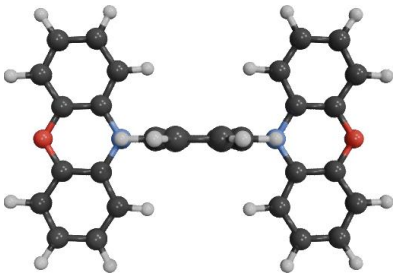
A Report On The Calculation Of The Excited States Of 1_4_Phx_nap_phx At The PBE1PBE/6-31G(d,p) Level

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 calculation was performed using the Gaussian software package at the PBE1PBE/6-31G(d,p) level of theory. The total self-consistent field (SCF) energy of the system was found to be -42643.99 eV after 1 step. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -5.04 and -1.75 eV respectively, corresponding to a HOMO-LUMO band gap of 3.30 eV. The permanent dipole moment (PDM) was calculated to be 2.01 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
16/07/2025 17:55:58 (25 m, 7 s)	14 (27 GB)	True (N/A)	Gaussian (2016+C.01)	PBE1PBE/ 6-31G(d,p)	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	-42643.9930 eV
Final energy	-4,114,520 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}	-1.75 eV

Permanent Dipole Moment

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

Total	2.01 D
X axis angle	89.34 °
XY plane angle	89.34 °

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
$\theta_{\mu,x}$	90.00 °
$\theta_{\mu,xy}$	0.00 °
m[d]	0.26 a.u.
$\theta_{m,x}$	0.00 °
$\theta_{m,xy}$	0.00 °
μ (Gaussian-CGS)	2.54e-20 esu·cm
m (Gaussian-CGS)	2.43e-21 erg·G^{-1}
$\theta_{\mu,m}$	90.00 °
cos($\theta_{\mu,m}$)	-0.00
g_{lum}	-0.000

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}	0.00
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

Spin-Orbit Coupling

Table 8: *Summary of the calculated spin-orbit coupling values. <S\|H_{SO}\|T>: SOC between singlet state S and triplet state T. <S\|λ\|T>: First-order mixing coefficient between the same.*

<S_0|H_{SO}|T_1>	1.91 cm^{-1}
<S_0|λ|T_1>	0.00
<S_1|H_{SO}|T_1>	0.00 cm^{-1}
<S_1|λ|T_1>	0.00

Methodology

Metadata

The calculation of the excited states was performed using the **Gaussian (2016+C.01)** program, the **DFT** method with the **PBE1PBE** functional and the **6-31G(d,p)** basis set. It was completed on the **16th July 2025** after a total duration of **25 m, 7 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.

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] Spin-orbit coupling (SOC, H_{SO}) was calculated using a custom implementation of the PySOC program.[4] Three-dimensional plots of atom positions and calculated densities, including molecular orbitals, were rendered using Visual Molecular Dynamics (VMD)[5] and the Tachyon ray-tracer.[6] Finally, two-dimensional graphs were plotted using the MatPlotlib library,[7] while this report itself was prepared using the Mako template library[8] and the Weasyprint library[9], 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 -42643.99 eV, corresponding to -4,114,520 $KJmol^{-1}$. A plot of the total SCF electron density is shown in figure 1.

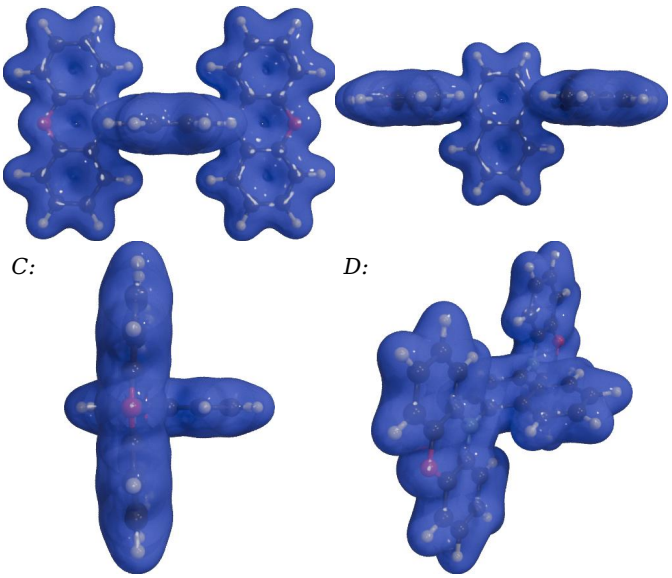


Figure 1: *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Geometry

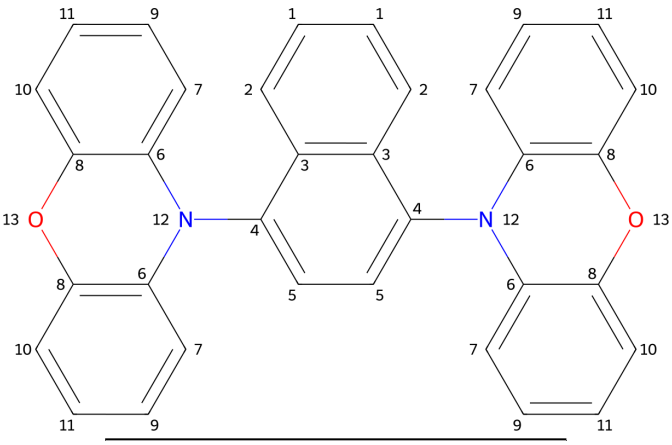


Figure 2: *Labelled structure of 1_4_Phx_nap_phx.*

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.

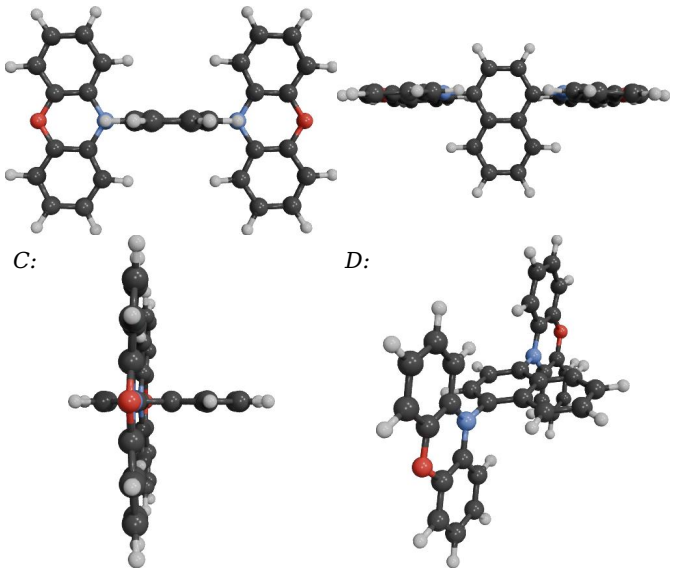


Figure 3: *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Permanent Dipole Moment

The calculated **permanent dipole moment** was 2.01 D, with a vector (x,y,z) of -0.02, 0.00, -2.01 D. The angle between the dipole moment vector and the x-axis was 89.34 °, while the angle between the dipole moment and the xy-plane was 89.34 °. A plot of the permanent dipole moment is shown in figure 4.

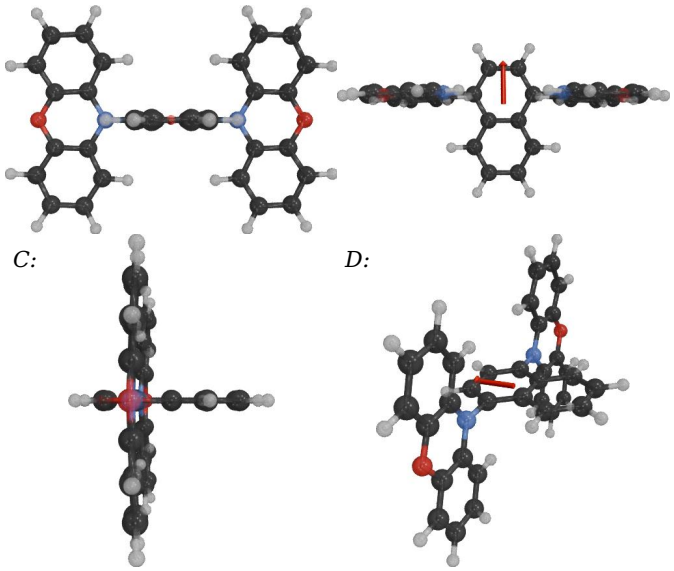


Figure 4: *The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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 $\theta_{\mu,x}$ = 90.00 ° 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 = 2.54e-20 esu·cm and m = 2.43e-21 erg·G^{-1}, while the **angle between the two dipole moments** was $\theta_{\mu,m}$ = 90.00 °. 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} = -0.000. A plot of the electric and magnetic transition dipole moments is shown in figure 5.

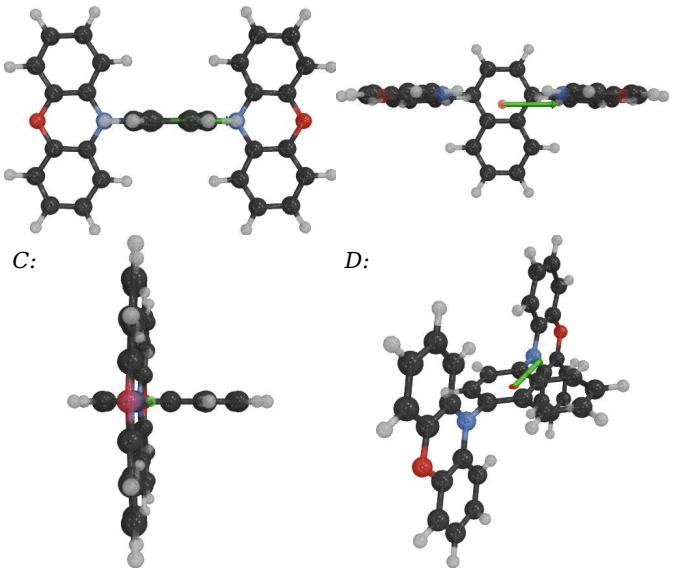


Figure 5: *The electric (red arrow) and magnetic (green arrow) transition (S_1) dipole moment plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D = 0.1 au. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Molecular Orbitals

In total, 680 doubly occupied molecular orbitals were calculated, divided into 128 occupied orbitals and 552 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO and LUMO** were -5.04 and -1.75 eV respectively, corresponding to a **HOMO-LUMO band gap** of 3.30 eV (figure 20). Plots of the orbital density for the HOMO-3, HOMO-4, 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.

