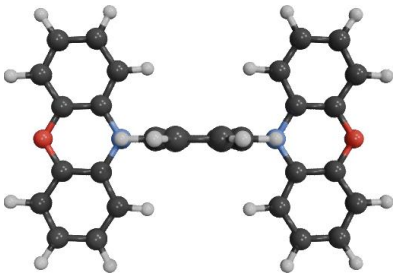
A Report On The Calculation Of The Excited States Of 1_4_Phx_nap_phx At The PBE0/6-31G** Level

osl - 16th July 2025



Abstract

The calculation of excited states for the system '1_4_Phx_nap_phx' is presented, accompanied by automated analysis and image generation provided by the Digichem software package. The calculations were performed using the Turbomole software package(s) at the PBE0/6-31G** level of theory. The total self-consistent field (SCF) energy of the system was found to be -42643.47 eV after 1 step. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -5.04 and -1.74 eV respectively, corresponding to a HOMO-LUMO band gap of 3.30 eV. The permanent dipole moment (PDM) was calculated to be 0.96 D. In total, 20 excited states were calculated with singlet and triplet multiplicity. The most intense absorption peaks were calculated to be at 285, 347 and 473 nm. The lowest energy singlet and triplet excited states (S_1 and T_1) were calculated to be 2.42 and 2.41 eV (512 and 514 nm) respectively, corresponding to a singlet/triplet splitting energy (ΔE_{ST}) of 0.01 eV.

Table 1: *Summary of overall calculation metadata.*

Calculation no.	Date[a] (Duration[b])	CPUs (Memory)	Success (Converged)	Computational package	Level of theory	Solvent (model)	Calculations	Wavefunction	Multiplicity	T[c] / K	p[d] / atm
Combined	16/07/2025 09:56:48 (7 m, 33 s)	28 (53993275392 B)	True (N/A)	Turbomole (7.5.0)	PBE0/6-31G**	Gas-phase (N/A)	Excited States	restricted	1 (singlet)	N/A	N/A
1	16/07/2025 09:49:03 (3 m, 58 s)	14 (26996637696 B)	True (N/A)	Turbomole (7.5.0)	PBE0/6-31G**	Gas-phase (N/A)	Excited States	restricted	1 (singlet)	N/A	N/A
2	16/07/2025 09:56:48 (3 m, 35 s)	14 (26996637696 B)	True (N/A)	Turbomole (7.5.0)	PBE0/6-31G**	Gas-phase (N/A)	Excited States	restricted	1 (singlet)	N/A	N/A

[a]: The date and time at which the calculation was completed. [b]: Total combined duration in real-time (wall-time) for all components of the calculation. [c]: Temperature used for thermochemistry analysis. [d]: Pressure used for thermochemistry analysis.

Summary Of Results

SCF Energy

Table 2: *Summary of SCF energy properties.*

No. of steps	1
Final energy	-42643.4651 eV
Final energy	-4,114,469 kJ·mol^{-1}

Geometry

Table 3: *Summary of geometry properties.*

Formula	$C_{34}H_{22}N_2O_2$
SMILES	c1ccc2c(c1)Oc1ccccc1N2c1ccc(N2c3ccccc3Oc3ccccc32)c2ccccc12
Molar mass	490.5507 g·mol^{-1}
Alignment method	Minimal
X extension	13.66 Å
Y extension	9.25 Å
Z extension	6.79 Å
Linearity ratio	0.32
Planarity ratio	0.27

Molecular Orbitals

Table 4: *Summary of HOMO & LUMO properties.*

$E_{HOMO,LUMO}$	3.30 eV
E_{HOMO}	-5.04 eV
E_{LUMO}	-1.74 eV

Permanent Dipole Moment

Table 5: *Summary of the permanent dipole moment properties.*

Total	0.96 D
X axis angle	90.00 °
XY plane angle	90.00 °

S_1 Transition Dipole Moment

Table 6: *Summary of the transition (S_1) dipole moment (TDM) properties μ: Electric TDM. m: Magnetic TDM. $\theta_{\mu,x}$ and $\theta_{m,x}$: Angle between μ or m and the x-axis. $\theta_{\mu,xy}$ and $\theta_{m,xy}$: Angle between μ or m and the xy-plane. $\theta_{\mu,m}$: Angle between the electric and magnetic TDM. g_{lum}: Dissymmetry factor.*

μ	0.03 D
$\theta_{\mu,x}$	89.90 °
$\theta_{\mu,xy}$	0.00 °
m[d]	0.26 a.u.
$\theta_{m,x}$	0.00 °
$\theta_{m,xy}$	0.00 °
μ (Gaussian-CGS)	2.55e-20 esu·cm
m (Gaussian-CGS)	2.42e-21 erg·G^{-1}
$\theta_{\mu,m}$	89.90 °
$\cos(\theta_{\mu,m})$	0.00
g_{lum}	0.001

Excited States

Table 7: *Summary of the calculated excited states. E_x: The energy of excited state x. λ_x: The wavelength of a photon of equivalent energy to excited state x. f_x: The oscillator strength of the excited state transition x. ΔE_{xy}: The difference in energy between the lowest excited states of multiplicity x and y.*

No. calculated singlets	10
E_{S_1}	2.42 eV
λ_{S_1} (colour, CIE)	512 nm (Green, (0.02, 0.78))
f_{S_1}	< 0.01
No. calculated triplets	10
E_{T_1}	2.41 eV
λ_{T_1} (colour, CIE)	514 nm (Green, (0.04, 0.81))
f_{T_1}	< 0.01
ΔE_{ST}	0.01 eV
Simulated Absorption Peaks	285, 347 and 473 nm

Methodology

Metadata

This report was generated from the combined results of two individual calculations. The individual metadatas for each separate calculation are presented in the following sections, and the overall calculation was performed using the **Turbomole (7.5.0)** program, the **DFT** method with the **PBE0** functional and the **6-31G**** basis set. It was completed on the **16th July 2025** after a total duration of **7 m, 33 s** and **finished successfully**. The base multiplicity of the system under study was **1 (singlet)**. Finally, a **restricted wavefunction** was used, resulting in a single set of doubly occupied orbitals. The full calculation metadata is tabulated in table 1.

The calculation of the excited states was performed using the **Turbomole (7.5.0)** program, the **DFT** method with the **PBE0** functional and the **6-31G**** basis set. It was completed on the **16th July 2025** after a total duration of **3 m, 58 s** and **finished successfully**. The base multiplicity of the system under study was **1 (singlet)**. Finally, a **restricted wavefunction** was used, resulting in a single set of doubly occupied orbitals.

