Hole-transfer induced energy transfer in perylene diimide dyads with a donor-spacer-acceptor motif (Electronic Supplementary Information)

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1. Details Experiments

1.1 Materials

Structural formulae and abbreviations for the full names of the perylene diimide dyads investigated in this work are shown in Charts 1 and Chart S1. The synthesis of all dyads has been described in detail in reference S1-S4 except for D-(Null)-A, D-(Ph)-A and D-(Me2-Ph)-A, which will be presented in a separate dedicated publication. The solvent used for the spectroscopic investigation was Chloroform of the highest spectroscopic grade commercially available.

1.2 Femtosecond UV/Vis Transient Absorption Measurements

To monitor the energy transfer kinetics of the perylene diimide dyads we used a femtosecond broadband pump-probe setup that has been described in detail in references S5 and S6. Solutions of the dyads (OD 0.3, ca. 2×10^{-4} to 3×10^{-4} M) were pumped through a flow cell of 120 μm path length and irradiated with 28-fs pulses (λ_{exc} = 435 nm, 50 nJ/pulse) from the frequency-doubled output of a noncollinear optical parametric amplifier (NOPA). For the donor spacer systems and the dyads with more complex synthetic routs and therefore less material availability we used an excitation wavelength of 465 nm as the molar absorption coefficient of the dyads at 435 nm was around 40,000 L/mol cm^{-1} while at 465 nm around 80,000 L/mol cm^{-1}. The 465 nm pulses were generated with the NOPA directly. Although the donor/acceptor excitation ratio at this wavelength is 5:1, we did not see any noticeable difference in the energy transfer dynamics compared to the 435 nm excitation were the ratio was 10:1. The pulses were focused down to a FWHM diameter of about 100 μm inside the sample. A CaF_2 white light continuum spanning from 290 to 720 nm and polarized at the magic angle was used as probe light. The time-dependent transient spectra were recorded with temporal resolutions of 100 fs, which is well below all observed decay rates.

1.3 Time resolved fluorescence Measurements

The time resolved fluorescence data were measured with a Hamamatsu streak camera system (C5680-24 C). The femtosecond excitation pulses centered at 389 nm wavelength with 100 nJ were generated by second harmonic generation of the output of a CPA-system (CPA-2001; Clark MXR) at 778 nm with 180 fs pulse duration. Solutions of the dyads (OD 0.4, ca. 3×10^{-4} M) were pumped through a flow cell of 0.5 mm.

The vertically polarized excitation light was used in a front face geometry (beam diameter 30 μm at the sample position). The fluorescence light was collected with an achromat

(f = 80 mm, 20 mm diameter, Type OUV 4.20, Bernhard Halle Nachfl. GmbH) in combination with a wire grid polarizer (Moxtek UBB01C, diameter 36 mm) in magic angle position. The collimated fluorescence light was focused with an achromatic lens (f = 75 mm NUV, diameter 25 mm; Edmund Optics) onto the entrance slit of the spectrograph (Princeton Instruments, Acton Series SP2356, f = 300 mm, 50 lines per mm grating blazed at 600 nm). A slit width of 10 μm was used, resulting in a relative wavelength resolution of 1.5 nm. The focal plane of the spectrograph was imaged onto the photocathode of the streak camera system. The time window was set by a fast single-sweep unit (Hamamatsu, M5677-01) with sweep velocities adopted to the investigated sample. The time windows were changed between 20 ns and 200 ps. For the shortest time windows a time resolution of 3.5 ps could be achieved after correcting for the electronic jitter. For a more detailed explanation of the streak camera operation see reference S7.

1.4 Analysis of the data: Maximum Entropy and global fit

The temporal evolution of the absorption changes in the transient absorption measurements have been quantified with a maximum entropy and a global fit analysis [S8]. For the time-resolved fluorescence measurements single line and global fit analyses were employed.

A detailed explanation of the mathematical principles behind the maximum entropy method can be found in reference S9-S11, The software implementation used in this work is described in reference S12.

In the maximum entropy analysis the time traces of all available wavelengths are inverse Laplace transformed and the transformation is stabilized by the maximum entropy method. The time-resolved spectra are converted to lifetime density maps (see Figure S12 as example),

In a lifetime density map a cut along a certain wavelength channel yields bands of negative and/or positive amplitude at various pump-probe delays (e.g. left profile graph of Figure S12). The positions of the maxima represent the time constants present at this wavelength. The width of the bands represents the uncertainty in the time constant. The absolute value of the amplitude represents the contribution of the time constant at the given pump-probe delay. The sign indicates appearance or disappearance of the spectral signal.

A spectral cut along a certain pump probe delay (e.g. top profile graph of Figure S12) also yields bands at different wavelengths. These profiles can be interpreted just like the decay associated difference spectra (DADS) obtained from global analyses. The bands are located at coordinates corresponding to their spectroscopic maxima. The sign of the amplitude indicates

appearance or disappearance of the spectral signal at the chosen pump-probe delay.

From the lifetime-resolved spectra, the number of exponentially decaying components, their time constants, and their decay-associated spectra are readily available by a direct visual evaluation of the lifetime density map. Unlike global analysis, maximum entropy analysis is model free, and it additionally yields the uncertainties in the time constants. For this reason in this work the maximum entropy analysis was used prior to the global analysis in order to obtain a good set of starting values for the time constants of the global fit and for a posthumous assessment of the quality of the global fit.

2. Stationary absorption and fluorescence

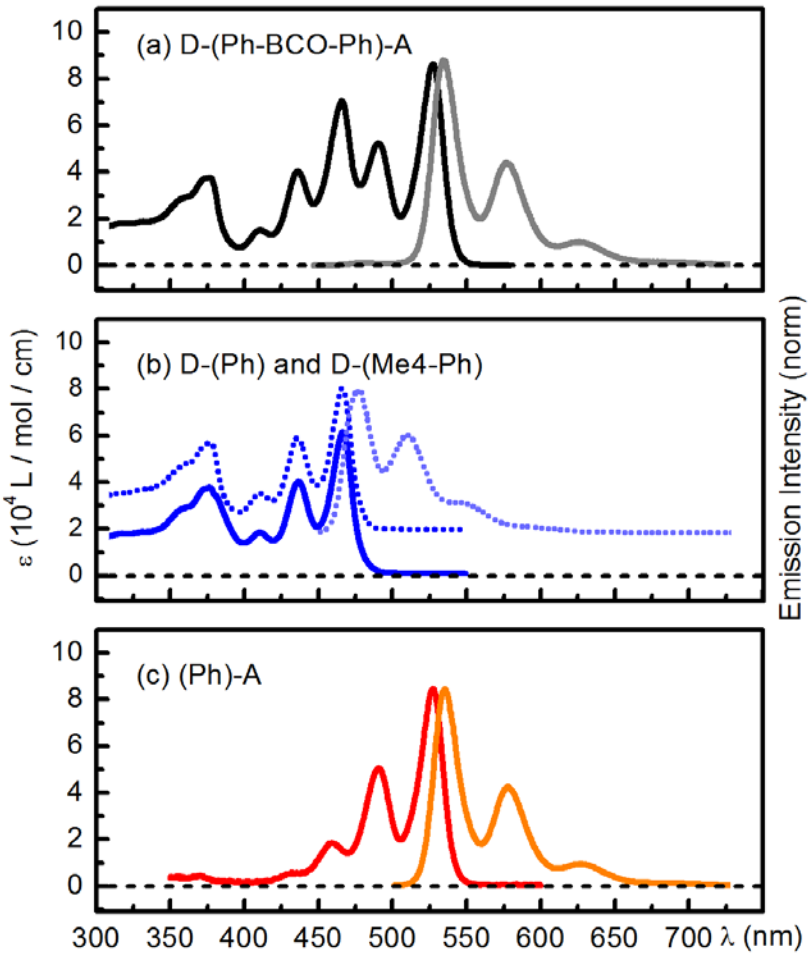

Figure S1: Stationary absorption and fluorescence spectra of (a) the dyad D-(Ph-BCO-Ph)-A, (b) the donor spacer systems D-(Ph) in solid line and D-(Me4-Ph) in dotted line offset by 20,000 L/mol/cm, and (c) the spacer acceptor system (Ph)-A in chloroform. The fluorescence spectra for D-(Ph-BCO-Ph)-A and D-(Me4-Ph) were obtained with an excitation at 436 nm, for (Ph)-A at 491 nm. For D-(Ph) no fluorescence could be detected.

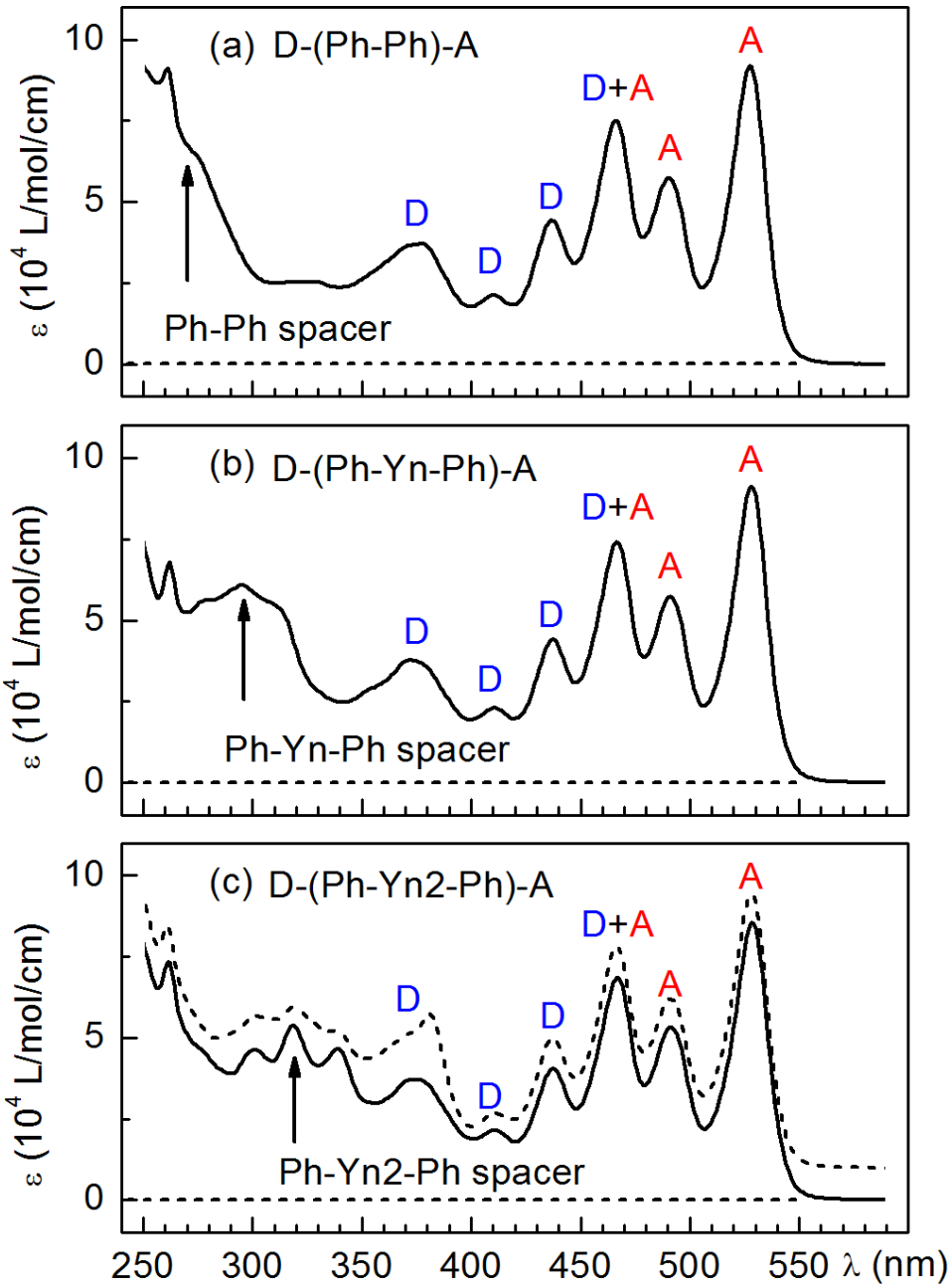

Figure S2: Stationary absorption spectra of the dyads undergoing coupled HT-FRET in chloroform. The spectral contributions of donor, spacer and acceptor are indicated for clarity. In (c) the dashed line represents the absorption spectrum offset by 10,000 L/mol/cm of the dyad D-(Py-Yn2-Py)-A that undergoes direct FRET.

3. Noise Induced FRET Distance Dependence

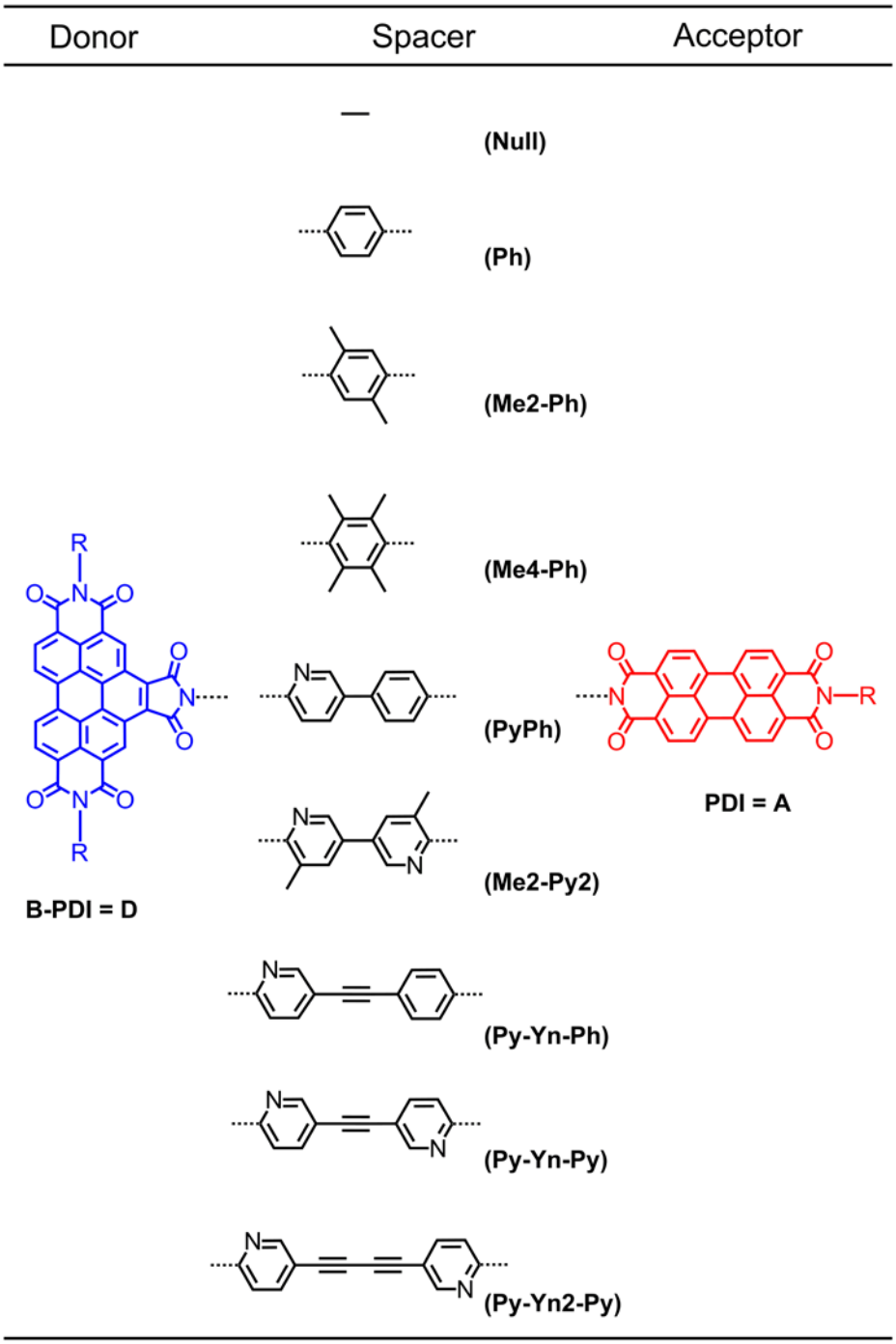

Chart S1: Perylene diimide dyads undergoing direct noise induced FRET together with the associated abbreviation. B-PDI = benzoperylene diimide; PDI = Perylene diimide; Ph = Phenyl; Me = Methyl; Py = Pyridine; Yn = Alkyne; R = 1-hexylheptyl.

Table S1. Measured energy transfer times in chloroform for all the dyads presented in Chart S1 together with theoretically determined donor-acceptor distances.

dyad	τ_{FRET} / ps	D-A distance / Å [(a)]
D-(Null)-A	1.2	13
D-(Ph)-A	5.4	17
D-(Me2-Ph)-A	9.2	17
D-(Me4-Ph)-A	9.4	17
D-(Py-Ph)-A	22	22
D-(Me2-Py2)-A	23	22
D-(Py-Yn-Ph)-A	30	24
D-(Py-Yn-Py)-A	36	24
D-(Py-Yn2-Py)-A	54	27
	53 [(b)]	

(a) Distance between the middle points of the transition dipole moments of the energy donor and acceptor obtained from ground state dyad geometries optimized at the B3LYP/6-311G** level of theory.

(b) Result from time resolved fluorescence measurements for D-(Py-Yn2-Py)-A. The excited state lifetime of the populated acceptor was 3.3 ns

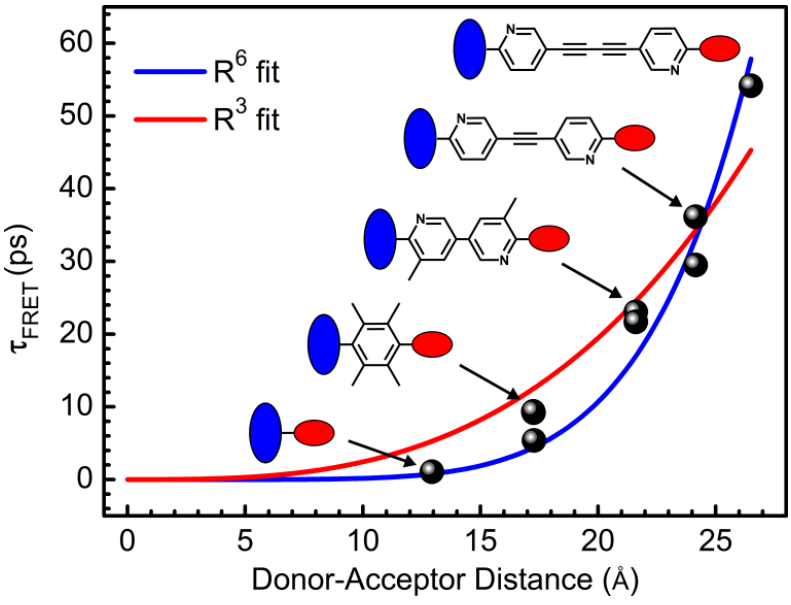

Figure S3: Noise induced FRET times (data: black dots; fits: blue and red lines) from transient measurements of the dyads in Chart S1 in chloroform versus donor-acceptor distances. The left (blue) and right (red) hatched ellipses depict the donor and acceptor of some representative dyads of Chart S1, while the spacer is shown with its structural formula. The FRET times are listed in Table S1.

4. Time resolved fluorescence spectra of D-(Py-Yn2-Py)-A

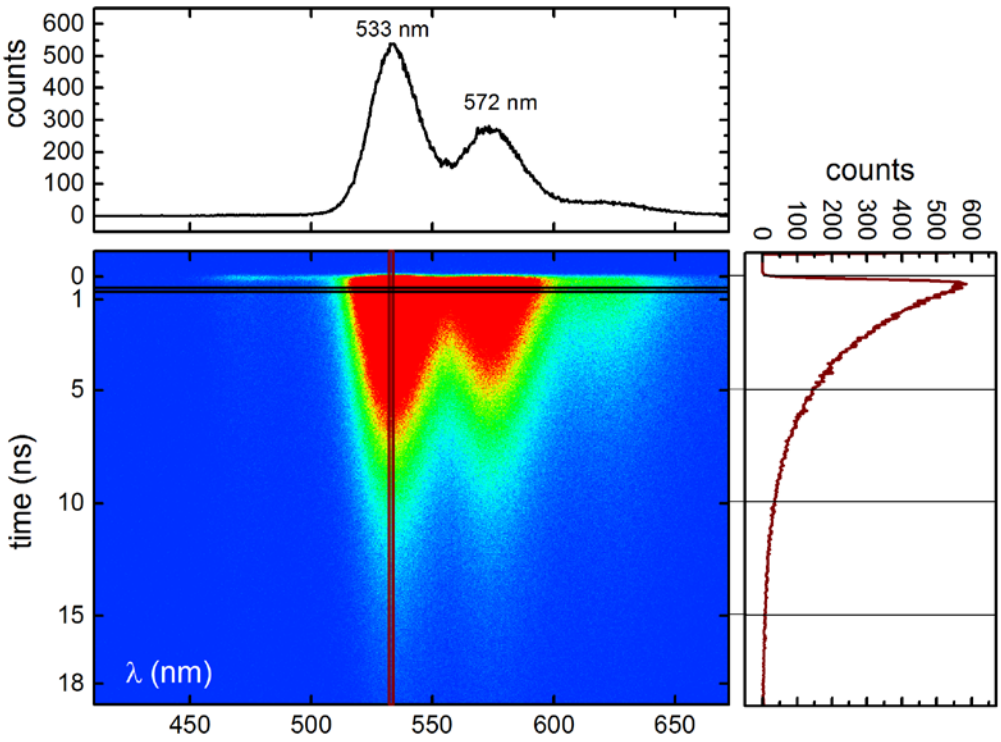

Figure S4: Time resolved fluorescence of **D-(Py-Yn2-Py)-A** dissolved in chloroform after excitation at 389 nm. In this 20 ns window, only the two strong bands of ns-fluorescence of the energy acceptor are resolved. The fluorescence of the energy donor is quenched by the 53 ps noise induced FRET within the instrument response function.

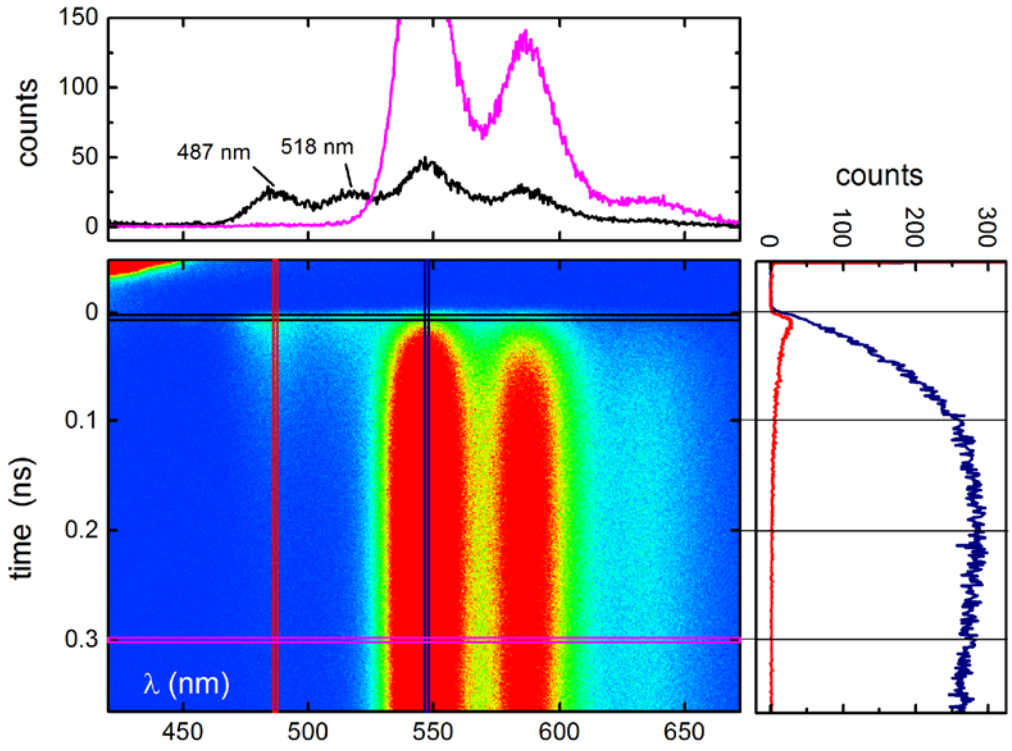

Figure S5: Time resolved fluorescence of **D-(Py-Yn2-Py)-A** dissolved in chloroform in the 0.5 ns window after excitation at 389 nm. At about 300 ps (magenta spectral cut), the energy donor fluorescence has died out and the energy acceptor fluorescence decays slowly as depicted in the navy blue temporal profile. The black spectral cut shows the initial fluorescence immediately after excitation. Both donor and acceptor contributions are present. The spot in the upper left corner is scattered light from the excitation.

5. Time resolved fluorescence spectra of D-(Ph-Yn2-Ph)-A

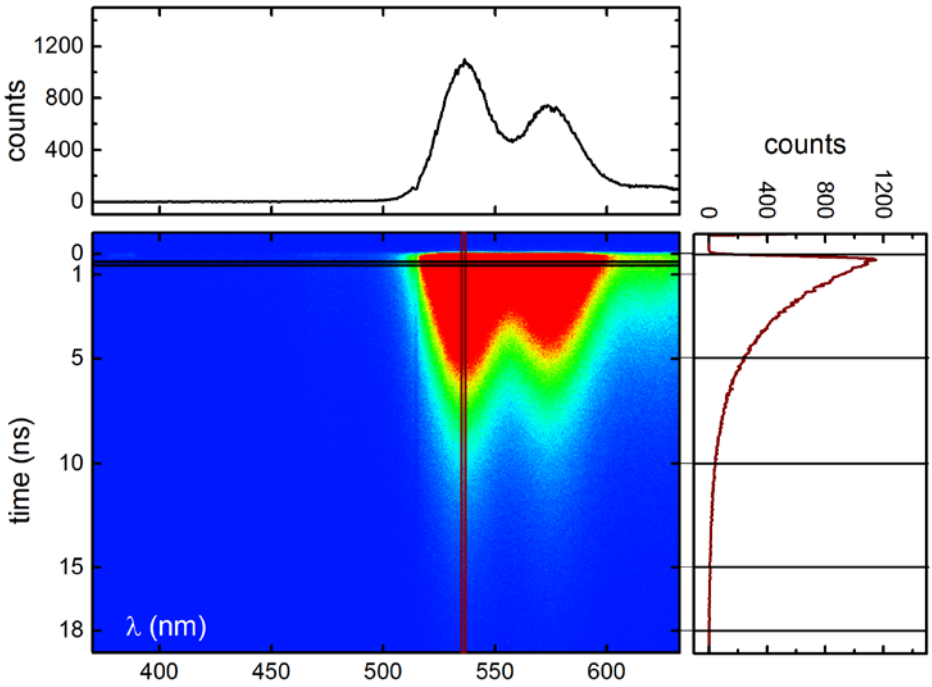

Figure S6: Time resolved fluorescence of **D-(Ph-Yn2-Ph)-A** dissolved in chloroform in the 20 ns window excited at 389 nm. Here, only the ns energy acceptor fluorescence decay can be temporally resolved.

