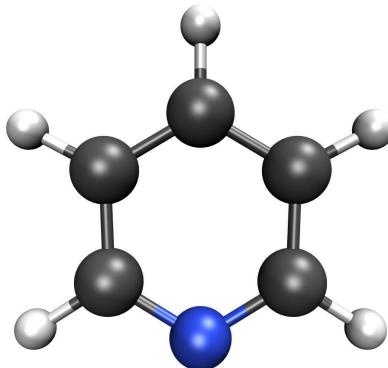




A Report On The Calculation Of The Excited States Of Pyridine At The PBE1PBE/6-31G(d,p) Level

osl - 15th June 2022



Abstract

The calculation of excited states for the system 'Pyridine' is presented, accompanied by automated analysis and image generation provided by the Silico 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 -6748.61 eV after 1 step. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -7.28 and -0.51 eV respectively, corresponding to a HOMO-LUMO band gap of 6.77 eV. The permanent dipole moment (PDM) was calculated to be 0.44 D. In total, 20 excited states were calculated with singlet and triplet multiplicity. The most intense absorption peaks were calculated to be at 154, 180, 213 and 243 nm. The lowest energy singlet and triplet excited states (S_1 and T_1) were calculated to be 5.07 and 4.28 eV (244 and 290 nm) respectively, corresponding to a singlet/triplet splitting energy (ΔE_{ST}) of 0.80 eV.

Table 1: Summary of overall calculation metadata. [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. [b]: Pressure used for thermochemistry analysis.

Date ^[a]	Duration ^[b]	Success (Converged)	Computational package	Level of theory	Calculations	Wavefunction	Multiplicity	T ^[c] / K	P ^[d] / atm
15/06/2022 23:33:59	4 m, 13 s	True (N/A)	Gaussian (2016+C. 01)	PBE1PBE/ 6-31G(d,p)	Excited States	restricted	1 (singlet)	N/A	N/A

Summary Of Results

Scf Energy

Table 2: Summary of SCF energy properties.

No. of steps	1
Final energy	-6748.6129 eV
Final energy	-651,142 kJ·mol ⁻¹

Geometry

Table 3: Summary of geometry properties.

Formula	C ₅ NH ₅
Exact mass	79.0422 g·mol ⁻¹
Molar mass	79.0999 g·mol ⁻¹
Alignment method	Minimal
X extension	4.31 Å
Y extension	3.89 Å
Z extension	0.00 Å
Linearity ratio	0.10
Planarity ratio	1.00

Molecular Orbitals

Table 4: Summary of HOMO & LUMO properties.

E _{HOMO,LUMO}	6.77 eV
E _{HOMO}	-7.28 eV
E _{LUMO}	-0.51 eV

Permanent Dipole Moment

Table 5: Summary of the permanent dipole moment properties.

Total	0.44 D
X axis angle	90.00 °

XY plane angle

0.13 °

S₁ 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	0.59 D
$\theta_{\mu,x}$	90.00 °
$\theta_{\mu,xy}$	89.98 °
$m^{[d]}$	0.69 a.u.
$\theta_{m,x}$	0.00 °
$\theta_{m,xy}$	0.00 °
μ (Gaussian-CGS)	5.88e-19 esu·cm
m (Gaussian-CGS)	6.41e-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 _{S₁}	5.07 eV
λ_{S_1} (colour, CIE)	244 nm (Ultraviolet ■, (0.00, 0.00))
	0.01

f_{S_1}	
No. calculated triplets	10
E_{T_1}	4.28 eV
λ_{T_1} (colour, CIE)	290 nm (Ultraviolet ■ (0.00, 0.00))
f_{T_1}	0.00
ΔE_{ST}	0.80 eV
Simulated Absorption Peaks	154, 180, 213 and 243 nm

Spin-Orbit Coupling

Table 8: Summary of the calculated spin-orbit coupling values.

$\langle S_0 H_{SO} T_1 \rangle:$	23.86 cm ⁻¹
$\langle S_0 \lambda T_1 \rangle:$	0.00
$\langle S_1 H_{SO} T_1 \rangle:$	0.02 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 **6-31G(d,p)** basis set. It was completed on the **15th June 2022** after a total duration of **4 m, 13 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 Silico 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 library⁸ and the Weasyprint library⁹, 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 -6748.61 eV, corresponding to -651,142 KJmol⁻¹. A plot of the total SCF electron density is shown in figure 1.

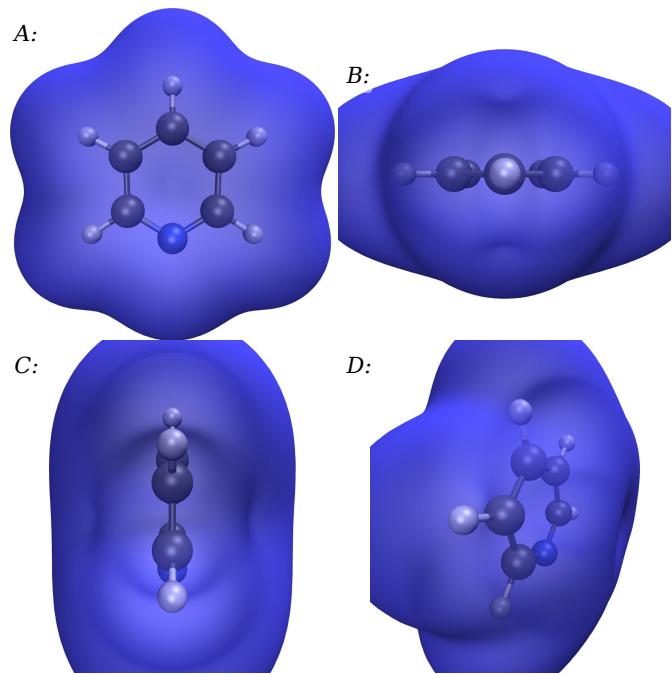


Figure 1: Plot of the total SCF electron density, plotted with an isovalue of 0.0004. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Geometry

The **empirical formula** of the studied system was C_5NH_5 , corresponding to a **molecular mass** of 79.10 gmol⁻¹ and an **exact mass**, considering only specific atomic isotopes, of 79.04 gmol⁻¹. The molecular geometry was aligned to the cartesian (X, Y and Z) axes by the **Minimal (MIN)** method. 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 4.31, 3.89 and 0.00 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 0.10 and 1.00 respectively.

Permanent Dipole Moment

The calculated **permanent dipole moment** was 0.44 D, with a vector (x,y,z) of 0.00, -0.44, 0.00 D. The angle between the dipole moment vector and the x-axis was 90.00 °, while the angle between the dipole moment and the xy-plane was 0.13 °. A plot of the permanent dipole moment is shown in figure 2.

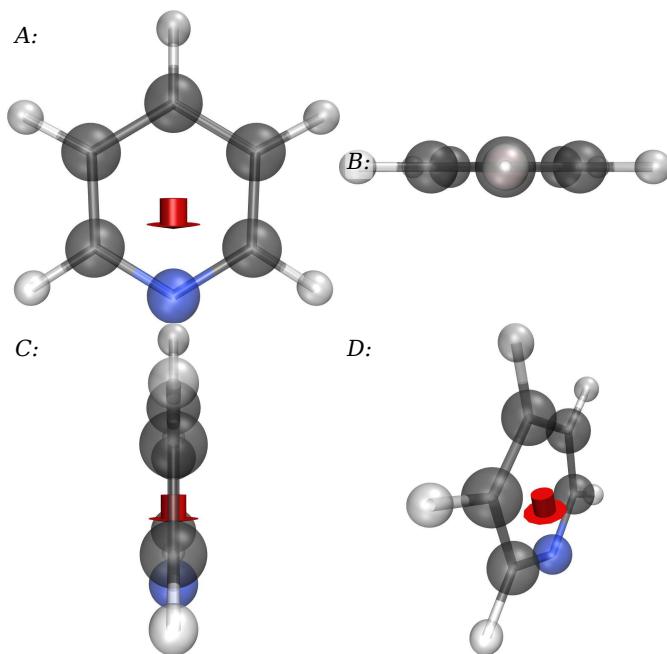


Figure 2: The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of $1 \text{ \AA} = 1.0 \text{ D}$. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

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 0.59 D and 0.69 au respectively. The corresponding vector components (x,y,z) were $\mu = 0.00, -0.00, 0.59 \text{ D}$ and $m = 0.69, 0.00, 0.00 \text{ au}$. In comparison to the molecular geometry, the angle between each dipole moment and the longest axis of the molecule (the x-axis) was $\theta_{\mu,x} = 90.00^\circ$ and $\theta_{m,x} = 0.00^\circ$, while the angle between each dipole moment and the xy-plane was $\theta_{\mu,xy} = 89.98^\circ$ and $\theta_{m,xy} = 0.00^\circ$. In Gaussian-CGS units, in which the magnetic and electric transition dipole moments can be directly compared, the magnitude of each dipole moment was $\mu = 5.88e-19 \text{ esu}\cdot\text{cm}$ and $m = 6.41e-21 \text{ erg}\cdot\text{G}^{-1}$, while the **angle between the two dipole moments** was $\theta_{\mu,m} = 90.00^\circ$. 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 3.

