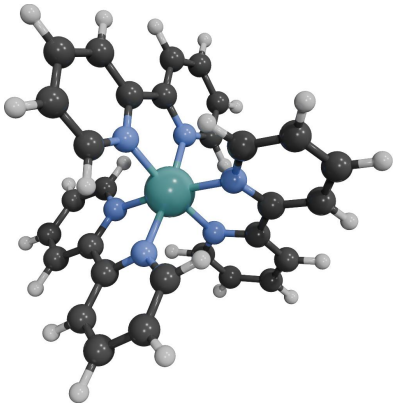
A Report On The Calculation Of The Excited States Of Ru_bpy_3 At The PBE1PBE Level

osl - 28th May 2025



Abstract

The calculation of excited states for the system 'Ru_bpy_3' 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 level of theory. The total self-consistent field (SCF) energy of the system was found to be -42951.50 eV after 1 step. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -6.46 and -2.59 eV respectively, corresponding to a HOMO-LUMO band gap of 3.87 eV. The permanent dipole moment (PDM) was calculated to be 5.29 D. In total, 20 excited states were calculated with singlet and triplet multiplicity. The most intense absorption peak was calculated to be at 398 nm. The lowest energy singlet and triplet excited states (S_1 and T_1) were calculated to be 2.81 and 2.64 eV (442 and 469 nm) respectively, corresponding to a singlet/triplet splitting energy (ΔE_{ST}) of 0.16 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 11:29:49 (1 h, 21 m, 52 s)	40 (20 GB)	True (N/A)	Gaussian (2016+C.01)	PBE1PBE	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	-42951.5016 eV
Final energy	-4,144,190 kJ·mol^{-1}

Geometry

Table 3: *Summary of geometry properties.*

Formula	$RuN_6C_{30}H_{24}{}^{+2}$
SMILES	[CH]1[CH][CH]N2[C]([CH]1)[C]1[CH][CH][CH][CH]N1[Ru]213(N2[CH][CH][CH][CH][C]2[C]2[CH][CH][CH][CH]N21)N1[CH][CH][CH][CH][C]1[C]1[CH][CH][CH][CH]N13
Exact mass	570.1099 g·mol^{-1}
Molar mass	569.6218 g·mol^{-1}
Alignment method	Minimal
X extension	10.20 Å
Y extension	10.01 Å
Z extension	7.20 Å
Linearity ratio	0.02
Planarity ratio	0.28

Molecular Orbitals

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

$E_{HOMO,LUMO}$	3.87 eV
E_{HOMO}	-6.46 eV
E_{LUMO}	-2.59 eV

Permanent Dipole Moment

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

Total	5.29 D
X axis angle	54.92 °
XY plane angle	0.04 °

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	0.11 D
$\theta_{\mu,x}$	62.70 °
$\theta_{\mu,xy}$	13.66 °
m[d]	0.07 a.u.
$\theta_{m,x}$	64.89 °
$\theta_{m,xy}$	27.10 °
μ (Gaussian-CGS)	1.13e-19 esu·cm
m (Gaussian-CGS)	6.86e-22 erg·G^{-1}
$\theta_{\mu,m}$	40.75 °
cos($\theta_{\mu,m}$)	0.76
g_{lum}	0.018

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}	2.81 eV
λ_{S_1} (colour, CIE)	442 nm (Blue ■, (0.16, 0.01))
f_{S_1}	< 0.01
No. calculated triplets	10
E_{T_1}	2.64 eV
λ_{T_1} (colour, CIE)	469 nm (Blue ■, (0.13, 0.05))
f_{T_1}	0.00
ΔE_{ST}	0.16 eV
Simulated Absorption Peaks	398 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. $<S|\lambda|T>$: First-order mixing coefficient between the same.*

$<S_0\|H_{SO}\|T_1>$	298.98 cm^{-1}
$<S_0\|\lambda\|T_1>$	0.01
$<S_1\|H_{SO}\|T_1>$	53.94 cm^{-1}
$<S_1\|\lambda\|T_1>$	0.04

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 using a basis set that could not be determined. It was completed on the **28th May 2025** after a total duration of **1 h, 21 m, 52 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 -42951.50 eV, corresponding to -4,144,190 $KJmol^{-1}$. A plot of the total SCF electron density is shown in figure 1.

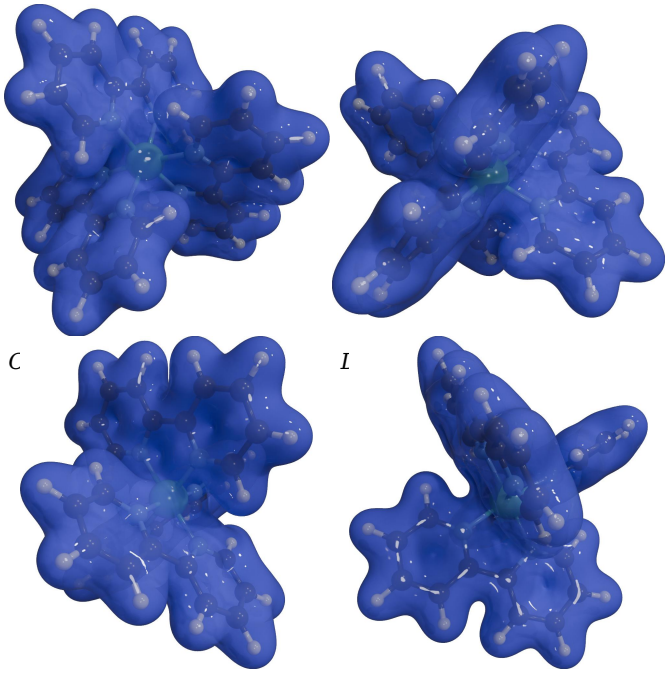


Figure 1: *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Geometry

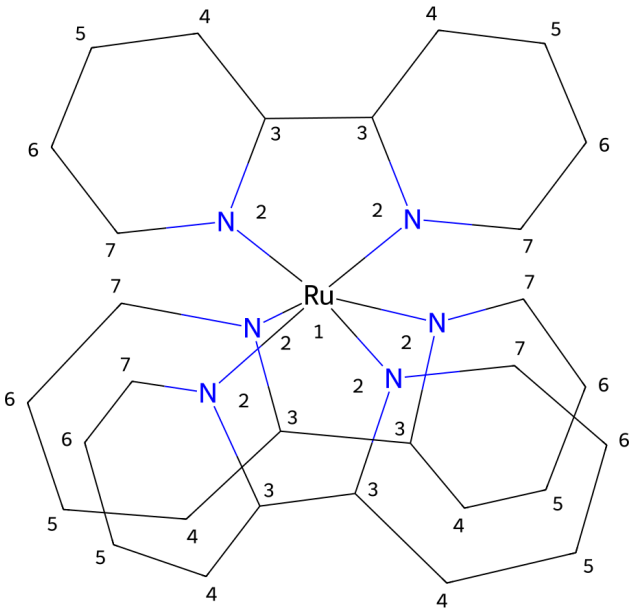


Figure 2: *Labelled structure of Ru_bpy_3.*

The **empirical formula** of the studied system was $RuN_6C_{30}H_{24}{}^{+2}$, corresponding to a **molecular mass** of 569.62 $gmol^{-1}$ and an **exact mass**, considering only specific atomic isotopes, of 570.11 $gmol^{-1}$. 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 10.20, 10.01 and 7.20 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 0.28 respectively.

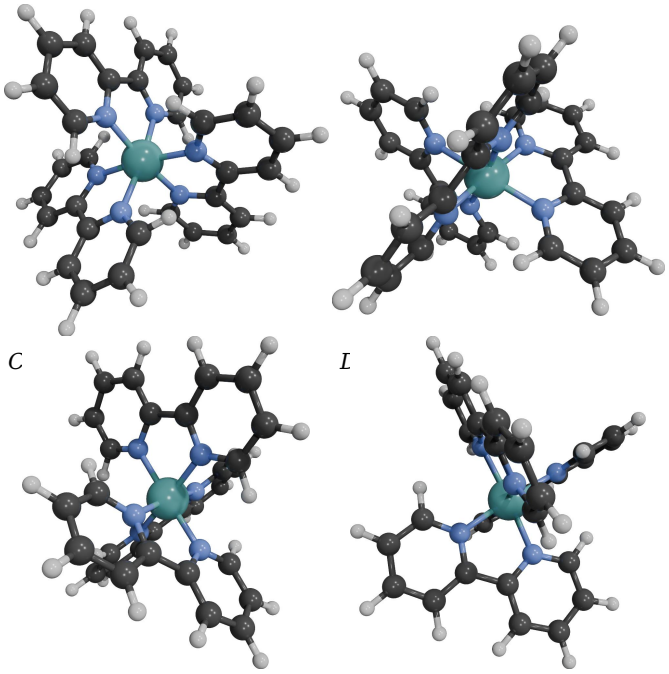


Figure 3: *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Permanent Dipole Moment

The calculated **permanent dipole moment** was 5.29 D, with a vector (x,y,z) of 3.04, 4.33, 0.00 D. The angle between the dipole moment vector and the x-axis was 54.92 °, while the angle between the dipole moment and the xy-plane was 0.04 °. A plot of the permanent dipole moment is shown in figure 4.

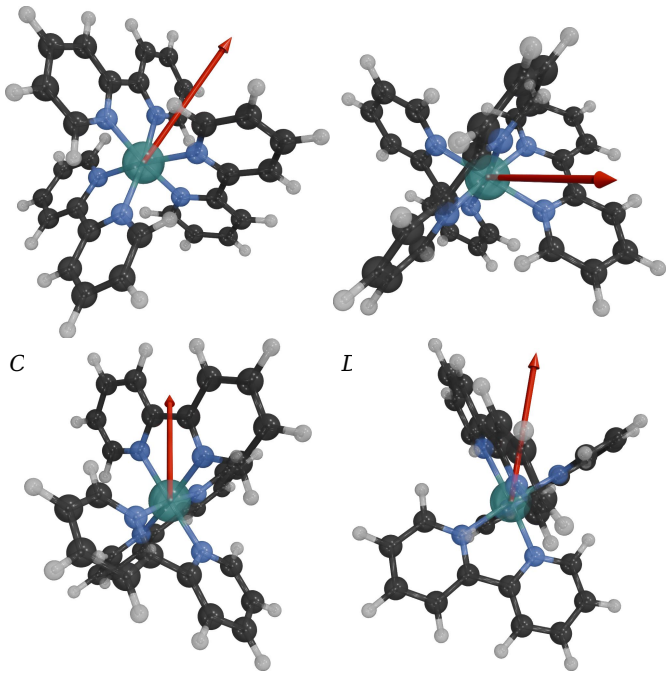


Figure 4: *The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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 0.11 D and 0.07 au respectively. The corresponding vector components (x,y,z) were μ = 0.05, -0.10, 0.03 D and m = -0.03, 0.06, 0.03 au. In comparison to the molecular geometry, the angle between each dipole moment and the longest axis of the molecule (the x-axis) was $\theta_{\mu,x}$ = 62.70 ° and $\theta_{m,x}$ = 64.89 °, while the angle between each dipole moment and the xy-plane was $\theta_{\mu,xy}$ = 13.66 ° and $\theta_{m,xy}$ = 27.10 °. 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 = 1.13e-19 esu·cm and m = 6.86e-22 erg·G^{-1}, while the **angle between the two dipole moments** was $\theta_{\mu,m}$ = 40.75 °. Correspondingly, the cosine of the angle was $\cos(\theta_{\mu,m})$ = 0.76, and the **dissymmetry factor** of the excited state transition was g_{lum} = 0.018. A plot of the electric and magnetic transition dipole moments is shown in figure 5.