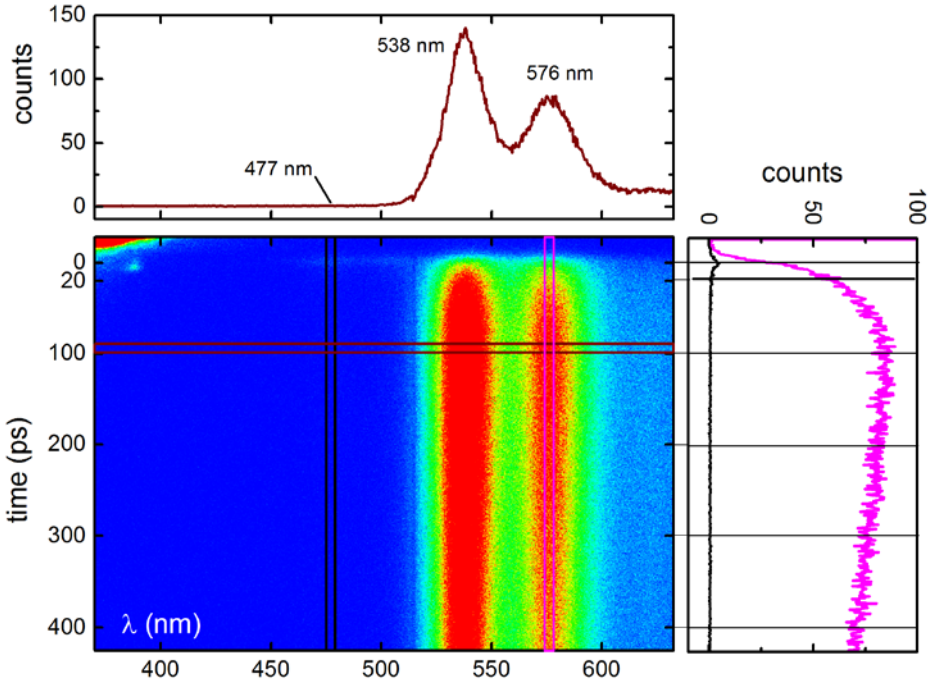

Figure S7: Time resolved fluorescence of **D-(Ph-Yn2-Ph)-A** dissolved in chloroform in the 0.5 ns window excited at 389 nm. The magenta temporal profile shows the build

up and decay of the energy acceptor fluorescence; the ps decay of the energy donor can be made out in the black temporal profile around time zero. The spot in the upper left corner is scattered light from the excitation.

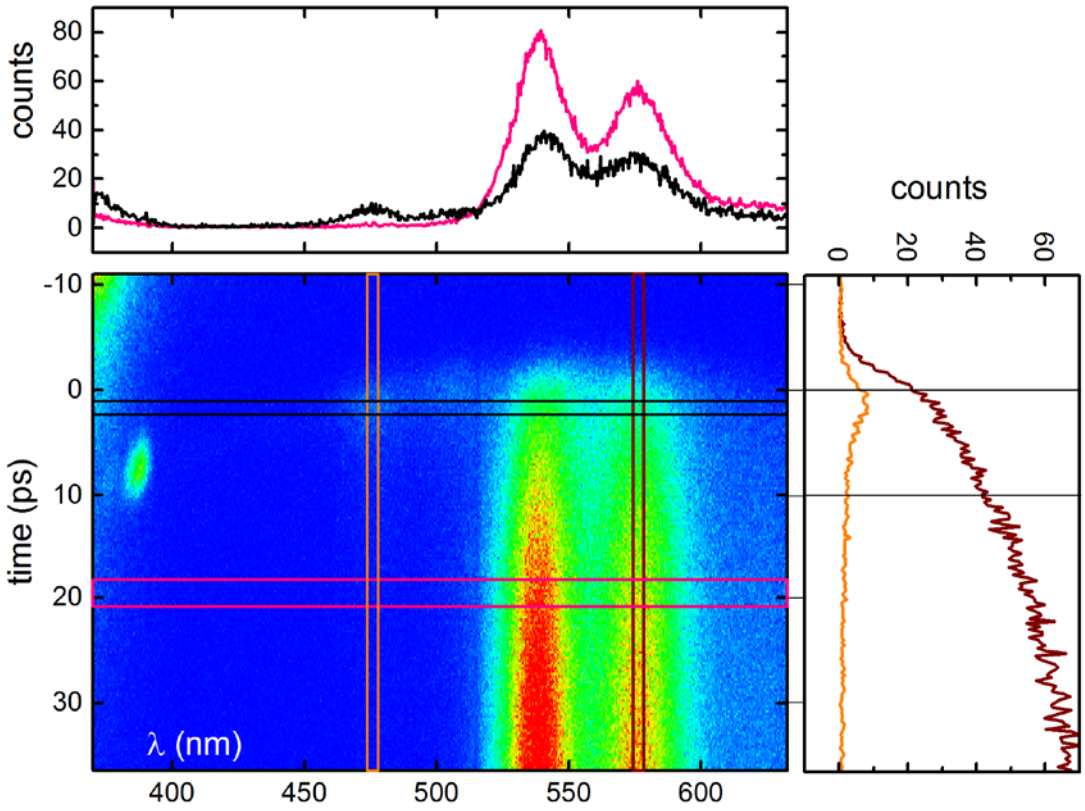

Figure S8: The 0.2 ns window for D-(Ph-Yn2-Ph)-A dissolved in chloroform and excited at 389 nm. At early times, the bands of the energy donor and the energy acceptor can be distinguished (black spectral cut). The two spots on the left are scattered light from the excitation.

6. Transient absorption and Maximum Entropy Analysis of D-(Me4-Ph)

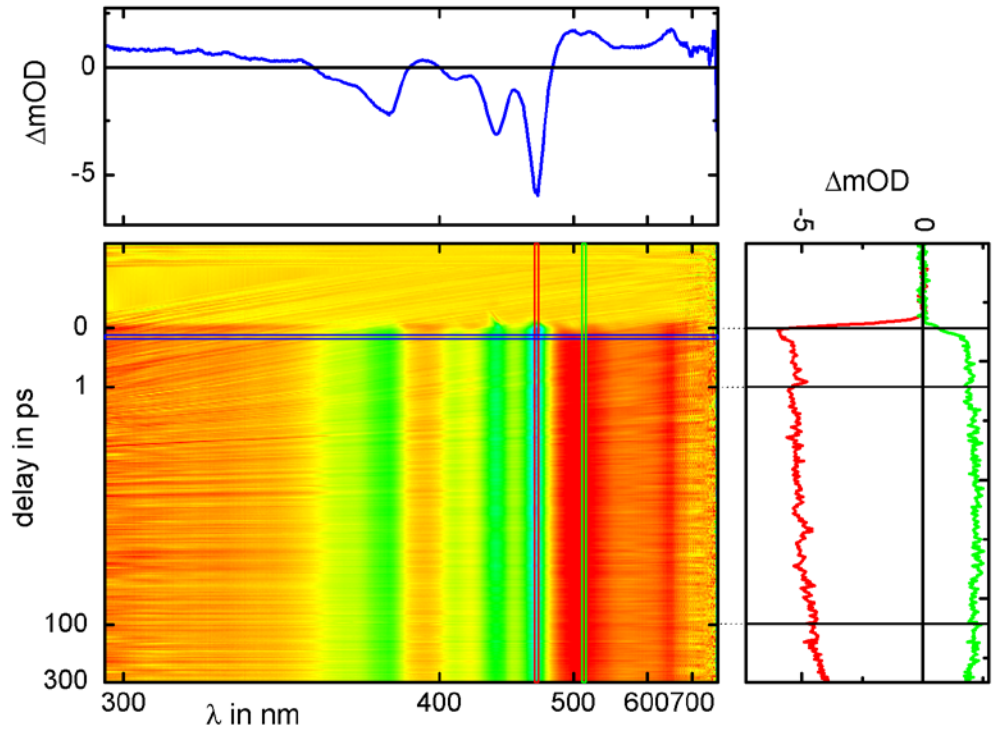

Figure S9: Transient absorption of **D-(Me4-Ph)** in chloroform excited at 435 nm.

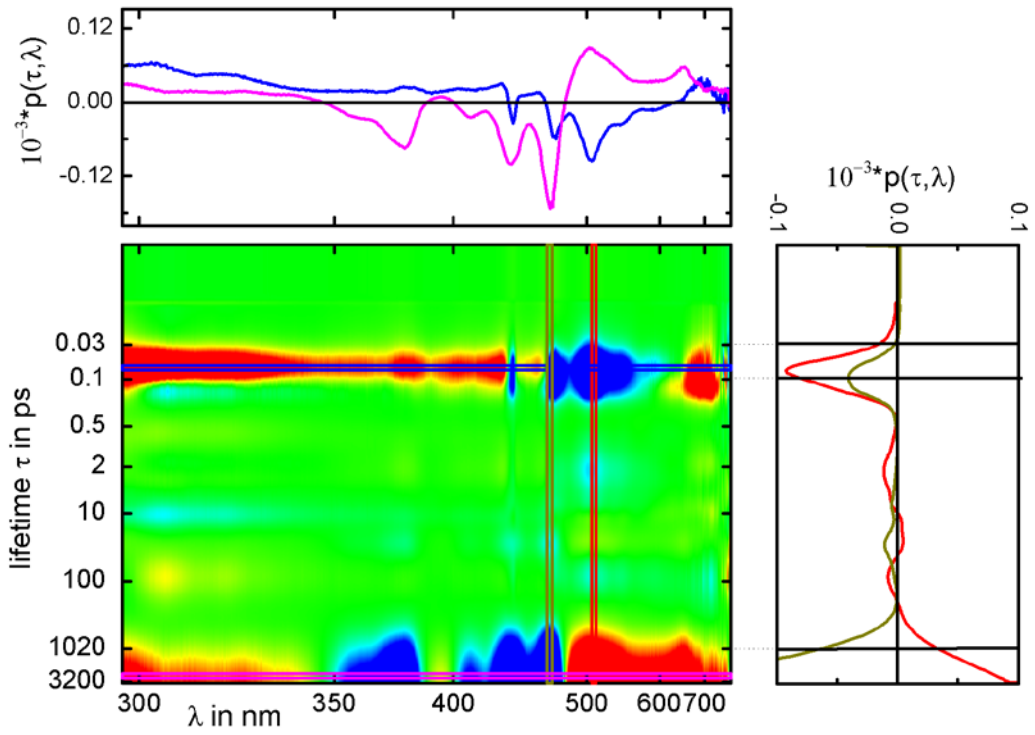

Figure S10: Maximum Entropy analysis of the TA measurement in figure S8 **D-(Me4-Ph).**

7. Transient absorption and Maximum Entropy Analysis of D-(Ph)

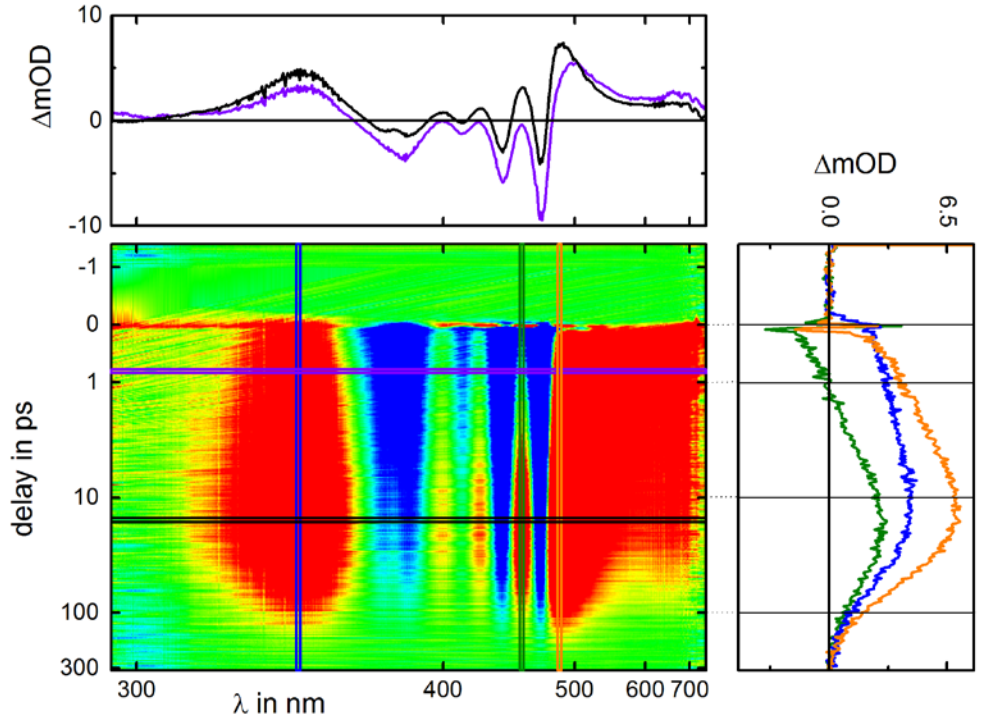

Figure S11: Transient absorption of **D-(Ph)** in chloroform after excitation at 465 nm.

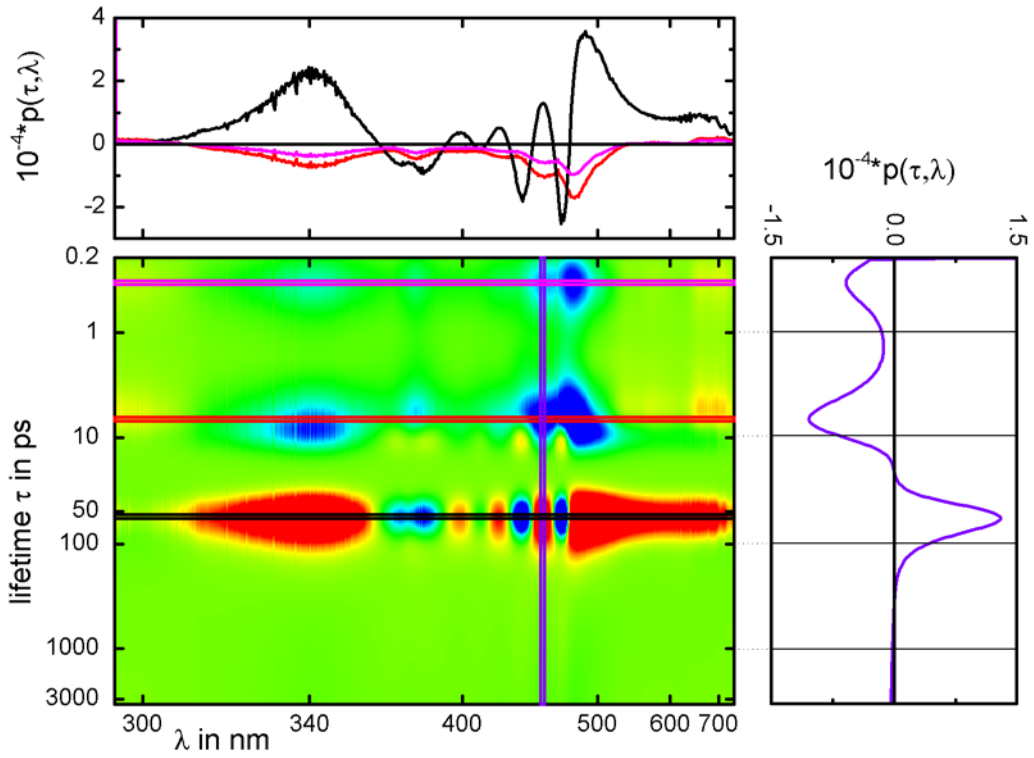

Figure S12: Maximum Entropy analysis of the TA measurement in figure S11 of **D-(Ph).**

8. Spectroelectrochemistry of D-(Me4-Ph)

Spectroelectrochemical measurements were carried out in a 0.8 mM dichloromethane (CH_2Cl_2) solution of D-(Me4-Ph) with 150 mM tetrabutylammonium tetrafluoroborate (Bu4N+ BF4-) as the supporting electrolyte. Bulk electrolysis was performed using a computer controlled potentiostat (Gamry Interface 100) and a three-electrode arrangement in a 0.2 mm glass cuvette utilizing a platinum wire mesh working electrode, a platinum wire mesh auxiliary electrode, and a silver wire pseudoreference electrode. The cuvette was placed in a computer controlled diode array spectrophotometer (Jenoptik Specord S 100) to measure the full optical spectral range at once. Spectra of the electrochemically generated anions were recorded by passing the light from the spectrophotometer through the platinum mesh working electrode. A blank spectrum consisting of the cuvette filled with solvent and supporting electrolyte was subtracted from each data set.

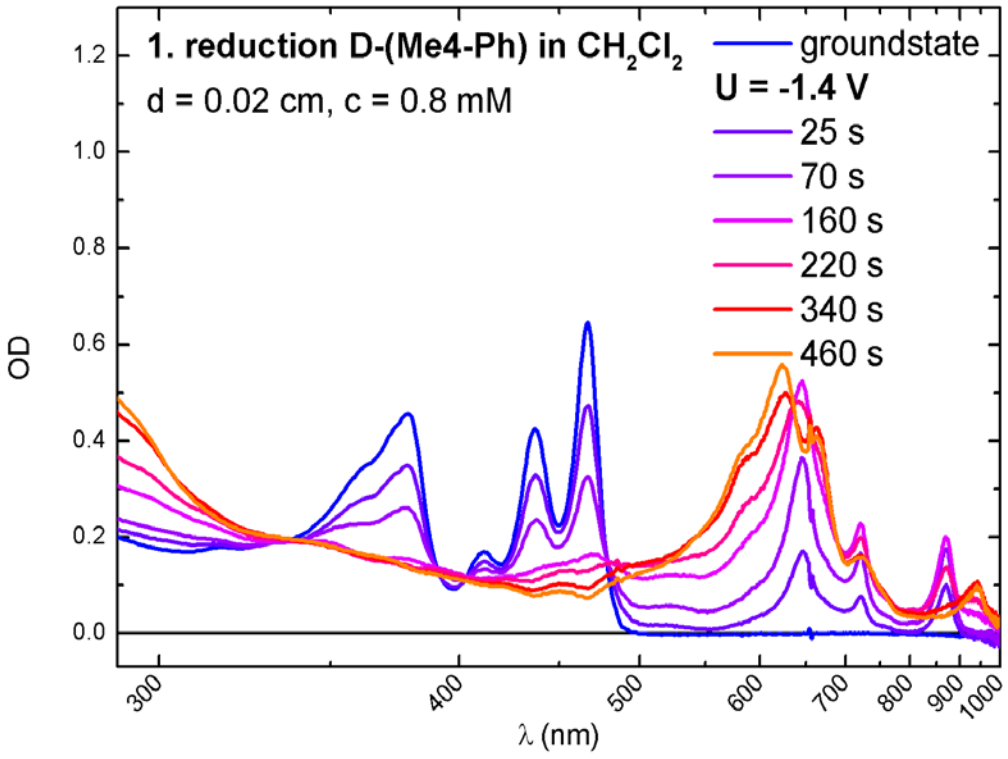

Figure S13: Change of steady state absorption of **D-(Me4-Ph)** in dichloromethane with a reducing voltage -1.4 V to produce the **D-(Me4-Ph)** monoanion.

9. Transient absorption and Maximum Entropy of D-(Ph-Yn2-Ph)-A

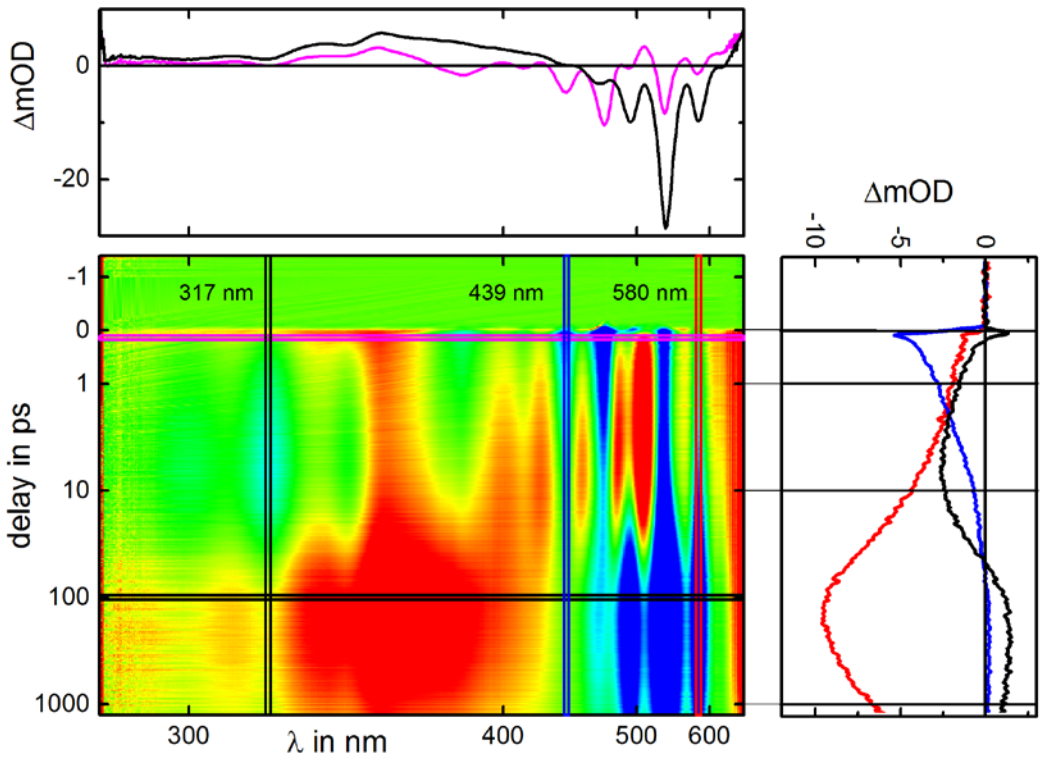

Figure S14: Transient absorption of **D-(Ph-Yn2-Ph)-A** in chloroform excited at 465 nm

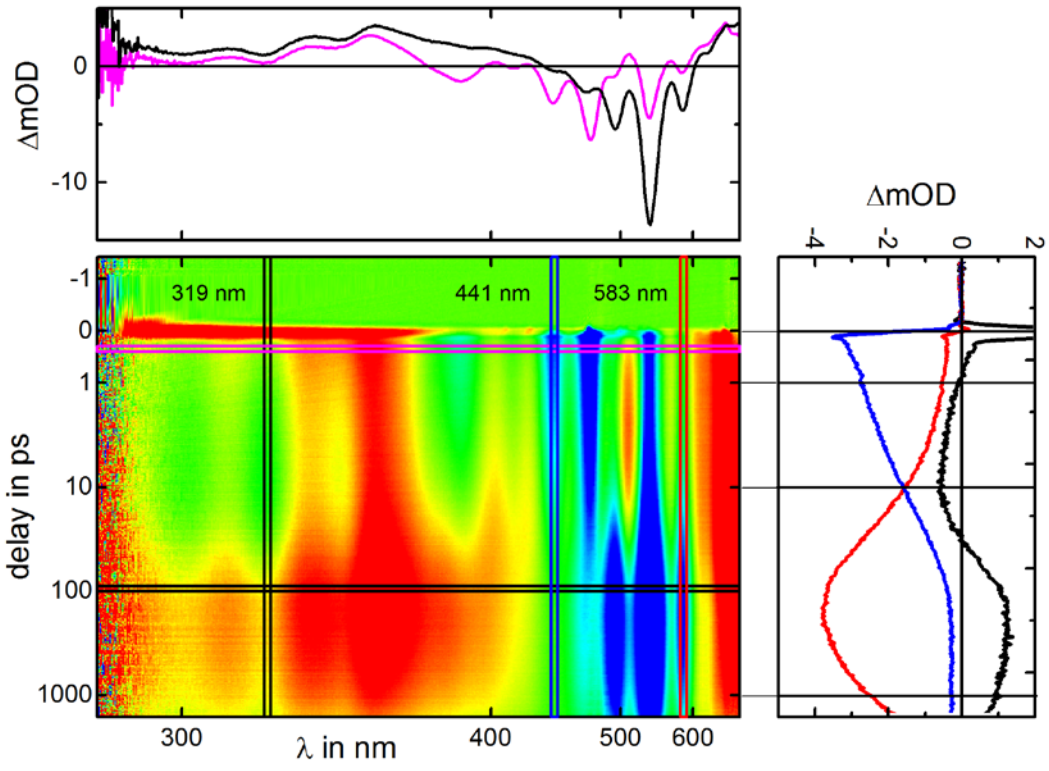

Figure S15: Transient absorption of **D-(Ph-Yn2-Ph)-A** in benzonitrile excited at 465 nm

