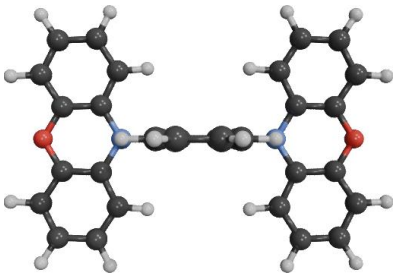
A Report On The Calculation Of The Excited States Of 1_4_Phx_nap_phx At The PBE0-d3bj/6-31G** Level

osl



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 calculation was performed using the PySCF software package at the PBE0-d3bj/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 peak was calculated to be at 292 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 515 nm) respectively, corresponding to a singlet/triplet splitting energy (ΔE_{ST}) of 0.01 eV.

Table 1: *Summary of overall calculation metadata.*

Date[a] (Duration[b])	CPUs (Memory)	Success (Converged)	Computational package	Level of theory	Solvent (model)	Calculations	Wavefunction	Multiplicity	T[c] / K	p[d] / atm
N/A (N/A)	14 (27 GB)	True (N/A)	PySCF (2.9.0)	PBE0-d3bj/ 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	-42643.4658 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
Exact mass	490.1681 g·mol^{-1}
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 °

Excited States

Table 6: *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)	515 nm (Green, (0.04, 0.81))
f_{T_1}	0.00
ΔE_{ST}	0.01 eV
Simulated Absorption Peaks	292 nm

Methodology

Metadata

The calculation of the excited states was performed using the **PySCF (2.9.0)** program, the **DFT** method with the **PBE0-d3bj** functional and the **6-31G**** basis set. The calculation **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.

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.

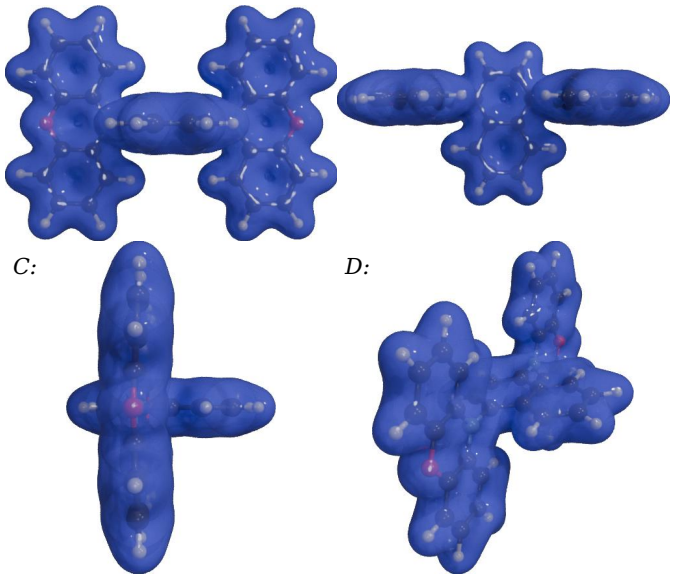


Figure 1: *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Geometry

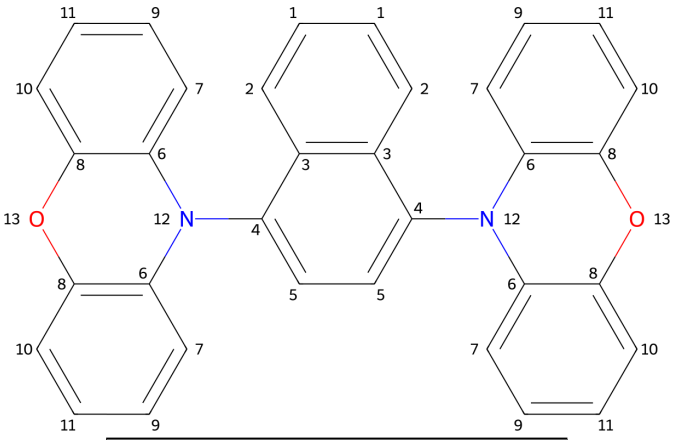


Figure 2: *Labelled structure of 1_4_Phx_nap_phx.*

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} and an **exact mass**, considering only specific atomic isotopes, of 490.17 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.