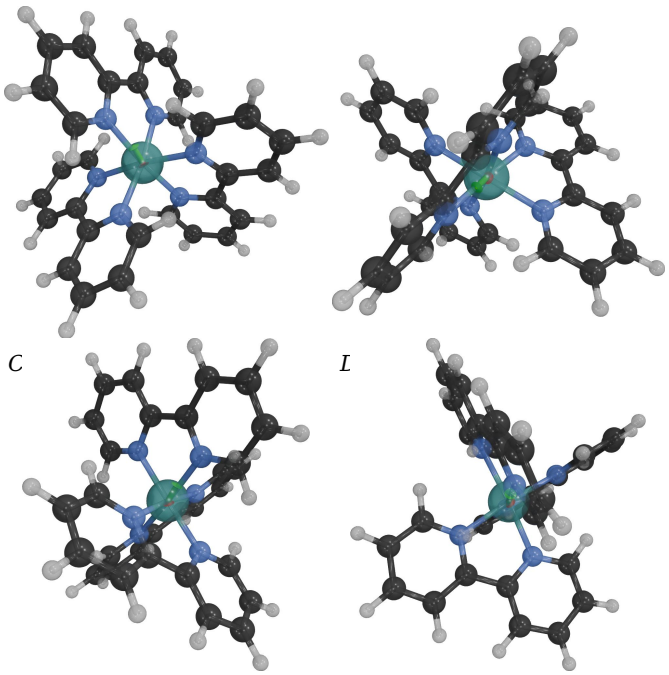


Figure 5: *The electric (red arrow) and magnetic (green arrow) transition (S_1) dipole moment plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D = 0.1 au. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

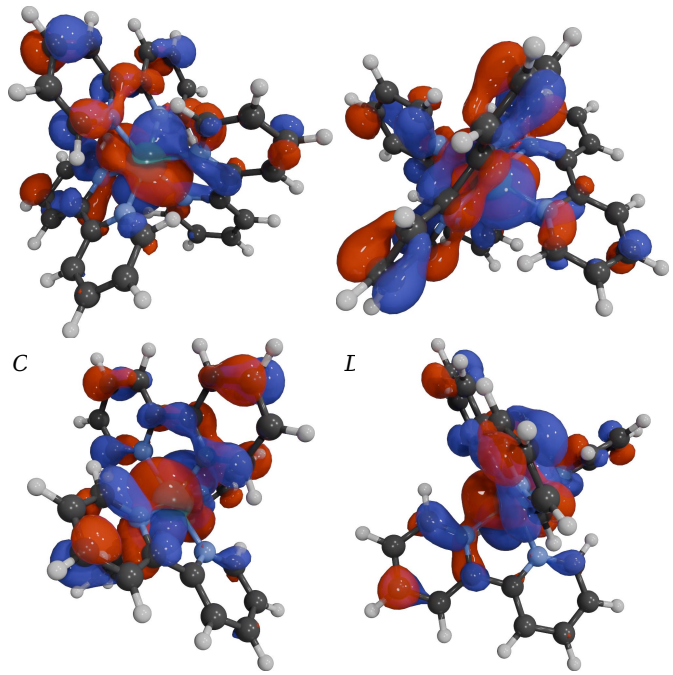


Figure 6: *Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Molecular Orbitals

In total, 828 doubly occupied molecular orbitals were calculated, divided into 130 occupied orbitals and 698 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO and LUMO** were -6.46 and -2.59 eV respectively, corresponding to a **HOMO-LUMO band gap** of 3.87 eV (figure 17). Plots of the orbital density for the HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2, LUMO+3, LUMO+6, LUMO+13 and LUMO+14 are shown in figures 6-9 and 11-16 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 10.