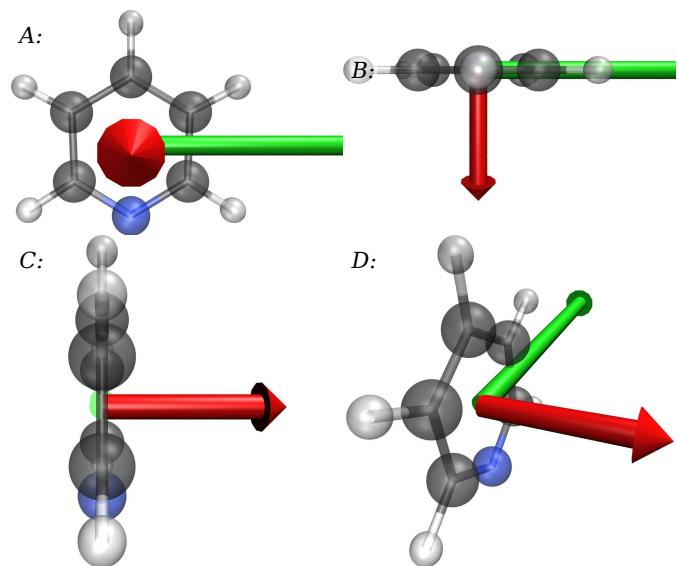


Figure 3: The electric (red arrow) and magnetic (green arrow) transition (S_1) dipole moment plotted against the aligned molecular geometry with a scale of $1 \text{ \AA} = 0.2 \text{ D} = 0.1 \text{ au}$. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Molecular Orbitals

In total, 115 doubly occupied molecular orbitals were calculated, divided into 21 occupied orbitals and 94 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO** and **LUMO** were -7.28 and -0.51 eV respectively, corresponding to a **HOMO-LUMO band gap** of 6.77 eV (figure 15). Plots of the orbital density for the HOMO-5, HOMO-4, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2 and LUMO+4 are shown in figures 4-10 and 12-14 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 11.

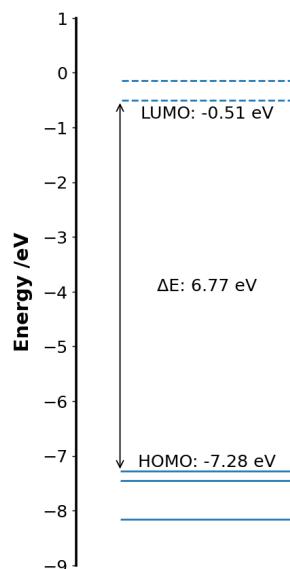


Figure 15: Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.

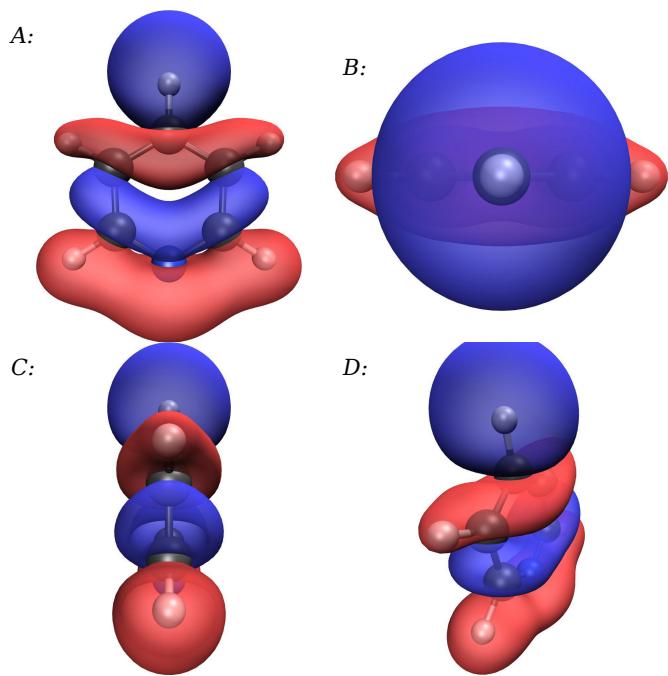


Figure 4: Orbital density plots of the HOMO-5, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

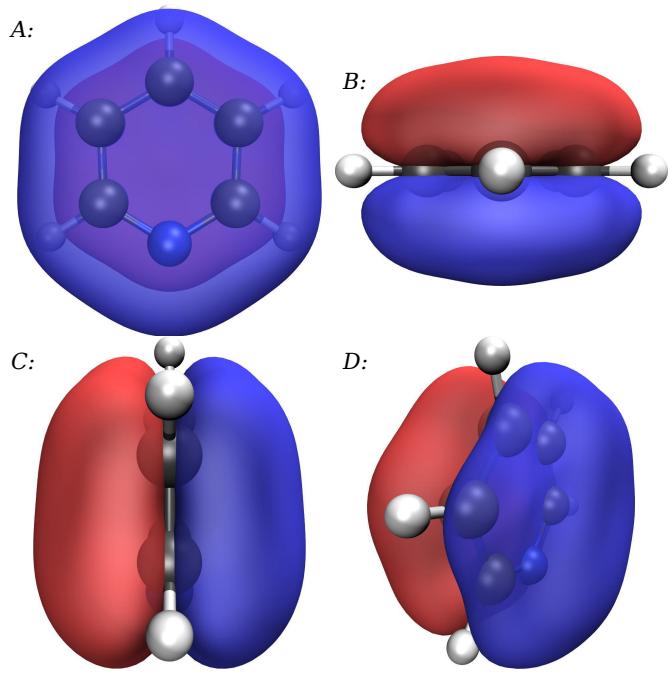


Figure 5: Orbital density plots of the HOMO-4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

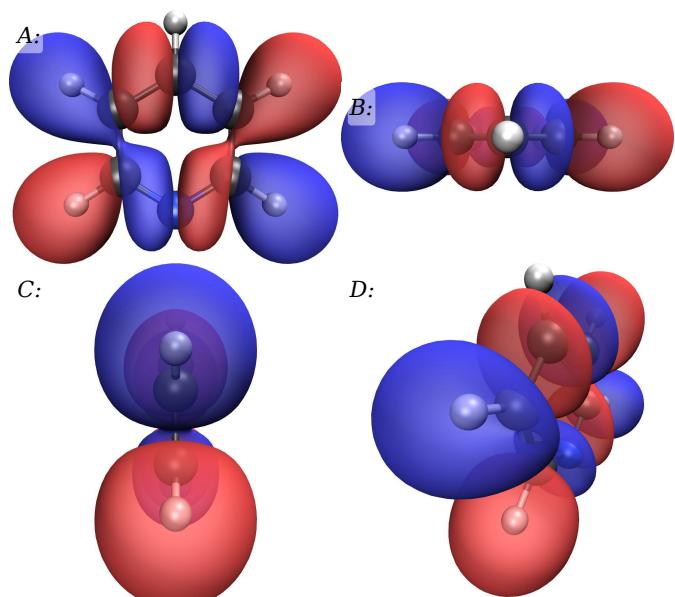


Figure 6: Orbital density plots of the HOMO-3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