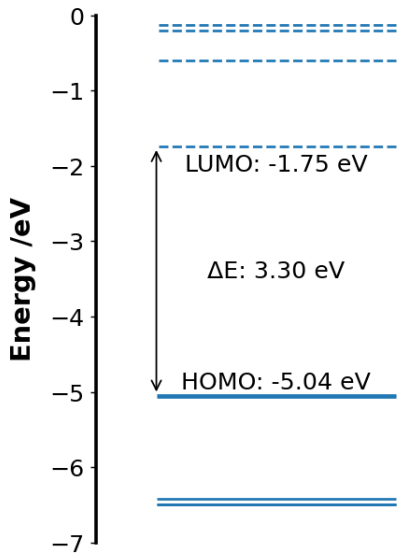


Figure 20: *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

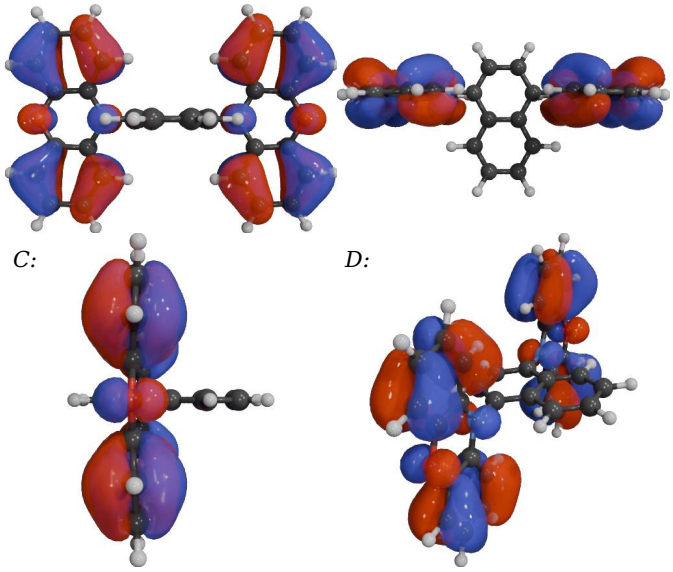


Figure 6: *Orbital density plots of the HOMO-3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

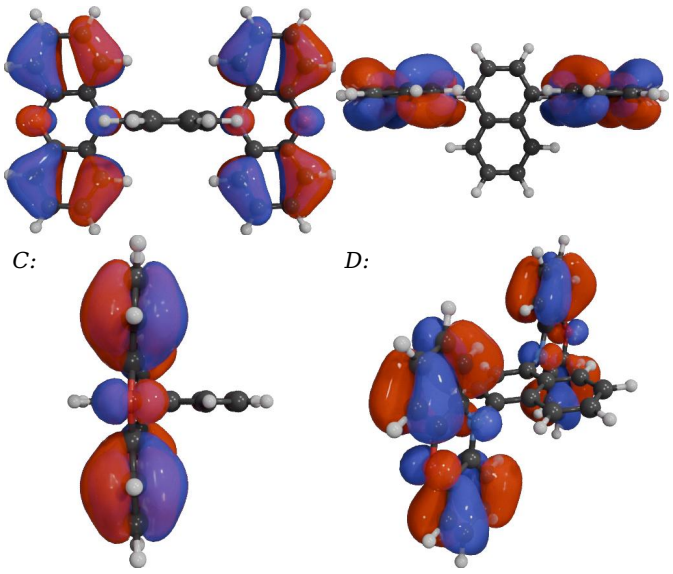


Figure 7: *Orbital density plots of the HOMO-4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