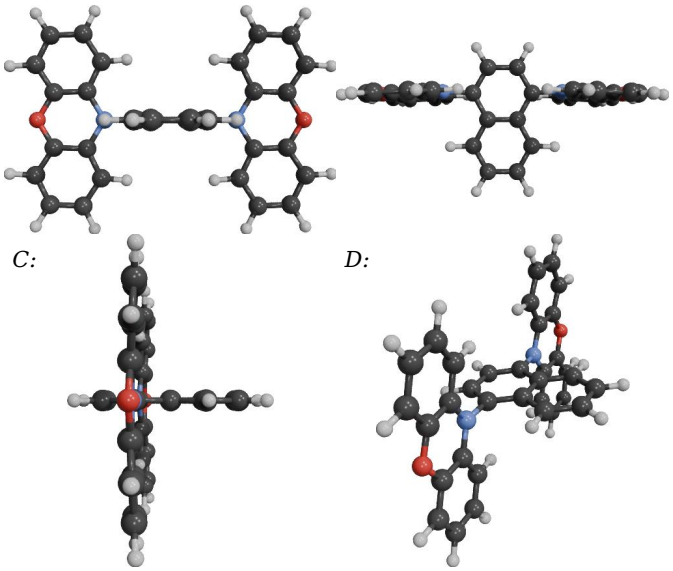


Figure 3: *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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.

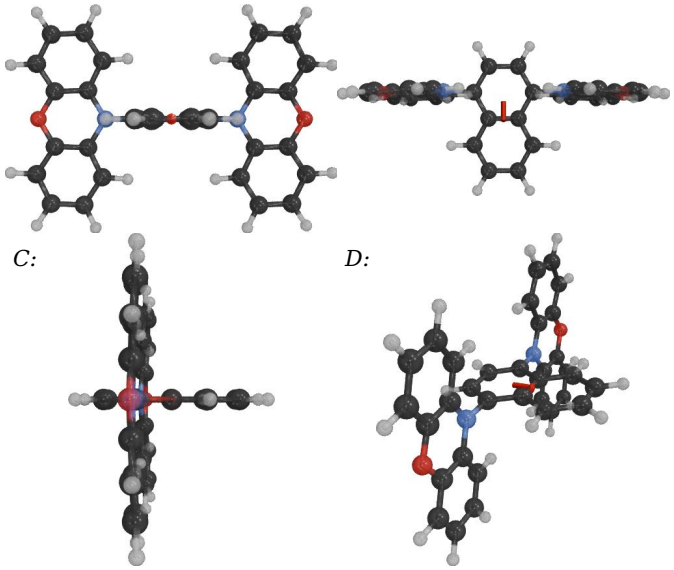


Figure 4: *The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

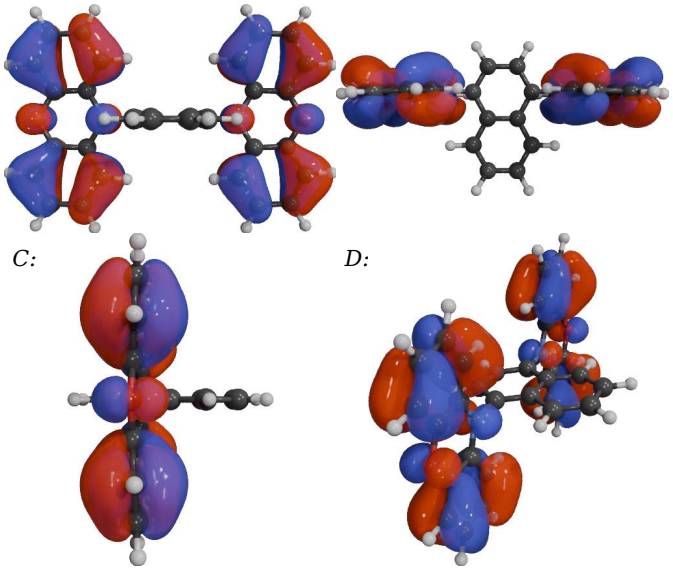


Figure 5: *Orbital density plots of the HOMO-4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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 19). 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 5-10 and 12-18 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 11.

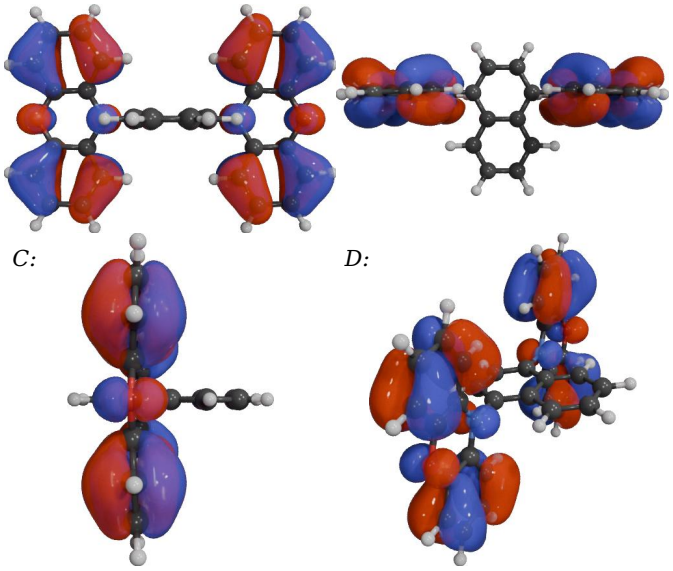


Figure 6: *Orbital density plots of the HOMO-3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