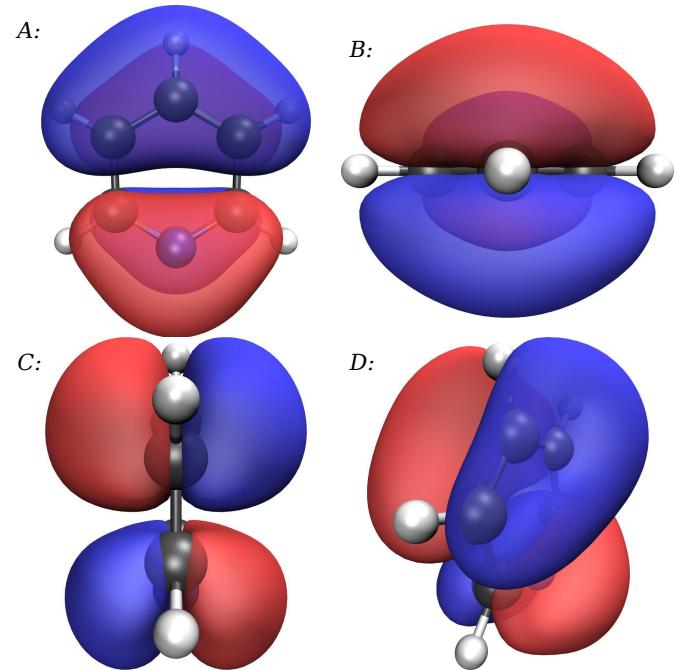


Figure 7: Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

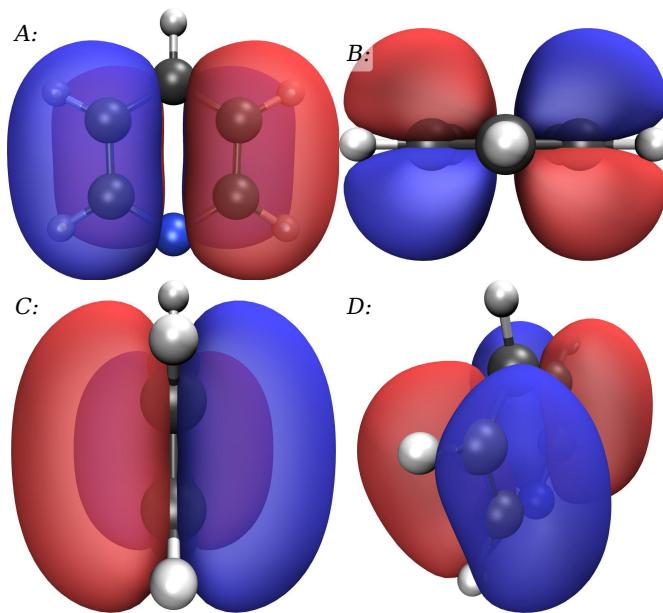


Figure 8: Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

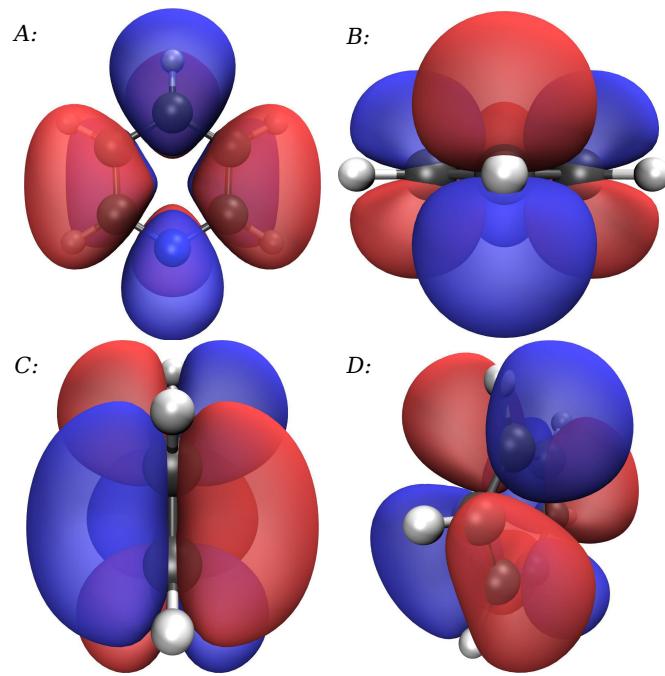


Figure 10: Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

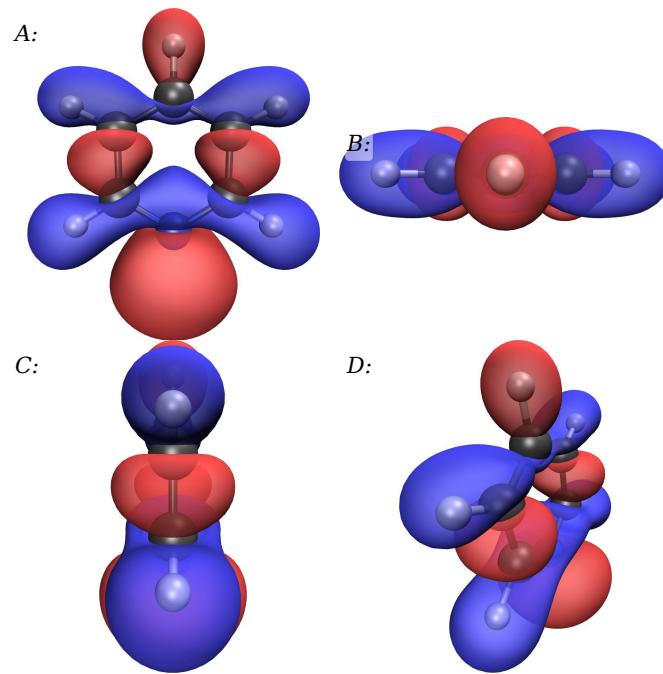


Figure 9: Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

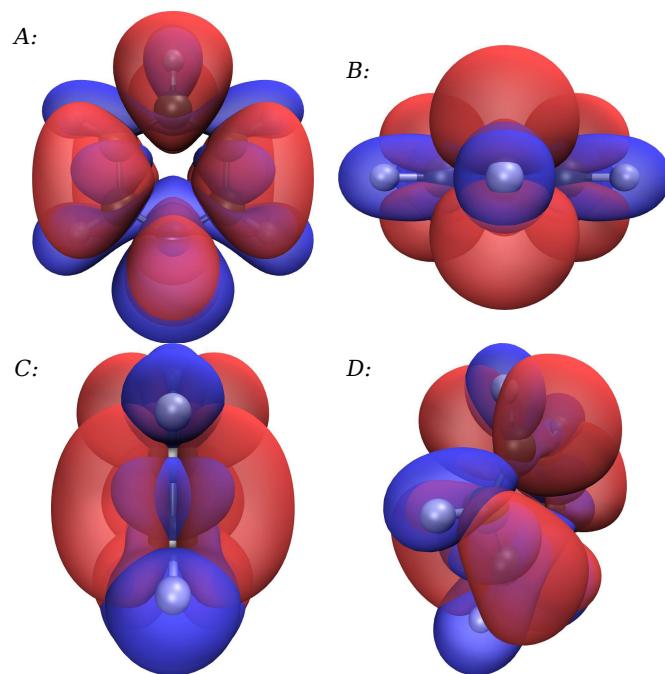


Figure 11: Orbital density plots of the HOMO (blue) and LUMO (red), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

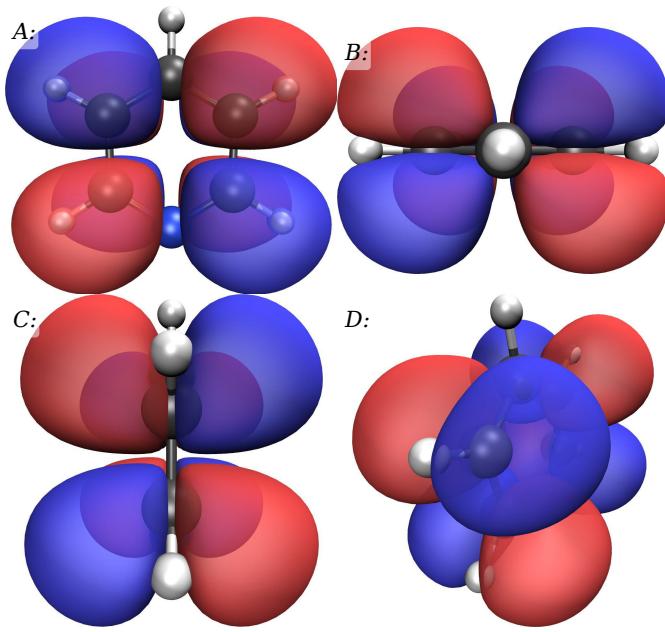


Figure 12: Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

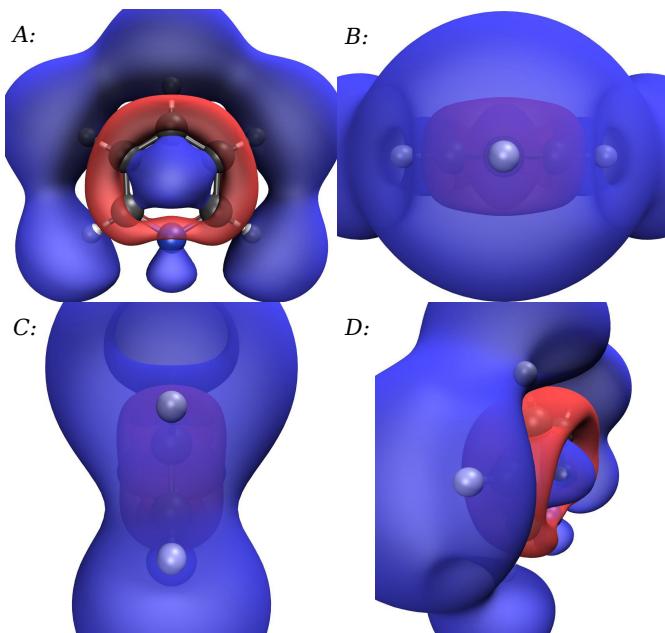


Figure 13: Orbital density plots of the LUMO+2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

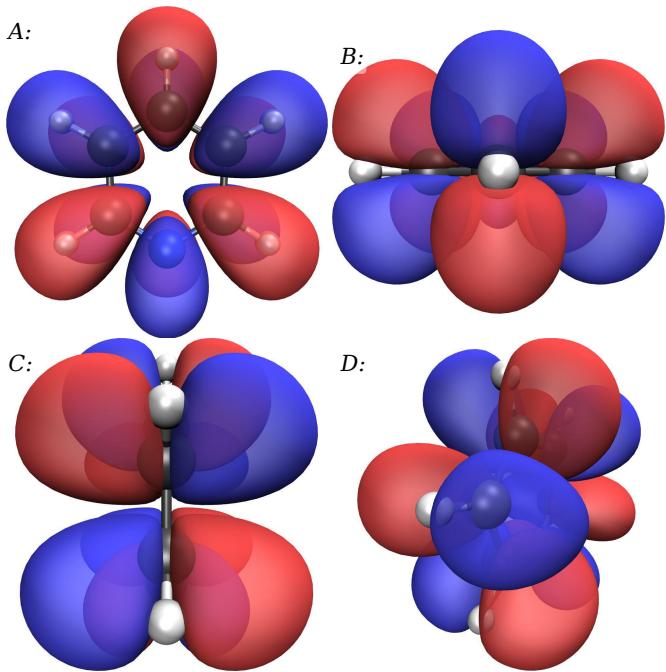


Figure 14: Orbital density plots of the LUMO+4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Excited States

In total, the energies of 20 electronic excited states were calculated (figure 16), 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 5.07 eV, corresponding to absorption by a photon with a wavelength of 244 nm, an ultraviolet 'color' ■ and CIE coordinates of (0.00, 0.00), while the energy of the T_1 was 4.28 eV (290 nm, ultraviolet ■, CIE: (0.00, 0.00)). The difference in energy between the S_1 and T_1 excited states (ΔE_{ST}) was therefore 0.80 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 **four most intense peaks** were found at 154, 180, 213 and 243 nm. The full simulated absorption spectrum is shown in figure 17. Finally, **natural transition orbitals (NTOs)** were calculated for each excited state and are shown in figures 18-37.

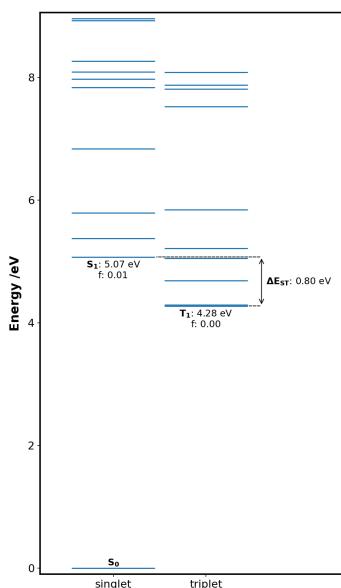


Figure 16: Graph of the calculated excited states. *f*: oscillator strength of the relevant ground to excited state transition.