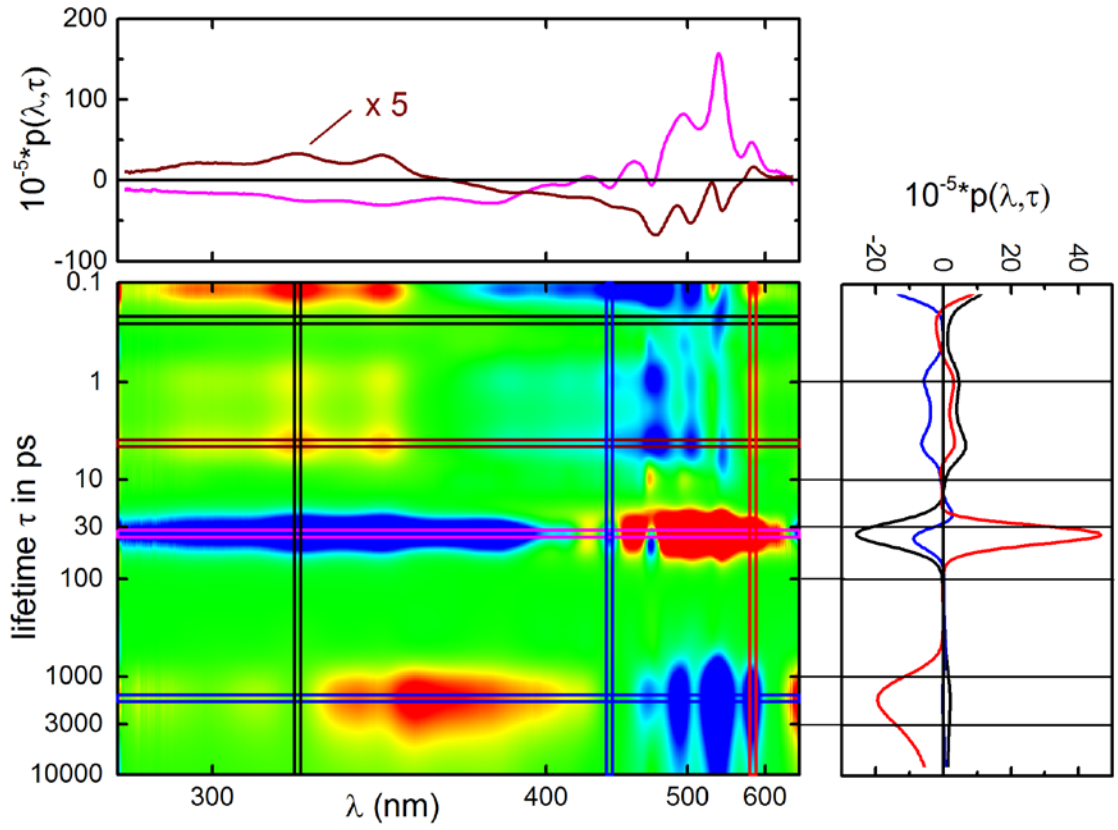

Figure S16: Maximum Entropy analysis of **D-(Ph-Yn2-Ph)-A** in chloroform

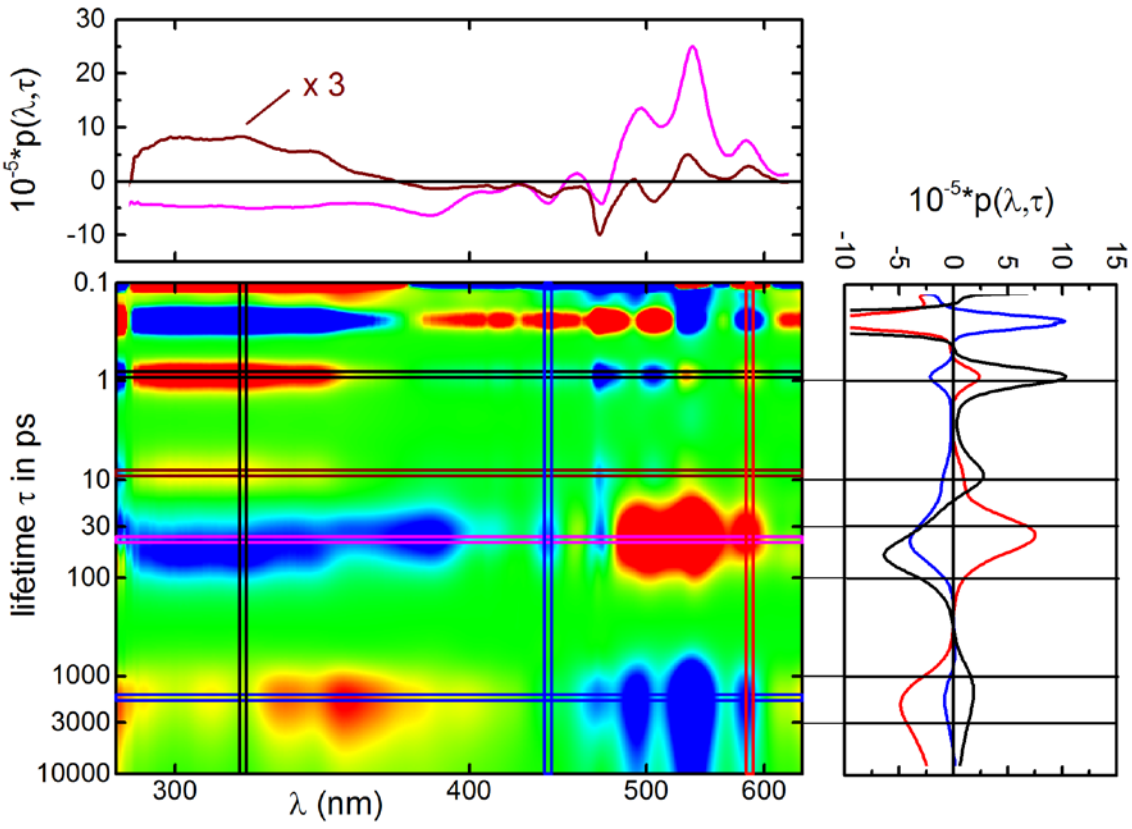

Figure S17: Maximum Entropy analysis of **D-(Ph-Yn2-Ph)-A** in benzonitrile

10. Transient absorption and Maximum Entropy of D-(Ph-BCO-Ph)-A

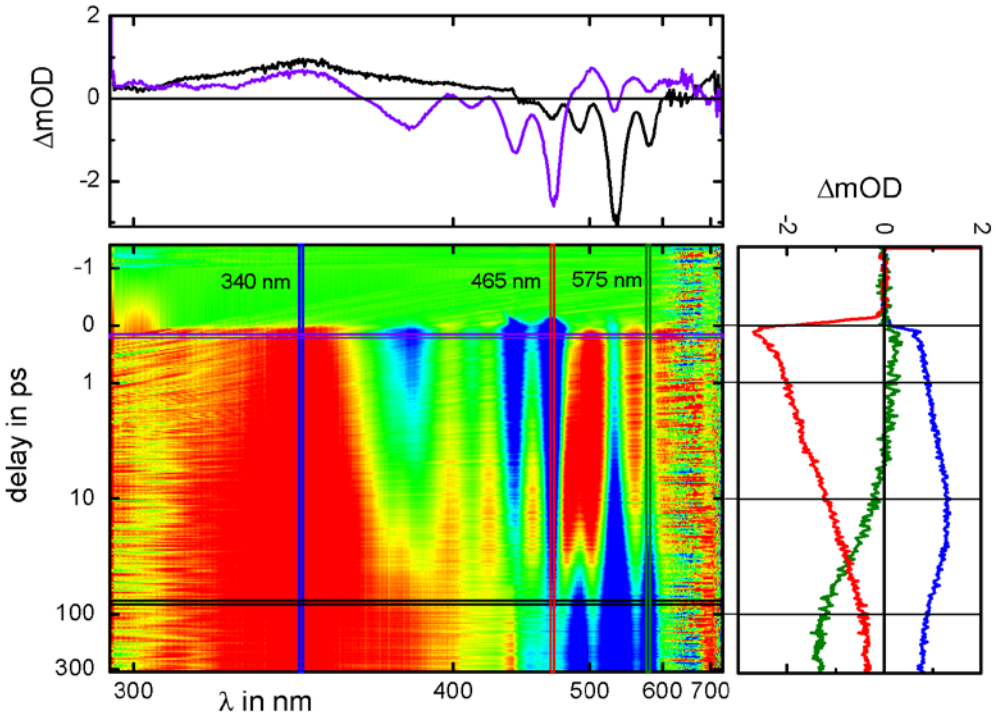

Figure S18: Transient absorption of **D-(Ph-BCO-Ph)-A** in chloroform excited at 435 nm.

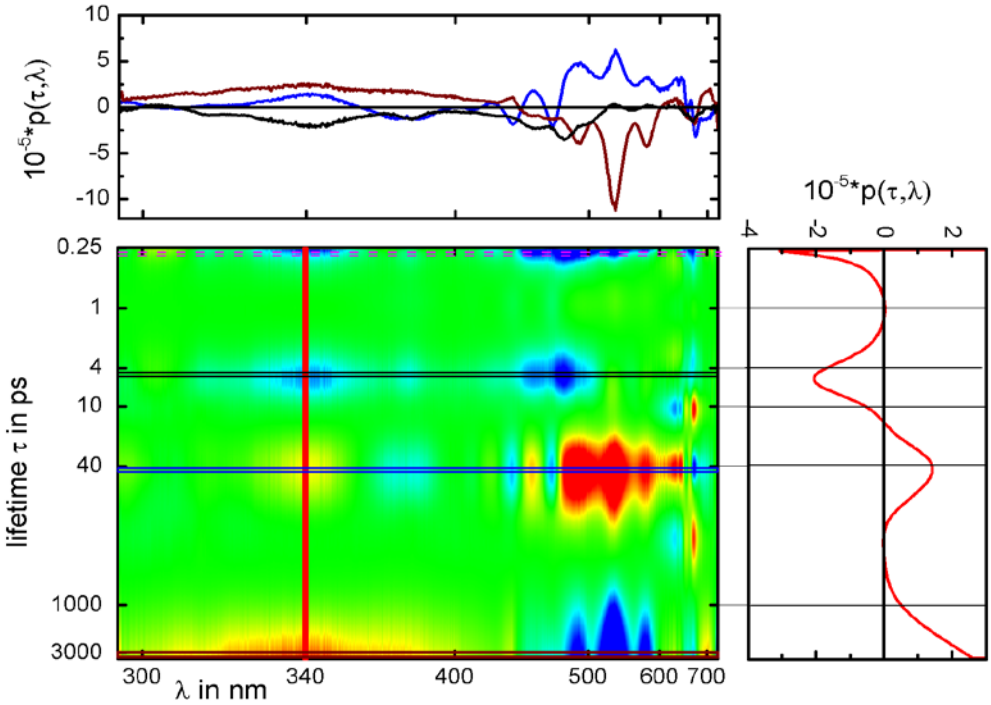

Figure S19: Maximum Entropy analysis of D-(Ph-BCO-Ph)-A, showing four lifetimes. The dashed magenta spectral cut indicating the fs-lifetime is omitted in the top part for clarity

11. Quantum Chemical Calculations of D-(Me4-Ph) and D-(Ph)

The ground state geometries of the donor spacer systems D-(Me4-Ph) and D-(Ph) were optimized at the MP2/def2-SV(P) level of theory [S13]. The vertical excitation energies at the S_0 equilibrium geometry and the excited-state potential energy surfaces have been determined with the coupled cluster (CC2) method and the def2-SV(P) basis set. For the coupled cluster (CC2) and second-order Møller-Plesset (MP2) calculations the resolution-of-the-identity (RI) approximation [S14, S15] implemented in the TURBOMOL software package [S16] was used. All reported energy differences (ΔE) are the differences of the calculated total electronic energies.

The optimization of the conical intersections were carried out with the complete active space self consistent field (CASSCF) method implemented in the Molpro software package [S17] and the 6-31G(d) basis set. A state-averaged CASSCF wavefunction over three roots and an active space comprising four π orbitals (CAS(4/4)) was used for the geometry optimization. Excitation energies and oscillator strengths at these geometries were then calculated using a state-averaged CASSCF wavefunction over four roots.

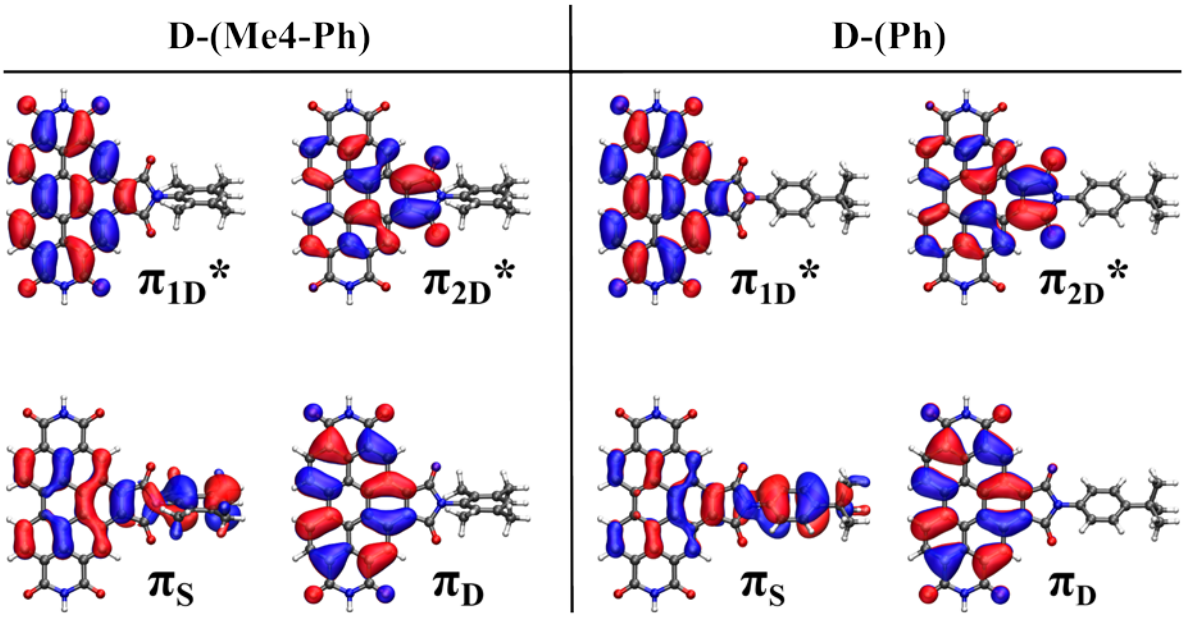

Figure S20: Hartree-Fock molecular orbitals of D-(Me4-Ph) (left) and D-(Ph) (right), obtained with the def2-SV(P) basis set at the MP2-optimized ground state equilibrium geometries.

Table S2. Energy differences and main configurations at the CC2/def2-SV(P) level of theory for the first five electronic states of D-(Me4-Ph) and D-(Ph) at the relevant points discussed in the paper. Oscillator strengths for the corresponding excitations are also given. Ground state minimum energies were chosen as reference points. For each point the electronic state for which the geometry was optimized is highlighted in bold.

			D-(Me4-Ph)		**D-(Ph)**	
Point	State	Main configuration	ΔE (eV)	*f*	ΔE (eV)	*f*
Franck-Condon	**S_0**	**closed shell (π_D^2)**	**0.00**	**-**	**0.00**	**-**
	S_1	$\pi_D^1\pi_{2D}^{*1}$	2.99	0.001	2.99	0.004
	S_2	$\pi_D^1\pi_{1D}^{*1}$ (LE)	3.07	0.545	3.07	0.542
	S_3	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	3.56	0.006	3.48	0.024
	S_4	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	3.70	0.548	3.64	0.574
π-Minimum	S_0	closed shell (π_D^2)	0.12	-	0.12	-
	S_1	**$\pi_D^1\pi_{1D}^{*1}$ (LE)**	**2.87**	**0.571**	**2.87**	**0.570**
	S_2	$\pi_D^1\pi_{2D}^{*1}$	2.94	0.001	2.93	0.004
	S_3	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	3.60	0.001	3.50	0.004
	S_4	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	3.61	0.423	3.53	0.495
d-CT-Minimum	S_0	closed shell (π_S^2)	-	-	0.89	-
	S_1	**$\pi_S^1\pi_{2D}^{*1}$ (d-CT)**	-	-	**2.47**	**0.003**
	S_2	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	-	-	3.07	0.213
	S_3	$\pi_D^1\pi_{2D}^{*1}$	-	-	3.70	0.266
	S_4	$\pi_D^1\pi_{1D}^{*1}$ (LE)	-	-	3.93	0.468
b-CT-Minimum	S_0	closed shell (π_S^2)	-	-	0.50	-
	S_1	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	-	-	2.73	0.004
	S_2	**$\pi_S^1\pi_{1D}^{*1}$ (b-CT)**	-	-	**2.86**	**0.192**
	S_3	$\pi_D^1\pi_{1D}^{*1}$ (LE)	-	-	3.37	0.537
	S_4	$\pi_D^1\pi_{2D}^{*1}$	-	-	3.60	0.003

Table S3. Energy differences and main configurations at the CASSCF/6-31G(d) level of theory for the first four electronic states of D-(Ph) at the relevant points discussed in the paper. Oscillator strengths for the corresponding excitations are also given. The ground state minimum energy was chosen as reference point. For each point the electronic state for which the geometry was optimized is highlighted in bold.

Point	State	Main configuration	ΔE (eV)	*f*
Franck-Condon	**S_0**	**closed shell (π_D^2)**	**0.00**	**-**
	S_1	$\pi_D^1\pi_{2D}^{*1}$	4.52	0.005
	S_2	$\pi_D^1\pi_{1D}^{*1}$ (LE)	4.60	1.135
	S_3	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	5.72	0.004
π-Minimum	S_0	closed shell (π_D^2)	0.22	-
	S_1	**$\pi_D^1\pi_{1D}^{*1}$ (LE)**	**4.30**	**1.253**
	S_2	$\pi_D^1\pi_{2D}^{*1}$	4.36	0.001
	S_3	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	5.88	0.003
d-CT-Minimum	S_0	closed shell (π_D^2)	1.53	-
	S_1	**$\pi_S^1\pi_{2D}^{*1}$ (d-CT)**	**3.54**	**0.005**
	S_2	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	4.78	0.233
	S_3	$\pi_D^1\pi_{2D}^{*1}$	6.05	0.210
b-CT-Minimum	S_0	closed shell (π_S^2)	1.21	-
	S_1	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	4.07	0.014
	S_2	**$\pi_S^1\pi_{1D}^{*1}$ (b-CT)**	**4.37**	**0.256**
	S_3	$\pi_D^1\pi_{1D}^{*1}$ (LE)	5.50	1.611
S_2/S_1 Conical Intersection	S_0	closed shell (π_S^2)	1.31	-
	S_1	**$\pi_S^1\pi_{2D}^{*1}$ (d-CT)**	**4.39**	**0.018**
	S_2	**$\pi_S^1\pi_{1D}^{*1}$ (b-CT)**	**4.41**	**0.249**
	S_3	$\pi_D^1\pi_{1D}^{*1}$ (LE)	5.49	1.640
S_1/S_0 Conical Intersection	**S_0**	**closed shell (π_S^2)**	**4.14**	**-**
	S_1	**$\pi_S^1\pi_{2D}^{*1}$ (d-CT)**	**4.18**	**0.001**
	S_2	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	6.12	0.372
	S_3	$\pi_D^1\pi_{2D}^{*1}$	8.03	0.818

Table S4. Calculated vertical excitation energies and oscillator strengths of the D-(Me4-Ph) and D-(Ph) radical anion at the CAM-B3LYP/def2-TZVP level of theory at the UB3LYP/def2-SV(P)-optimized radical anion ground state equilibrium geometries. The calculated energies are compared with the two strong experimental absorption bands of the spectroelectrochemically derived radical anion D-(Me4-Ph).

		D-(Me4-Ph) anion		**D-(Ph) anion**	
transition	Character	ΔE (eV)	*f*	ΔE (eV)	*f*
$D_0 \rightarrow D_5$	$\pi_D^2\pi_{1D}^{*1} \rightarrow \pi_D^1\pi_{1D}^{*2}$	2.07	0.375	2.08	0.378
$D_0 \rightarrow D_{27}$	$\pi_D^2\pi_{1D}^{*1} \rightarrow \pi_D^2\pi_{3D}^{*1}$	4.19	0.118	4.18	0.118
Exp.	-	**1.99**	-	-	-
		4.13	-	-	-

Optimized geometries of D-(Me4-Ph)

S_0-Minimum

MP2/def2-SV(P) optimized

C	6.721342	0.530889	-1.110563
C	5.311962	0.501662	-1.134723
C	4.643319	0.000020	-0.000061
C	5.311961	-0.501626	1.134596
C	6.721340	-0.530841	1.110450
N	3.220833	0.000017	0.000007
C	2.439993	-1.165609	-0.025133
C	1.019193	-0.692346	-0.033066
C	1.019188	0.692350	0.033236
C	2.439980	1.165634	0.025191
C	-0.174996	1.448362	0.019486
C	-1.407543	0.714852	0.042729
C	-1.407537	-0.714870	-0.042366
C	-0.174983	-1.448367	-0.019119
C	-0.184616	2.871625	0.077830
C	-1.380963	3.554024	0.087286
C	-2.630117	2.854781	0.102878
C	-2.647057	1.426327	0.018824
C	-1.350828	5.044720	0.143143
N	-2.602331	5.654748	0.162286
C	-3.857924	5.055672	0.165757
C	-3.845828	3.568938	0.100966
C	-5.062339	2.881594	0.103922
C	-5.083288	1.487605	0.051199
C	-3.895031	0.727783	0.041848
C	-3.895021	-0.727814	-0.041689
C	-2.647047	-1.426353	-0.018524
C	-2.630088	-2.854800	-0.102692
C	-3.845794	-3.568965	-0.101036
C	-5.062306	-2.881623	-0.104178
C	-5.083273	-1.487641	-0.051275
C	-0.184584	-2.871649	-0.077030
C	-1.380931	-3.554034	-0.087080
C	-1.350780	-5.044719	-0.143248
N	-2.602277	-5.654772	-0.162089
C	-3.857867	-5.055692	-0.165987
O	-4.877872	-5.720695	-0.209661
O	-0.325909	-5.700926	-0.164172
O	-4.877941	5.720678	0.209070
O	-0.325963	5.700948	0.163739
O	2.868985	-2.301245	-0.045113
O	2.868958	2.301276	0.045137
H	-2.597168	-6.676251	-0.205768
H	-2.597233	6.676238	0.205706
H	-5.992000	-3.461778	-0.123867
H	-6.056733	-0.988088	-0.056117
H	-6.056746	0.988048	0.055916
H	-5.992040	3.461746	0.123418
H	0.757816	-3.430157	-0.084346
H	0.757775	3.430167	0.084179
C	4.545177	1.029202	-2.319167
C	7.505378	1.088635	-2.271864
C	4.545156	-1.029223	2.319002
C	7.505374	-1.088578	2.271758
H	5.082137	0.824646	-3.260312
H	4.393140	2.121644	-2.239747
H	3.551032	0.557494	-2.392577

H	8.580584	1.127448	-2.028021
H	7.388013	0.466778	-3.178853
H	7.176898	2.112021	-2.526830
H	5.082083	-0.824704	3.260173
H	3.551003	-0.557525	2.392397
H	4.393131	-2.121664	2.239532
H	8.580584	-1.127365	2.027928
H	7.387985	-0.466729	3.178753
H	7.176915	-2.111973	2.526713
C	7.392452	0.000030	-0.000054
H	8.490754	0.000038	-0.000050

π-Minimum

CC2/def2-SV(P) optimized

C	6.749890	0.553874	-1.101406
C	5.338681	0.524468	-1.126306
C	4.670046	-0.000011	-0.000006
C	5.338754	-0.524462	1.126265
C	6.749965	-0.553743	1.101330
N	3.247279	-0.000016	0.000037
C	2.458990	-1.168050	-0.025182
C	1.041791	-0.689570	-0.033543
C	1.041791	0.689535	0.033673
C	2.458988	1.168017	0.025283
C	-0.161960	1.459751	0.014303
C	-1.410049	0.708476	0.041670
C	-1.410050	-0.708501	-0.041637
C	-0.161964	-1.459780	-0.014204
C	-0.180752	2.857839	0.069767
C	-1.405399	3.554219	0.072620
C	-2.639827	2.852449	0.092536
C	-2.649931	1.417575	0.014169
C	-1.376444	5.030598	0.122176
N	-2.635949	5.640351	0.133178
C	-3.892800	5.040745	0.135585
C	-3.871193	3.561238	0.082108
C	-5.098577	2.863426	0.088561
C	-5.117107	1.478907	0.042201
C	-3.895943	0.715522	0.039430
C	-3.895943	-0.715534	-0.039554
C	-2.649937	-1.417594	-0.014209
C	-2.639835	-2.852468	-0.092564
C	-3.871205	-3.561251	-0.082211
C	-5.098585	-2.863433	-0.088766
C	-5.117111	-1.478914	-0.042407
C	-0.180760	-2.857870	-0.069648
C	-1.405411	-3.554244	-0.072556
C	-1.376461	-5.030624	-0.122093
N	-2.635968	-5.640372	-0.133114
C	-3.892815	-5.040758	-0.135689
O	-4.928995	-5.706822	-0.171576
O	-0.344396	-5.701735	-0.144389
O	-4.928981	5.706815	0.171368
O	-0.344378	5.701704	0.144535
O	2.885355	-2.315176	-0.045298
O	2.885353	2.315144	0.045398
H	-2.630948	-6.664318	-0.170511
H	-2.630927	6.664299	0.170514

H	-6.025895	-3.449071	-0.103862
H	-6.084839	-0.967755	-0.051527
H	-6.084838	0.967753	0.051258
H	-6.025886	3.449069	0.103575
H	0.755634	-3.429678	-0.076515
H	0.755646	3.429642	0.076698
C	4.570409	1.071019	-2.301143
C	7.533512	1.134425	-2.251856
C	4.570559	-1.071099	2.301112
C	7.533665	-1.134325	2.251711
H	5.111251	0.890516	-3.245611
H	4.408505	2.160391	-2.198387
H	3.579473	0.592441	-2.385663
H	8.609162	1.170112	-2.006826
H	7.417407	0.529531	-3.171007
H	7.203455	2.162308	-2.488134
H	5.111410	-0.890564	3.245569
H	3.579583	-0.592609	2.385665
H	4.408747	-2.160484	2.198343
H	8.609312	-1.169897	2.006651
H	7.417530	-0.529520	3.170916
H	7.203703	-2.162257	2.487907
C	7.421358	0.000125	-0.000031
H	8.520342	0.000243	-0.000009