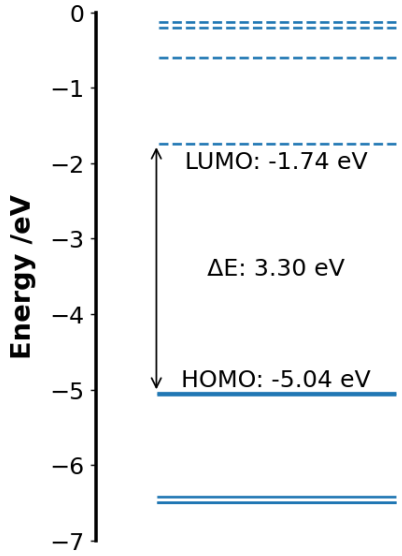


Figure 19: *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

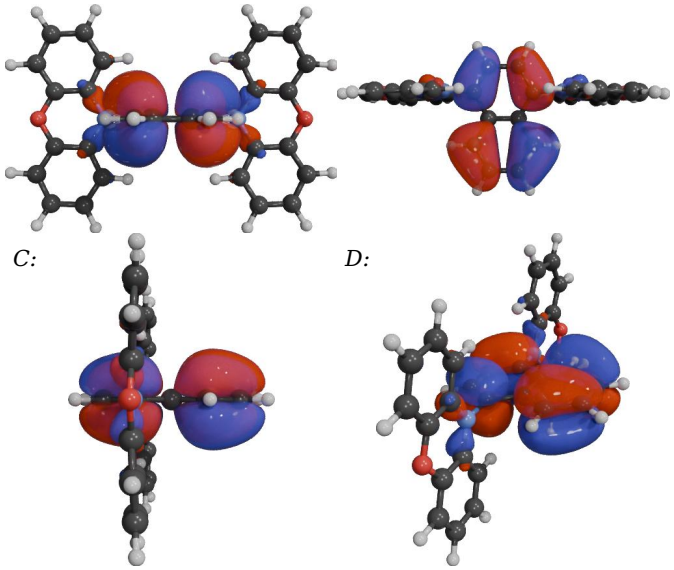


Figure 7: *Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

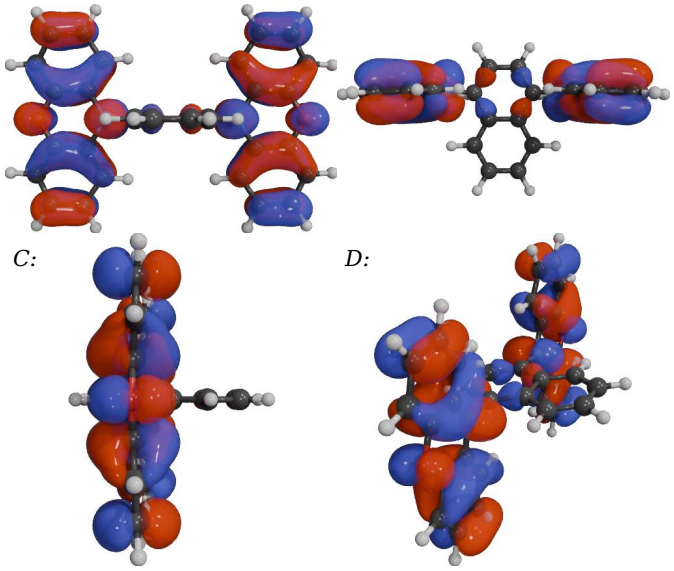


Figure 8: *Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

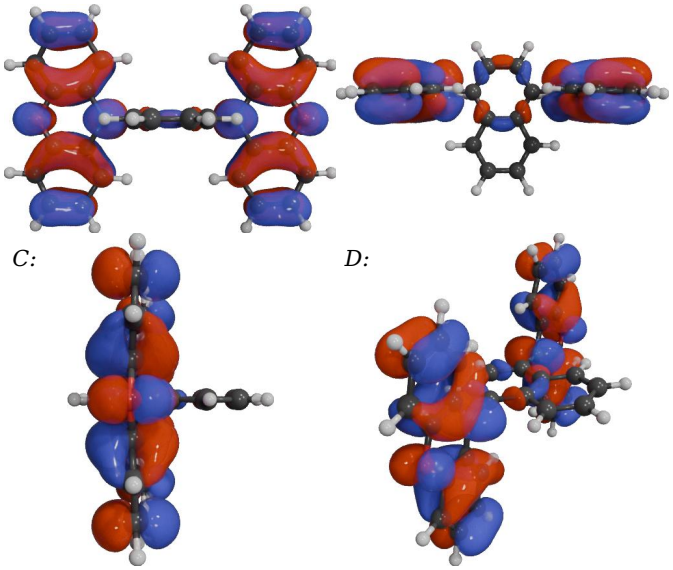


