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Supporting information available for

Synthesis and Conformation of a Novel Fluorescein-Zn-Porphyrin Dyad and Intramolecular Energy Transfer

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1. NOESY spectrum of dyad 1 at 323 K

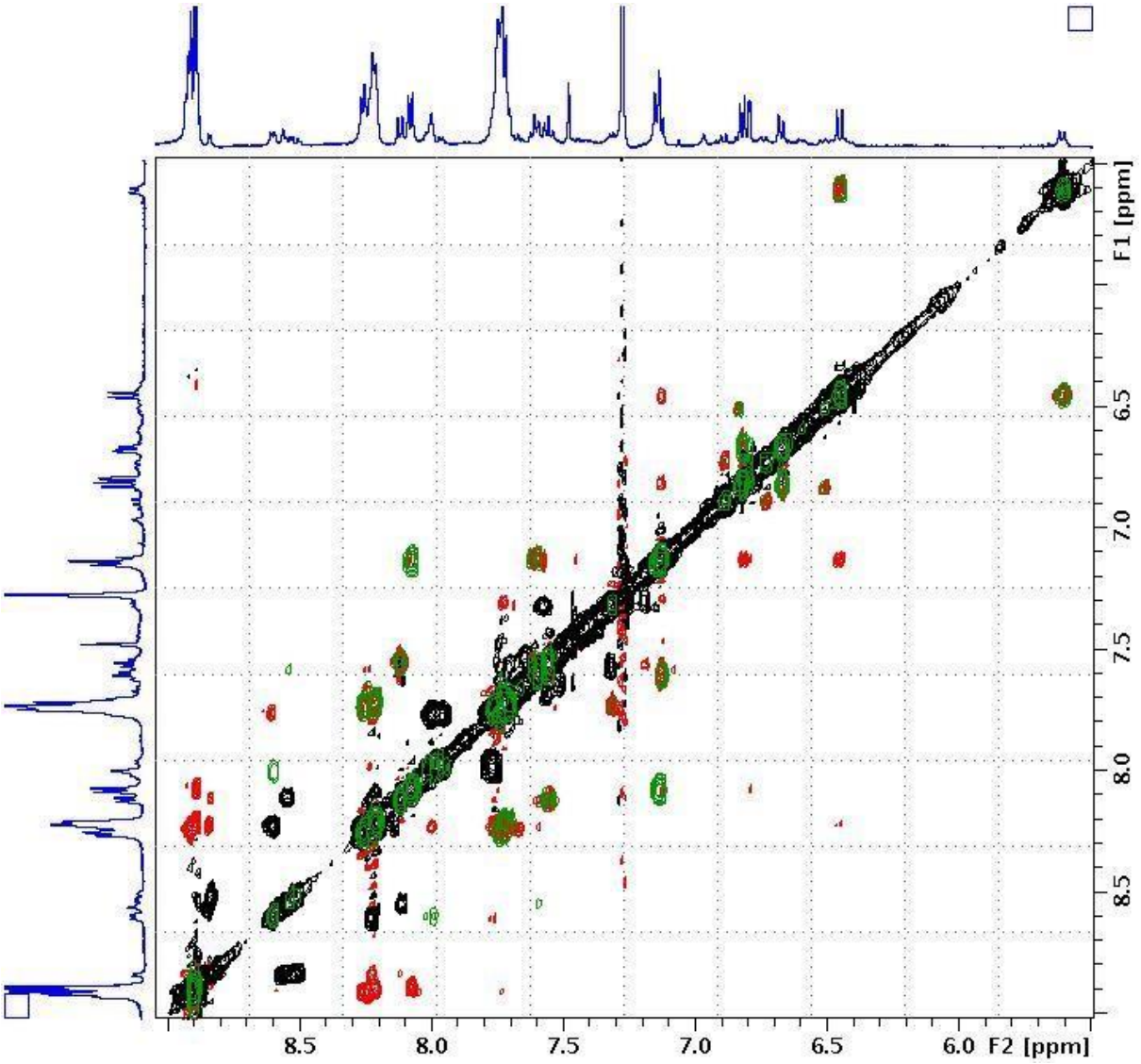

Figure 1: Aromatic region of the NOESY spectrum of **1** at 323 K.

2. Excitation and emission spectra of dyad 1

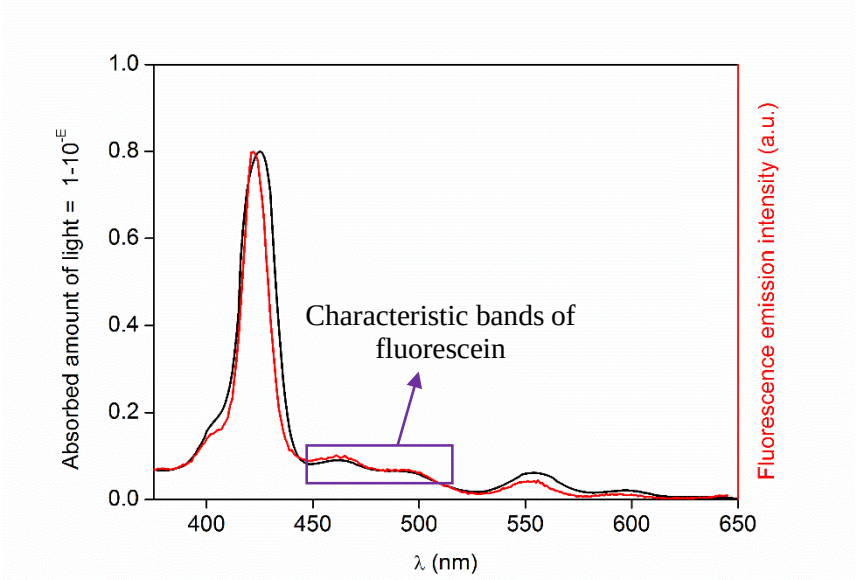

Figure 2: Comparison between excitation (red line, λ_{obs} = 650 nm) and absorption (black line) spectra of dyad **1** in $CHCl_3$ (conc. 2 x 10^{-6} mol.L^{-1}, room temp.).

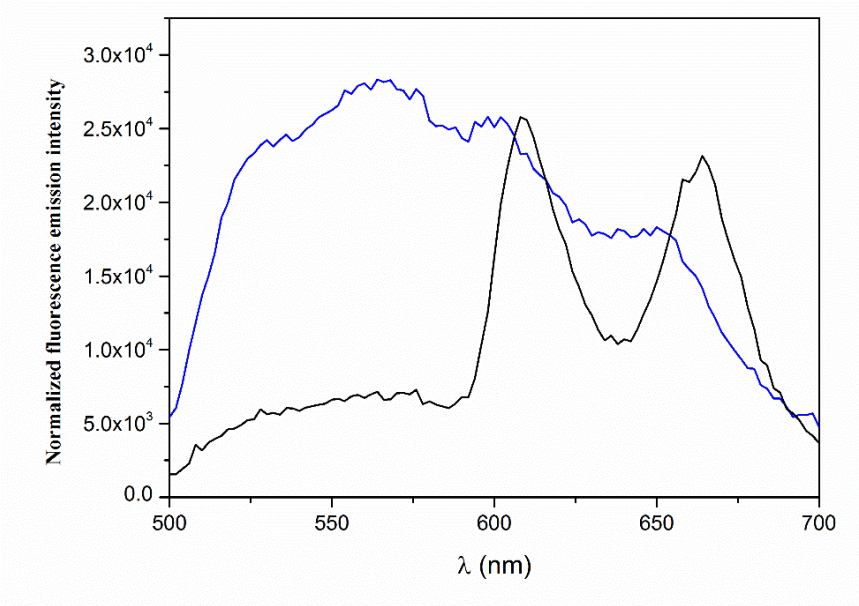

Figure 3: Normalized emission spectra λ_{em} = 490 nm (relative to porphyrin emission maximum) of dyad 1 in $CHCl_3$ (blue line) and DMSO (black line) at 298 K (conc. 2.10^{-6} M).

3. DFT calculations of dyad 1 (linear and folded form).

Table 1: Total energies of dyad **1** in two conformations (linear and folded form), in different solvents using PCM method. Energies are given in Hartrees and in eV.

	Gas phase		Chloroform		DMSO		Water	
	Linear	**Folded**	**Linear**	**Folded**	**Linear**	**Folded**	**Linear**	**Folded**
	Energy (Hartree)							
B3LYP	-3635.3078	-3635.3140	-3635.4699	-3635.4986	-3635.3564	-3635.3890	-3635.3572	-3635.3949
ωB97XD	-3634.1359	-3634.1359	-3634.2429	-3634.2827	-3634.1566	-3634.2086	-3634.1574	-3634.2156
	Energy (eV)							
B3LYP	-98922.5407	-98922.7108	-98926.9529	-98927.7348	-98923.8654	-98924.7511	-98923.8867	-98924.9106
ωB97XD	-98889.8368	-98890.6517	-98893.5632	-98894.6479	-98891.2161	-98892.6314	-98891.2381	-98892.8207

Table 2: Energy gap between linear and fold form in dyad **1** in different solvents using PCM method.