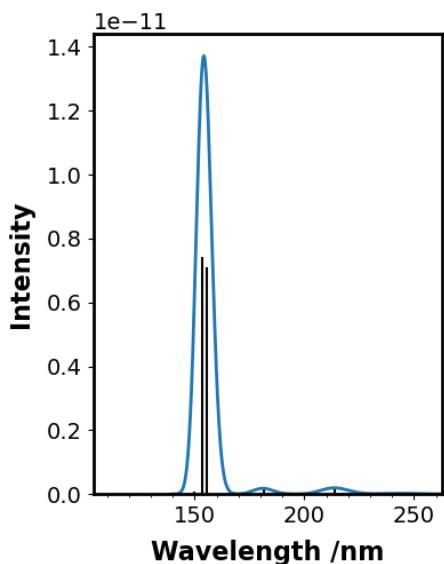


Figure 17: Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 154, 180, 213 and 243 nm.

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 **S₀** and **T₁** states was found to be 23.86 cm^{-1} , while the H_{SO} between the **S₁** and **T₁** excited states was 0.02 cm^{-1} . These values correspond to a first-order mixing coefficient ($\lambda = H_{SO}/\Delta E_{ST}$) of < 0.01 and < 0.01 respectively.

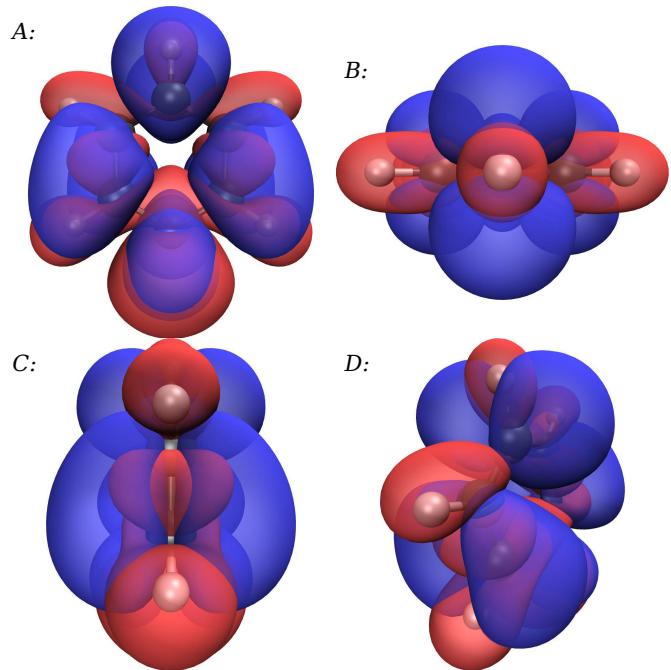


Figure 18: Density plot of the NTO hole (blue) & electron (red) of the **T₁** state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

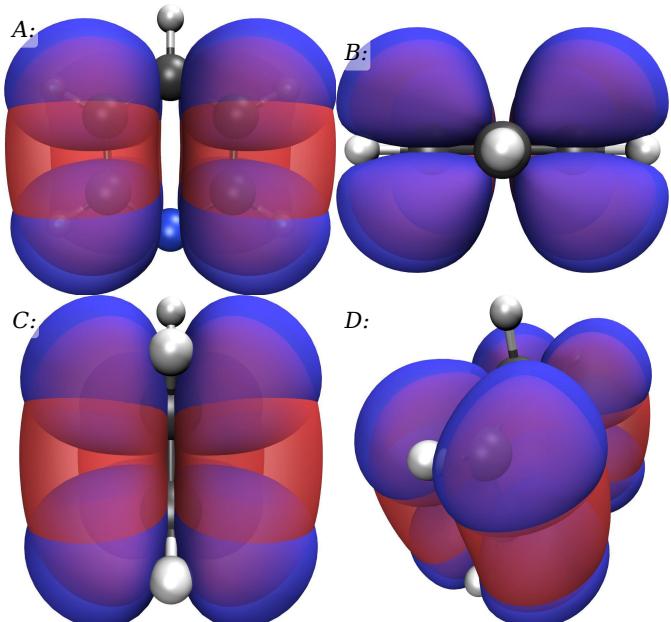


Figure 19: Density plot of the NTO hole (blue) & electron (red) of the **T₂** state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

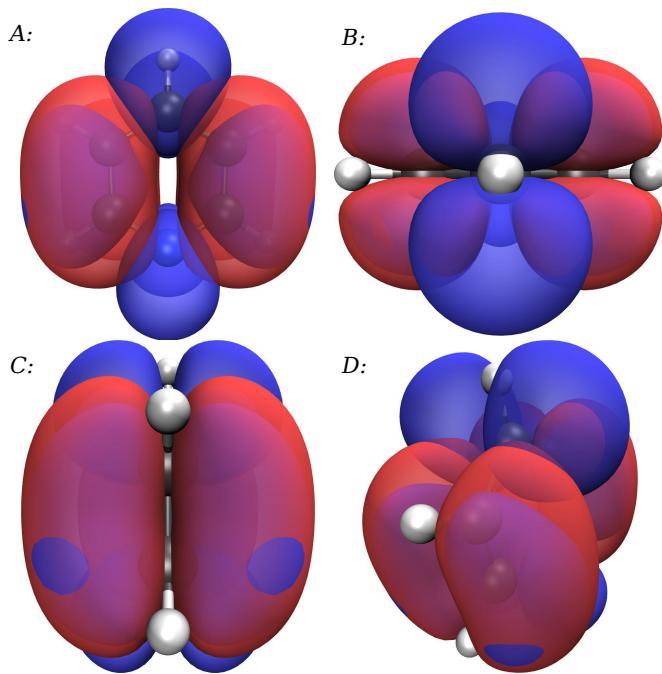


Figure 20: Density plot of the NTO hole (blue) & electron (red) of the T_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

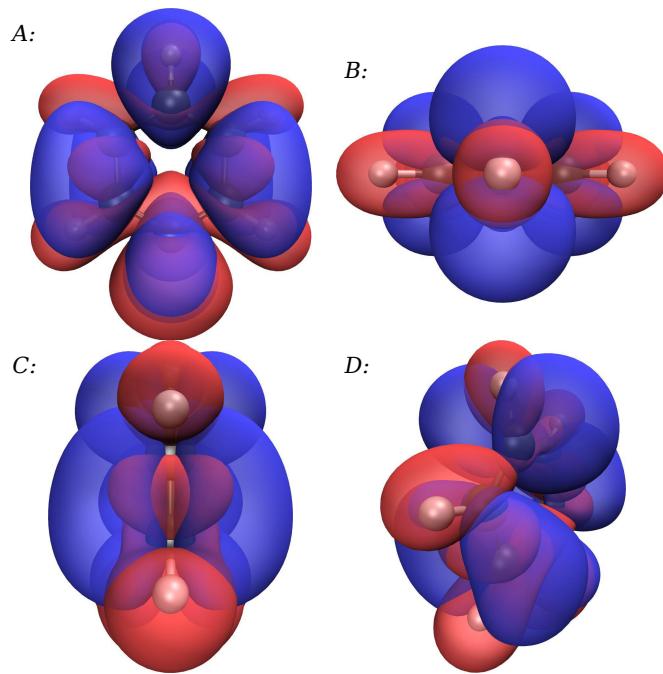


Figure 22: Density plot of the NTO hole (blue) & electron (red) of the S_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

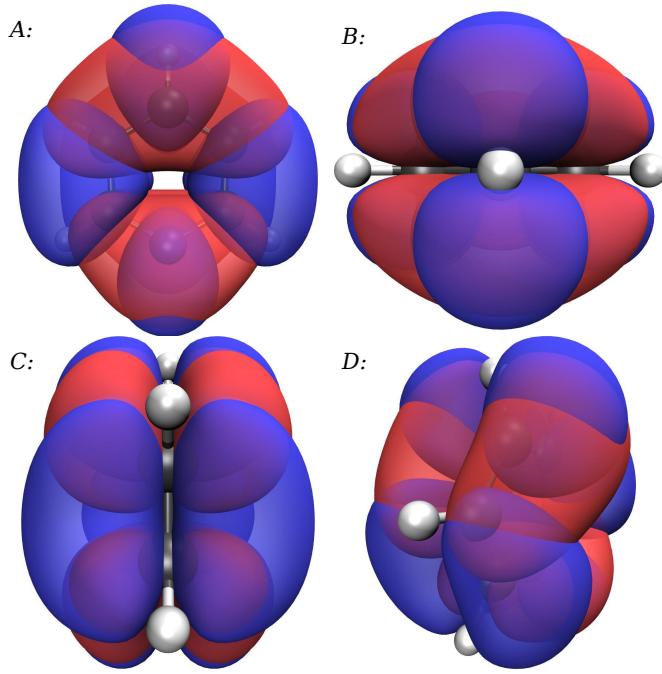


Figure 21: Density plot of the NTO hole (blue) & electron (red) of the T_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

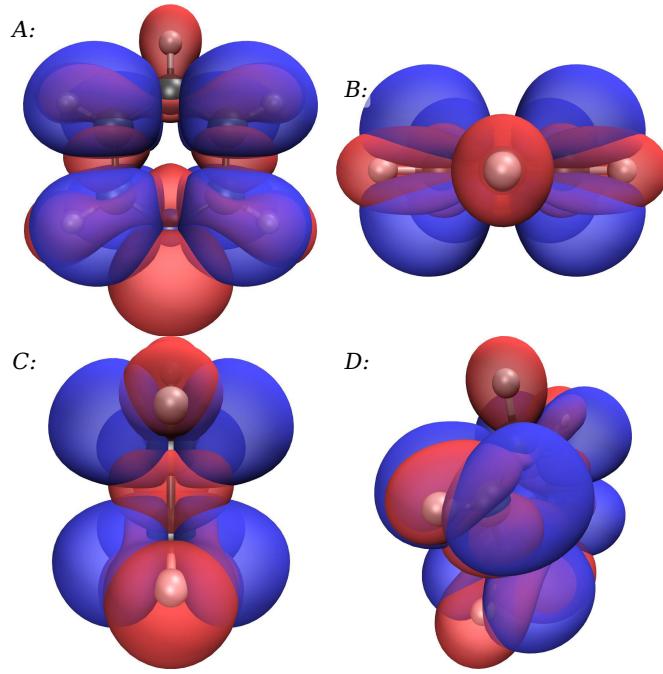


Figure 23: Density plot of the NTO hole (blue) & electron (red) of the T_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