Figure 9: *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

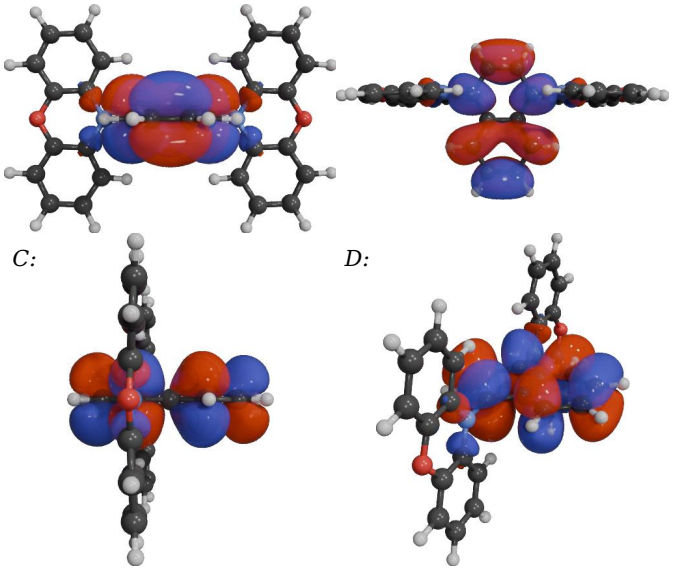


Figure 10: *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

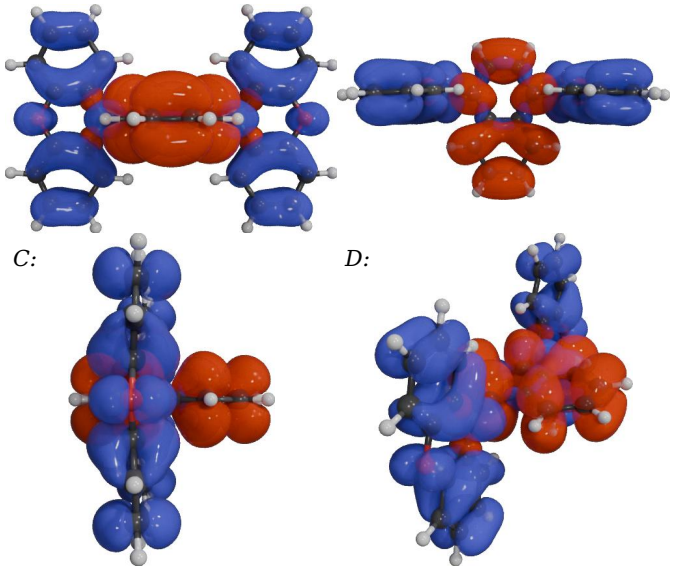


Figure 11: *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

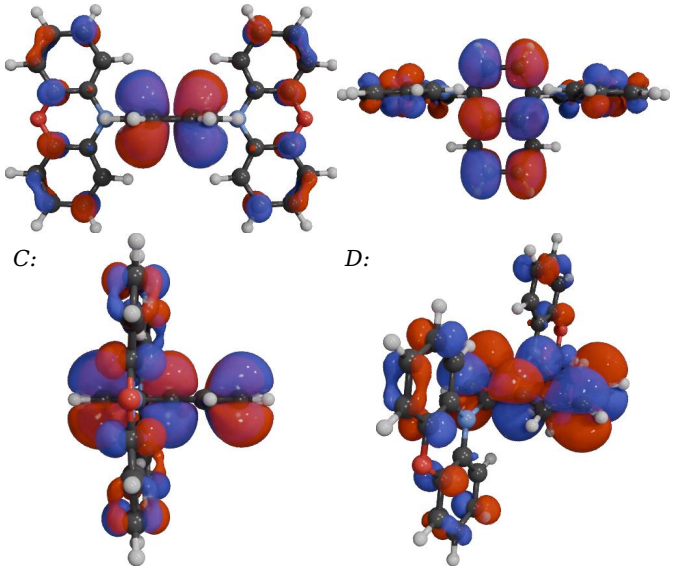


Figure 12: *Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

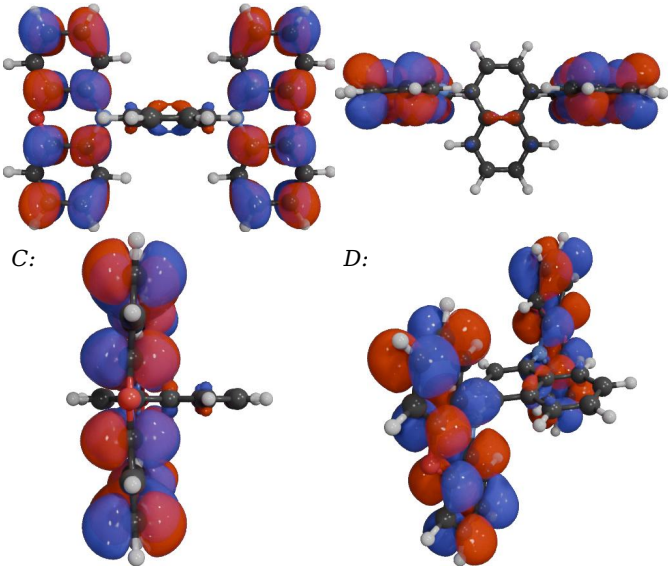