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Analysis

The report presented here was generated using the Digichem software package. This toolset relies upon a number of third-party applications and libraries which should be cited appropriately in derivative works. In particular, the calculation results described within were parsed by the cclib library.[1] Scientific constants which were used, among other things, for the interconversion of scientific units were provided by SciPy.[2] Commission internationale de l'éclairage (CIE) coordinates, along with visual representations of the equivalent colour, were calculated using the Colour Science library.[3] Three-dimensional plots of atom positions and calculated densities, including molecular orbitals, were rendered using Visual Molecular Dynamics (VMD)[4] and the Tachyon ray-tracer.[5] Finally, two-dimensional graphs were plotted using the MatPlotlib library,[6] while this report itself was prepared using the Mako template library[7] and the Weasyprint library[8], the latter of which was responsible for generation of the PDF file.

Discussion

Total SCF Energy

The total energy of the system was calculated at the **self-consistent field (SCF)** level, corresponding to the energy calculated by the density-functional theory (DFT) method, with a value of -42643.47 eV, corresponding to -4,114,469 KJmol^{-1}. A plot of the total SCF electron density is shown in figure 1.

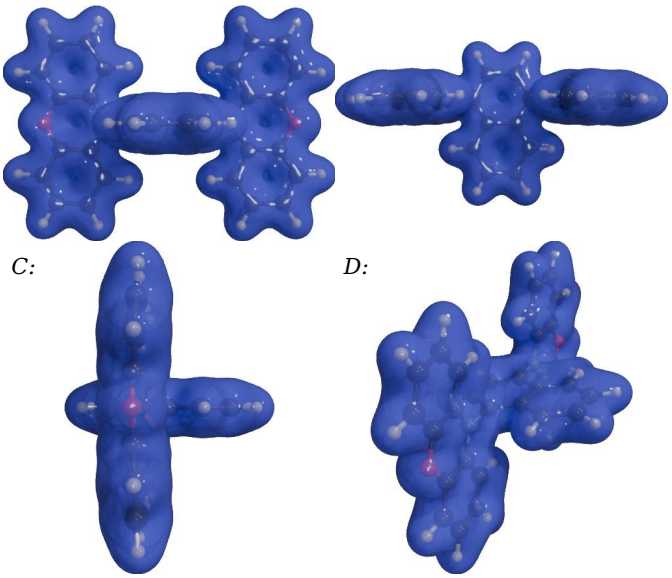

Figure 1: *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Geometry

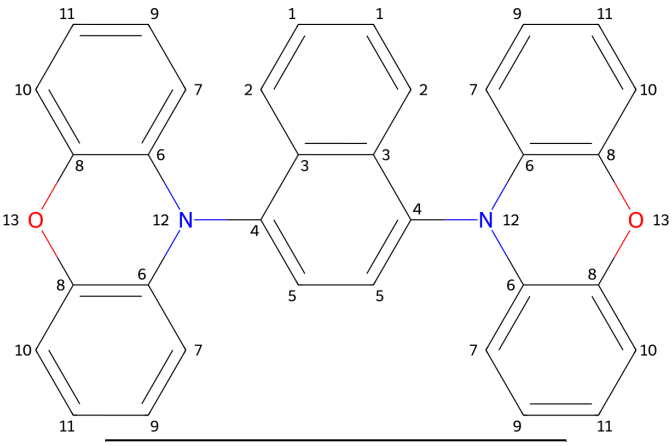

Figure 2: *Labelled structure of 1_4_Phx_nap_phx.*

The **empirical formula** of the studied system was $C_{34}H_{22}N_2O_2$, corresponding to a **molecular mass** of 490.55 gmol^{-1}. The molecular structure, with atom labelling, is shown in figure 2. The molecular geometry was aligned to the cartesian (X, Y and Z) axes by the **Minimal (MIN)** method, and the resulting atomic position are displayed in figure 3. Using this method, the **extent of the molecular system** in the X, Y and Z axes (L_X, L_Y and L_Z, corresponding to the molecular width, length and height respectively) was determined to be 13.66, 9.25 and 6.79 Å

respectively. These extensions give rise to a **molecular linearity ratio** (1-(L_Y/L_X)) and **planarity ratio** (1-(L_X/L_Y)) of 0.32 and 0.27 respectively.

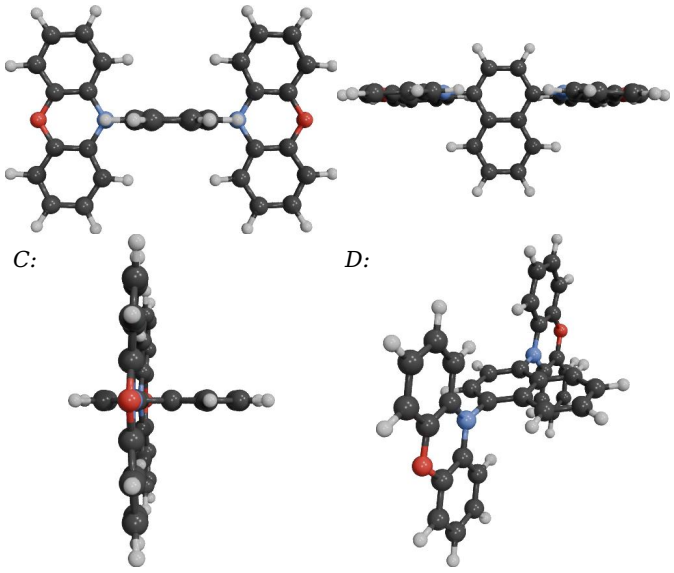

Figure 3: *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Permanent Dipole Moment

The calculated **permanent dipole moment** was 0.96 D, with a vector (x,y,z) of -0.00, 0.00, 0.96 D. The angle between the dipole moment vector and the x-axis was 90.00 °, while the angle between the dipole moment and the xy-plane was 90.00 °. A plot of the permanent dipole moment is shown in figure 4.

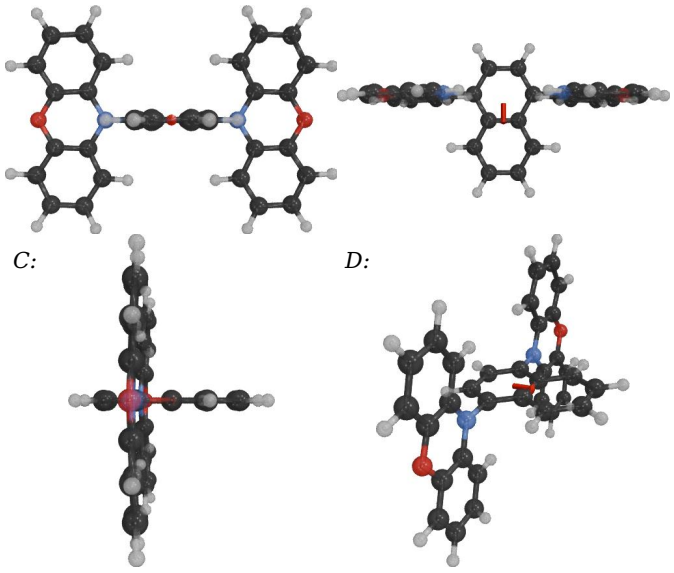

Figure 4: *The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Transition (S_1) Dipole Moment

