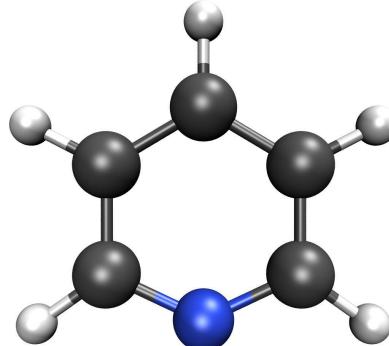




A Report On The Calculation Of The Optimised Structure And Excited States Of Pyridine At The PBE1PBE/6-31G(d,p) Level

osl - 16th June 2022



Abstract

The calculation of optimised structure and 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 -6748.11 eV after 5 steps. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -6.49 and -0.59 eV respectively, corresponding to a HOMO-LUMO band gap of 5.90 eV. The permanent dipole moment (PDM) was calculated to be 0.61 D. In total, 10 excited states were calculated with singlet multiplicity. The most intense absorption peaks were calculated to be at 145, 157 and 215 nm. The lowest energy singlet excited state (S_1) was calculated to be 4.12 eV (301 nm).

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
16/06/2022 00:14:35	9 m, 42 s	True (True)	Gaussian (2016+C. 01)	PBE1PBE/ 6-31G(d,p)	Optimisation, Excited States	restricted	1 (singlet)	N/A	N/A

Summary Of Results

Scf Energy

Table 2: Summary of SCF energy properties.

No. of steps	5
Final energy	-6748.1068 eV
Final energy	-651,093 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	4.38 Å
Y extension	3.81 Å
Z extension	0.00 Å
Linearity ratio	0.13
Planarity ratio	1.00

Molecular Orbitals

Table 4: Summary of HOMO & LUMO properties.

E _{HOMO,LUMO}	5.90 eV
E _{HOMO}	-6.49 eV
E _{LUMO}	-0.59 eV

Permanent Dipole Moment

Table 5: Summary of the permanent dipole moment properties.

Total	0.61 D
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X axis angle 89.99 °

XY plane angle 0.01 °

S₁ Transition Dipole Moment

Table 6: Summary of the transition (S₁) 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	0.50 D
$\theta_{\mu,x}$	90.00 °
$\theta_{\mu,xy}$	90.00 °
$m^{[d]}$	0.74 a.u.
$\theta_{m,x}$	0.00 °
$\theta_{m,xy}$	0.00 °
μ (Gaussian-CGS)	4.95e-19 esu·cm
m (Gaussian-CGS)	6.86e-21 erg·G ⁻¹
$\theta_{\mu,m}$	90.00 °
$\cos(\theta_{\mu,m})$	-0.00
g_{lum}	-0.000

Excited States

Table 7: Summary of the calculated excited states. E_x : The energy of excited state x . λ_x : The wavelength of a photon of equivalent energy to excited state x . f_x : The oscillator strength of the excited state transition x . ΔE_{xy} : The difference in energy between the lowest excited states of multiplicity x and y .

No. calculated singlets	10
E_{S_1}	4.12 eV

λ_{S_1} (colour, CIE)	301 nm (Ultraviolet ■ (0.00, 0.00))
f_{S_1}	< 0.01
Simulated Absorption Peaks	145, 157 and 215 nm

Vertical S₁ Emission

Table 8: Summary of the vertical emission from the S₁ state.

Excited energy	-6743.99 eV
Excited multiplicity	Singlet
Ground energy	-6748.11 eV
Ground multiplicity	Singlet
Emission type	Fluorescence
S ₁ energy	4.12 eV
S ₁ wavelength (colour, CIE)	301 nm (Ultraviolet ■ (0.00, 0.00))
S ₁ oscillator strength	0.00
S ₁ rate	3.54e+07 /s ¹

Methodology

Metadata

The calculation of the optimised structure and excited states was performed using the **Gaussian (2016+C.01)** program, the **DFT** method with the **PBE1PBE** functional and the **6-31G(d,p)** basis set. It was completed on the **16th June 2022** after a total duration of **9 m, 42 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 Emission rate constants (k_e) were calculated according to the method developed by Shizu and Kaji⁴ as described by formula 1, where ΔE_e is the energy of emission, ϵ_0 is the vacuum permittivity constant, \hbar is the reduced Planck constant (the Dirac constant), c is the speed of light and μ_e is the transition dipole moment of the emission.

$$k_e = \frac{4 \Delta E_e}{3 \epsilon_0 \hbar^4 c^3} \mu_e \quad 1$$

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, over a total of five steps, the results of which are displayed in figure 1. The energy calculated by the final step was -6748.11 eV, corresponding to -651,093 KJmol⁻¹. A plot of the total SCF electron density is shown in figure 2.