Figure 13: *Orbital density plots of the LUMO+2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

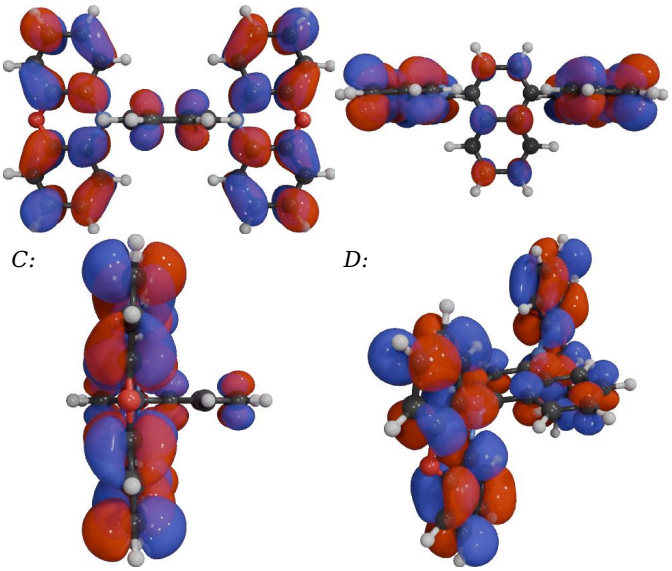


Figure 14: *Orbital density plots of the LUMO+3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

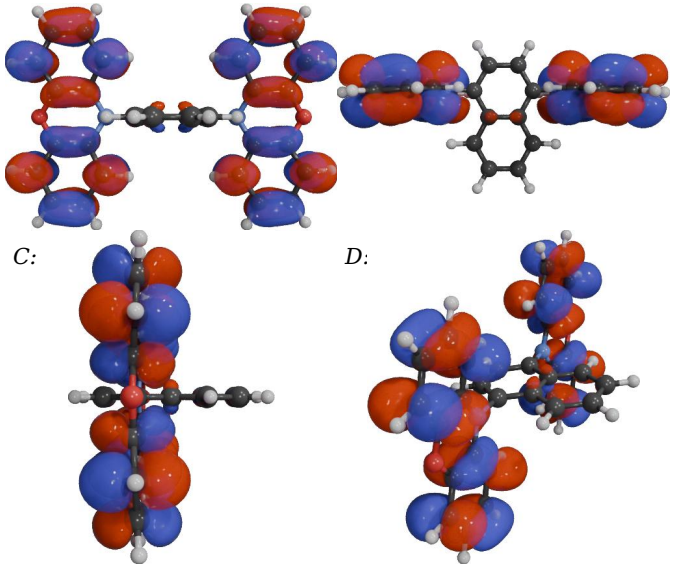


Figure 15: *Orbital density plots of the LUMO+4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