The calculated **electric (TEDM, μ)** and **magnetic (TMDM, m)** transition dipole moments between the ground state and the S_1 excited state were 0.03 D and 0.26 au respectively. The corresponding vector components (x,y,z) were μ = -0.00, -0.03, 0.00 D and m = 0.26, 0.00, 0.00 au. In comparison to the molecular geometry, the angle between each dipole moment and the longest axis of the molecule (the x-axis) was $\theta_{\mu,x}$ = 89.90 ° and $\theta_{m,x}$ = 0.00 °, while the angle between each dipole moment and the xy-plane was $\theta_{\mu,xy}$ = 0.00 ° and $\theta_{m,xy}$ = 0.00 °. In Gaussian-CGS units, in which the magnetic and electric transition dipole moments can be directly compared, the magnitude of each dipole moment was μ = 2.55e-20 esu·cm and m = 2.42e-21 erg·G^{-1}, while the **angle between the two dipole moments** was $\theta_{\mu,m}$ = 89.90 °. Correspondingly, the cosine of the angle was cos($\theta_{\mu,m}$) = 0.00, and the **dissymmetry factor** of the excited state transition was g_{lum} = 0.001. A plot of the electric and magnetic transition dipole moments is shown in figure 5.

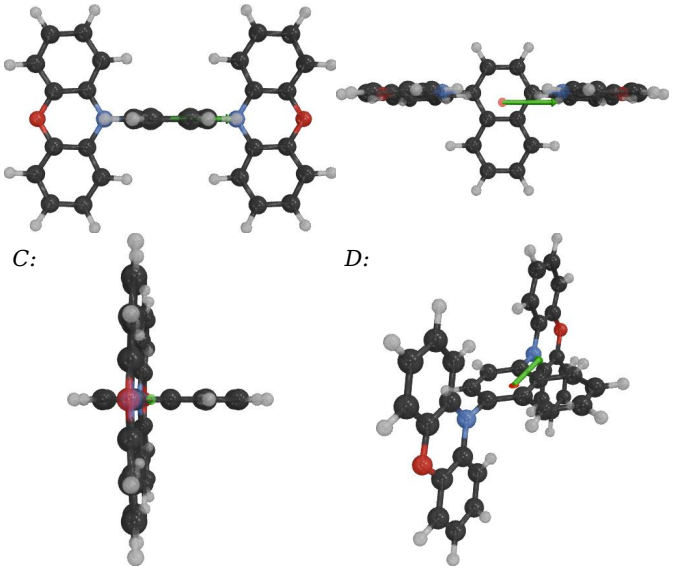

Figure 5: *The electric (red arrow) and magnetic (green arrow) transition (S_1) dipole moment plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D = 0.1 au. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Molecular Orbitals

In total, 642 doubly occupied molecular orbitals were calculated, divided into 128 occupied orbitals and 514 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO and LUMO** were -5.04 and -1.74 eV respectively, corresponding to a **HOMO-LUMO band gap** of 3.30 eV (figure 20). Plots of the orbital density for the HOMO-4, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2, LUMO+3, LUMO+4, LUMO+5, LUMO+6 and LUMO+7 are shown in figures 6-11 and 13-19 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 12.

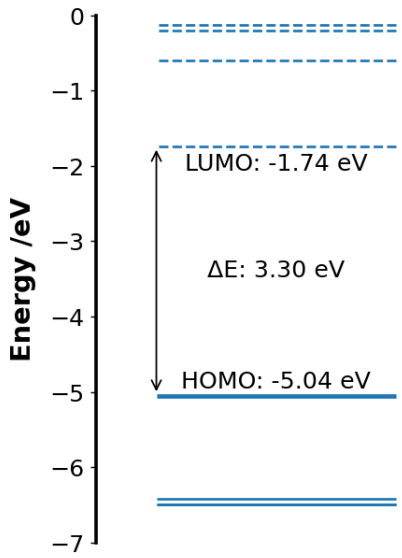

Figure 20: *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

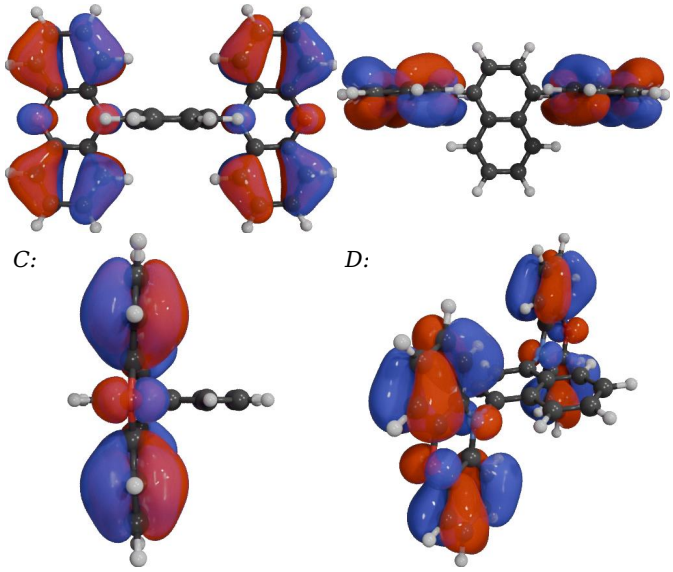

Figure 6: *Orbital density plots of the HOMO-4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

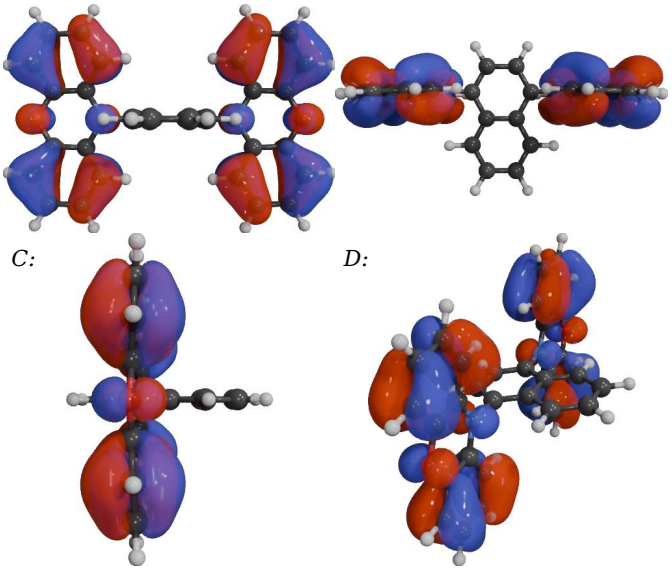

Figure 7: *Orbital density plots of the HOMO-3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

