.481439	1.003563
H	7.300335	-0.445082	-1.298508
H	6.605362	-2.057174	-3.066376
H	4.192339	-2.479832	-3.458923
H	2.494861	-1.357078	-2.071715
H	1.537386	1.608045	1.757640
H	2.403165	3.183695	3.443193
H	4.830802	3.688116	3.549546
H	6.394522	2.537918	1.988237

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63 atoms

derivative para, ground state

O	-2.764132	-4.156098	1.077950
N	-2.442194	-0.403915	-0.541088
C	-2.671330	-3.014030	0.629425
C	-3.837768	-2.205762	0.287787
C	-5.113266	-2.724275	0.532606
C	-6.245016	-1.998308	0.249803
C	-6.104077	-0.715302	-0.282939
C	-4.860995	-0.180152	-0.537828
C	-3.695325	-0.920359	-0.269966
C	-1.305082	-1.074108	-0.146747
C	-0.033036	-0.493497	-0.298723
C	1.096476	-1.171001	0.098271
C	1.022526	-2.449463	0.656928
C	-0.214772	-3.024547	0.809492
C	-1.381869	-2.358831	0.423654
H	-5.166828	-3.719525	0.956644
H	-7.228834	-2.406903	0.444438
H	-6.983326	-0.118294	-0.496310
H	-4.801392	0.825152	-0.927885
H	0.098356	0.499389	-0.701653
H	1.927759	-2.958849	0.962338
H	-0.329793	-4.011205	1.240791
C	-2.316382	0.883926	-1.212662
H	-3.151615	0.988129	-1.903266
H	-1.428368	0.849159	-1.843065
C	-2.253356	2.060407	-0.254106
H	-1.427425	1.909287	0.448320
H	-3.166113	2.083474	0.349421
C	-2.075788	3.380982	-0.982305
H	-1.162763	3.342692	-1.588582
H	-2.903387	3.524447	-1.687279
C	-2.003680	4.571023	-0.040692
H	-1.177887	4.423580	0.665466
H	-2.917610	4.610493	0.563959
C	-1.818567	5.897511	-0.758974
H	-0.904404	5.855197	-1.361242
H	-2.642900	6.041660	-1.466120
C	-1.748993	7.079902	0.192220
H	-1.615206	8.020419	-0.346083
H	-0.913831	6.973335	0.889672
H	-2.664634	7.161808	0.784160
N	2.355052	-0.523019	-0.050871
O	4.925910	0.552972	-0.203258
C	4.169255	0.717819	0.933162
C	4.721060	1.448924	1.963672
C	3.985365	1.691650	3.118999
C	2.703349	1.182096	3.228785
C	2.153789	0.433938	2.194020
C	2.876038	0.196916	1.029983
C	3.238475	-0.964094	-1.041282
C	2.880301	-1.898119	-2.006668
C	3.784565	-2.283301	-2.989648
C	5.059358	-1.745327	-3.016709
C	5.427882	-0.810790	-2.054615
C	4.525258	-0.420682	-1.088156
H	5.727691	1.831007	1.842648

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H         4.420066    2.273571    3.922244
H         2.117864    1.358499    4.123028
H         1.152327    0.033873    2.286160
H         1.884290   -2.321273   -1.990070
H         3.479958   -3.009419   -3.733614
H         5.769148   -2.042606   -3.778698
H         6.414603   -0.363307   -2.048458


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  63 atoms
derivative para, singlet excited state S1
O        -2.866680   -4.148105    1.208675
N        -2.353657   -0.456822   -0.537002
C        -2.701307   -3.003828    0.705109
C        -3.833560   -2.182785    0.301205
C        -5.134402   -2.649970    0.511431
C        -6.239832   -1.893069    0.166494
C        -6.051847   -0.636448   -0.392618
C        -4.767840   -0.148047   -0.613591
C        -3.645771   -0.914626   -0.287691
C        -1.244376   -1.135926   -0.058928
C         0.032419   -0.593553   -0.162244
C         1.139022   -1.333059    0.294622
C         1.003821   -2.589772    0.863255
C        -0.260141   -3.121105    0.984346
C        -1.410536   -2.417391    0.539346
H        -5.232390   -3.631791    0.958417
H        -7.240612   -2.273806    0.337256
H        -6.902957   -0.019213   -0.657211
H        -4.660938    0.843083   -1.031238
H         0.205048    0.391195   -0.568969
H         1.879820   -3.131168    1.203238
H        -0.421748   -4.096747    1.423131
C        -2.168983    0.803837   -1.226431
H        -2.965700    0.910824   -1.963491
H        -1.245537    0.743409   -1.805539
C        -2.141974    2.002386   -0.292074
H        -1.339518    1.866848    0.440570
H        -3.074873    2.025844    0.279922
C        -1.956195    3.314659   -1.030908
H        -1.015898    3.289579   -1.595556
H        -2.753636    3.430145   -1.775032
C        -1.957062    4.519389   -0.105492
H        -1.154563    4.409128    0.634010
H        -2.893693    4.534149    0.464478
C        -1.792645    5.843599   -0.832314
H        -0.854793    5.829978   -1.398739
H        -2.593551    5.947916   -1.572553
C        -1.806613    7.038331    0.105905
H        -1.688458    7.978196   -0.437342
H        -0.997102    6.971808    0.838001
H        -2.747818    7.089556    0.659947
N         2.440768   -0.742182    0.163865
O         4.957984    0.416657   -0.094608
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C         4.212346    0.637920    1.012805
C         4.750705    1.448824    1.996788
C         4.016370    1.693437    3.138644
C         2.745302    1.129194    3.300247
C         2.206035    0.322619    2.327511
C         2.935573    0.060899    1.160334
C         3.190535   -0.966576   -0.963512
C         2.726244   -1.774821   -2.009358
C         3.516734   -1.977203   -3.114632
C         4.781591   -1.384356   -3.208437
C         5.256253   -0.583196   -2.190738
C         4.463918   -0.374606   -1.075249
H         5.735964    1.869699    1.845223
H         4.429522    2.325878    3.913784
H         2.179520    1.328660    4.200910
H         1.227643   -0.123703    2.435438
H         1.748711   -2.226460   -1.917428
H         3.156054   -2.603475   -3.920079
H         5.394535   -1.554460   -4.084147
H         6.229542   -0.112507   -2.235265