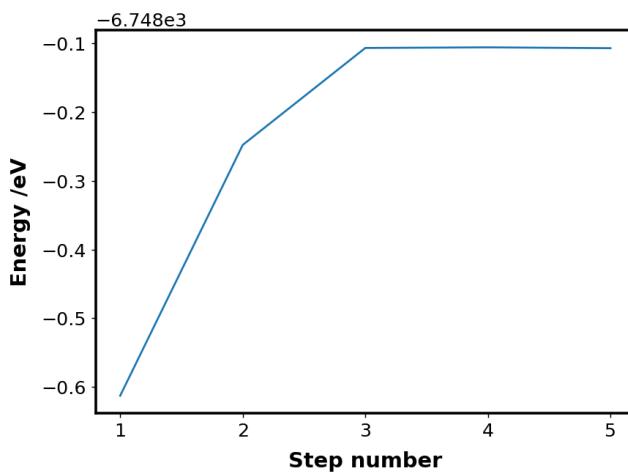


Figure 1: Graph of calculated energies at the self-consistent field (SCF) level.

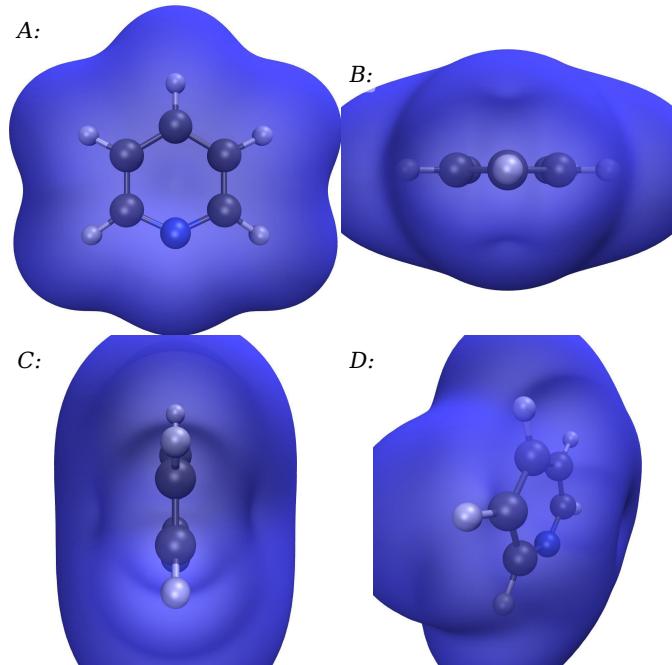


Figure 2: Plot of the total SCF electron density, plotted with an isovalue of 0.0004. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Geometry

The **empirical formula** of the studied system was C₅NH₅, 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 4.38, 3.81 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 0.13 and 1.00 respectively.

Permanent Dipole Moment

The calculated **permanent dipole moment** was 0.61 D, with a vector (x,y,z) of 0.00, -0.61, 0.00 D. The angle between the dipole moment vector and the x-axis was 89.99 °, while the angle between the dipole moment and the xy-plane was 0.01 °. A plot of the permanent dipole moment is shown in figure 3.

