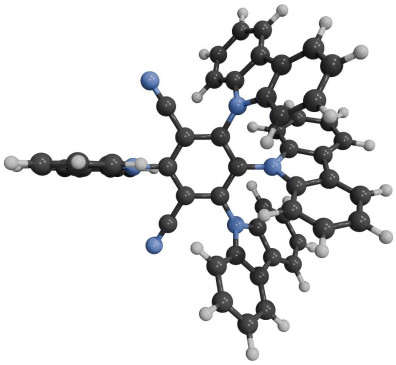
A Report On The Calculation Of The Excited States Of 4CzIPN At The PBE1PBE/def2SVP Level

osl - 28th May 2025



Abstract

The calculation of excited states for the system '4CzIPN' 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/def2SVP level of theory. The total self-consistent field (SCF) energy of the system was found to be -67416.40 eV after 1 step. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -6.26 and -2.71 eV respectively, corresponding to a HOMO-LUMO band gap of 3.55 eV. The permanent dipole moment (PDM) was calculated to be 17.34 D. In total, 20 excited states were calculated with singlet and triplet multiplicity. The most intense absorption peak was calculated to be at 399 nm. The lowest energy singlet and triplet excited states (S_1 and T_1) were calculated to be 2.75 and 2.62 eV (451 and 474 nm) respectively, corresponding to a singlet/triplet splitting energy (ΔE_{ST}) of 0.13 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
28/05/2025 11:42:34 (1 h, 20 m, 5 s)	40 (20 GB)	True (N/A)	Gaussian (2016+C.01)	PBE1PBE/ def2SVP	Water (IEFPCM)	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	-67416.4030 eV
Final energy	-6,504,694 kJ·mol^{-1}

Geometry

Table 3: *Summary of geometry properties.*

Formula	$C_{56}H_{32}N_6$
SMILES	N#Cc1c(-n2c3ccccc3c3ccccc32)c(C#N)c(-n2c3ccccc3c3ccccc32)c(-n2c3ccccc3c3ccccc32)c1-n1c2ccccc2c2ccccc21
Exact mass	788.2688 g·mol^{-1}
Molar mass	788.8935 g·mol^{-1}
Alignment method	Minimal
X extension	14.08 Å
Y extension	13.73 Å
Z extension	8.97 Å
Linearity ratio	0.02
Planarity ratio	0.35

Molecular Orbitals

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

$E_{HOMO,LUMO}$	3.55 eV
E_{HOMO}	-6.26 eV
E_{LUMO}	-2.71 eV

Permanent Dipole Moment

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

Total	17.34 D
X axis angle	0.00 °
XY plane angle	0.00 °

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	3.79 D
$\theta_{\mu,x}$	90.00 °
$\theta_{\mu,xy}$	13.46 °
m[d]	0.36 a.u.
$\theta_{m,x}$	90.00 °
$\theta_{m,xy}$	67.89 °
μ (Gaussian-CGS)	3.79e-18 esu·cm
m (Gaussian-CGS)	3.37e-21 erg·G^{-1}
$\theta_{\mu,m}$	81.35 °
$\cos(\theta_{\mu,m})$	0.15
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}	2.75 eV
λ_{S_1} (colour, CIE)	451 nm (Blue, (0.16, 0.02))
f_{S_1}	0.15
No. calculated triplets	10
E_{T_1}	2.62 eV
λ_{T_1} (colour, CIE)	474 nm (Cyan, (0.11, 0.08))
f_{T_1}	0.00
ΔE_{ST}	0.13 eV
Simulated Absorption Peaks	399 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.*

$\langle S_0\|H_{SO}\|T_1\rangle$	0.64 cm^{-1}
$\langle S_0\|\lambda\|T_1\rangle$	0.00
$\langle S_1\|H_{SO}\|T_1\rangle$	0.17 cm^{-1}
$\langle S_1\|\lambda\|T_1\rangle$	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 **def2SVP** basis set. It was completed on the **28th May 2025** after a total duration of **1 h, 20 m, 5 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 -67416.40 eV, corresponding to -6,504,694 $KJmol^{-1}$. A plot of the total SCF electron density is shown in figure 1.

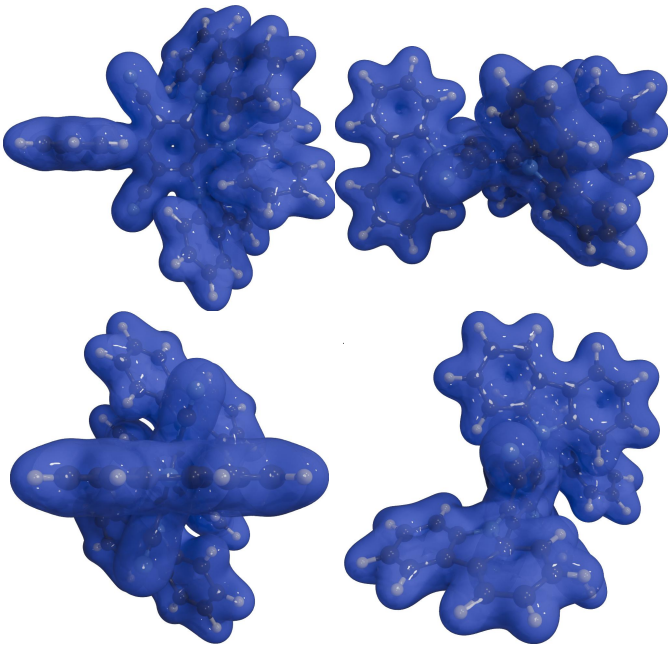


Figure 1: *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Geometry

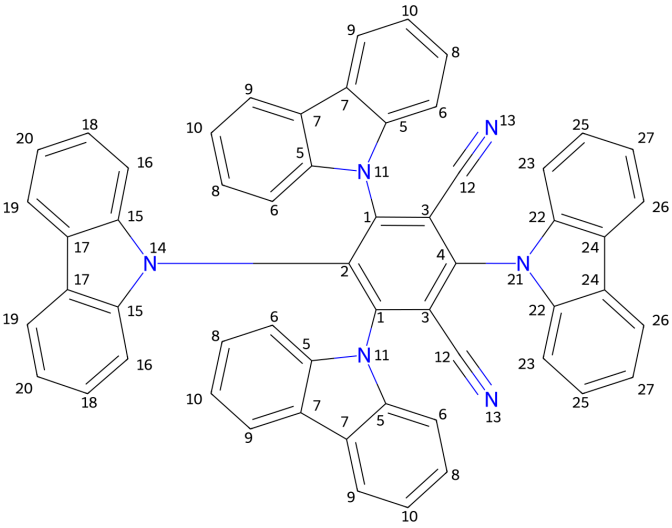


Figure 2: *Labelled structure of 4CzIPN.*

The **empirical formula** of the studied system was $C_{56}H_{32}N_6$, corresponding to a **molecular mass** of 788.89 $gmol^{-1}$ and an **exact mass**, considering only specific atomic isotopes, of 788.27 $gmol^{-1}$. 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 14.08, 13.73 and 8.97 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 0.02 and 0.35 respectively.

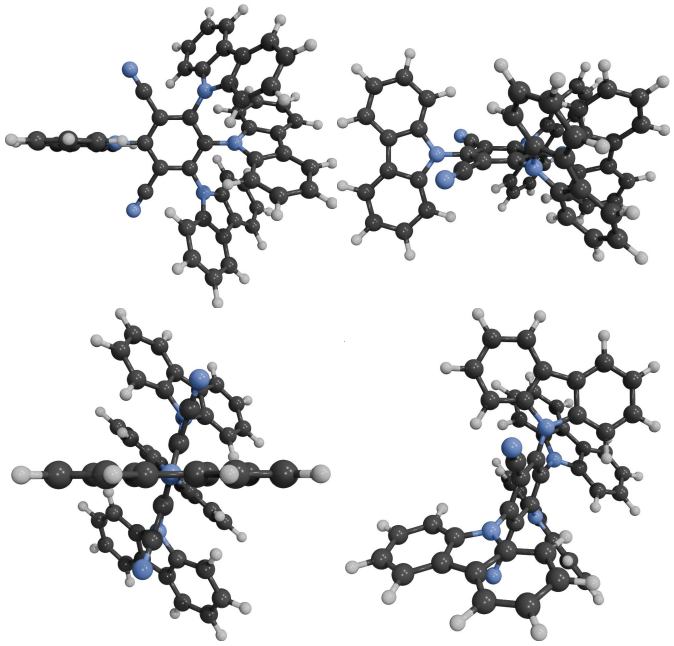


Figure 3: *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Permanent Dipole Moment

The calculated **permanent dipole moment** was 17.34 D, with a vector (x,y,z) of 17.34, 0.00, 0.00 D. The angle between the dipole moment vector and the x-axis was 0.00 °, while the angle between the dipole moment and the xy-plane was 0.00 °. A plot of the permanent dipole moment is shown in figure 4.

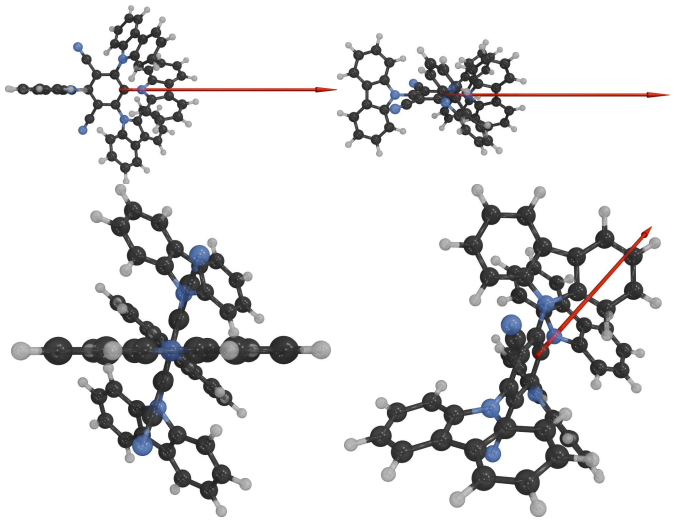


Figure 4: *The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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 3.79 D and 0.36 au respectively. The corresponding vector components (x,y,z) were μ = 0.00, -3.68, -0.88 D and m = 0.00, 0.14, -0.34 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 $\theta_{m,x}$ = 90.00 °, while the angle between each dipole moment and the xy-plane was $\theta_{\mu,xy}$ = 13.46 ° and $\theta_{m,xy}$ = 67.89 °. 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 = 3.79e-18 esu·cm and m = 3.37e-21 erg·G^{-1}, while the **angle between the two dipole moments** was $\theta_{\mu,m}$ = 81.35 °. Correspondingly, the cosine of the angle was $\cos(\theta_{\mu,m})$ = 0.15, 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.