Optimized geometries of D-(Ph)

S_0-Minimum

MP2/def2-SV(P) optimized

C	2.9560790	2.8505630	-0.0050240
C	1.7095020	3.5531590	-0.0455160
C	2.9676580	1.4199500	-0.0353340
C	4.1742300	3.5599540	-0.0342300
C	1.7255840	0.7143240	0.0166900
C	4.2132400	0.7185150	0.0134600
C	5.4041690	1.4739310	-0.0061350
C	5.3882840	2.8689990	-0.0062040
C	0.4956200	1.4508520	-0.0330490
C	0.5107090	2.8752690	-0.0303320
C	4.2081580	-0.7391300	-0.0169490
C	1.7205650	-0.7176750	-0.0135630
C	2.9578560	-1.4319520	0.0338100
C	0.4857080	-1.4456840	0.0395880
C	5.3938450	-1.5028170	-0.0000920
C	2.9362640	-2.8624280	0.0023540
C	5.3682730	-2.8977390	-0.0018520
C	0.4908380	-2.8701620	0.0344750
C	4.1495220	-3.5802920	0.0284170
C	1.6849320	-3.5563940	0.0452400
C	4.1565480	-5.0685400	0.0210400
C	1.6494850	-5.0481350	0.0416280
N	2.8987600	-5.6627660	0.0361600
O	5.1744320	-5.7381370	0.0093940
O	0.6222540	-5.7009710	0.0474360
H	2.8901850	-6.6851450	0.0354280
C	4.1916080	5.0481290	-0.0285040
C	1.6844360	5.0451150	-0.0453700
N	2.9379580	5.6510570	-0.0423160
O	5.2141360	5.7106480	-0.0191420
O	0.6617600	5.7050630	-0.0511960
H	2.9364930	6.6734680	-0.0440800
H	6.2960280	-3.4812980	0.0000580
H	6.3689170	-1.0070020	-0.0245330
H	6.3758090	0.9714020	0.0177570
H	6.3200550	3.4461120	-0.0096050
H	-0.4527310	-3.4262120	0.0534490
H	-0.4290070	3.4378400	-0.0481940
C	-0.7057800	-0.6859440	-0.0023050
C	-0.7009480	0.6994860	0.0150710
C	-2.1263100	-1.1551600	0.0402020
C	-2.1184210	1.1785640	-0.0193510
N	-2.9089450	0.0143190	0.0127750
O	-2.5520520	-2.2911830	0.0765580
O	-2.5361660	2.3174700	-0.0536100
C	-4.3267900	0.0188320	0.0157940
C	-5.0229300	0.8556530	0.8954750
C	-5.0327030	-0.8142700	-0.8642310
C	-6.4224470	0.8642970	0.8840930
C	-6.4285010	-0.8072610	-0.8454660
C	-7.1583790	0.0318430	0.0212280
H	-4.4736480	1.5073150	1.5818410
H	-6.9340280	1.5362380	1.5787340
H	-4.4913310	-1.4705070	-1.5524850
H	-6.9555040	-1.4734080	-1.5377820
C	-8.6849340	0.0041100	-0.0122120
C	-9.1699210	-1.4148920	0.3269040

H	-10.2755520	-1.4517700	0.3244900
H	-8.8040400	-2.1564290	-0.4046620
H	-8.8130550	-1.7175130	1.3280910
C	-9.3044110	0.9785970	0.9941300
H	-9.0093670	2.0219990	0.7844480
H	-10.4062500	0.9216860	0.9312170
H	-9.0141270	0.7316890	2.0307040
C	-9.1650340	0.3929950	-1.4200690
H	-8.8039720	1.4027090	-1.6873920
H	-8.8001440	-0.3146550	-2.1849550
H	-10.2705580	0.3957840	-1.4597200

π-Minimum

CC2/def2-SV(P) optimized

C	2.966789	2.847841	0.007975
C	1.734970	3.553353	-0.030050
C	2.971406	1.411398	-0.028879
C	4.200528	3.551615	-0.024785
C	1.729038	0.707890	0.021239
C	4.214951	0.706058	0.015328
C	5.438697	1.464587	-0.006055
C	5.425368	2.850014	-0.000137
C	0.483749	1.462628	-0.025923
C	0.508027	2.861847	-0.012445
C	4.209815	-0.726692	-0.021956
C	1.723952	-0.710942	-0.018776
C	2.961487	-1.423229	0.026652
C	0.473562	-1.456852	0.033362
C	5.428233	-1.493866	-0.005011
C	2.946583	-2.859605	-0.010252
C	5.405089	-2.879166	-0.011027
C	0.487883	-2.856213	0.019499
C	4.175426	-3.572092	0.017998
C	1.709968	-3.556394	0.032239
C	4.191863	-5.052727	0.007424
C	1.675784	-5.033509	0.022439
N	2.933131	-5.647822	0.026151
O	5.225840	-5.722696	-0.009229
O	0.641530	-5.701288	0.018587
H	2.924477	-6.672364	0.017841
C	4.227477	5.032105	-0.014566
C	1.711277	5.030681	-0.020657
N	2.972929	5.636080	-0.028664
O	5.266218	5.694751	-0.001870
O	0.681797	5.705762	-0.013254
H	2.971549	6.660663	-0.020858
H	6.330407	-3.468118	-0.010843
H	6.397640	-0.986499	-0.031145
H	6.404578	0.950378	0.016617
H	6.354817	3.432414	-0.003689
H	-0.449817	-3.425554	0.033461
H	-0.425663	3.437806	-0.022959
C	-0.727282	-0.682668	-0.008632
C	-0.722351	0.696972	0.021444
C	-2.144087	-1.157062	0.031610
C	-2.135941	1.181424	-0.011250
N	-2.934611	0.014860	0.012308
O	-2.566260	-2.305087	0.060081

O	-2.549945	2.332391	-0.036949
C	-4.352492	0.019634	0.015294
C	-5.049745	0.886545	0.867769
C	-5.059750	-0.843714	-0.837526
C	-6.451113	0.894540	0.856000
C	-6.457071	-0.835979	-0.818792
C	-7.188310	0.032649	0.020655
H	-4.501029	1.560719	1.533032
H	-6.962859	1.589507	1.528484
H	-4.518781	-1.522462	-1.504378
H	-6.984147	-1.525039	-1.489258
C	-8.714808	0.004091	-0.012471
C	-9.199649	-1.403497	0.370396
H	-10.305883	-1.440672	0.367672
H	-8.832684	-2.167988	-0.337434
H	-8.844130	-1.674878	1.381557
C	-9.334180	1.009845	0.962386
H	-9.039088	2.046673	0.719858
H	-10.436668	0.951047	0.901404
H	-9.043688	0.796021	2.006822
C	-9.193443	0.347960	-1.432240
H	-8.833217	1.349626	-1.731284
H	-8.826664	-0.383453	-2.174354
H	-10.299541	0.348217	-1.473307

d-CT-Minimum

CC2/def2-SV(P) optimized

C	2.952927	2.857187	0.133563
C	1.713174	3.561476	0.133593
C	2.952093	1.425130	0.032418
C	4.179982	3.565140	0.135583
C	1.709061	0.723058	0.051214
C	4.201742	0.719426	0.046446
C	5.395989	1.467786	0.062072
C	5.389145	2.866235	0.128671
C	0.482202	1.456891	0.045708
C	0.508608	2.875531	0.123196
C	4.195891	-0.740274	-0.051411
C	1.703251	-0.724207	-0.052127
C	2.940723	-1.436083	-0.035332
C	0.470628	-1.448333	-0.044615
C	5.384163	-1.498043	-0.068994
C	2.930066	-2.868117	-0.136379
C	5.366148	-2.896406	-0.135222
C	0.485696	-2.867147	-0.122098
C	4.151487	-3.585739	-0.140167
C	1.684788	-3.562590	-0.134382
C	4.162798	-5.067763	-0.219187
C	1.645839	-5.046622	-0.211422
N	2.900047	-5.662288	-0.229990
O	5.185908	-5.748673	-0.263927
O	0.613386	-5.712442	-0.249459
H	2.891274	-6.684633	-0.285750
C	4.203116	5.047009	0.214994
C	1.686062	5.045754	0.211088
N	2.945116	5.651488	0.227982
O	5.231638	5.719804	0.258347
O	0.658948	5.719672	0.250970

H	2.944509	6.673856	0.284035
H	6.297485	-3.475356	-0.159202
H	6.357585	-0.996813	-0.070156
H	6.365425	0.958888	0.061226
H	6.325068	3.437781	0.151699
H	-0.456466	-3.428105	-0.139328
H	-0.429055	3.443928	0.142150
C	-0.750596	-0.706492	-0.063946
C	-0.744830	0.724709	0.067173
C	-2.070245	-1.232611	-0.058921
C	-2.060214	1.261225	0.062864
N	-2.956928	0.017925	0.003820
O	-2.555409	-2.366682	-0.070299
O	-2.536449	2.399232	0.072850
C	-4.300512	0.023144	0.005564
C	-5.032979	1.182566	0.452091
C	-5.047333	-1.129751	-0.435989
C	-6.417376	1.171501	0.453107
C	-6.427397	-1.093704	-0.434197
C	-7.161056	0.044913	0.011120
H	-4.479394	2.053737	0.807879
H	-6.935240	2.062574	0.819847
H	-4.506896	-2.009579	-0.790060
H	-6.963900	-1.976895	-0.798861
C	-8.677534	0.008340	-0.008215
C	-9.151891	-1.158268	0.877943
H	-10.257388	-1.188881	0.887356
H	-8.789014	-2.133280	0.507936
H	-8.799232	-1.028607	1.917541
C	-9.301674	1.306507	0.510969
H	-9.011952	2.175320	-0.106793
H	-10.402661	1.221372	0.472904
H	-9.017973	1.505572	1.559977
C	-9.141560	-0.217000	-1.459587
H	-8.780550	0.595406	-2.116573
H	-8.779469	-1.178233	-1.864784
H	-10.246862	-0.227998	-1.495846

b-CT-Minimum

CC2/def2-SV(P) optimized

C	2.9640882	2.8569813	0.0146457
C	1.7231763	3.5625637	-0.0262539
C	2.9694561	1.4148799	-0.0248754
C	4.1887479	3.5613970	-0.0061302
C	1.7287629	0.7117477	0.0209651
C	4.2164837	0.7066819	0.0192251
C	5.4253859	1.4667950	0.0121672
C	5.4093908	2.8535112	0.0260379
C	0.4835448	1.4719498	-0.0285280
C	0.5081427	2.8769783	-0.0133071
C	4.2098207	-0.7333188	-0.0298527
C	1.7221542	-0.7161108	-0.0148538
C	2.9567839	-1.4303248	0.0224547
C	0.4703822	-1.4650964	0.0432237
C	5.4118687	-1.5042627	-0.0311647
C	2.9382504	-2.8723040	-0.0176376
C	5.3833533	-2.8907602	-0.0452568
C	0.4824239	-2.8703125	0.0267163

C	4.1566257	-3.5876810	-0.0053051
C	1.6913372	-3.5667125	0.0313909
C	4.1687097	-5.0628461	-0.0258173
C	1.6500029	-5.0443257	0.0177562
N	2.9033139	-5.6578693	0.0061552
O	5.1896906	-5.7530688	-0.0582340
O	0.6133181	-5.7132045	0.0231194
H	2.8965032	-6.6815116	-0.0072920
C	4.2141920	5.0364002	0.0135716
C	1.6951823	5.0404872	-0.0131154
N	2.9539911	5.6427541	-0.0101806
O	5.2415095	5.7174619	0.0387567
O	0.6645025	5.7186115	-0.0118657
H	2.9564631	6.6664191	0.0030908
H	6.3097783	-3.4784008	-0.0606359
H	6.3843480	-1.0030311	-0.0677799
H	6.3935666	0.9568750	0.0420828
H	6.3411341	3.4328142	0.0352738
H	-0.4501517	-3.4454469	0.0457231
H	-0.4193904	3.4603973	-0.0275112
C	-0.7216061	-0.6931834	-0.0032872
C	-0.7149842	0.7109381	0.0296098
C	-2.0906250	-1.1904135	0.0696254
C	-2.0797621	1.2196399	-0.0386930
N	-2.9585388	0.0192771	0.0411298
O	-2.5254937	-2.3265804	0.1389299
O	-2.5052683	2.3573529	-0.1345423
C	-4.3261428	0.0253221	0.0107075
C	-5.0618307	1.2564958	0.1178205
C	-5.0760909	-1.1992889	-0.0779710
C	-6.4484310	1.2494721	0.1034278
C	-6.4587470	-1.1655762	-0.0918076
C	-7.1962153	0.0484842	-0.0000924
H	-4.5264299	2.2019247	0.2076669
H	-6.9610473	2.2122183	0.1892828
H	-4.5539053	-2.1531052	-0.1533561
H	-6.9896278	-2.1207789	-0.1744599
C	-8.7117010	0.0096172	-0.0191211
C	-9.1951915	-0.8459336	1.1669811
H	-10.3007823	-0.8711321	1.1765558
H	-8.8333393	-1.8871248	1.1009426
H	-8.8493820	-0.4175879	2.1255370
C	-9.3339024	1.4040676	0.0922993
H	-9.0361546	2.0532772	-0.7505397
H	-10.4349053	1.3140168	0.0718926
H	-9.0570512	1.9009311	1.0394275
C	-9.1667828	-0.6321666	-1.3435751
H	-8.8007906	-0.0482486	-2.2078587
H	-8.8037554	-1.6699986	-1.4462338
H	-10.2718358	-0.6537851	-1.3817955

S_0-Minimum

CASSCF(4/4)/6-31G(d) optimized

C	2.951726	2.826309	-0.085466
C	1.694694	3.522924	-0.102531
C	2.965412	1.415705	-0.043306
C	4.153769	3.532733	-0.110137
C	1.719190	0.707473	-0.018915
C	4.199849	0.724782	-0.025820
C	5.375446	1.465641	-0.051660
C	5.354257	2.848498	-0.093208
C	0.503563	1.428798	-0.037395
C	0.520165	2.858066	-0.079836
C	4.195647	-0.744759	0.018709
C	1.715133	-0.712890	0.023581
C	2.957276	-1.428426	0.042055
C	0.495409	-1.427068	0.047846
C	5.366984	-1.492508	0.038977
C	2.935506	-2.838927	0.084297
C	5.337876	-2.875219	0.080639
C	0.503803	-2.856403	0.090233
C	4.133488	-3.552396	0.103268
C	1.674504	-3.528151	0.107345
C	4.127320	-5.022960	0.147317
C	1.658441	-5.008338	0.150424
N	2.886821	-5.624689	0.166863
O	5.143231	-5.701520	0.166201
O	0.629604	-5.663730	0.170424
H	2.880684	-6.621239	0.196695
C	4.156024	5.003308	-0.154179
C	1.687115	5.003179	-0.145572
N	2.919002	5.612307	-0.167885
O	5.175801	5.675893	-0.177878
O	0.662063	5.664604	-0.160698
H	2.918573	6.608877	-0.197670
H	6.248301	-3.439517	0.096015
H	6.320546	-1.010699	0.022731
H	6.326231	0.978243	-0.039924
H	6.267894	3.407444	-0.112908
H	-0.422779	-3.392504	0.108761
H	-0.403324	3.399604	-0.093949
C	-0.691262	-0.675844	0.027319
C	-0.687389	0.684545	-0.011231
C	-2.108233	-1.139997	0.044943
C	-2.101722	1.157115	-0.022059
N	-2.889842	0.010756	0.013160
O	-2.521076	-2.277538	0.070898
O	-2.507635	2.297131	-0.045912
C	-4.319711	0.014304	0.016420
C	-5.010618	0.655690	1.025781
C	-5.018084	-0.625791	-0.996047
C	-6.398718	0.664798	1.019419
C	-6.399875	-0.624155	-0.984039
C	-7.125303	0.023765	0.020164
H	-4.476342	1.157467	1.807512
H	-6.900034	1.178700	1.811875
H	-4.487002	-1.130378	-1.778106
H	-6.914364	-1.133631	-1.773936
C	-8.663188	0.004983	-0.014282
C	-9.161247	-1.456534	0.050623
H	-10.245624	-1.482192	0.033001
H	-8.803055	-2.041979	-0.786904
H	-8.825589	-1.937516	0.962228

C	-9.283030	0.773567	1.167281
H	-8.994415	1.818370	1.163008
H	-10.363664	0.731379	1.096528
H	-8.999833	0.342067	2.120485
C	-9.157089	0.660964	-1.323512
H	-8.816948	1.687959	-1.391628
H	-8.800922	0.131997	-2.198683
H	-10.241432	0.660018	-1.355070

π-Minimum

CASSCF(4/4)/6-31G(d) optimized

C	2.950911	2.821600	-0.083730
C	1.725224	3.520717	-0.100374
C	2.956600	1.401895	-0.041960
C	4.179200	3.514849	-0.107764
C	1.714965	0.701784	-0.018229
C	4.182244	0.708688	-0.024738
C	5.398756	1.452891	-0.050600
C	5.385626	2.824969	-0.091048
C	0.491138	1.443499	-0.036718
C	0.519059	2.837496	-0.077047
C	4.178120	-0.728515	0.017913
C	1.710921	-0.707080	0.022895
C	2.948504	-1.414494	0.040813
C	0.482859	-1.441572	0.047129
C	5.390320	-1.479854	0.038131
C	2.934641	-2.834138	0.082628
C	5.369293	-2.851840	0.078633
C	0.502731	-2.835716	0.087324
C	4.158919	-3.534600	0.100945
C	1.704934	-3.526023	0.105003
C	4.161473	-5.004947	0.144143
C	1.692294	-4.988004	0.146693
N	2.929072	-5.604868	0.162825
O	5.192629	-5.667422	0.162644
O	0.669515	-5.661749	0.166891
H	2.920167	-6.601355	0.192039
C	4.190207	4.985153	-0.151015
C	1.720990	4.982744	-0.142064
N	2.961286	5.592319	-0.164020
O	5.225151	5.641544	-0.174321
O	0.702107	5.662492	-0.157511
H	2.958111	6.588843	-0.193155
H	6.277761	-3.418068	0.094095
H	6.335846	-0.985449	0.022090
H	6.341413	0.952917	-0.038916
H	6.297332	3.385836	-0.110729
H	-0.414058	-3.389301	0.105765
H	-0.394519	3.396486	-0.091204
C	-0.713271	-0.671194	0.026362
C	-0.709399	0.680183	-0.010307
C	-2.129227	-1.137834	0.043868
C	-2.122700	1.155282	-0.021094
N	-2.915037	0.010951	0.013103
O	-2.538042	-2.277315	0.068641
O	-2.524508	2.297233	-0.043837
C	-4.343739	0.014497	0.016394
C	-5.035285	0.660581	1.022531

C	-5.042743	-0.630362	-0.992860
C	-6.423446	0.669838	1.016077
C	-6.424571	-0.628871	-0.980847
C	-7.150124	0.023951	0.020066
H	-4.500839	1.165822	1.801893
H	-6.924679	1.187703	1.806085
H	-4.511445	-1.138409	-1.772509
H	-6.938994	-1.142361	-1.768285
C	-8.688012	0.004948	-0.014267
C	-9.186357	-1.456123	0.057996
H	-10.270798	-1.481891	0.040313
H	-8.827944	-2.045746	-0.776515
H	-8.850781	-1.932536	0.972038
C	-9.308022	0.779501	1.163345
H	-9.019181	1.824221	1.153808
H	-10.388716	0.737084	1.092803
H	-9.024765	0.352812	2.118705
C	-9.182278	0.654193	-1.326721
H	-8.842145	1.680838	-1.400151
H	-8.826031	0.120741	-2.199152
H	-10.266690	0.653001	-1.358260

d-CT-Minimum

CASSCF(4/4)/6-31G(d) optimized

C	2.934665	2.830872	0.116493
C	1.691850	3.533682	0.145686
C	2.934568	1.421781	0.057757
C	4.152074	3.530960	0.145523
C	1.687215	0.721219	0.029172
C	4.173238	0.727314	0.028967
C	5.349936	1.456175	0.059375
C	5.342011	2.846036	0.117089
C	0.486287	1.439135	0.059122
C	0.514337	2.863558	0.117590
C	4.167820	-0.747092	-0.032099
C	1.681922	-0.722881	-0.029741
C	2.924095	-1.432496	-0.059610
C	0.475708	-1.432009	-0.058436
C	5.339152	-1.484515	-0.063711
C	2.913878	-2.841559	-0.118322
C	5.321051	-2.874259	-0.121407
C	0.493342	-2.856700	-0.116925
C	4.126088	-3.550478	-0.148605
C	1.665895	-3.535317	-0.146219
C	4.123053	-5.021961	-0.209738
C	1.652202	-5.007642	-0.207357
N	2.885923	-5.623260	-0.233096
O	5.142296	-5.698057	-0.239050
O	0.631322	-5.679232	-0.235075
H	2.879357	-6.618951	-0.275290
C	4.159806	5.002410	0.206630
C	1.688912	5.006040	0.206829
N	2.927093	5.612683	0.231271
O	5.183961	5.671097	0.234871
O	0.672948	5.685024	0.235618
H	2.927806	6.608395	0.273455
H	6.235826	-3.431001	-0.145180
H	6.290745	-0.999089	-0.044370

H	6.297951	0.963839	0.039049
H	6.260854	3.396084	0.139897
H	-0.433438	-3.392510	-0.137694
H	-0.408474	3.406136	0.139290
C	-0.737660	-0.695932	-0.027768
C	-0.732538	0.711765	0.029697
C	-2.061121	-1.178756	-0.047851
C	-2.052184	1.203870	0.051021
N	-2.915078	0.015389	0.002074
O	-2.514197	-2.328636	-0.092470
O	-2.497388	2.357062	0.095885
C	-4.262463	0.019790	0.002869
C	-5.011626	1.248025	0.090641
C	-5.023437	-1.202640	-0.083903
C	-6.376104	1.236326	0.090803
C	-6.380447	-1.170281	-0.081857
C	-7.115676	0.041079	0.005340
H	-4.476229	2.166972	0.154965
H	-6.882291	2.174334	0.159145
H	-4.498167	-2.127063	-0.148828
H	-6.905263	-2.100151	-0.149508
C	-8.642949	0.003523	0.002629
C	-9.126135	-0.838021	1.209476
H	-10.209224	-0.863726	1.218330
H	-8.772463	-1.859659	1.163904
H	-8.792394	-0.404932	2.145036
C	-9.267213	1.406408	0.106864
H	-8.988730	2.036873	-0.729263
H	-10.346023	1.315304	0.100702
H	-8.987708	1.906733	1.026506
C	-9.125423	-0.650255	-1.315749
H	-8.791824	-0.083094	-2.176715
H	-8.770910	-1.667122	-1.421832
H	-10.208498	-0.675109	-1.328590

b-CT-Minimum

CASSCF(4/4)/6-31G(d) optimized

C	2.957607	2.826259	0.182704
C	1.710551	3.526048	0.227227
C	2.964305	1.404321	0.090070
C	4.165855	3.520346	0.228571
C	1.719775	0.701246	0.043730
C	4.194764	0.712481	0.045821
C	5.393100	1.458252	0.095151
C	5.375323	2.823633	0.183734
C	0.490904	1.450378	0.091313
C	0.521520	2.848149	0.181624
C	4.189017	-0.733141	-0.047654
C	1.714157	-0.702185	-0.045808
C	2.953061	-1.415181	-0.092019
C	0.479381	-1.441518	-0.093546
C	5.381367	-1.488410	-0.096815
C	2.935006	-2.837030	-0.184632
C	5.352681	-2.853638	-0.185361
C	0.498853	-2.839360	-0.183827
C	4.137779	-3.540732	-0.230332
C	1.682518	-3.526827	-0.229278
C	4.133692	-4.997842	-0.325090
C	1.661556	-4.980674	-0.324324
N	2.892622	-5.596327	-0.364025
O	5.149975	-5.687809	-0.370403

O	0.632999	-5.657063	-0.369493
H	2.886017	-6.590236	-0.428722
C	4.173343	4.977488	0.323348
C	1.701167	4.980070	0.322306
N	2.937078	5.585876	0.362156
O	5.195073	5.659305	0.368786
O	0.678008	5.664567	0.367380
H	2.938411	6.579807	0.426865
H	6.260570	-3.421153	-0.222603
H	6.330375	-0.999419	-0.065207
H	6.338176	0.961694	0.063631
H	6.287688	3.383908	0.221079
H	-0.413983	-3.396214	-0.219387
H	-0.386841	3.412269	0.217035
C	-0.702467	-0.673061	-0.045527
C	-0.696889	0.691498	0.043155
C	-2.081805	-1.154093	-0.075597
C	-2.072367	1.183683	0.073037
N	-2.939183	0.018551	-0.001062
O	-2.511465	-2.279015	-0.136863
O	-2.492690	2.312306	0.133840
C	-4.297907	0.023529	-0.001128
C	-5.043617	1.234144	0.230047
C	-5.054380	-1.180129	-0.231805
C	-6.404872	1.224884	0.228313
C	-6.409933	-1.150373	-0.229486
C	-7.150929	0.044881	0.000122
H	-4.518503	2.144145	0.402416
H	-6.911421	2.147239	0.409815
H	-4.539612	-2.095914	-0.403418
H	-6.933736	-2.064959	-0.410909
C	-8.674344	0.008479	-0.008996
C	-9.156862	-0.973584	1.089142
H	-10.239528	-0.998987	1.090827
H	-8.804706	-1.983046	0.921998
H	-8.827063	-0.655552	2.070953
C	-9.298624	1.389093	0.260114
H	-9.020896	2.114833	-0.495158
H	-10.376802	1.298320	0.241016
H	-9.023117	1.776599	1.233920
C	-9.152554	-0.486636	-1.398171
H	-8.819966	0.178187	-2.186393
H	-8.800063	-1.484786	-1.622790
H	-10.235188	-0.509104	-1.412738