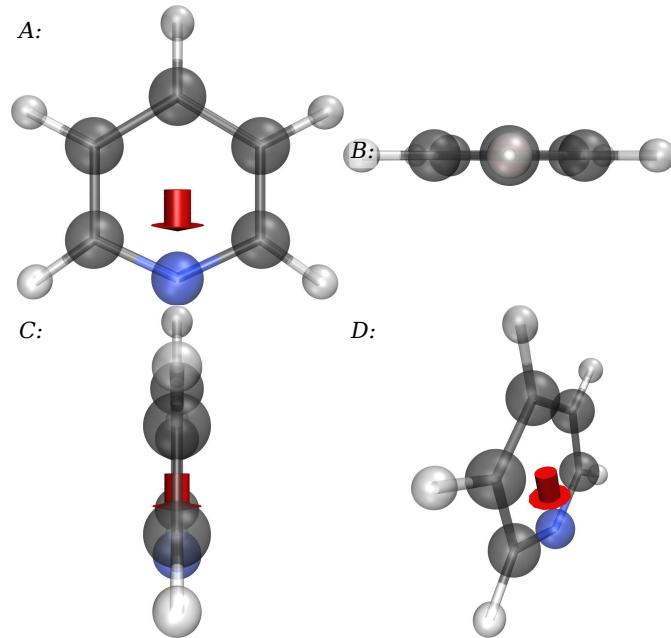


Figure 3: The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

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 0.50 D and 0.74 au respectively. The corresponding vector components (x,y,z) were $\mu = 0.00, 0.00, 0.50$ D and $m = 0.74, 0.00, 0.00$ au. In comparison to the molecular geometry, the angle between each dipole moment and the longest axis of the molecule (the x-axis) was $\theta_{\mu,x} = 90.00$ ° and $\theta_{m,x} = 0.00$ °, while the angle between each dipole moment and the xy-plane was $\theta_{\mu,xy} = 90.00$ ° and $\theta_{m,xy} = 0.00$ °. In Gaussian-CGS units, in which the magnetic and electric transition dipole moments can be directly compared, the magnitude of each dipole moment was $\mu = 4.95e-19$ esu·cm and $m = 6.86e-21$ erg·G⁻¹, while the **angle between the two dipole moments** was $\theta_{\mu,m} = 90.00$ °. Correspondingly, the cosine of the angle was $\cos(\theta_{\mu,m}) = -0.00$, and the **dissymmetry factor** of the excited state transition was $g_{lum} = -0.000$. A plot of the electric and magnetic transition dipole moments is shown in figure 4.

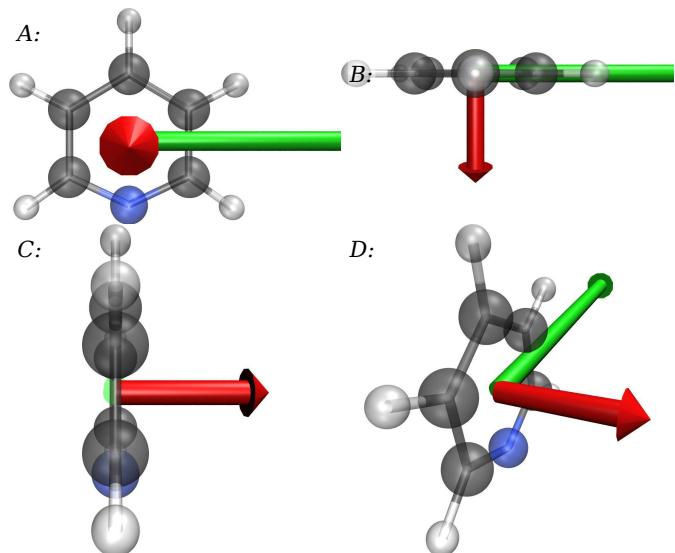


Figure 4: The electric (red arrow) and magnetic (green arrow) transition (S_1) dipole moment plotted against the aligned molecular geometry with a scale of 1 Å = 0.2 D = 0.1 au. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Molecular Orbitals

In total, 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 -6.49 and -0.59 eV respectively, corresponding to a **HOMO-LUMO band gap** of 5.90 eV (figure 15). Plots of the orbital density for the HOMO-5, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2 and LUMO+3 are shown in figures 5-10 and 12-14 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 11.

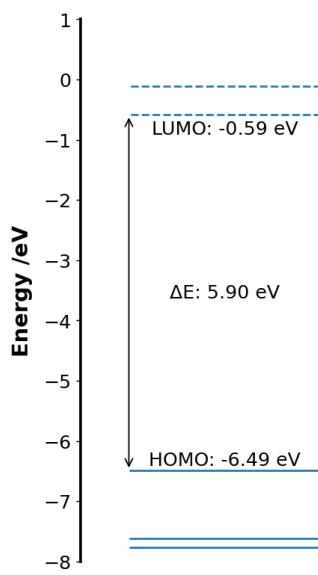


Figure 15: Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.