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  63 atoms
derivative para, triplet excited state T1
O        -2.562201   -6.072956    6.278575
N        -2.061486   -2.426629    4.439652
C        -2.401373   -4.941543    5.747415
C        -3.536454   -4.139742    5.311457
C        -4.835466   -4.610127    5.524511
C        -5.942900   -3.871371    5.149276
C        -5.758367   -2.629343    4.556324
C        -4.476722   -2.138321    4.332044
C        -3.351875   -2.887953    4.688230
C        -0.952151   -3.084175    4.945576
C         0.320469   -2.533205    4.840802
C         1.431953   -3.251469    5.324630
C         1.299879   -4.498505    5.919209
C         0.040089   -5.035423    6.046278
C        -1.113406   -4.350568    5.576356
H        -4.930579   -5.579330    5.998842
H        -6.942502   -4.253578    5.323140
H        -6.611619   -2.025859    4.268056
H        -4.372183   -1.157969    3.889093
H         0.487194   -1.560356    4.404148
H         2.176380   -5.024547    6.281183
H        -0.117392   -5.998625    6.512980
C        -1.875599   -1.195699    3.698559
H        -2.669577   -1.121217    2.954724
H        -0.949029   -1.279954    3.127158
C        -1.851913    0.044332    4.577797
H        -1.065667   -0.066073    5.331934
H        -2.795295    0.107985    5.129122
C        -1.631760    1.315967    3.779313
H        -0.681085    1.248110    3.235944
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H	-2.412336	1.405568	3.014055
C	-1.630693	2.566057	4.642067
H	-0.847015	2.479653	5.404660
H	-2.579328	2.627565	5.188589
C	-1.423864	3.847243	3.851648
H	-0.474655	3.785602	3.307755
H	-2.206513	3.928099	3.089263
C	-1.433046	5.089526	4.725821
H	-1.284298	5.997024	4.136978
H	-0.640450	5.045912	5.477888
H	-2.384362	5.188113	5.255634
N	2.726384	-2.655198	5.186259
O	5.244609	-1.491479	4.928831
C	4.382039	-1.057087	5.877104
C	4.806202	-0.032436	6.705747
C	3.959002	0.424149	7.694703
C	2.692630	-0.146374	7.862797
C	2.266831	-1.165743	7.044142
C	3.107079	-1.636093	6.026111
C	3.591252	-3.087514	4.209776
C	3.242225	-4.101374	3.307549
C	4.145163	-4.507059	2.354472
C	5.412366	-3.918129	2.272221
C	5.771867	-2.910699	3.143894
C	4.865215	-2.495336	4.103322
H	5.795466	0.380935	6.559492
H	4.282896	1.224202	8.347887
H	2.040856	0.213028	8.648402
H	1.295367	-1.623176	7.164864
H	2.260538	-4.546395	3.384493
H	3.870130	-5.290182	1.660032
H	6.115304	-4.249380	1.518803
H	6.740477	-2.430283	3.099513

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Cartesian coordinates calculated by means of the COSMO-(TD)PBE0-GD3BJ/TZP method in dichloromethane (in Angstroms):

63 atoms
derivative ortho, ground state

O	1.862317	1.496079	-0.111138
N	-2.031674	0.547085	0.672893
C	0.688362	1.158672	0.034829
C	-0.400523	2.108438	-0.176664
C	-0.096956	3.371212	-0.698423
C	-1.078567	4.307897	-0.914204
C	-2.400994	3.981735	-0.601774
C	-2.727662	2.748974	-0.083393
C	-1.728665	1.784195	0.144625
C	-1.084259	-0.452196	0.724951
C	-1.467282	-1.756384	1.095934
C	-0.546513	-2.770937	1.155896
C	0.790816	-2.536304	0.840692
C	1.188494	-1.273594	0.474191
C	0.272564	-0.197052	0.409609

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H         0.941607    3.576614   -0.925945
H        -0.835909    5.280352   -1.324571
H        -3.191740    4.702507   -0.774869
H        -3.765123    2.532172    0.123099
H        -2.499243   -1.983244    1.314609
H        -0.869835   -3.766079    1.435633
H         1.524333   -3.331662    0.869157
C        -3.386193    0.291097    1.154783
H        -3.772339    1.223259    1.564330
H        -3.320568   -0.388674    2.002903
C        -4.320543   -0.256008    0.089454
H        -3.913033   -1.189936   -0.309743
H        -4.360360    0.443500   -0.751152
C        -5.718537   -0.491530    0.634441
H        -5.667389   -1.188195    1.479652
H        -6.115095    0.448277    1.036776
C        -6.677805   -1.036384   -0.409920
H        -6.281017   -1.976916   -0.810514
H        -6.725394   -0.340162   -1.255788
C        -8.080479   -1.271075    0.126411
H        -8.029970   -1.966025    0.971914
H        -8.473363   -0.330272    0.527577
C        -9.032477   -1.814813   -0.925387
H       -10.032589   -1.975125   -0.517018
H        -8.675942   -2.770270   -1.320005
H        -9.122577   -1.122934   -1.767327
N         2.563111   -1.104065    0.145089
O         5.170879   -0.357543   -0.547487
C         4.228113   -0.599969   -1.520121
C         4.631436   -0.479412   -2.833035
C         3.739802   -0.753339   -3.866225
C         2.446729   -1.142107   -3.560838
C         2.041759   -1.254233   -2.235540
C         2.924265   -0.983085   -1.196237
C         3.431892   -0.609686    1.117527
C         3.066067   -0.483830    2.452438
C         3.969651   -0.008568    3.396513
C         5.250169    0.355604    3.016953
C         5.623801    0.241623    1.680993
C         4.727235   -0.237944    0.749689
H         5.651815   -0.174562   -3.034062
H         4.062934   -0.662267   -4.895984
H         1.739001   -1.362052   -4.351293
H         1.028657   -1.556706   -2.003420
H         2.064188   -0.761835    2.753542
H         3.659441    0.075897    4.431233
H         5.959807    0.728049    3.745541
H         6.616451    0.520032    1.346871