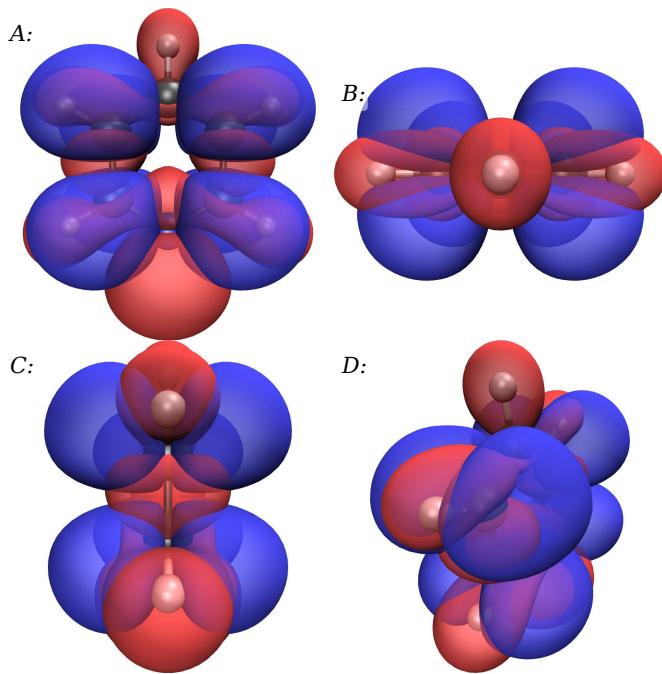


Figure 24: Density plot of the NTO hole (blue) & electron (red) of the S_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

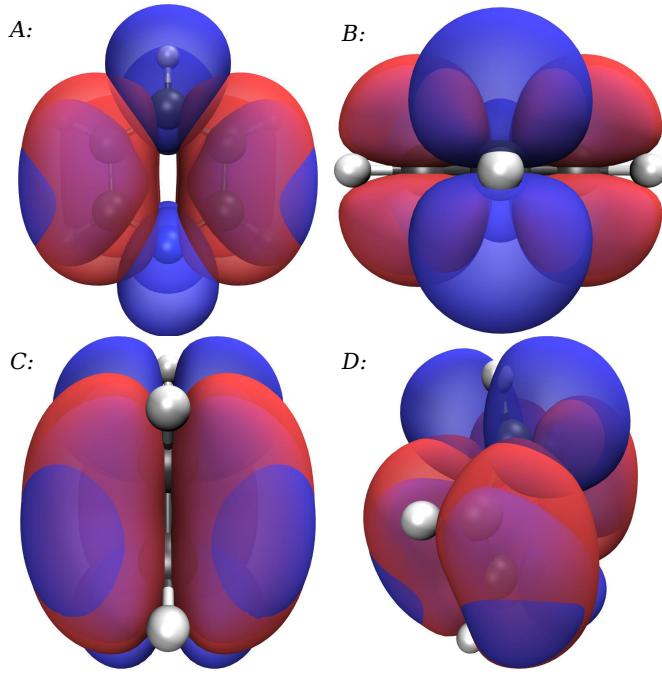


Figure 25: Density plot of the NTO hole (blue) & electron (red) of the S_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

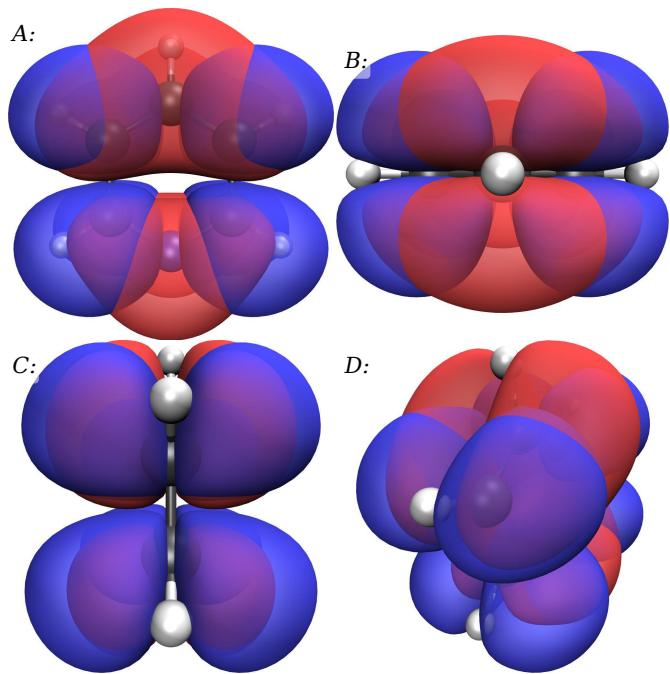


Figure 26: Density plot of the NTO hole (blue) & electron (red) of the T_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

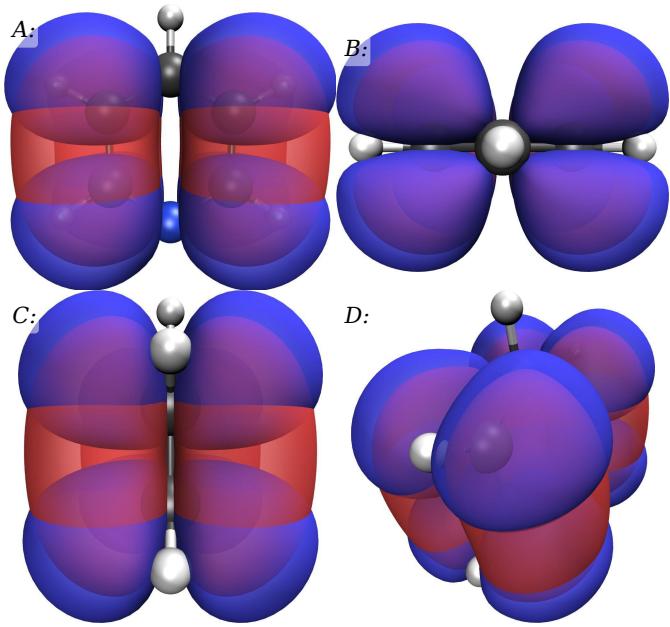


Figure 27: Density plot of the NTO hole (blue) & electron (red) of the S_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

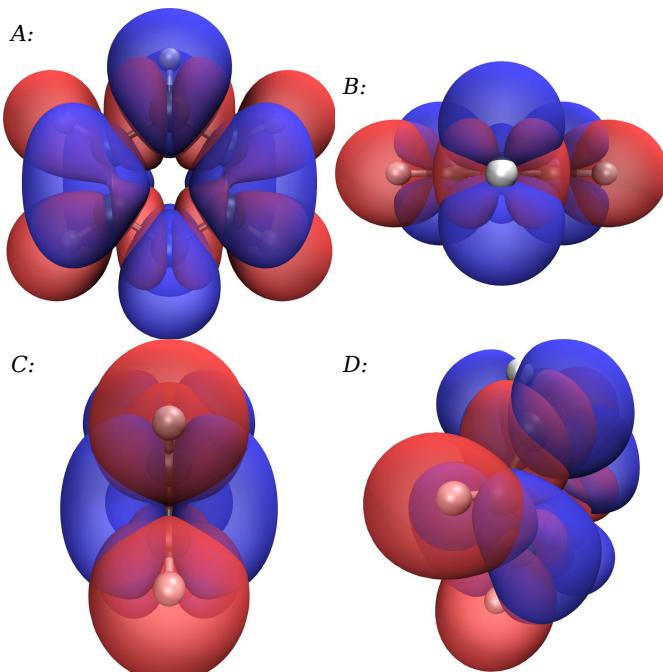


Figure 28: Density plot of the NTO hole (blue) & electron (red) of the T_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

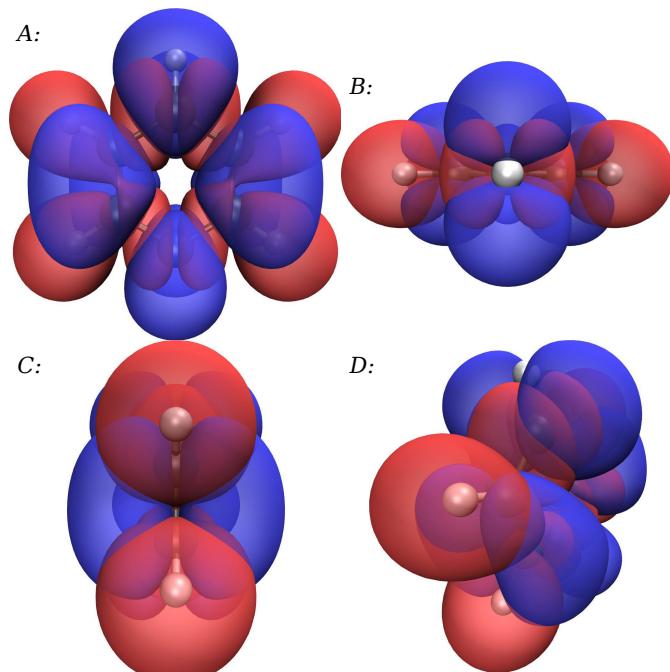


Figure 30: Density plot of the NTO hole (blue) & electron (red) of the S_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