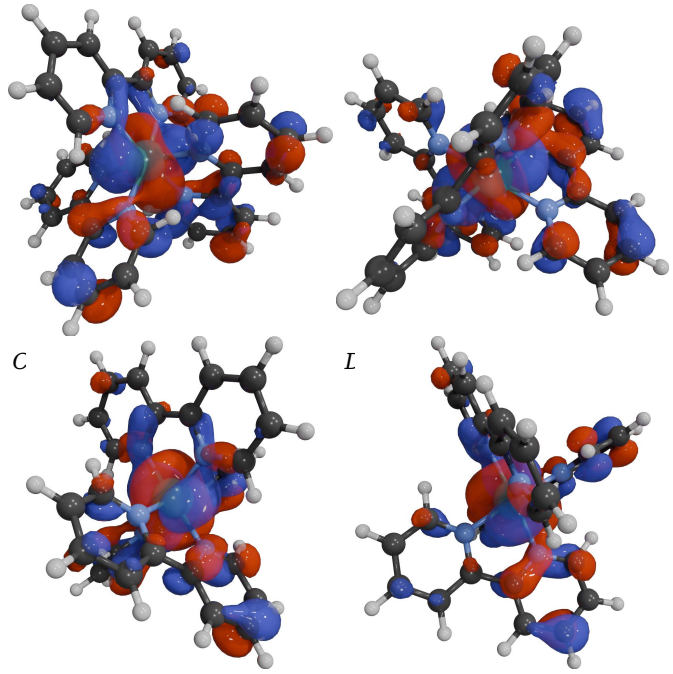


Figure 7: *Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

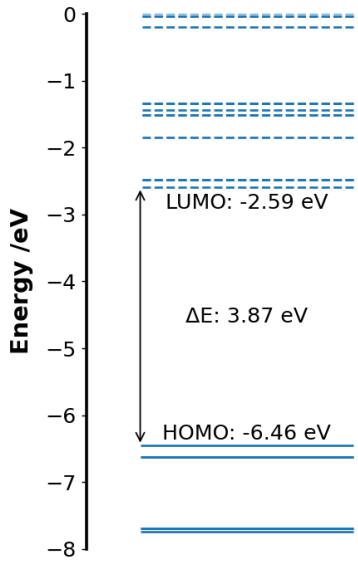


Figure 17: *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

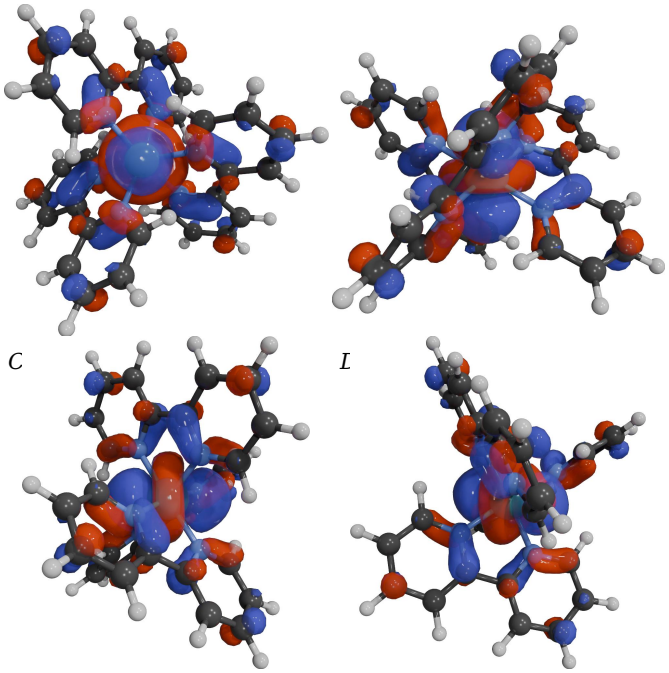


Figure 8: *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

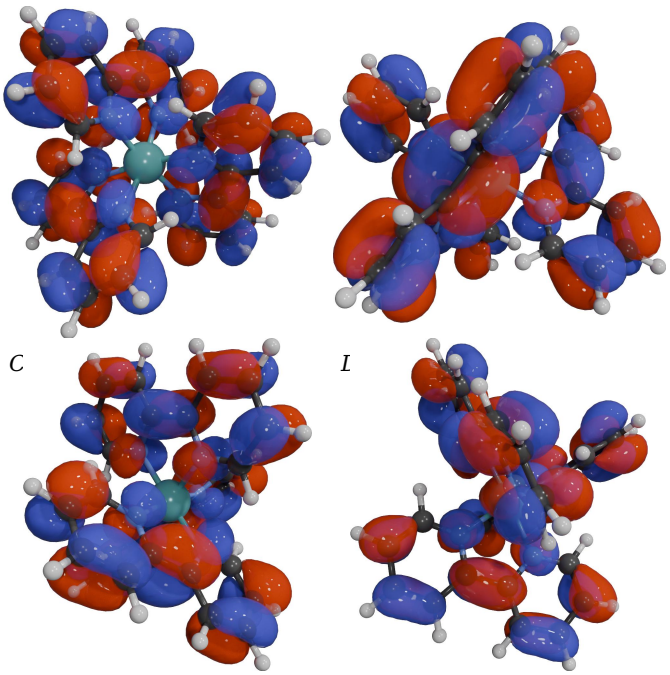


Figure 9: *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

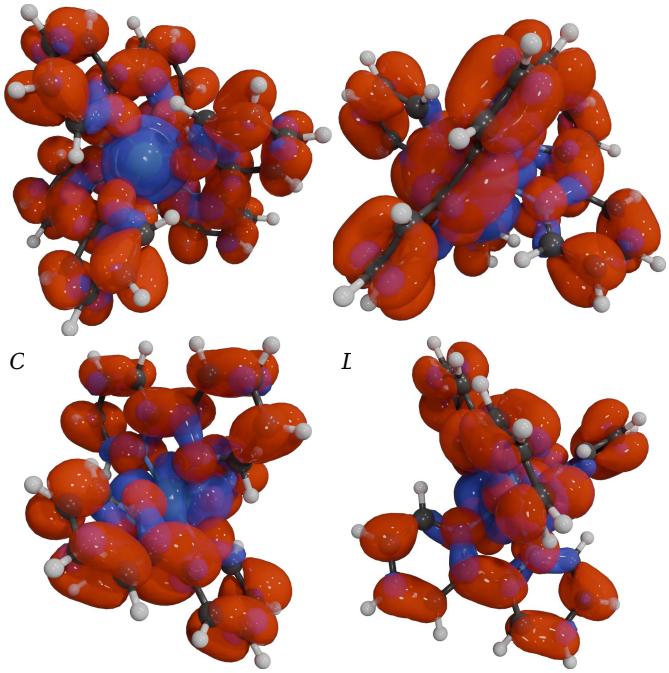


Figure 10: *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

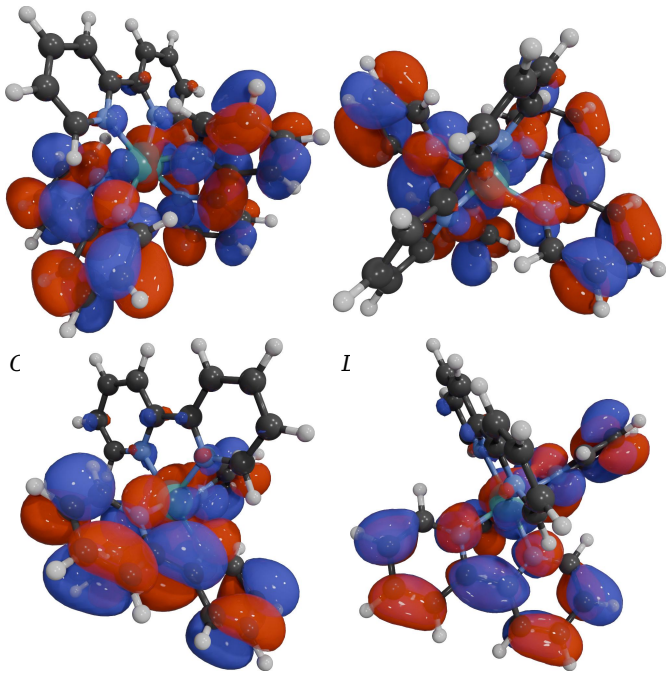


Figure 11: *Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

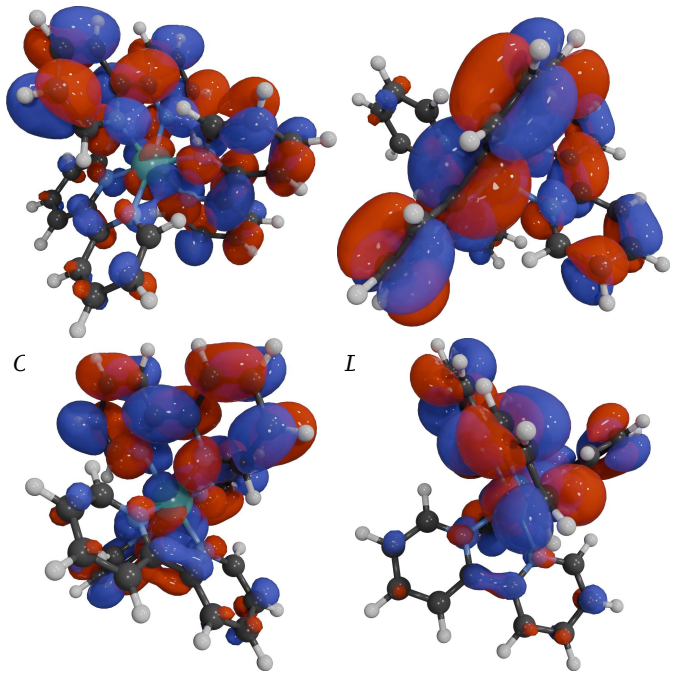


Figure 12: *Orbital density plots of the LUMO+2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

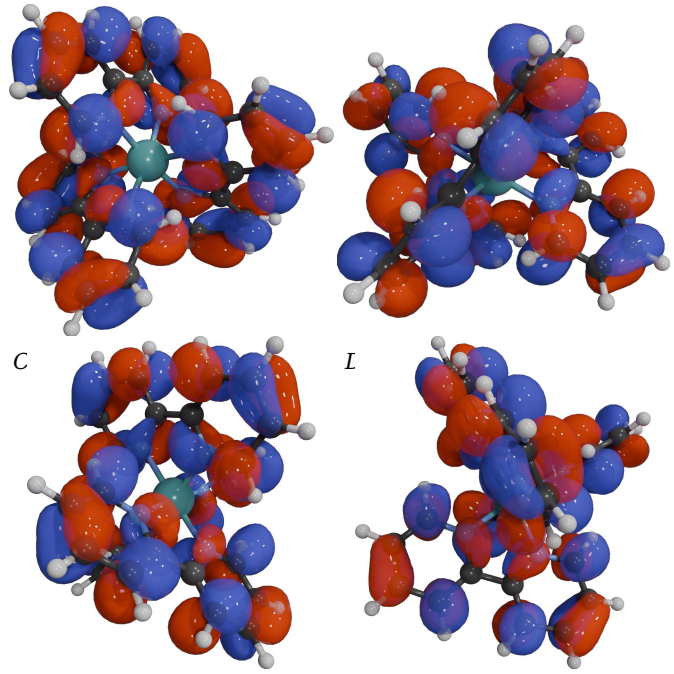


Figure 13: *Orbital density plots of the LUMO+3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

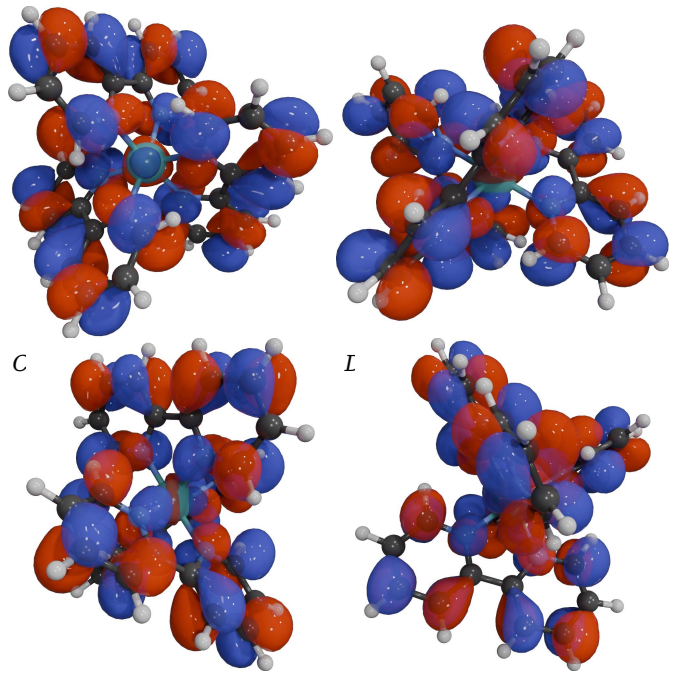


Figure 14: *Orbital density plots of the LUMO+6, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

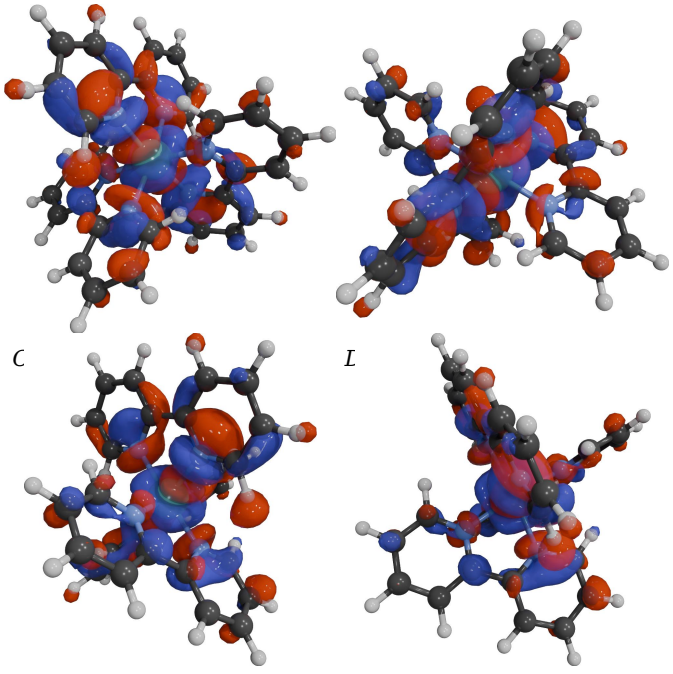


Figure 15: *Orbital density plots of the LUMO+13, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

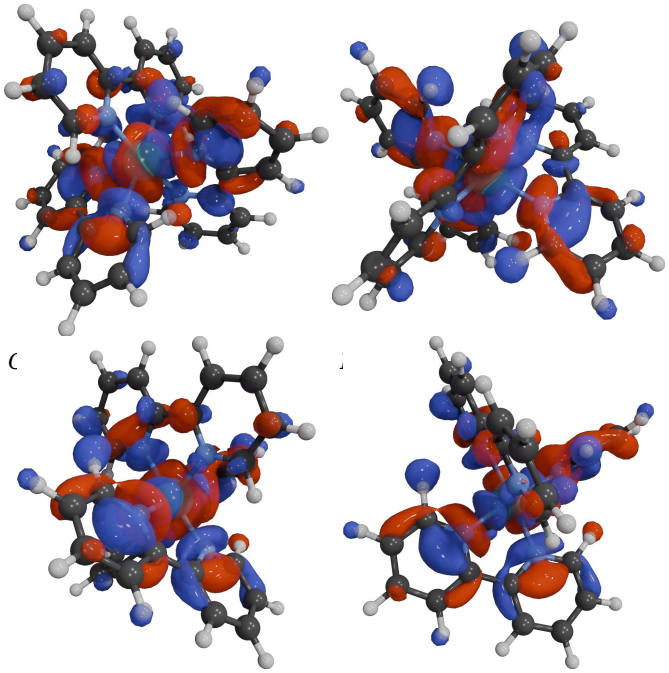


Figure 16: *Orbital density plots of the LUMO+14, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Excited States

In total, the energies of 20 electronic excited states were calculated (figure 18), 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 2.81 eV, corresponding to absorption by a photon with a wavelength of 442 nm, a blue 'color' and CIE coordinates of (0.16, 0.01), while the energy of the **T_1** was 2.64 eV (469 nm, blue , CIE: (0.13, 0.05)). The difference in energy between the S_1 and T_1 excited states **(ΔE_{ST})** was therefore 0.16 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 398 nm. The full simulated absorption spectrum is shown in figure 19. Finally, **natural transition orbitals (NTOs)** were calculated for each excited state and are shown in figures 20-39.

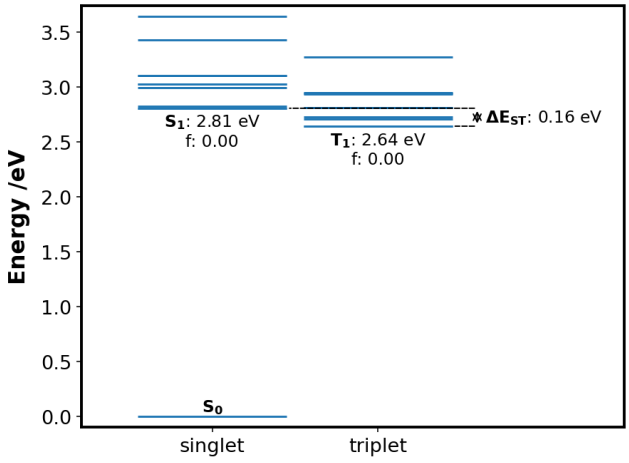


Figure 18: *Graph of the calculated excited states. f: oscillator strength of the relevant ground to excited state transition.*

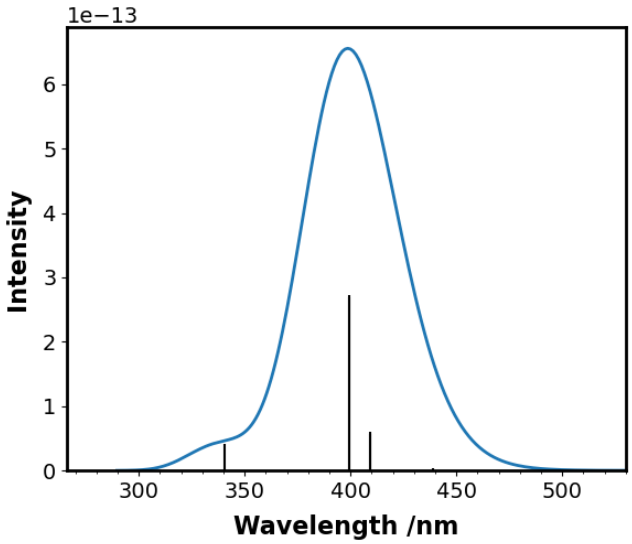


Figure 19: *Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 398 nm.*

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 298.98 cm^{-1}, while the H_{SO} between the **S_1 and T_1** excited states was 53.94 cm^{-1}. These values correspond to a first-order mixing coefficient ($\lambda = H_{SO}/\Delta E_{ST}$) of 0.01 and 0.04 respectively.