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  63 atoms
derivative ortho, singlet excited state S1
O         1.743237    1.635166   -0.220402
N        -2.078571    0.513914    0.815480
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C	0.561055	1.253285	0.049667
C	-0.558113	2.166409	-0.082751
C	-0.341465	3.455845	-0.582203
C	-1.381162	4.356571	-0.737684
C	-2.668993	3.967383	-0.395493
C	-2.910832	2.691049	0.104913
C	-1.864901	1.780162	0.281936
C	-1.084241	-0.454679	0.815855
C	-1.360442	-1.770104	1.176419
C	-0.350637	-2.745026	1.230417
C	0.944175	-2.411217	0.896248
C	1.223284	-1.107835	0.510649
C	0.245958	-0.079549	0.451081
H	0.676832	3.717169	-0.842826
H	-1.191412	5.350571	-1.127747
H	-3.501408	4.650790	-0.520001
H	-3.929298	2.419371	0.342325
H	-2.369722	-2.071472	1.414907
H	-0.596552	-3.758055	1.524085
H	1.744033	-3.142832	0.916068
C	-3.412463	0.171693	1.276282
H	-3.849571	1.063344	1.727434
H	-3.323066	-0.549188	2.089065
C	-4.310047	-0.357718	0.169895
H	-3.903096	-1.300369	-0.209723
H	-4.286005	0.345261	-0.668910
C	-5.743615	-0.551816	0.627658
H	-5.775455	-1.275820	1.450452
H	-6.122590	0.392698	1.037132
C	-6.660247	-1.012990	-0.492313
H	-6.298976	-1.970065	-0.887440
H	-6.598934	-0.298459	-1.322193
C	-8.111192	-1.158629	-0.066165
H	-8.174900	-1.878718	0.757086
H	-8.463070	-0.202299	0.336570
C	-9.018166	-1.597839	-1.203041
H	-10.055963	-1.692296	-0.876463
H	-8.704064	-2.565794	-1.603262
H	-8.990927	-0.876804	-2.024822
N	2.571993	-0.819729	0.119041
O	5.181108	-0.247800	-0.657243
C	4.262637	-0.640152	-1.570673
C	4.674082	-0.743316	-2.887918
C	3.764045	-1.137961	-3.847640
C	2.442434	-1.428607	-3.494046
C	2.029684	-1.327386	-2.186371
C	2.939096	-0.933658	-1.197733
C	3.501204	-0.442616	1.054987
C	3.175973	-0.318718	2.410462
C	4.140539	0.064053	3.312719
C	5.445178	0.334923	2.887778
C	5.783281	0.225291	1.554263
C	4.815118	-0.158912	0.642997
H	5.702415	-0.512205	-3.132792
H	4.079714	-1.222481	-4.879506
H	1.736983	-1.735607	-4.255060
H	1.011238	-1.545340	-1.898727

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H         2.162794   -0.527406    2.722872
H         3.885870    0.157339    4.360280
H         6.197669    0.634046    3.606055
H         6.783550    0.431429    1.196747


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  63 atoms
derivative ortho, triplet excited state T1
O         1.751754    1.663825   -0.138860
N        -2.090042    0.537238    0.799512
C         0.560698    1.279865    0.086564
C        -0.560428    2.177699   -0.108704
C        -0.342049    3.454082   -0.639734
C        -1.386047    4.338298   -0.850458
C        -2.679270    3.945611   -0.532519
C        -2.922517    2.682454   -0.000917
C        -1.873267    1.788174    0.231434
C        -1.088950   -0.421948    0.852507
C        -1.357051   -1.726786    1.256362
C        -0.336020   -2.685633    1.363748
C         0.959825   -2.352161    1.033683
C         1.231164   -1.060789    0.601243
C         0.243331   -0.047140    0.501365
H         0.680461    3.719474   -0.878858
H        -1.195400    5.322709   -1.263596
H        -3.514311    4.616531   -0.699757
H        -3.944265    2.406968    0.217469
H        -2.366544   -2.030754    1.490851
H        -0.575328   -3.689820    1.691358
H         1.764179   -3.077295    1.083875
C        -3.428817    0.202687    1.252045
H        -3.877580    1.106819    1.665412
H        -3.346804   -0.489454    2.090180
C        -4.308325   -0.370616    0.152853
H        -3.894845   -1.326492   -0.184217
H        -4.272976    0.299577   -0.711947
C        -5.748029   -0.549308    0.597849
H        -5.790664   -1.244302    1.444793
H        -6.132068    0.408709    0.969524
C        -6.650755   -1.048839   -0.516894
H        -6.284277   -2.018108   -0.875818
H        -6.580466   -0.362111   -1.369222
C        -8.106390   -1.181834   -0.102540
H        -8.179053   -1.876060    0.741902
H        -8.462752   -0.213639    0.266513
C        -9.000958   -1.656382   -1.235001
H       -10.042076   -1.741757   -0.916575
H        -8.682149   -2.635804   -1.602212
H        -8.965549   -0.960682   -2.078016
N         2.568966   -0.780570    0.174850
O         5.169679   -0.259337   -0.670924
C         4.208333   -0.591001   -1.565667
C         4.573141   -0.660081   -2.898570
C         3.621980   -0.999758   -3.840193
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C         2.306991   -1.271570   -3.451373
C         1.940613   -1.203413   -2.127230
C         2.890749   -0.860981   -1.158377
C         3.545779   -0.479713    1.092810
C         3.272756   -0.400075    2.462825
C         4.281561   -0.090731    3.345700
C         5.578900    0.152168    2.885544
C         5.864855    0.089588    1.536407
C         4.852802   -0.221925    0.645346
H         5.599237   -0.449145   -3.169891
H         3.901636   -1.058030   -4.884233
H         1.569609   -1.539442   -4.196822
H         0.927622   -1.409421   -1.812834
H         2.263487   -0.583107    2.802890
H         4.065943   -0.032682    4.404569
H         6.366766    0.393867    3.587380
H         6.858288    0.278652    1.151264