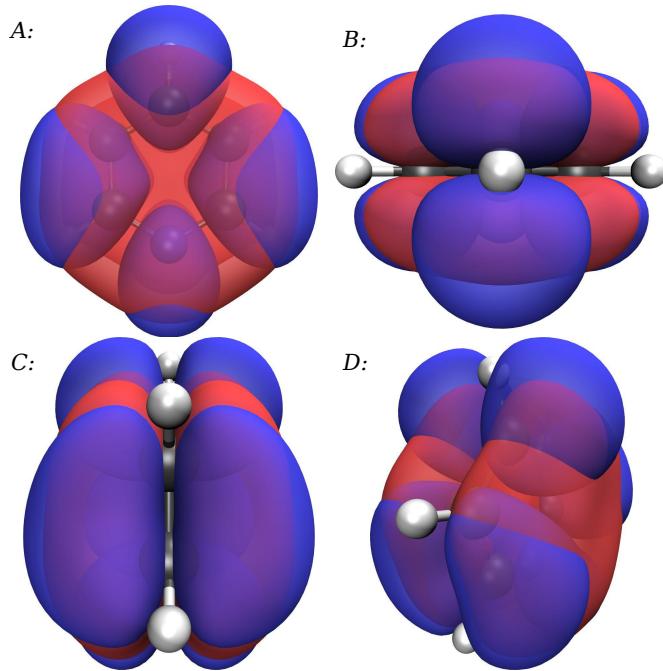


Figure 29: Density plot of the NTO hole (blue) & electron (red) of the T_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

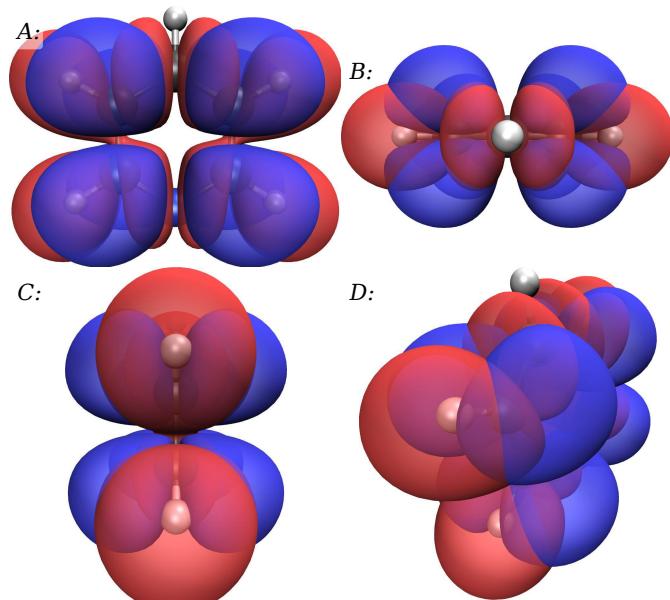


Figure 31: Density plot of the NTO hole (blue) & electron (red) of the T_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

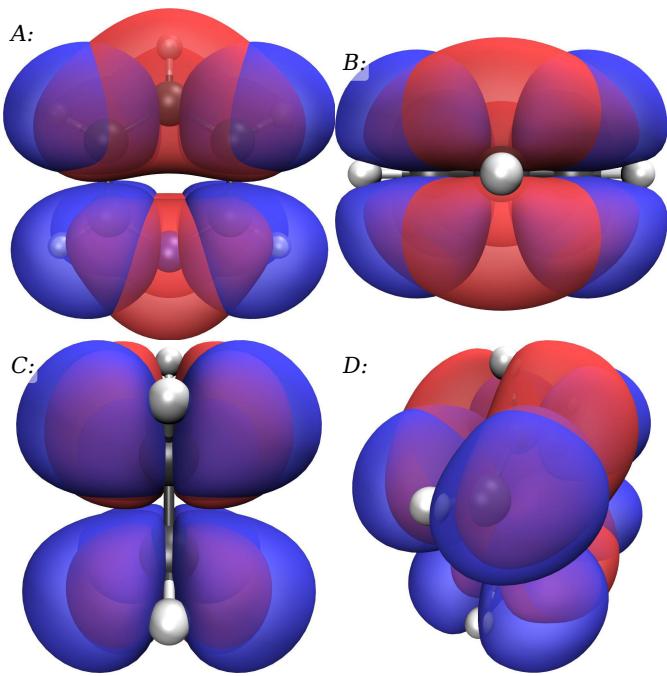


Figure 32: Density plot of the NTO hole (blue) & electron (red) of the S_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

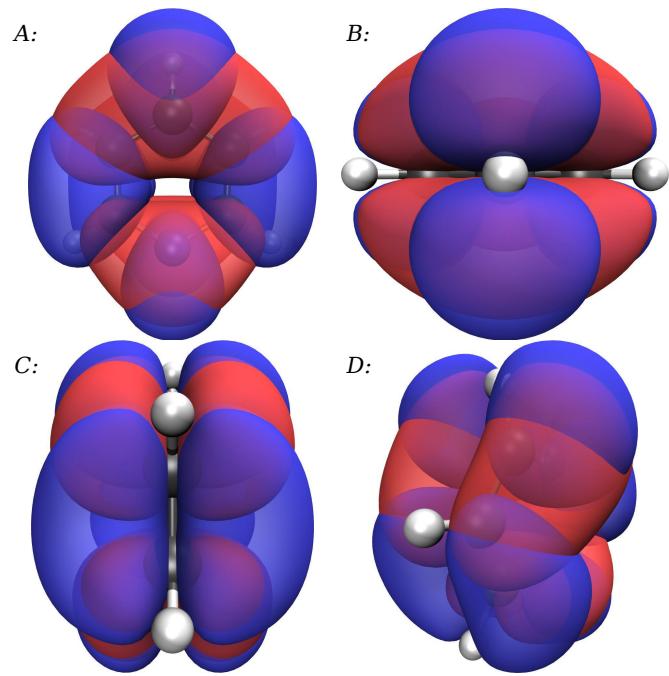


Figure 34: Density plot of the NTO hole (blue) & electron (red) of the S_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

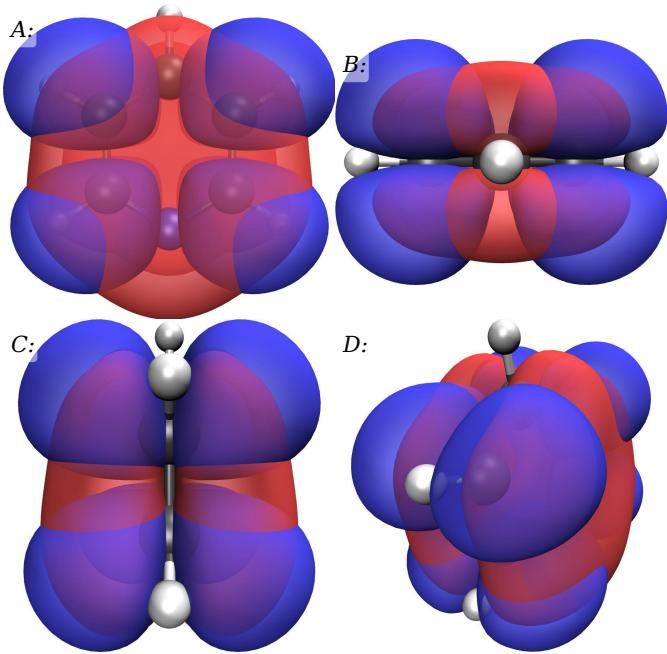


Figure 33: Density plot of the NTO hole (blue) & electron (red) of the T_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

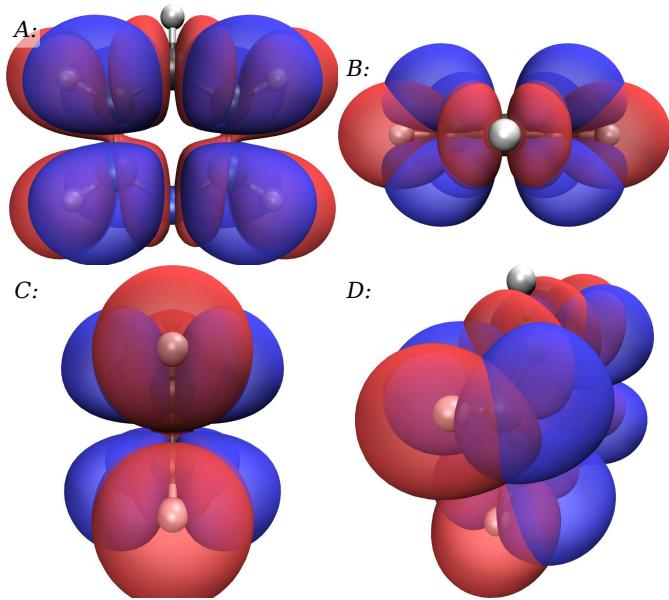


Figure 35: Density plot of the NTO hole (blue) & electron (red) of the S_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

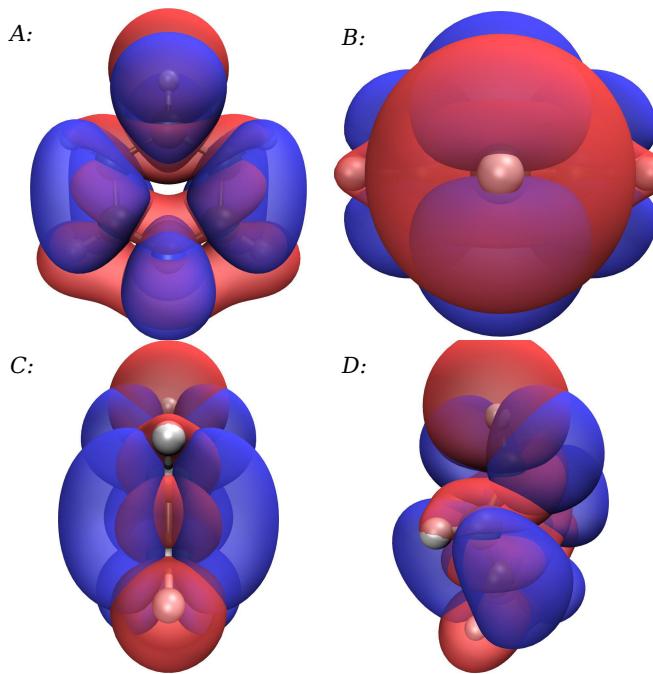


Figure 36: Density plot of the NTO hole (blue) & electron (red) of the S_g state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