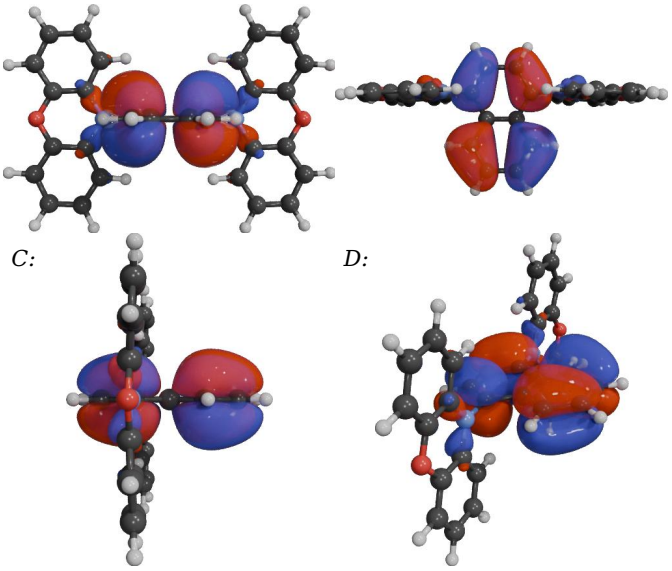

Figure 8: *Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

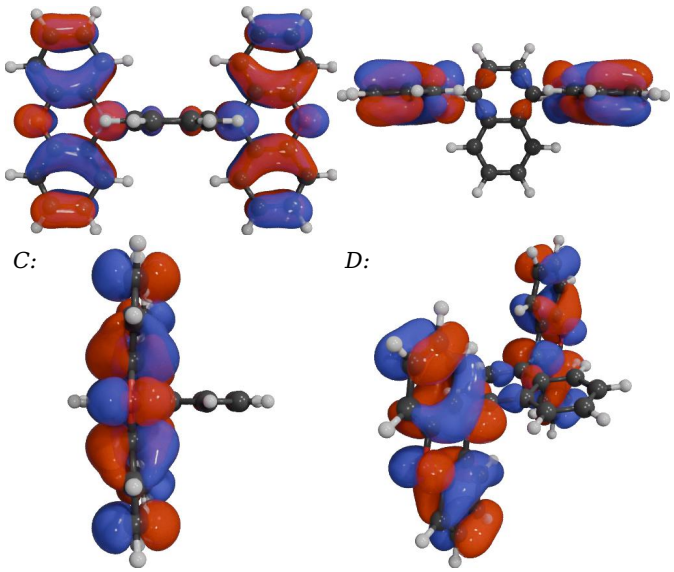

Figure 9: *Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

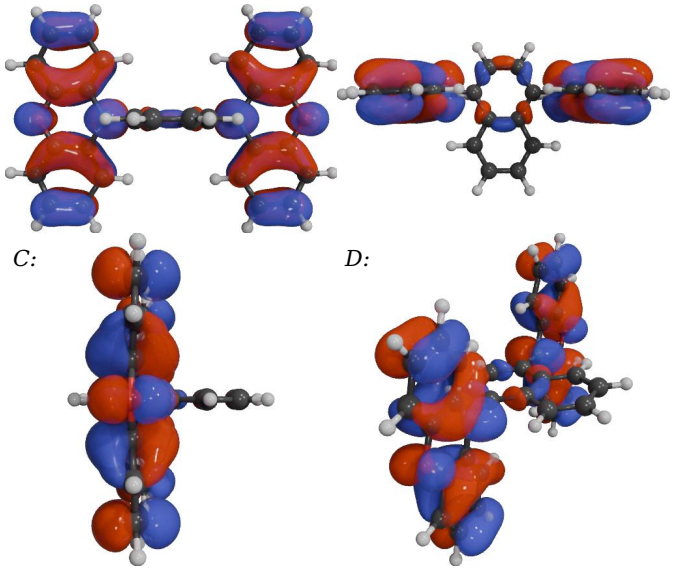

Figure 10: *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

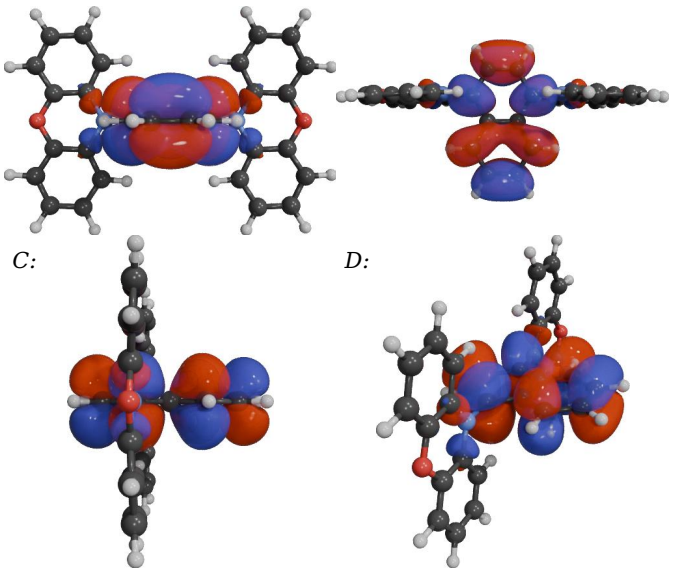

Figure 11: *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

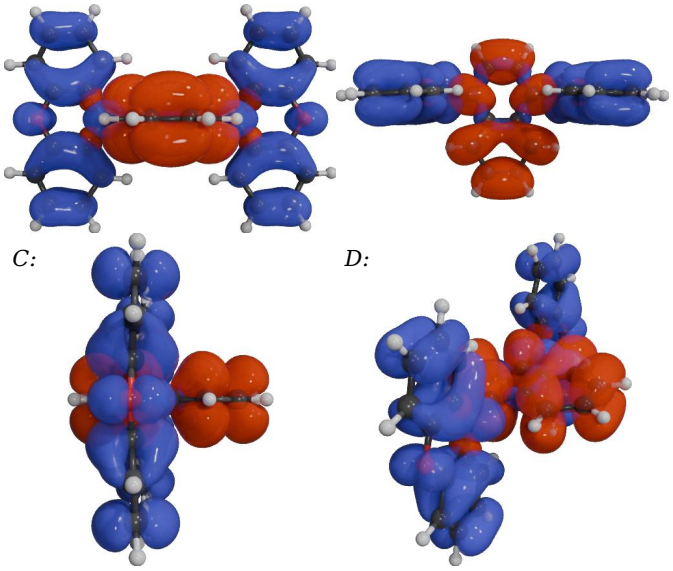

Figure 12: *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

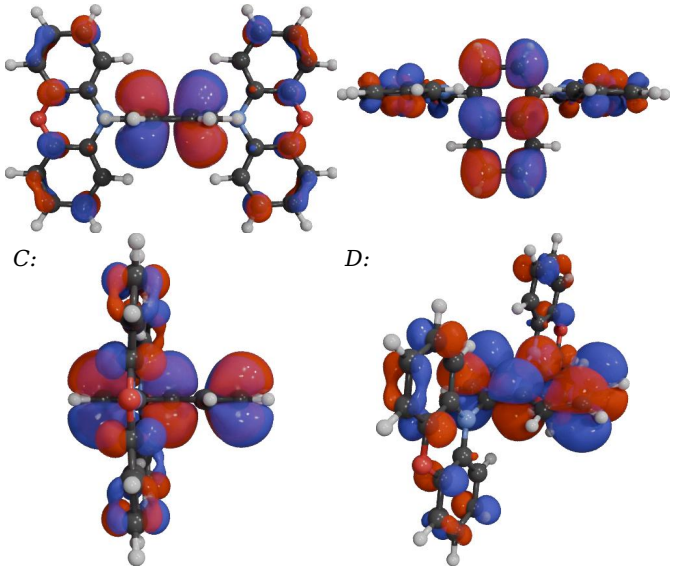

Figure 13: *Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

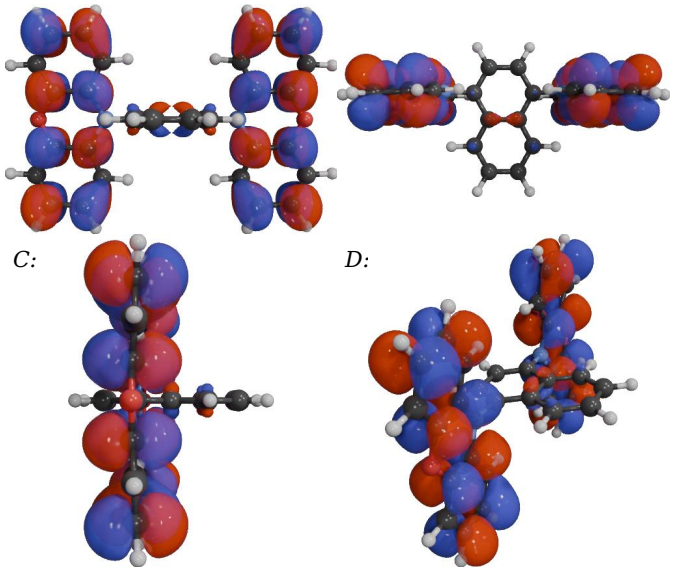