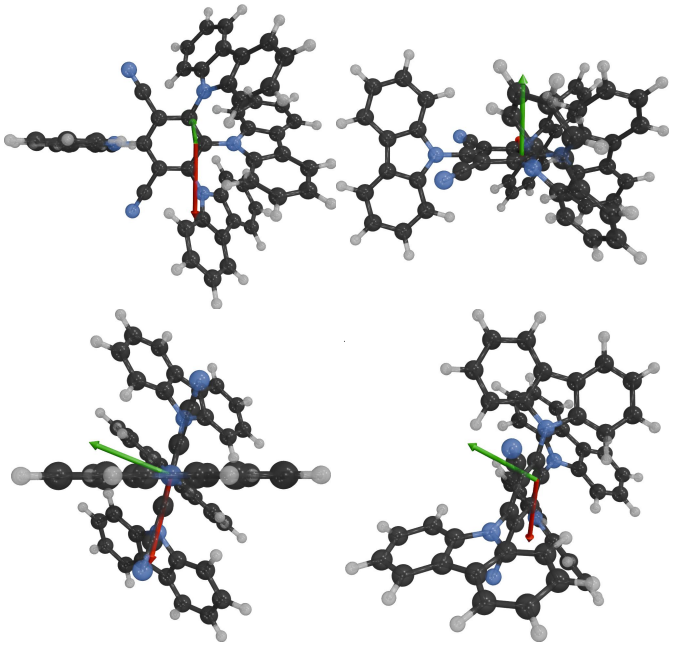


Figure 5: *The electric (red arrow) and magnetic (green arrow) transition (S_1) dipole moment plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D = 0.1 au. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Molecular Orbitals

In total, 1090 doubly occupied molecular orbitals were calculated, divided into 205 occupied orbitals and 885 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO and LUMO** were -6.26 and -2.71 eV respectively, corresponding to a **HOMO-LUMO band gap** of 3.55 eV (figure 16). Plots of the orbital density for the HOMO-6, HOMO-5, HOMO-4, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO and LUMO+1 are shown in figures 6-13 and 15 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 14.

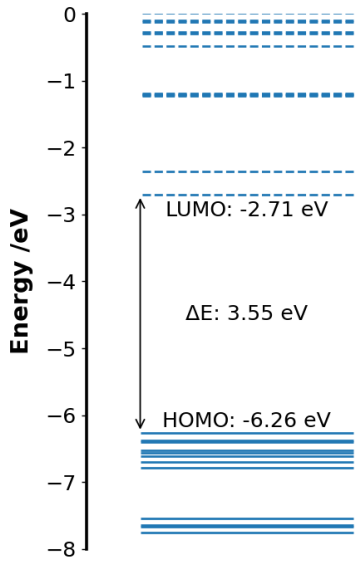


Figure 16: *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

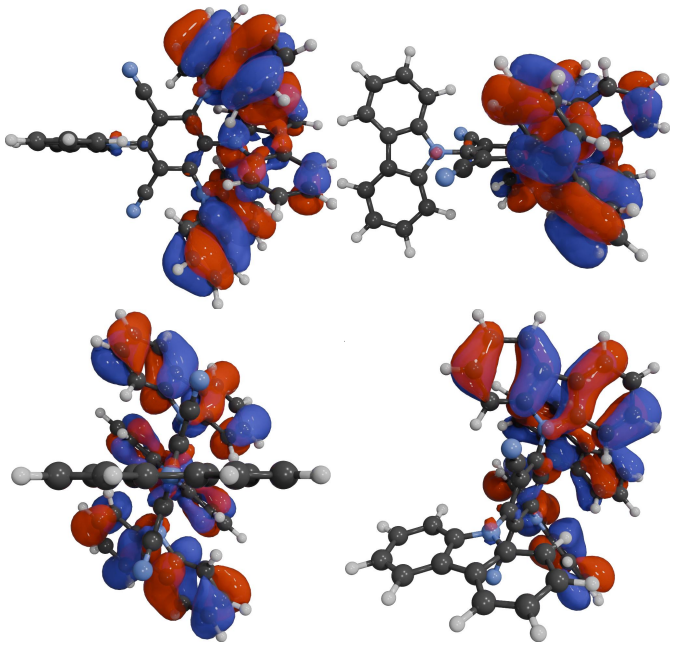


Figure 6: *Orbital density plots of the HOMO-6, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

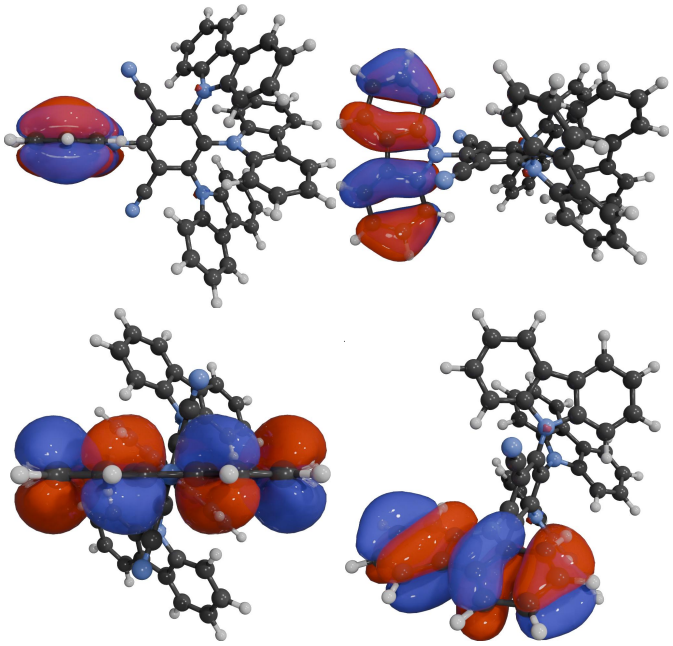


Figure 7: *Orbital density plots of the HOMO-5, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

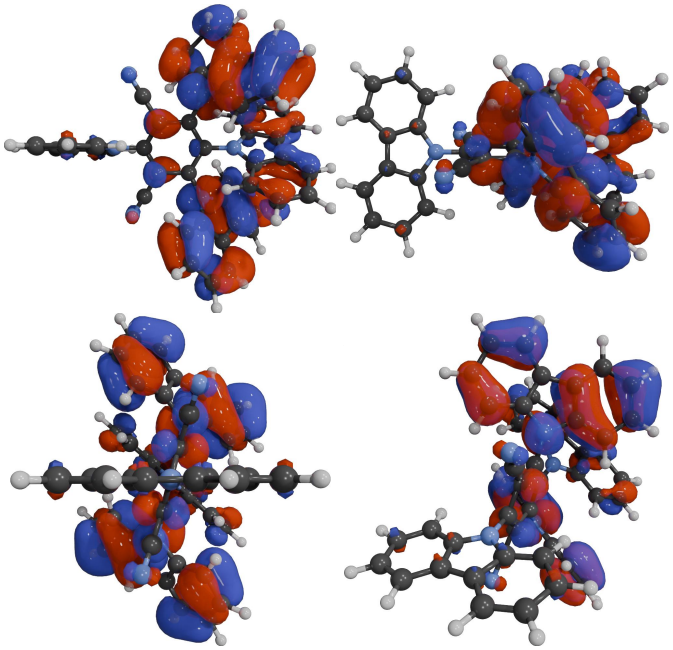


Figure 8: *Orbital density plots of the HOMO-4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

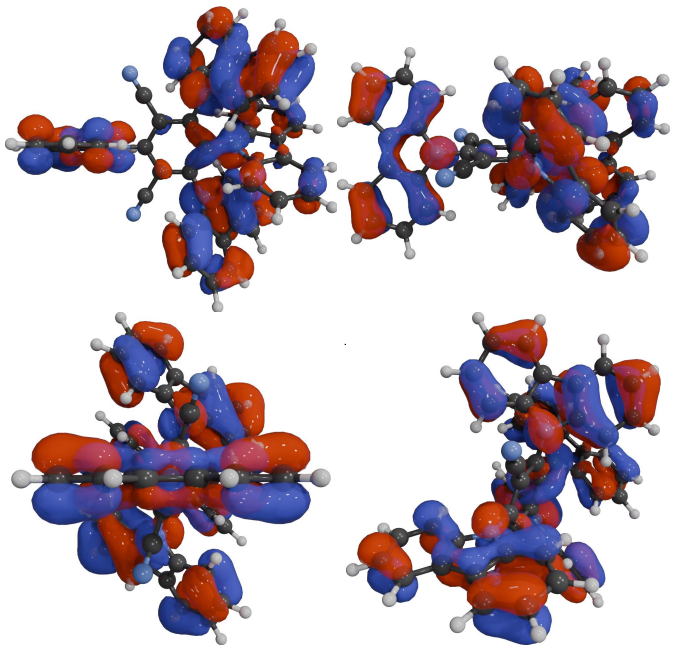


Figure 9: *Orbital density plots of the HOMO-3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