	Gas phase	Chloroform	DMSO	Water	Gas phase	Chloroform	DMSO	Water
	ΔE (linear-folded) in Hartrees				**ΔE (linear-folded) in kJ/mol**			
B3LYP	0.01	0.03	0.03	0.04	16.41	75.44	85.45	98.79
ωB97XD	0.03	0.04	0.05	0.06	78.62	104.66	136.56	152.70
	ΔE (linear-folded) in eV				**ΔE (linear-folded) in kcal/mol**			
B3LYP	0.17	0.78	0.89	1.02	3.92	18.03	20.42	23.61
ωB97XD	0.81	1.08	1.42	1.58	18.79	25.01	32.64	36.50

4. TD-DFT calculations of compounds 1, 2 and 3

4-1. Excited states data

Table 3: Calculated optical properties (vertical transition wavelengths and energies, oscillator strength, configuration interaction description) as obtained with a) B3LYP and b) ωB97XD functionals for compound **1** (folded form).

A) B3LYP

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	566.9	2.19	0.01	H-1→L+2 (14%) **H→L (68%)** H→L+1 (-13%)
2	555.3	2.23	0.07	H-1→L+1 (35%) H-1→L+2 (19%) H→L+1 (-28%) H→L+2 (50%)
3	553.9	2.28	0.05	H-1→L+1 (19%) H-1→L+2 (-32%) **H→L (19%)** H→L+1 (50%) H→L+2 (28%)
4	492.0	2.52	0.01	**H-1→L (70%)**
5	422.3	2.94	0.06	H-4→L (63%) *H-2→L (-25%)*
6	417.1	2.97	0.40	*H-4→L (26%)* *H-2→L (54%)* **H-2→L+1 (-18%)** H-1→L+1 (19%) H-1→L+2 (-14%) H→L+2 (-12%)
7	407.6	3.04	1.18	**H-2→L+1 (42%)** **H-2→L+2 (-22%)** H-1→L+1 (35%) H-1→L+2 (24%) H→L+1 (16%) H→L+2 (-25%)
8	406.9	3.05	0.38	*H-2→L (13%)* **H-2→L+1 (53%)** H-1→L+1 (-19%) H-1→L+2 (-30%) H→L+1 (-20%) H→L+2 (13%)
9	402.8	3.08	0.58	*H-2→L (-15%)* *H-2→L+2 (54%)* H-1→L+1 (31%) H-1→L+2 (-14%) H→L+2 (-22%) *H→L+3 (12%)*
10	401.7	3.09	0.78	*H-2→L (-20%)* H-2→L+2 (-37%) H-1→L+1 (13%) H-1→L+2 (-30%)

				H→L+1 (-21%) *H→L+3 (38%)*
11	400.8	3.09	0.50	*H-2→L (15%)* **H-2→L+2 (13%)** H-1→L+1 (-14%) H-1→L+2 (23%) H→L+1 (16%) H→L+3 (58%)

*In black : transfer from porphyrin to porphyrin. In **red** : transfer from fluorescein to porphyrin orbitals. In *blue* : from fluorescein to fluorescein.

B) ωB97XD

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	572.8	2.16	0.04	H-1→L+1 (43%) H→L (54%)
2	571.6	2.17	0.07	H-1→L (-43%) H→L+1 (54%)
3	388.8	3.19	1.16	*H-2→L+2 (44%)* H-1→L (34%) H-1→L+1 (25%) H→L (-19%) H→L+1 (28%)
4	384.5	3.22	1.77	H-1→L (-35%) H-1→L+1 (42%) H→L (-32%) H→L+1 (-28%)
5	377.0	3.29	1.61	H-2→L (-10%) *H-2→L+2 (50%)* H-1→L (-24%) H-1→L+1 (-27%) H→L (21%) H→L+1 (-19%)
8	306.5	4.04	0.12	H-9→L+2 (10%) H-7→L+2 (-23%) H-5→L+2 (-14%) H-4→L (-14%) *H-4→L+2 (55%)* *H-2→L+2 (11%)*

*In black : transfer from porphyrin to porphyrin. In **red** : transfer from fluorescein to porphyrin orbitals. In *blue* : from fluorescein to fluorescein.

C) CAM-B3LYP

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	553.4	2.24	0.03	H-1→L+1 (-44%) H→L (53%) H→L (-12%)
2	553.2	2.24	0.03	H-1→L (44%) H→L (12%) H→L+1 (53%)
3	384.3	3.23	1.09	*H-2→L+2 (36%)* H-1→L (-18%) H-1→L+1 (43%)

				H→L (35%) H→L+1 (15%)
4	382.1	3.24	2.07	H-1→L (50%) H-1→L+1 (22%) H→L (18%) H→L+1 (-41%)
5	373.8	3.32	1.39	*H-2→L+2 (59%)* H-1→L (12%) H-1→L+1 (-25%) H→L (-21%) H→L+1 (-10%)
9	302.8	4.09	0.15	H-6→L+2 (-27%) H-5→L+2 (57%) *H-4→L+2 (-17%)* *H-2→L+2 (10%)*

*In black : transfer from porphyrin to porphyrin. In **red** : transfer from fluorescein to porphyrin orbitals. In *blue* : from fluorescein to fluorescein.

Table 4: Calculated optical properties (vertical transition wavelengths and energies, oscillator strength, configuration interaction description) as obtained with a) B3LYP and b) ωB97XD functionals for compound **1** (linear form).

A) B3LYP

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	542.7	2.28	0.04	H-1→L+2 (42%) H→L+1 (56%)
2	542.4	2.29	0.04	H-1→L+1 (-42%) H→L+2 (56%)
3	491.5	2.52	0.00	H→L (71%)
4	446.3	2.78	0.00	H-1→L (71%)
5	426.0	2.91	0.00	H-4→L (70%)
6	412.1	3.01	0.64	H-5→L (-16%) *H-2→L (67%)*
7	399.4	3.10	1.66	H-3→L+2 (16%) H-1→L+1 (52%) H-1→L+2 (-15%) H→L+1 (11%) H→L+2 (40%)
8	397.4	3.12	1.59	H-1→L+1 (16%) H-1→L+2 (54%) H→L+1 (-40%) H→L+2 (12%)

*In black : transfer from porphyrin to porphyrin. In **red** : transfer from fluorescein to porphyrin orbitals. In *blue* : from fluorescein to fluorescein.

B) ωB97XD

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	561.2	2.21	0.02	H-1→L (-44%) H-1→L+1 (-11%) H→L (-13%) H→L+1 (-52%)
2	561.1	2.21	0.02	H-1→L (11%) H-1→L+1 (44%) H→L (52%) H→L+1 (13%)
3	380.0	3.26	1.41	*H-4→L+2 (-10%)* *H-2→L+2 (64%)* H-1→L (19%) H→L+1 (16%)
4	377.7	3.28	1.28	*H-2→L+2 (-24%)* H-1→L (47%) H-1→L+1 (-17%) H→L (14%) H→L+1 (40%)
5	377.3	3.29	1.93	H-1→L (17%) H-1→L+1 (51%) H→L (-43%) H→L+1 (14%)

*In black : transfer from porphyrin to porphyrin. In **red** : transfer from fluorescein to porphyrin orbitals. In *blue* : from fluorescein to fluorescein.

C) CAM-B3LYP

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	546.5	2.27	0.01	H-1→L (-19%) H-1→L+1 (-42%) H→L (48%) H→L+1 (-22%)
2	546.3	2.26	0.01	H-1→L (42%) H-1→L+1 (-19%) H→L (21%) H→L+1 (48%)
3	378.2	3.28	2.12	*H-2→L+2 (25%)* H-1→L (48%) H-1→L+1 (13%) H→L (11%) H→L+1 (-42%)
4	377.1	3.29	1.78	H-1→L (-13%) H-1→L+1 (52%) H→L (45%) H→L+1 (11%)
5	375.8	3.30	0.72	*H-2→L+2 (64%)* H-1→L (-19%) H→L+1 (17%)

*In black : transfer from porphyrin to porphyrin. In **red** : transfer from fluorescein to porphyrin orbitals. In *blue* : from fluorescein to fluorescein.

Table 5: Computed optical properties obtained with a) B3LYP and b) ωB97XD (absorption wavelength, vertical transition energies, oscillator strength, configuration interaction (CI) description) for compound **2** (porphyrin).

A) B3LYP

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	555.3	2.23	0.05	H-1→L+1 (40%) H→L (58%)
2	554.3	2.24	0.06	H-1→L (-41%) H→L+1 (58%)
3	408.8	3.03	1.62	H-2→L+1 (24%) H-1→L (53%) H→L+1 (38%)
4	405.3	3.06	1.45	H-2→L (-15%) H-1→L+1 (56%) H→L (-39%)

B) ωB97XD

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	564.3	2.20	0.03	H→L (54%) H→L+1 (-45%)
2	564.1	2.20	0.03	H-1→L (45%) H→L+1 (54%)
3	380.0	3.26	1.96	H-1→L (54%) H→L (10%) H→L+1 (-45%)
4	379.0	3.27	1.85	H-1→L+1 (54%) H→L (45%) H→L+1 (-10%)

C) CAM-B3LYP

Excited states	λ (nm)	E (eV)	f	MO contribution*
1	547.6	2.26	0.01	H-1→L+1 (-46%) H→L (53%)
2	547.5	2.26	0.01	H-1→L (46%) H→L+1 (53%)
3	378.7	3.27	1.96	H-1→L (53%) H→L+1 (-46%)
4	377.8	3.28	1.85	H-1→L+1 (53%) H→L (46%)

Table 6: Computed optical properties obtained with a) B3LYP and b) ωB97XD (absorption wavelength, vertical transition energies, oscillator strength, configuration interaction (CI) description) for compound **3** (fluorescein).