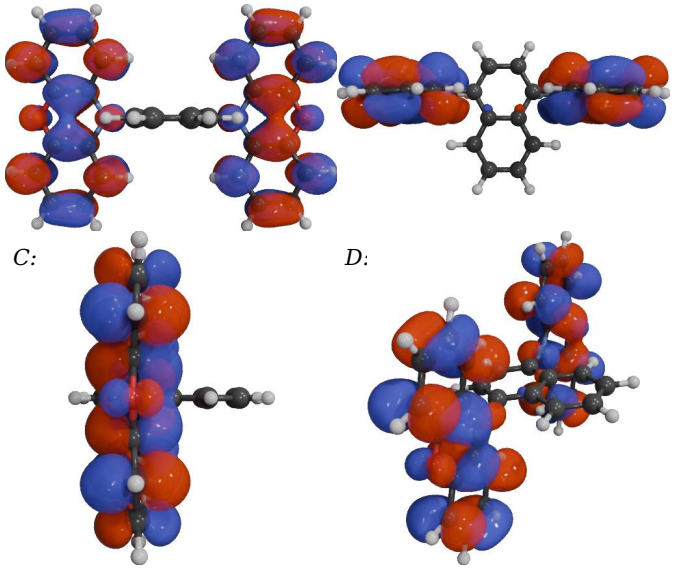


Figure 16: *Orbital density plots of the LUMO+5, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

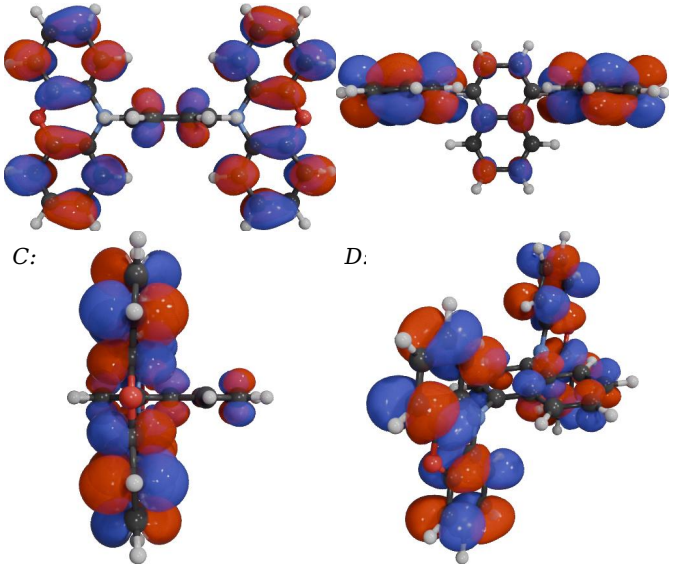


Figure 17: *Orbital density plots of the LUMO+6, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

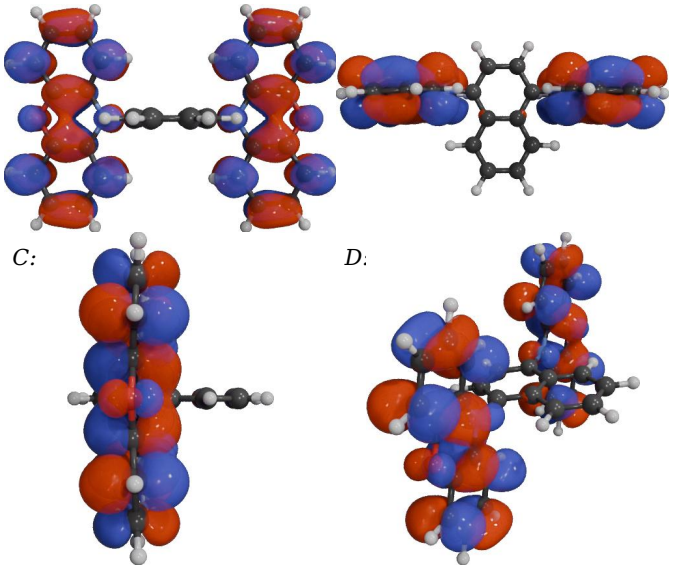


Figure 18: *Orbital density plots of the LUMO+7, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Excited States

In total, the energies of 20 electronic excited states were calculated (figure 20), 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 (515 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 7. 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 **one most intense peak** was found at 292 nm. The full simulated absorption spectrum is shown in figure 21.