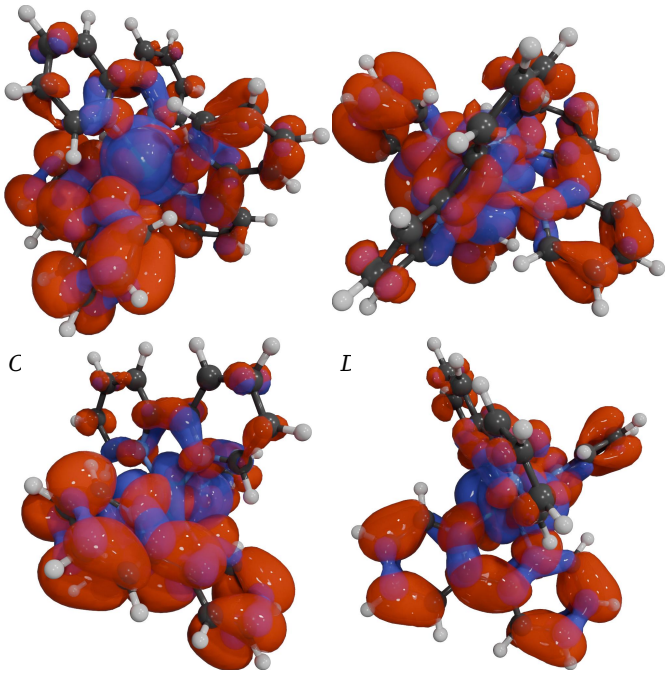


Figure 20: *Density plot of the NTO hole (red) & electron (blue) of the T_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

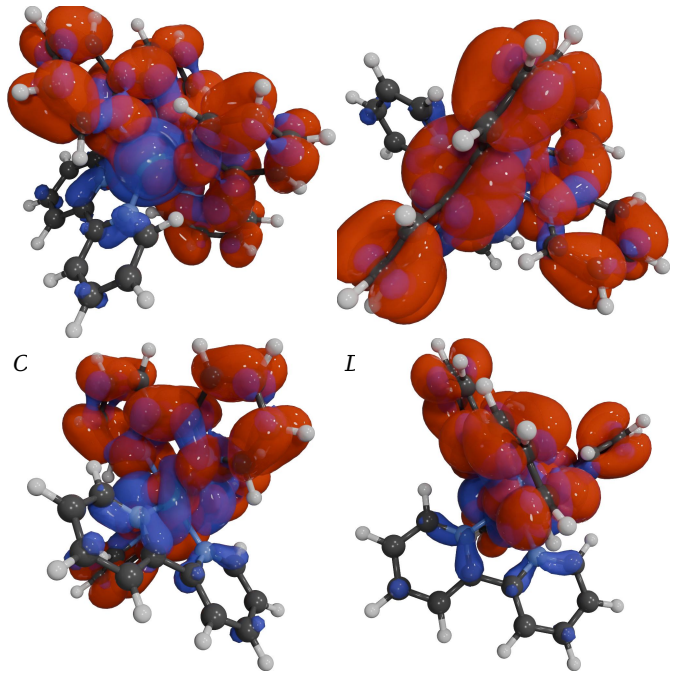


Figure 21: *Density plot of the NTO hole (red) & electron (blue) of the T_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

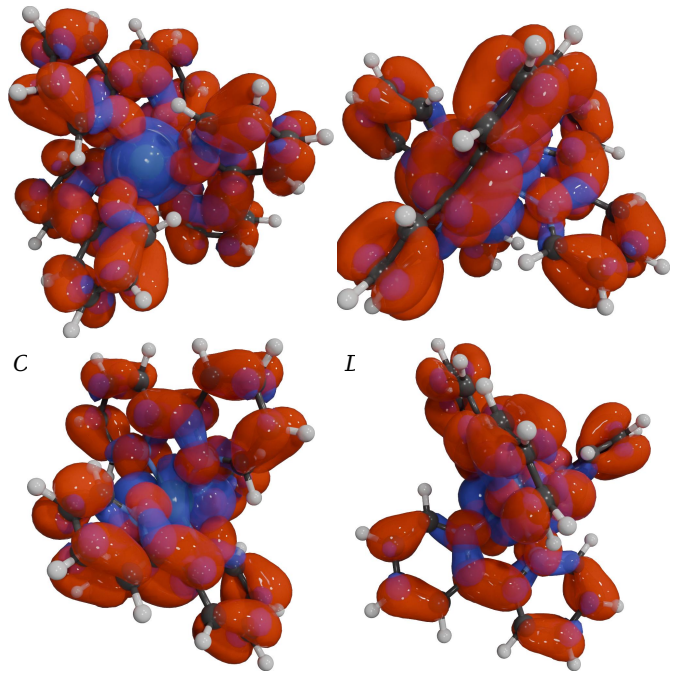


Figure 22: *Density plot of the NTO hole (red) & electron (blue) of the T_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

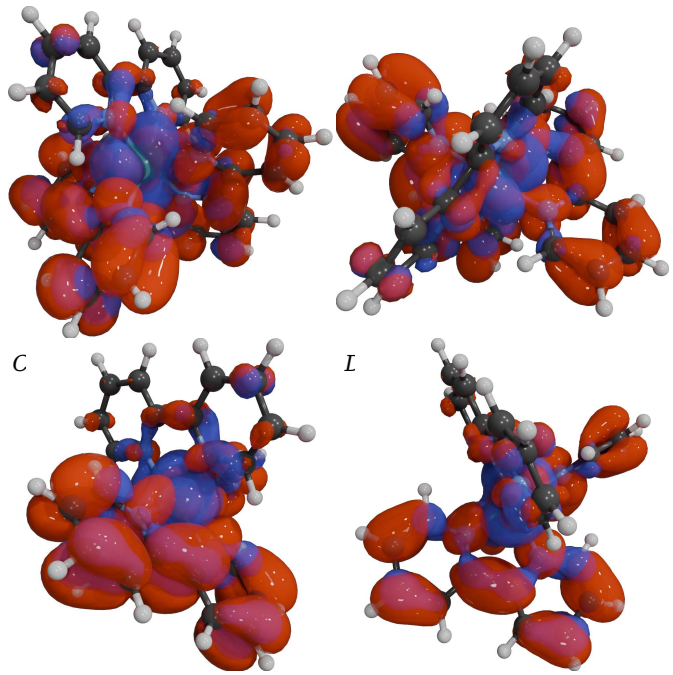


Figure 23: *Density plot of the NTO hole (red) & electron (blue) of the T_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

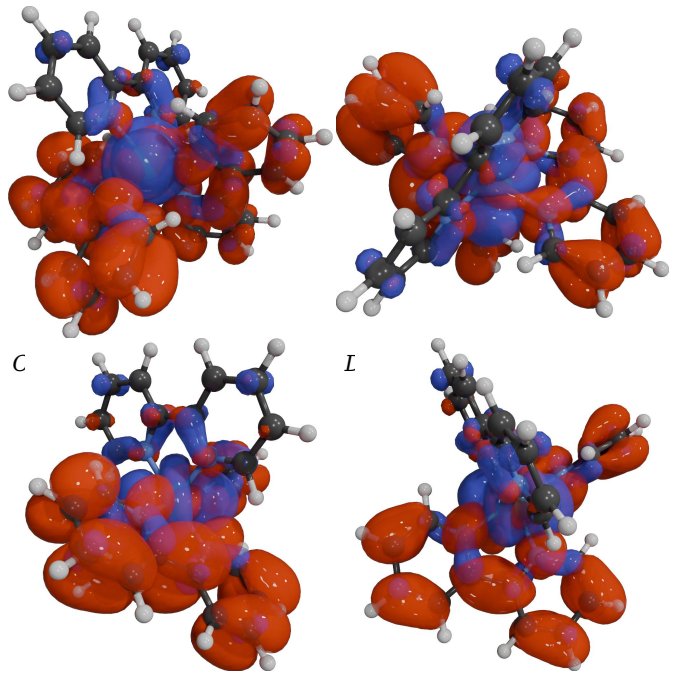


Figure 24: *Density plot of the NTO hole (red) & electron (blue) of the S_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

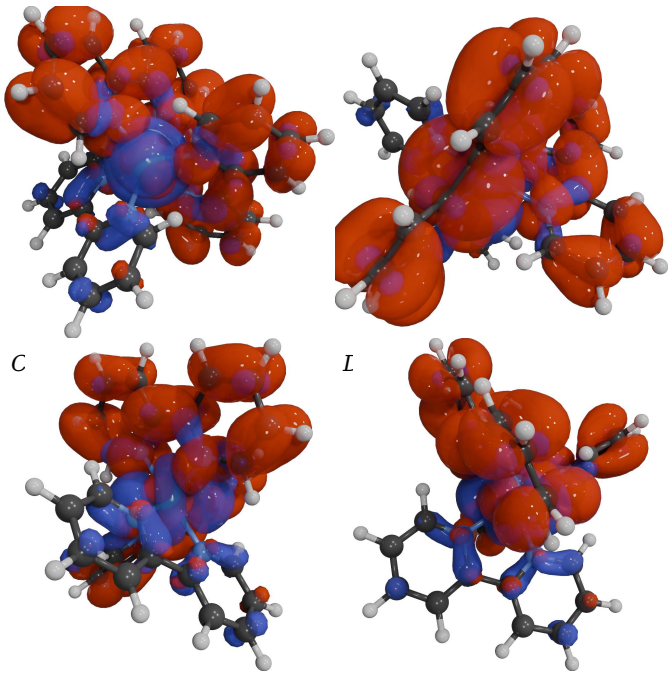


Figure 25: *Density plot of the NTO hole (red) & electron (blue) of the S_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