A) B3LYP

Excited state	λ (nm)	E (eV)	f	MO contribution*
1	428.8	2.89	0.59	H-2→L (15%) H→L (68%)

.

B) ωB97XD

Excited state	λ (nm)	E (eV)	f	MO contribution*
1	387.0	3.20	0.80	H-1→L (-11%) H→L (69%)

C) CAM-B3LYP

Excited state	λ (nm)	E (eV)	f	MO contribution*
1	386.03	3.2118	0.8230	H→L (69%)

4-2. Excited states diagram

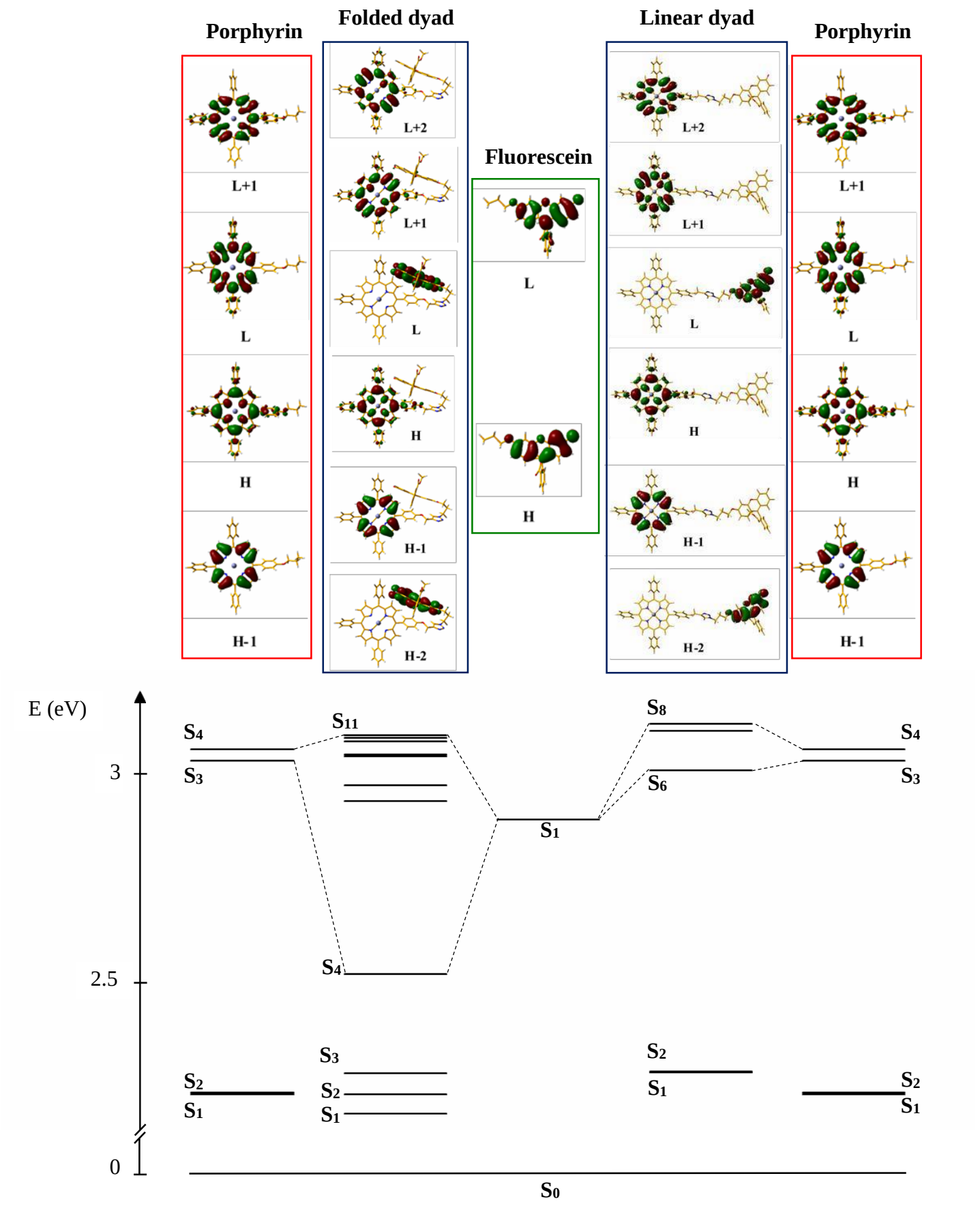

Figure 4: Molecular orbitals and excited states involved in dyad **1** and reference compounds **2** and **3** with B3LYP functionals.

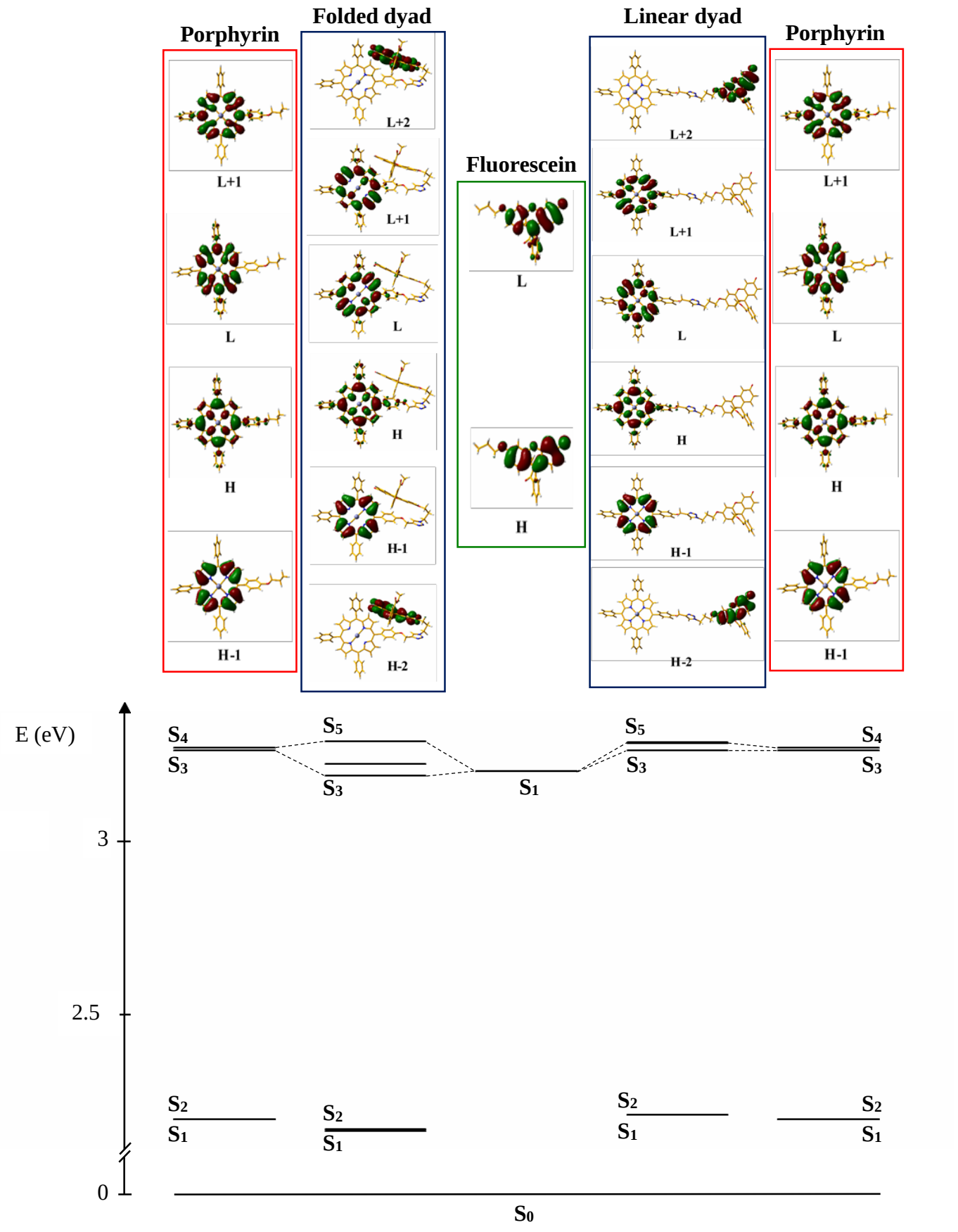

Figure 5: Molecular orbitals and excited states involved in dyad **1** and reference compounds **2** and **3** with ωB97XD functionals.