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  63 atoms
derivative meta, ground state
O        -0.083447   -3.827202    1.142503
N        -2.502188   -0.942382   -0.483556
C        -0.820271   -2.944199    0.689255
C        -2.265136   -3.096742    0.604650
C        -2.856474   -4.262353    1.106449
C        -4.216796   -4.445618    1.067418
C        -5.015906   -3.437468    0.521264
C        -4.462861   -2.282635    0.016710
C        -3.069225   -2.088753    0.036103
C        -1.156970   -0.696099   -0.340042
C        -0.594060    0.531051   -0.746951
C         0.751593    0.762245   -0.610900
C         1.597173   -0.210224   -0.064445
C         1.065813   -1.404895    0.346752
C        -0.302903   -1.664585    0.223153
H        -2.197348   -5.010657    1.528929
H        -4.665912   -5.349339    1.460254
H        -6.093125   -3.554469    0.496636
H        -5.122608   -1.522903   -0.375017
H        -1.211707    1.317794   -1.152849
H         1.165901    1.714052   -0.922395
H         1.695426   -2.172203    0.779435
C        -3.343271    0.032119   -1.172370
H        -4.137257   -0.510574   -1.682423
H        -2.751096    0.484245   -1.966570
C        -3.915368    1.094186   -0.250422
H        -3.095807    1.612493    0.257401
H        -4.506409    0.612458    0.534739
C        -4.771434    2.095332   -1.005684
H        -4.174281    2.557919   -1.800557
H        -5.591896    1.568465   -1.507160
C        -5.342319    3.181431   -0.109808
H        -4.519874    3.706686    0.390449
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H        -5.938223    2.718822    0.686011
C        -6.199403    4.188815   -0.858365
H        -5.602873    4.644732   -1.656288
H        -7.021811    3.662076   -1.354950
C        -6.759376    5.275040    0.044321
H        -7.370634    5.986273   -0.515294
H        -5.954714    5.835109    0.528676
H        -7.383920    4.846033    0.832757
N         2.990643    0.044975    0.074517
O         5.667227    0.813287    0.231669
C         5.142217    0.368319   -0.960427
C         5.992524    0.295682   -2.043216
C         5.533005   -0.205260   -3.257312
C         4.216243   -0.617814   -3.368008
C         3.357616   -0.529813   -2.277871
C         3.808232   -0.036701   -1.058260
C         3.426193    0.846348    1.136017
C         2.583653    1.259123    2.162345
C         3.069414    2.033294    3.210196
C         4.399929    2.414233    3.241504
C         5.250169    2.012368    2.215962
C         4.768300    1.232918    1.185896
H         7.017702    0.623892   -1.918734
H         6.206278   -0.269609   -4.103195
H         3.842395   -1.012519   -4.305159
H         2.329757   -0.855959   -2.369569
H         1.542864    0.963029    2.144115
H         2.394030    2.335647    4.001546
H         4.783763    3.018672    4.054084
H         6.298047    2.288373    2.209227

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  63 atoms
derivative meta, singlet excited state S1
O        -0.031803   -3.498419    1.063364
N        -2.396464   -0.603944   -0.665090
C        -0.760383   -2.586936    0.557415
C        -2.197451   -2.739732    0.466708
C        -2.809532   -3.889866    0.980412
C        -4.181079   -4.064151    0.929924
C        -4.967875   -3.070771    0.361636
C        -4.384488   -1.918278   -0.157034
C        -2.997845   -1.737961   -0.125684
C        -1.045143   -0.347366   -0.493617
C        -0.473855    0.862364   -0.885215
C         0.907706    1.090583   -0.756826
C         1.689846    0.090864   -0.212746
C         1.165865   -1.109427    0.212850
C        -0.222892   -1.355526    0.089913
H        -2.160953   -4.637115    1.421292
H        -4.635472   -4.961716    1.335164
H        -6.045955   -3.178930    0.321536
H        -5.033640   -1.161613   -0.573248
H        -1.080915    1.659622   -1.287778
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H         1.348604    2.028716   -1.068504
H         1.792775   -1.876957    0.646041
C        -3.239736    0.373768   -1.329516
H        -4.005933   -0.167934   -1.886023
H        -2.645693    0.889435   -2.083457
C        -3.881852    1.356007   -0.362750
H        -3.111172    2.005003    0.065382
H        -4.306854    0.792488    0.473922
C        -4.973462    2.186357   -1.012036
H        -4.550271    2.798342   -1.817087
H        -5.698508    1.514538   -1.488255
C        -5.701307    3.076298   -0.019344
H        -4.990262    3.778461    0.432211
H        -6.080791    2.456788    0.802447
C        -6.856362    3.849647   -0.632478
H        -6.478743    4.480719   -1.444507
H        -7.553714    3.141910   -1.094538
C        -7.596399    4.705333    0.381421
H        -8.425232    5.247794   -0.078360
H        -6.927204    5.440286    0.837196
H        -8.006389    4.088913    1.186357
N         3.106338    0.306984   -0.069917
O         5.838496    0.714249    0.209122
C         5.350966    0.068517   -0.874054
C         6.259852   -0.371632   -1.820926
C         5.795299   -1.031131   -2.939525
C         4.424016   -1.249942   -3.117651
C         3.516517   -0.814258   -2.181886
C         3.968676   -0.146449   -1.036392
C         3.593622    0.945753    1.043064
C         2.752743    1.400740    2.066793
C         3.293123    2.038336    3.157892
C         4.675360    2.237349    3.257006
C         5.520219    1.791835    2.262254
C         4.982209    1.146415    1.162121
H         7.313312   -0.187211   -1.657866
H         6.499262   -1.380702   -3.683492
H         4.073294   -1.768172   -4.000233
H         2.456172   -0.979501   -2.306165
H         1.688112    1.239381    1.978828
H         2.642239    2.388057    3.948186
H         5.088053    2.742123    4.120749
H         6.592159    1.928224    2.314135