Figure 14: *Orbital density plots of the LUMO+2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

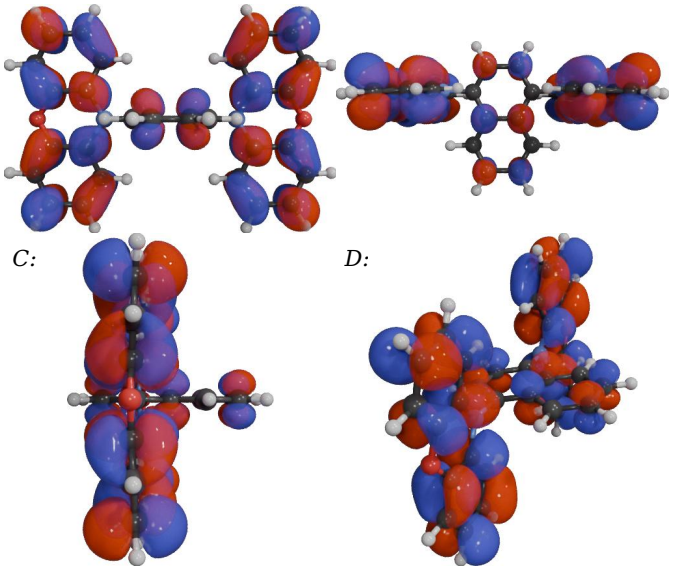

Figure 15: *Orbital density plots of the LUMO+3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

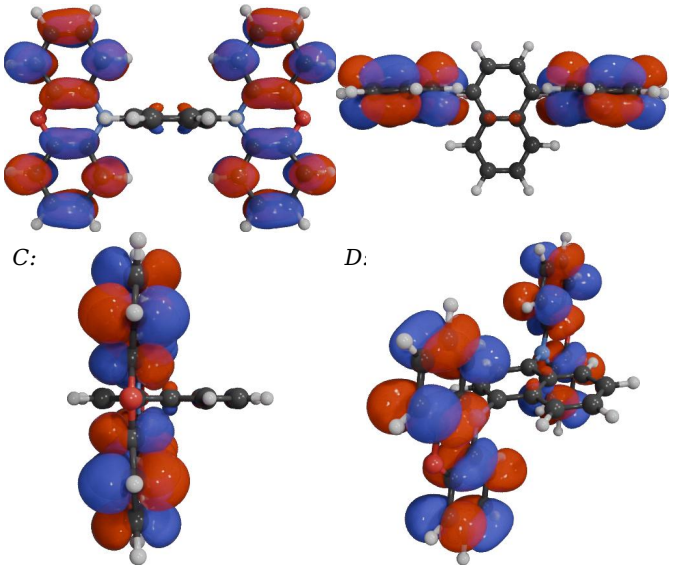

Figure 16: *Orbital density plots of the LUMO+4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

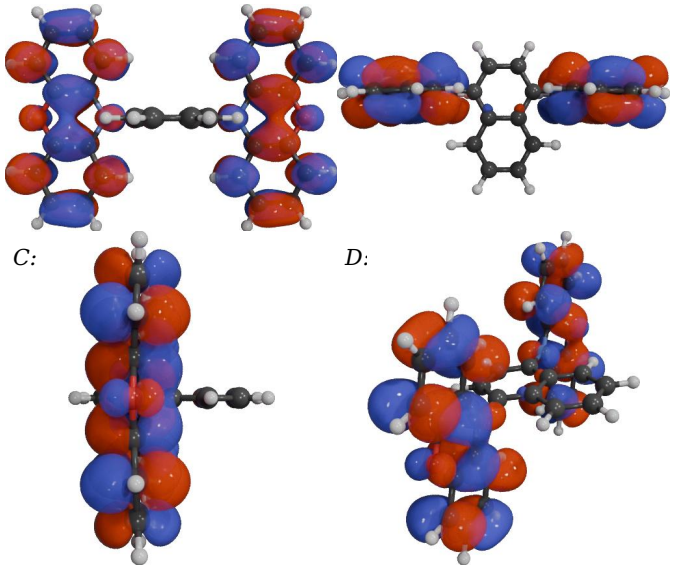

Figure 17: *Orbital density plots of the LUMO+5, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

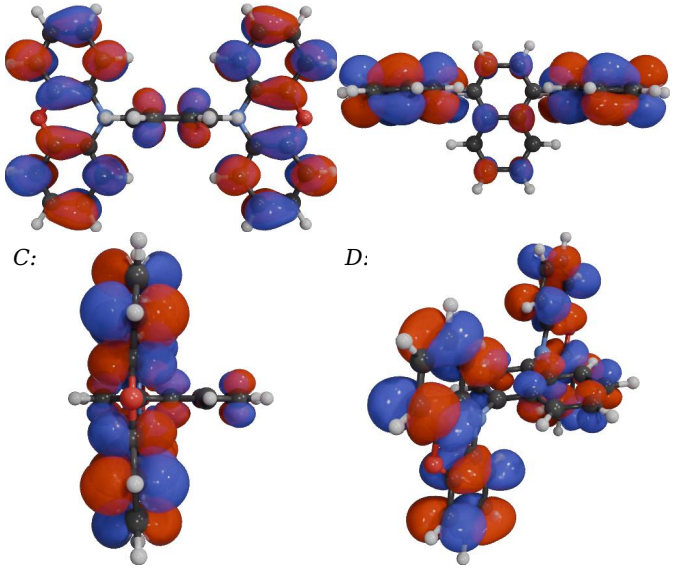

Figure 18: *Orbital density plots of the LUMO+6, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