5. CT state between porphyrin and fluorescein patterns (B3LYP functional)

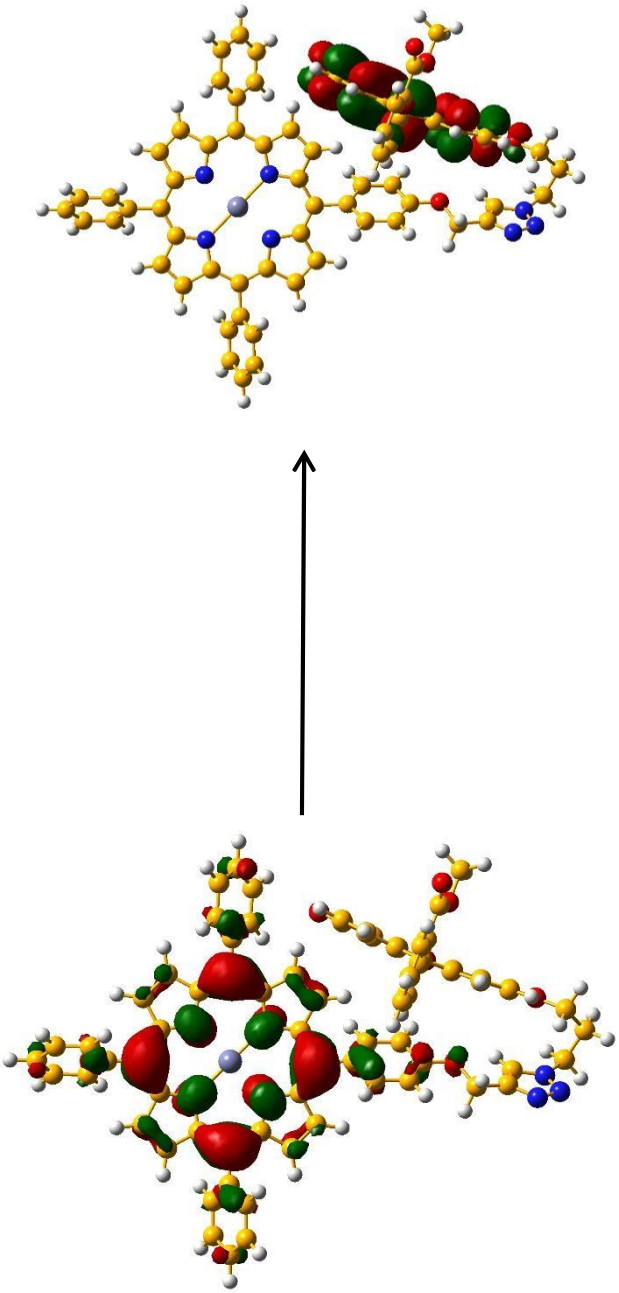

Figure 6: Internal charge transfer between porphyrin and fluorescein patterns in the $S_0 \rightarrow S_1$ transition, with B3LYP functional.

6. Computational data

All calculations were performed with GaussianG09[1]. DFT and TD-DFT calculations were obtained in chloroform, which was described with PCM method.

6-1. Ground states

Compound 1 (linear form) ground state configuration (DFT-ωB97XD/6-31+G(d,p))

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

N	6.65768900	1.48101300	-0.04781700
C	6.80728700	2.83903500	0.00136300
C	5.33493500	1.22290600	-0.28026100
C	5.52267100	3.46831100	-0.20735100
C	4.61428900	2.47286400	-0.37136300
C	8.01578500	3.52739100	0.20837600
C	9.27678400	2.93434300	0.38999700
N	9.54323900	1.59323800	0.36479100
C	10.49687700	3.65841900	0.66980100
C	10.87923200	1.43737100	0.61094600
C	11.48360900	2.73650200	0.80556700
C	11.56385700	0.21307700	0.70260300
C	10.98203000	-1.06176500	0.59087900
N	9.65690200	-1.32015600	0.37561800
C	11.70221000	-2.31188300	0.68897000
C	9.50512500	-2.67883100	0.34213200
C	10.79063900	-3.30753400	0.54783500
C	8.29614400	-3.36669600	0.14291600
C	7.03694000	-2.77289200	-0.05303200
N	6.77034800	-1.43198200	-0.03494900
C	5.82322400	-3.49751800	-0.35457400
C	5.43978900	-1.27602100	-0.31030200
C	4.84046500	-2.57540800	-0.51716400
C	4.75578500	-0.05115500	-0.41376700
C	7.95384200	5.02102500	0.24161500
C	8.52463500	5.77864200	-0.78613100
C	7.32481200	5.68473700	1.29986900
C	8.46696900	7.16954900	-0.75722000
C	7.26574400	7.07549900	1.32953200
C	7.83683400	7.82137500	0.30060200
C	3.29544800	-0.11773400	-0.72111300
C	2.38432800	-0.64883800	0.20174900
C	2.80375500	0.32069700	-1.95008900
C	1.03626700	-0.75308500	-0.10188600
C	1.45054700	0.22659600	-2.27135200
C	0.56261400	-0.32391400	-1.34636800
C	8.35302700	-4.86072300	0.12786400
C	7.77084500	-5.60209700	1.16110000

C	8.98621400	-5.54115400	-0.91717700
C	7.82239500	-6.99344400	1.15134300
C	9.03900700	-6.93247000	-0.92779300
C	8.45722700	-7.66198000	0.10684500
C	13.03625500	0.27448900	0.95506800
C	13.90605300	0.76224300	-0.02562800
C	13.56793200	-0.15023700	2.17715600
C	15.27686200	0.82453700	0.20976100
C	14.93867200	-0.09033000	2.41303700
C	15.79681200	0.39746800	1.42977500
O	-0.76887900	-0.49147300	-1.56262800
H	5.34213400	4.53367900	-0.22661300
H	3.55146000	2.57359400	-0.53883600
H	10.58095500	4.73150800	0.76651300
H	12.52524900	2.91507800	1.03133000
H	12.76631600	-2.41274300	0.84781200
H	10.96988900	-4.37278300	0.57973800
H	5.74114300	-4.57079900	-0.45081700
H	3.80520200	-2.75581800	-0.76875700
H	9.01280100	5.27025600	-1.61293100
H	6.88199500	5.10297700	2.10346300
H	8.91190800	7.74362400	-1.56460600
H	6.77651300	7.57611500	2.15987100
H	2.74400400	-0.99248200	1.16749000
H	3.49223800	0.73506900	-2.68104900
H	0.33172000	-1.16944600	0.61088000
H	1.11427100	0.57554300	-3.24076000
H	7.27874900	-5.08046500	1.97727000
H	9.43717100	-4.97232800	-1.72546300
H	7.36899500	-7.55458700	1.96310500
H	9.53176900	-7.44626500	-1.74793200
H	13.50002800	1.09355100	-0.97733900
H	12.89753600	-0.52570300	2.94521400
H	15.94007100	1.20341700	-0.56226500
H	15.33647300	-0.42200200	3.36761500
C	-1.28392800	-0.14092700	-2.83211200
H	-1.17985500	0.93971400	-3.00081600
H	-0.74091200	-0.66052700	-3.63225700
C	-2.72098700	-0.54650200	-2.86244500
C	-3.55004700	-0.94544900	-1.84230100
H	-3.40074500	-1.07304000	-0.78251200
N	-4.72518300	-1.20577000	-2.45914100
N	-4.63806600	-0.97595600	-3.77288000
N	-3.42292300	-0.57942500	-4.02414700
C	-5.99117900	-1.63096000	-1.88331500
H	-5.77159100	-2.10792200	-0.92505800
H	-6.40823700	-2.38781900	-2.55272000
C	-6.95294700	-0.45565000	-1.71821800
H	-6.53327200	0.27539600	-1.01922900
H	-7.08210900	0.04010400	-2.68523200

C	-8.30744800	-0.92330200	-1.21385500
H	-8.74935700	-1.64603300	-1.91229200
H	-8.22070000	-1.40030000	-0.22852300
O	-9.13171600	0.23066200	-1.12392800
C	-10.42446300	0.08794300	-0.77345900
C	-11.02331100	-1.13701300	-0.42932900
C	-11.17858900	1.26035200	-0.77195600
C	-12.36308000	-1.16676200	-0.08900300
H	-10.45632000	-2.05951800	-0.42865200
C	-12.51891800	1.20235000	-0.42724500
H	-10.72265500	2.20478300	-1.04432900
C	-13.14775300	-0.00263500	-0.07009500
H	-12.81879700	-2.11787200	0.16528900
O	-13.19898700	2.37396800	-0.45907500
C	-14.54676900	0.03297200	0.29189200
C	-14.52301400	2.43134100	-0.15260600
C	-15.22179800	1.22126300	0.24027800
C	-15.23610100	-1.23747800	0.65401200
C	-15.12882100	3.64164800	-0.22502400
C	-16.61835600	1.37513000	0.59618900
C	-14.99387300	-1.93426100	1.85211800
C	-16.12051000	-1.78591800	-0.27835200
C	-16.53645000	3.79552200	0.10353800
H	-14.56716400	4.51918400	-0.52522100
C	-17.23692500	2.56943000	0.53043100
H	-17.15901700	0.49302300	0.92321900
C	-15.62967600	-3.15589300	2.08267800
C	-14.06712200	-1.45537100	2.92423800
C	-16.76126600	-2.99626700	-0.03162900
H	-16.29850500	-1.25680400	-1.20947100
O	-17.12101300	4.88102200	0.04239200
H	-18.28340400	2.67774900	0.79787000
C	-16.51478400	-3.68523400	1.15206900
H	-15.42122500	-3.67912300	3.00959300
O	-13.56137600	-2.18693700	3.74876300
O	-13.87038900	-0.13795400	2.88594500
H	-17.44901200	-3.39930800	-0.76816600
H	-17.00793400	-4.63136900	1.34914900
C	-12.92876700	0.38943300	3.82294700
H	-12.87263400	1.45561000	3.60924800
H	-13.27421100	0.22058600	4.84504900
H	-11.95305900	-0.08164400	3.68406000
H	8.49898600	-8.74710900	0.09915200
H	16.86590200	0.44641900	1.61365900
H	7.79044900	8.90609700	0.32322900
Zn	8.15714300	0.08049800	0.16495000