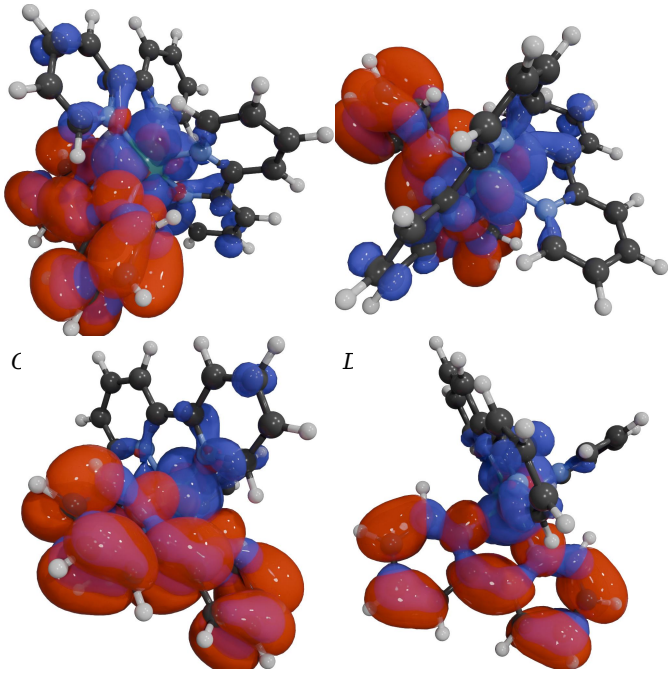


Figure 26: *Density plot of the NTO hole (red) & electron (blue) of the T_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

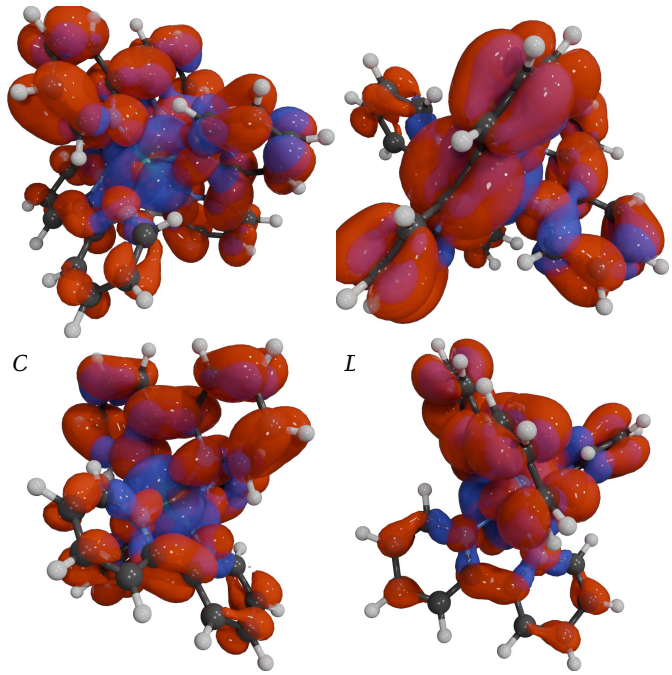


Figure 27: *Density plot of the NTO hole (red) & electron (blue) of the T_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

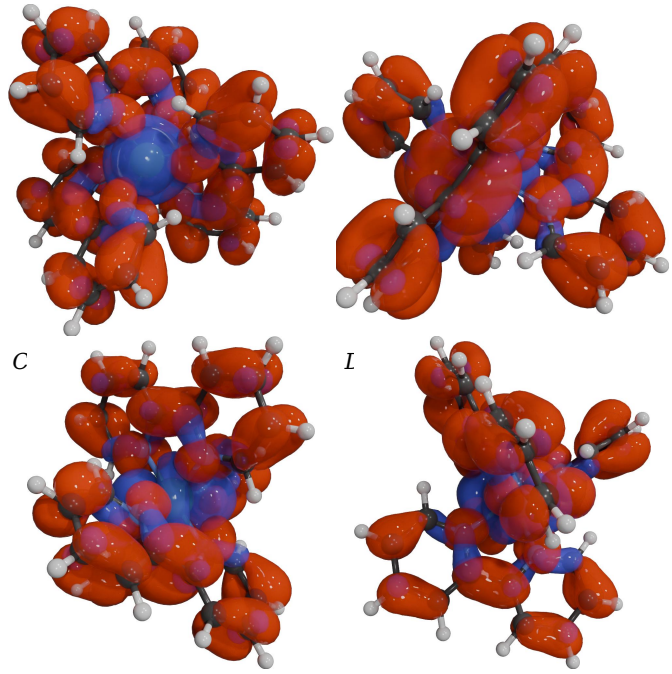


Figure 28: *Density plot of the NTO hole (red) & electron (blue) of the S_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

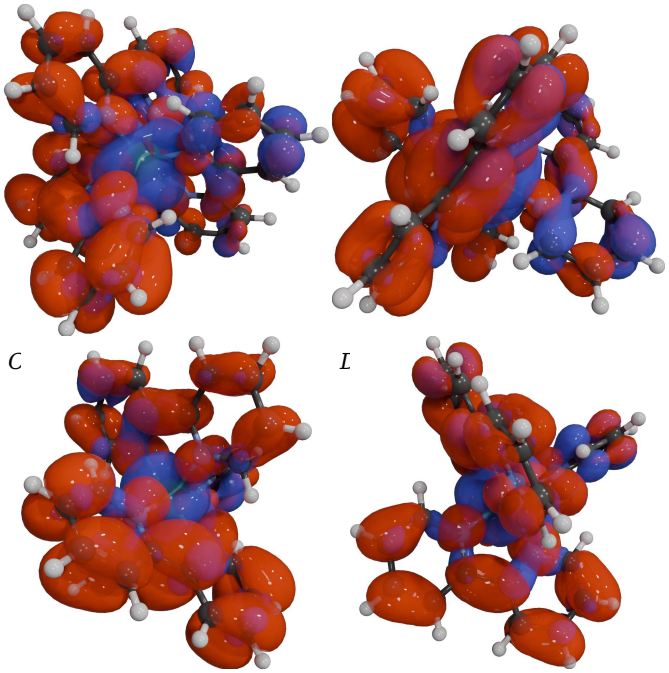


Figure 29: *Density plot of the NTO hole (red) & electron (blue) of the T_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

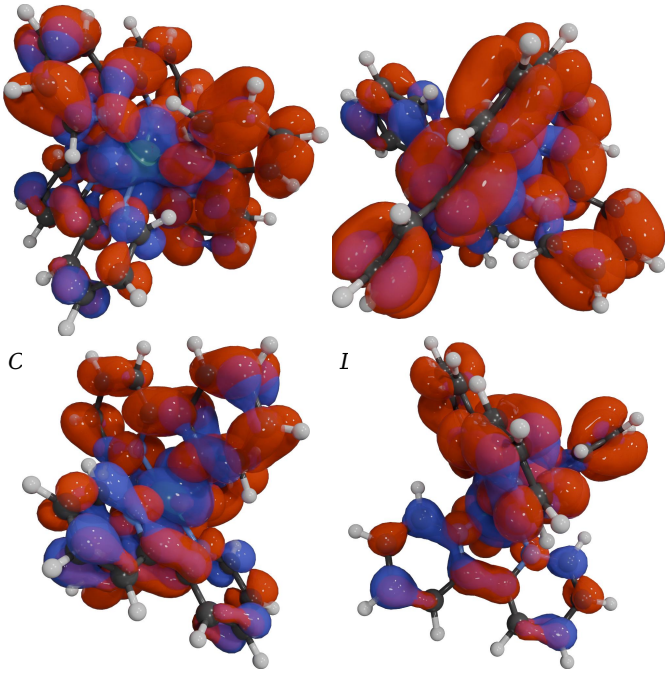


Figure 30: *Density plot of the NTO hole (red) & electron (blue) of the T_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

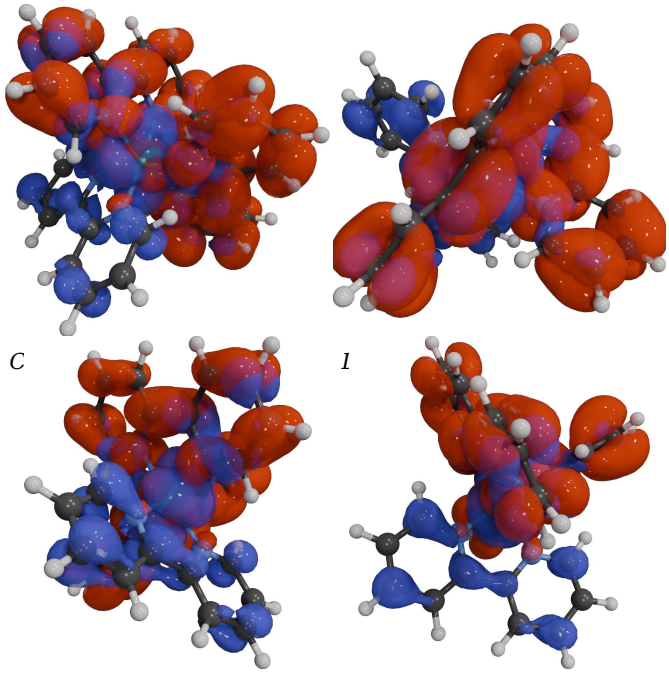


Figure 31: *Density plot of the NTO hole (red) & electron (blue) of the T_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

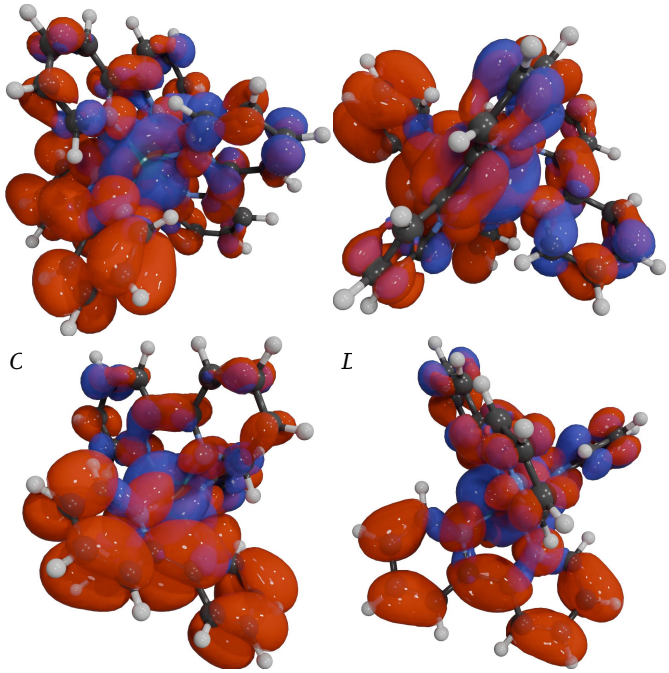


Figure 32: *Density plot of the NTO hole (red) & electron (blue) of the S_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

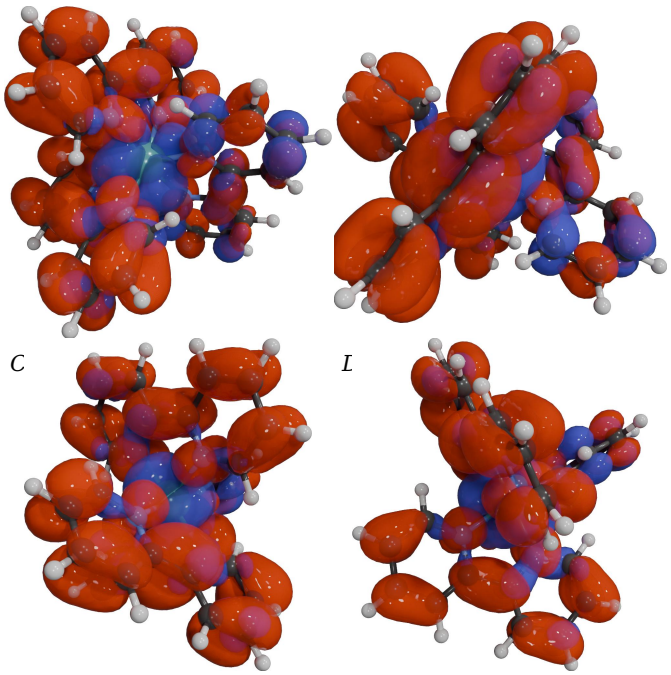


Figure 33: *Density plot of the NTO hole (red) & electron (blue) of the S_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