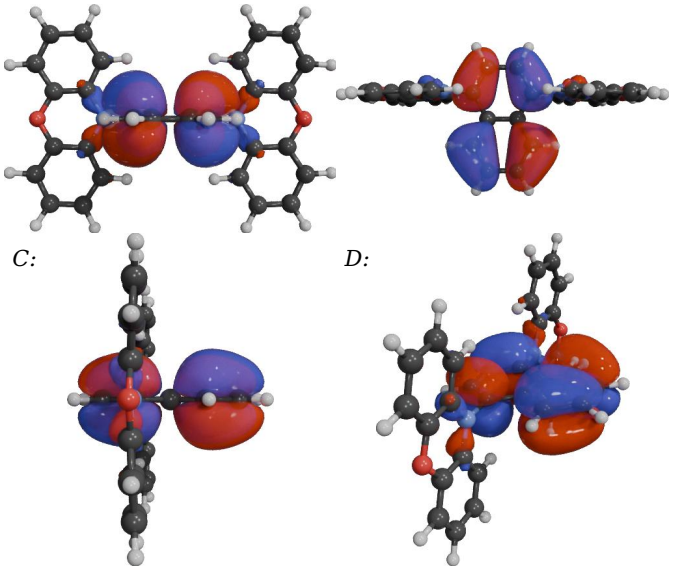


Figure 8: *Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

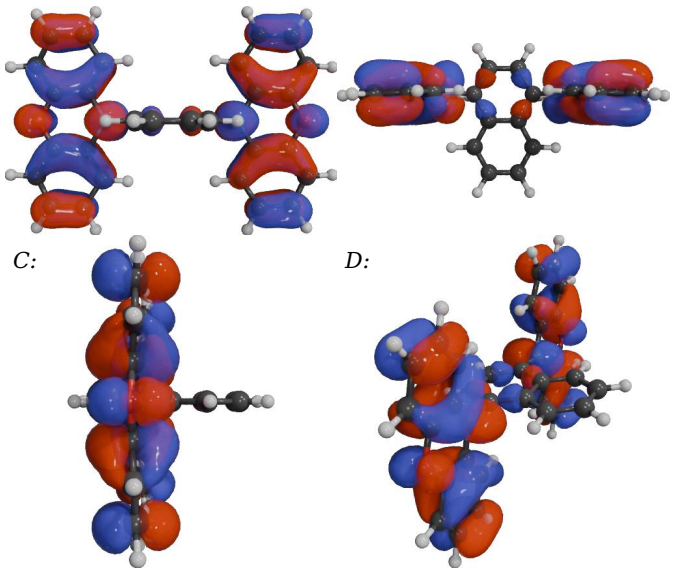


Figure 9: *Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

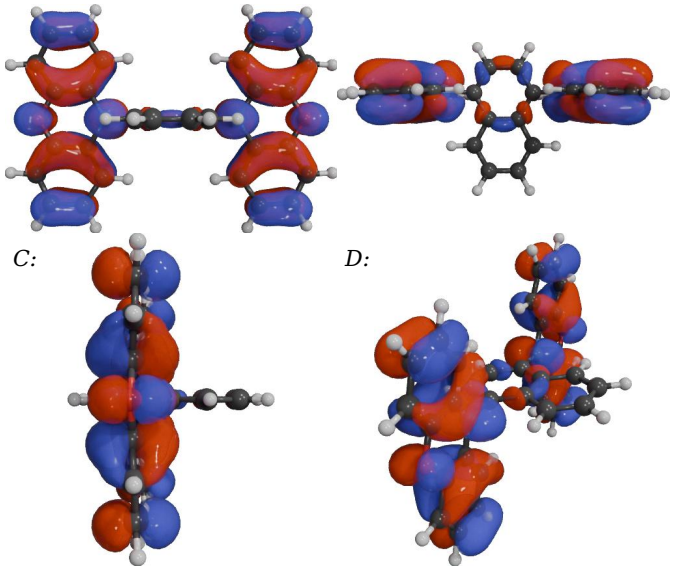


Figure 10: *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

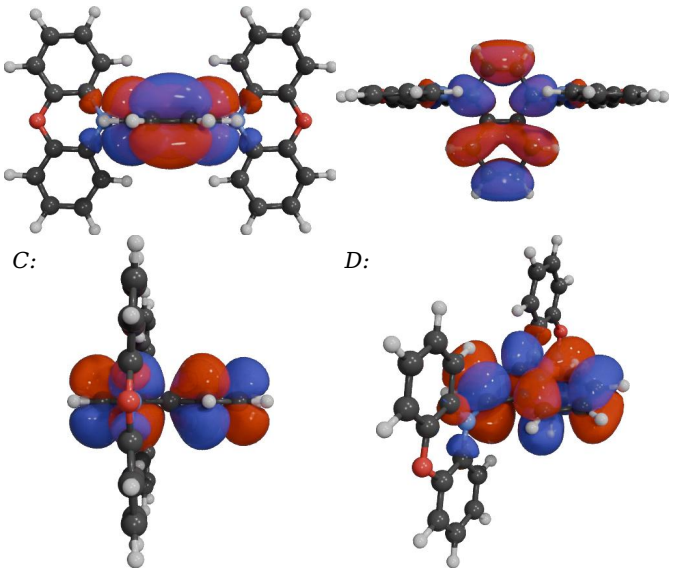


Figure 11: *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

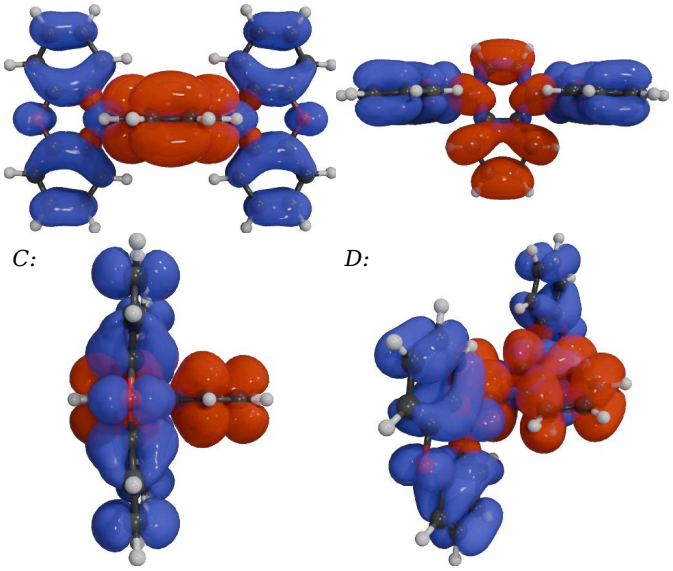


Figure 12: *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

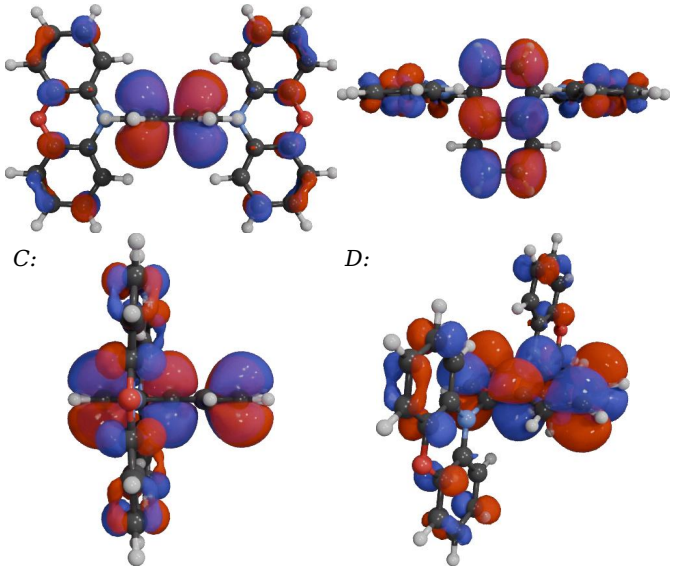


Figure 13: *Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

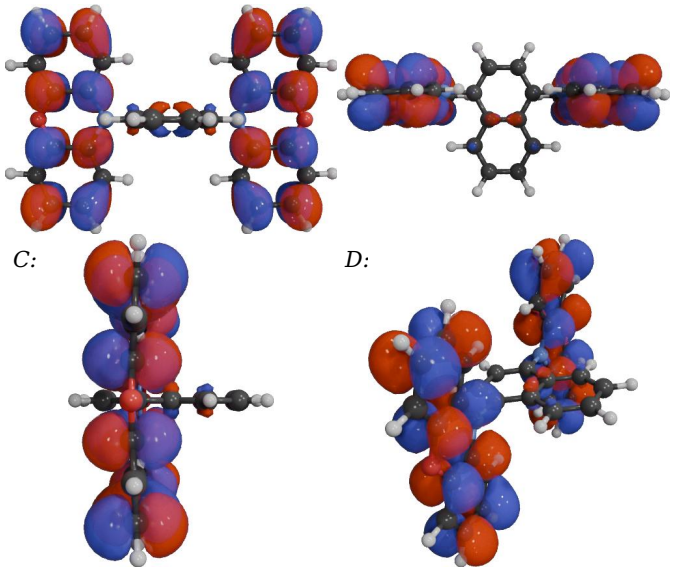


Figure 14: *Orbital density plots of the LUMO+2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

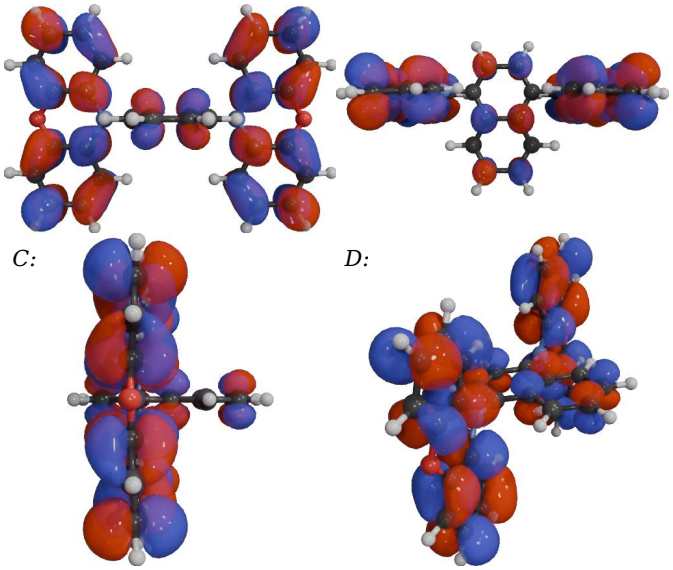


Figure 15: *Orbital density plots of the LUMO+3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

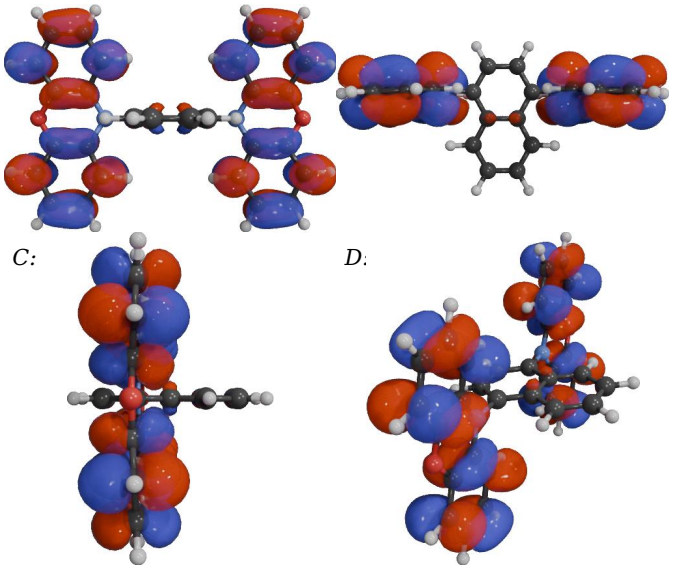


Figure 16: *Orbital density plots of the LUMO+4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

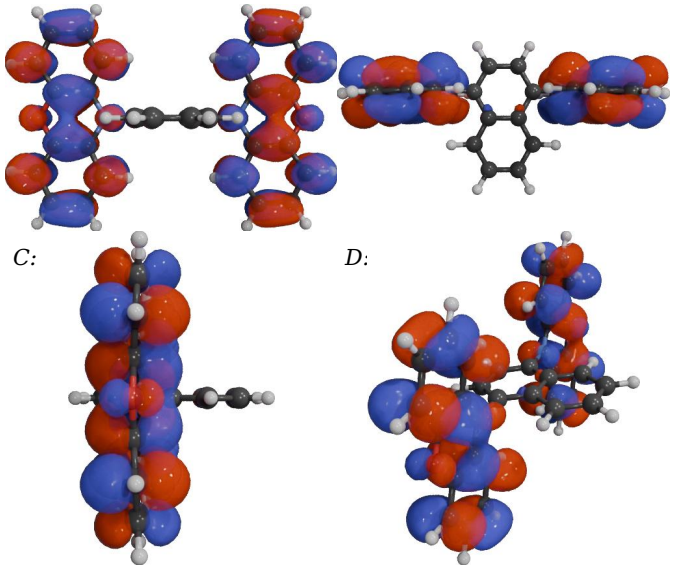


Figure 17: *Orbital density plots of the LUMO+5, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

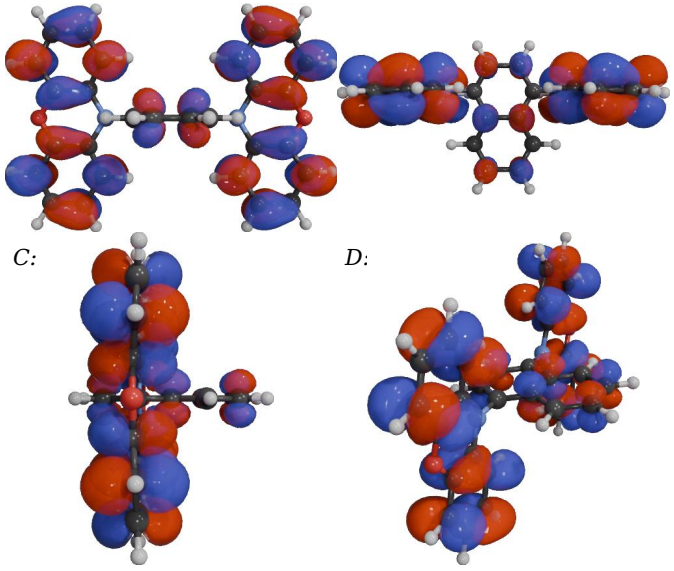


Figure 18: *Orbital density plots of the LUMO+6, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

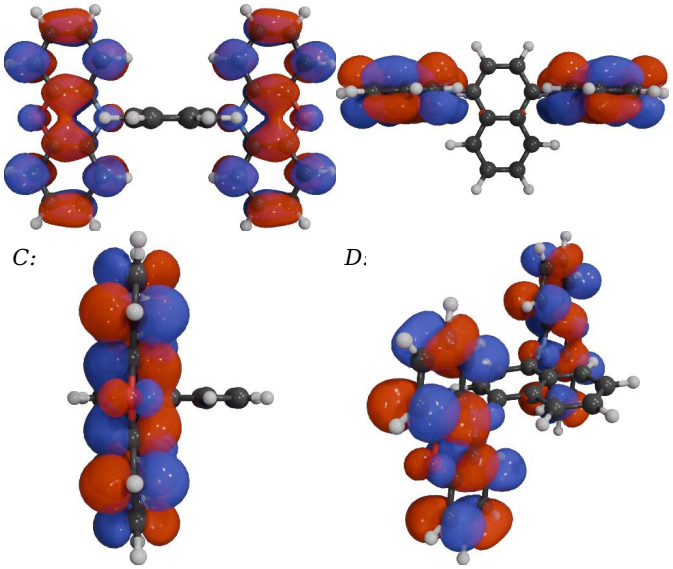


Figure 19: *Orbital density plots of the LUMO+7, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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 (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 9. 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 22. Finally, **natural transition orbitals (NTOs)** were calculated for each excited state and are shown in figures 23-42.