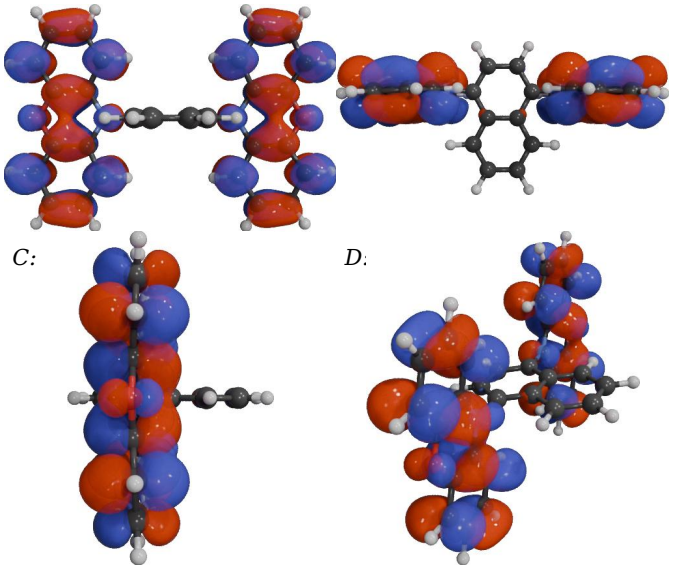

Figure 19: *Orbital density plots of the LUMO+7, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Excited States

In total, the energies of 20 electronic excited states were calculated (figure 21), consisting of 10 states with a multiplicity of singlet and 10 of multiplicity triplet. The energy of the lowest **singlet excited state (S_1)** was 2.42 eV, corresponding to absorption by a photon with a wavelength of 512 nm, a green 'color' and CIE coordinates of (0.02, 0.78), while the energy of the **T_1** was 2.41 eV (514 nm, green , CIE: (0.04, 0.81)). The difference in energy between the S_1 and T_1 excited states **(ΔE_{ST})** was therefore 0.01 eV. A complete table of the calculated excited state properties is available in table 8. In addition, an electronic transition spectrum was simulated using a gaussian function with full-width at half maximum (FWHM) of 0.40 eV, from which the **three most intense peaks** were found at 285, 347 and 473 nm. The full simulated absorption spectrum is shown in figure 22.

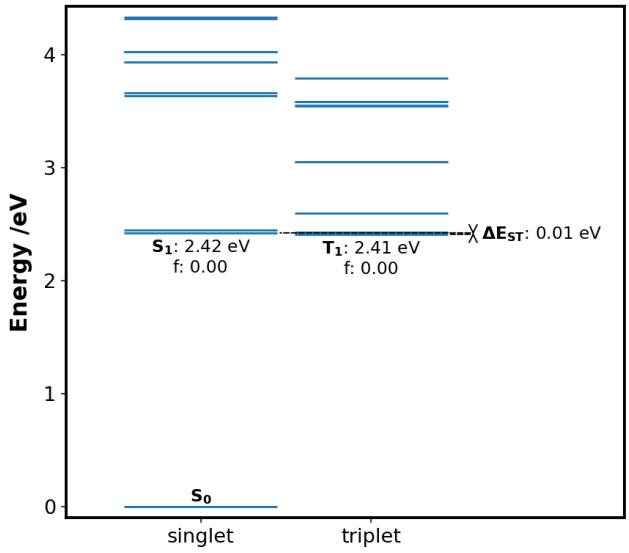

Figure 21: *Graph of the calculated excited states. f: oscillator strength of the relevant ground to excited state transition.*

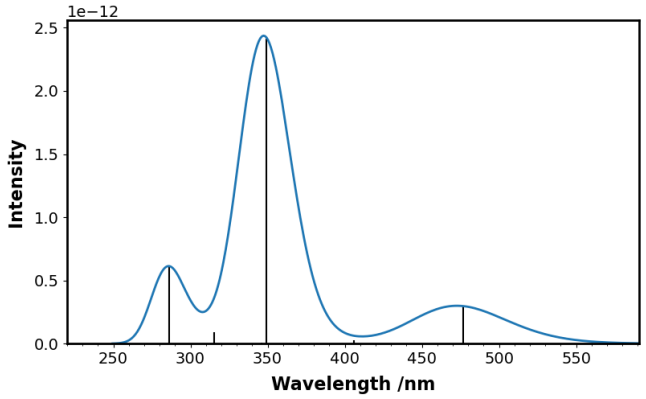

Figure 22: *Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 285, 347 and 473 nm.*

Tables Of Results

Atom Coordinates

Table 9: *Coordinates of the atoms of the system under study, as aligned to the cartesian axes by the Minimal method. Atoms that are chemically equivalent have been assigned the same group number.s*