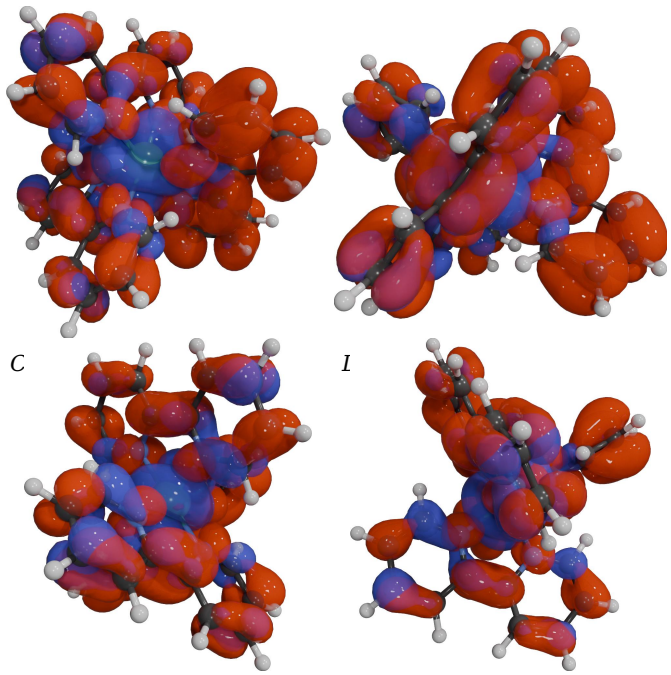


Figure 34: *Density plot of the NTO hole (red) & electron (blue) of the S_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

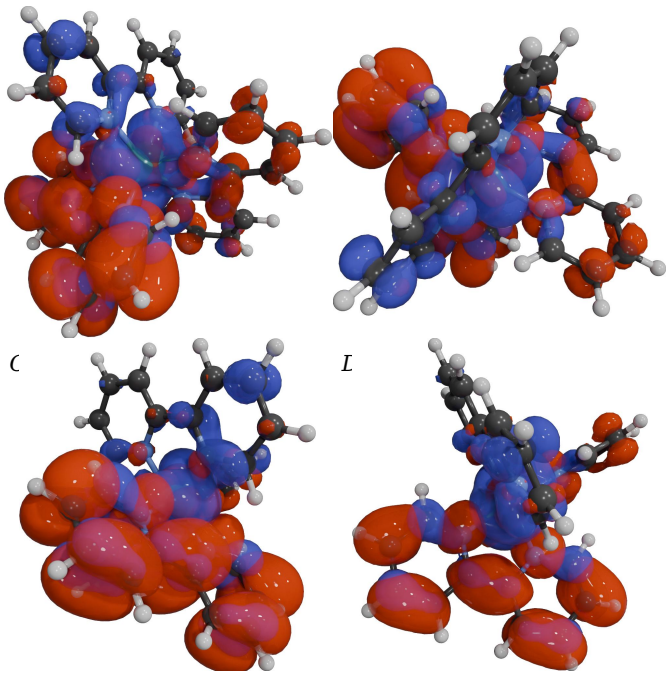


Figure 35: *Density plot of the NTO hole (red) & electron (blue) of the S_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

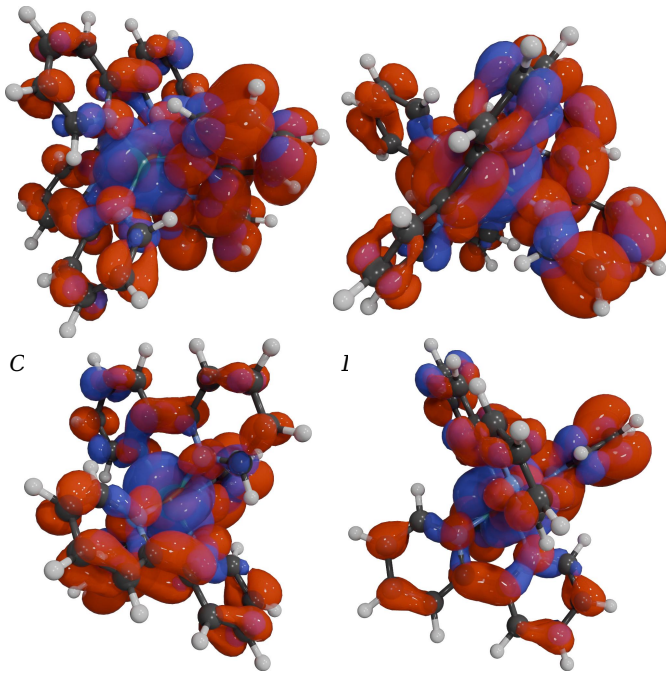


Figure 36: *Density plot of the NTO hole (red) & electron (blue) of the S_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

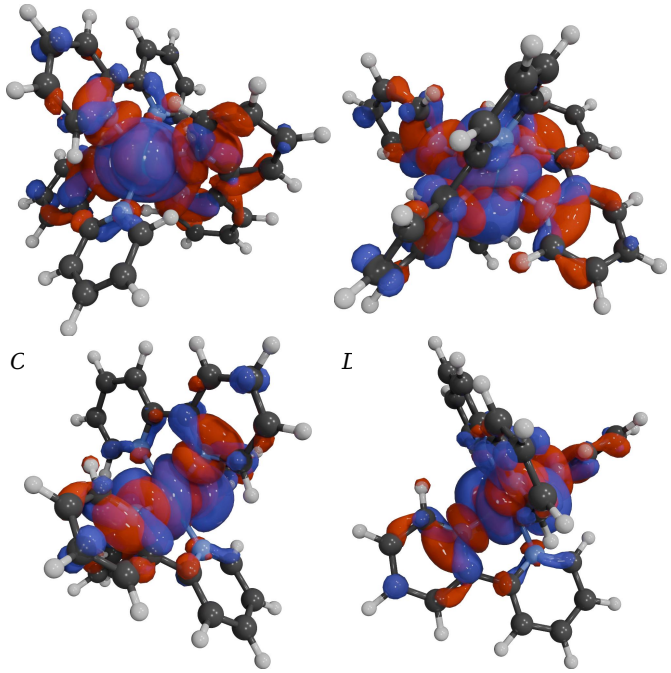


Figure 37: *Density plot of the NTO hole (red) & electron (blue) of the T_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

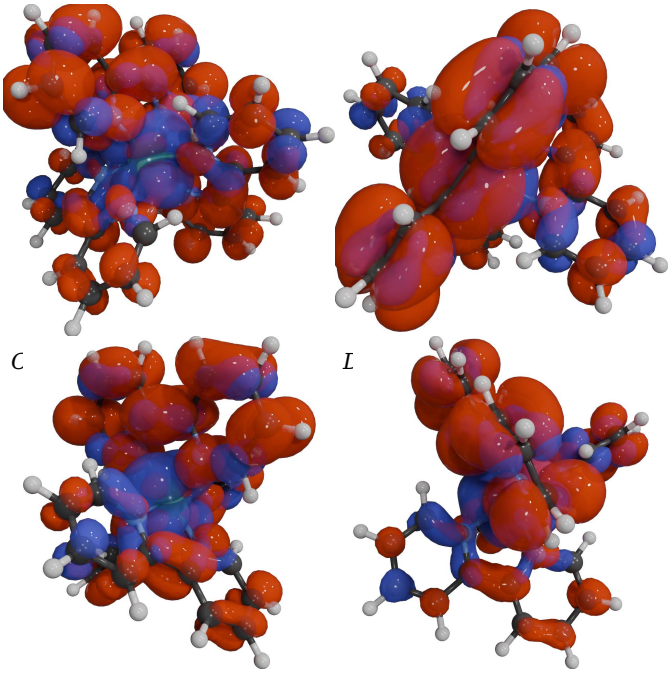


Figure 38: *Density plot of the NTO hole (red) & electron (blue) of the S_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