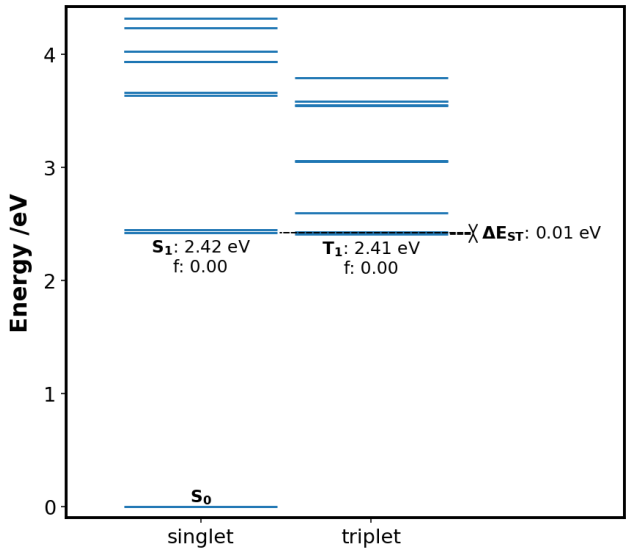


Figure 21: *Graph of the calculated excited states. f: oscillator strength of the relevant ground to excited state transition.*

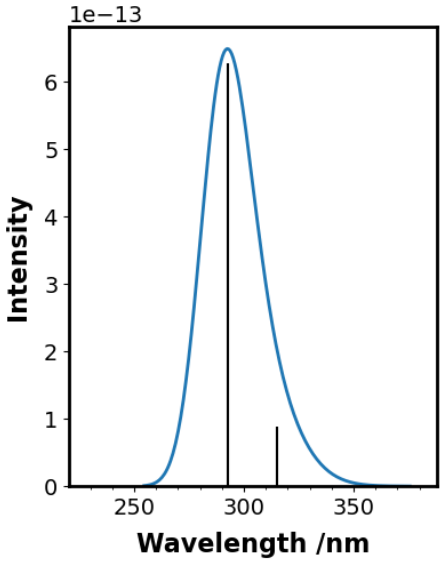


Figure 22: *Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 292 nm.*

Spin-Orbit Coupling

The **spin-orbit coupling** between each singlet state (including the ground state) and each triplet excited state was then calculated using a custom implementation of the PySOC program, the results of which are displayed in table 10. From this analysis, the H_{SO} between the **S_0 and T_1** states was found to be 1.91 cm^{-1}, while the H_{SO} between the **S_1 and T_1** excited states was < 0.01 cm^{-1}. These values correspond to a first-order mixing coefficient ($\lambda = H_{SO}/\Delta E_{ST}$) of < 0.01 and < 0.01 respectively.

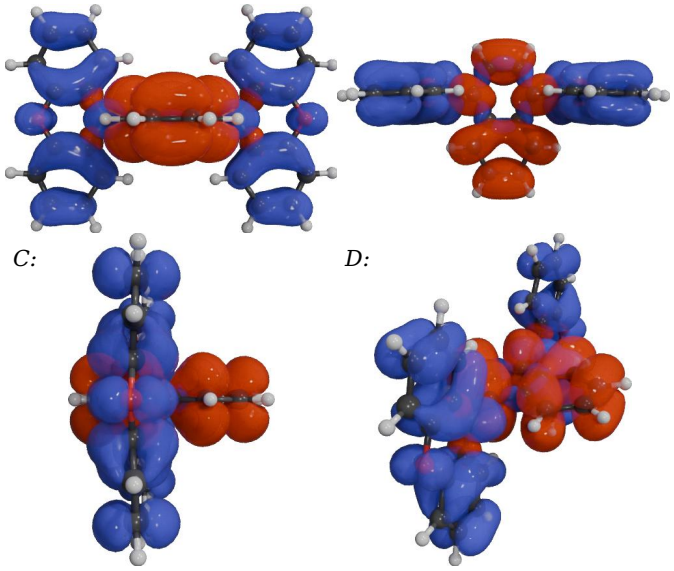


Figure 23: *Density plot of the NTO hole (red) & electron (blue) of the T_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

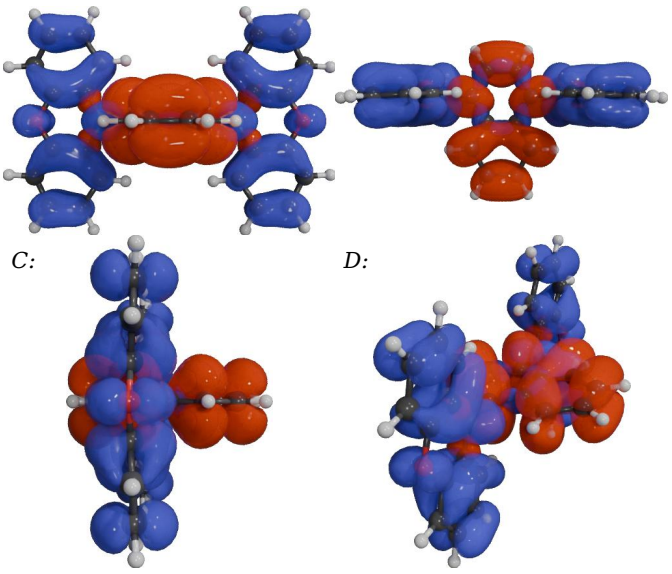


Figure 24: *Density plot of the NTO hole (red) & electron (blue) of the S_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

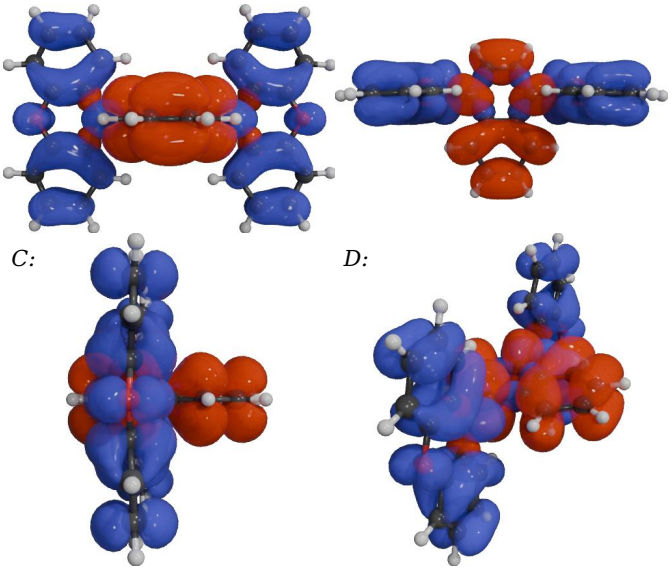


Figure 25: *Density plot of the NTO hole (red) & electron (blue) of the T_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

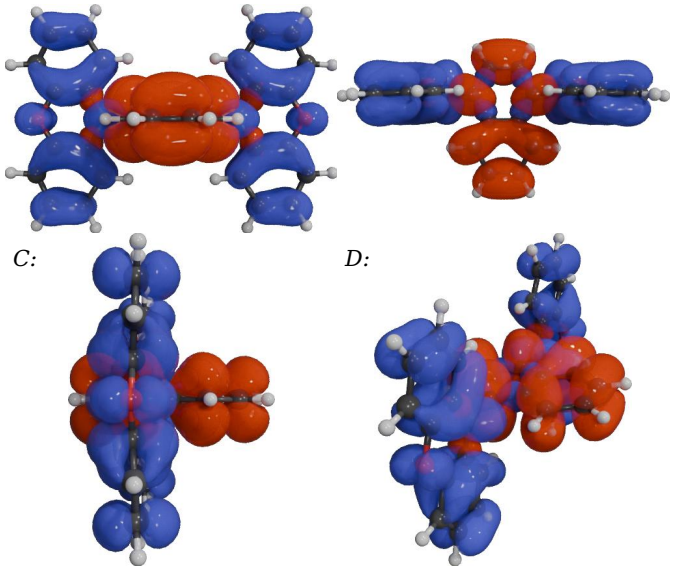


Figure 26: *Density plot of the NTO hole (red) & electron (blue) of the S_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

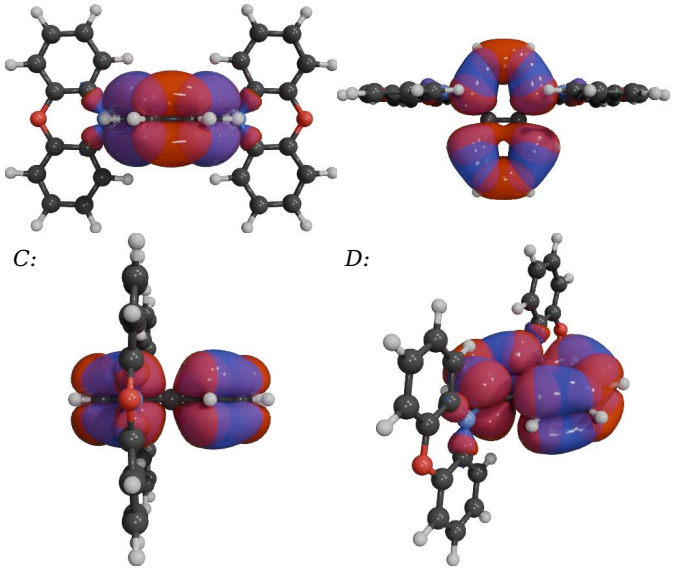


Figure 27: *Density plot of the NTO hole (red) & electron (blue) of the T_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

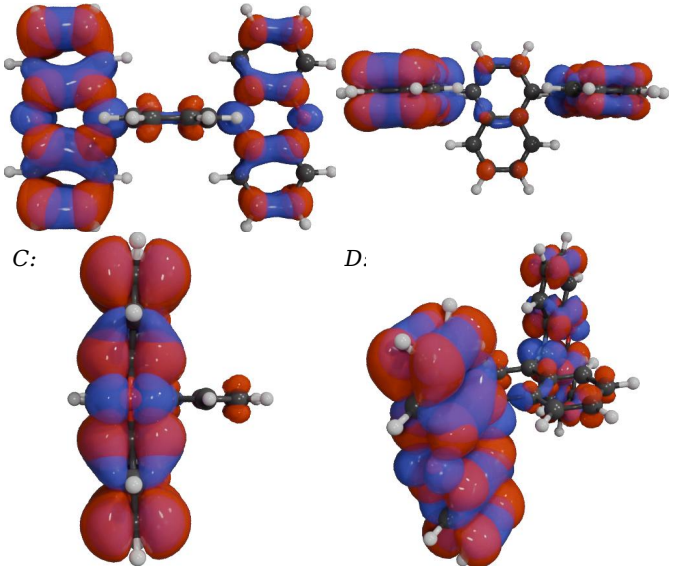


Figure 28: *Density plot of the NTO hole (red) & electron (blue) of the T_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

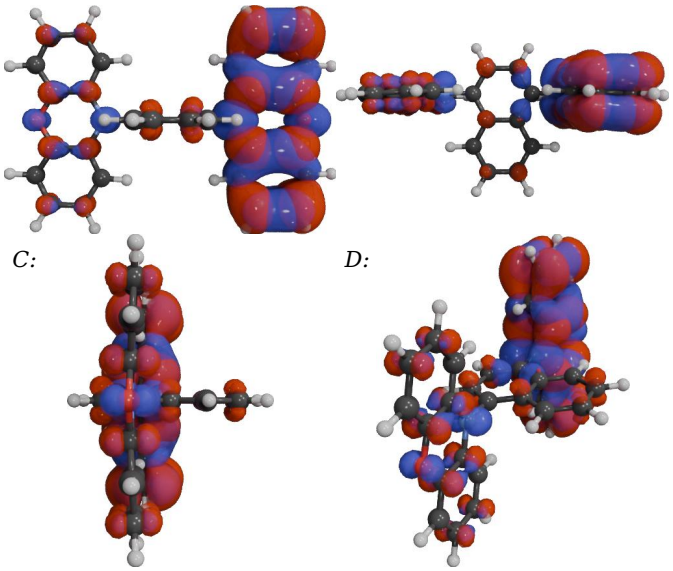


Figure 29: *Density plot of the NTO hole (red) & electron (blue) of the T_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