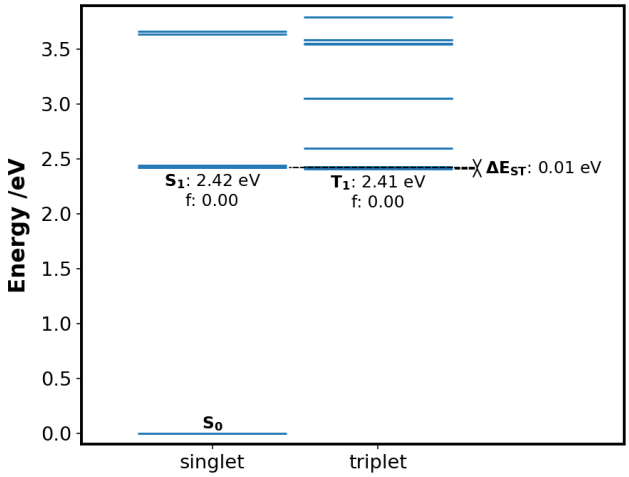


Figure 20: *Graph of the calculated excited states. f: oscillator strength of the relevant ground to excited state transition.*

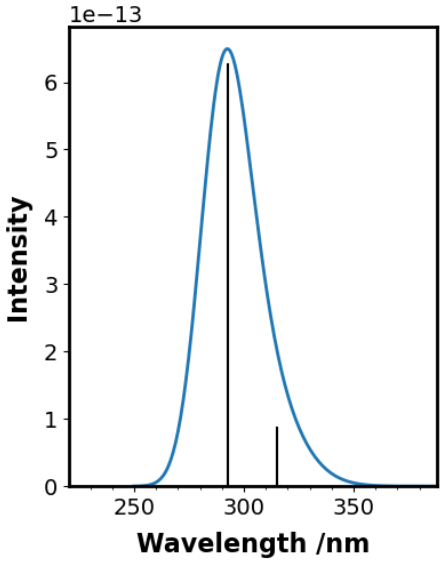


Figure 21: *Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 292 nm.*

Tables Of Results

Atom Coordinates

Table 8: *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 9: *Energies of the calculated molecular orbitals.*

Level	Label	Symmetry	Energy /eV
144	LUMO+15	None	2.8901
143	LUMO+14	None	2.8630
142	LUMO+13	None	2.4530
141	LUMO+12	None	2.2790
140	LUMO+11	None	2.1706
139	LUMO+10	None	1.1527
138	LUMO+9	None	1.1498
137	LUMO+8	None	0.5040
136	LUMO+7	None	0.1767
135	LUMO+6	None	0.1689
134	LUMO+5	None	0.1559
133	LUMO+4	None	0.1052
132	LUMO+3	None	-0.1275
131	LUMO+2	None	-0.2050
130	LUMO+1	None	-0.6058
129	**LUMO**	**None**	**-1.7445**
128	**HOMO**	**None**	**-5.0432**
127	HOMO-1	None	-5.0667
126	HOMO-2	None	-6.4166
125	HOMO-3	None	-6.4939
124	HOMO-4	None	-6.4941
123	HOMO-5	None	-7.2223
122	HOMO-6	None	-7.2735
121	HOMO-7	None	-7.2859
120	HOMO-8	None	-7.3128
119	HOMO-9	None	-7.5827
118	HOMO-10	None	-8.3414
117	HOMO-11	None	-8.9587
116	HOMO-12	None	-8.9940
115	HOMO-13	None	-9.3324
114	HOMO-14	None	-9.4424
113	HOMO-15	None	-9.6177