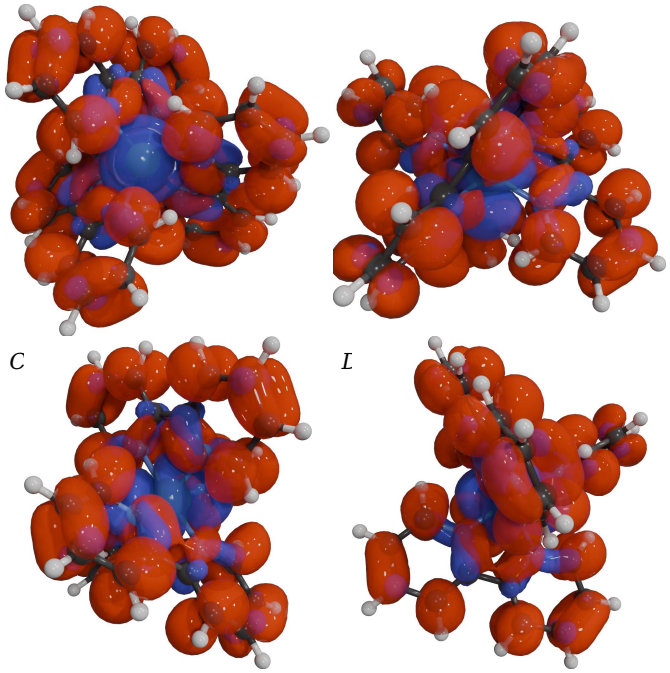


Figure 39: *Density plot of the NTO hole (red) & electron (blue) of the S_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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	Ru	Ru_1	0.0001900	-0.0002900	-0.0014390
2	N	N_2	1.3117040	-1.2320590	-1.0471890
3	C	C_3	2.5844240	-1.2636520	-0.5794290
4	C	C_4	3.5513710	-2.0681420	-1.1801290
5	C	C_5	3.2056320	-2.8511040	-2.2740590
6	C	C_6	1.8966270	-2.8128370	-2.7441890
7	C	C_7	0.9816510	-1.9915310	-2.1016890
8	H	H_4	4.5648980	-2.0875240	-0.7989790
9	H	H_5	3.9490750	-3.4816060	-2.7500690
10	H	H_6	1.5795840	-3.4064170	-3.5940390
11	H	H_7	-0.0478260	-1.9263790	-2.4340090
12	N	N_2	0.4098490	1.7503290	-1.0483090
13	N	N_2	-1.7221340	-0.5186900	-1.0477190
14	N	N_2	1.7745210	0.2879650	1.0455810
15	N	N_2	-0.6388630	-1.6805670	1.0455910
16	N	N_2	-1.1348780	1.3925420	1.0465410
17	C	C_3	2.8479170	-0.3978660	0.5801010
18	C	C_3	-0.1976700	2.8689110	-0.5800190
19	C	C_7	1.2301600	1.8424760	-2.1047790
20	C	C_3	-2.3880030	-1.6033690	-0.5790890
21	C	C_7	-2.2123340	0.1463450	-2.1037690
22	C	C_7	1.9234500	1.1022260	2.1003510
23	C	C_3	-1.7713400	-2.2647680	0.5811310
24	C	C_7	-0.0077390	-2.2187160	2.0991110
25	C	C_3	-1.0773950	2.6652040	0.5812010
26	C	C_7	-1.9127830	1.1141970	2.1024210
27	C	C_4	4.0979810	-0.2720540	1.1836510
28	C	C_4	0.0145300	4.1077210	-1.1828290
29	C	C_6	1.4831360	3.0447680	-2.7489690
30	H	H_7	1.6867080	0.9175330	-2.4374390
31	C	C_4	-3.5677110	-2.0378780	-1.1810890
32	C	C_6	-3.3809660	-0.2344910	-2.7470790
33	H	H_7	-1.6393160	1.0039760	-2.4364990
34	C	C_6	3.1399720	1.2713110	2.7453710
35	H	H_7	1.0329560	1.6242660	2.4306510
36	C	C_4	-2.2896080	-3.4090150	1.1854210
37	C	C_6	-0.4713830	-3.3558790	2.7443910
38	H	H_7	0.8913170	-1.7108610	2.4283910
39	C	C_4	-1.8095200	3.6852990	1.1866110
40	C	C_6	-2.6657310	2.0834360	2.7490510
41	H	H_7	-1.9188460	0.0818710	2.4323810
42	C	C_5	4.2473490	0.5705670	2.2777110
43	H	H_4	4.9490650	-0.8238380	0.8044510
44	C	C_5	0.8633800	4.1982390	-2.2785290
45	H	H_4	-0.4750220	4.9955950	-0.8022590
46	H	H_6	2.1537810	3.0659240	-3.6003490
47	C	C_5	-4.0706430	-1.3475250	-2.2764090
48	H	H_4	-4.0920250	-2.9057510	-0.8006090
49	H	H_6	-3.7347780	0.3360930	-3.5981490
50	H	H_6	3.2074960	1.9407560	3.5952810
51	C	C_5	-1.6342540	-3.9613590	2.2784510
52	H	H_4	-3.1949420	-3.8679450	0.8078310
53	H	H_6	0.0749760	-3.7506310	3.5933510
54	C	C_5	-2.6123340	3.3929510	2.2818110
55	H	H_4	-1.7572190	4.6988850	0.8087010
56	H	H_6	-3.2779940	1.8074210	3.5999310
57	H	H_5	5.2152690	0.6770260	2.7558310
58	H	H_5	1.0368850	5.1567040	-2.7560590
59	H	H_5	-4.9879310	-1.6757970	-2.7535390
60	H	H_5	-2.0275840	-4.8518390	2.7571910
61	H	H_5	-3.1872540	4.1778810	2.7615410

Molecular Orbitals

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

Level	Label	Symmetry	Energy /eV
146	LUMO+15	A	0.3293
145	LUMO+14	A	0.0291
144	LUMO+13	A	0.0286
143	LUMO+12	A	0.0125
142	LUMO+11	A	-0.0370
141	LUMO+10	A	-0.0381
140	LUMO+9	A	-0.1940
139	LUMO+8	A	-1.3377
138	LUMO+7	A	-1.3391
137	LUMO+6	A	-1.4384
136	LUMO+5	A	-1.5110
135	LUMO+4	A	-1.5121
134	LUMO+3	A	-1.8526
133	LUMO+2	A	-2.4811
132	LUMO+1	A	-2.4828
131	**LUMO**	**A**	**-2.5897**
130	**HOMO**	**A**	**-6.4570**
129	HOMO-1	A	-6.6252
128	HOMO-2	A	-6.6254
127	HOMO-3	A	-7.6929
126	HOMO-4	A	-7.6943
125	HOMO-5	A	-7.7482
124	HOMO-6	A	-9.0456
123	HOMO-7	A	-9.0462
122	HOMO-8	A	-9.0592
121	HOMO-9	A	-9.2075
120	HOMO-10	A	-9.2089
119	HOMO-11	A	-9.3773
118	HOMO-12	A	-9.4451
117	HOMO-13	A	-9.4538
116	HOMO-14	A	-9.6176
115	HOMO-15	A	-9.6181

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	2.6430	469.10	Blue (0.13, 0.05)	0.0000	HOMO → LUMO+1 (0.86) HOMO → LUMO+2 (0.04)
2	T_2	Triplet-A	2.6441	468.91	Blue (0.13, 0.05)	0.0000	HOMO → LUMO+2 (0.86) HOMO → LUMO+1 (0.04)
3	T_3	Triplet-A	2.7086	457.74	Blue (0.15, 0.03)	0.0000	HOMO → LUMO (0.89)
4	T_4	Triplet-A	2.7261	454.80	Blue (0.15, 0.02)	0.0000	HOMO-1 → LUMO+1 (0.40) HOMO-2 → LUMO+2 (0.39) HOMO-2 → LUMO+1 (0.07) HOMO-1 → LUMO+2 (0.07)
5	S_1	Singlet-A	2.8061	441.84	Blue (0.16, 0.01)	0.0001	HOMO → LUMO+1 (0.96)
6	S_2	Singlet-A	2.8077	441.59	Blue (0.16, 0.01)	0.0001	HOMO → LUMO+2 (0.96)
7	T_5	Triplet-A	2.8122	440.88	Blue (0.16, 0.01)	0.0000	HOMO-1 → LUMO+2 (0.31) HOMO-2 → LUMO+1 (0.30) HOMO-1 → LUMO (0.10) HOMO-2 → LUMO+2 (0.09) HOMO-1 → LUMO+1 (0.08) HOMO-2 → LUMO (0.06)
8	T_6	Triplet-A	2.8131	440.74	Blue (0.16, 0.01)	0.0000	HOMO-2 → LUMO+2 (0.31) HOMO-1 → LUMO+1 (0.31) HOMO-2 → LUMO (0.09) HOMO-2 → LUMO+1 (0.09) HOMO-1 → LUMO+2 (0.08) HOMO-1 → LUMO (0.06)
9	S_3	Singlet-A	2.8231	439.18	Blue (0.16, 0.01)	0.0033	HOMO → LUMO (0.98)
10	T_7	Triplet-A	2.9377	422.05	Blue (0.17, 0.01)	0.0000	HOMO-1 → LUMO (0.53) HOMO-2 → LUMO (0.27) HOMO-2 → LUMO+1 (0.04) HOMO-1 → LUMO+1 (0.04) HOMO-2 → LUMO+2 (0.03) HOMO-1 → LUMO+2 (0.02)
11	T_8	Triplet-A	2.9385	421.93	Blue (0.17, 0.01)	0.0000	HOMO-2 → LUMO (0.52) HOMO-1 → LUMO (0.26) HOMO-1 → LUMO+2 (0.04) HOMO-1 → LUMO+1 (0.04) HOMO-2 → LUMO+2 (0.03) HOMO-2 → LUMO+1 (0.03)
12	T_9	Triplet-A	2.9488	420.46	Blue (0.17, 0.01)	0.0000	HOMO-1 → LUMO+2 (0.39) HOMO-2 → LUMO+1 (0.38) HOMO-2 → LUMO+2 (0.08) HOMO-1 → LUMO+1 (0.06) HOMO → LUMO (0.05)
13	S_4	Singlet-A	2.9932	414.22	Violet (0.17, 0.00)	0.0002	HOMO-2 → LUMO+1 (0.42) HOMO-1 → LUMO+2 (0.41) HOMO-1 → LUMO+1 (0.08) HOMO-2 → LUMO+2 (0.07)
14	S_5	Singlet-A	3.0280	409.46	Violet (0.17, 0.00)	0.0481	HOMO-1 → LUMO (0.75) HOMO-2 → LUMO (0.13) HOMO-1 → LUMO+2 (0.04) HOMO-2 → LUMO+1 (0.03)
15	S_6	Singlet-A	3.0289	409.34	Violet (0.17, 0.00)	0.0503	HOMO-2 → LUMO (0.75) HOMO-1 → LUMO (0.13) HOMO-2 → LUMO+2 (0.04) HOMO-1 → LUMO+1 (0.03)
16	S_7	Singlet-A	3.1036	399.49	Ultraviolet (0.17, 0.00)	0.2167	HOMO-1 → LUMO+2 (0.24) HOMO-2 → LUMO+1 (0.24) HOMO-1 → LUMO+1 (0.20) HOMO-2 → LUMO+2 (0.20) HOMO-2 → LUMO (0.06) HOMO-1 → LUMO (0.04)
17	S_8	Singlet-A	3.1043	399.40	Ultraviolet (0.17, 0.00)	0.2192	HOMO-1 → LUMO+1 (0.24) HOMO-2 → LUMO+2 (0.24) HOMO-1 → LUMO+2 (0.20) HOMO-2 → LUMO+1 (0.20) HOMO-1 → LUMO (0.06) HOMO-2 → LUMO (0.04)

18	T_{10}	Triplet-A	3.2733	378.77	Ultraviolet ■ (0.17, 0.00)	0.0000	HOMO → LUMO+14 (0.42) HOMO → LUMO+13 (0.24) HOMO → LUMO+18 (0.08) HOMO → LUMO+10 (0.04) HOMO-2 → LUMO+13 (0.03) HOMO-1 → LUMO+14 (0.03) HOMO → LUMO+11 (0.02)
19	S_9	Singlet-A	3.4282	361.66	Ultraviolet ■ (0.18, 0.01)	0.0000	HOMO-2 → LUMO+2 (0.34) HOMO-1 → LUMO+1 (0.33) HOMO → LUMO+6 (0.13) HOMO-1 → LUMO+2 (0.06) HOMO-2 → LUMO+1 (0.06)
20	S_{10}	Singlet-A	3.6419	340.44	Ultraviolet ■ (0.00, 0.00)	0.0240	HOMO → LUMO+3 (0.98)

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	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
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
S_1	0.05, -0.10, 0.03	0.11	62.70	13.66	-0.03, 0.06, 0.03	0.07	64.89	27.10	1.13e-19	6.86e-22	40.75	0.76	0.018
S_2	0.10, 0.05, -0.00	0.11	27.09	1.71	-0.06, -0.03, -0.00	0.06	29.07	2.47	1.11e-19	6.02e-22	4.61	1.00	0.022
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
S_3	-0.00, -0.00, -0.55	0.55	89.82	89.59	-0.00, 0.00, -0.71	0.71	89.78	89.75	5.51e-19	6.60e-21	179.50	-1.00	-0.048
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_4	-0.00, 0.03, 0.13	0.13	88.14	76.74	-0.00, 0.01, 0.16	0.16	88.29	86.73	1.33e-19	1.49e-21	169.66	-0.98	-0.044
S_5	1.92, -0.72, 0.00	2.05	20.51	0.02	0.38, -0.15, 0.00	0.41	20.95	0.45	2.05e-18	3.77e-21	179.39	-1.00	-0.007
S_6	-0.76, -1.95, 0.00	2.09	68.80	0.07	-0.14, -0.38, 0.00	0.40	69.17	0.40	2.09e-18	3.76e-21	179.51	-1.00	-0.007
S_7	-2.51, -3.48, 0.00	4.29	54.21	0.00	0.16, 0.23, 0.00	0.28	54.23	0.10	4.29e-18	2.60e-21	0.10	1.00	0.002
S_8	3.50, -2.52, -0.00	4.32	35.74	0.00	-0.22, 0.16, -0.00	0.28	35.75	0.23	4.32e-18	2.55e-21	0.23	1.00	0.002
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_9	-0.01, -0.01, 0.00	0.01	51.65	3.95	-0.00, 0.00, 0.00	< 0.01	87.39	24.20	1.11e-20	2.04e-23	49.07	0.66	0.005
S_{10}	0.00, -0.00, 1.32	1.32	89.96	89.93	-0.00, -0.00, -0.15	0.15	89.48	89.15	1.32e-18	1.42e-21	0.87	1.00	0.004