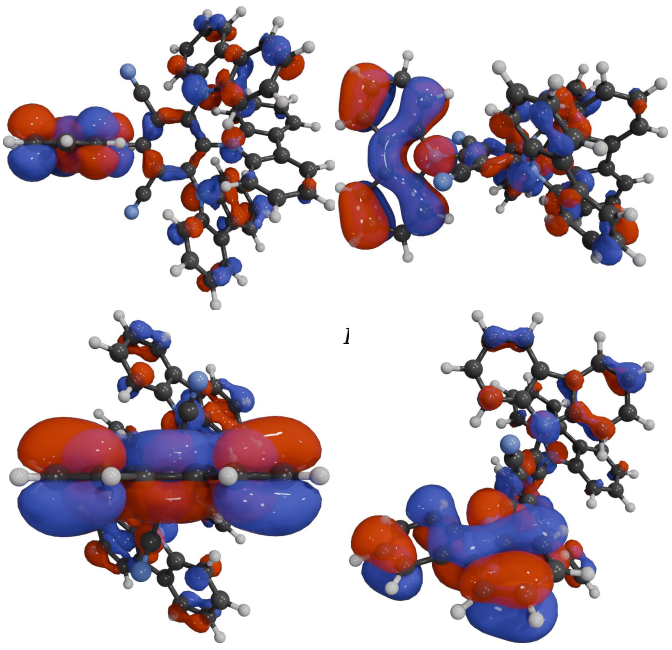


Figure 11: *Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

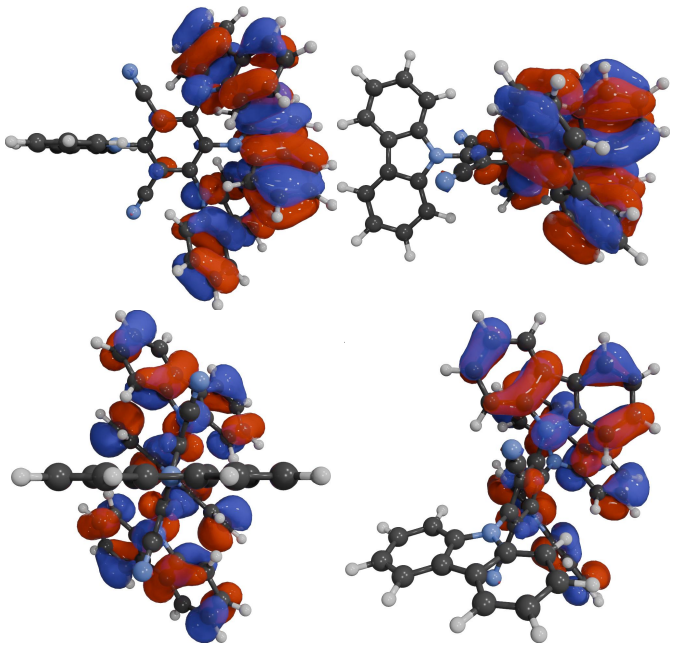


Figure 10: *Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

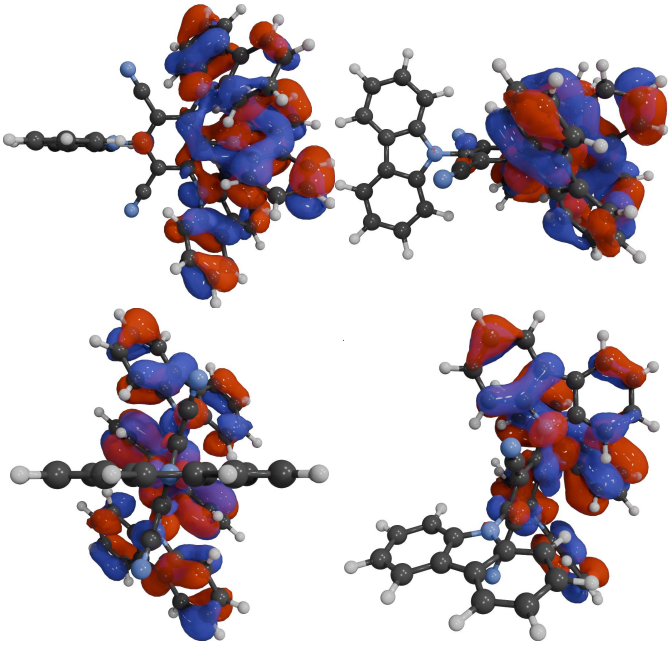


Figure 12: *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

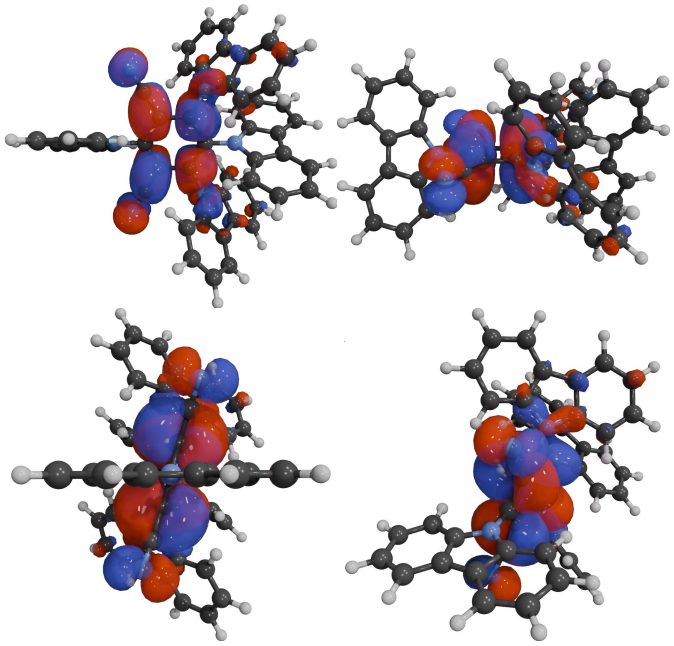


Figure 13: *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

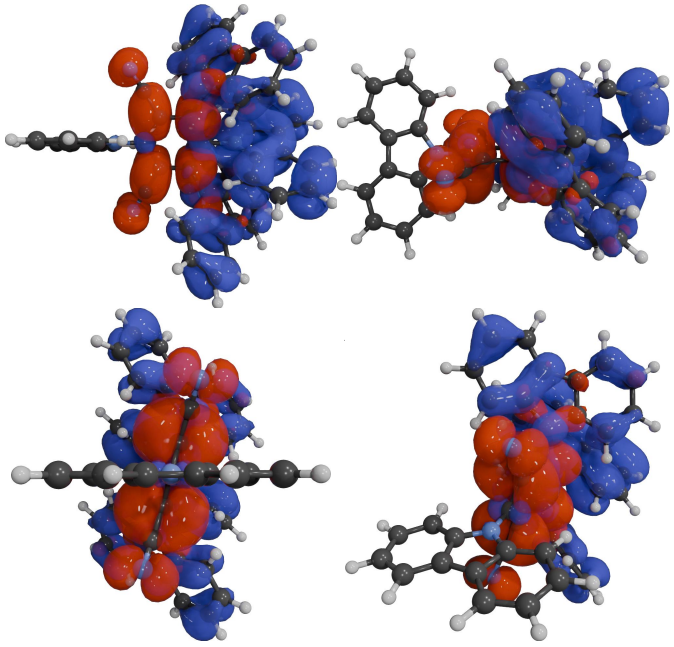


Figure 14: *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

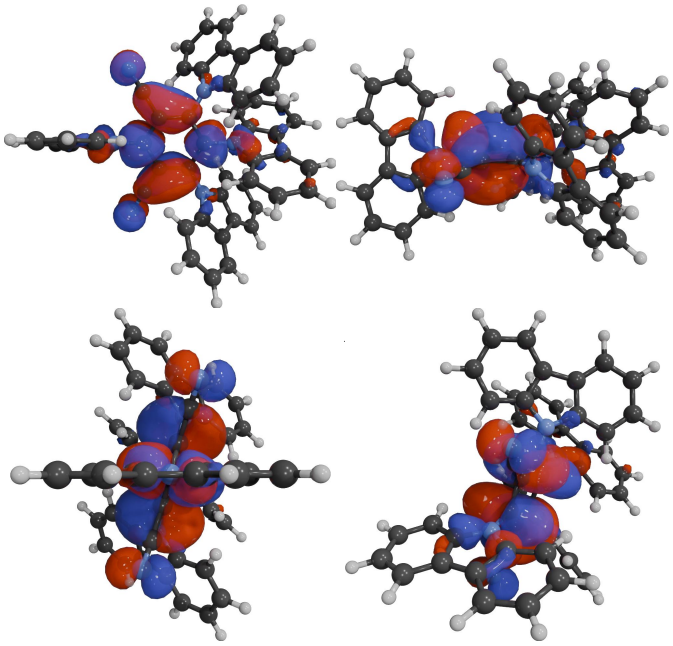


Figure 15: *Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Excited States

In total, the energies of 20 electronic excited states were calculated (figure 17), 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 2.75 eV, corresponding to absorption by a photon with a wavelength of 451 nm, a blue 'color' and CIE coordinates of (0.16, 0.02), while the energy of the **T_1** was 2.62 eV (474 nm, cyan , CIE: (0.11, 0.08)). The difference in energy between the S_1 and T_1 excited states **(ΔE_{ST})** was therefore 0.13 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 399 nm. The full simulated absorption spectrum is shown in figure 18. Finally, **natural transition orbitals (NTOs)** were calculated for each excited state and are shown in figures 19-38.

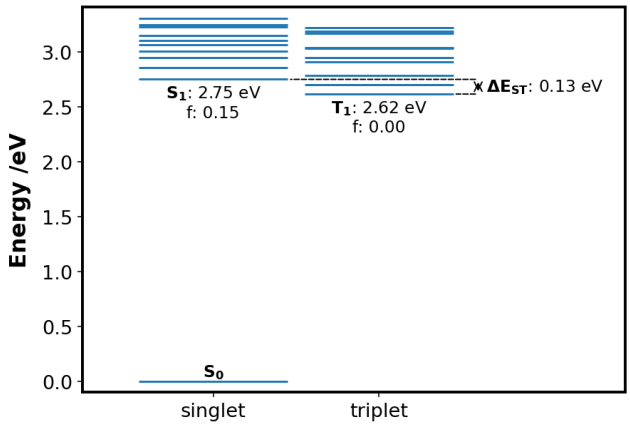


Figure 17: *Graph of the calculated excited states. f: oscillator strength of the relevant ground to excited state transition.*

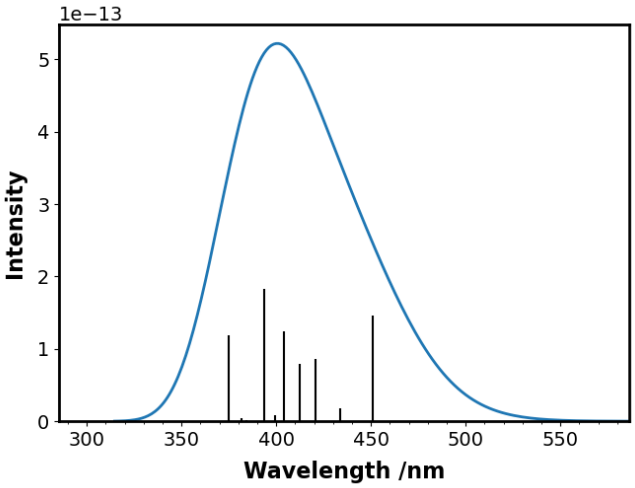


Figure 18: *Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 399 nm.*

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 $\mathbf{S_0}$ **and** $\mathbf{T_1}$ states was found to be 0.64 cm^{-1}, while the H_{SO} between the $\mathbf{S_1}$ **and** $\mathbf{T_1}$ excited states was 0.17 cm^{-1}. These values correspond to a first-order mixing coefficient ($\lambda = H_{SO}/\Delta E_{ST}$) of < 0.01 and < 0.01 respectively.