S_2/S_1 Conical Intersection

CASSCF(4/4)/6-31G(d) optimized

C	2.965410	2.826646	0.182843
C	1.717545	3.525750	0.227445
C	2.974280	1.400527	0.090209
C	4.171473	3.519506	0.228672
C	1.730613	0.696554	0.043817
C	4.202550	0.708795	0.045914
C	5.407229	1.459664	0.095429
C	5.386599	2.819189	0.183812
C	0.494512	1.454980	0.091834
C	0.524670	2.844613	0.181820
C	4.196812	-0.729642	-0.047646

C	1.725001	-0.697593	-0.045970
C	2.963022	-1.411542	-0.092147
C	0.482917	-1.446120	-0.094188
C	5.395445	-1.490093	-0.096948
C	2.942693	-2.837563	-0.184765
C	5.363895	-2.849444	-0.185324
C	0.501916	-2.835738	-0.184147
C	4.143308	-3.540068	-0.230383
C	1.689428	-3.526590	-0.229568
C	4.138849	-4.993599	-0.324964
C	1.666202	-4.975248	-0.324426
N	2.896633	-5.591310	-0.364230
O	5.154323	-5.687950	-0.370029
O	0.635317	-5.653640	-0.369650
H	2.889834	-6.585011	-0.429178
C	4.178611	4.973096	0.323268
C	1.705925	4.974641	0.322317
N	2.941223	5.580795	0.362333
O	5.199590	5.659237	0.368507
O	0.680484	5.661177	0.367376
H	2.942417	6.574522	0.427288
H	6.269885	-3.420082	-0.222437
H	6.343613	-0.999738	-0.064983
H	6.351437	0.961711	0.063617
H	6.297106	3.382569	0.221079
H	-0.406879	-3.398930	-0.219801
H	-0.379575	3.415078	0.217291
C	-0.691404	-0.665944	-0.044706
C	-0.685788	0.684462	0.042192
C	-2.089668	-1.146961	-0.074625
C	-2.080304	1.176985	0.071917
N	-2.948660	0.018908	-0.001107
O	-2.510255	-2.266223	-0.135594
O	-2.491341	2.299936	0.132396
C	-4.311173	0.023923	-0.001171
C	-5.055383	1.234918	0.229761
C	-5.065838	-1.179731	-0.231532
C	-6.415737	1.226440	0.228058
C	-6.421009	-1.150903	-0.229149
C	-7.163753	0.045273	0.000160
H	-4.532791	2.146122	0.402412
H	-6.922444	2.148671	0.409158
H	-4.553736	-2.096739	-0.403560
H	-6.944553	-2.065533	-0.410120
C	-8.685885	0.008912	-0.008844
C	-9.167572	-0.973660	1.089974
H	-10.250074	-0.999016	1.090608
H	-8.815616	-1.983179	0.923168
H	-8.838895	-0.655152	2.071884
C	-9.310409	1.389435	0.259488
H	-9.033568	2.114910	-0.496305
H	-10.388366	1.297995	0.240303
H	-9.035787	1.777586	1.233224
C	-9.163390	-0.487861	-1.398287
H	-8.831925	0.176555	-2.187149
H	-8.811187	-1.486201	-1.622197
H	-10.245864	-0.510614	-1.411765

S_1/S_0 Conical Intersection

CASSCF(4/4)/6-31G(d) optimized

C	2.926172	2.836541	0.125217
C	1.694505	3.541747	0.156986
C	2.915482	1.428481	0.062690
C	4.154018	3.533625	0.155741
C	1.665183	0.734967	0.032282
C	4.156630	0.730297	0.031329
C	5.331376	1.449258	0.062824
C	5.333913	2.845795	0.124795
C	0.478601	1.451747	0.064566
C	0.512751	2.868208	0.127489
C	4.150150	-0.750827	-0.034318
C	1.658753	-0.733994	-0.032997
C	2.903008	-1.438230	-0.064538
C	0.465859	-1.440562	-0.064206
C	5.318676	-1.479897	-0.066884
C	2.901501	-2.846383	-0.127062
C	5.309109	-2.876314	-0.128843
C	0.487794	-2.857471	-0.127147
C	4.123202	-3.553936	-0.158700
C	1.663681	-3.541044	-0.157699
C	4.123041	-5.024722	-0.224006
C	1.651294	-5.010705	-0.222986
N	2.886965	-5.626172	-0.250490
O	5.142826	-5.701954	-0.254263
O	0.633927	-5.689350	-0.253000
H	2.880383	-6.621500	-0.294728
C	4.166494	5.004340	0.221048
C	1.694722	5.011463	0.222308
N	2.935576	5.616349	0.248675
O	5.192004	5.672890	0.250371
O	0.683116	5.698654	0.253278
H	2.937560	6.611698	0.292927
H	6.228239	-3.426004	-0.153425
H	6.269136	-0.992450	-0.045440
H	6.277591	0.953664	0.040510
H	6.257810	3.387479	0.148530
H	-0.438649	-3.394383	-0.150810
H	-0.408819	3.413429	0.151997
C	-0.785541	-0.717166	-0.031821
C	-0.779126	0.738521	0.033297
C	-2.030627	-1.243923	-0.055384
C	-2.018698	1.275577	0.057729
N	-2.960867	0.015298	0.001455
O	-2.550628	-2.380232	-0.105410
O	-2.533840	2.413452	0.107827
C	-4.236768	0.016976	0.002161
C	-5.019009	1.284894	0.061951
C	-5.030966	-1.240597	-0.056416
C	-6.363086	1.265221	0.061435
C	-6.365558	-1.194213	-0.053919
C	-7.103039	0.047622	0.004567
H	-4.452791	2.189655	0.103942
H	-6.885083	2.194956	0.105238
H	-4.478415	-2.153015	-0.099083
H	-6.909699	-2.112910	-0.096838
C	-8.624667	0.005926	0.002704
C	-9.094041	-0.810289	1.234166
H	-10.175941	-0.835205	1.244189
H	-8.742381	-1.832945	1.213022
H	-8.762162	-0.353404	2.158844

C	-9.257802	1.406753	0.070537
H	-8.987299	2.018124	-0.781957
H	-10.334735	1.304016	0.066036
H	-8.986498	1.933192	0.977714
C	-9.093623	-0.687463	-1.302070
H	-8.762101	-0.142911	-2.178129
H	-8.741165	-1.707103	-1.380050
H	-10.175510	-0.712030	-1.314444

12. Quantum Chemical Calculations of D-(Ph-BCO-Ph)-A, D-(Ph-Ph)-A, D-(Ph-Yn-Ph)-A and D-(Ph-Yn2-Ph)-A

The ground state geometries of the donor spacer acceptor dyads D-(Ph-BCO-Ph)-A, D-(Ph-Ph)-A, D-(Ph-Yn-Ph)-A and D-(Ph-Yn2-Ph)-A were optimized at the B3LYP/6-31G(d) level of theory [S18]. The vertical excitation energies at the S_0 equilibrium geometries have been determined with the coupled cluster (CC2) method and the def2-SV(P) basis set. Due to the large size of the investigated systems geometry optimization of the electronically excited singlet states were performed with the TDDFT method using the CAM-B3LYP functional [S19] and the def2-SV(P) basis set. Excitation energies and oscillator strengths at these geometries were then calculated at the CC2/def2-SV(P) level of theory. The density functional theory (DFT) and time-dependent DFT (TDDFT) calculations were carried out using the Gaussian 09 software package [S20]. For the coupled cluster (CC2) calculations the resolution-of-the-identity (RI) approximation [S14, S15] implemented in the TURBOMOL software package [S16] was used. All reported energy differences (ΔE) are the differences of the calculated total electronic energies.

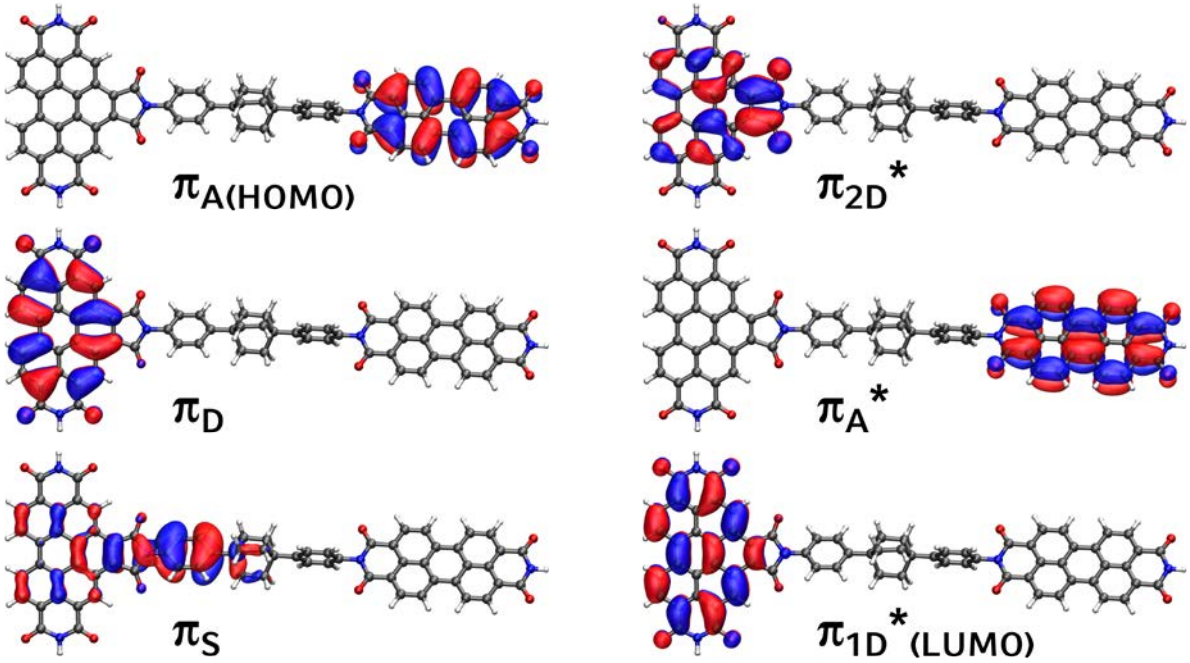

Figure S21: Hartree-Fock molecular orbitals of D-(Ph-BCO-Ph)-A, obtained with the def2-SV(P) basis set at the B3LYP/6-31G(d)-optimized ground state equilibrium geometry.

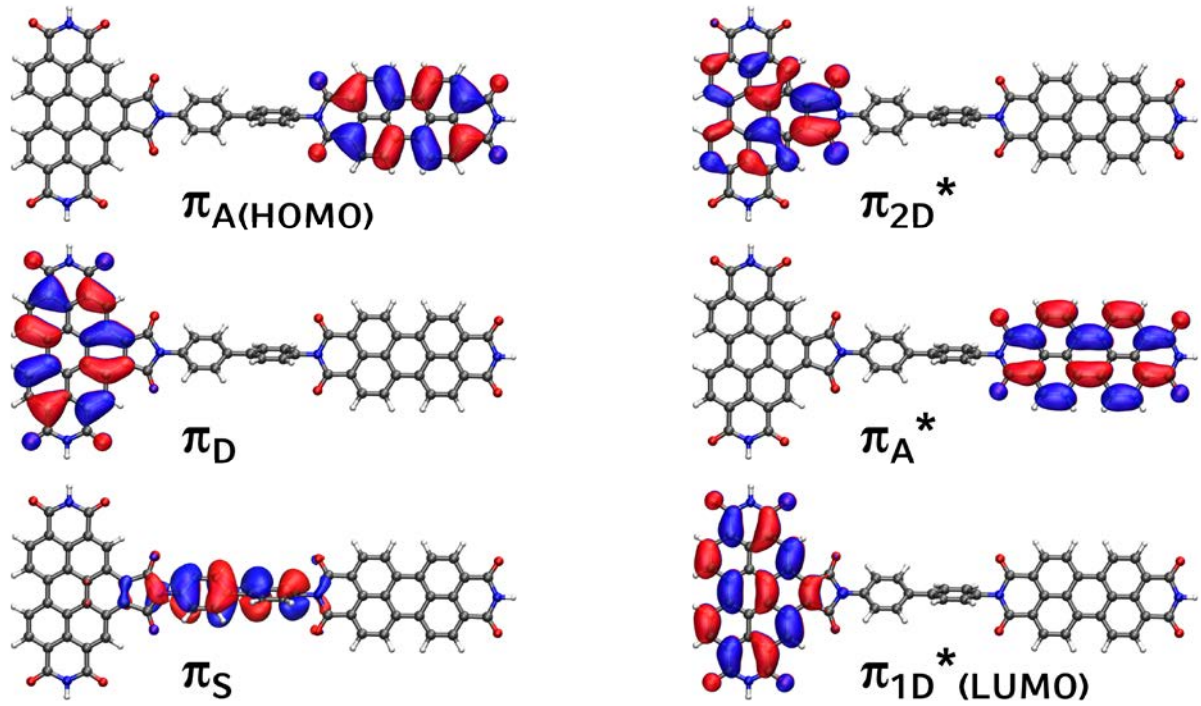

Figure S22: Hartree-Fock molecular orbitals of D-(Ph-Ph)-A, obtained with the def2-SV(P) basis set at the B3LYP/6-31G(d)-optimized ground state equilibrium geometry.

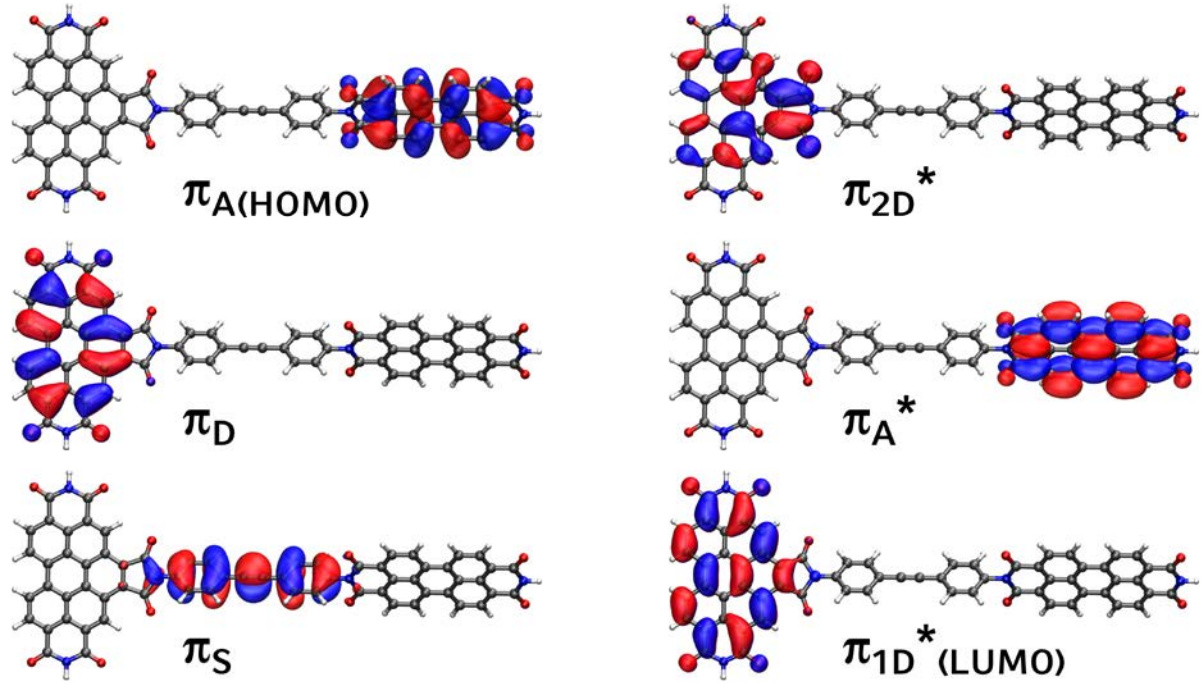

Figure S23: Hartree-Fock molecular orbitals of D-(Ph-Yn-Ph)-A, obtained with the def2-SV(P) basis set at the B3LYP/6-31G(d)-optimized ground state equilibrium geometry.

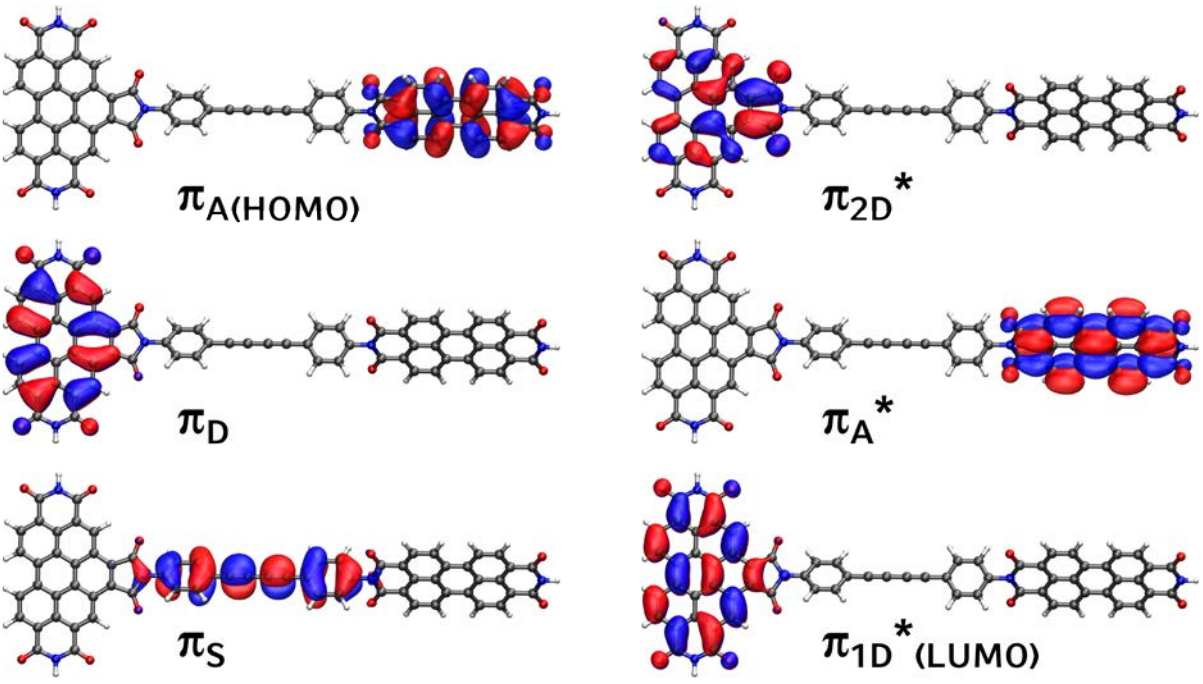

Figure S24: Hartree-Fock molecular orbitals of D-(Ph-Yn2-Ph)-A, obtained with the def2-SV(P) basis set at the B3LYP/6-31G(d)-optimized ground state equilibrium geometry.

Table S5. Energy differences and main configurations at the CC2/def2-SV(P) level of theory for the first five electronic states of D-(Ph-BCO-Ph)-A and D-(Ph-Ph)-A at the relevant points discussed in the paper. For the CC2 calculations the reduced-virtual-space (RVS) approach [S21] was used. All virtual orbitals above 20 eV were omitted in the correlation calculation. Oscillator strengths for the corresponding excitations are also given. Ground state minimum energies were chosen as reference points. For each point the electronic state for which the geometry was optimized is highlighted in bold.

			D-(Ph-BCO-Ph)-A		**D-(Ph-Ph)-A**	
Point	State	Main configuration	ΔE (eV)	*f*	ΔE (eV)	*f*
Franck-Condon	**S_0**	**closed shell (π_D^2)**	**0.00**	**-**	**0.00**	**-**
	S_1	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	2.99	1.024	2.99	1.081
	S_2	$\pi_D^1\pi_{2D}^{*1}$	3.28	0.008	3.27	0.009
	S_3	$\pi_D^1\pi_{1D}^{*1}$ (LE-donor)	3.36	0.586	3.35	0.580
	S_4	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	3.84	0.036	3.75	0.031
π-Minimum	S_0	closed shell (π_D^2)	0.25	-	0.28	-
	S_1	**$\pi_D^1\pi_{1D}^{*1}$ (LE-donor)**	**3.16**	**0.622**	**3.14**	**0.618**
	S_2	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	3.17	1.019	3.15	1.083
	S_3	$\pi_D^1\pi_{2D}^{*1}$	3.26	0.007	3.25	0.005
	S_4	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	3.96	0.660	4.00	0.630
d-CT-Minimum	S_0	closed shell	0.86	-	0.94	-
	S_1	**$\pi_S^1\pi_{2D}^{*1}$ (d-CT)**	**2.66**	**0.001**	**2.67**	**0.001**
	S_2	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	3.20	0.160	3.20	0.291
	S_3	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	3.44	1.039	3.53	1.180
	S_4	$\pi_D^1\pi_{2D}^{*1}$	3.66	0.410	3.68	0.008
b-CT-Minimum	S_0	closed shell	0.44	-	0.61	-
	S_1	**$\pi_S^1\pi_{1D}^{*1}$ (b-CT)**	**3.00**	**0.144**	**3.06**	**0.270**
	S_2	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	3.01	0.926	3.11	0.976
	S_3	$\pi_D^1\pi_{1D}^{*1}$ (LE-donor)	3.16	0.451	3.31	0.518
	S_4	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	3.28	0.136	3.43	0.015

Table S6. Energy differences and main configurations at the CC2/def2-SV(P) level of theory for the first five electronic states of D-(Ph-Yn-Ph)-A and D-(Ph-Yn2-Ph)-A at the relevant points discussed in the paper. For the CC2 calculations the reduced-virtual-space (RVS) approach [S21] was used. All virtual orbitals above 20 eV were omitted in the correlation calculation. Oscillator strengths for the corresponding excitations are also given. Ground state minimum energies were chosen as reference points. For each point the electronic state for which the geometry was optimized is highlighted in bold.

			D-(Ph-Yn-Ph)-A		**D-(Ph-Yn2-Ph)-A**	
Point	State	Main configuration	ΔE (eV)	*f*	ΔE (eV)	*f*
Franck-Condon	**S_0**	**closed shell (π_D^2)**	**0.00**	**-**	**0.00**	**-**
	S_1	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	2.99	1.115	2.98	1.151
	S_2	$\pi_D^1\pi_{2D}^{*1}$	3.26	0.012	3.26	0.011
	S_3	$\pi_D^1\pi_{1D}^{*1}$ (LE-donor)	3.35	0.579	3.35	0.577
	S_4	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	3.69	0.028	3.80	0.001
π-Minimum	S_0	closed shell (π_D^2)	0.29	-	0.29	-
	S_1	**$\pi_D^1\pi_{1D}^{*1}$ (LE-donor)**	**3.05**	**0.618**	**3.10**	**0.617**
	S_2	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	3.06	1.120	3.11	1.138
	S_3	$\pi_D^1\pi_{2D}^{*1}$	3.14	0.008	3.20	0.006
	S_4	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	3.65	0.437	3.73	0.560
d-CT-Minimum	S_0	closed shell	0.69	-	0.67	-
	S_1	**$\pi_S^1\pi_{2D}^{*1}$ (d-CT)**	**2.50**	**0.001**	**2.58**	**0.001**
	S_2	$\pi_S^1\pi_{1D}^{*1}$ (b-CT)	3.03	0.314	3.09	0.289
	S_3	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	3.35	1.212	3.35	1.246
	S_4	$\pi_D^1\pi_{2D}^{*1}$	3.49	0.287	3.49	0.482
b-CT-Minimum	S_0	closed shell	0.40	-	0.39	-
	S_1	**$\pi_S^1\pi_{1D}^{*1}$ (b-CT)**	**2.88**	**0.363**	**2.97**	**0.374**
	S_2	$\pi_A^1\pi_A^{*1}$ (LE-acceptor)	2.95	1.112	3.05	1.150
	S_3	$\pi_D^1\pi_{1D}^{*1}$ (LE-donor)	3.08	0.587	3.32	0.583
	S_4	$\pi_S^1\pi_{2D}^{*1}$ (d-CT)	3.28	0.007	3.43	0.008

Optimized geometries of D-(Ph-BCO-Ph)-A

S_0-Minimum

B3LYP/6-31G(d) optimized

C	8.4468490	2.7072880	-0.4697960
C	7.2156080	3.4323870	-0.6022990
C	8.4178690	1.3013210	-0.2318120
C	9.6843050	3.3729270	-0.5723660
C	7.1539600	0.6367180	-0.1288130
C	9.6428550	0.5798970	-0.0990710
C	10.8501780	1.2883500	-0.2091480
C	10.8724390	2.6590510	-0.4415500
C	5.9487980	1.3906510	-0.2656660
C	6.0079210	2.7953370	-0.5037420
C	9.5976430	-0.8626880	0.1459650
C	7.1097770	-0.7734570	0.1114870
C	8.3295620	-1.5110070	0.2462930
C	5.8596100	-1.4550400	0.2192090
C	10.7582550	-1.6403230	0.2877900
C	8.2700480	-2.9158840	0.4849610
C	10.6941980	-3.0095570	0.5209670
C	5.8301970	-2.8606350	0.4575410
C	9.4633190	-3.6525490	0.6204930
C	6.9955210	-3.5674380	0.5854420
C	9.4301260	-5.1152760	0.8697690
C	6.9235910	-5.0343130	0.8325520
N	8.1564480	-5.6743430	0.9522070
O	10.4281650	-5.8064510	0.9974070
O	5.8820990	-5.6605570	0.9282850
H	8.1209470	-6.6748170	1.1220610
C	9.7429640	4.8354470	-0.8190770
C	7.2358610	4.9006300	-0.8500160
N	8.5067050	5.4677470	-0.9350590
O	10.7825760	5.4675390	-0.9178420
O	6.2355470	5.5863000	-0.9736490
H	8.5341360	6.4685980	-1.1041930
H	11.5970890	-3.6011990	0.6292920
H	11.7360890	-1.1793930	0.2166630
H	11.7970560	0.7708770	-0.1129200
H	11.8108610	3.1970210	-0.5249790
H	4.8777730	-3.3719740	0.5386190
H	5.0893180	3.3616100	-0.6068960
C	4.6887380	-0.6754040	0.0792120
C	4.7310240	0.6817940	-0.1506100
C	3.2568200	-1.1012260	0.1504710
C	3.3278920	1.1922260	-0.2420860
N	2.4930280	0.0693500	-0.0512030
O	2.8102580	-2.2138960	0.3396420
O	2.9513870	2.3297450	-0.4357040
C	1.0643740	0.1120760	-0.0479940
C	0.3931320	1.1391450	0.6164730
C	0.3303290	-0.8782420	-0.7085870
C	-1.0013150	1.1720470	0.6157310
C	-1.0595520	-0.8363600	-0.6843090
C	-1.7641380	0.1851760	-0.0239010
H	0.9524130	1.9164400	1.1231600
H	-1.4884130	1.9889060	1.1354640
H	0.8416600	-1.6819620	-1.2245510
H	-1.6031000	-1.6220090	-1.2005740
C	-3.2950760	0.1937400	-0.0363170
C	-3.9028590	1.3670460	0.7657540
C	-3.8186430	0.3113820	-1.4934830