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	211.4079	0.1242	211.4079	298.9760	0.0371	0.0140
S_0	T_2	211.7685	0.0781	211.7685	299.4859	0.0371	0.0140
S_0	T_3	2.9288	6.3637	2.9288	7.5929	0.0009	0.0003
S_0	T_4	0.4139	1.1408	0.4139	1.2822	0.0002	0.0001
S_0	T_5	102.3924	0.0207	102.3924	144.8047	0.0180	0.0064
S_0	T_6	102.7291	0.2861	102.7291	145.2812	0.0180	0.0064
S_0	T_7	99.4613	5.0107	99.4613	140.7488	0.0175	0.0059
S_0	T_8	101.3224	3.0430	101.3224	143.3238	0.0178	0.0060

S_0	T_9	7.2515	75.7552	7.2515	76.4462	0.0095	0.0032
S_0	T_{10}	697.7951	0.3430	697.7951	986.8314	0.1224	0.0374
S_1	T_1	38.1278	1.2821	38.1278	53.9361	0.0067	0.0410
S_1	T_2	35.3152	11.3073	35.3152	51.2072	0.0063	0.0392
S_1	T_3	37.5791	0.0240	37.5791	53.1449	0.0066	0.0676
S_1	T_4	209.1139	1.0302	209.1139	295.7336	0.0367	0.4583
S_1	T_5	197.5265	34.6701	197.5265	281.4880	0.0349	5.7213
S_1	T_6	189.1665	6.4044	189.1665	267.5985	0.0332	4.7397
S_1	T_7	104.5409	9.0737	104.5409	148.1214	0.0184	0.1395
S_1	T_8	70.5623	17.6249	70.5623	101.3346	0.0126	0.0949
S_1	T_9	200.7486	0.2575	200.7486	283.9016	0.0352	0.2467
S_1	T_{10}	71.3554	97.5969	71.3554	140.3864	0.0174	0.0373
S_2	T_1	36.4708	11.3492	36.4708	52.8114	0.0065	0.0398
S_2	T_2	37.0964	1.4116	37.0964	52.4812	0.0065	0.0398
S_2	T_3	37.8892	0.3156	37.8892	53.5843	0.0066	0.0670
S_2	T_4	205.1946	0.4381	205.1946	290.1893	0.0360	0.4409
S_2	T_5	195.5533	6.1274	195.5533	276.6220	0.0343	7.6215
S_2	T_6	194.8670	34.5697	194.8670	277.7433	0.0344	6.3770
S_2	T_7	71.8072	17.3429	71.8072	103.0210	0.0128	0.0983
S_2	T_8	84.8499	8.9382	84.8499	120.3283	0.0149	0.1141
S_2	T_9	209.9434	1.4001	209.9434	296.9081	0.0368	0.2609
S_2	T_{10}	71.2210	128.9131	71.2210	163.5954	0.0203	0.0436
S_3	T_1	28.5080	0.1857	28.5080	40.3169	0.0050	0.0278
S_3	T_2	31.6124	0.5694	31.6124	44.7103	0.0055	0.0310
S_3	T_3	2.1579	0.1005	2.1579	3.0534	0.0004	0.0033
S_3	T_4	8.5556	13.6183	8.5556	18.2168	0.0023	0.0233
S_3	T_5	110.1942	1.7049	110.1942	155.8474	0.0193	1.7727
S_3	T_6	125.1098	0.6273	125.1098	176.9330	0.0219	2.1937
S_3	T_7	258.4974	0.2153	258.4974	365.5706	0.0453	0.3955
S_3	T_8	266.0052	1.0885	266.0052	376.1898	0.0466	0.4042
S_3	T_9	26.0525	0.2880	26.0525	36.8450	0.0046	0.0363
S_3	T_{10}	15.0694	3.7417	15.0694	21.6374	0.0027	0.0060
S_4	T_1	201.0719	0.3150	201.0719	284.3588	0.0353	0.1007
S_4	T_2	196.8504	0.3907	196.8504	278.3889	0.0345	0.0989
S_4	T_3	3.1392	3.2945	3.1392	5.5284	0.0007	0.0024
S_4	T_4	0.4241	292.7140	0.4241	292.7147	0.0363	0.1359
S_4	T_5	12.5077	2.3497	12.5077	17.8440	0.0022	0.0122
S_4	T_6	13.4156	1.2595	13.4156	19.0143	0.0024	0.0131
S_4	T_7	45.4381	1.5045	45.4381	64.2768	0.0080	0.1436
S_4	T_8	44.5218	3.0702	44.5218	63.0382	0.0078	0.1429
S_4	T_9	1.5432	0.0857	1.5432	2.1841	0.0003	0.0061
S_4	T_{10}	41.7381	0.7664	41.7381	59.0316	0.0073	0.0261
S_5	T_1	67.6202	8.1802	67.6202	95.9787	0.0119	0.0309
S_5	T_2	73.0399	12.7943	73.0399	104.0833	0.0129	0.0336
S_5	T_3	262.7646	0.3247	262.7646	371.6054	0.0461	0.1442
S_5	T_4	5.0550	2.8454	5.0550	7.6943	0.0010	0.0032
S_5	T_5	12.9349	181.2835	12.9349	182.2041	0.0226	0.1047
S_5	T_6	12.6069	100.2605	12.6069	101.8334	0.0126	0.0588
S_5	T_7	15.9554	48.1407	15.9554	53.1665	0.0066	0.0730
S_5	T_8	17.7493	211.3870	17.7493	212.8721	0.0264	0.2949
S_5	T_9	68.8440	9.6253	68.8440	97.8348	0.0121	0.1532
S_5	T_{10}	8.9026	23.3135	8.9026	26.4958	0.0033	0.0134
S_6	T_1	64.9058	13.4651	64.9058	92.7730	0.0115	0.0298

S_6	T_2	67.3788	7.9199	67.3788	95.6166	0.0119	0.0308
S_6	T_3	264.8289	0.6842	264.8289	374.5253	0.0464	0.1450
S_6	T_4	4.8672	2.9945	4.8672	7.5064	0.0009	0.0031
S_6	T_5	12.7101	101.1102	12.7101	102.6955	0.0127	0.0588
S_6	T_6	12.2511	177.1181	12.2511	177.9635	0.0221	0.1022
S_6	T_7	12.6501	214.4609	12.6501	215.2058	0.0267	0.2926
S_6	T_8	12.4084	46.8154	12.4084	49.9962	0.0062	0.0686
S_6	T_9	70.5789	9.3017	70.5789	100.2460	0.0124	0.1552
S_6	T_{10}	9.4300	4.9143	9.4300	14.2127	0.0018	0.0072
S_7	T_1	196.6403	30.1123	196.6403	279.7169	0.0347	0.0753
S_7	T_2	194.5490	10.1651	194.5490	275.3216	0.0341	0.0743
S_7	T_3	84.2138	0.2299	84.2138	119.0965	0.0148	0.0374
S_7	T_4	6.8932	0.3961	6.8932	9.7565	0.0012	0.0032
S_7	T_5	31.4730	57.8156	31.4730	72.9640	0.0090	0.0310
S_7	T_6	31.5324	226.9085	31.5324	231.2489	0.0287	0.0987
S_7	T_7	40.8742	195.1003	40.8742	203.4835	0.0252	0.1521
S_7	T_8	40.6442	7.6861	40.6442	57.9911	0.0072	0.0435
S_7	T_9	12.4189	10.2631	12.4189	20.3418	0.0025	0.0163
S_7	T_{10}	26.4394	51.5846	26.4394	63.7107	0.0079	0.0465
S_8	T_1	192.6165	9.4027	192.6165	272.5632	0.0338	0.0733
S_8	T_2	195.0215	30.7147	195.0215	277.5071	0.0344	0.0748
S_8	T_3	91.5890	0.1102	91.5890	129.5265	0.0161	0.0406
S_8	T_4	7.0584	1.0640	7.0584	10.0386	0.0012	0.0033
S_8	T_5	31.2831	223.2485	31.2831	227.5898	0.0282	0.0966
S_8	T_6	31.1075	57.6486	31.1075	72.5171	0.0090	0.0309
S_8	T_7	39.2107	8.7248	39.2107	56.1345	0.0070	0.0418
S_8	T_8	40.0552	198.8434	40.0552	206.7548	0.0256	0.1546
S_8	T_9	18.5921	6.9184	18.5921	27.1882	0.0034	0.0217
S_8	T_{10}	26.4440	95.6161	26.4440	102.6694	0.0127	0.0753
S_9	T_1	188.2838	0.4235	188.2838	266.2739	0.0330	0.0420
S_9	T_2	189.2836	0.3257	189.2836	267.6876	0.0332	0.0423
S_9	T_3	2.4643	52.2183	2.4643	52.3344	0.0065	0.0090
S_9	T_4	0.0690	0.5185	0.0690	0.5276	0.0001	0.0001
S_9	T_5	23.4105	0.5685	23.4105	33.1123	0.0041	0.0067
S_9	T_6	23.1784	0.1856	23.1784	32.7797	0.0041	0.0066
S_9	T_7	34.7382	13.7705	34.7382	51.0207	0.0063	0.0129
S_9	T_8	34.9168	9.4731	34.9168	50.2803	0.0062	0.0127
S_9	T_9	2.3275	271.0705	2.3275	271.0905	0.0336	0.0701
S_9	T_{10}	2.6316	0.1233	2.6316	3.7237	0.0005	0.0030
S_{10}	T_1	1.6672	0.2525	1.6672	2.3713	0.0003	0.0003
S_{10}	T_2	1.6028	0.0406	1.6028	2.2670	0.0003	0.0003
S_{10}	T_3	0.0238	0.0181	0.0238	0.0383	< 0.0001	< 0.0001
S_{10}	T_4	0.1631	1.9249	0.1631	1.9387	0.0002	0.0003
S_{10}	T_5	6.4014	0.0526	6.4014	9.0531	0.0011	0.0014
S_{10}	T_6	6.2870	0.1515	6.2870	8.8925	0.0011	0.0013
S_{10}	T_7	6.3587	0.0078	6.3587	8.9925	0.0011	0.0016
S_{10}	T_8	6.3019	0.0092	6.3019	8.9122	0.0011	0.0016
S_{10}	T_9	0.3921	0.2034	0.3921	0.5906	0.0001	0.0001
S_{10}	T_{10}	4.6862	0.2868	4.6862	6.6335	0.0008	0.0022

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