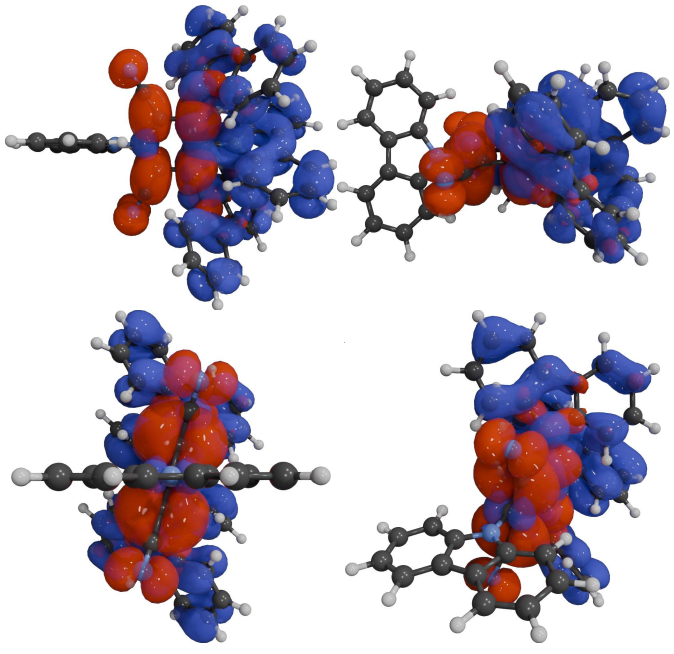


Figure 19: *Density plot of the NTO hole (red) & electron (blue) of the T_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

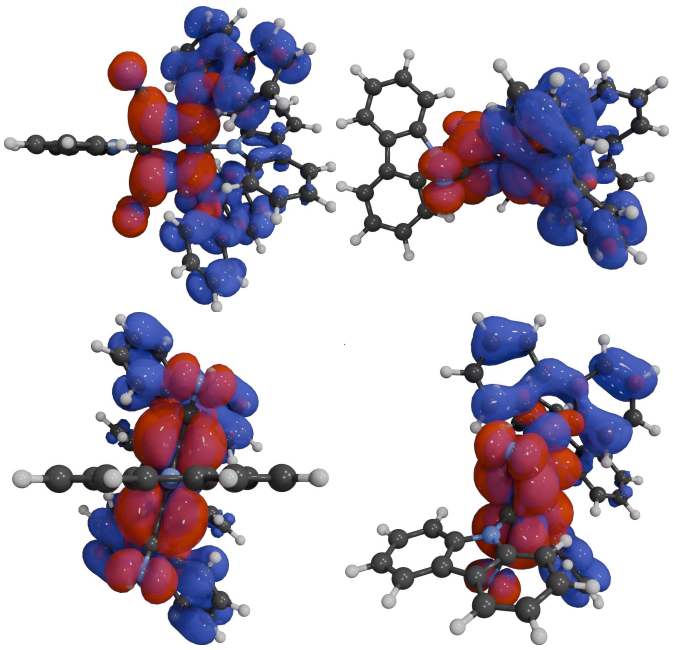


Figure 20: *Density plot of the NTO hole (red) & electron (blue) of the T_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

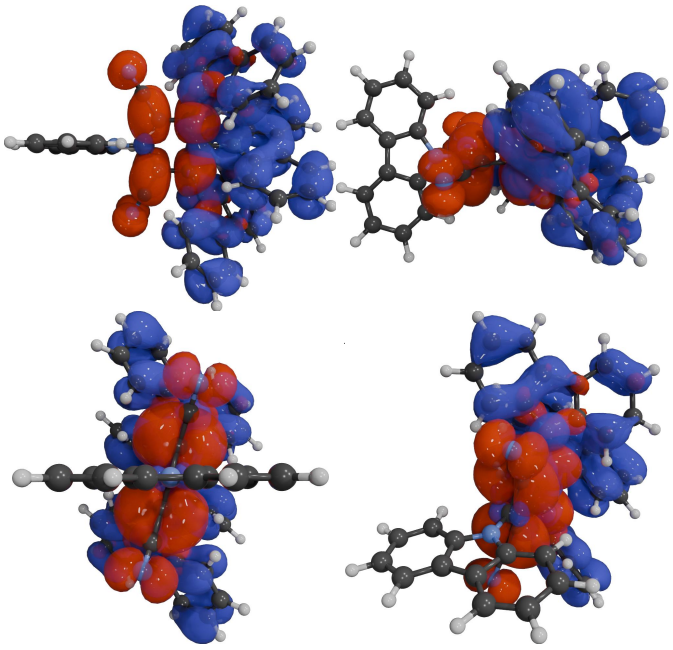


Figure 21: *Density plot of the NTO hole (red) & electron (blue) of the S_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

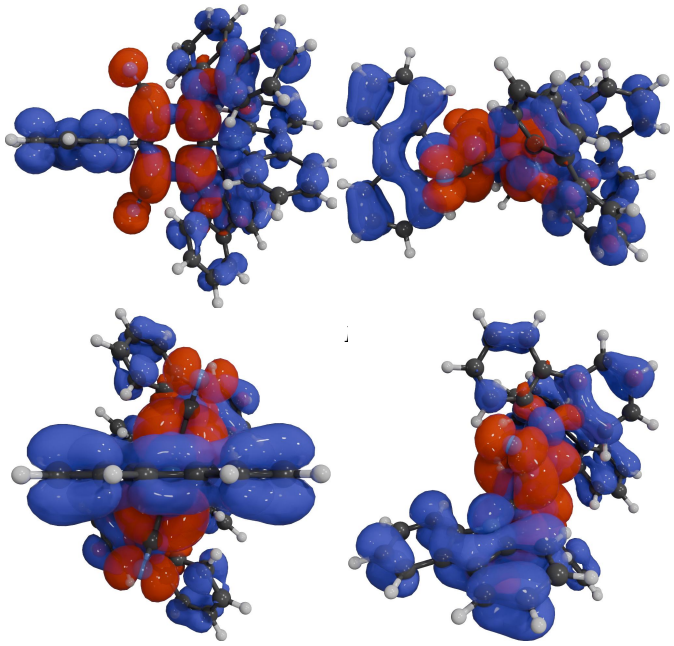


Figure 22: *Density plot of the NTO hole (red) & electron (blue) of the T_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

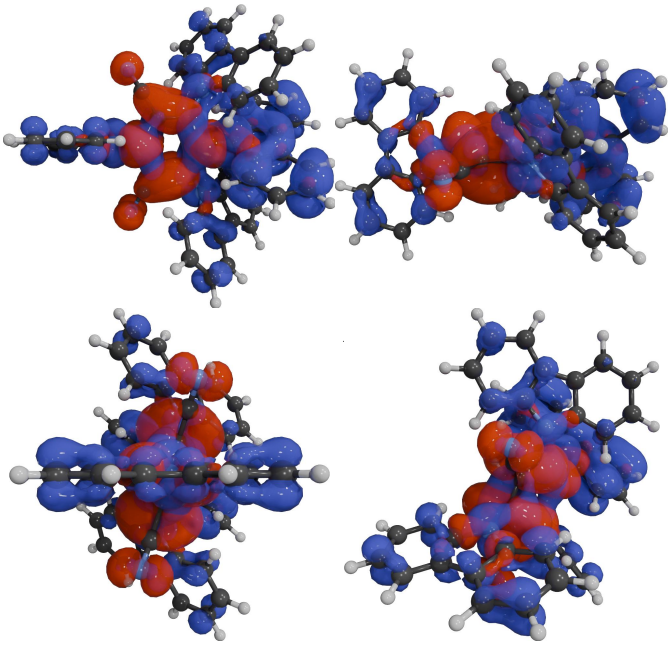


Figure 24: *Density plot of the NTO hole (red) & electron (blue) of the T_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

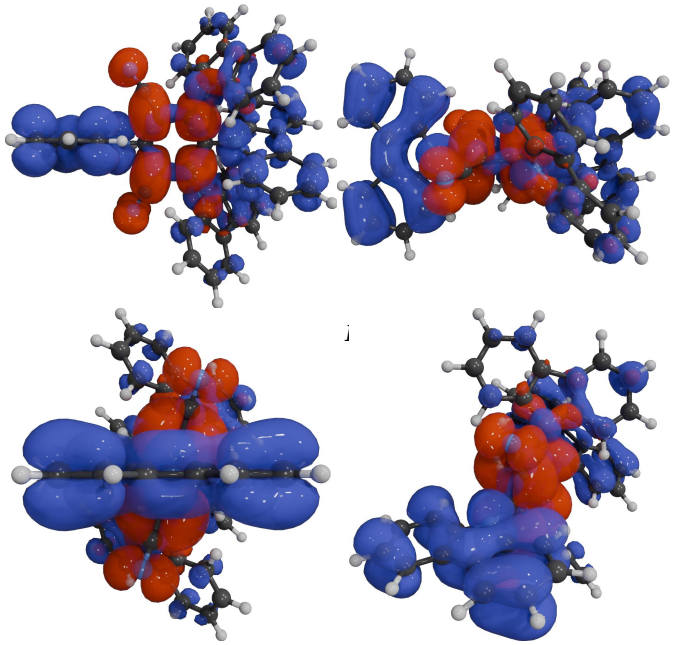


Figure 23: *Density plot of the NTO hole (red) & electron (blue) of the S_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

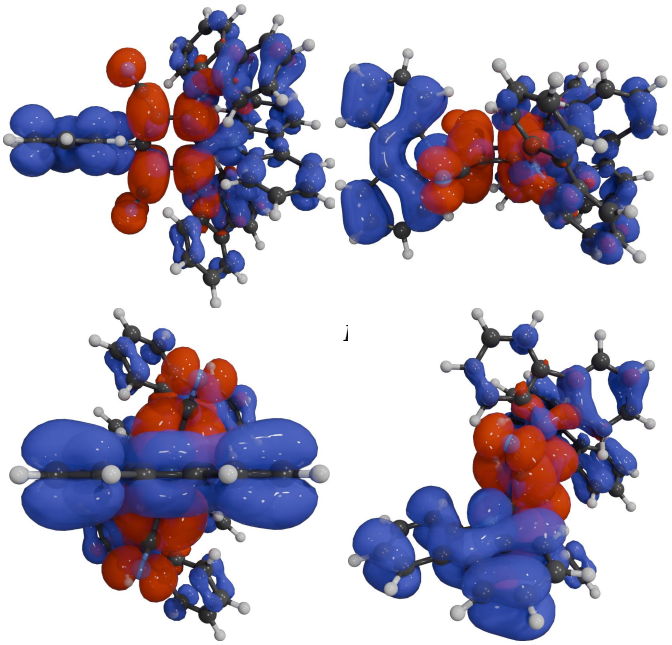


Figure 25: *Density plot of the NTO hole (red) & electron (blue) of the T_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

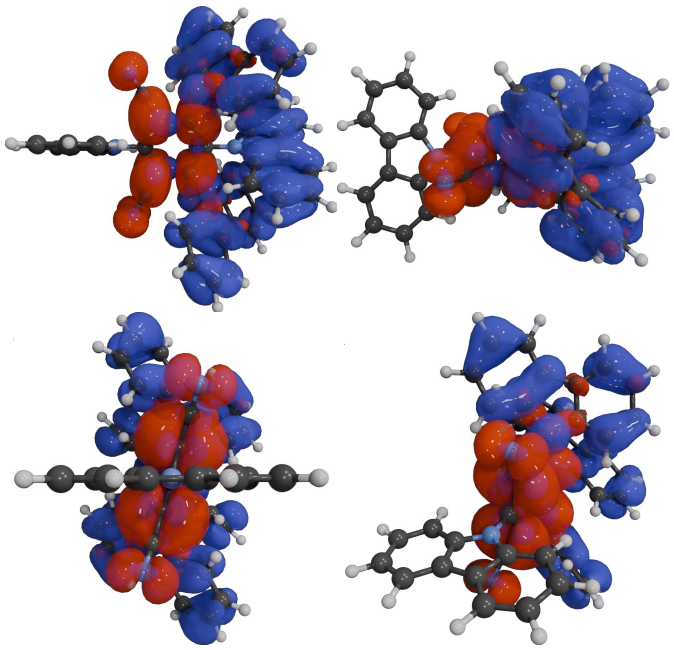


Figure 26: *Density plot of the NTO hole (red) & electron (blue) of the S_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