Compound 1 (folded form) ground state configuration (DFT-ωB97XD/6-31+G(d,p))

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

N	2.30164800	-0.71947900	0.19952800
C	2.17264100	-2.07955900	0.22236700
C	1.06260100	-0.18929800	0.42408100
C	0.80982300	-2.42203100	0.54552800
C	0.12276600	-1.25753200	0.65990500
C	3.18586300	-3.01342200	-0.06789300
C	4.54402800	-2.70487700	-0.25421200
N	5.10231100	-1.46365100	-0.11023900
C	5.57416400	-3.64976800	-0.62261900
C	6.44189500	-1.58718200	-0.34507400
C	6.74444800	-2.96301500	-0.67168100
C	7.38479700	-0.54337200	-0.29641800
C	7.09089300	0.81523600	-0.08641500
N	5.84076600	1.35850500	0.02092000
C	8.07743100	1.86408100	0.05193000
C	5.99058000	2.70724500	0.19265800
C	7.40082900	3.02750600	0.22634000
C	4.94788000	3.64261700	0.30395600
C	3.57224000	3.34023200	0.32359000
N	3.02600800	2.08925100	0.36780500
C	2.51331300	4.32097800	0.25468700
C	1.66432500	2.23320500	0.34300500
C	1.33905300	3.63908400	0.25218800
C	0.73362500	1.17967500	0.40274900
C	2.75188600	-4.43208500	-0.23306700
C	3.25175000	-5.45052800	0.58577100
C	1.80721100	-4.76126200	-1.21392200
C	2.81951400	-6.76487000	0.42599700
C	1.37151200	-6.07308100	-1.37189000
C	1.87791400	-7.07969700	-0.55180000
C	-0.71751500	1.52073700	0.36604600
C	-1.52254300	1.02693500	-0.67383600
C	-1.31428200	2.35542100	1.31247800
C	-2.85449700	1.38729800	-0.78450700
C	-2.65511000	2.72925600	1.21524600
C	-3.42333100	2.26027600	0.14891300
C	5.32409100	5.08585100	0.39129000
C	5.04121900	5.82118500	1.54766300
C	5.95759700	5.72960200	-0.67725900
C	5.38512500	7.16719800	1.63524100
C	6.30157000	7.07603400	-0.59128400
C	6.01646900	7.79833700	0.56550800
C	8.82000500	-0.90695700	-0.49678400
C	9.49168400	-1.70699600	0.43388100
C	9.51792500	-0.45054000	-1.62020200
C	10.83059800	-2.03992200	0.24719400

C	10.85643100	-0.78306100	-1.80837000
C	11.51661900	-1.57838000	-0.87415800
O	-4.72142300	2.58513700	-0.06598400
H	0.43166700	-3.42367600	0.67950100
H	-0.92359000	-1.13485400	0.89635500
H	5.41796200	-4.69907600	-0.82839500
H	7.72269700	-3.34735200	-0.92346400
H	9.14864600	1.72236200	0.03113200
H	7.81671000	4.01382800	0.37510400
H	2.65302200	5.39038500	0.18505400
H	0.34427500	4.05390800	0.17699800
H	3.97501400	-5.20538900	1.35841900
H	1.39953000	-3.98560800	-1.85583600
H	3.21227600	-7.54215800	1.07497700
H	0.62944900	-6.29180400	-2.13386000
H	-1.08855900	0.36506800	-1.41736300
H	-0.72186700	2.72990300	2.14222000
H	-3.46524900	1.02677500	-1.60568100
H	-3.08204000	3.37840800	1.97150300
H	4.55178100	5.32863900	2.38320900
H	6.17497600	5.16875800	-1.58192700
H	5.16266600	7.72179900	2.54211500
H	6.78826100	7.56190300	-1.43181900
H	8.95857500	-2.06379000	1.31065000
H	9.00161200	0.16719400	-2.34959200
H	11.33963600	-2.65767100	0.98117000
H	11.38229500	-0.42267000	-2.68751700
C	-5.27619800	3.67323700	0.65068700
H	-5.45824200	3.40629000	1.69957200
H	-4.58713500	4.52832400	0.63146200
C	-6.56305200	4.00602100	-0.02870700
C	-6.98289800	3.63412900	-1.28120300
H	-6.53434100	3.02888900	-2.05146100
N	-8.21447400	4.17722400	-1.39229600
N	-8.54556400	4.84222700	-0.27855900
N	-7.54212500	4.74640600	0.55076200
C	-9.22005500	3.88114000	-2.40400800
H	-8.68702300	3.46193400	-3.25807900
H	-9.68875500	4.81675300	-2.71387100
C	-10.26877800	2.89142200	-1.87349400
H	-10.99601000	3.42182700	-1.25092800
H	-10.80795400	2.46567300	-2.72529500
C	-9.65745900	1.79355500	-1.02009700
H	-9.19735700	2.24494900	-0.13586700
H	-10.41850700	1.07919400	-0.68784500
O	-8.67390800	1.11539800	-1.79865800
C	-7.67410500	0.45126500	-1.18157800
C	-7.54711300	0.32160900	0.21309500
C	-6.72371300	-0.11889100	-2.02879000
C	-6.46520800	-0.35831600	0.73550300

H	-8.28443000	0.73628700	0.88775600
C	-5.66337500	-0.82178000	-1.47843200
H	-6.82373300	-0.02610800	-3.10386700
C	-5.49974500	-0.95251600	-0.09025800
H	-6.36752900	-0.45571700	1.81161400
O	-4.78029500	-1.37592700	-2.34839000
C	-4.40022800	-1.74148800	0.40101000
C	-3.78160800	-2.19397600	-1.91224500
C	-3.58578900	-2.38360300	-0.48873200
C	-4.11791800	-1.76513000	1.86572800
C	-2.99293300	-2.78408700	-2.84575000
C	-2.54246700	-3.30520300	-0.09737300
C	-4.63892500	-2.69824600	2.77824800
C	-3.26195500	-0.76437200	2.33395100
C	-1.92562700	-3.69222200	-2.45490100
H	-3.15666500	-2.59837700	-3.90135300
C	-1.78492900	-3.94051600	-1.01077100
H	-2.39697900	-3.48588200	0.96350300
C	-4.27854200	-2.61429700	4.12664700
C	-5.57094800	-3.80991200	2.41359900
C	-2.91236300	-0.69029500	3.67738800
H	-2.87007600	-0.03600400	1.63103800
O	-1.17734900	-4.23840900	-3.27407500
H	-1.01860900	-4.65016700	-0.71643400
C	-3.42112500	-1.62068300	4.57921900
H	-4.68569300	-3.34927600	4.81219200
O	-5.95201400	-4.65190200	3.19921300
O	-5.94860700	-3.77424900	1.13635200
H	-2.23967400	0.09333800	4.01140300
H	-3.15327600	-1.57224800	5.62953500
C	-6.83228500	-4.81091300	0.70472600
H	-7.00681700	-4.62036700	-0.35302300
H	-6.36788900	-5.78905700	0.84641100
H	-7.77018300	-4.76749800	1.26260400
H	12.56141400	-1.83620700	-1.01958400
H	6.28346800	8.84877100	0.63330900
H	1.53848300	-8.10431300	-0.67205200
Zn	4.07127900	0.31838100	0.11538200

Compound 2 ground state configuration (DFT-ωB97XD/6-31+G(d,p))

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

N	0.52784600	-1.50593900	0.05322400
C	0.27896900	-2.85793300	0.05122600
C	1.89207600	-1.33565500	0.08113400
C	1.53935400	-3.57105000	0.06573600
C	2.53019400	-2.63555300	0.09704000
C	-0.99706300	-3.46583400	0.03678500
C	-2.23456400	-2.78358400	0.00913700
N	-2.40474900	-1.42060800	-0.05258500
C	-3.53346800	-3.41997100	0.08045200
C	-3.75650100	-1.17098700	-0.03275200
C	-4.46888500	-2.42886600	0.05470000
C	-4.36526900	0.10449900	-0.06354400
C	-3.68232700	1.34228200	-0.06145800
N	-2.32104100	1.51244200	0.02770200
C	-4.31472300	2.63967900	-0.18094500
C	-2.06889500	2.86305600	-0.01904000
C	-3.32299400	3.57439200	-0.15458100
C	-0.79416200	3.47146300	0.01936400
C	0.44288900	2.79007700	0.06684500
N	0.61261500	1.42566600	0.07870500
C	1.74189800	3.42881800	0.10673200
C	1.96443800	1.17668400	0.11045300
C	2.67706700	2.43739900	0.12020700
C	2.57515700	-0.09835900	0.10991800
C	-1.04392700	-4.96429400	0.06466200
C	-1.50966800	-5.68791700	-1.04537500
C	-0.62667400	-5.67696600	1.20084900
C	-1.55534600	-7.08319400	-1.02123700
C	-0.67318800	-7.07215800	1.22651900
C	-1.13720600	-7.77998500	0.11506300
C	4.07281600	-0.13935700	0.14051700
C	4.78868300	0.27961200	1.27734400
C	4.80914800	-0.59085600	-0.96217900
C	6.17759700	0.24989000	1.30680900
C	6.20652600	-0.62707700	-0.94941100
C	6.90050700	-0.20234200	0.19109900
C	-0.75299500	4.97032400	-0.00329300
C	-0.25075000	5.66103800	-1.11836200
C	-1.22028700	5.71599000	1.09130100
C	-0.21555400	7.05670100	-1.13812800
C	-1.18423700	7.11164400	1.07311400
C	-0.68172200	7.78661200	-0.04196500
C	-5.86276400	0.14831900	-0.09843500
C	-6.57156200	-0.33946700	-1.20892600
C	-6.59118900	0.67769000	0.97988600
C	-7.96672300	-0.29828100	-1.24106300