C	-3.8590460	-1.1192890	0.5714970
C	-5.4531440	1.2662720	0.8125810
H	-3.5993990	2.3169280	0.3086030
H	-3.5010270	1.3667640	1.7856870
C	-5.3697600	0.4071760	-1.5274760
H	-3.4805520	-0.5556930	-2.0722570
H	-3.3678570	1.1907300	-1.9678700
H	-3.3721990	-1.9878950	0.1165370
H	-3.6012200	-1.1488860	1.6375870
C	-5.3972510	-1.2070590	0.3735250
C	-5.9719480	0.1453000	-0.1279080
H	-5.9102180	2.2192340	0.5223840
H	-5.7886410	1.0661730	1.8364020
H	-5.7690610	-0.3183670	-2.2456260
H	-5.6795240	1.3993770	-1.8781160
H	-5.6520520	-1.9861430	-0.3557490
H	-5.8799640	-1.4992940	1.3116460
C	-7.5033240	0.1207870	-0.1250020
C	-8.1983040	-0.1236130	1.0724910
C	-8.2698030	0.3477000	-1.2766680
C	-9.5883790	-0.1492970	1.1198070
H	-7.6472820	-0.2985980	1.9917710
C	-9.6646340	0.3272080	-1.2402890
H	-7.7858400	0.5465730	-2.2258530
C	-10.3237110	0.0761130	-0.0423410
H	-10.1038180	-0.3409410	2.0559790
H	-10.2382410	0.5026610	-2.1452920
N	-11.7697700	0.0473070	-0.0009550
C	-12.4119050	-1.1177620	-0.4681110
C	-13.8950030	-1.1253830	-0.4096310
O	-11.7686470	-2.0629140	-0.8949500
C	-14.5798000	-2.2444980	-0.8499180
C	-14.6158790	-0.0123280	0.0868310
C	-15.9775240	-2.2833370	-0.8068050
H	-14.0109550	-3.0876040	-1.2272340
C	-13.9129400	1.1306930	0.5390290
C	-16.0447180	-0.0426690	0.1317970
C	-16.7320280	-1.2111530	-0.3263640
H	-16.4684380	-3.1812640	-1.1623250
C	-12.4300080	1.1847450	0.5067320
C	-14.6155210	2.2206300	1.0223720
C	-16.7507160	1.0961580	0.6340700
C	-18.2016920	-1.2446050	-0.2758490
O	-11.8013830	2.1556450	0.8961370
C	-16.0135980	2.2002540	1.0669660
H	-14.0603150	3.0874440	1.3646720
C	-18.2206740	1.0663080	0.6779790
C	-18.9097240	-0.1042250	0.2236780
C	-18.9346830	-2.3547050	-0.6999490
H	-16.5188160	3.0771670	1.4535850
C	-18.9719010	2.1444010	1.1499530
C	-20.3392880	-0.1352030	0.2701400
C	-20.3320210	-2.3798690	-0.6509030
H	-18.4262090	-3.2321400	-1.0808520
C	-20.3692650	2.1090760	1.1916490
H	-18.4781630	3.0434480	1.4984360
C	-21.0368870	-1.2892690	-0.1743170
C	-21.0557920	0.9883060	0.7604500
H	-20.8852110	-3.2515840	-0.9847440
H	-20.9368060	2.9565520	1.5618170
C	-22.5181290	-1.3423370	-0.1340830
C	-22.5374300	0.9770220	0.8170590
N	-23.1375470	-0.1959250	0.3614960
O	-23.1786250	-2.3026100	-0.4998530
O	-23.2136380	1.9082800	1.2265530
H	-24.1519780	-0.2179920	0.3947110

π-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	8.417235	2.713393	-0.495420
C	7.200480	3.427125	-0.628001
C	8.392197	1.308255	-0.247987
C	9.656650	3.380405	-0.605550
C	7.136554	0.643667	-0.136759
C	9.612363	0.595318	-0.115483
C	10.840262	1.314074	-0.235019
C	10.856237	2.670606	-0.473684
C	5.918830	1.404451	-0.277576
C	5.972243	2.778212	-0.520627
C	9.576487	-0.820255	0.133810
C	7.101248	-0.750338	0.110831
C	8.321589	-1.474148	0.243823
C	5.846506	-1.451813	0.231588
C	10.766418	-1.596557	0.275868
C	8.275149	-2.878719	0.491386
C	10.713388	-2.952131	0.514651
C	5.829902	-2.826548	0.474458
C	9.479158	-3.603934	0.624242
C	7.023619	-3.533525	0.602003
C	9.457738	-5.061226	0.880758
C	6.962883	-4.990742	0.856680
N	8.194260	-5.623086	0.973096
O	10.458280	-5.733278	1.003917
O	5.929350	-5.611964	0.960194
H	8.163274	-6.624832	1.148897
C	9.709222	4.837195	-0.860891
C	7.213800	4.885321	-0.883508
N	8.475806	5.458388	-0.976539
O	10.742655	5.461051	-0.964444
O	6.213061	5.554861	-1.006251
H	8.495708	6.460434	-1.152236
H	11.621172	-3.548382	0.623650
H	11.741293	-1.117845	0.195363
H	11.789509	0.789409	-0.136733
H	11.793182	3.223056	-0.565369
H	4.883220	-3.360338	0.566631
H	5.053824	3.356728	-0.627721
C	4.662044	-0.663618	0.088888
C	4.695725	0.674496	-0.150878
C	3.233461	-1.097825	0.167039
C	3.290393	1.177959	-0.239695
N	2.464636	0.059479	-0.039087
O	2.806067	-2.203814	0.363262
O	2.919097	2.303718	-0.437404
C	1.040966	0.094267	-0.033049
C	0.364055	1.151960	0.568395
C	0.308443	-0.933868	-0.629429
C	-1.028540	1.178561	0.570224
C	-1.079066	-0.897580	-0.604595
C	-1.786047	0.154837	-0.005935
H	0.920812	1.968013	1.028157
H	-1.518581	2.029181	1.043857
H	0.822267	-1.771287	-1.100506
H	-1.621568	-1.721075	-1.074678
C	-3.312064	0.155118	-0.018916
C	-3.923523	1.374381	0.692704
C	-3.833047	0.165740	-1.473103
C	-3.871760	-1.106386	0.675406
C	-5.462083	1.247574	0.776775
H	-3.641517	2.291836	0.149418

H	-3.502304	1.466408	1.706355
C	-5.373333	0.292914	-1.511577
H	-3.513932	-0.759939	-1.978951
H	-3.360223	0.996061	-2.022377
H	-3.360697	-2.006939	0.301962
H	-3.637392	-1.045625	1.751908
C	-5.395897	-1.227563	0.448916
C	-5.974641	0.091122	-0.109812
H	-5.947884	2.186408	0.465364
H	-5.774291	1.070776	1.818756
H	-5.790927	-0.450698	-2.208736
H	-5.667593	1.284565	-1.893933
H	-5.624979	-2.039259	-0.262423
H	-5.897497	-1.496719	1.390881
C	-7.501095	0.066416	-0.108827
C	-8.196945	-0.133815	1.092259
C	-8.263658	0.257304	-1.265131
C	-9.584392	-0.151937	1.138048
H	-7.646314	-0.280296	2.024283
C	-9.656079	0.245196	-1.228292
H	-7.777920	0.423171	-2.226612
C	-10.319430	0.037783	-0.027727
H	-10.102817	-0.309326	2.086174
H	-10.229905	0.393273	-2.145540
N	-11.758277	0.018786	0.012345
C	-12.407042	-1.105984	-0.518909
C	-13.892165	-1.106431	-0.462526
O	-11.780494	-2.021865	-0.995355
C	-14.580157	-2.188921	-0.963111
C	-14.603399	-0.017895	0.091801
C	-15.980989	-2.216058	-0.925544
H	-14.012437	-3.019272	-1.387126
C	-13.890546	1.088689	0.606988
C	-16.024560	-0.035968	0.131049
C	-16.719702	-1.168873	-0.392474
H	-16.483613	-3.092885	-1.332316
C	-12.405109	1.125843	0.581282
C	-14.577110	2.153610	1.145724
C	-16.718280	1.079242	0.692989
C	-18.194126	-1.189055	-0.349564
O	-11.776304	2.056835	1.024542
C	-15.978121	2.145180	1.185375
H	-14.008150	2.998273	1.538671
C	-18.192856	1.061827	0.731647
C	-18.889843	-0.072503	0.210338
C	-18.930408	-2.259824	-0.836822
H	-16.479658	3.009216	1.619921
C	-18.928078	2.113876	1.259541
C	-20.311832	-0.090651	0.249770
C	-20.330864	-2.272611	-0.794268
H	-18.425793	-3.123713	-1.267898
C	-20.328613	2.090938	1.294602
H	-18.422545	2.990658	1.662588
C	-21.019664	-1.207387	-0.260707
C	-21.018535	1.008054	0.799405
H	-20.898064	-3.121636	-1.181102
H	-20.895002	2.925555	1.712706
C	-22.503941	-1.244492	-0.227595
C	-22.502835	1.007146	0.848860
N	-23.110748	-0.126486	0.327591
O	-23.162374	-2.167601	-0.646353
O	-23.160377	1.913418	1.304197
H	-24.127616	-0.139529	0.355894

d-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	8.343654	2.794470	0.155033
C	7.113499	3.513411	0.196081
C	8.324751	1.375735	0.069373
C	9.575086	3.481006	0.198704
C	7.071171	0.694117	0.026082
C	9.559679	0.661901	0.028518
C	10.750960	1.382302	0.073808
C	10.762473	2.775844	0.158105
C	5.870592	1.435113	0.068210
C	5.915630	2.854135	0.153864
C	9.534752	-0.806509	-0.060078
C	7.046522	-0.754042	-0.061210
C	8.276234	-1.477895	-0.102853
C	5.821310	-1.453728	-0.104703
C	10.700929	-1.566987	-0.103531
C	8.247059	-2.896437	-0.188591
C	10.665162	-2.960083	-0.188010
C	5.818323	-2.873547	-0.190534
C	9.454479	-3.624405	-0.230578
C	6.993134	-3.573122	-0.231328
C	9.443550	-5.106284	-0.320961
C	6.945827	-5.056590	-0.321560
N	8.184078	-5.686172	-0.358131
O	10.443559	-5.785177	-0.360927
O	5.924046	-5.699777	-0.362055
H	8.163321	-6.701208	-0.419876
C	9.614302	4.962500	0.288771
C	7.116351	4.997526	0.286247
N	8.375186	5.584787	0.324218
O	10.636721	5.607092	0.329747
O	6.116896	5.674973	0.325368
H	8.388791	6.599955	0.385754
H	11.584697	-3.547603	-0.221873
H	11.675287	-1.080709	-0.071981
H	11.708229	0.863172	0.043801
H	11.701402	3.331748	0.193340
H	4.868786	-3.408757	-0.224224
H	4.984777	3.421254	0.186424
C	4.613444	-0.696963	-0.060090
C	4.637691	0.719766	0.022993
C	3.276678	-1.174029	-0.087503
C	3.318420	1.242319	0.050958
N	2.442182	0.048532	-0.017392
O	2.818213	-2.301193	-0.157184
O	2.899113	2.384771	0.120124
C	1.085788	0.071623	-0.013806
C	0.359621	1.309287	-0.007944
C	0.314287	-1.140076	-0.016952
C	-1.016277	1.316359	-0.000565
C	-1.056118	-1.090654	-0.005226
C	-1.775252	0.128803	0.007094
H	0.919266	2.239094	-0.009215
H	-1.517505	2.283307	-0.002130
H	0.838439	-2.090219	-0.028597
H	-1.599694	-2.036878	-0.006710
C	-3.288856	0.119268	-0.001310
C	-3.912786	1.524567	0.046434
C	-3.791818	-0.569147	-1.295372
C	-3.847674	-0.676613	1.203713
C	-5.447321	1.430369	0.201405
H	-3.651648	2.070851	-0.875383

H	-3.488951	2.098428	0.885698
C	-5.328707	-0.453645	-1.407957
H	-3.486759	-1.627781	-1.286116
H	-3.303140	-0.111715	-2.170718
H	-3.318598	-1.634693	1.319130
H	-3.648653	-0.100897	2.123217
C	-5.362097	-0.924821	1.025532
C	-5.945257	-0.006476	-0.070960
H	-5.949046	2.128448	-0.487159
H	-5.746694	1.731518	1.218006
H	-5.747576	-1.425863	-1.710379
H	-5.600988	0.268549	-2.195015
H	-5.556407	-1.973840	0.745585
H	-5.880925	-0.761621	1.981724
C	-7.471309	-0.040107	-0.070553
C	-8.177462	0.309352	1.089322
C	-8.221854	-0.382438	-1.199139
C	-9.565220	0.310494	1.125316
H	-7.637459	0.592171	1.995978
C	-9.614564	-0.379489	-1.173323
H	-7.728230	-0.657839	-2.131248
C	-10.289528	-0.035259	-0.011077
H	-10.092085	0.588121	2.040383
H	-10.179247	-0.653623	-2.066670
N	-11.727634	-0.033783	0.020216
C	-12.379095	-1.276927	-0.008160
C	-13.863412	-1.250438	0.035408
O	-11.752376	-2.307856	-0.064304
C	-14.554295	-2.441547	0.021064
C	-14.572054	-0.028401	0.088461
C	-15.955168	-2.447743	0.059243
H	-13.988982	-3.374438	-0.020688
C	-13.857113	1.190944	0.107112
C	-15.993537	-0.025667	0.123187
C	-16.691476	-1.272159	0.109532
H	-16.459773	-3.413178	0.047193
C	-12.372465	1.211518	0.079949
C	-14.541844	2.384724	0.154956
C	-16.685175	1.223493	0.171058
C	-18.166142	-1.269664	0.149649
O	-11.739566	2.239972	0.107123
C	-15.942853	2.396286	0.185205
H	-13.971574	3.315418	0.169367
C	-18.160002	1.226658	0.204247
	-18.859363	-0.020170	0.194482
C	-18.904806	-2.444457	0.144866
H	-16.442603	3.363616	0.222194
C	-18.893003	2.404286	0.245356
C	-20.281489	-0.017444	0.230333
C	-20.305604	-2.435686	0.181792
H	-18.402314	-3.410492	0.112025
C	-20.293895	2.400883	0.279198
H	-18.385832	3.368400	0.252224
C	-20.991917	-1.243721	0.223560
C	-20.985978	1.211545	0.272725
H	-20.874634	-3.367559	0.177746
H	-20.858439	3.334925	0.311628
C	-22.476806	-1.260746	0.261507
C	-22.470797	1.234245	0.310594
N	-23.081389	-0.012090	0.301543
O	-23.136569	-2.273298	0.258498
O	-23.125672	2.249316	0.347107
H	-24.098448	-0.010151	0.327458

b-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	12.338302	-2.827385	0.001047
C	11.103878	-3.540537	0.007943
C	12.331613	-1.392341	-0.010247
C	13.562276	-3.518509	0.005264
C	11.096055	-0.705445	-0.014430
C	13.571923	-0.682341	-0.016985
C	14.768992	-1.423507	-0.012426
C	14.764610	-2.811816	-0.001523
C	9.862165	-1.461933	-0.007150
C	9.898873	-2.872496	0.003957
C	13.553225	0.767683	-0.028215
C	11.077390	0.726672	-0.025667
C	12.294779	1.445415	-0.032406
C	9.824064	1.450989	-0.030102
C	14.730793	1.539461	-0.035100
C	12.264215	2.880176	-0.043578
C	14.690185	2.927088	-0.045879
C	9.824354	2.861903	-0.041214
C	13.469940	3.602580	-0.050199
C	11.011713	3.561052	-0.047802
C	13.465614	5.082653	-0.061837
C	10.968256	5.042209	-0.059380
N	12.208031	5.668168	-0.065319
O	14.470823	5.757343	-0.067810
O	9.944530	5.686957	-0.063473
H	12.191011	6.685282	-0.073200
C	13.596011	-4.998372	0.016988
C	11.098543	-5.022405	0.019731
N	12.353964	-5.616205	0.023138
O	14.618265	-5.646850	0.021038
O	10.091689	-5.693082	0.026168
H	12.363247	-6.633425	0.031184
H	15.606974	3.519801	-0.051215
H	15.704534	1.051618	-0.032009
H	15.729703	-0.910536	-0.017465
H	15.696494	-3.380472	0.001998
H	8.881991	3.409775	-0.044619
H	8.970966	-3.444493	0.009543
C	8.648769	0.674568	-0.022634
C	8.667260	-0.716670	-0.011497
C	7.244914	1.125920	-0.024115
C	7.275657	-1.205640	-0.005256
N	6.438981	-0.051150	-0.012900
O	6.843011	2.261025	-0.032401
O	6.904970	-2.351366	0.004373
C	5.024004	-0.070652	-0.009514
C	4.313548	-1.285400	0.014094
C	4.278662	1.126800	-0.027836
C	2.925335	-1.291606	0.016438
C	2.895153	1.089219	-0.025621
C	2.170444	-0.113278	-0.006492
H	4.849379	-2.228452	0.030834
H	2.429882	-2.262233	0.039026
H	4.787768	2.084619	-0.043198
H	2.365395	2.044383	-0.037603
C	0.649409	-0.097648	0.018609
C	0.027072	-1.504301	-0.007749
C	0.152719	0.599493	1.306701
C	0.075903	0.679524	-1.188454
C	-1.509939	-1.418491	-0.144782
H	0.301726	-2.040953	0.915855

H	0.444084	-2.084916	-0.845894
C	-1.383917	0.492282	1.433224
H	0.463130	1.656875	1.288437
H	0.647102	0.146874	2.181438
H	0.600226	1.638954	-1.314946
H	0.274302	0.097207	-2.104315
C	-1.439345	0.923000	-1.007862
C	-2.010154	0.021251	0.108947
H	-2.002025	-2.105927	0.561807
H	-1.821885	-1.737495	-1.152452
H	-1.801380	1.470387	1.719651
H	-1.654142	-0.214770	2.235086
H	-1.639401	1.975619	-0.744883
H	-1.964860	0.739813	-1.957161
C	-3.536181	0.049453	0.121139
C	-4.252466	-0.316007	-1.027804
C	-4.278495	0.402700	1.252105
C	-5.640529	-0.321697	-1.051490
H	-3.719127	-0.607860	-1.935424
C	-5.671360	0.394897	1.239275
H	-3.776486	0.690902	2.175768
C	-6.355660	0.035159	0.087250
H	-6.174718	-0.611699	-1.958554
H	-6.228826	0.677891	2.134516
N	-7.794686	0.029726	0.069028
C	-8.449160	1.270982	0.087668
C	-9.934452	1.240859	0.060181
O	-7.826331	2.305075	0.123481
C	-10.627718	2.430509	0.068124
C	-10.641002	0.017027	0.028436
C	-12.029049	2.433186	0.044770
H	-10.063851	3.364860	0.093229
C	-9.922995	-1.200457	0.017029
C	-12.062685	0.010677	0.007850
C	-12.763253	1.255626	0.015199
H	-12.535695	3.397636	0.051392
C	-8.437416	-1.217064	0.031344
C	-10.605059	-2.396278	-0.010839
C	-12.751605	-1.240484	-0.019832
C	-14.238207	1.249403	-0.009088
O	-7.804282	-2.245438	0.012107
C	-12.006396	-2.411467	-0.028033
H	-10.032390	-3.325560	-0.019833
C	-14.226638	-1.247377	-0.039057
	-14.928980	-0.002092	-0.034487
C	-14.979647	2.422540	-0.007791
H	-12.504029	-3.380397	-0.049518
C	-14.957262	-2.427062	-0.061948
C	-16.351451	-0.008412	-0.055789
C	-16.380621	2.410148	-0.029848
H	-14.479026	3.389929	0.010525
C	-16.358325	-2.427133	-0.081940
H	-14.447750	-3.389955	-0.064844
C	-17.064680	1.216284	-0.053221
C	-17.053367	-1.239409	-0.079532
H	-16.951787	3.340730	-0.028655
H	-16.920905	-3.362754	-0.100017
C	-18.549653	1.229580	-0.075803
C	-18.538186	-1.265889	-0.102004
N	-19.151581	-0.020853	-0.098135
O	-19.212256	2.240432	-0.075273
O	-19.191463	-2.282587	-0.122551
H	-20.168809	-0.025367	-0.113563

Optimized geometries of D-(Ph-Ph)-A

S_0-Minimum

B3LYP/6-31G(d) optimized

C	9.017643	-5.001336	0.631267
C	9.043548	-3.523802	0.446366
C	10.296926	-2.830884	0.357539
C	11.512829	-3.537131	0.444610
C	11.525674	-5.009759	0.629894
N	10.270099	-5.609310	0.706685
C	7.856397	-2.847236	0.363282
C	7.841397	-1.432753	0.183909
C	9.069589	-0.710066	0.090797
C	10.312033	-1.415992	0.179182
C	6.646609	-0.683159	0.087605
C	6.646644	0.682803	-0.087480
C	7.841471	1.432328	-0.183838
C	9.069626	0.709570	-0.090783
C	5.229262	1.154336	-0.150830
N	4.427760	-0.000118	0.000091
C	5.229203	-1.154612	0.151016
C	10.312107	1.415424	-0.179226
C	10.297073	2.830317	-0.357583
C	9.043730	3.523308	-0.446352
C	7.856545	2.846810	-0.363213
C	11.559192	0.725887	-0.091173
C	11.559155	-0.726526	0.091070
C	12.722931	-2.854208	0.356629
C	12.743735	-1.474830	0.183038
C	11.513012	3.536494	-0.444713
C	12.723079	2.853501	-0.356788
C	12.743811	1.474121	-0.183197
C	9.017902	5.000843	-0.631253
N	10.270389	5.608744	-0.706731
C	11.525934	5.009120	-0.629999
C	2.999355	-0.000081	0.000090
C	2.297968	1.009245	0.668254
C	0.906754	1.007374	0.656335
C	0.180696	-0.000010	0.000086
C	0.906705	-1.007431	-0.656161
C	2.297918	-1.009372	-0.668076
O	4.817978	-2.286806	0.299008
O	4.818096	2.286548	-0.298848
O	7.996285	5.660672	-0.713719
O	12.545492	5.675181	-0.712397
O	12.545198	-5.675879	0.712243
O	7.995992	-5.661107	0.713779
C	-1.303285	0.000029	0.000082
C	-2.026245	-0.409367	-1.132866
C	-3.417905	-0.409082	-1.136098
C	-4.113466	0.000103	0.000073
C	-3.417890	0.409251	1.136248
C	-2.026230	0.409463	1.133025
N	-5.559233	0.000143	0.000068
C	-6.211697	1.248274	-0.085547
C	-7.695020	1.220724	-0.090087
C	-8.407223	0.000221	0.000069
C	-7.695088	-1.220321	0.090223
C	-6.211766	-1.247953	0.085677
C	-9.837115	0.000261	0.000072
C	-10.534374	-1.245317	0.100055

C	-9.788225	-2.422258	0.188701
C	-8.389439	-2.414051	0.182714
C	-12.005286	-1.245106	0.106279
C	-12.704243	0.000341	0.000077
C	-12.005217	1.245749	-0.106126
C	-10.534305	1.245878	-0.099908
C	-14.134883	0.000380	0.000080
C	-14.842516	-1.225743	0.108618
C	-14.146379	-2.416391	0.213799
C	-12.747899	-2.422644	0.212040
C	-14.842448	1.226543	-0.108457
C	-16.325173	1.248903	-0.111007
N	-16.935559	0.000458	0.000084
C	-16.325242	-1.248021	0.111173
C	-12.747765	2.423328	-0.211885
C	-14.146246	2.417152	-0.213639
C	-8.389306	2.414493	-0.182573
C	-9.788091	2.422778	-0.188556
O	-16.993818	-2.266183	0.202214
O	-16.993693	2.267102	-0.202046
O	-5.574751	2.287034	-0.152099
O	-5.574878	-2.286747	0.152248
H	10.266453	6.616297	-0.832839
H	10.266110	-6.616863	0.832792
H	13.644322	3.422215	-0.426661
H	13.706606	0.981610	-0.119070
H	13.706555	-0.982374	0.118865
H	13.644144	-3.422976	0.426457
H	6.920920	3.389675	-0.433856
H	6.920745	-3.390047	0.433969
H	2.835303	1.802447	1.172977
H	2.835215	-1.802602	-1.172797
H	0.376601	-1.816714	-1.149255
H	0.376690	1.816684	1.149426
H	-1.493775	0.705646	2.031856
H	-3.965233	0.720620	2.020241
H	-1.493800	-0.705578	-2.031694
H	-3.965258	-0.720420	-2.020095
H	-7.827386	-3.339431	0.250263
H	-7.827202	3.339842	-0.250124
H	-10.286714	-3.381218	0.263311
H	-10.286527	3.381766	-0.263163
H	-12.246470	-3.379170	0.296618
H	-12.246283	3.379826	-0.296465
H	-14.707052	-3.341657	0.296698
H	-14.706868	3.342449	-0.296537
H	-17.950785	0.000486	0.000086

π-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	9.034432	-4.960813	0.742488
C	9.058171	-3.496571	0.524750
C	10.292629	-2.809047	0.420974
C	11.514709	-3.508279	0.524607
C	11.530300	-4.971957	0.743423
N	10.281538	-5.566198	0.832141
C	7.846838	-2.815692	0.424596
C	7.828372	-1.435153	0.217230
C	9.064949	-0.700467	0.105645
C	10.303317	-1.397826	0.209762
C	6.624347	-0.672433	0.102276