Index	Element	Group	X Coord /Å	Y Coord /Å	Z Coord /Å
1	C	C_1	-0.6924000	-0.0000100	3.3249400
2	C	C_2	-1.3815300	-0.0000100	2.1132400
3	C	C_3	-0.7089500	0.0000000	0.8684400
4	C	C_3	0.7089500	0.0000000	0.8684300
5	C	C_2	1.3815400	-0.0000100	2.1132400
6	C	C_1	0.6924100	-0.0000100	3.3249400
7	H	H_1	-1.2418600	-0.0000200	4.2621100
8	H	H_2	-2.4696600	-0.0000100	2.1485900
9	C	C_4	-1.4025500	0.0000000	-0.3765700
10	C	C_4	1.4025500	0.0000000	-0.3765800
11	H	H_2	2.4696600	-0.0000100	2.1485800
12	H	H_1	1.2418800	-0.0000200	4.2621000
13	C	C_5	0.6946900	0.0000100	-1.5895900
14	C	C_5	-0.6946900	0.0000100	-1.5895900
15	H	H_5	1.2365800	0.0000100	-2.5324900
16	H	H_5	-1.2365900	0.0000100	-2.5324900
17	C	C_6	3.5807400	1.2261000	-0.3748500
18	C	C_6	3.5807400	-1.2260900	-0.3748400
19	C	C_7	2.9650900	2.4897200	-0.3511000
20	C	C_8	4.9830400	1.1776300	-0.3181000
21	C	C_8	4.9830400	-1.1776200	-0.3181000
22	C	C_7	2.9650900	-2.4897100	-0.3510900
23	C	C_9	3.7255000	3.6601000	-0.2605100
24	H	H_7	1.8833700	2.5844000	-0.3901800
25	C	C_{10}	5.7445300	2.3474700	-0.2338700
26	C	C_{10}	5.7445300	-2.3474600	-0.2338600
27	H	H_7	1.8833700	-2.5844000	-0.3901700
28	C	C_9	3.7255000	-3.6601000	-0.2604900
29	C	C_{11}	5.1145000	3.5890200	-0.2003600
30	H	H_9	3.2280700	4.6264200	-0.2313900
31	H	H_{10}	6.8282000	2.2861500	-0.1850100
32	C	C_{11}	5.1145000	-3.5890200	-0.2003500
33	H	H_{10}	6.8282000	-2.2861500	-0.1850000
34	H	H_9	3.2280700	-4.6264200	-0.2313700
35	H	H_{11}	5.7050300	4.4981800	-0.1242400
36	H	H_{11}	5.7050300	-4.4981700	-0.1242200
37	C	C_6	-3.5807400	1.2261000	-0.3748300
38	C	C_6	-3.5807400	-1.2260900	-0.3748500
39	C	C_7	-2.9650900	2.4897200	-0.3510800
40	C	C_8	-4.9830500	1.1776200	-0.3180700
41	C	C_8	-4.9830400	-1.1776200	-0.3180900
42	C	C_7	-2.9650900	-2.4897100	-0.3511200
43	C	C_9	-3.7255000	3.6601000	-0.2604700
44	H	H_7	-1.8833700	2.5844000	-0.3901600
45	C	C_{10}	-5.7445300	2.3474700	-0.2338300
46	C	C_{10}	-5.7445300	-2.3474700	-0.2338700
47	H	H_7	-1.8833700	-2.5844000	-0.3902000
48	C	C_9	-3.7254900	-3.6601000	-0.2605300
49	C	C_{11}	-5.1145000	3.5890200	-0.2003200
50	H	H_9	-3.2280700	4.6264200	-0.2313500
51	H	H_{10}	-6.8282000	2.2861500	-0.1849700
52	C	C_{11}	-5.1145000	-3.5890200	-0.2003800
53	H	H_{10}	-6.8282000	-2.2861500	-0.1850000
54	H	H_9	-3.2280600	-4.6264200	-0.2314300
55	H	H_{11}	-5.7050300	4.4981700	-0.1241800
56	H	H_{11}	-5.7050300	-4.4981800	-0.1242600
57	N	N_{12}	-2.8391600	0.0000000	-0.4303400
58	O	O_{13}	5.6952200	0.0000000	-0.3258600
59	O	O_{13}	-5.6952200	0.0000000	-0.3258400
60	N	N_{12}	2.8391600	0.0000000	-0.4303500

Molecular Orbitals

Table 10: *Energies of the calculated molecular orbitals.*

Level	Label	Symmetry	Energy /eV
144	LUMO+15	A	2.8871
143	LUMO+14	A	2.8614
142	LUMO+13	A	2.4551
141	LUMO+12	A	2.2792
140	LUMO+11	A	2.1711
139	LUMO+10	A	1.1530
138	LUMO+9	A	1.1501
137	LUMO+8	A	0.5075
136	LUMO+7	A	0.1793
135	LUMO+6	A	0.1691
134	LUMO+5	A	0.1587
133	LUMO+4	A	0.1058
132	LUMO+3	A	-0.1277
131	LUMO+2	A	-0.2045
130	LUMO+1	A	-0.6050
129	**LUMO**	**A**	**-1.7421**
128	**HOMO**	**A**	**-5.0413**
127	HOMO-1	A	-5.0647
126	HOMO-2	A	-6.4170
125	HOMO-3	A	-6.4945
124	HOMO-4	A	-6.4947
123	HOMO-5	A	-7.2227
122	HOMO-6	A	-7.2743
121	HOMO-7	A	-7.2858
120	HOMO-8	A	-7.3122
119	HOMO-9	A	-7.5818
118	HOMO-10	A	-8.3405
117	HOMO-11	A	-8.9574
116	HOMO-12	A	-8.9927
115	HOMO-13	A	-9.3321
114	HOMO-14	A	-9.4421
113	HOMO-15	A	-9.6151

Excited States

Table 8: *Energies and other properties of the calculated excited states.*

Number	Symbol	Symmetry	Energy /eV	Wavelength /nm	Colour (CIE x,y)	Oscillator Strength	Transitions (Probability)
1	T_1	Triplet-A	2.4102	514.42	Green (0.04, 0.81)	< 0.0001	HOMO → LUMO (0.99)
2	S_1	Singlet-A	2.4228	511.75	Green (0.02, 0.78)	< 0.0001	HOMO → LUMO (0.99)
3	T_2	Triplet-A	2.4315	509.91	Green (0.01, 0.75)	< 0.0001	HOMO-1 → LUMO (0.99)
4	S_2	Singlet-A	2.4450	507.09	Green (0.01, 0.70)	< 0.0001	HOMO-1 → LUMO (0.99)
5	T_3	Triplet-A	2.5998	476.89	Cyan (0.10, 0.10)	0.3390	HOMO-2 → LUMO (0.93)
6	T_4	Triplet-A	3.0523	406.20	Violet (0.17, 0.00)	< 0.0001	HOMO-1 → LUMO+2 (0.42) HOMO → LUMO+3 (0.31) HOMO → LUMO+1 (0.17) HOMO-7 → LUMO+9 (0.02)
7	T_5	Triplet-A	3.0534	406.05	Violet (0.17, 0.00)	0.0215	HOMO → LUMO+2 (0.43) HOMO-1 → LUMO+3 (0.30) HOMO-1 → LUMO+1 (0.16) HOMO-7 → LUMO+10 (0.02)
8	T_6	Triplet-A	3.5441	349.83	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO → LUMO+1 (0.35) HOMO-1 → LUMO+4 (0.28) HOMO → LUMO+6 (0.18) HOMO → LUMO+3 (0.13)
9	T_7	Triplet-A	3.5513	349.12	Ultraviolet (0.00, 0.00)	1.4802	HOMO-1 → LUMO+1 (0.32) HOMO → LUMO+4 (0.31) HOMO-1 → LUMO+6 (0.19) HOMO-1 → LUMO+3 (0.12)
10	T_8	Triplet-A	3.5821	346.13	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO → LUMO+5 (0.49) HOMO-1 → LUMO+7 (0.46)
11	T_9	Triplet-A	3.5823	346.10	Ultraviolet (0.00, 0.00)	0.0038	HOMO → LUMO+7 (0.47) HOMO-1 → LUMO+5 (0.47)
12	S_3	Singlet-A	3.6369	340.91	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO → LUMO+1 (0.94)
13	S_4	Singlet-A	3.6629	338.49	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-1 → LUMO+1 (0.92)
14	T_{10}	Triplet-A	3.7928	326.89	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO → LUMO+1 (0.46) HOMO → LUMO+6 (0.26) HOMO-1 → LUMO+4 (0.19)
15	S_5	Singlet-A	3.9326	315.27	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-1 → LUMO+2 (0.48) HOMO → LUMO+3 (0.44)
16	S_6	Singlet-A	3.9342	315.15	Ultraviolet (0.00, 0.00)	0.0441	HOMO → LUMO+2 (0.51) HOMO-1 → LUMO+3 (0.39)
17	S_7	Singlet-A	4.0276	307.84	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-4 → LUMO (0.99)
18	S_8	Singlet-A	4.0289	307.73	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-3 → LUMO (0.99)
19	S_9	Singlet-A	4.3181	287.13	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-1 → LUMO+4 (0.43) HOMO → LUMO+6 (0.34) HOMO → LUMO+3 (0.07) HOMO-4 → LUMO+2 (0.06) HOMO-3 → LUMO+3 (0.04)
20	S_{10}	Singlet-A	4.3288	286.42	Ultraviolet (0.00, 0.00)	0.2499	HOMO → LUMO+4 (0.45) HOMO-1 → LUMO+6 (0.29) HOMO-1 → LUMO+3 (0.08) HOMO-3 → LUMO+2 (0.07) HOMO-4 → LUMO+3 (0.05)