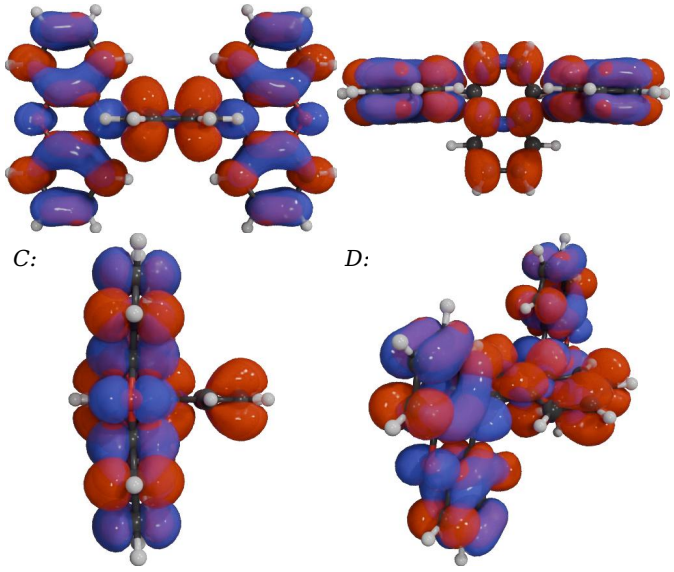


Figure 30: *Density plot of the NTO hole (red) & electron (blue) of the T_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

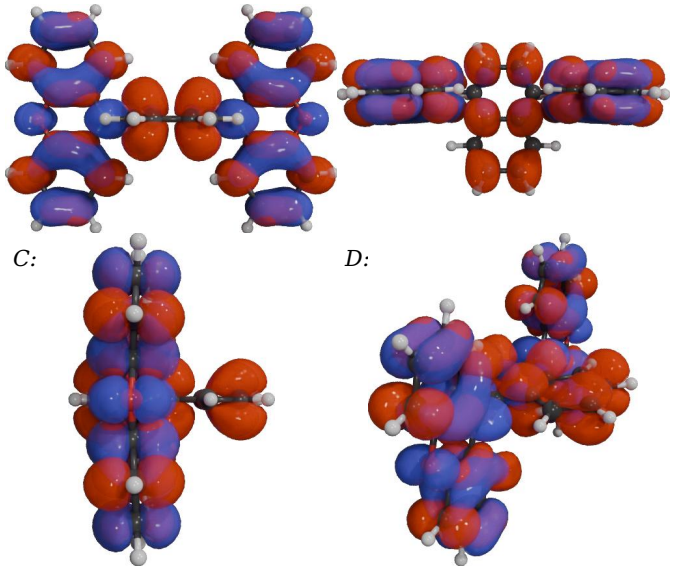


Figure 31: *Density plot of the NTO hole (red) & electron (blue) of the T_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

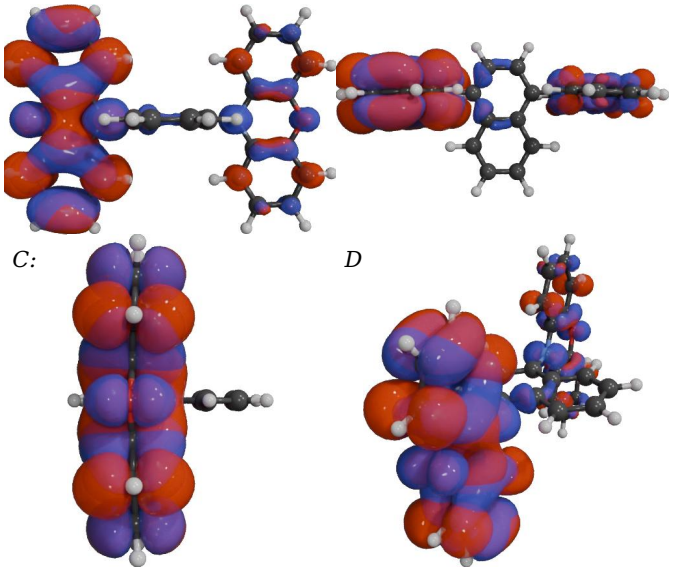


Figure 32: *Density plot of the NTO hole (red) & electron (blue) of the T_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

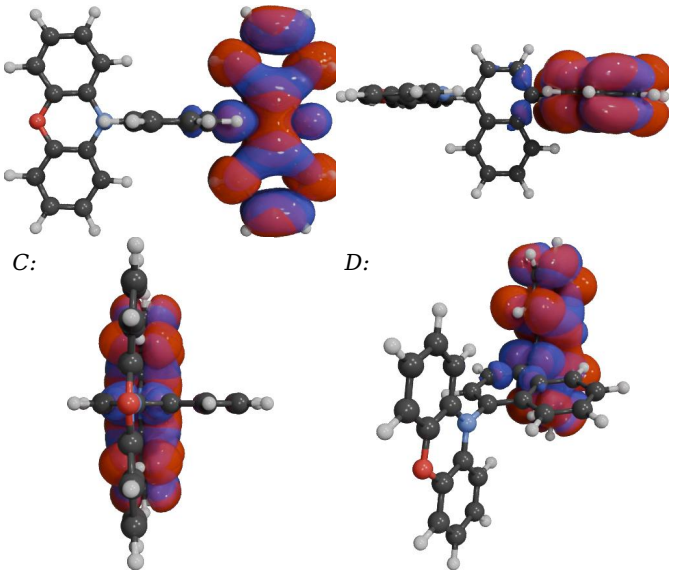


Figure 33: *Density plot of the NTO hole (red) & electron (blue) of the T_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

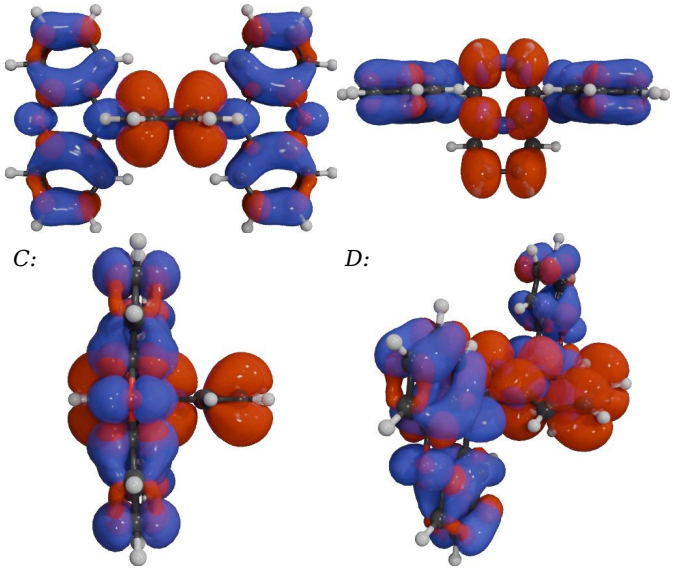


Figure 34: *Density plot of the NTO hole (red) & electron (blue) of the S_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

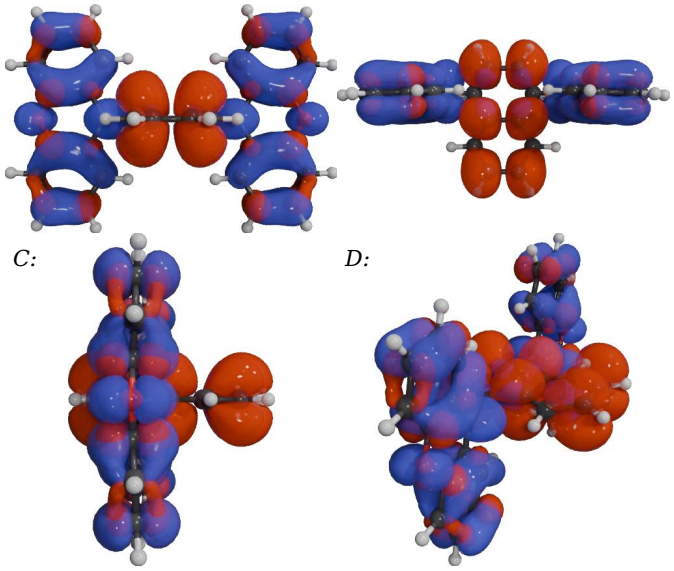


Figure 35: *Density plot of the NTO hole (red) & electron (blue) of the S_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

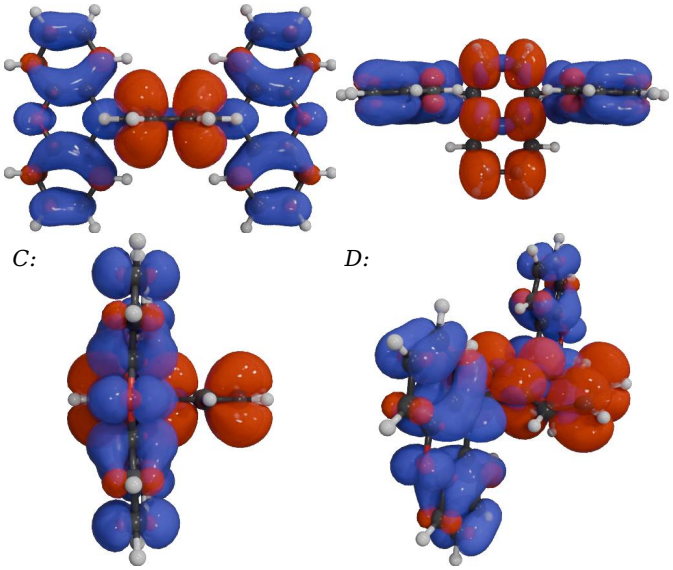


Figure 36: *Density plot of the NTO hole (red) & electron (blue) of the T_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