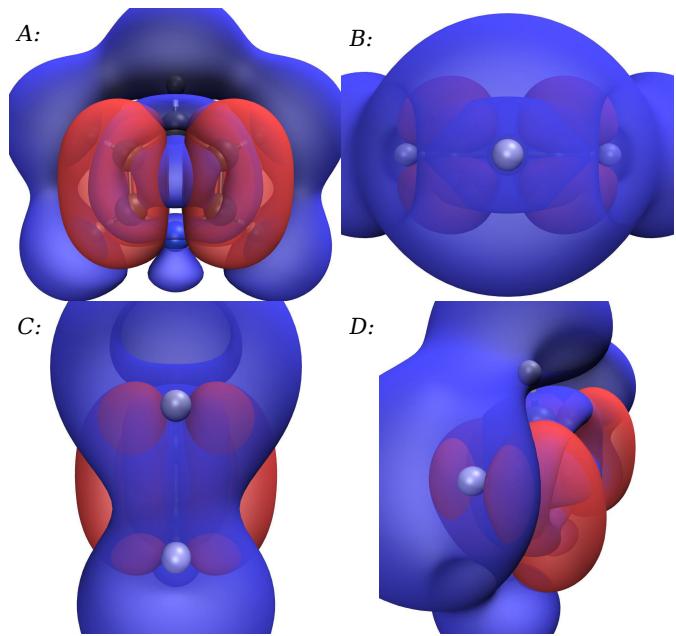


Figure 37: Density plot of the NTO hole (blue) & electron (red) of the S_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

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.

Element	X Coord /Å	Y Coord /Å	Z Coord /Å				
C	1.1386510	-0.7199620	-0.0000210	26	LUMO+4	A	4.2561
C	1.1954040	0.6709180	0.0000190	25	LUMO+3	A	4.2020
C	0.0000400	1.3817880	0.0000190	24	LUMO+2	A	2.9309
C	-1.1953660	0.6709790	0.0000190	23	LUMO+1	A	-0.1420
C	-1.1386990	-0.7199010	0.0000290	22	LUMO	A	-0.5097
N	-0.0000350	-1.4172120	-0.0000610	21	HOMO	A	-7.2829
H	2.0570560	-1.3046500	-0.0000410	20	HOMO-1	A	-7.4475
H	2.1540580	1.1793990	0.0000390	19	HOMO-2	A	-8.1539
H	0.0000600	2.4678180	0.0000490	18	HOMO-3	A	-10.1324
H	-2.1539920	1.1795280	0.0000190	17	HOMO-4	A	-11.2402
H	-2.0571240	-1.3045430	-0.0000410	16	HOMO-5	A	-11.2780
				15	HOMO-6	A	-11.9507

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

Level	Label	Symmetry	Energy /eV				
37	LUMO+15	A	14.9940	11	HOMO-10	A	-17.5726
36	LUMO+14	A	14.5273	10	HOMO-11	A	-17.6352
35	LUMO+13	A	12.7428	9	HOMO-12	A	-21.3397
34	LUMO+12	A	12.6081	8	HOMO-13	A	-22.5449
33	LUMO+11	A	9.0029	7	HOMO-14	A	-26.3953
				6	HOMO-15	A	-278.8609

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	4.2757	289.97	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO → LUMO (0.97) HOMO → LUMO+4 (0.02)
2	T ₂	Triplet-A	4.2914	288.91	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-1 → LUMO+1 (0.67) HOMO-2 → LUMO (0.30) HOMO-4 → LUMO+4 (0.02)
3	T ₃	Triplet-A	4.6850	264.64	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-1 → LUMO (0.97) HOMO-2 → LUMO+1 (0.03)
4	T ₄	Triplet-A	5.0511	245.46	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-2 → LUMO (0.68) HOMO-1 → LUMO+1 (0.32)
5	S ₁	Singlet-A	5.0737	244.37	Ultraviolet [■] (0.00, 0.00)	0.0066	HOMO → LUMO (0.99)
6	T ₅	Triplet-A	5.2125	237.86	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO → LUMO+1 (1.00)
7	S ₂	Singlet-A	5.3747	230.68	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO → LUMO+1 (1.00)
8	S ₃	Singlet-A	5.7931	214.02	Ultraviolet [■] (0.00, 0.00)	0.0445	HOMO-1 → LUMO (0.69) HOMO-2 → LUMO+1 (0.30)
9	T ₆	Triplet-A	5.8469	212.05	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-2 → LUMO+1 (0.96) HOMO-1 → LUMO (0.03)
10	S ₄	Singlet-A	6.8391	181.29	Ultraviolet [■] (0.00, 0.00)	0.0294	HOMO-1 → LUMO+1 (0.62) HOMO-2 → LUMO (0.35)
11	T ₇	Triplet-A	7.5290	164.68	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.98)
12	T ₈	Triplet-A	7.8093	158.76	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-4 → LUMO (0.83) HOMO-2 → LUMO+4 (0.16)
13	S ₅	Singlet-A	7.8387	158.17	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.99)
14	T ₉	Triplet-A	7.8738	157.46	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-3 → LUMO+1 (0.98)
15	S ₆	Singlet-A	7.9756	155.45	Ultraviolet [■] (0.00, 0.00)	0.8636	HOMO-2 → LUMO+1 (0.66) HOMO-1 → LUMO (0.27)
16	T ₁₀	Triplet-A	8.0844	153.36	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-4 → LUMO+1 (0.65) HOMO-1 → LUMO+4 (0.34)
17	S ₇	Singlet-A	8.0937	153.19	Ultraviolet [■] (0.00, 0.00)	0.8783	HOMO-2 → LUMO (0.58) HOMO-1 → LUMO+1 (0.32) HOMO → LUMO+2 (0.02)
18	S ₈	Singlet-A	8.2671	149.97	Ultraviolet [■] (0.00, 0.00)	0.0069	HOMO-3 → LUMO+1 (0.99)
19	S ₉	Singlet-A	8.9279	138.87	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-5 → LUMO (0.96) HOMO → LUMO+4 (0.03)
20	S ₁₀	Singlet-A	8.9578	138.41	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-1 → LUMO+2 (0.99)

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
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	0.00, -0.00, 0.59	0.59	90.00	89.98	0.69, 0.00, 0.00	0.69	0.00	0.00	5.88e-19	6.41e-21	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 ₂	0.00, 0.00, 0.00	0.00	0.00	0.00	-0.00, -0.03, 0.00	0.03	89.80	0.00	0.00e+00	2.68e-22	90.00	0.00	0.000
S ₃	-1.42, 0.00, 0.00	1.42	0.00	0.00	-0.00, 0.00, -0.18	0.18	89.97	89.97	1.42e-18	1.65e-21	90.03	-0.00	< 0.001
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 ₄	-0.00, -1.07, 0.00	1.07	89.99	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	1.07e-18	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
S ₅	-0.00, -0.00, 0.00	< 0.01	33.69	0.00	0.00, -0.16, 0.00	0.16	90.00	0.00	9.16e-22	1.47e-21	123.69	-0.55	-0.995
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 ₆	5.34, -0.00, 0.00	5.34	0.01	0.00	0.00, 0.00, 0.04	0.04	90.00	90.00	5.34e-18	3.64e-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 ₇	-0.00, -5.35, -0.00	5.35	89.99	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	5.35e-18	0.00e+00	90.00	0.00	0.000
S ₈	-0.00, 0.00, -0.47	0.47	89.94	89.93	-0.33, 0.00, 0.00	0.33	0.00	0.00	4.68e-19	3.10e-21	90.06	-0.00	< 0.001
S ₉	0.00, -0.00, -0.00	< 0.01	90.00	86.42	1.25, -0.00, 0.00	1.25	0.00	0.00	4.07e-21	1.16e-20	90.00	-0.00	< 0.001
S ₁₀	0.00, -0.00, 0.00	< 0.01	90.00	0.00	0.00, 0.53, 0.00	0.53	89.99	0.00	2.54e-22	4.87e-21	0.01	1.00	0.208