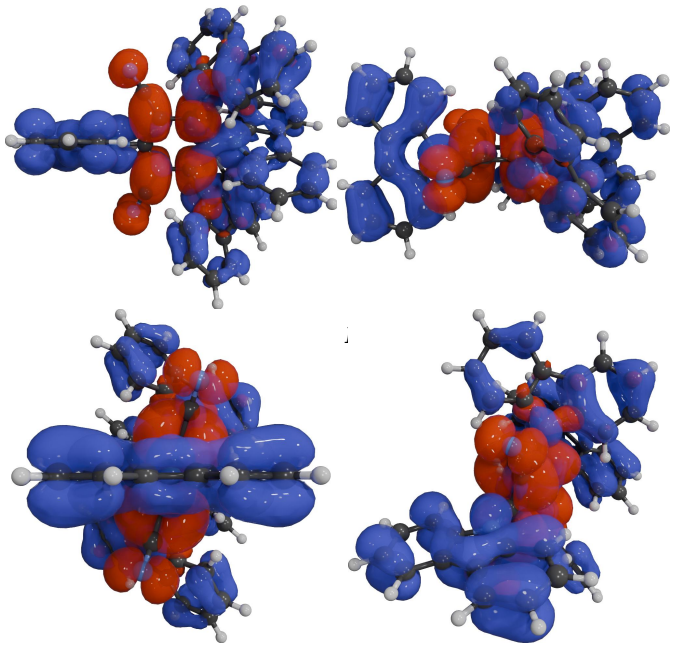


Figure 27: *Density plot of the NTO hole (red) & electron (blue) of the S_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

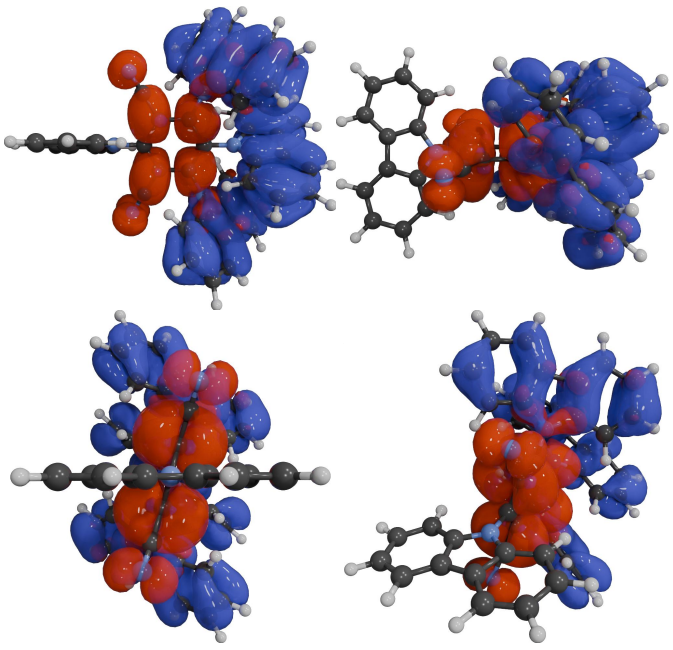


Figure 28: *Density plot of the NTO hole (red) & electron (blue) of the T_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

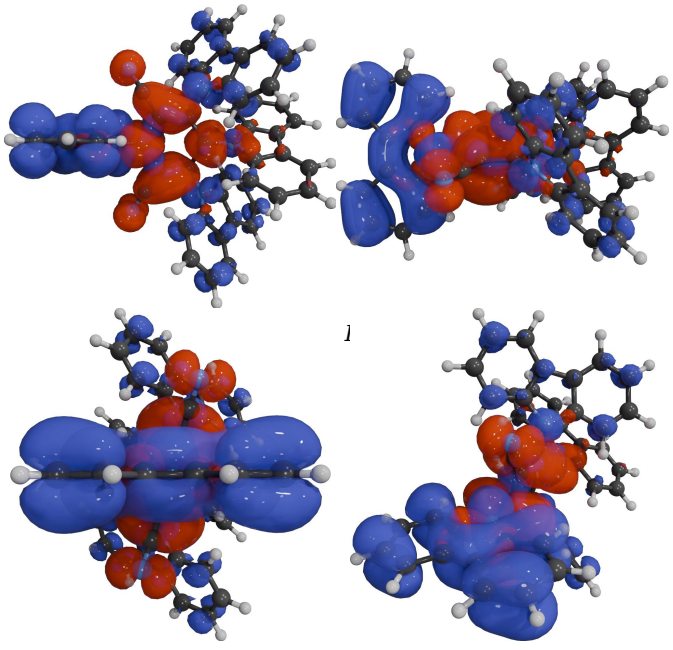


Figure 29: *Density plot of the NTO hole (red) & electron (blue) of the T_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

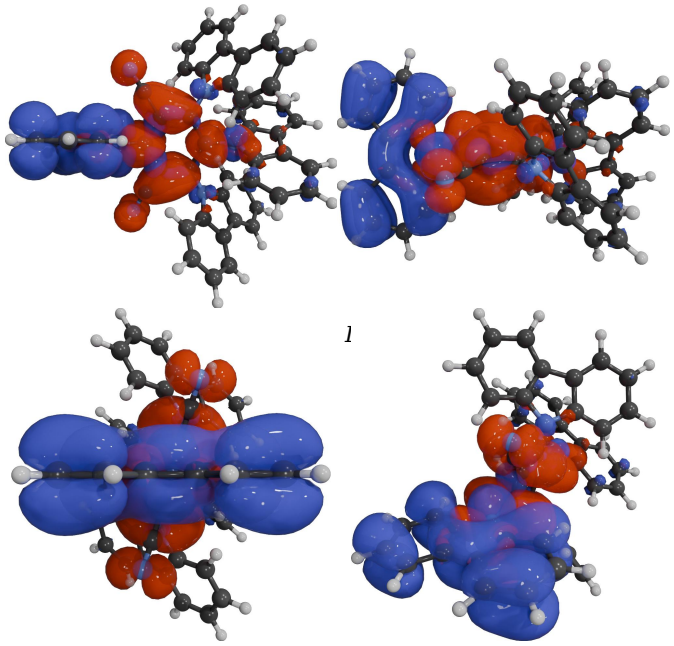


Figure 30: *Density plot of the NTO hole (red) & electron (blue) of the S_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

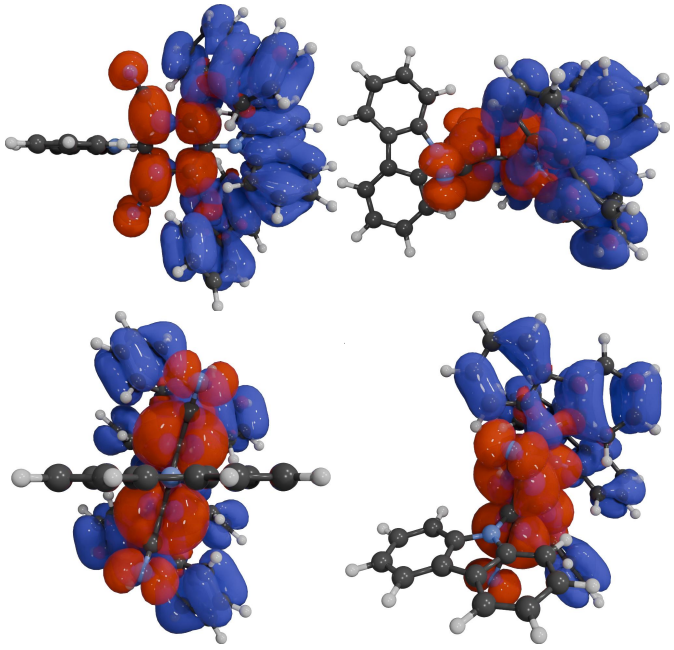


Figure 31: *Density plot of the NTO hole (red) & electron (blue) of the S_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

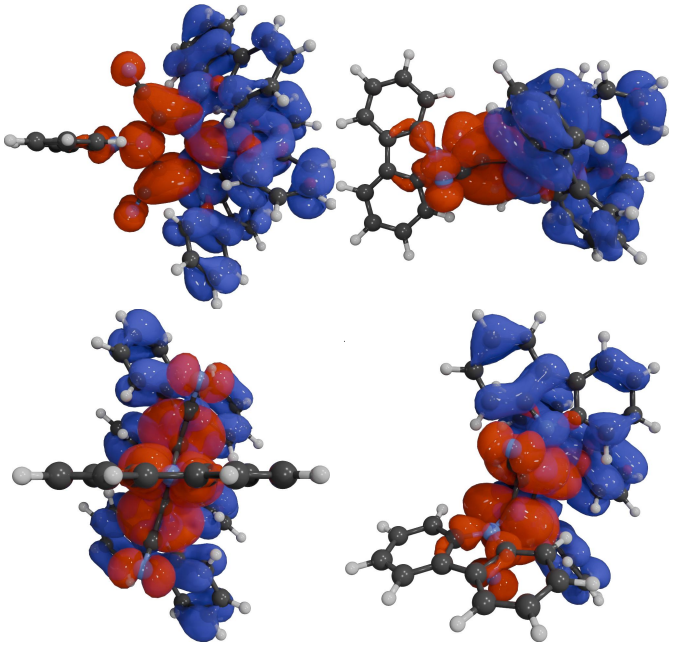


Figure 32: *Density plot of the NTO hole (red) & electron (blue) of the S_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

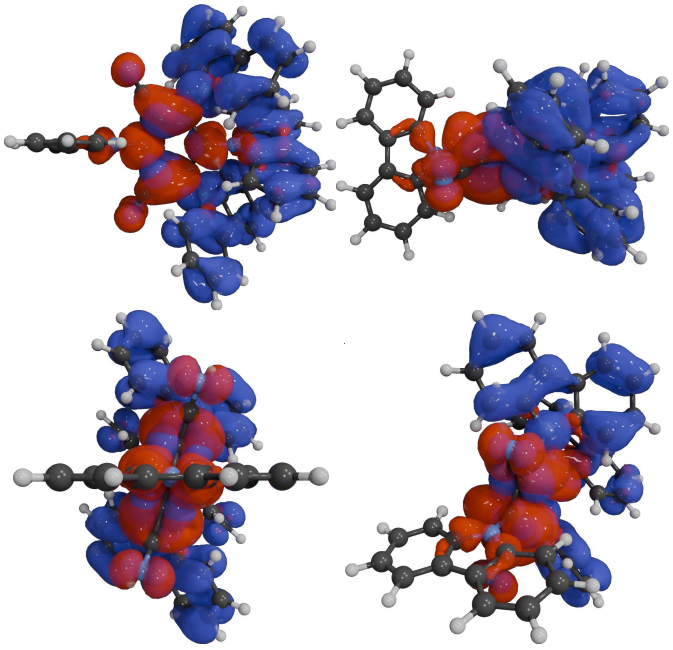


Figure 33: *Density plot of the NTO hole (red) & electron (blue) of the T_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