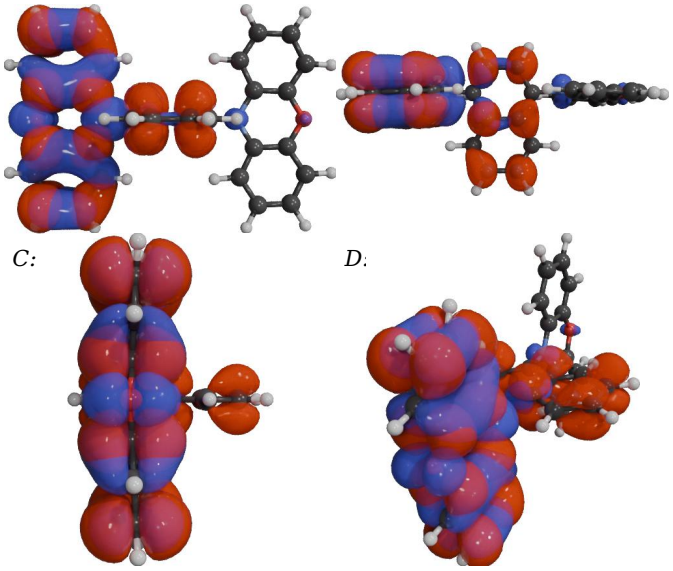


Figure 37: *Density plot of the NTO hole (red) & electron (blue) of the S_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

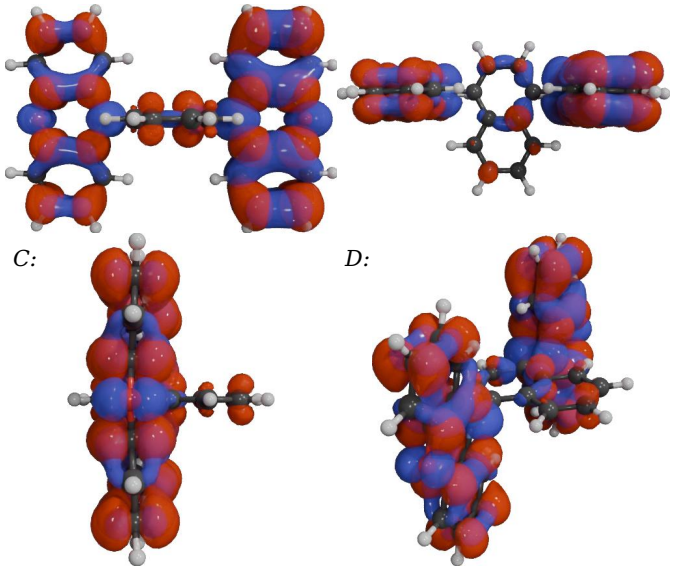


Figure 38: *Density plot of the NTO hole (red) & electron (blue) of the S_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

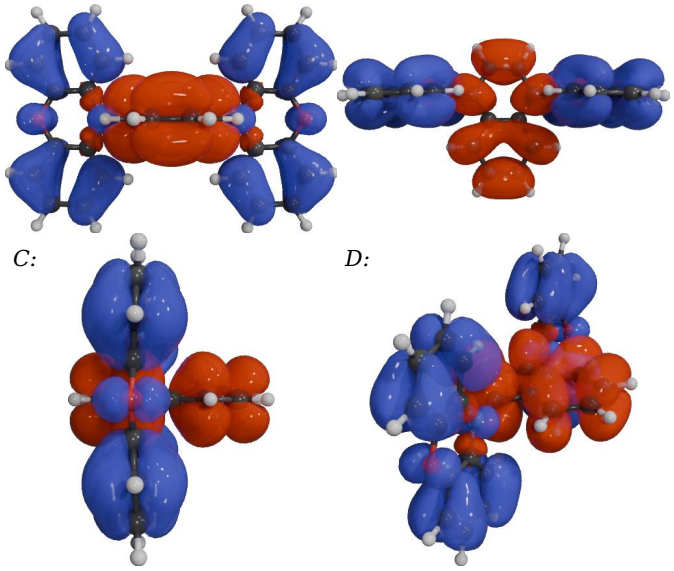


Figure 39: *Density plot of the NTO hole (red) & electron (blue) of the S_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

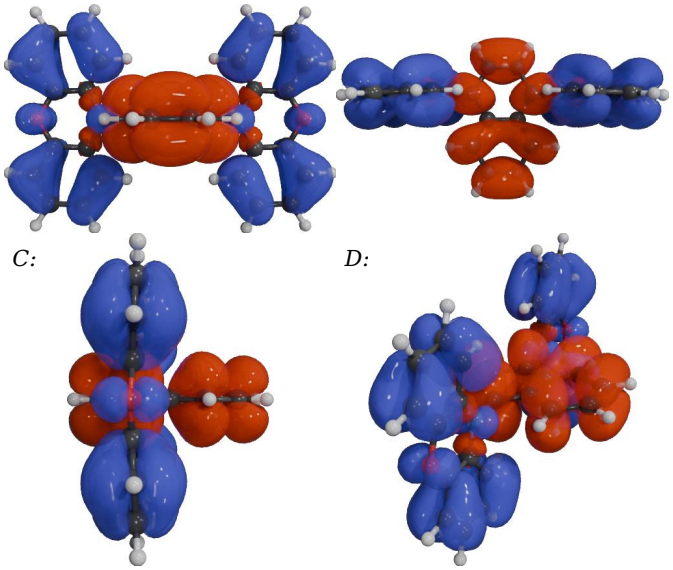


Figure 40: *Density plot of the NTO hole (red) & electron (blue) of the S_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

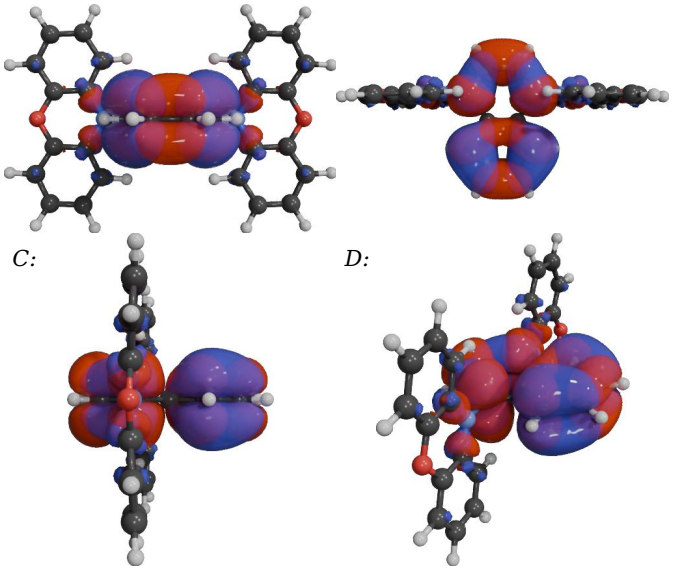


Figure 41: *Density plot of the NTO hole (red) & electron (blue) of the S_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

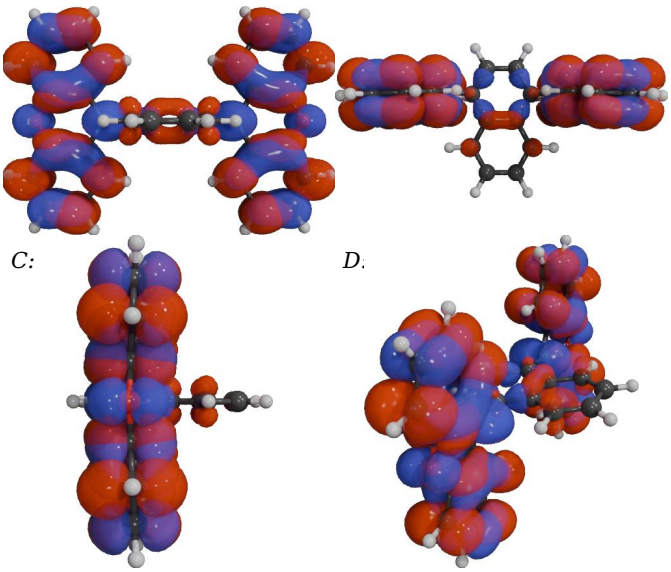


Figure 42: *Density plot of the NTO hole (red) & electron (blue) of the S_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Tables Of Results

Atom Coordinates

Table 11: *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	-0.6924010	-0.0000110	3.3126330
2	C	C_2	-1.3815310	-0.0000110	2.1009330
3	C	C_3	-0.7089510	-0.0000010	0.8561330
4	C	C_3	0.7089490	-0.0000010	0.8561230
5	C	C_2	1.3815390	-0.0000110	2.1009330
6	C	C_1	0.6924090	-0.0000110	3.3126330
7	H	H_1	-1.2418610	-0.0000210	4.2498030
8	H	H_2	-2.4696610	-0.0000100	2.1362830
9	C	C_4	-1.4025510	-0.0000010	-0.3888770
10	C	C_4	1.4025490	-0.0000010	-0.3888870
11	H	H_2	2.4696590	-0.0000110	2.1362730
12	H	H_1	1.2418790	-0.0000210	4.2497930
13	C	C_5	0.6946890	0.0000090	-1.6018970
14	C	C_5	-0.6946910	0.0000090	-1.6018970
15	H	H_5	1.2365790	0.0000090	-2.5447970
16	H	H_5	-1.2365910	0.0000090	-2.5447970
17	C	C_6	3.5807400	1.2260990	-0.3871570
18	C	C_6	3.5807390	-1.2260910	-0.3871470
19	C	C_7	2.9650900	2.4897190	-0.3634070
20	C	C_8	4.9830400	1.1776280	-0.3304070
21	C	C_8	4.9830390	-1.1776220	-0.3304070
22	C	C_7	2.9650890	-2.4897110	-0.3633970
23	C	C_9	3.7255000	3.6600990	-0.2728170
24	H	H_7	1.8833700	2.5843990	-0.4024870
25	C	C_{10}	5.7445300	2.3474680	-0.2461770
26	C	C_{10}	5.7445290	-2.3474620	-0.2461670
27	H	H_7	1.8833690	-2.5844010	-0.4024770
28	C	C_9	3.7254990	-3.6601010	-0.2727970
29	C	C_{11}	5.1145000	3.5890180	-0.2126670
30	H	H_9	3.2280700	4.6264190	-0.2436970
31	H	H_{10}	6.8282000	2.2861480	-0.1973170
32	C	C_{11}	5.1144990	-3.5890220	-0.2126570
33	H	H_{10}	6.8281990	-2.2861520	-0.1973070
34	H	H_9	3.2280690	-4.6264210	-0.2436770
35	H	H_{11}	5.7050300	4.4981780	-0.1365470
36	H	H_{11}	5.7050290	-4.4981720	-0.1365270
37	C	C_6	-3.5807400	1.2261000	-0.3871370
38	C	C_6	-3.5807410	-1.2260900	-0.3871570
39	C	C_7	-2.9650900	2.4897200	-0.3633870
40	C	C_8	-4.9830500	1.1776200	-0.3303770
41	C	C_8	-4.9830410	-1.1776200	-0.3303970
42	C	C_7	-2.9650910	-2.4897100	-0.3634270
43	C	C_9	-3.7255000	3.6601000	-0.2727770
44	H	H_7	-1.8833700	2.5844000	-0.4024670
45	C	C_{10}	-5.7445300	2.3474700	-0.2461370
46	C	C_{10}	-5.7445310	-2.3474700	-0.2461770
47	H	H_7	-1.8833710	-2.5844000	-0.4025070
48	C	C_9	-3.7254910	-3.6601000	-0.2728370
49	C	C_{11}	-5.1145000	3.5890200	-0.2126270
50	H	H_9	-3.2280700	4.6264200	-0.2436570
51	H	H_{10}	-6.8282000	2.2861500	-0.1972770
52	C	C_{11}	-5.1145010	-3.5890200	-0.2126870
53	H	H_{10}	-6.8282010	-2.2861500	-0.1973070
54	H	H_9	-3.2280610	-4.6264200	-0.2437370
55	H	H_{11}	-5.7050300	4.4981700	-0.1364870
56	H	H_{11}	-5.7050310	-4.4981800	-0.1365670
57	N	N_{12}	-2.8391610	-0.0000000	-0.4426470
58	O	O_{13}	5.6952190	-0.0000020	-0.3381670
59	O	O_{13}	-5.6952210	0.0000000	-0.3381470
60	N	N_{12}	2.8391590	-0.0000010	-0.4426570