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  63 atoms
derivative meta, triplet excited state T1
O        -0.004792   -3.658968    0.521118
N        -2.419565   -0.599015   -0.810779
C        -0.753192   -2.705140    0.131591
C        -2.183983   -2.870991    0.014196
C        -2.778308   -4.088415    0.364167
C        -4.149050   -4.271433    0.280347
C        -4.953367   -3.226133   -0.150834
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C	-4.385878	-2.004664	-0.506193
C	-3.004638	-1.814380	-0.440539
C	-1.082149	-0.348862	-0.613167
C	-0.532851	0.918608	-0.834562
C	0.831834	1.155637	-0.657823
C	1.657726	0.107873	-0.267798
C	1.140943	-1.165408	-0.030218
C	-0.234724	-1.414940	-0.174289
H	-2.121617	-4.879693	0.703011
H	-4.589377	-5.223694	0.554878
H	-6.028569	-3.346241	-0.211427
H	-5.043942	-1.207712	-0.819352
H	-1.152309	1.744917	-1.147398
H	1.245454	2.136782	-0.847064
H	1.773697	-1.974189	0.305774
C	-3.281409	0.452623	-1.331153
H	-4.049077	-0.018387	-1.943646
H	-2.698933	1.066921	-2.015208
C	-3.907984	1.290807	-0.229561
H	-3.121767	1.838224	0.299681
H	-4.365397	0.621168	0.505161
C	-4.955359	2.251855	-0.760339
H	-4.495570	2.946150	-1.473181
H	-5.708750	1.688185	-1.323924
C	-5.641888	3.034038	0.346063
H	-4.895081	3.619040	0.895982
H	-6.069864	2.329281	1.069297
C	-6.737546	3.958514	-0.156899
H	-6.309688	4.670322	-0.871404
H	-7.473469	3.369569	-0.715492
C	-7.432251	4.711786	0.964684
H	-8.217614	5.367429	0.582723
H	-6.721697	5.329539	1.520714
H	-7.891952	4.018124	1.674232
N	3.039419	0.333481	-0.086545
O	5.784416	0.772116	0.278156
C	5.342009	-0.189152	-0.573984
C	6.307152	-0.917490	-1.246222
C	5.923746	-1.868984	-2.172469
C	4.572294	-2.067577	-2.444728
C	3.608653	-1.342054	-1.774551
C	3.975217	-0.414383	-0.794166
C	3.489172	1.295313	0.814405
C	2.621148	2.015474	1.640515
C	3.112408	2.964042	2.513538
C	4.482016	3.203863	2.599696
C	5.359207	2.464232	1.829884
C	4.867478	1.509267	0.957436
H	7.348715	-0.713006	-1.033754
H	6.677969	-2.439583	-2.699281
H	4.269079	-2.785452	-3.195836
H	2.562398	-1.485096	-2.000805
H	1.560459	1.818771	1.590304
H	2.423542	3.513426	3.142155
H	4.865409	3.950855	3.282982
H	6.431257	2.599369	1.895054

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  63 atoms
derivative para, ground state

O	-2.753600	-4.141119	1.105599
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5. X-ray diffraction studies

Crystals of compounds ***o*-A**, ***m*-A** and ***p*-A** were crystallized from mixtures of toluene and chloroform by slow solvent evaporation. Single crystals suitable for X-ray diffraction measurements were selected under a polarizing microscope and mounted on nylon loops using Paratone Oil. Diffraction data were collected using graphite-monochromated Mo Kα radiation on a Rigaku Oxford Diffraction Gemini A Ultra diffractometer equipped with an Atlas CCD detector at room temperature. Data collection and reduction were carried out using the CrysAlisPRO software suite.[21] Crystal structures were solved by intrinsic phasing using SHELXT and refined by least squares minimizations using SHELXL.[22,23] Both programs

were invoked from within the Olex2 program suite.[24] Crystal structure of ***m*-A** contained heavily disordered solvent molecules which were treated using the SQUEEZE procedure implemented in PLATON.[25,26] Two symmetry equivalent solvent accessible voids of 118 Å^3 were found in the unit cell each containing 12 e$^-$ which cannot be assigned to any of the solvents used in crystallization. This might be due to partial occupancy of solvent accessible voids. Data collection as well as crystal structure refinement details are given in Table S2. Crystal structures were analyzed using PLATON and intermolecular interaction energies were estimated using CrystalExplorer17 by scaling the interaction energies computed at the B3LYP/6-31G(d,p) level of theory for electron density calculated using Tonto.[25,27-29]

CCDC 1949980-1949982 contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

Table S2. Data collection and crystal structure refinement details for all phenoxazine-acridone isomers.