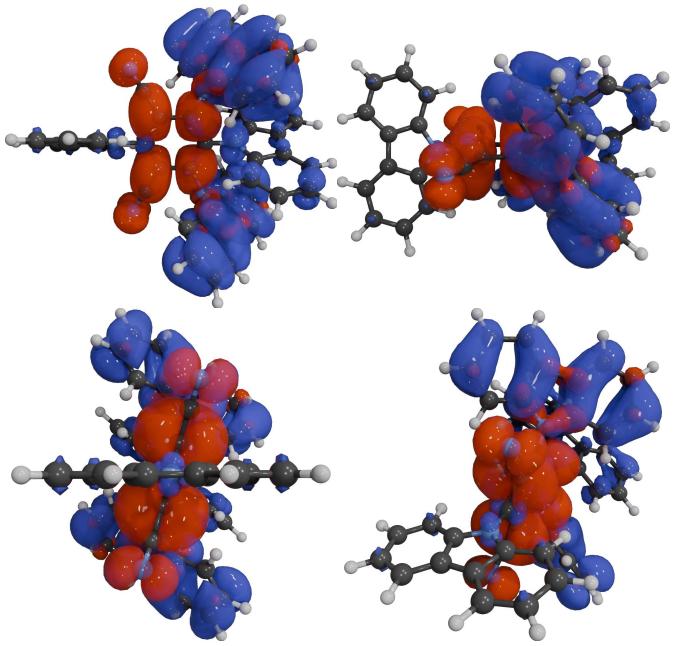


Figure 34: *Density plot of the NTO hole (red) & electron (blue) of the T_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

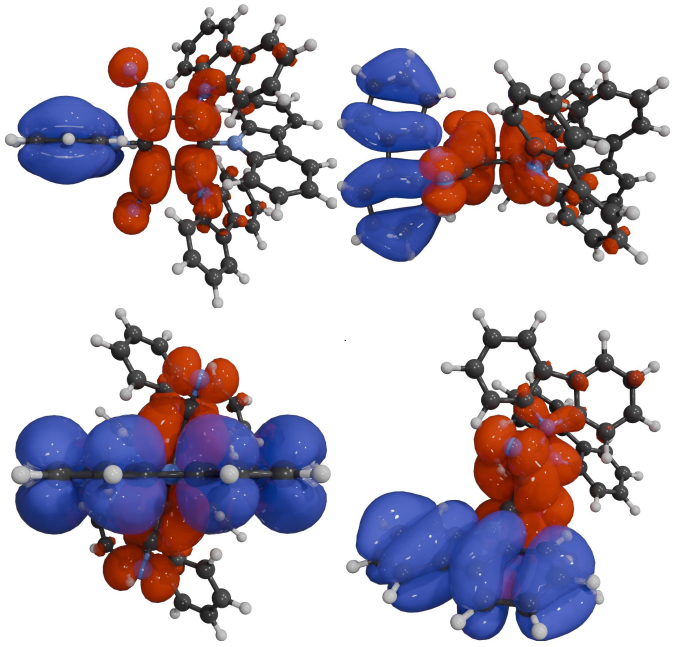


Figure 35: *Density plot of the NTO hole (red) & electron (blue) of the T_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

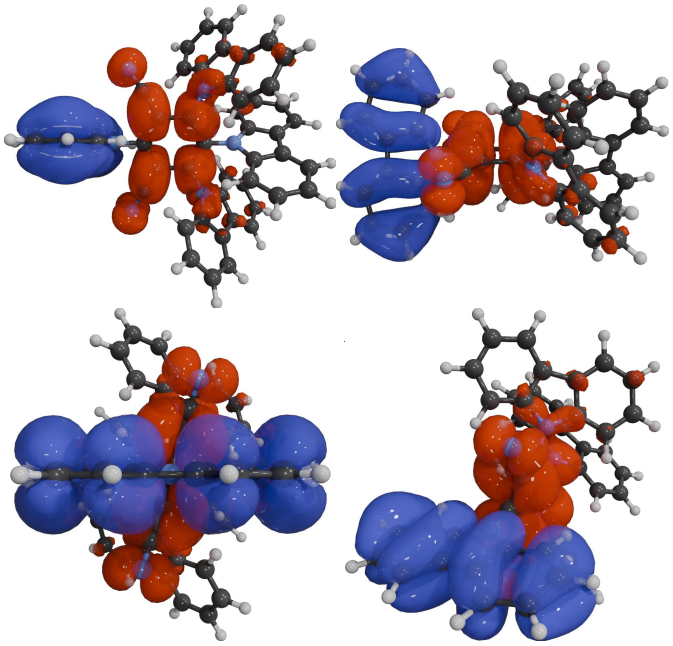


Figure 36: *Density plot of the NTO hole (red) & electron (blue) of the S_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

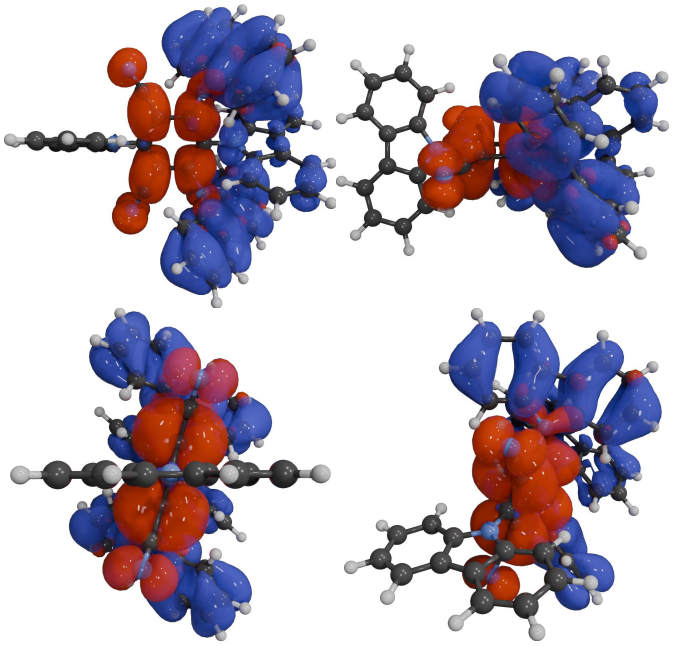


Figure 37: *Density plot of the NTO hole (red) & electron (blue) of the S_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

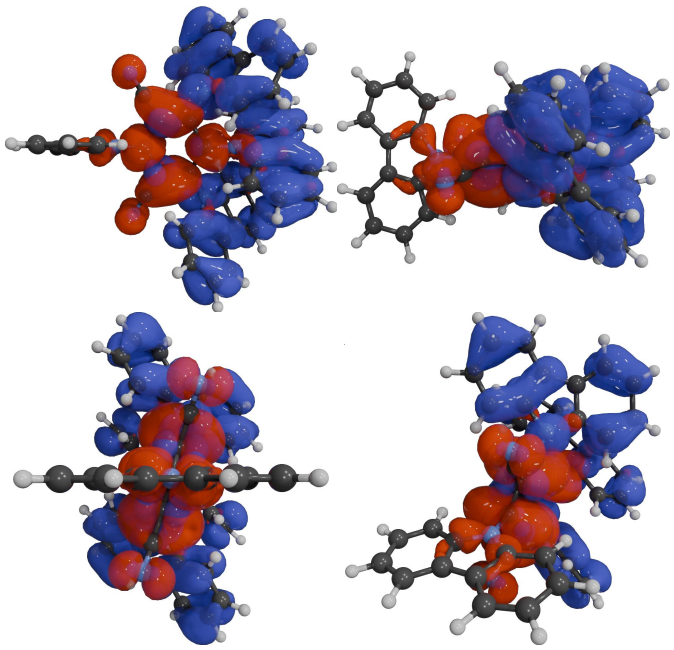


Figure 38: *Density plot of the NTO hole (red) & electron (blue) of the S_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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}	-0.1953400	-1.1883600	-0.2801610
2	C	C_{2}	0.5149500	0.0000500	-0.0000710
3	C	C_{1}	-0.1954010	1.1884200	0.2799990
4	C	C_{3}	-1.6047310	1.1718390	0.2981490
5	C	C_{4}	-2.3124500	-0.0000210	-0.0000810
6	C	C_{3}	-1.6046700	-1.1718510	-0.2983210
7	C	C_{5}	1.4805810	-2.5625800	-1.5000210
8	C	C_{5}	0.4177210	-3.5279000	0.2647590
9	C	C_{6}	1.8539210	-1.7282800	-2.5508210
10	C	C_{7}	2.0822510	-3.8244990	-1.2964110
11	C	C_{6}	-0.3832490	-3.7880000	1.3756390
12	C	C_{7}	1.4054020	-4.4388100	-0.1727910
13	C	C_{8}	2.8937810	-2.1551190	-3.3722110
14	H	H_{6}	1.3529200	-0.7776600	-2.7335310
15	C	C_{9}	3.1189920	-4.2370190	-2.1391110
16	C	C_{8}	-0.1922380	-4.9992200	2.0366790
17	H	H_{6}	-1.1261990	-3.0730910	1.7339890
18	C	C_{9}	1.5773820	-5.6487300	0.5058690
19	C	C_{10}	3.5272810	-3.3905090	-3.1655610
20	H	H_{8}	3.2157710	-1.5137790	-4.1957510
21	H	H_{9}	3.5968120	-5.2084090	-1.9938910
22	C	C_{10}	0.7722120	-5.9233000	1.6069890
23	H	H_{8}	-0.8080880	-5.2288710	2.9089890
24	H	H_{9}	2.3394120	-6.3606190	0.1808390
25	H	H_{10}	4.3401310	-3.6951790	-3.8281810
26	H	H_{10}	0.8948730	-6.8638100	2.1481390
27	C	C_{5}	1.4803990	2.5626500	1.5000090
28	C	C_{5}	0.4176190	3.5280100	-0.2648010
29	C	C_{6}	1.8537290	1.7282900	2.5507690
30	C	C_{7}	2.0819780	3.8246410	1.2965390
31	C	C_{6}	-0.3832520	3.7881200	-1.3757610
32	C	C_{7}	1.4051880	4.4389800	0.1729090
33	C	C_{8}	2.8934990	2.1551710	3.3722690
34	H	H_{6}	1.3528000	0.7776200	2.7333590
35	C	C_{9}	3.1186180	4.2371810	2.1393590
36	C	C_{8}	-0.1922720	4.9993900	-2.0367010
37	H	H_{6}	-1.1261010	3.0731590	-1.7342310
38	C	C_{9}	1.5771380	5.6489500	-0.5056510
39	C	C_{10}	3.5268990	3.3906210	3.1657790
40	H	H_{8}	3.2154690	1.5137910	4.1957890
41	H	H_{9}	3.5963680	5.2086210	1.9942490
42	C	C_{10}	0.7720580	5.9235200	-1.6068510
43	H	H_{8}	-0.8080420	5.2290490	-2.9090710
44	H	H_{9}	2.3390770	6.3608810	-0.1805110
45	H	H_{10}	4.3396680	3.6953110	3.8284790
46	H	H_{10}	0.8946970	6.8640800	-2.1479210
47	N	N_{11}	0.4761610	-2.3826000	-0.5434810
48	N	N_{11}	0.4760590	2.3826700	0.5433790
49	C	C_{12}	-2.3335690	-2.3436010	-0.6688510
50	C	C_{12}	-2.3337110	2.3435090	0.6688090
51	N	N_{13}	-2.9361890	-3.2821610	-0.9819210
52	N	N_{13}	-2.9364110	3.2819690	0.9819790
53	N	N_{14}	1.9119500	0.0000600	-0.0000110
54	C	C_{15}	2.7268300	-0.7750790	0.8300590
55	C	C_{15}	2.7269100	0.7751410	-0.8300810
56	C	C_{16}	2.3698110	-1.6451590	1.8578290
57	C	C_{17}	4.0788900	-0.4960590	0.5271990
58	C	C_{16}	2.3699790	1.6452310	-1.8578710
59	C	C_{17}	4.0789400	0.4960110	-0.5271810
60	C	C_{18}	3.3961910	-2.2778490	2.5541790
61	H	H_{16}	1.3286310	-1.8244000	2.1251190
62	C	C_{19}	5.0934900	-1.1396280	1.2421490
63	C	C_{18}	3.3964290	2.2778210	-2.5542010
64	H	H_{16}	1.3288190	1.8245400	-2.1251910
65	C	C_{19}	5.0936090	1.1394920	-1.2421110
66	C	C_{20}	4.7440910	-2.0372180	2.2466090
67	H	H_{18}	3.1404410	-2.9722090	3.3576990
68	H	H_{19}	6.1427100	-0.9342480	1.0182090
69	C	C_{20}	4.7442990	2.0371020	-2.2465910
70	H	H_{18}	3.1407490	2.9721910	-3.3577410
71	H	H_{19}	6.1428000	0.9340320	-1.0181510
72	H	H_{20}	5.5251010	-2.5509980	2.8110790
73	H	H_{20}	5.5253690	2.5508020	-2.8110610
74	N	N_{21}	-3.7131600	-0.0000620	-0.0000610
75	C	C_{22}	-4.5211200	0.0104380	1.1353890
76	C	C_{22}	-4.5211600	-0.0105920	-1.1354810
77	C	C_{23}	-4.1490800	0.0076980	2.4786890
78	C	C_{24}	-5.8750700	0.0065770	0.7243490
79	C	C_{23}	-4.1491700	-0.0078320	-2.4787910
80	C	C_{24}	-5.8751000	-0.0067930	-0.7243910
81	C	C_{25}	-5.1724800	0.0108980	3.4230990
82	H	H_{23}	-3.0998100	0.0014680	2.7811890
83	C	C_{26}	-6.8831600	0.0079170	1.6943190
84	C	C_{25}	-5.1726100	-0.0110720	-3.4231610
85	H	H_{23}	-3.0999200	-0.0015520	-2.7813310
86	C	C_{26}	-6.8832200	-0.0081830	-1.6943210
87	C	C_{27}	-6.5233300	0.0125070	3.0386390
88	H	H_{25}	-4.9157400	0.0105680	4.4848890
89	H	H_{26}	-7.9349000	0.0037370	1.3990590
90	C	C_{27}	-6.5234400	-0.0127530	-3.0386510
91	H	H_{25}	-4.9159000	-0.0107420	-4.4849610
92	H	H_{26}	-7.9349500	-0.0040530	-1.3990210
93	H	H_{27}	-7.2995900	0.0144570	3.8067990
94	H	H_{27}	-7.2997300	-0.0147430	-3.8067810