C	-7.98638900	0.71730700	0.94961700
C	-8.67888500	0.22975300	-0.16142000
O	8.25732300	-0.19083500	0.31606200
H	1.65225800	-4.64539900	0.05690300
H	3.59588600	-2.80953400	0.12802100
H	-3.70691000	-4.48359200	0.15674600
H	-5.54231200	-2.53906100	0.10735400
H	-5.37576300	2.81228800	-0.28848300
H	-3.42985700	4.64644700	-0.23539100
H	1.91621600	4.49494000	0.11727900
H	3.75133700	2.54992500	0.13467600
H	-1.83084000	-5.14999900	-1.93308400
H	-0.27122600	-5.13026200	2.06990400
H	-1.91439600	-7.62506400	-1.89219800
H	-0.35053500	-7.60501300	2.11705800
H	-1.17303900	-8.86584100	0.13448700
H	4.24496100	0.62841000	2.15097100
H	4.28344900	-0.91524700	-1.85611900
H	6.72600500	0.57046700	2.18745600
H	6.73589000	-0.97910800	-1.82717000
H	0.10658300	5.09742200	-1.97577300
H	-1.60724000	5.19461500	1.96249900
H	0.17240300	7.57289100	-2.01227500
H	-1.54593300	7.67062300	1.93208100
H	-0.65409200	8.87277900	-0.05685700
H	-6.02150200	-0.74516700	-2.05345900
H	-6.05690000	1.05165700	1.84883300
H	-8.49629400	-0.67552700	-2.11188300
H	-8.53166600	1.12553500	1.79644300
H	-9.76478000	0.26101900	-0.18568100
C	9.05767400	-0.62495900	-0.78885600
H	8.82559300	-1.67318700	-1.02213600
H	8.82447300	-0.01765400	-1.67527100
C	10.52244400	-0.46865300	-0.40065700
H	10.71535700	-1.07759500	0.49160500
H	11.12454800	-0.89837300	-1.21170200
C	10.93743000	0.98466300	-0.14960700
H	10.35078600	1.42479800	0.66285900
H	11.99654500	1.04763600	0.12296800
H	10.78431700	1.59823000	-1.04613200
Zn	-0.89654300	0.00313800	0.04053400

Compound 3 ground state configuration (DFT-ωB97XD/6-31+G(d,p))

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

C	4.28989400	-1.91861500	-0.13275300
C	3.48621400	-0.85116300	-0.29474500
C	2.04014200	-0.97995000	-0.31033000
C	1.51220200	-2.31894200	-0.09694300
C	2.30074300	-3.40625700	0.06437500
C	3.75322000	-3.28452200	0.04514800
C	1.18272000	0.07054300	-0.46687700
C	-0.70153200	-1.47519800	-0.20195200
C	-0.24623400	-0.16561400	-0.43335300
C	-1.21969100	0.82931500	-0.60579900
H	-0.90773300	1.84978500	-0.80175300
C	-2.57343900	0.54857900	-0.53178200
C	-2.99282100	-0.77042700	-0.28550000
C	-2.04983900	-1.78448300	-0.12495300
H	5.37028700	-1.81935700	-0.11733700
H	3.90886500	0.14122000	-0.41165400
H	1.86695800	-4.38713100	0.21887500
H	-3.28881000	1.34933800	-0.66670900
H	-2.36747200	-2.80420200	0.05613000
O	0.16227300	-2.50659800	-0.04337400
O	-4.28326200	-1.15131200	-0.19152400
O	4.50237200	-4.25140000	0.18022600
C	1.68004200	1.45332100	-0.71447200
C	1.53961200	2.49782000	0.21629700
C	2.25296900	1.73416800	-1.95817800
C	1.96344600	3.78692700	-0.11423400
C	2.69071100	3.01706500	-2.27263200
H	2.34798200	0.93284400	-2.68440200
C	2.54578200	4.04798400	-1.34829200
H	1.82823700	4.57670900	0.61698200
H	3.14010500	3.20845500	-3.24166400
H	2.88113900	5.05157200	-1.58775800
C	0.92046500	2.32589200	1.56808100
O	0.35329000	3.21746300	2.16172400
O	1.07049500	1.09134100	2.05288200
C	-5.30606800	-0.17329300	-0.33960400
H	-5.22681500	0.29814000	-1.32904100
H	-5.18658200	0.60594300	0.42614900
C	-6.64630800	-0.86746100	-0.18572800
H	-6.72572300	-1.65282100	-0.94463500
H	-6.67714000	-1.36084400	0.79129500
C	-7.80493300	0.11996000	-0.31850400
H	-8.76459500	-0.39051600	-0.20567800
H	-7.75231500	0.90080500	0.44759600
H	-7.80200200	0.60962400	-1.29811600
C	0.40947300	0.81348300	3.29028900

H	0.78052900	1.47324600	4.07689400
H	-0.66795100	0.95278000	3.17589400
H	0.64108200	-0.22633100	3.51410300

6-2. Excited states calculations

Absorption spectra calculations for compounds **1**, **2** and **3** were performed using B3LYP, CAM-B3LYP and wB97XD methods, and 6-31+G(d,p) as basis set.

Compound 1 (linear form) absorption spectrum calculation and input keywords

#p scrf=(solvent=chloroform) geom=connectivity gfinput gfprint iop(6/7=3) pop=full

pseudo=read td=(nstates=30)

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

N	-4.76903200	1.47531700	0.32992800
C	-4.97688400	2.82510000	0.29139400
C	-3.44562200	1.27077200	0.60592800
C	-3.72778900	3.50749900	0.54917400
C	-2.78338900	2.54983400	0.73551300
C	-6.21116500	3.46094700	0.06148200
C	-7.44248000	2.81542700	-0.14927500
N	-7.65220200	1.46455400	-0.13309300
C	-8.68709300	3.48747100	-0.45475700
C	-8.97314100	1.25109700	-0.41074600
C	-9.62964600	2.52421500	-0.61527200
C	-9.59908000	-0.00306600	-0.52722600
C	-8.96404200	-1.25340400	-0.41512300
N	-7.63403700	-1.45667500	-0.17621600
C	-9.62646600	-2.53348400	-0.54295600
C	-7.42121300	-2.80712800	-0.16050900
C	-8.67423400	-3.48991000	-0.39870700
C	-6.18428100	-3.44178200	0.04618100
C	-4.95529800	-2.79626700	0.27589900
N	-4.74953700	-1.44569900	0.28596700
C	-3.71664700	-3.47094200	0.59480600
C	-3.43627100	-1.23317300	0.60137800
C	-2.78228700	-2.50764700	0.80153700
C	-2.81513000	0.02111400	0.74700400
C	-6.21645500	4.95537700	0.04034700
C	-6.87247600	5.67714200	1.04232900
C	-5.56591800	5.65835300	-0.98011400
C	-6.88670800	7.06845700	1.02300300
C	-5.57503600	7.04852100	-1.00182600
C	-6.23842400	7.75493600	-0.00002000
C	-1.36890000	0.02243500	1.12317200
C	-0.38267700	-0.43028900	0.23682100
C	-0.96696300	0.45929400	2.38523100
C	0.95381200	-0.45451300	0.60545000
C	0.37189800	0.44378000	2.77214200
C	1.33784500	-0.02322000	1.87980400
C	-6.17161400	-4.93635700	0.02609000
C	-5.53273400	-5.62361900	-1.01087400

C	-6.79098900	-5.67284900	1.04158900
C	-5.51955000	-7.01448900	-1.03952000
C	-6.77955400	-7.06330500	1.01744700
C	-6.14495100	-7.73521100	-0.02531700
C	-11.06558300	-0.00619400	-0.81650000
C	-11.98167300	0.44656000	0.13882500
C	-11.54839000	-0.46606500	-2.04644300
C	-13.34706000	0.44145000	-0.12694800
C	-12.91262300	-0.47533600	-2.31564700
C	-13.81390200	-0.02144800	-1.35517100
O	2.66694000	-0.09552200	2.15602900
H	-3.59183900	4.57903000	0.58655800
H	-1.73247100	2.69505700	0.94142400
H	-8.81784600	4.55585600	-0.55135300
H	-10.67249300	2.66120800	-0.86371000
H	-10.68184300	-2.68110800	-0.72235100
H	-8.80773000	-4.56121500	-0.44890100
H	-3.58571400	-4.54097800	0.67251700
H	-1.74609600	-2.64615000	1.07553200
H	-7.37242000	5.14249600	1.84495500
H	-5.05054200	5.10828500	-1.76229500
H	-7.38777800	7.62491500	1.80800600
H	-5.06093700	7.58641100	-1.79209700
H	-0.66974900	-0.77217300	-0.75352800
H	-1.71384900	0.81496000	3.08919500
H	1.71627200	-0.80815200	-0.08109000
H	0.63625900	0.79172000	3.76373600
H	-5.04351000	-5.06164100	-1.80134800
H	-7.28002200	-5.14973900	1.85839300
H	-5.01758100	-7.54310300	-1.84317600
H	-7.24881500	-7.62904600	1.81586900
H	-11.61839100	0.80021900	1.09959700
H	-10.84620500	-0.82094200	-2.79535300
H	-14.05344500	0.77933600	0.62418900
H	-13.28239400	-0.84512500	-3.26649000
C	3.08836500	0.23103400	3.46645500
H	2.90100900	1.29064300	3.68416700
H	2.53685800	-0.36777600	4.20361000
C	4.54999300	-0.06353700	3.55463600
C	5.37294000	-0.72057700	2.67184400
H	5.20676700	-1.16431300	1.70378800
N	6.57564500	-0.72904500	3.28925600
N	6.51084300	-0.11465600	4.47311800
N	5.28222600	0.29045300	4.64145300
C	7.84943800	-1.23983300	2.80373200
H	7.63028200	-1.98364900	2.03457700
H	8.33355300	-1.74801300	3.64133500
C	8.72848200	-0.11495800	2.26063000
H	8.22042300	0.38390200	1.42864500
H	8.89382100	0.62678500	3.04838700