C	6.624397	0.672117	-0.102186
C	7.828480	1.434741	-0.217183
C	9.065001	0.699955	-0.105641
C	5.207709	1.143653	-0.172571
N	4.409042	-0.000073	0.000065
C	5.207624	-1.143856	0.172712
C	10.303422	1.397214	-0.209802
C	10.292840	2.808436	-0.421015
C	9.058434	3.496059	-0.524747
C	7.847049	2.815278	-0.424549
C	11.541360	0.710670	-0.106333
C	11.541306	-0.711381	0.106249
C	12.732023	-2.824508	0.421374
C	12.750557	-1.462291	0.217554
C	11.514973	3.507569	-0.524694
C	12.732236	2.823700	-0.421503
C	12.750667	1.461483	-0.217682
C	9.034805	4.960303	-0.742485
N	10.281956	5.565588	-0.832186
C	11.530673	4.971246	-0.743514
C	2.985726	-0.000023	0.000062
C	2.283120	1.037510	0.615298
C	0.893789	1.034345	0.605579
C	0.170032	0.000067	0.000065
C	0.893721	-1.034256	-0.605452
C	2.283052	-1.037510	-0.615174
O	4.807904	-2.264769	0.339331
O	4.808072	2.264592	-0.339220
O	8.017342	5.608515	-0.838754
O	12.548177	5.621691	-0.840374
O	12.547755	-5.622484	0.840248
O	8.016920	-5.608943	0.838789
C	-1.315055	0.000110	0.000071
C	-2.036064	-0.447655	-1.114023
C	-3.425445	-0.445434	-1.117821
C	-4.122876	0.000175	0.000088
C	-3.425410	0.445756	1.117988
C	-2.036029	0.447913	1.114172
N	-5.561566	0.000199	0.000101
C	-6.211660	1.244780	0.014633
C	-7.696964	1.220895	0.007399
C	-8.409385	0.000242	0.000097
C	-7.697000	-1.220433	-0.007202
C	-6.211697	-1.244363	-0.014420
C	-9.831183	0.000262	0.000091
C	-10.525971	-1.247926	-0.003032
C	-9.786149	-2.422348	-0.007554
C	-8.384693	-2.413430	-0.010698
C	-12.001139	-1.248204	-0.001459
C	-12.697745	0.000304	0.000080
C	-12.001102	1.248793	0.001624
C	-10.525935	1.248472	0.003208
C	-14.120372	0.000325	0.000075
C	-14.828046	-1.227604	-0.000493
C	-14.138446	-2.418488	-0.001124
C	-12.737240	-2.424678	-0.001737
C	-14.828010	1.228274	0.000637
C	-16.313107	1.248175	0.000487
N	-16.920857	0.000366	0.000063
C	-16.313143	-1.247461	-0.000355
C	-12.737169	2.425287	0.001895
C	-14.138375	2.419138	0.001272
C	-8.384622	2.413912	0.010887
C	-9.786077	2.422872	0.007734
O	-16.971181	-2.261284	-0.000604
O	-16.971115	2.262016	0.000729

O	-5.584560	2.276706	0.031711
O	-5.584628	-2.276306	-0.031542
H	10.276459	6.571980	-0.982303
H	10.275966	-6.572591	0.982257
H	13.654927	3.400583	-0.507082
H	13.713034	0.957512	-0.141063
H	13.712962	-0.958398	0.140901
H	13.654671	-3.401465	0.506918
H	6.914452	3.374432	-0.509682
H	6.914198	-3.374771	0.509764
H	2.821228	1.860621	1.083943
H	2.821107	-1.860655	-1.083820
H	0.361167	-1.869258	-1.066418
H	0.361289	1.869381	1.066547
H	-1.501906	0.783248	2.006119
H	-3.973450	0.792301	1.996090
H	-1.501968	-0.783016	-2.005976
H	-3.973511	-0.791956	-1.995916
H	-7.816433	-3.345432	-0.016536
H	-7.816335	3.345898	0.016728
H	-10.288258	-3.389186	-0.009869
H	-10.288158	3.389724	0.010043
H	-12.232126	-3.389896	-0.002388
H	-12.232028	3.390491	0.002549
H	-14.705387	-3.351650	-0.001316
H	-14.705289	3.352316	0.001459
H	-17.938211	0.000380	0.000059

d-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	8.986809	-5.026344	-0.324668
C	9.008927	-3.542933	-0.228917
C	10.251488	-2.845437	-0.182553
C	11.471069	-3.552578	-0.226072
C	11.485222	-5.033972	-0.321176
N	10.235754	-5.634779	-0.361671
C	7.822549	-2.863389	-0.186489
C	7.801075	-1.443899	-0.094402
C	9.014548	-0.724004	-0.047035
C	10.256449	-1.426932	-0.091571
C	6.581022	-0.707893	-0.046729
C	6.581060	0.707553	0.046474
C	7.801152	1.443486	0.094279
C	9.014586	0.723519	0.047040
C	5.251435	1.205791	0.079529
N	4.396760	-0.000107	-0.000196
C	5.251370	-1.206050	-0.079924
C	10.256524	1.426374	0.091711
C	10.251638	2.844879	0.182694
C	9.009113	3.542448	0.228925
C	7.822700	2.862975	0.186369
C	11.503315	0.733852	0.046591
C	11.503276	-0.734485	-0.046317
C	12.670455	-2.867971	-0.180380
C	12.682435	-1.474945	-0.091508
C	11.471256	3.551947	0.226344
C	12.670606	2.867268	0.180781
C	12.682513	1.474242	0.091910
C	8.987072	5.025860	0.324672
N	10.236050	5.634222	0.361813
C	11.485486	5.033340	0.321453

C	3.040148	-0.000075	-0.000192
C	2.292177	1.224943	0.041334
C	0.921389	1.206893	0.045751
C	0.182071	-0.000016	-0.000167
C	0.921338	-1.206956	-0.046103
C	2.292126	-1.225062	-0.041712
O	4.813585	-2.341569	-0.157723
O	4.813714	2.341334	0.157343
O	7.976791	5.686929	0.368887
O	12.496743	5.695602	0.362542
O	12.496444	-5.696293	-0.362158
O	7.976492	-5.687353	-0.368985
C	-1.283085	0.000015	-0.000146
C	-2.010027	-1.064850	-0.563097
C	-3.395415	-1.061174	-0.572955
C	-4.095897	0.000075	-0.000098
C	-3.395350	1.061296	0.572735
C	-2.009963	1.064912	0.562830
N	-5.528819	0.000107	-0.000073
C	-6.183701	1.092321	-0.604374
C	-7.665240	1.067087	-0.594527
C	-8.376388	0.000199	0.000020
C	-7.665269	-1.066738	0.594518
C	-6.183731	-1.092074	0.604253
C	-9.798300	0.000248	0.000074
C	-10.493541	-1.090625	0.606919
C	-9.754504	-2.116193	1.180913
C	-8.353819	-2.108343	1.177099
C	-11.968679	-1.092441	0.603829
C	-12.664650	0.000347	0.000181
C	-11.968648	1.093088	-0.603518
C	-10.493511	1.091169	-0.606718
C	-14.086953	0.000396	0.000235
C	-14.794616	-1.075648	0.591578
C	-14.106001	-2.119295	1.165560
C	-12.704400	-2.123717	1.169881
C	-14.794586	1.076490	-0.591055
C	-16.280802	1.094091	-0.599920
N	-16.888655	0.000494	0.000340
C	-16.280832	-1.093146	0.600554
C	-12.704341	2.124415	-1.169513
C	-14.105942	2.120091	-1.165087
C	-8.353761	2.108743	-1.177053
C	-9.754446	2.116688	-1.180764
O	-16.936909	-1.982573	1.088449
O	-16.936854	1.983565	-1.087763
O	-5.553213	1.993552	-1.103061
O	-5.553268	-1.993313	1.102959
H	10.232493	6.649200	0.426927
H	10.232144	-6.649758	-0.426785
H	13.599971	3.439001	0.215854
H	13.648320	0.971379	0.058089
H	13.648269	-0.972140	-0.057584
H	13.599790	-3.439759	-0.215352
H	6.882225	3.413730	0.222915
H	6.882046	-3.414089	-0.223135
H	2.836059	2.163934	0.060670
H	2.835970	-2.164075	-0.061055
H	0.394081	-2.161874	-0.050766
H	0.394171	2.161833	0.050426
H	-1.485734	1.897509	1.034416
H	-3.939352	1.890206	1.025652
H	-1.485850	-1.897470	-1.034700
H	-3.939468	-1.890061	-1.025853
H	-7.787159	-2.922997	1.631829
H	-7.787079	2.923358	-1.631823

H	-10.256964	-2.959995	1.652139
H	-10.256883	2.960526	-1.651950
H	-12.199638	-2.969559	1.635246
H	-12.199555	2.970222	-1.634916
H	-14.673119	-2.937269	1.614370
H	-14.673037	2.938104	-1.613854
H	-17.906163	0.000529	0.000379

b-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	9.008846	-5.004554	-0.426662
C	9.034263	-3.535244	-0.301295
C	10.280536	-2.838359	-0.240108
C	11.494637	-3.541929	-0.298071
C	11.509433	-5.010358	-0.423111
N	10.256916	-5.609893	-0.476109
C	7.838899	-2.852548	-0.244949
C	7.818263	-1.451895	-0.125054
C	9.052308	-0.707777	-0.059909
C	10.292140	-1.413114	-0.118748
C	6.627375	-0.687767	-0.060429
C	6.626667	0.686263	0.058671
C	7.816736	1.451465	0.124949
C	9.051567	0.708497	0.061467
C	5.241820	1.171577	0.101329
N	4.391298	-0.001739	-0.002336
C	5.243013	-1.174350	-0.104984
C	10.290640	1.415007	0.121936
C	10.277531	2.840245	0.243276
C	9.030505	3.535945	0.302827
C	7.835881	2.852126	0.244868
C	11.533280	0.723259	0.063479
C	11.534040	-0.720191	-0.058681
C	12.707690	-2.848051	-0.237362
C	12.728606	-1.473525	-0.120783
C	11.490873	3.544968	0.302813
C	12.704665	2.852233	0.243669
C	12.727042	1.477727	0.127116
C	9.003525	5.005229	0.428180
N	10.250947	5.611748	0.479246
C	11.504111	5.013407	0.427871
C	3.015164	-0.001848	-0.003048
C	2.273226	1.216054	0.060350
C	0.900981	1.201611	0.065465
C	0.154094	-0.001227	-0.004228
C	0.900513	-1.204389	-0.073415
C	2.272753	-1.219460	-0.067158
O	4.837085	-2.297613	-0.205684
O	4.834543	2.294419	0.201230
O	7.988010	5.668385	0.485231
O	12.512964	5.685293	0.484711
O	12.519011	-5.681260	-0.478630
O	7.994047	-5.668695	-0.485039
C	-1.304544	-0.000928	-0.004572
C	-2.036579	-1.096460	-0.510980
C	-3.419287	-1.092656	-0.520567
C	-4.120035	-0.001005	-0.004168
C	-3.419071	1.091004	0.511523
C	-2.036379	1.094885	0.501545
H	10.248105	6.624704	0.565370
H	10.255164	-6.622851	-0.562230

H	13.628504	3.432035	0.292640
H	13.692085	0.975109	0.084079
H	13.693113	-0.969978	-0.076504
H	13.632152	-3.426965	-0.285133
H	6.907660	3.420050	0.293518
H	6.911292	-3.421345	-0.294873
H	2.804296	2.161061	0.098383
H	2.803381	-2.164703	-0.104785
H	0.381827	-2.163101	-0.097708
H	0.382673	2.160541	0.089310
H	-1.515127	1.950875	0.930543
H	-3.963182	1.942267	0.919899
H	-1.515498	-1.952453	-0.940166
H	-3.963476	-1.943740	-0.929245
N	-5.549830	-0.001011	-0.003778
H	-7.805902	-2.903934	1.669886
C	-6.203830	1.084063	-0.623019
C	-7.684010	1.058833	-0.611808
C	-8.394048	-0.000692	-0.001911
C	-7.683436	-1.060443	0.606914
C	-6.203264	-1.086156	0.615957
C	-9.816016	-0.000461	-0.000819
C	-10.510923	-1.083228	0.620910
C	-9.771630	-2.102574	1.208861
C	-8.372119	-2.095068	1.204400
C	-11.984560	-1.084816	0.618772
C	-12.680456	0.000071	0.001534
C	-11.985170	1.084686	-0.616880
C	-10.511531	1.082547	-0.621443
C	-14.102713	0.000355	0.002753
C	-14.809914	-1.067851	0.608642
C	-14.121181	-2.104939	1.195921
C	-12.720265	-2.109571	1.199263
C	-14.810523	1.068846	-0.601912
C	-16.296811	1.086453	-0.609775
N	-16.904283	0.000933	0.005189
C	-16.296193	-1.084843	0.619089
C	-12.721464	2.109726	-1.196123
C	-14.122377	2.105651	-1.190381
C	-8.373281	2.093652	-1.208287
C	-9.772801	2.101626	-1.210578
O	-16.951207	-1.968228	1.119079
O	-16.952327	1.970104	-1.108637
O	-5.568164	1.975813	-1.132488
O	-5.567197	-1.978200	1.124402
H	-7.807517	2.902338	-1.674637
H	-10.274125	-2.939780	1.691551
H	-10.275766	2.939003	-1.692480
H	-12.215357	-2.949427	1.675244
H	-12.217043	2.949394	-1.672948
H	-14.688238	-2.916856	1.655664
H	-14.689893	2.917800	-1.649147
H	-17.921843	0.001144	0.006073

Optimized geometries of D-(Ph-Yn-Ph)-A

S_0-Minimum

B3LYP/6-31G(d) optimized

N	-18.310677	-0.001134	0.000009
C	-17.700424	0.749878	-1.003416
C	-16.217641	0.736338	-0.985565
C	-15.509824	-0.000950	-0.000052
C	-16.217501	-0.738331	0.985491
C	-17.700282	-0.752065	1.003408
C	-15.521521	1.452372	-1.942559
C	-14.122986	1.455432	-1.947953
C	-13.380194	0.746703	-1.001791
C	-14.079260	-0.000857	-0.000084
C	-13.380052	-0.748325	1.001593
C	-11.909141	-0.746055	1.002780
C	-11.211644	-0.000667	-0.000144
C	-11.909282	0.744628	-1.003041
C	-11.163400	1.446942	-1.951819
C	-9.764600	1.440734	-1.946031
C	-9.069989	0.727891	-0.984429
C	-9.781705	-0.000571	-0.000174
C	-9.069851	-0.728939	0.984052
C	-7.586666	-0.743638	1.006735
N	-6.937083	-0.000379	-0.000230
C	-7.586806	0.742789	-1.007171
C	-11.163126	-1.448274	1.951525
C	-9.764327	-1.441879	1.945680
C	-15.521246	-1.454275	1.942455
C	-14.122710	-1.457152	1.947787
C	-5.491055	-0.000290	-0.000266
C	-4.798317	0.948630	0.750918
C	-3.408329	0.950787	0.752593
C	-2.691018	-0.000120	-0.000332
C	-3.408248	-0.951111	-0.753225
C	-4.798237	-0.949125	-0.751481
O	-6.945760	-1.359446	1.842780
O	-6.946017	1.358660	-1.843261
O	-18.369000	1.362446	-1.821764
O	-18.368742	-1.364717	1.821787
C	-1.267022	-0.000031	-0.000359
C	-0.050661	0.000010	-0.000334
C	1.372483	0.000080	-0.000314
C	2.093696	-0.956186	-0.742135
C	3.482759	-0.953954	-0.749335
C	4.182575	0.000214	-0.000267
C	3.482643	0.954316	0.748777
C	2.093580	0.956413	0.741534
N	5.609349	0.000279	-0.000242
C	6.411482	1.163807	-0.056471
C	7.828241	0.688252	-0.033338
C	7.828301	-0.687491	0.033086
C	6.411584	-1.163178	0.056042
C	9.023137	-1.442187	0.072369
C	10.251256	-0.714234	0.036206
C	10.251193	0.715223	-0.036157
C	9.023011	1.443060	-0.072472
C	11.493624	1.425690	-0.072636
C	12.740792	0.731547	-0.037839
C	12.740856	-0.730325	0.038198
C	11.493749	-1.424585	0.072842

C	11.478710	-2.848901	0.144977
C	12.694627	-3.559425	0.183029
C	13.904668	-2.871617	0.150289
C	13.925427	-1.483119	0.079327
C	9.038219	-2.866224	0.143475
C	10.225440	-3.546761	0.178527
C	10.199603	-5.034128	0.251585
N	11.451976	-5.645707	0.285728
C	12.707513	-5.041867	0.257618
C	11.478460	2.850005	-0.144768
C	10.225129	3.547748	-0.178469
C	9.037968	2.867099	-0.143569
C	12.694316	3.560643	-0.182668
C	13.904417	2.872948	-0.149781
C	13.925297	1.484453	-0.078820
C	12.707072	5.043087	-0.257249
N	11.451481	5.646810	-0.285508
C	10.199162	5.035113	-0.251520
O	9.177866	-5.698243	0.280792
O	13.727060	-5.712004	0.293051
O	5.999432	2.303900	-0.110370
O	5.999634	-2.303306	0.109964
O	13.726560	5.713320	-0.292558
O	9.177366	5.699133	-0.280845
H	11.448065	-6.659867	0.336336
H	11.447481	6.660969	-0.336112
H	14.825890	-3.443786	0.181382
H	14.888235	-0.987022	0.056530
H	14.888150	0.988445	-0.055905
H	14.825590	3.445204	-0.180759
H	8.102773	-3.413260	0.170774
H	8.102473	3.414047	-0.170981
H	4.022600	-1.696307	-1.323702
H	4.022395	1.696720	1.323162
H	1.552593	1.699121	1.318779
H	1.552798	-1.698948	-1.319395
H	-2.864358	-1.687241	-1.336123
H	-5.349329	-1.682188	-1.332216
H	-2.864500	1.686978	1.335470
H	-5.349472	1.681620	1.331685
H	-9.202793	1.992511	-2.692207
H	-9.202416	-1.993583	2.691831
H	-11.661588	2.019908	-2.724627
H	-11.661206	-2.021309	2.724351
H	-13.622247	2.031081	-2.717048
H	-13.621863	-2.032736	2.716860
H	-16.082098	2.009271	-2.686178
H	-16.081717	-2.011249	2.686098
H	-19.325884	-0.001199	0.000032

π-Minimum

CAM-B3LYP/def2-SV(P) optimized

N	-18.301967	-0.001580	-0.000300
C	-17.694319	0.889605	-0.873681
C	-16.209137	0.875782	-0.859494
C	-15.501343	-0.001221	-0.000164
C	-16.208995	-0.878405	0.859097
C	-17.694175	-0.892608	0.873141
C	-15.519620	1.726606	-1.692745
C	-14.118360	1.731890	-1.696278
C	-13.382178	0.891990	-0.872567

C	-14.078780	-0.001040	-0.000096
C	-13.382034	-0.893892	0.872441
C	-11.906882	-0.895344	0.870437
C	-11.212018	-0.000679	0.000038
C	-11.907026	0.893812	-0.870426
C	-11.167371	1.737433	-1.687666
C	-9.765944	1.733868	-1.678780
C	-9.078090	0.878168	-0.847620
C	-9.790231	-0.000503	0.000101
C	-9.077947	-0.879002	0.847879
C	-7.592963	-0.901271	0.859533
N	-6.943425	-0.000182	0.000195
C	-7.593109	0.900796	-0.859150
C	-11.167090	-1.738784	1.687741
C	-9.765664	-1.734876	1.678975
C	-15.519342	-1.729054	1.692415
C	-14.118081	-1.733980	1.696082
C	-5.505144	-0.000065	0.000197
C	-4.810190	1.095825	0.503823
C	-3.422303	1.098682	0.502146
C	-2.707714	0.000154	0.000195
C	-3.422132	-1.098487	-0.501751
C	-4.810018	-1.095848	-0.503426
O	-6.964383	-1.650655	1.567735
O	-6.964654	1.650242	-1.567397
O	-18.352316	1.613431	-1.583546
O	-18.352056	-1.616607	1.582937
C	-1.276061	0.000267	0.000193
C	-0.064167	0.000339	0.000169
C	1.366862	0.000379	0.000122
C	2.084979	-1.015097	-0.649002
C	3.472551	-1.014292	-0.656682
C	4.173863	0.000445	0.000037
C	3.472544	1.015148	0.656801
C	2.084971	1.015887	0.649206
N	5.595834	0.000465	0.000000
C	6.395830	1.153186	-0.101306
C	7.811752	0.677885	-0.060463
C	7.811765	-0.676924	0.060305
C	6.395853	-1.152243	0.101258
C	9.015710	-1.445333	0.127603
C	10.252162	-0.704934	0.061802
C	10.252150	0.705921	-0.062154
C	9.015683	1.446306	-0.127857
C	11.490498	1.408360	-0.122654
C	12.728506	0.716776	-0.062026
C	12.728518	-0.715763	0.061477
C	11.490522	-1.407360	0.122203
C	11.479988	-2.828939	0.245347
C	12.702071	-3.533200	0.304948
C	13.919342	-2.844375	0.243977
C	13.937761	-1.472083	0.125350
C	9.034359	-2.836100	0.248981
C	10.245656	-3.521784	0.306490
C	10.221963	-4.996679	0.433231
N	11.469108	-5.606454	0.485235
C	12.717781	-5.007730	0.432684
C	11.479939	2.829939	-0.245800
C	10.245595	3.522771	-0.306845
C	9.034309	2.837074	-0.249238
C	12.702010	3.534212	-0.305502
C	13.919293	2.845400	-0.244626
C	13.937736	1.473108	-0.125997
C	12.717696	5.008741	-0.433246
N	11.469012	5.607452	-0.485695
C	10.221877	4.997666	-0.433584

O	9.204410	-5.649411	0.489250
O	13.735394	-5.662675	0.488639
O	5.996297	2.282201	-0.198364
O	5.996341	-2.281264	0.198330
O	13.735298	5.663695	-0.489287
O	9.204314	5.650387	-0.489528
H	11.463644	-6.620233	0.572560
H	11.463532	6.621231	-0.573025
H	14.842047	-3.425487	0.293063
H	14.900150	-0.964424	0.079840
H	14.900134	0.965459	-0.080563
H	14.841988	3.426521	-0.293789
H	8.101973	-3.399748	0.299554
H	8.101914	3.400713	-0.299735
H	4.012543	-1.812531	-1.163922
H	4.012530	1.813409	1.164014
H	1.541774	1.813591	1.159657
H	1.541789	-1.812829	-1.159416
H	-2.876406	-1.959253	-0.892987
H	-5.360993	-1.953915	-0.892648
H	-2.876712	1.959530	0.893387
H	-5.361299	1.953804	0.893051
H	-9.197915	2.405056	-2.325658
H	-9.197526	-2.405926	2.325901
H	-11.669334	2.430610	-2.361806
H	-11.668942	-2.432088	2.361833
H	-13.613610	2.421750	-2.371684
H	-13.613220	-2.423712	2.371535
H	-16.086526	2.392890	-2.346118
H	-16.086141	-2.395483	2.345732
H	-19.319324	-0.001712	-0.000351

d-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

N	-18.257232	0.007395	-0.026283
C	-17.645392	-0.382948	-1.209092
C	-16.159265	-0.375839	-1.185672
C	-15.455460	0.008426	-0.017178
C	-16.167130	0.392160	1.146718
C	-17.653381	0.398140	1.160491
C	-15.466754	-0.747738	-2.314831
C	-14.065161	-0.748520	-2.316124
C	-13.333108	-0.380359	-1.196352
C	-14.033166	0.008939	-0.012544
C	-13.341095	0.398728	1.175794
C	-11.865967	0.398371	1.180771
C	-11.166638	0.009900	-0.003205
C	-11.857988	-0.378983	-1.191723
C	-11.115202	-0.744017	-2.306388
C	-9.714543	-0.742406	-2.293115
C	-9.029747	-0.371804	-1.156460
C	-9.744713	0.010342	0.001432
C	-9.037496	0.392972	1.163927
C	-7.555892	0.407813	1.192059
N	-6.898645	0.010948	0.010744
C	-7.548018	-0.385848	-1.174949
C	-11.130662	0.763973	2.300205
C	-9.729933	0.763256	2.296053
C	-15.482246	0.764543	2.280359
C	-14.080688	0.766348	2.290778
C	-5.464877	0.010956	0.015282
C	-4.770065	1.194303	0.266025

C	-3.384558	1.196477	0.273362
C	-2.671660	0.010917	0.022324
C	-3.383369	-1.174718	-0.231864
C	-4.768847	-1.172507	-0.231517
O	-6.927315	0.737195	2.169199
O	-6.912971	-0.714659	-2.148097
O	-18.298213	-0.701008	-2.174626
O	-18.312692	0.715627	2.121793
C	-1.250622	0.010634	0.024620
C	-0.031331	0.009407	0.025542
C	1.373511	0.006647	0.025019
C	2.098296	-1.180590	-0.254726
C	3.467152	-1.194664	-0.260509
C	4.213932	0.000300	0.021090
C	3.473269	1.198393	0.305587
C	2.104297	1.190476	0.303505
N	5.570724	-0.002578	0.018046
C	6.429098	1.159960	0.336606
C	7.758059	0.676507	0.199868
C	7.754130	-0.689662	-0.179524
C	6.422493	-1.168383	-0.306060
C	8.971703	-1.401883	-0.384243
C	10.187497	-0.709062	-0.195958
C	10.191596	0.687409	0.195294
C	8.979870	1.384396	0.394388
C	11.435618	1.363269	0.380964
C	12.680430	0.692868	0.188219
C	12.676235	-0.722946	-0.211671
C	11.427477	-1.389164	-0.392872
C	11.418621	-2.757442	-0.777572
C	12.636218	-3.440767	-0.977153
C	13.837618	-2.781611	-0.799132
C	13.853449	-1.438239	-0.420665
C	8.989506	-2.771813	-0.768059
C	10.173849	-3.428830	-0.959045
C	10.147655	-4.859981	-1.360175
N	11.394955	-5.448134	-1.532711
C	12.646085	-4.869785	-1.378782
C	11.434916	2.731538	0.765780
C	10.194120	3.407101	0.958699
C	9.005848	2.754172	0.778287
C	12.656600	3.410761	0.954100
C	13.854087	2.747614	0.764886
C	13.861910	1.404220	0.386257
C	12.674980	4.839713	1.355650
N	11.427273	5.422206	1.521293
C	10.176459	4.838256	1.360294
O	9.135821	-5.497333	-1.532700
O	13.655225	-5.510060	-1.565415
O	5.995983	2.257973	0.644257
O	5.983278	-2.265045	-0.609877
O	13.687943	5.476622	1.532854
O	9.168414	5.478967	1.542299
H	11.388454	-6.427272	-1.807732
H	11.426589	6.401326	1.796457
H	14.765249	-3.334089	-0.960595
H	14.820603	-0.953979	-0.290581
H	14.826181	0.916732	0.247140
H	14.785017	3.296991	0.917712
H	8.047452	-3.301951	-0.911502
H	8.066945	3.287529	0.930244
H	4.014252	-2.106518	-0.478083
H	4.025078	2.107745	0.521789
H	1.558819	2.110827	0.519574
H	1.548095	-2.098494	-0.469218
H	-2.836805	-2.099103	-0.427415