Molecular Orbitals

Table 12: *Energies of the calculated molecular orbitals.*

Level	Label	Symmetry	Energy /eV
144	LUMO+15	A	2.8866
143	LUMO+14	A	2.8596
142	LUMO+13	A	2.4406
141	LUMO+12	A	2.2776
140	LUMO+11	A	2.1590
139	LUMO+10	A	1.1516
138	LUMO+9	A	1.1486
137	LUMO+8	A	0.5034
136	LUMO+7	A	0.1758
135	LUMO+6	A	0.1682
134	LUMO+5	A	0.1548
133	LUMO+4	A	0.1045
132	LUMO+3	A	-0.1284
131	LUMO+2	A	-0.2057
130	LUMO+1	A	-0.6063
129	**LUMO**	**A**	**-1.7453**
128	**HOMO**	**A**	**-5.0444**
127	HOMO-1	A	-5.0681
126	HOMO-2	A	-6.4173
125	HOMO-3	A	-6.4951
124	HOMO-4	A	-6.4951
123	HOMO-5	A	-7.2230
122	HOMO-6	A	-7.2744
121	HOMO-7	A	-7.2867
120	HOMO-8	A	-7.3136
119	HOMO-9	A	-7.5833
118	HOMO-10	A	-8.3419
117	HOMO-11	A	-8.9599
116	HOMO-12	A	-8.9950
115	HOMO-13	A	-9.3346
114	HOMO-14	A	-9.4448
113	HOMO-15	A	-9.6184

Excited States

Table 9: *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	2.4097	514.52	Green (0.04, 0.81)	0.0000	HOMO → LUMO (0.99)
2	S_1	Singlet-A	2.4224	511.82	Green (0.02, 0.78)	0.0000	HOMO → LUMO (0.99)
3	T_2	Triplet-A	2.4313	509.95	Green (0.01, 0.75)	0.0000	HOMO-1 → LUMO (0.99)
4	S_2	Singlet-A	2.4448	507.13	Green (0.01, 0.70)	0.0000	HOMO-1 → LUMO (0.99)
5	T_3	Triplet-A	2.5977	477.28	Cyan (0.10, 0.11)	0.0000	HOMO-2 → LUMO (0.93) HOMO-10 → LUMO+8 (0.03)
6	T_4	Triplet-A	3.0541	405.96	Violet (0.17, 0.00)	0.0000	HOMO-1 → LUMO+2 (0.42) HOMO → LUMO+3 (0.31) HOMO → LUMO+1 (0.17)
7	T_5	Triplet-A	3.0553	405.80	Violet (0.17, 0.00)	0.0000	HOMO → LUMO+2 (0.43) HOMO-1 → LUMO+3 (0.30) HOMO-1 → LUMO+1 (0.16)
8	T_6	Triplet-A	3.5461	349.64	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)
9	T_7	Triplet-A	3.5534	348.92	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)
10	T_8	Triplet-A	3.5822	346.11	Ultraviolet (0.00, 0.00)	0.0000	HOMO → LUMO+5 (0.49) HOMO-1 → LUMO+7 (0.46)
11	T_9	Triplet-A	3.5825	346.08	Ultraviolet (0.00, 0.00)	0.0000	HOMO → LUMO+7 (0.47) HOMO-1 → LUMO+5 (0.47)
12	S_3	Singlet-A	3.6387	340.74	Ultraviolet (0.00, 0.00)	0.0000	HOMO → LUMO+1 (0.94) HOMO-1 → LUMO+2 (0.05)
13	S_4	Singlet-A	3.6649	338.30	Ultraviolet (0.00, 0.00)	0.0000	HOMO-1 → LUMO+1 (0.92) HOMO → LUMO+2 (0.06)
14	T_{10}	Triplet-A	3.7950	326.70	Ultraviolet (0.00, 0.00)	0.0000	HOMO → LUMO+1 (0.46) HOMO → LUMO+6 (0.26) HOMO-1 → LUMO+4 (0.19) HOMO-1 → LUMO+2 (0.04)
15	S_5	Singlet-A	3.9348	315.10	Ultraviolet (0.00, 0.00)	0.0000	HOMO-1 → LUMO+2 (0.48) HOMO → LUMO+3 (0.44) HOMO → LUMO+1 (0.04)
16	S_6	Singlet-A	3.9364	314.97	Ultraviolet (0.00, 0.00)	0.0442	HOMO → LUMO+2 (0.51) HOMO-1 → LUMO+3 (0.39) HOMO-1 → LUMO+1 (0.05)
17	S_7	Singlet-A	4.0246	308.07	Ultraviolet (0.00, 0.00)	0.0000	HOMO-4 → LUMO (0.99)
18	S_8	Singlet-A	4.0260	307.96	Ultraviolet (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.99)
19	S_9	Singlet-A	4.2336	292.86	Ultraviolet (0.00, 0.00)	0.2708	HOMO-2 → LUMO (0.82) HOMO → LUMO+5 (0.05) HOMO-1 → LUMO+7 (0.04)
20	S_{10}	Singlet-A	4.3191	287.06	Ultraviolet (0.00, 0.00)	0.0000	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)

Transition Dipole Moments

Table 13: *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, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000

S_1	0.00, 0.03, 0.00	0.03	90.00	0.00	0.26, 0.00, 0.00	0.26	0.00	0.00	2.54e-20	2.43e-21	90.00	-0.00	-0.000
T_2	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
S_2	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, -0.01	0.01	89.21	89.21	0.00e+00	1.34e-22	90.00	0.00	0.000
T_3	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
T_4	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
T_5	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
T_6	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
T_7	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
T_8	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
T_9	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
S_3	0.00, 0.00, 0.00	0.00	0.00	0.00	-0.00, 0.00, -1.53	1.53	90.00	90.00	0.00e+00	1.42e-20	90.00	0.00	0.000
S_4	0.00, 0.04, 0.00	0.04	90.00	0.00	0.07, 0.00, -0.00	0.07	0.93	0.93	3.61e-20	6.31e-22	90.00	0.00	0.000
T_{10}	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00e+00	0.00e+00	90.00	0.00	0.000
S_5	0.00, 0.03, 0.00	0.03	90.00	0.00	-0.00, 0.00, -2.07	2.07	89.94	89.94	2.90e-20	1.92e-20	90.00	0.00	0.000
S_6	0.00, -1.72, 0.00	1.72	90.00	0.00	0.13, 0.00, -0.04	0.14	14.68	14.68	1.72e-18	1.28e-21	90.00	0.00	0.000
S_7	0.00, -0.00, 0.00	< 0.01	90.00	0.00	-0.00, 0.00, -0.04	0.04	89.33	89.33	2.54e-22	3.97e-22	90.00	0.00	0.000
S_8	0.00, 0.04, 0.00	0.04	90.00	0.00	0.12, 0.00, -0.00	0.12	0.05	0.05	3.89e-20	1.10e-21	90.00	0.00	0.000
S_9	-4.11, 0.00, 0.00	4.11	0.00	0.00	0.00, -0.10, 0.00	0.10	90.00	0.00	4.11e-18	9.31e-22	90.00	0.00	0.000
S_{10}	0.00, -0.00, 0.00	< 0.01	90.00	0.00	0.00, 0.00, -0.87	0.87	90.00	90.00	2.54e-21	8.10e-21	90.00	0.00	0.000

Spin-Orbit Coupling

Table 10: *Calculated SOC values between singlet and triplet states. [a]: SOC between the singlet state and triplet sub-state with quantum number +1. [b]: The same with the triplet sub-state with quantum number 0. [c]: The same with the triplet sub-state with quantum number +1. [d]: Root sum square of the SOC between the singlet state and all three triplet sub-states. [e]: The first order mixing coefficient ($H_{SO}/\Delta E_{ST}$) between the singlet and triplet state.*