C	10.06797800	-0.65280600	1.78878500
H	10.58931300	-1.16980100	2.60465700
H	9.93732300	-1.35661100	0.95728500
O	10.83552500	0.46788500	1.36223500
C	12.08844000	0.26815000	0.91422500
C	12.69320800	-0.99770200	0.79341000
C	12.79071600	1.41929300	0.55745500
C	13.98596700	-1.09026700	0.31688200
H	12.16152500	-1.90116800	1.06390400
C	14.08675200	1.29809000	0.08391100
H	12.32739400	2.39440500	0.65028700
C	14.71999300	0.05034900	-0.04783600
H	14.44747200	-2.06715000	0.21879600
O	14.71974500	2.44994700	-0.25063100
C	16.06240900	0.01281300	-0.56504300
C	15.98996000	2.44287700	-0.73258800
C	16.69021600	1.18480600	-0.89133700
C	16.77146900	-1.29635600	-0.66331300
C	16.54875600	3.64044700	-1.04574700
C	18.03619900	1.25874900	-1.41650400
C	16.82542300	-2.07708800	-1.83122900
C	17.43925500	-1.74000300	0.48076000
C	17.89859000	3.72035000	-1.57145200
H	15.98848200	4.55865700	-0.90735100
C	18.60469100	2.43798700	-1.73724100
H	18.58161900	0.32950700	-1.54783200
C	17.55524400	-3.26885900	-1.82858700
C	16.14847300	-1.71915300	-3.11552600
C	18.15170200	-2.93506100	0.47510800
H	17.40184700	-1.13466000	1.38130100
O	18.43903900	4.79493400	-1.86611500
H	19.61450700	2.48544900	-2.13316500
C	18.21206800	-3.70251900	-0.68474200
H	17.59339800	-3.85030700	-2.74326000
O	16.40767000	-2.24268000	-4.17969900
O	15.21624700	-0.78094200	-2.96616300
H	18.66144100	-3.26085100	1.37600300
H	18.76750800	-4.63438100	-0.69844900
C	14.53763400	-0.35796400	-4.15174600
H	13.83252200	0.40429300	-3.82481200
H	15.24925200	0.05909200	-4.86749300
H	14.01022700	-1.19901600	-4.60648100
H	-6.13817689	-8.80497436	-0.04677557
H	-14.86395629	-0.02837100	-1.56069002
H	-6.24942506	8.82474084	-0.01724132
Zn	-6.20090500	0.00935400	0.07699100

Compound 1 (folded form) absorption spectrum calculation and input keywords

#p scrf=(solvent=chloroform) geom=connectivity gfinput gfprint iop(6/7=3) pop=full pseudo=read td=(nstates=30)

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

N	1.08125900	-0.72998900	0.26426000
C	0.85722200	-2.07351800	0.34644300
C	-0.11645300	-0.10140600	0.45642500
C	-0.52977400	-2.30386100	0.66986000
C	-1.13189600	-1.08836800	0.73126700
C	1.81050300	-3.08774800	0.11605100
C	3.19374600	-2.88708200	-0.03189800
N	3.83816000	-1.68561300	0.09275300
C	4.16518000	-3.91674000	-0.33025000
C	5.17169700	-1.91252000	-0.08562100
C	5.38392000	-3.31873600	-0.35391300
C	6.18635700	-0.93571900	-0.04341000
C	5.98493800	0.45168200	0.07553600
N	4.77491000	1.08659000	0.08958300
C	7.03909400	1.43701300	0.19463800
C	5.01368900	2.43011700	0.17824300
C	6.44168100	2.65378200	0.25712900
C	4.03719300	3.44135800	0.18419000
C	2.64175000	3.23846500	0.18813900
N	2.01091000	2.03434200	0.30658200
C	1.65250800	4.28189100	0.03484900
C	0.66256200	2.26680800	0.25445300
C	0.43421000	3.68242500	0.06672500
C	-0.34187200	1.28594900	0.36733700
C	1.27085100	-4.47124400	-0.02936700
C	1.67955400	-5.51854900	0.80561500
C	0.31238700	-4.73809600	-1.01469900
C	1.14362000	-6.79323200	0.65967500
C	-0.23288200	-6.00916000	-1.15874100
C	0.18336000	-7.03952300	-0.32107100
C	-1.76250800	1.73610000	0.32130400
C	-2.61504400	1.26622900	-0.69107600
C	-2.27883600	2.65638300	1.23546600
C	-3.91322900	1.73280400	-0.80968400
C	-3.58470600	3.13531000	1.13150100
C	-4.39918400	2.68794200	0.08999000
C	4.51335300	4.85648600	0.16704500
C	4.21954200	5.71928300	1.22941400
C	5.24446900	5.35313100	-0.91770600
C	4.64448100	7.04286900	1.20949000
C	5.67263300	6.67642800	-0.94159300
C	5.37151200	7.52323700	0.12229900
C	7.59628100	-1.41635400	-0.14867000

C	8.13996800	-2.25137300	0.83397000
C	8.39789900	-1.05033200	-1.23609100
C	9.45126900	-2.70460800	0.73736000
C	9.70987400	-1.50035300	-1.33650100
C	10.23852200	-2.32796300	-0.34838200
O	-5.66700600	3.11062000	-0.13034000
H	-0.98196100	-3.26774600	0.84573300
H	-2.16791000	-0.88197400	0.95638900
H	3.94467800	-4.95945300	-0.50950100
H	6.33857100	-3.78410600	-0.55402500
H	8.09777000	1.22421000	0.23839600
H	6.92259800	3.61600100	0.36122700
H	1.86144600	5.33300200	-0.10478100
H	-0.52997600	4.15726500	-0.04426400
H	2.41554000	-5.32827600	1.58136500
H	-0.02285500	-3.94243600	-1.67348000
H	1.47247800	-7.59765800	1.31015000
H	-0.98191100	-6.19320800	-1.92152500
H	-2.24456300	0.54111500	-1.40972900
H	-1.64951300	3.01587000	2.04426700
H	-4.55983600	1.39114800	-1.61124000
H	-3.94834000	3.84763400	1.86321500
H	3.65091300	5.34699100	2.07660900
H	5.46955400	4.69725400	-1.75375800
H	4.40156600	7.70852500	2.03131500
H	6.22245200	7.06035000	-1.79449300
H	7.52753800	-2.54594000	1.68139500
H	7.98495500	-0.41245200	-2.01223400
H	9.86310000	-3.35910900	1.49857000
H	10.32016300	-1.22414400	-2.19018400
C	-6.12643300	4.26656800	0.54869500
H	-6.31116100	4.05586200	1.60948000
H	-5.37515900	5.06485600	0.48473000
C	-7.39546000	4.66596600	-0.12895600
C	-7.85467000	4.28115200	-1.36419500
H	-7.45661800	3.62441100	-2.11978500
N	-9.04850500	4.90010800	-1.48215100
N	-9.32136400	5.62358400	-0.39060200
N	-8.31585500	5.48967200	0.43310400
C	-10.07962700	4.63800700	-2.47883200
H	-9.57874600	4.16378400	-3.32340900
H	-10.49195900	5.59135500	-2.81339900
C	-11.18359200	3.73109300	-1.91373100
H	-11.87323300	4.32333700	-1.30425300
H	-11.75373900	3.31657400	-2.75048800
C	-10.64031900	2.62167400	-1.03008200
H	-10.14546200	3.06549500	-0.16120200
H	-11.44372500	1.96833200	-0.67423100
O	-9.70767600	1.85670200	-1.79340500
C	-8.75619600	1.13880600	-1.16464300