H	-5.317851	-2.093080	-0.431166
H	-2.838971	2.120876	0.471564
H	-5.320056	2.114895	0.462845
H	-9.144872	-1.033911	-3.177471
H	-9.166240	1.055210	3.184085
H	-11.614521	-1.044206	-3.226772
H	-11.636147	1.063909	3.217302
H	-13.557441	-1.049941	-3.231642
H	-13.579154	1.068134	3.209578
H	-16.030840	-1.039846	-3.202878
H	-16.052315	1.056202	3.164726
H	-19.274736	0.006984	-0.029575

b-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

N	-18.271144	0.012658	0.012408
C	-17.659957	0.859948	0.925635
C	-16.173326	0.843342	0.909004
C	-15.468714	0.007195	0.007744
C	-16.179579	-0.826172	-0.891176
C	-17.666311	-0.836956	-0.902883
C	-15.481930	1.651905	1.781635
C	-14.080507	1.652743	1.784054
C	-13.347458	0.851116	0.920039
C	-14.046434	0.004414	0.005374
C	-13.353811	-0.845001	-0.911609
C	-11.879324	-0.847220	-0.914712
C	-11.180317	-0.001176	0.000604
C	-11.872976	0.847571	0.918239
C	-11.131224	1.644139	1.781231
C	-9.731433	1.636939	1.771613
C	-9.044966	0.826227	0.892974
C	-9.758084	-0.003950	-0.001760
C	-9.051147	-0.836910	-0.898824
C	-7.571839	-0.863984	-0.917198
N	-6.914473	-0.009338	-0.006583
C	-7.565533	0.847592	0.906443
C	-11.143534	-1.646686	-1.780126
C	-9.743693	-1.644958	-1.775144
C	-15.494252	-1.637410	-1.766108
C	-14.092857	-1.643736	-1.773189
C	-5.484195	-0.011868	-0.008962
C	-4.789649	-1.207328	0.197081
C	-3.406795	-1.213814	0.194077
C	-2.691053	-0.016280	-0.012397
C	-3.403558	1.183450	-0.217491
C	-4.786394	1.181332	-0.217094
O	-6.938903	-1.568751	-1.666478
O	-6.927439	1.549801	1.653746
O	-18.312213	1.551825	1.670536
O	-18.323730	-1.526238	-1.645649
C	-1.280244	-0.017930	-0.013269
C	-0.055363	-0.018140	-0.013647
C	1.340919	-0.015712	-0.014030
C	2.070380	1.188637	-0.198752
C	3.440536	1.199537	-0.198032
C	4.182740	-0.009282	-0.012726
C	3.445806	-1.221532	0.171099
C	2.075581	-1.216868	0.170672
N	5.558625	-0.006371	-0.011099
C	6.416901	-1.175737	0.117480

C	7.800716	-0.686546	0.066042
C	7.798303	0.682439	-0.078013
C	6.412808	1.166230	-0.136490
C	8.988294	1.449610	-0.152777
C	10.223552	0.709254	-0.071543
C	10.226164	-0.703077	0.073689
C	8.993659	-1.448791	0.147444
C	11.468574	-1.406300	0.149108
C	12.708627	-0.711530	0.081621
C	12.705918	0.728635	-0.063978
C	11.463282	1.417917	-0.139304
C	11.448456	2.840235	-0.284764
C	12.660947	3.546181	-0.350774
C	13.876109	2.855577	-0.274049
C	13.900041	1.484665	-0.134643
C	9.005888	2.847090	-0.296883
C	10.199764	3.532630	-0.361742
C	10.170886	4.998064	-0.512736
N	11.417910	5.605261	-0.568850
C	12.672225	5.010904	-0.500751
C	11.459101	-2.828683	0.294403
C	10.213050	-3.526520	0.363503
C	9.016531	-2.846129	0.291417
C	12.674312	-3.529284	0.368029
C	13.886837	-2.833296	0.299036
C	13.905607	-1.462267	0.159833
C	12.691140	-4.993919	0.518009
N	11.439040	-5.593769	0.578062
C	10.189714	-4.992061	0.514126
O	9.155149	5.660618	-0.586094
O	13.679405	5.686043	-0.564238
O	6.016963	-2.299097	0.234554
O	6.009393	2.288037	-0.256332
O	13.700875	-5.664624	0.587876
O	9.176475	-5.659134	0.580982
H	11.413625	6.616437	-0.672520
H	11.438532	-6.604967	0.681602
H	14.799598	3.435447	-0.328151
H	14.865619	0.984337	-0.078309
H	14.869297	-0.957662	0.109653
H	14.812517	-3.409086	0.358977
H	8.077282	3.412686	-0.359394
H	8.090037	-3.415784	0.348177
H	3.974118	2.132684	-0.339119
H	3.983597	-2.152282	0.312327
H	1.533738	-2.153216	0.315134
H	1.524415	2.122481	-0.343883
H	-2.855601	2.113215	-0.379961
H	-5.335313	2.109643	-0.373680
H	-2.861389	-2.145309	0.355223
H	-5.341112	-2.133908	0.354972
H	-9.163184	2.270501	2.455198
H	-9.180206	-2.280766	-2.460588
H	-11.631613	2.300306	2.492114
H	-11.648828	-2.300904	-2.489337
H	-13.573628	2.308136	2.491385
H	-13.590896	-2.301095	-2.482199
H	-16.046875	2.287494	2.466443
H	-16.063958	-2.270757	-2.449047
H	-19.288741	0.014657	0.014085

Optimized geometries of D-(Ph-Yn2-Ph)-A

S_0-Minimum

B3LYP/6-31G(d) optimized

C	15.131270	-1.493746	0.022472
C	13.947166	-0.739209	0.010801
C	12.699642	-1.433524	0.019905
C	12.683793	-2.859534	0.038449
C	13.899253	-3.571751	0.048567
C	15.109694	-2.883941	0.040772
C	11.430170	-3.557430	0.046915
C	11.403410	-5.046552	0.063866
N	12.655359	-5.659759	0.073420
C	13.911256	-5.056015	0.066921
C	11.457559	-0.721590	0.010298
C	10.229038	-1.449746	0.020345
C	10.243330	-2.875436	0.038587
C	11.458350	0.709609	-0.009349
C	10.230634	1.439120	-0.019503
C	9.035458	0.683969	-0.008301
C	9.034697	-0.693276	0.009020
C	12.701217	1.420173	-0.018844
C	13.947975	0.724482	-0.009646
C	7.619459	1.161079	-0.015618
N	6.815650	-0.003427	0.000209
C	7.618171	-1.168821	0.016144
C	12.686944	2.846199	-0.037374
C	11.434092	3.545477	-0.045932
C	10.246501	2.864793	-0.037719
C	15.132911	1.477712	-0.021223
C	15.112869	2.867930	-0.039511
C	13.903189	3.557075	-0.047387
C	13.916832	5.041325	-0.065715
N	12.661602	5.646454	-0.072303
C	11.408976	5.034630	-0.062856
O	14.930441	-5.727512	0.075901
O	10.381150	-5.710441	0.069166
O	7.208493	2.302655	-0.031250
O	7.205943	-2.309942	0.031726
O	14.936757	5.711698	-0.074604
O	10.387449	5.699645	-0.068216
C	5.389427	-0.002637	0.000047
H	12.650863	-6.675118	0.085605
H	12.658226	6.661818	-0.084467
H	16.030582	-3.457423	0.049291
H	16.094379	-0.997743	0.017562
H	16.095471	0.980647	-0.016247
H	16.034391	3.440396	-0.047954
H	9.307730	-3.422795	0.046330
H	9.311505	3.413185	-0.045535
C	4.689807	0.941536	0.762791
C	4.688913	-0.946019	-0.762859
C	3.300181	-0.948274	-0.755874
C	3.301079	0.945359	0.755500
C	2.579853	-0.001055	-0.000259
C	1.159825	-0.000259	-0.000423
C	-0.061699	0.000402	-0.000549
C	-1.420619	0.001071	-0.000654
C	-2.642034	0.001681	-0.000698
C	-4.062880	0.002385	-0.000767
C	-4.780497	-1.147401	-0.388896

C	-4.779348	1.152924	0.387272
C	-6.168745	1.149977	0.388488
C	-6.169889	-1.143017	-0.390257
C	-6.863159	0.003837	-0.000920
N	-8.307786	0.004592	-0.000992
C	-8.962638	-0.799138	0.958203
C	-8.961708	0.809037	-0.960224
C	-10.444326	0.788370	-0.941682
C	-10.445233	-0.776814	0.939616
C	-11.157019	0.006182	-0.001041
O	-8.326660	-1.470677	1.754246
O	-8.324953	1.479907	-1.756211
C	-11.138306	1.551810	-1.864495
C	-11.140099	-1.539461	1.862419
C	-12.586815	0.006997	-0.001054
C	-12.536996	1.555437	-1.873531
C	-12.538794	-1.541492	1.871430
C	-13.284666	-0.787721	0.962888
C	-13.283742	0.802516	-0.965001
C	-14.754596	0.801075	-0.967319
C	-14.755518	-0.784582	0.965193
C	-15.454105	0.008654	-0.001062
C	-15.498631	-1.531945	1.880850
C	-15.496837	1.549293	-1.882984
C	-16.895414	1.545381	-1.879000
C	-16.884632	0.009488	-0.001062
C	-16.897202	-1.526398	1.876870
C	-17.591922	0.789089	-0.953822
C	-17.592829	-0.769288	0.951699
C	-19.074824	0.803950	-0.971403
C	-19.075748	-0.782412	0.969287
N	-19.685628	0.011127	-0.001055
O	-19.742745	1.451243	-1.763032
O	-19.744422	-1.428919	1.760923
H	5.227967	-1.680403	-1.347721
H	5.229562	1.675312	1.347770
H	2.760221	1.679756	1.343234
H	2.758623	-1.682057	-1.343730
H	-4.237147	-2.037738	-0.687698
H	-6.719673	-2.029957	-0.686946
H	-4.235106	2.042701	0.686116
H	-6.717644	2.037491	0.685100
H	-10.576163	2.145046	-2.577811
H	-10.578644	-2.133329	2.575750
H	-13.034480	2.168645	-2.615267
H	-13.036988	-2.154125	2.613164
H	-14.995678	2.157097	-2.626651
H	-14.998180	-2.140346	2.624505
H	-17.455637	2.133428	-2.598507
H	-17.458109	-2.113792	2.596378
H	-20.700851	0.011723	-0.001052

π-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	15.145485	-1.483558	0.068686
C	13.936516	-0.724884	0.034302
C	12.698248	-1.417927	0.066369
C	12.687211	-2.843274	0.131899
C	13.909018	-3.549776	0.164101
C	15.126566	-2.859503	0.132000
C	11.452690	-3.537728	0.163886
C	11.428430	-5.016523	0.230955

N	12.675340	-5.628349	0.259638
C	13.924189	-5.028344	0.232316
C	11.460174	-0.713184	0.033916
C	10.223490	-1.455344	0.068468
C	10.241669	-2.849889	0.133022
C	11.460705	0.701523	-0.032106
C	10.224580	1.444588	-0.067113
C	9.020385	0.674462	-0.031428
C	9.019869	-0.684338	0.032307
C	12.699304	1.405362	-0.064115
C	13.937053	0.711414	-0.031619
C	7.605032	1.151928	-0.051265
N	6.804155	-0.004115	-0.000045
C	7.604149	-1.160755	0.051538
C	12.689332	2.830718	-0.129640
C	11.455331	3.526074	-0.162060
C	10.243797	2.839119	-0.131647
C	15.146586	1.469204	-0.065582
C	15.128696	2.845164	-0.128893
C	13.911665	3.536328	-0.161409
C	13.927937	5.014887	-0.229601
N	12.679535	5.615803	-0.257354
C	11.432170	5.004885	-0.229120
O	14.941655	-5.685110	0.262746
O	10.410567	-5.670497	0.259590
O	7.205346	2.283925	-0.099170
O	7.203597	-2.292454	0.099233
O	14.945892	5.670912	-0.259664
O	10.414794	5.659600	-0.258108
C	5.382973	-0.003564	-0.000401
H	12.669514	-6.644835	0.306037
H	12.674467	6.632293	-0.303742
H	16.049062	-3.442415	0.158509
H	16.108081	-0.974830	0.044689
H	16.108800	0.959771	-0.041255
H	16.051627	3.427402	-0.155077
H	9.309210	-3.415052	0.159748
H	9.311760	3.404958	-0.158716
C	4.682176	0.984108	0.697434
C	4.681734	-0.990659	-0.698606
C	3.294410	-0.991363	-0.692280
C	3.294861	0.985981	0.690332
C	2.577686	-0.002383	-0.001182
C	1.149044	-0.001726	-0.001584
C	-0.066358	-0.001079	-0.001863
C	-1.440249	-0.000268	-0.002100
C	-2.655579	0.000504	-0.002284
C	-4.084868	0.001400	-0.002421
C	-4.798968	-1.117559	-0.458835
C	-4.797593	1.121262	0.453934
C	-6.185238	1.118708	0.455907
C	-6.186613	-1.113289	-0.460833
C	-6.880844	0.003131	-0.002450
N	-8.318706	0.003997	-0.002326
C	-8.969450	-0.890044	0.864376
C	-8.968562	0.898878	-0.868823
C	-10.453223	0.877637	-0.856216
C	-10.454082	-0.866728	0.852391
C	-11.165809	0.005974	-0.001738
O	-8.341384	-1.634063	1.578653
O	-8.339752	1.641966	-1.583414
C	-11.140644	1.727938	-1.693391
C	-11.142331	-1.716050	1.689878
C	-12.587590	0.007019	-0.001382
C	-12.542003	1.733123	-1.701415
C	-12.543691	-1.719176	1.698603

C	-13.282981	-0.881177	0.875223
C	-13.282113	0.896244	-0.877631
C	-14.757257	0.896393	-0.878580
C	-14.758121	-0.879088	0.876984
C	-15.454318	0.009188	-0.000598
C	-15.494616	-1.714192	1.705250
C	-15.492944	1.732622	-1.706429
C	-16.894234	1.728917	-1.702113
C	-16.876854	0.010287	-0.000183
C	-16.895901	-1.708321	1.701752
C	-17.584161	0.883269	-0.863982
C	-17.585007	-0.861599	0.864030
C	-19.069416	0.898443	-0.877636
C	-19.070275	-0.874463	0.878562
N	-19.677581	0.012464	0.000644
O	-19.726854	1.619232	-1.591033
O	-19.728412	-1.594228	1.592348
H	5.221816	-1.767562	-1.237747
H	5.222608	1.760559	1.236873
H	2.751427	1.761772	1.233127
H	2.750627	-1.766692	-1.235384
H	-4.253544	-1.993787	-0.814320
H	-6.737790	-1.986312	-0.814385
H	-4.251090	1.996807	0.809444
H	-6.735342	1.992406	0.809466
H	-10.572361	2.393693	-2.345630
H	-10.574701	-2.382638	2.341835
H	-13.043553	2.421972	-2.380261
H	-13.045911	-2.407296	2.377692
H	-14.987848	2.418303	-2.385820
H	-14.990184	-2.400651	2.384350
H	-17.460768	2.392267	-2.358779
H	-17.463079	-2.370795	2.358746
H	-20.694948	0.013256	0.000946

d-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	15.064588	-1.484218	0.010567
C	13.885490	-0.742116	0.005243
C	12.638511	-1.435718	0.006878
C	12.633330	-2.857124	0.012788
C	13.852685	-3.565798	0.018098
C	15.052342	-2.879935	0.017130
C	11.390428	-3.555814	0.013310
C	11.368012	-5.042201	0.019555
N	12.616914	-5.652012	0.025180
C	13.866503	-5.050138	0.025046
C	11.396809	-0.730978	0.002940
C	10.182806	-1.452070	0.003401
C	10.204278	-2.874730	0.008280
C	11.397218	0.719281	-0.001666
C	10.183621	1.441050	-0.003089
C	8.963841	0.703876	-0.000304
C	8.963437	-0.714216	-0.000383
C	12.639315	1.423330	-0.004622
C	13.885903	0.729034	-0.002016
C	7.633771	1.203182	0.001994
N	6.778132	-0.004538	-0.001189
C	7.633080	-1.212761	-0.003760
C	12.634928	2.844739	-0.010525
C	11.392416	3.544122	-0.012015
C	10.205885	2.863698	-0.007933

C	15.065418	1.470481	-0.006418
C	15.053953	2.866205	-0.012983
C	13.854679	3.552736	-0.014878
C	13.869326	5.037070	-0.021801
N	12.620072	5.639637	-0.022900
C	11.370828	5.030518	-0.018257
O	14.877547	-5.714102	0.030327
O	10.357715	-5.704772	0.020050
O	7.197364	2.342146	-0.000323
O	7.196029	-2.351479	-0.001666
O	14.880742	5.700472	-0.026289
O	10.360899	5.693649	-0.019524
C	5.421867	-0.004090	-0.001666
H	12.613045	-6.669045	0.029843
H	12.616771	6.656672	-0.027551
H	15.981529	-3.452995	0.021531
H	16.030497	-0.980423	0.009908
H	16.031044	0.966148	-0.005008
H	15.983462	3.438747	-0.016654
H	9.263684	-3.426460	0.008674
H	9.265598	3.415948	-0.009070
C	4.679105	1.223455	0.077505
C	4.678256	-1.231095	-0.081326
C	3.309396	-1.219489	-0.084202
C	3.310241	1.212852	0.079494
C	2.582935	-0.003053	-0.002579
C	1.180647	-0.002487	-0.002971
C	-0.042697	-0.001812	-0.003250
C	-1.404515	-0.001109	-0.003311
C	-2.623599	-0.000307	-0.003326
C	-4.046942	0.000649	-0.003292
C	-4.758699	-1.181355	-0.267495
C	-4.757004	1.183646	0.261042
C	-6.143208	1.180450	0.265482
C	-6.144902	-1.176249	-0.271567
C	-6.839485	0.002572	-0.002921
N	-8.274051	0.003556	-0.002583
C	-8.928043	-0.854111	0.903384
C	-8.927307	0.862190	-0.908155
C	-10.409380	0.842666	-0.890768
C	-10.410087	-0.832108	0.887143
C	-11.121135	0.005895	-0.001514
O	-8.297898	-1.563712	1.650298
O	-8.296536	1.570801	-1.655483
C	-11.097571	1.660472	-1.760074
C	-11.098959	-1.648743	1.757009
C	-12.543009	0.007138	-0.000904
C	-12.498368	1.668310	-1.765280
C	-12.499760	-1.654135	1.763412
C	-13.238684	-0.849078	0.907095
C	-13.237965	0.864580	-0.908294
C	-14.713057	0.868601	-0.905256
C	-14.713783	-0.850439	0.905403
C	-15.409613	0.009719	0.000402
C	-15.450025	-1.661964	1.756729
C	-15.448614	1.681470	-1.755890
C	-16.850188	1.679770	-1.749783
C	-16.831921	0.011028	0.001079
C	-16.851598	-1.657684	1.751955
C	-17.539366	0.858847	-0.887187
C	-17.540081	-0.835484	0.890021
C	-19.025448	0.874325	-0.900355
C	-19.026176	-0.848207	0.904619
N	-19.633701	0.013623	0.002426
O	-19.681370	1.575556	-1.633677
O	-19.682692	-1.548218	1.638575

H	5.227326	-2.165734	-0.138296
H	5.228824	2.157691	0.134852
H	2.762477	2.154666	0.144369
H	2.760985	-2.160902	-0.149416
H	-4.213497	-2.104360	-0.473116
H	-6.694467	-2.095505	-0.475950
H	-4.210475	2.105888	0.466564
H	-6.691450	2.100454	0.470060
H	-10.530496	2.299146	-2.439843
H	-10.532420	-2.288408	2.436293
H	-13.000129	2.331226	-2.469144
H	-13.002074	-2.316181	2.467701
H	-14.943944	2.346955	-2.455401
H	-14.945915	-2.328371	2.455766
H	-17.416861	2.324545	-2.424546
H	-17.418817	-2.301412	2.427258
H	-20.651183	0.014568	0.002917

b-CT-Minimum

CAM-B3LYP/def2-SV(P) optimized

C	12.646728	-2.834358	-0.282467
C	11.399681	-3.529647	-0.353336
C	12.658415	-1.411636	-0.139311
C	13.860739	-3.537307	-0.352288
C	11.417270	-0.706151	-0.069263
C	13.899807	-0.719638	-0.068886
C	15.095667	-1.472617	-0.143616
C	15.074656	-2.843712	-0.281566
C	10.183395	-1.449263	-0.144867
C	10.204268	-2.847007	-0.285516
C	13.899649	0.720492	0.075885
C	11.417131	0.706835	0.072880
C	12.658109	1.412390	0.144629
C	10.183082	1.449882	0.146784
C	15.095343	1.473576	0.152234
C	12.646135	2.835104	0.287768
C	15.074052	2.844653	0.290160
C	10.203672	2.847703	0.287476
C	13.859946	3.538134	0.359235
C	11.398891	3.530349	0.356927
C	13.873900	5.002992	0.506819
C	11.372558	4.996386	0.504636
N	12.620554	5.600884	0.566232
O	14.882370	5.675690	0.575247
O	10.357774	5.661136	0.571004
H	12.618209	6.612221	0.668087
C	13.875022	-5.002140	-0.499849
C	11.373660	-4.995653	-0.501068
N	12.621789	-5.600077	-0.560996
O	14.883639	-5.674782	-0.566901
O	10.359015	-5.660494	-0.568846
H	12.619636	-6.611412	-0.662861
H	15.998360	3.422767	0.348876
H	16.059751	0.970400	0.102101
H	16.059965	-0.969364	-0.092179
H	15.999090	-3.421754	-0.339028
H	9.276283	3.415932	0.344097
H	9.276984	-3.415275	-0.343406
C	8.991429	0.685508	0.069096
C	8.991509	-0.684820	-0.068833
C	7.606930	1.171936	0.117137
C	7.607158	-1.171158	-0.118841

N	6.753190	0.000433	-0.001488
O	7.199454	2.293475	0.229837
O	7.199792	-2.292700	-0.232130
C	5.378787	0.000495	-0.002545
C	4.642711	-1.218284	-0.124659
C	4.642673	1.219366	0.118414
C	3.272606	-1.211568	-0.125179
C	3.272567	1.212825	0.116757
C	2.541688	0.000673	-0.004798
H	5.180917	-2.155604	-0.217588
H	2.728875	-2.153239	-0.219533
H	5.180842	2.156627	0.212187
H	2.728806	2.154565	0.210242
C	1.148576	0.000750	-0.005927
C	-0.081087	0.000739	-0.006939
C	-1.432385	0.000679	-0.008054
C	-2.656952	0.000408	-0.009065
C	-4.072012	-0.000830	-0.010091
C	-4.780340	-1.211870	-0.137724
C	-4.782639	1.208984	0.116430
C	-6.168348	1.201817	0.116534
C	-6.166069	-1.207284	-0.139523
C	-6.860966	-0.003419	-0.011797
H	-4.228851	-2.148710	-0.236213
H	-6.714109	-2.146022	-0.237808
H	-4.232939	2.146809	0.215585
H	-6.718222	2.139573	0.213812
N	-8.294404	-0.003094	-0.009457
C	-8.945960	-0.756759	0.986654
C	-8.948975	0.750813	-1.003391
C	-10.430484	0.731872	-0.982119
C	-10.427516	-0.736340	0.970977
C	-11.140047	-0.001860	-0.004208
O	-8.311817	-1.378812	1.804884
O	-8.317280	1.372091	-1.824104
C	-11.120591	1.447753	-1.936063
C	-11.114711	-1.451573	1.927504
C	-12.561927	-0.001122	-0.001490
C	-12.521163	1.453908	-1.940018
C	-12.515262	-1.456260	1.936824
C	-13.255743	-0.751345	0.997294
C	-13.258778	0.749830	-0.997608
C	-14.733678	0.753345	-0.992787
C	-14.730654	-0.753227	0.998193
C	-15.428192	0.000457	0.004063
C	-15.465076	-1.465076	1.936023
C	-15.470947	1.466024	-1.927748
C	-16.872462	1.464381	-1.919362
C	-16.850459	0.001275	0.006846
C	-16.866610	-1.461818	1.933124
C	-17.559694	0.744447	-0.969369
C	-17.556724	-0.741077	0.985835
C	-19.045920	0.757731	-0.981782
C	-19.042904	-0.752623	1.004083
N	-19.652282	0.002910	0.012345
O	-19.703019	1.372554	-1.787856
O	-19.697553	-1.366672	1.812738
H	-10.555238	2.007511	-2.683471
H	-10.547087	-2.011951	2.672721
H	-13.024629	2.034095	-2.712335
H	-13.016370	-2.035955	2.711042
H	-14.967654	2.049569	-2.697841
H	-14.959443	-2.049196	2.704143
H	-17.440621	2.029582	-2.660913
H	-17.432514	-2.026367	2.676891
H	-20.669791	0.003507	0.014344

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