Identification code	***o*-A**	***m*-A**	***p*-A**
Empirical formula	$C_{31}H_{28}N_2O_2$	$C_{31}H_{28}N_2O_2$	$C_{31}H_{28}N_2O_2$
Formula weight	460.55	460.55	460.55
T /K	293(2)	293(2)	293(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/c$	$P2_1/n$
a /Å	9.3283(7)	12.0942(9)	7.9995(3)
b /Å	10.2674(8)	14.5020(9)	14.2069(6)
c /Å	13.0289(9)	28.554(2)	21.3942(9)
α /°	79.338(6)	90	90
β /°	87.728(6)	90.589(7)	100.552(4)
γ /°	73.749(7)	90	90
V /Å^3	1177.24(16)	5007.8(6)	2390.29(17)
Z	2	8	4
ρ_{calc} /g/cm^3	1.30	1.22	1.28
μ /mm^{-1}	0.081	0.076	0.080
F(000)	488	1952	976
Crystal size/mm^3	0.72 × 0.40 × 0.13	0.53 × 0.32 × 0.03	0.76 × 0.51 × 0.09
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.586 to 51.996	5.618 to 51.998	5.736 to 51.998
Index ranges	$-11 \le h \le 11$,	$-14 \le h \le 13$,	$-9 \le h \le 9$,

	$-12 \le k \le 12$, $-16 \le l \le 16$	$-17 \le k \le 17$, $-31 \le l \le 35$	$-17 \le k \le 17$, $-25 \le l \le 26$
Reflections collected	16699	52508	25561
Independent reflections	4629 [R_{int} = 0.0380, R_{sigma} = 0.0371]	9828 [R_{int} = 0.0958, R_{sigma} = 0.0867]	4692 [R_{int} = 0.0327, R_{sigma} = 0.0230]
Data/restraints/parameters	4629/0/317	9828/34/633	4692/0/317
Goodness−of−fit on F^2	1.011	1.004	1.022
Final R indexes [I>=2σ(I)]	R_1 = 0.0512, wR_2 = 0.1261	R_1 = 0.0883, wR_2 = 0.2591	R_1 = 0.0494, wR_2 = 0.1291
Final R indexes [all data]	R_1 = 0.0951, wR_2 = 0.1545	R_1 = 0.1862, wR_2 = 0.3320	R_1 = 0.0762, wR_2 = 0.1452
Largest diff. peak/hole / eÅ^{-3}	+0.22/−0.16	+0.51/−0.41	+0.38/−0.21

Table S3. Intermolecular interactions' details for ***m*-A** molecules and their closest neighbours in crystal structure. E_{ele}, E_{pol}, E_{dis} and E_{rep} stand for electrostatic, polarization, dispersion and repulsive components of the total intermolecular interaction energy (E_{tot}), respectively.

	most significant interaction(s)/shortest contacts	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	Molecule 1 (C1 through C31, N1 through N2, O1 through O2)					
Pair 1	C6−H6···O41^{i} H···O = 2.38 Å; C···O = 3.202(4) Å; C−H···O = 148º	−20.7	−2.9	−91.8	54.8	−70.1
Pair 2	-	−16.6	−7.8	−88.4	53.4	−67.4
Pair 3	C10−H10···*Cg*6^{ii} H···*Cg* = 2.71 Å; C−H···*Cg* = 141º; C···*Cg* = 3.478(5) Å	−16.4	−3.7	−50.8	25.9	−48.4
Pair 4	C1=O1···C41=O41 C···O = 3.020(5) Å; C1=O1···C31 = 102.6(2)º C11−H11···*Cg18* H···*Cg* = 2.73 Å; C−H···*Cg* = 167º; C···*Cg* = 3.645(5) Å	−14.6	−2.1	−59.8	39.5	−44.6
Pair 5	-	−3.3	−1.2	−41.3	19.6	−28.2
Pair 6	-	−3.3	−0.6	−8.5	3.0	−9.5
Pair 7	-	−0.2	−0.3	−12.9	5.9	−8.1
Pair 8	-	−3.9	−0.5	−13.4	13.3	−8.0
	Molecule 2 (C41 through C71, N41 through N42, O41 through O42)					
Pair 1	C46−H46···O1^{iii} H···O = 2.48 Å; C···O = 3.125(5) Å; C−H···O = 127º	−20.7	−7.4	−91.8	54.8	−73.4
Pair 2	C69−H69A···*Cg4*^{iii} H···*Cg* = 2.78 Å; C−H···*Cg* = 170º; C···*Cg* = 3.744(11) Å	−16.6	−6.5	−88.4	53.4	−66.4
Pair 3		−12.8	−3.1	−47.2	15.9	−47.1

Pair 4	C1=O1···C41=O41 C···O = 3.020(5) Å; C1=O1···C31 = 102.6(2)º	−14.6	−5.0	−59.8	39.5	−46.8
Pair 5	-	−3.3	−1.2	−41.3	19.6	−28.2
Pair 6	-	−1.3	−0.5	−16.2	6.5	−11.8
Pair 7	-	−4.2	−2.4	−8.1	6.7	−9.2
Pair 8	-	−0.2	−0.3	−12.9	5.9	−8.1
Pair 9	-	−3.9	−0.5	−13.4	13.3	−8.0

i = $1-x,-\frac{1}{2}+y,\frac{3}{2}-z$; ii = $1-x,\frac{1}{2}+y,\frac{3}{2}-z$; iii = $2-x,\frac{1}{2}+y,\frac{3}{2}-z$; iv = $2-x,\frac{1}{2}+y,\frac{3}{2}-z$

ring6 = C20C21C22C23C24C25; ring18 = C60C61C62C63C64C65.

Table S4. Intermolecular interactions' details for ***p*-A** molecule and its closest neighbours in crystal structure. E_{ele}, E_{pol}, E_{dis} and E_{rep} stand for electrostatic, polarization, dispersion and repulsive components of the total intermolecular interaction energy (E_{tot}), respectively.

	most significant interaction(s)/shortest contacts	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
Pair 1	*Cg*4···*Cg*2[i] *Cg*···*Cg* = 3.8776(10) Å; slippage = 1.595 Å	−11.0	−2.3	−71.6	32.0	−55.9
Pair 2	C23−H23···*Cg*3[ii] H···*Cg* = 2.82 Å; C−H···*Cg* = 155º; C···*Cg* = 3.679(2) Å C30−H30A···*Cg*6[iii] H···*Cg* = 2.93 Å; C−H···*Cg* = 154º; C···*Cg* = 3.830(3) Å	−14.4	−2.6	−67.4	44.5	−48.3
Pair 3	C6−H6···O1[iv] H···O = 2.58 Å; C···O = 3.480(2) Å; C−H···O = 165º C26−H26A···O1[iv] H···O = 2.58 Å; C···O = 3.513(2) Å; C−H···O = 162º	−16.3	−6.6	−36.6	23.8	−39.3
Pair 4	-	−7.3	−1.7	−37.6	18.7	−30.2
Pair 5	-	−0.8	−1.3	−31.9	14.1	−20.8
Pair 6	-	−6.0	−1.7	−11.4	6.1	−13.8
Pair 7	-	−1.2	−0.4	−14.7	8.8	−8.9

i = $1-x,1-y,1-z$; ii = $\frac{3}{2}-x,\frac{1}{2}-y,\frac{3}{2}-z$; iii = $\frac{3}{2}-x,-\frac{1}{2}+y,\frac{3}{2}-z$; iv = $1+x,y,z$.

ring2 = N1C1C2C7C8C13; ring3 = C2C3C4C5C6C7; ring4 = C8C9C10C11C12C13; ring6 = C20C21C22C23C24C25.