C	-8.62360500	1.04450400	0.23370100
C	-7.86256900	0.46949700	-2.00154100
C	-7.59263400	0.30034400	0.76890700
H	-9.32021400	1.53578900	0.90000500
C	-6.85462100	-0.29562900	-1.43731000
H	-7.96641000	0.53772600	-3.07807200
C	-6.68487800	-0.39423300	-0.04645900
H	-7.49163700	0.22891900	1.84669100
O	-6.02725100	-0.94602900	-2.29577100
C	-5.64730600	-1.24978500	0.45999500
C	-5.08724600	-1.81863700	-1.84193500
C	-4.89163900	-1.98057300	-0.41701300
C	-5.35064000	-1.25110000	1.92209900
C	-4.35029200	-2.49189400	-2.76499100
C	-3.91300600	-2.96077100	-0.00721700
C	-5.86957100	-2.16786700	2.85160600
C	-4.46903600	-0.26106400	2.36458000
C	-3.34813800	-3.45920700	-2.35569700
H	-4.51238000	-2.32327100	-3.82391100
C	-3.21080200	-3.67470900	-0.90827600
H	-3.76595900	-3.12111300	1.05655700
C	-5.47985900	-2.08177900	4.19145000
C	-6.83039100	-3.26098000	2.50975300
C	-4.09322200	-0.18207400	3.70098500
H	-4.07674200	0.45412700	1.64829600
O	-2.64400800	-4.08025700	-3.16613300
H	-2.49124600	-4.42437200	-0.59579500
C	-4.59834800	-1.09818800	4.61959100
H	-5.88437600	-2.80423200	4.89178200
O	-7.14231100	-4.14692100	3.27884300
O	-7.32076500	-3.15252100	1.27695900
H	-3.40360200	0.59415800	4.01703200
H	-4.30992600	-1.04537600	5.66412200
C	-8.22980600	-4.17341500	0.85724000
H	-8.46188700	-3.94501900	-0.18160300
H	-7.76043700	-5.15582400	0.93817600
H	-9.13553500	-4.14767600	1.46698000
H	11.24825629	-2.67396222	-0.42335670
H	5.69824977	8.54197903	0.10477443
H	-0.23279867	-8.01931088	-0.42936537
Zn	2.92439600	0.17357000	0.19136700

Compound 2 absorption spectrum calculation and input keywords

#p scrf=(solvent=chloroform) geom=connectivity gfinput gfprint iop(6/7=3) pop=full

pseudo=read td=(nstates=30)

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

N	0.51945400	-1.50380500	0.06922700
C	0.26645800	-2.84716700	0.07057400
C	1.87670700	-1.34171800	0.10533700
C	1.51937700	-3.56826400	0.10136100
C	2.51037300	-2.64106800	0.13260500
C	-1.00585200	-3.44460900	0.04542700
C	-2.23373600	-2.76124800	0.00489000
N	-2.39573800	-1.40486100	-0.05391600
C	-3.53248800	-3.39441100	0.05731200
C	-3.73920500	-1.15183300	-0.04781600
C	-4.45969000	-2.40356000	0.02426400
C	-4.33752600	0.12020300	-0.07786000
C	-3.65331400	1.34889200	-0.06525400
N	-2.29902300	1.51102900	0.02802700
C	-4.28185900	2.64647300	-0.17460200
C	-2.04329700	2.85362400	-0.00782600
C	-3.29052600	3.57310700	-0.13855900
C	-0.77199300	3.45161400	0.03875400
C	0.45600700	2.76867200	0.08861500
N	0.61812700	1.41104800	0.09367000
C	1.75413700	3.40337500	0.13656500
C	1.96130800	1.15822500	0.12899500
C	2.68132500	2.41196800	0.14867400
C	2.56147900	-0.11373000	0.13009900
C	-1.06169600	-4.93860000	0.07959200
C	-1.48615700	-5.66031300	-1.04059800
C	-0.69791400	-5.63836000	1.23458300
C	-1.54714500	-7.05095900	-1.00662100
C	-0.75788500	-7.02895100	1.26973500
C	-1.18326600	-7.73891700	0.14893200
C	4.05482100	-0.16450800	0.15284900
C	4.77542900	0.22579200	1.28953100
C	4.77255100	-0.59969900	-0.96042700
C	6.16038900	0.18665000	1.30712400
C	6.16588500	-0.64859100	-0.95897500
C	6.86818300	-0.24907400	0.18016700
C	-0.72205900	4.94607200	0.01955900
C	-0.22961100	5.62823900	-1.09775200
C	-1.16792900	5.68619000	1.11926400
C	-0.18079700	7.01955700	-1.11453200
C	-1.12046700	7.07773600	1.10345400
C	-0.62566900	7.74790700	-0.01324100
C	-5.83046000	0.17210900	-0.12580300

C	-6.52333200	-0.28630900	-1.25115400
C	-6.56030600	0.68272100	0.95288500
C	-7.91382200	-0.23355800	-1.29863400
C	-7.95072500	0.73649100	0.90653200
C	-8.63119200	0.27877700	-0.21975100
O	8.21818600	-0.24853300	0.29184100
H	1.62443400	-4.64392600	0.10220600
H	3.57577700	-2.81728000	0.17374500
H	-3.70823200	-4.45838700	0.12858800
H	-5.53476700	-2.50687500	0.06432100
H	-5.34255500	2.82209900	-0.28356700
H	-3.39047600	4.64678100	-0.21134200
H	1.93094900	4.46937500	0.15502700
H	3.75661600	2.51777600	0.17052900
H	-1.76888600	-5.12378800	-1.94201600
H	-0.37040700	-5.08444600	2.10992200
H	-1.87725800	-7.59700800	-1.88542200
H	-0.47636500	-7.55735400	2.17579900
H	-1.23258700	-8.82340200	0.17663200
H	4.23820200	0.56498100	2.17077000
H	4.23454200	-0.90694900	-1.85294800
H	6.71783300	0.48873900	2.18798600
H	6.68330500	-0.99384300	-1.84635200
H	0.11495700	5.06017100	-1.95730900
H	-1.55143100	5.16370000	1.99111500
H	0.20316700	7.53413300	-1.99038200
H	-1.46704100	7.63809800	1.96674800
H	-0.58672800	8.83310800	-0.02551600
H	-5.96409200	-0.68204000	-2.09424400
H	-6.03030500	1.03758400	1.83228200
H	-8.43612600	-0.58966700	-2.18164400
H	-8.50230100	1.13402900	1.75332000
H	-9.71563500	0.32218500	-0.25716700
C	8.99382300	-0.63653200	-0.83385500
H	8.78292700	-1.68477300	-1.08545000
H	8.72799500	-0.01357600	-1.70001400
C	10.45939200	-0.45015700	-0.48114400
H	10.69872400	-1.08311200	0.38141500
H	11.05159600	-0.82407500	-1.32478400
C	10.82123600	1.00455800	-0.18675800
H	10.25461200	1.38102700	0.66973600
H	11.88762000	1.10500600	0.03794900
H	10.59622400	1.64453400	-1.04809300
Zn	-0.88944300	0.00335600	0.02951000

Compound 3 absorption spectrum calculation and input keywords

#p scrf=(solvent=chloroform) geom=connectivity gfinput gfprint iop(6/7=3) pop=full

pseudo=read td=(nstates=30)

Charge=0, Multiplicity=1

Cartesian coordinates (Angströms)

C	4.27293700	-1.92996200	-0.15254800
C	3.47103600	-0.85742400	-0.31322000
C	2.02874200	-0.98151000	-0.31884400
C	1.49889600	-2.31327100	-0.10403200
C	2.28871000	-3.40686800	0.05702300
C	3.73229900	-3.28639300	0.03296400
C	1.16927800	0.07475200	-0.46915700
C	-0.71142400	-1.46905400	-0.20139200
C	-0.25367100	-0.15963800	-0.43204000
C	-1.22798500	0.83902900	-0.60305600
H	-0.91550800	1.85864400	-0.80172400
C	-2.57905800	0.55908000	-0.52750400
C	-3.00056700	-0.76220600	-0.28046100
C	-2.05905400	-1.77878400	-0.12224600
H	5.35328700	-1.82845000	-0.14748000
H	3.89957000	0.13124600	-0.43827200
H	1.84727500	-4.38425800	0.21429000
H	-3.29457700	1.35946500	-0.66266900
H	-2.37719300	-2.79854200	0.05875500
O	0.15407900	-2.50116500	-0.04618800
O	-4.28880000	-1.13842200	-0.18574300
O	4.48577500	-4.26342300	0.17114400
C	1.67254700	1.45500500	-0.71789800
C	1.55563500	2.49518300	0.22147100
C	2.22799600	1.73417000	-1.96939500
C	1.99019000	3.78080200	-0.10882400
C	2.67246900	3.01518400	-2.28432000
H	2.30386400	0.93745200	-2.70263400
C	2.55473200	4.04209800	-1.35161600
H	1.88409600	4.57006200	0.62738100
H	3.10770400	3.20718400	-3.25933100
H	2.89871600	5.04268700	-1.59030200
C	0.95778700	2.31465700	1.58038900
O	0.40370200	3.20570500	2.19289500
O	1.10624300	1.07745200	2.04942800
C	-5.31595500	-0.15567700	-0.33299200
H	-5.23584500	0.31130500	-1.32308300
H	-5.19155400	0.62086600	0.43284100
C	-6.65469100	-0.85060500	-0.17496100
H	-6.73896700	-1.63507300	-0.93442700
H	-6.68561100	-1.34151500	0.80342400
C	-7.81198200	0.13888800	-0.30556400
H	-8.77122400	-0.37173700	-0.18970500

H	-7.75452400	0.91932800	0.46035500
H	-7.80920400	0.62713400	-1.28568500
C	0.46387700	0.77863500	3.29537300
H	0.86127700	1.41362200	4.08875200
H	-0.61338600	0.93089600	3.20325700
H	0.68735000	-0.26805500	3.49105900

7. References

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