Transition Dipole Moments

Table 11: *Properties of the calculated transition dipole moments. [a]: The electric transition dipole moment (TEDM), in Debye (D). [b]: Angle between the TEDM and the x-axis of the molecule. [c]: Angle between the TEDM and xy-plane of the molecule. [d]: The magnetic transition dipole moment (TMDM), in atomic units (au). [e]: Angle between the TMDM and the x-axis of the molecule. [f]: Angle between the TMDM and xy-plane of the molecule. [g]: The TEDM, in Gaussian CGS (centimetre, gram, second) units. [h]: The TMDM, in Gaussian CGS (centimetre, gram, second) units. [i]: The angle between the electric and magnetic transition dipole moments, in Gaussian CGS units. [j]: The cosine of the angle between the electric and magnetic transition dipole moments, in Gaussian CGS units. [k]: The dissymmetry factor of the transition dipole moment.*

Excited State	$\mu^{[a]}$ Vector /D	$\mu^{[a]}$ /D	$\theta_{\mu,x}{}^{[b]}$ /	$\theta_{\mu,xy}{}^{[c]}$ /	$m^{[d]}$ Vector /au	$m^{[d]}$ /au	$\theta_{m,x}{}^{[e]}$ /	$\theta_{m,xy}{}^{[f]}$ /	$\mu^{[g]}$ /esu·cm	$m^{[h]}$ /erg·G^{-1}	$\theta_{\mu,m}{}^{[i]}$ /	$\cos(\theta_{\mu,m})^{[j]}$	$g_{lum}{}^{[k]}$
T_1	-0.00, -0.03, 0.00	0.03	89.65	0.02	0.28, 0.00, 0.00	0.28	0.00	0.00	2.68e-20	2.58e-21	89.65	0.01	0.002
S_1	-0.00, -0.03, 0.00	0.03	89.90	0.00	0.26, 0.00, 0.00	0.26	0.00	0.00	2.55e-20	2.42e-21	89.90	0.00	0.001
T_2	0.00, 0.00, -0.00	< 0.01	18.54	2.01	-0.00, 0.00, 0.06	0.06	89.75	89.75	7.24e-23	5.82e-22	87.75	0.04	0.019

S_2	-0.00, -0.00, 0.00	< 0.01	48.19	19.47	0.00, 0.00, -0.01	0.01	88.90	88.90	3.05e-23	1.32e-22	69.75	0.35	0.303
T_3	5.86, 0.00, 0.00	5.86	0.00	0.00	0.00, 0.37, 0.00	0.37	90.00	0.00	5.86e-18	3.46e-21	90.00	-0.00	-0.000
T_4	0.00, -0.04, 0.00	0.04	89.94	0.03	-0.01, 0.00, -2.58	2.58	89.88	89.88	3.96e-20	2.39e-20	89.97	0.00	0.001
T_5	0.00, 1.36, 0.00	1.36	90.00	0.00	0.18, 0.00, -0.08	0.19	23.12	23.12	1.36e-18	1.78e-21	90.00	-0.00	< 0.001
T_6	0.00, -0.01, -0.00	0.01	89.69	0.23	-0.00, 0.00, 4.95	4.95	89.99	89.99	1.13e-20	4.59e-20	89.77	0.00	0.004
T_7	-0.00, 10.48, -0.00	10.48	90.00	0.00	0.44, 0.00, 0.01	0.44	0.71	0.71	1.05e-17	4.10e-21	90.00	0.00	< 0.001
T_8	-0.04, -0.00, 0.01	0.04	19.02	19.01	0.00, 0.25, -0.00	0.25	90.00	0.19	3.80e-20	2.29e-21	89.21	0.01	0.003
T_9	-0.00, -0.00, -0.53	0.53	89.90	89.78	0.00, 0.01, -0.00	0.01	90.00	2.73	5.27e-19	5.34e-23	92.53	-0.04	< 0.001
S_3	0.00, 0.00, -0.00	< 0.01	39.79	19.23	0.00, 0.00, -1.53	1.53	90.00	90.00	2.32e-23	1.42e-20	109.23	-0.33	-0.002
S_4	0.00, 0.04, 0.00	0.04	90.00	0.00	-0.07, 0.00, 0.00	0.07	0.92	0.92	3.83e-20	6.30e-22	90.00	0.00	0.000
T_{10}	-0.00, 0.01, 0.00	0.01	89.76	0.97	0.00, 0.00, -3.60	3.60	90.00	90.00	7.21e-21	3.34e-20	89.03	0.02	0.014
S_5	0.00, -0.03, -0.00	0.03	89.91	0.01	-0.00, 0.00, -2.08	2.08	89.94	89.94	2.92e-20	1.93e-20	90.01	-0.00	< 0.001
S_6	0.00, 1.72, 0.00	1.72	90.00	0.00	0.13, 0.00, -0.04	0.14	14.98	14.98	1.72e-18	1.27e-21	90.00	0.00	< 0.001
S_7	0.00, -0.00, -0.00	< 0.01	72.18	4.39	0.00, 0.00, 0.04	0.04	89.24	89.24	1.66e-22	3.81e-22	85.85	0.07	0.106
S_8	-0.00, 0.04, 0.00	0.04	89.96	0.03	-0.12, 0.00, 0.00	0.12	0.00	0.00	3.77e-20	1.10e-21	90.04	-0.00	< 0.001
S_9	0.00, 0.00, 0.00	< 0.01	86.36	0.30	0.00, 0.00, -0.86	0.86	90.00	90.00	2.40e-21	8.01e-21	89.70	0.01	0.006
S_{10}	0.00, 3.90, -0.00	3.90	89.98	0.00	0.05, 0.00, 0.00	0.05	0.64	0.64	3.90e-18	4.52e-22	90.02	-0.00	< 0.001

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