Table S5. Intermolecular interactions' details for ***o*-A** molecule and its closest neighbours in crystal structure. E_{ele}, E_{pol}, E_{dis} and E_{rep} stand for electrostatic, polarization, dispersion and repulsive components of the total intermolecular interaction energy (E_{tot}), respectively.

	most significant interaction(s)/shortest contacts	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}

Pair 1	*Cg*4···*Cg*4[i] *Cg*···*Cg* = 3.9294(13) Å; slippage = 0.763 Å	−10.1	−1.9	−55.8	20.9	−47.7
Pair 2	-	−17.1	−5.0	−53.6	33.9	−47.5
Pair 3	C5−H5···*Cg*6[ii] H···*Cg* = 2.95 Å; C−H···Cg = 142º; C···*Cg* = 3.725(2) Å	−16.2	−7.4	−38.2	22.6	−41.9
Pair 4	*Cg*5···*Cg*5[iii] *Cg*···*Cg* = 3.8207(11) Å; slippage = 1.955 Å C17−H17···O1[iii] H···O = 2.49 Å; C···O = 3.173(2) Å; C−H···O = 130º	−12.0	−3.2	−59.8	48.0	−37.5
Pair 5	-	−7.9	0.0	−53.7	30.8	−36.1
Pair 6	-	−1.8	−1.2	−45.8	21.2	−29.5

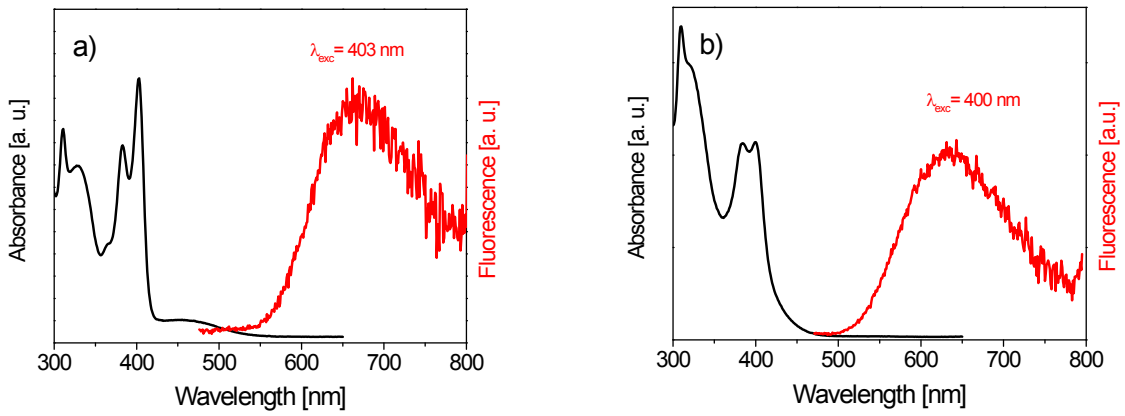
i = $1-x, 1-y, 1-z$; ii = $2-x, -y, 2-z$; iii = $2-x, -y, 1-z$.

ring4 = C8C9C10C11C12C13; ring5 = C14C15C16C17C18C19; ring6 = C20C21C22C23C24C25.

6. Optical studies

Absorption spectra at room temperature were measured on a Perkin-Elmer Lambda 35 spectrophotometer. Emission spectra and fluorescence lifetimes at room temperature were collected on a Horiba Fluorolog 3 fluorimeter. Excitation for fluorescence lifetimes measurements was provided by Delta Diode 336 nm.

Solutions of the compounds diluted in toluene (T) and in dichloromethane (DCM) were first frozen in liquid nitrogen (77 K) and next inserted into a liquid helium cryostat, which temperature could be stabilized at any value between 5 and 300 K. Fluorescence and phosphorescence spectra at low temperatures (5 - 175 K) were detected using a Parker-type disc-chopper phosphorimeter.[30] Samples were excited by the 405 nm line emitted by a diode laser (50 mW). Emission spectra were collected at right angle and dispersed using a McPherson 207 monochromator and detected with an EMI9659 photomultiplier operating in photons counting mode. Transients were accumulated with the aid of a Stanford Research SR430 multi-channel scaler.



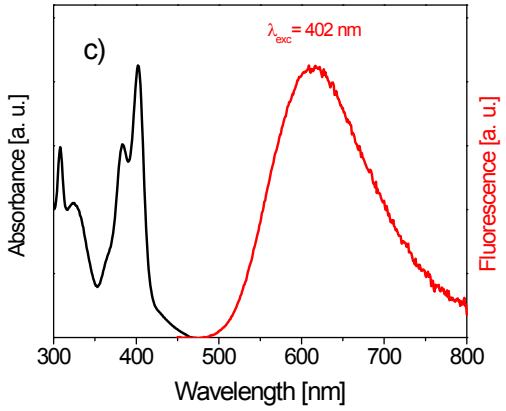


Figure S4. Absorption and fluorescence spectra of ***o*-A** (a), ***m*-A** (b) and ***p*-A** (c) in dichloromethane (DCM).