Singlet State	Triplet State	H_{SO} +1[a] /cm^{-1}	H_{SO} 0[b] /cm^{-1}	H_{SO} -1[c] /cm^{-1}	H_{SO} Root Sum Square[d] /cm^{-1}	H_{SO} Root Sum Square[d] /eV	λ[e]
S_0	T_1	1.3481	0.0004	1.3481	1.9065	0.0002	0.0001
S_0	T_2	0.0008	0.1209	0.0008	0.1209	< 0.0001	< 0.0001
S_0	T_3	0.2110	0.0002	0.2110	0.2984	< 0.0001	< 0.0001
S_0	T_4	0.0036	1.8423	0.0036	1.8423	0.0002	0.0001
S_0	T_5	0.0860	0.0543	0.0860	0.1332	< 0.0001	< 0.0001
S_0	T_6	0.0003	2.3258	0.0003	2.3258	0.0003	0.0001
S_0	T_7	0.3056	0.0023	0.3056	0.4322	0.0001	< 0.0001
S_0	T_8	0.3225	0.0002	0.3225	0.4561	0.0001	< 0.0001
S_0	T_9	0.0053	0.0001	0.0053	0.0075	< 0.0001	< 0.0001
S_0	T_{10}	0.0003	1.8181	0.0003	1.8181	0.0002	0.0001
S_1	T_1	< 0.0001	< 0.0001	< 0.0001	< 0.0001	< 0.0001	< 0.0001
S_1	T_2	0.0363	0.0000	0.0363	0.0514	< 0.0001	0.0007
S_1	T_3	0.0006	0.6191	0.0006	0.6191	0.0001	0.0004
S_1	T_4	0.7941	0.0000	0.7941	1.1231	0.0001	0.0002
S_1	T_5	0.0225	< 0.0001	0.0225	0.0317	< 0.0001	< 0.0001
S_1	T_6	0.4489	< 0.0001	0.4489	0.6348	0.0001	0.0001
S_1	T_7	0.0001	0.0000	0.0001	0.0002	< 0.0001	< 0.0001
S_1	T_8	0.0052	0.0767	0.0052	0.0771	< 0.0001	< 0.0001
S_1	T_9	0.2151	0.0017	0.2151	0.3042	< 0.0001	< 0.0001
S_1	T_{10}	0.3520	0.0000	0.3520	0.4978	0.0001	< 0.0001
S_2	T_1	0.0221	0.0000	0.0221	0.0312	< 0.0001	0.0001
S_2	T_2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
S_2	T_3	0.7458	0.0005	0.7458	1.0547	0.0001	0.0009
S_2	T_4	0.0219	< 0.0001	0.0219	0.0310	< 0.0001	< 0.0001
S_2	T_5	0.7804	0.0000	0.7804	1.1037	0.0001	0.0002
S_2	T_6	0.0001	0.0000	0.0001	0.0002	< 0.0001	< 0.0001
S_2	T_7	0.4440	< 0.0001	0.4440	0.6279	0.0001	0.0001
S_2	T_8	0.2090	0.0017	0.2090	0.2955	< 0.0001	< 0.0001

S_2	T_9	0.0050	0.0767	0.0050	0.0770	< 0.0001	< 0.0001
S_2	T_{10}	0.0001	0.0000	0.0001	0.0001	< 0.0001	< 0.0001
S_3	T_1	0.9506	0.0000	0.9506	1.3444	0.0002	0.0001
S_3	T_2	< 0.0001	0.0000	< 0.0001	< 0.0001	< 0.0001	< 0.0001
S_3	T_3	0.0021	< 0.0001	0.0021	0.0030	< 0.0001	< 0.0001
S_3	T_4	0.0009	< 0.0001	0.0009	0.0012	< 0.0001	< 0.0001
S_3	T_5	0.0169	0.0000	0.0169	0.0239	< 0.0001	< 0.0001
S_3	T_6	0.0001	< 0.0001	0.0001	0.0001	< 0.0001	< 0.0001
S_3	T_7	0.0094	0.0001	0.0094	0.0134	< 0.0001	< 0.0001
S_3	T_8	0.0435	0.0050	0.0435	0.0617	< 0.0001	0.0001
S_3	T_9	0.0009	0.2132	0.0009	0.2132	< 0.0001	0.0005
S_3	T_{10}	0.0001	0.0000	0.0001	0.0001	< 0.0001	< 0.0001
S_4	T_1	< 0.0001	< 0.0001	< 0.0001	0.0001	< 0.0001	< 0.0001
S_4	T_2	0.9392	< 0.0001	0.9392	1.3282	0.0002	0.0001
S_4	T_3	< 0.0001	0.0372	< 0.0001	0.0372	< 0.0001	< 0.0001
S_4	T_4	0.0094	0.0000	0.0094	0.0133	< 0.0001	< 0.0001
S_4	T_5	0.0004	0.0000	0.0004	0.0006	< 0.0001	< 0.0001
S_4	T_6	0.0281	< 0.0001	0.0281	0.0398	< 0.0001	< 0.0001
S_4	T_7	< 0.0001	< 0.0001	< 0.0001	0.0001	< 0.0001	< 0.0001
S_4	T_8	0.0008	0.1817	0.0008	0.1817	< 0.0001	0.0003
S_4	T_9	0.0421	0.0043	0.0421	0.0597	< 0.0001	0.0001
S_4	T_{10}	0.0139	0.0000	0.0139	0.0196	< 0.0001	< 0.0001
S_5	T_1	0.3485	0.0000	0.3485	0.4928	0.0001	< 0.0001
S_5	T_2	0.0047	< 0.0001	0.0047	0.0066	< 0.0001	< 0.0001
S_5	T_3	0.0132	0.0006	0.0132	0.0187	< 0.0001	< 0.0001
S_5	T_4	0.0020	0.0000	0.0020	0.0028	< 0.0001	< 0.0001
S_5	T_5	0.0352	0.0000	0.0352	0.0497	< 0.0001	< 0.0001
S_5	T_6	0.0003	< 0.0001	0.0003	0.0005	< 0.0001	< 0.0001
S_5	T_7	0.0229	0.0001	0.0229	0.0324	< 0.0001	< 0.0001
S_5	T_8	0.0192	0.0262	0.0192	0.0377	< 0.0001	< 0.0001
S_5	T_9	0.0003	0.6586	0.0003	0.6586	0.0001	0.0002
S_5	T_{10}	0.0006	0.0000	0.0006	0.0009	< 0.0001	< 0.0001
S_6	T_1	0.0056	< 0.0001	0.0056	0.0079	< 0.0001	< 0.0001
S_6	T_2	0.2940	0.0000	0.2940	0.4158	0.0001	< 0.0001
S_6	T_3	0.0002	0.0430	0.0002	0.0430	< 0.0001	< 0.0001
S_6	T_4	0.0461	< 0.0001	0.0461	0.0651	< 0.0001	< 0.0001
S_6	T_5	0.0023	0.0000	0.0023	0.0033	< 0.0001	< 0.0001
S_6	T_6	0.0158	0.0001	0.0158	0.0224	< 0.0001	< 0.0001
S_6	T_7	0.0005	< 0.0001	0.0005	0.0008	< 0.0001	< 0.0001
S_6	T_8	0.0003	0.6602	0.0003	0.6602	0.0001	0.0002
S_6	T_9	0.0160	0.0262	0.0160	0.0347	< 0.0001	< 0.0001
S_6	T_{10}	0.0274	< 0.0001	0.0274	0.0387	< 0.0001	< 0.0001
S_7	T_1	0.0643	< 0.0001	0.0643	0.0909	< 0.0001	< 0.0001
S_7	T_2	0.0002	0.0000	0.0002	0.0003	< 0.0001	< 0.0001
S_7	T_3	0.2642	0.0006	0.2642	0.3736	< 0.0001	< 0.0001
S_7	T_4	0.0021	0.0000	0.0021	0.0030	< 0.0001	< 0.0001
S_7	T_5	0.0779	0.0000	0.0779	0.1101	< 0.0001	< 0.0001
S_7	T_6	0.0002	0.0000	0.0002	0.0003	< 0.0001	< 0.0001
S_7	T_7	0.0874	0.0000	0.0874	0.1236	< 0.0001	< 0.0001
S_7	T_8	0.0588	0.0000	0.0588	0.0831	< 0.0001	< 0.0001
S_7	T_9	0.0018	0.0005	0.0018	0.0025	< 0.0001	< 0.0001
S_7	T_{10}	0.0001	0.0000	0.0001	0.0002	< 0.0001	< 0.0001
S_8	T_1	0.0003	< 0.0001	0.0003	0.0004	< 0.0001	< 0.0001

S_8	T_2	0.0230	< 0.0001	0.0230	0.0325	< 0.0001	< 0.0001
S_8	T_3	0.0009	0.1714	0.0009	0.1714	< 0.0001	< 0.0001
S_8	T_4	0.0780	0.0000	0.0780	0.1104	< 0.0001	< 0.0001
S_8	T_5	0.0021	0.0000	0.0021	0.0030	< 0.0001	< 0.0001
S_8	T_6	0.0856	0.0000	0.0856	0.1211	< 0.0001	< 0.0001
S_8	T_7	0.0002	0.0000	0.0002	0.0003	< 0.0001	< 0.0001
S_8	T_8	0.0017	0.0005	0.0017	0.0024	< 0.0001	< 0.0001
S_8	T_9	0.0593	< 0.0001	0.0593	0.0839	< 0.0001	< 0.0001
S_8	T_{10}	0.0813	0.0000	0.0813	0.1150	< 0.0001	0.0001
S_9	T_1	0.0008	0.6963	0.0008	0.6963	0.0001	< 0.0001
S_9	T_2	0.8543	0.0005	0.8543	1.2082	0.0001	0.0001
S_9	T_3	< 0.0001	< 0.0001	< 0.0001	< 0.0001	< 0.0001	< 0.0001
S_9	T_4	0.0149	0.0043	0.0149	0.0216	< 0.0001	< 0.0001
S_9	T_5	0.0003	0.1547	0.0003	0.1547	< 0.0001	< 0.0001
S_9	T_6	0.0253	0.0001	0.0253	0.0357	< 0.0001	< 0.0001
S_9	T_7	< 0.0001	0.0613	< 0.0001	0.0613	< 0.0001	< 0.0001
S_9	T_8	0.0004	< 0.0001	0.0004	0.0006	< 0.0001	< 0.0001
S_9	T_9	0.0233	< 0.0001	0.0233	0.0329	< 0.0001	< 0.0001
S_9	T_{10}	0.0543	0.0002	0.0543	0.0768	< 0.0001	< 0.0001
S_{10}	T_1	0.0149	< 0.0001	0.0149	0.0211	< 0.0001	< 0.0001
S_{10}	T_2	0.0001	0.0000	0.0001	0.0001	< 0.0001	< 0.0001
S_{10}	T_3	0.0034	< 0.0001	0.0034	0.0047	< 0.0001	< 0.0001
S_{10}	T_4	0.0025	< 0.0001	0.0025	0.0036	< 0.0001	< 0.0001
S_{10}	T_5	0.0842	< 0.0001	0.0842	0.1190	< 0.0001	< 0.0001
S_{10}	T_6	< 0.0001	< 0.0001	< 0.0001	0.0001	< 0.0001	< 0.0001
S_{10}	T_7	0.0007	< 0.0001	0.0007	0.0009	< 0.0001	< 0.0001
S_{10}	T_8	0.1477	0.0027	0.1477	0.2089	< 0.0001	< 0.0001
S_{10}	T_9	0.0031	0.1160	0.0031	0.1160	< 0.0001	< 0.0001
S_{10}	T_{10}	0.0001	< 0.0001	0.0001	0.0001	< 0.0001	< 0.0001

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