Molecular Orbitals

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

Level	Label	Symmetry	Energy /eV
221	LUMO+15	A	0.5513
220	LUMO+14	A	0.2542

219	LUMO+13	A	0.2155	204	HOMO-1	A	-6.3732
218	LUMO+12	A	0.1611	203	HOMO-2	A	-6.4012
217	LUMO+11	A	0.0169	202	HOMO-3	A	-6.5247
216	LUMO+10	A	-0.0971	201	HOMO-4	A	-6.5585
215	LUMO+9	A	-0.1246	200	HOMO-5	A	-6.6091
214	LUMO+8	A	-0.2735	199	HOMO-6	A	-6.6945
213	LUMO+7	A	-0.2952	198	HOMO-7	A	-6.7822
212	LUMO+6	A	-0.4901	197	HOMO-8	A	-7.5384
211	LUMO+5	A	-1.1929	196	HOMO-9	A	-7.6374
210	LUMO+4	A	-1.2052	195	HOMO-10	A	-7.6717
209	LUMO+3	A	-1.2166	194	HOMO-11	A	-7.7580
208	LUMO+2	A	-1.2319	193	HOMO-12	A	-8.3204
207	LUMO+1	A	-2.3571	192	HOMO-13	A	-8.3335
206	**LUMO**	**A**	**-2.7094**	191	HOMO-14	A	-8.3865
205	**HOMO**	**A**	**-6.2608**	190	HOMO-15	A	-8.4206

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	2.6163	473.89	Cyan (0.11, 0.08)	0.0000	HOMO → LUMO (0.94) HOMO-3 → LUMO (0.02)
2	T_2	Triplet-A	2.6997	459.25	Blue (0.15, 0.03)	0.0000	HOMO-2 → LUMO (0.44) HOMO-4 → LUMO (0.37) HOMO → LUMO+1 (0.07) HOMO-16 → LUMO (0.03) HOMO-13 → LUMO (0.03)
3	S_1	Singlet-A	2.7501	450.84	Blue (0.16, 0.02)	0.1496	HOMO → LUMO (0.94) HOMO-1 → LUMO (0.03)
4	T_3	Triplet-A	2.7877	444.75	Blue (0.16, 0.01)	0.0000	HOMO-1 → LUMO (0.85) HOMO-3 → LUMO (0.11)
5	S_2	Singlet-A	2.8584	433.75	Blue (0.17, 0.01)	0.0167	HOMO-1 → LUMO (0.93) HOMO → LUMO (0.04) HOMO-3 → LUMO (0.02)
6	T_4	Triplet-A	2.9105	425.99	Blue (0.17, 0.01)	0.0000	HOMO → LUMO+1 (0.70) HOMO-1 → LUMO+1 (0.10) HOMO-2 → LUMO (0.09) HOMO-17 → LUMO+1 (0.03) HOMO-4 → LUMO (0.02)
7	T_5	Triplet-A	2.9453	420.96	Blue (0.17, 0.01)	0.0000	HOMO-3 → LUMO (0.82) HOMO-1 → LUMO (0.13)
8	S_3	Singlet-A	2.9462	420.83	Blue (0.17, 0.01)	0.0769	HOMO-2 → LUMO (0.89) HOMO-4 → LUMO (0.08)
9	S_4	Singlet-A	3.0067	412.36	Violet (0.17, 0.00)	0.0676	HOMO-3 → LUMO (0.94) HOMO-1 → LUMO (0.03) HOMO-6 → LUMO (0.02)
10	T_6	Triplet-A	3.0308	409.08	Violet (0.17, 0.00)	0.0000	HOMO-4 → LUMO (0.51) HOMO-2 → LUMO (0.42)
11	T_7	Triplet-A	3.0375	408.18	Violet (0.17, 0.00)	0.0000	HOMO-1 → LUMO+1 (0.81) HOMO → LUMO+1 (0.12) HOMO-3 → LUMO+1 (0.05)
12	S_5	Singlet-A	3.0677	404.16	Violet (0.17, 0.00)	0.1024	HOMO-1 → LUMO+1 (0.91) HOMO-3 → LUMO+1 (0.05) HOMO → LUMO+1 (0.02)
13	S_6	Singlet-A	3.1056	399.23	Ultraviolet (0.17, 0.00)	0.0069	HOMO-4 → LUMO (0.73) HOMO → LUMO+1 (0.16) HOMO-2 → LUMO (0.09)
14	S_7	Singlet-A	3.1490	393.73	Ultraviolet (0.17, 0.00)	0.1425	HOMO → LUMO+1 (0.79) HOMO-4 → LUMO (0.17) HOMO-1 → LUMO+1 (0.03)
15	T_8	Triplet-A	3.1713	390.96	Ultraviolet (0.17, 0.00)	0.0000	HOMO-2 → LUMO+1 (0.50) HOMO-6 → LUMO (0.26) HOMO-4 → LUMO+1 (0.14) HOMO-3 → LUMO (0.02)
16	T_9	Triplet-A	3.1862	389.13	Ultraviolet (0.17, 0.00)	0.0000	HOMO-6 → LUMO (0.62) HOMO-2 → LUMO+1 (0.17) HOMO-4 → LUMO+1 (0.12)
17	T_{10}	Triplet-A	3.2210	384.92	Ultraviolet (0.17, 0.00)	0.0000	HOMO-5 → LUMO (0.98)
18	S_8	Singlet-A	3.2274	384.16	Ultraviolet (0.17, 0.00)	0.0008	HOMO-5 → LUMO (0.99)
19	S_9	Singlet-A	3.2499	381.50	Ultraviolet (0.17, 0.00)	0.0028	HOMO-6 → LUMO (0.93) HOMO-2 → LUMO+1 (0.03) HOMO-3 → LUMO (0.02)
20	S_{10}	Singlet-A	3.3058	375.05	Ultraviolet (0.17, 0.01)	0.0845	HOMO-2 → LUMO+1 (0.84) HOMO-4 → LUMO+1 (0.11) HOMO-6 → LUMO (0.04)

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. [jj]: 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	μ[a] Vector /D	μ[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] /	μ[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
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_1	0.00, -3.68, -0.88	3.79	90.00	13.46	0.00, 0.14, -0.34	0.36	90.00	67.89	3.79e-18	3.37e-21	81.35	0.15	0.001
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
S_2	0.00, 1.24, 0.10	1.24	89.98	4.41	-0.00, -0.20, -0.04	0.20	89.97	10.74	1.24e-18	1.89e-21	6.33	0.99	0.006
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
S_3	2.62, 0.00, 0.00	2.62	0.01	0.00	-0.09, 0.00, -0.00	0.09	0.06	0.06	2.62e-18	8.72e-22	0.06	1.00	0.001
S_4	0.00, -2.34, -0.68	2.43	89.98	16.19	0.00, 0.09, 0.18	0.20	90.00	62.80	2.43e-18	1.86e-21	46.61	0.69	0.002
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
S_5	-2.97, -0.00, 0.00	2.97	0.00	0.00	0.20, 0.00, 0.00	0.20	0.00	0.00	2.97e-18	1.85e-21	0.00	1.00	0.002
S_6	0.77, 0.00, 0.00	0.77	0.00	0.00	0.21, 0.00, 0.00	0.21	0.00	0.00	7.66e-19	1.94e-21	180.00	-1.00	-0.010
S_7	-3.45, 0.00, 0.00	3.45	0.00	0.00	-0.11, 0.00, 0.00	0.11	0.00	0.00	3.45e-18	1.06e-21	180.00	-1.00	-0.001
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
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_8	0.25, 0.00, 0.00	0.25	0.00	0.00	-0.02, 0.00, 0.00	0.02	0.00	0.00	2.52e-19	1.60e-22	0.00	1.00	0.003
S_9	0.00, -0.23, -0.41	0.47	89.97	61.30	0.00, -0.14, -0.25	0.29	89.98	60.94	4.73e-19	2.69e-21	179.64	-1.00	-0.023
S_{10}	-0.00, -2.50, -0.71	2.60	89.99	15.99	0.00, -0.03, -0.68	0.68	90.00	87.72	2.60e-18	6.28e-21	108.27	-0.31	-0.003