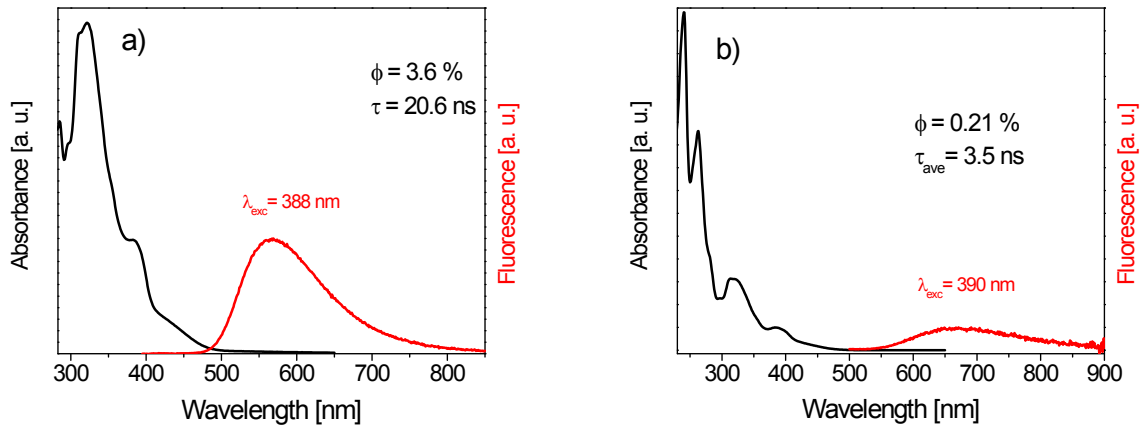
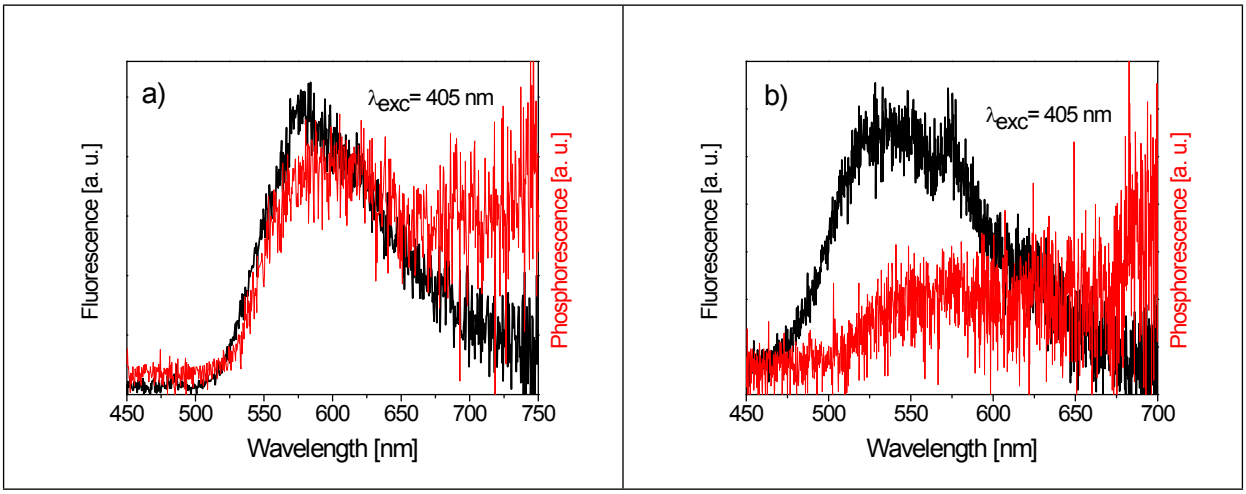


Figure S5. Absorption and fluorescence spectra of the compound **di-*m*-A**: a) in toluene and b) in dichloromethane at RT.



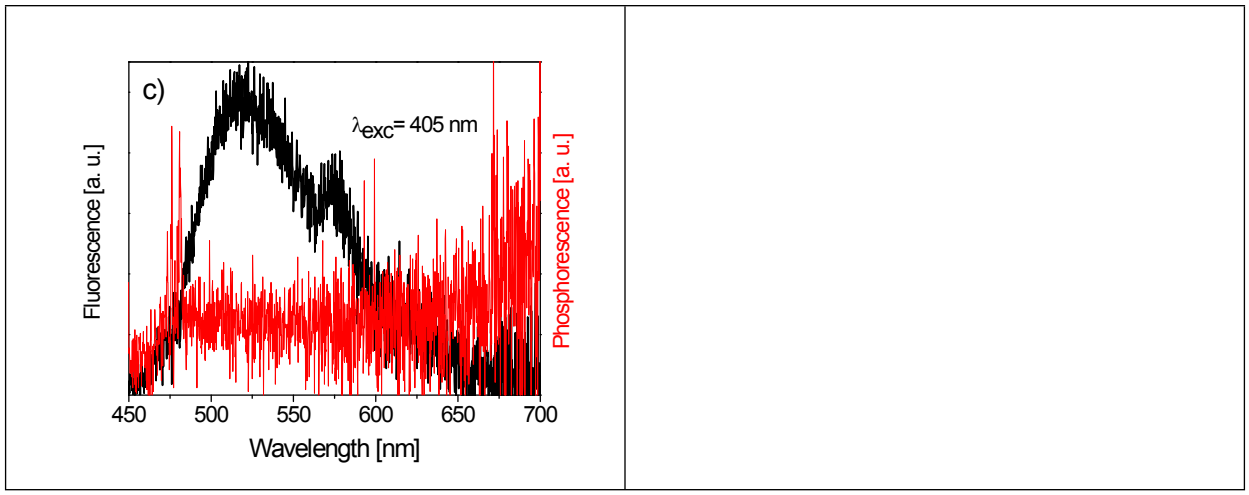


Figure S6. Fluorescence (black) and phosphorescence (red) spectra of ***o*-A** (a), ***m*-A** (c) and ***p*-A** (c) in DCM at 5 K.

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