Excited States

Table 7: *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	S_1	Singlet	2.4221	511.88	Green (0.02, 0.78)	< 0.0001	HOMO → LUMO (0.99)
2	S_2	Singlet	2.4445	507.20	Green (0.01, 0.70)	< 0.0001	HOMO-1 → LUMO (0.99)
3	S_3	Singlet	3.6380	340.81	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO → LUMO+1 (0.94) HOMO-1 → LUMO+2 (0.05)
4	S_4	Singlet	3.6640	338.38	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-1 → LUMO+1 (0.92) HOMO → LUMO+2 (0.06)
5	S_5	Singlet	3.9344	315.13	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-1 → LUMO+2 (0.48) HOMO → LUMO+3 (0.44) HOMO → LUMO+1 (0.04) HOMO → LUMO+6 (0.02)
6	S_6	Singlet	3.9360	315.00	Ultraviolet (0.00, 0.00)	0.0441	HOMO → LUMO+2 (0.51) HOMO-1 → LUMO+3 (0.39) HOMO-1 → LUMO+1 (0.05) HOMO-1 → LUMO+6 (0.02)
7	S_7	Singlet	4.0245	308.07	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-4 → LUMO (0.99) HOMO-1 → LUMO (0.01)
8	S_8	Singlet	4.0259	307.97	Ultraviolet (0.00, 0.00)	< 0.0001	HOMO-3 → LUMO (0.99) HOMO → LUMO (0.01)
9	S_9	Singlet	4.2344	292.80	Ultraviolet (0.00, 0.00)	0.2709	HOMO-2 → LUMO (0.82) HOMO → LUMO+5 (0.05) HOMO-1 → LUMO+7 (0.04) HOMO-9 → LUMO+1 (0.02) HOMO-10 → LUMO+8 (0.01) HOMO-5 → LUMO+1 (0.01) HOMO-2 → LUMO+8 (0.01) HOMO-10 → LUMO (0.01)
10	S_{10}	Singlet	4.3188	287.08	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) HOMO-1 → LUMO+2 (0.02) HOMO-3 → LUMO+1 (0.02)
11	T_1	Triplet	2.4095	514.57	Green (0.04, 0.81)	0.0000	HOMO → LUMO (0.99)
12	T_2	Triplet	2.4310	510.02	Green (0.01, 0.75)	0.0000	HOMO-1 → LUMO (0.99) HOMO-4 → LUMO (0.01)
13	T_3	Triplet	2.5978	477.27	Cyan (0.10, 0.11)	0.0000	HOMO-2 → LUMO (0.93) HOMO-10 → LUMO+8 (0.03) HOMO-9 → LUMO+1 (0.01) HOMO-15 → LUMO+12 (0.01) HOMO-8 → LUMO (0.01)
14	T_4	Triplet	3.0537	406.02	Violet (0.17, 0.00)	0.0000	HOMO-1 → LUMO+2 (0.42) HOMO → LUMO+3 (0.31) HOMO → LUMO+1 (0.17) HOMO-7 → LUMO+9 (0.02) HOMO-8 → LUMO+10 (0.01) HOMO-4 → LUMO+4 (0.01) HOMO-3 → LUMO+6 (0.01) HOMO → LUMO+6 (0.01) HOMO-6 → LUMO+10 (0.01) HOMO-5 → LUMO+5 (0.01) HOMO-6 → LUMO+7 (0.01)
15	T_5	Triplet	3.0548	405.87	Violet (0.17, 0.00)	0.0000	HOMO → LUMO+2 (0.43) HOMO-1 → LUMO+3 (0.30) HOMO-1 → LUMO+1 (0.16) HOMO-7 → LUMO+10 (0.02) HOMO-8 → LUMO+9 (0.01) HOMO-3 → LUMO+4 (0.01) HOMO-4 → LUMO+6 (0.01) HOMO-1 → LUMO+6 (0.01) HOMO-6 → LUMO+9 (0.01) HOMO-5 → LUMO+7 (0.01) HOMO-6 → LUMO+5 (0.01)

16	T_6	Triplet	3.5456	349.68	Ultraviolet ■ (0.00, 0.00)	0.0000	HOMO → LUMO+1 (0.35) HOMO-1 → LUMO+4 (0.28) HOMO → LUMO+6 (0.18) HOMO → LUMO+3 (0.13) HOMO-1 → LUMO+2 (0.02) HOMO-7 → LUMO+5 (0.01) HOMO-8 → LUMO+7 (0.01)
17	T_7	Triplet	3.5529	348.97	Ultraviolet ■ (0.00, 0.00)	0.0000	HOMO-1 → LUMO+1 (0.32) HOMO → LUMO+4 (0.31) HOMO-1 → LUMO+6 (0.19) HOMO-1 → LUMO+3 (0.12) HOMO → LUMO+2 (0.02) HOMO-7 → LUMO+7 (0.01) HOMO-8 → LUMO+5 (0.01)
18	T_8	Triplet	3.5819	346.14	Ultraviolet ■ (0.00, 0.00)	0.0000	HOMO → LUMO+5 (0.49) HOMO-1 → LUMO+7 (0.46) HOMO-7 → LUMO+6 (0.02) HOMO-8 → LUMO+4 (0.01) HOMO-6 → LUMO+4 (0.01)
19	T_9	Triplet	3.5822	346.12	Ultraviolet ■ (0.00, 0.00)	0.0000	HOMO → LUMO+7 (0.47) HOMO-1 → LUMO+5 (0.47) HOMO-7 → LUMO+4 (0.02) HOMO-8 → LUMO+6 (0.01) HOMO-6 → LUMO+6 (0.01)
20	T_{10}	Triplet	3.7943	326.76	Ultraviolet ■ (0.00, 0.00)	0.0000	HOMO → LUMO+1 (0.45) HOMO → LUMO+6 (0.26) HOMO-1 → LUMO+4 (0.19) HOMO-1 → LUMO+2 (0.04) HOMO → LUMO+3 (0.02) HOMO-3 → LUMO+1 (0.01) HOMO-7 → LUMO+5 (0.01)

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