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	0.3644	0.3764	0.3644	0.6381	0.0001	< 0.0001
S_0	T_2	0.1443	0.0002	0.1443	0.2040	< 0.0001	< 0.0001
S_0	T_3	2.8549	0.6217	2.8549	4.0850	0.0005	0.0002
S_0	T_4	0.9879	0.0001	0.9879	1.3971	0.0002	0.0001
S_0	T_5	0.1613	0.3893	0.1613	0.4512	0.0001	< 0.0001
S_0	T_6	0.0057	0.0002	0.0057	0.0081	< 0.0001	< 0.0001
S_0	T_7	2.2059	< 0.0001	2.2059	3.1197	0.0004	0.0001
S_0	T_8	0.1659	0.2010	0.1659	0.3089	< 0.0001	< 0.0001
S_0	T_9	0.3385	0.5384	0.3385	0.7205	0.0001	< 0.0001
S_0	T_{10}	0.2308	0.0001	0.2308	0.3265	< 0.0001	< 0.0001
S_1	T_1	0.1236	< 0.0001	0.1236	0.1747	< 0.0001	0.0002
S_1	T_2	0.2152	0.3521	0.2152	0.4654	0.0001	0.0011
S_1	T_3	0.1568	< 0.0001	0.1568	0.2217	< 0.0001	0.0007
S_1	T_4	0.1389	0.1316	0.1389	0.2364	< 0.0001	0.0002
S_1	T_5	0.1553	< 0.0001	0.1553	0.2197	< 0.0001	0.0001
S_1	T_6	0.0459	0.0249	0.0459	0.0695	< 0.0001	< 0.0001
S_1	T_7	0.1659	0.0519	0.1659	0.2403	< 0.0001	0.0001
S_1	T_8	0.1337	< 0.0001	0.1337	0.1891	< 0.0001	0.0001
S_1	T_9	0.2428	< 0.0001	0.2428	0.3433	< 0.0001	0.0001
S_1	T_{10}	0.0248	0.0844	0.0248	0.0914	< 0.0001	< 0.0001
S_2	T_1	0.1242	0.0001	0.1242	0.1756	< 0.0001	0.0001
S_2	T_2	0.0435	0.4590	0.0435	0.4631	0.0001	0.0004
S_2	T_3	0.0526	0.0001	0.0526	0.0744	< 0.0001	0.0001

S_2	T_4	0.1736	0.0482	0.1736	0.2502	< 0.0001	0.0006
S_2	T_5	0.3017	0.0001	0.3017	0.4267	0.0001	0.0006
S_2	T_6	0.1841	0.3021	0.1841	0.3988	< 0.0001	0.0003
S_2	T_7	0.2561	0.2227	0.2561	0.4251	0.0001	0.0003
S_2	T_8	0.0705	< 0.0001	0.0705	0.0996	< 0.0001	< 0.0001
S_2	T_9	0.1901	0.0001	0.1901	0.2688	< 0.0001	0.0001
S_2	T_{10}	0.3076	0.0712	0.3076	0.4408	0.0001	0.0002
S_3	T_1	0.3164	0.2845	0.3164	0.5302	0.0001	0.0002
S_3	T_2	0.2974	0.0003	0.2974	0.4206	0.0001	0.0002
S_3	T_3	0.0302	0.0456	0.0302	0.0625	< 0.0001	< 0.0001
S_3	T_4	0.0460	0.0001	0.0460	0.0651	< 0.0001	0.0002
S_3	T_5	0.0270	1.1239	0.0270	1.1245	0.0001	0.1549
S_3	T_6	0.2726	0.0001	0.2726	0.3856	< 0.0001	0.0006
S_3	T_7	0.0265	0.0001	0.0265	0.0375	< 0.0001	0.0001
S_3	T_8	0.1400	0.1748	0.1400	0.2641	< 0.0001	0.0001
S_3	T_9	0.3276	0.1522	0.3276	0.4877	0.0001	0.0003
S_3	T_{10}	0.0012	< 0.0001	0.0012	0.0017	< 0.0001	< 0.0001
S_4	T_1	0.2862	0.0001	0.2862	0.4047	0.0001	0.0001
S_4	T_2	0.0014	1.1010	0.0014	1.1010	0.0001	0.0004
S_4	T_3	0.3986	0.0001	0.3986	0.5636	0.0001	0.0003
S_4	T_4	0.0460	0.3963	0.0460	0.4016	< 0.0001	0.0005
S_4	T_5	0.0513	0.0002	0.0513	0.0726	< 0.0001	0.0001
S_4	T_6	0.1436	0.0770	0.1436	0.2172	< 0.0001	0.0011
S_4	T_7	0.1564	0.1104	0.1564	0.2472	< 0.0001	0.0010
S_4	T_8	0.0417	< 0.0001	0.0417	0.0590	< 0.0001	< 0.0001
S_4	T_9	0.0948	< 0.0001	0.0948	0.1340	< 0.0001	0.0001
S_4	T_{10}	0.2044	0.0370	0.2044	0.2914	< 0.0001	0.0002
S_5	T_1	0.0457	0.0389	0.0457	0.0755	< 0.0001	< 0.0001
S_5	T_2	0.1287	0.0001	0.1287	0.1820	< 0.0001	0.0001
S_5	T_3	0.3155	0.1652	0.3155	0.4758	0.0001	0.0002
S_5	T_4	0.3299	< 0.0001	0.3299	0.4665	0.0001	0.0004
S_5	T_5	0.1888	0.0411	0.1888	0.2702	< 0.0001	0.0003
S_5	T_6	0.0103	< 0.0001	0.0103	0.0146	< 0.0001	< 0.0001
S_5	T_7	0.1144	< 0.0001	0.1144	0.1618	< 0.0001	0.0007
S_5	T_8	0.0047	0.6072	0.0047	0.6073	0.0001	0.0007
S_5	T_9	0.0161	0.4981	0.0161	0.4987	0.0001	0.0005
S_5	T_{10}	0.0075	< 0.0001	0.0075	0.0106	< 0.0001	< 0.0001
S_6	T_1	0.1834	0.2429	0.1834	0.3553	< 0.0001	0.0001
S_6	T_2	0.0810	0.0001	0.0810	0.1145	< 0.0001	< 0.0001
S_6	T_3	0.2276	0.2837	0.2276	0.4290	0.0001	0.0002
S_6	T_4	0.1947	0.0000	0.1947	0.2754	< 0.0001	0.0002
S_6	T_5	0.1672	0.4443	0.1672	0.5033	0.0001	0.0004
S_6	T_6	0.1188	< 0.0001	0.1188	0.1681	< 0.0001	0.0003
S_6	T_7	0.0743	< 0.0001	0.0743	0.1050	< 0.0001	0.0002
S_6	T_8	0.0370	0.1778	0.0370	0.1854	< 0.0001	0.0003
S_6	T_9	0.2545	0.0599	0.2545	0.3649	< 0.0001	0.0006
S_6	T_{10}	0.0005	< 0.0001	0.0005	0.0008	< 0.0001	< 0.0001
S_7	T_1	0.2195	0.0732	0.2195	0.3189	< 0.0001	0.0001
S_7	T_2	0.1106	< 0.0001	0.1106	0.1564	< 0.0001	< 0.0001
S_7	T_3	0.1079	0.1356	0.1079	0.2042	< 0.0001	0.0001
S_7	T_4	0.2630	< 0.0001	0.2630	0.3720	< 0.0001	0.0002
S_7	T_5	0.1543	0.3836	0.1543	0.4414	0.0001	0.0003
S_7	T_6	0.1122	0.0001	0.1122	0.1587	< 0.0001	0.0002

S_7	T_7	0.1349	< 0.0001	0.1349	0.1907	< 0.0001	0.0002
S_7	T_8	0.1096	0.0031	0.1096	0.1551	< 0.0001	0.0009
S_7	T_9	0.0714	0.0526	0.0714	0.1138	< 0.0001	0.0004
S_7	T_{10}	0.0029	< 0.0001	0.0029	0.0040	< 0.0001	< 0.0001
S_8	T_1	0.0219	0.1528	0.0219	0.1559	< 0.0001	< 0.0001
S_8	T_2	0.0196	0.0000	0.0196	0.0278	< 0.0001	< 0.0001
S_8	T_3	0.2682	0.1148	0.2682	0.3962	< 0.0001	0.0001
S_8	T_4	0.0148	< 0.0001	0.0148	0.0209	< 0.0001	< 0.0001
S_8	T_5	0.2687	0.1052	0.2687	0.3943	< 0.0001	0.0002
S_8	T_6	0.0118	0.0000	0.0118	0.0166	< 0.0001	< 0.0001
S_8	T_7	0.0067	0.0000	0.0067	0.0095	< 0.0001	< 0.0001
S_8	T_8	0.0023	0.0111	0.0023	0.0116	< 0.0001	< 0.0001
S_8	T_9	0.0240	0.0806	0.0240	0.0874	< 0.0001	0.0003
S_8	T_{10}	0.0091	0.0000	0.0091	0.0129	< 0.0001	0.0003
S_9	T_1	0.1917	< 0.0001	0.1917	0.2711	< 0.0001	0.0001
S_9	T_2	0.1830	0.0085	0.1830	0.2589	< 0.0001	0.0001
S_9	T_3	0.2412	0.0001	0.2412	0.3412	< 0.0001	0.0001
S_9	T_4	0.1134	0.0892	0.1134	0.1836	< 0.0001	0.0001
S_9	T_5	0.1328	0.0001	0.1328	0.1878	< 0.0001	0.0001
S_9	T_6	0.2495	0.1603	0.2495	0.3875	< 0.0001	0.0002
S_9	T_7	0.0702	0.1264	0.0702	0.1607	< 0.0001	0.0001
S_9	T_8	0.0272	< 0.0001	0.0272	0.0385	< 0.0001	0.0001
S_9	T_9	0.0296	< 0.0001	0.0296	0.0419	< 0.0001	0.0001
S_9	T_{10}	0.0148	0.0640	0.0148	0.0674	< 0.0001	0.0003
S_{10}	T_1	0.0090	< 0.0001	0.0090	0.0127	< 0.0001	< 0.0001
S_{10}	T_2	0.4686	0.2834	0.4686	0.7207	0.0001	0.0001
S_{10}	T_3	0.0306	0.0001	0.0306	0.0433	< 0.0001	< 0.0001
S_{10}	T_4	0.0964	0.2719	0.0964	0.3041	< 0.0001	0.0001
S_{10}	T_5	0.0164	0.0001	0.0164	0.0232	< 0.0001	< 0.0001
S_{10}	T_6	0.0612	0.1179	0.0612	0.1463	< 0.0001	0.0001
S_{10}	T_7	0.1085	0.5587	0.1085	0.5794	0.0001	0.0003
S_{10}	T_8	0.1278	0.0001	0.1278	0.1807	< 0.0001	0.0002
S_{10}	T_9	0.1331	< 0.0001	0.1331	0.1882	< 0.0001	0.0002
S_{10}	T_{10}	0.0085	0.0400	0.0085	0.0418	< 0.0001	0.0001

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