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	$\lambda^{[e]}$
S ₀	T ₁	16.8740	0.0004	16.8740	23.8634	0.0030	0.0007
S ₀	T ₂	0.0549	< 0.0001	0.0549	0.0777	< 0.0001	< 0.0001
S ₀	T ₃	0.0013	0.0020	0.0013	0.0027	< 0.0001	< 0.0001
S ₀	T ₄	0.0013	< 0.0001	0.0013	0.0019	< 0.0001	< 0.0001
S ₀	T ₅	1.3715	0.0004	1.3715	1.9396	0.0002	< 0.0001
S ₀	T ₆	0.0002	0.2194	0.0002	0.2194	< 0.0001	< 0.0001
S ₀	T ₇	2.6921	0.0007	2.6921	3.8071	0.0005	0.0001
S ₀	T ₈	0.0013	0.0002	0.0013	0.0018	< 0.0001	< 0.0001
S ₀	T ₉	2.4312	0.0001	2.4312	3.4383	0.0004	0.0001
S ₀	T ₁₀	0.0008	0.1435	0.0008	0.1435	< 0.0001	< 0.0001
S ₁	T ₁	0.0134	0.0001	0.0134	0.0190	< 0.0001	< 0.0001
S ₁	T ₂	4.0883	0.0003	4.0883	5.7818	0.0007	0.0009
S ₁	T ₃	1.0593	0.0000	1.0593	1.4980	0.0002	0.0005
S ₁	T ₄	5.5698	0.0007	5.5698	7.8770	0.0010	0.0432
S ₁	T ₅	0.0008	1.4694	0.0008	1.4694	0.0002	0.0013
S ₁	T ₆	0.0284	0.0001	0.0284	0.0402	< 0.0001	< 0.0001
S ₁	T ₇	0.0005	14.9524	0.0005	14.9524	0.0019	0.0008
S ₁	T ₈	7.0308	0.0009	7.0308	9.9431	0.0012	0.0005
S ₁	T ₉	0.0005	0.0001	0.0005	0.0007	< 0.0001	< 0.0001
S ₁	T ₁₀	0.2621	0.0000	0.2621	0.3706	< 0.0001	< 0.0001
S ₂	T ₁	0.0027	1.1667	0.0027	1.1667	0.0001	0.0001
S ₂	T ₂	0.7498	0.0035	0.7498	1.0604	0.0001	0.0001
S ₂	T ₃	1.3330	< 0.0001	1.3330	1.8851	0.0002	0.0003
S ₂	T ₄	0.5194	0.0001	0.5194	0.7346	0.0001	0.0003
S ₂	T ₅	0.0001	0.0001	0.0001	0.0002	< 0.0001	< 0.0001
S ₂	T ₆	6.2743	0.0006	6.2743	8.8732	0.0011	0.0023
S ₂	T ₇	0.0001	0.0001	0.0001	0.0001	< 0.0001	< 0.0001
S ₂	T ₈	0.0155	0.0007	0.0155	0.0220	< 0.0001	< 0.0001
S ₂	T ₉	0.0007	14.5661	0.0007	14.5661	0.0018	0.0007
S ₂	T ₁₀	6.7335	0.0017	6.7335	9.5226	0.0012	0.0004
S ₃	T ₁	0.7876	0.0048	0.7876	1.1139	0.0001	0.0001
S ₃	T ₂	0.0026	1.5192	0.0026	1.5192	0.0002	0.0001
S ₃	T ₃	0.0003	0.0001	0.0003	0.0005	< 0.0001	< 0.0001
S ₃	T ₄	0.0009	0.1772	0.0009	0.1772	< 0.0001	< 0.0001
S ₃	T ₅	4.0364	0.0004	4.0364	5.7083	0.0007	0.0012
S ₃	T ₆	0.0002	< 0.0001	0.0002	0.0003	< 0.0001	< 0.0001
S ₃	T ₇	0.6281	0.0005	0.6281	0.8882	0.0001	0.0001
S ₃	T ₈	0.0003	0.0509	0.0003	0.0509	< 0.0001	< 0.0001

S ₃	T ₉	2.1150	0.0016	2.1150	2.9911	0.0004	0.0002
S ₃	T ₁₀	0.0010	< 0.0001	0.0010	0.0014	< 0.0001	< 0.0001
S ₄	T ₁	4.0865	0.0003	4.0865	5.7791	0.0007	0.0003
S ₄	T ₂	0.0129	0.0001	0.0129	0.0183	< 0.0001	< 0.0001
S ₄	T ₃	0.0005	0.9851	0.0005	0.9851	0.0001	0.0001
S ₄	T ₄	0.0002	0.0000	0.0002	0.0003	< 0.0001	< 0.0001
S ₄	T ₅	0.8023	0.0002	0.8023	1.1346	0.0001	0.0001
S ₄	T ₆	0.0002	1.2640	0.0002	1.2640	0.0002	0.0002
S ₄	T ₇	1.7093	0.0002	1.7093	2.4173	0.0003	0.0004
S ₄	T ₈	0.0002	0.0000	0.0002	0.0003	< 0.0001	< 0.0001
S ₄	T ₉	0.0024	0.0001	0.0024	0.0035	< 0.0001	< 0.0001
S ₄	T ₁₀	0.0001	0.1615	0.0001	0.1615	< 0.0001	< 0.0001
S ₅	T ₁	0.0053	14.3557	0.0053	14.3557	0.0018	0.0005
S ₅	T ₂	1.6926	0.0459	1.6926	2.3941	0.0003	0.0001
S ₅	T ₃	0.4370	0.0012	0.4370	0.6180	0.0001	< 0.0001
S ₅	T ₄	2.4429	0.0011	2.4429	3.4548	0.0004	0.0002
S ₅	T ₅	0.0008	0.0006	0.0008	0.0013	< 0.0001	< 0.0001
S ₅	T ₆	0.0207	0.0001	0.0207	0.0293	< 0.0001	< 0.0001
S ₅	T ₇	0.0001	< 0.0001	0.0001	0.0002	< 0.0001	< 0.0001
S ₅	T ₈	1.9123	0.0004	1.9123	2.7044	0.0003	0.0114
S ₅	T ₉	0.0003	1.2561	0.0003	1.2561	0.0002	0.0044
S ₅	T ₁₀	0.1062	0.0005	0.1062	0.1502	< 0.0001	0.0001
S ₆	T ₁	0.1908	0.0026	0.1908	0.2698	< 0.0001	< 0.0001
S ₆	T ₂	0.0009	0.2299	0.0009	0.2299	< 0.0001	< 0.0001
S ₆	T ₃	0.0003	< 0.0001	0.0003	0.0004	< 0.0001	< 0.0001
S ₆	T ₄	0.0006	0.5807	0.0006	0.5808	0.0001	< 0.0001
S ₆	T ₅	4.4927	0.0018	4.4927	6.3536	0.0008	0.0003
S ₆	T ₆	0.0005	0.0000	0.0005	0.0007	< 0.0001	< 0.0001
S ₆	T ₇	0.0075	0.0001	0.0075	0.0106	< 0.0001	< 0.0001
S ₆	T ₈	0.0001	0.0707	0.0001	0.0707	< 0.0001	0.0001
S ₆	T ₉	1.1001	0.0001	1.1001	1.5558	0.0002	0.0019
S ₆	T ₁₀	0.0005	< 0.0001	0.0005	0.0008	< 0.0001	< 0.0001
S ₇	T ₁	6.9229	0.0010	6.9229	9.7905	0.0012	0.0003
S ₇	T ₂	0.0218	< 0.0001	0.0218	0.0308	< 0.0001	< 0.0001
S ₇	T ₃	0.0004	0.2867	0.0004	0.2867	< 0.0001	< 0.0001
S ₇	T ₄	0.0004	< 0.0001	0.0004	0.0005	< 0.0001	< 0.0001
S ₇	T ₅	0.6701	0.0008	0.6701	0.9477	0.0001	< 0.0001
S ₇	T ₆	0.0003	0.4886	0.0003	0.4886	0.0001	< 0.0001
S ₇	T ₇	3.6241	0.0001	3.6241	5.1253	0.0006	0.0011
S ₇	T ₈	0.0004	< 0.0001	0.0004	0.0006	< 0.0001	< 0.0001
S ₇	T ₉	0.1942	0.0002	0.1942	0.2747	< 0.0001	0.0002
S ₇	T ₁₀	0.0003	0.0652	0.0003	0.0652	< 0.0001	0.0009
S ₈	T ₁	0.0009	0.0005	0.0009	0.0014	< 0.0001	< 0.0001
S ₈	T ₂	0.3708	0.0007	0.3708	0.5244	0.0001	< 0.0001
S ₈	T ₃	0.5478	0.0006	0.5478	0.7747	0.0001	< 0.0001
S ₈	T ₄	0.3810	0.0022	0.3810	0.5389	0.0001	< 0.0001
S ₈	T ₅	0.0004	14.7811	0.0004	14.7811	0.0018	0.0006
S ₈	T ₆	2.7755	0.0015	2.7755	3.9252	0.0005	0.0002
S ₈	T ₇	0.0001	0.9296	0.0001	0.9296	0.0001	0.0002
S ₈	T ₈	0.0761	0.0001	0.0761	0.1077	< 0.0001	< 0.0001
S ₈	T ₉	0.0004	< 0.0001	0.0004	0.0005	< 0.0001	< 0.0001
S ₈	T ₁₀	1.8787	0.0002	1.8787	2.6570	0.0003	0.0018
S ₉	T ₁	0.0066	0.0001	0.0066	0.0094	< 0.0001	< 0.0001

S ₉	T ₂	2.1664	0.0001	2.1664	3.0638	0.0004	0.0001
S ₉	T ₃	0.0986	0.0001	0.0986	0.1395	< 0.0001	< 0.0001
S ₉	T ₄	2.6693	< 0.0001	2.6693	3.7749	0.0005	0.0001
S ₉	T ₅	0.0003	0.0118	0.0003	0.0118	< 0.0001	< 0.0001
S ₉	T ₆	0.0442	< 0.0001	0.0442	0.0625	< 0.0001	< 0.0001
S ₉	T ₇	0.0004	4.8880	0.0004	4.8880	0.0006	0.0004
S ₉	T ₈	5.3454	0.0008	5.3454	7.5596	0.0009	0.0008
S ₉	T ₉	0.0004	0.0001	0.0004	0.0006	< 0.0001	< 0.0001
S ₉	T ₁₀	0.4233	0.0001	0.4233	0.5986	0.0001	0.0001
S ₁₀	T ₁	0.0020	0.6367	0.0020	0.6367	0.0001	< 0.0001
S ₁₀	T ₂	0.3465	0.0020	0.3465	0.4900	0.0001	< 0.0001
S ₁₀	T ₃	2.3635	< 0.0001	2.3635	3.3425	0.0004	0.0001
S ₁₀	T ₄	0.3420	< 0.0001	0.3420	0.4837	0.0001	< 0.0001
S ₁₀	T ₅	0.0001	0.0001	0.0001	0.0002	< 0.0001	< 0.0001
S ₁₀	T ₆	0.5086	< 0.0001	0.5086	0.7193	0.0001	< 0.0001
S ₁₀	T ₇	0.0001	0.0003	0.0001	0.0004	< 0.0001	< 0.0001
S ₁₀	T ₈	0.1447	< 0.0001	0.1447	0.2047	< 0.0001	< 0.0001
S ₁₀	T ₉	0.0001	0.3405	0.0001	0.3405	< 0.0001	< 0.0001
S ₁₀	T ₁₀	1.1089	< 0.0001	1.1089	1.5682	0.0002	0.0002

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