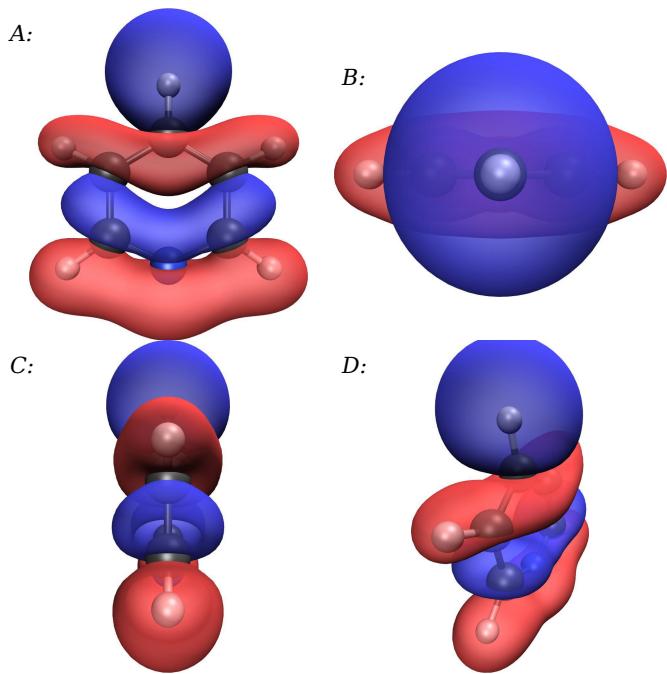


Figure 5: Orbital density plots of the HOMO-5, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

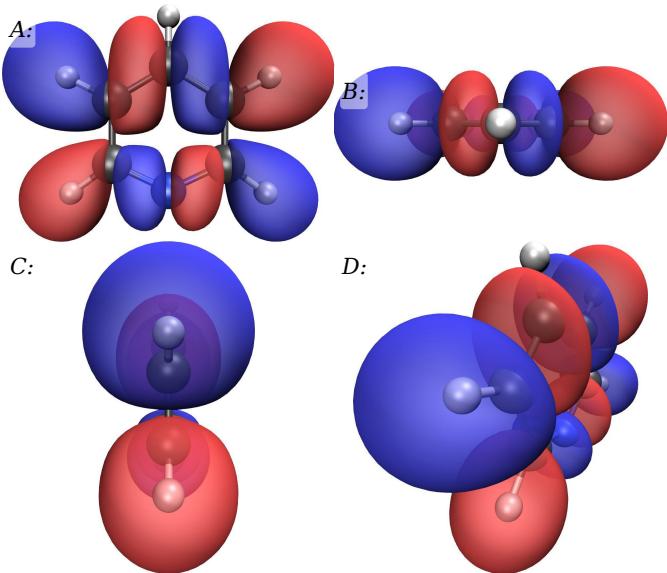


Figure 6: Orbital density plots of the HOMO-3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

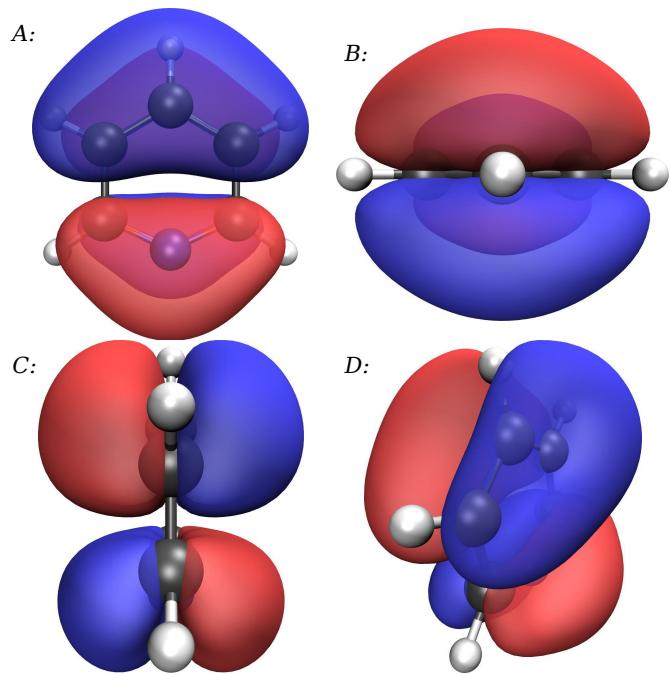


Figure 7: Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

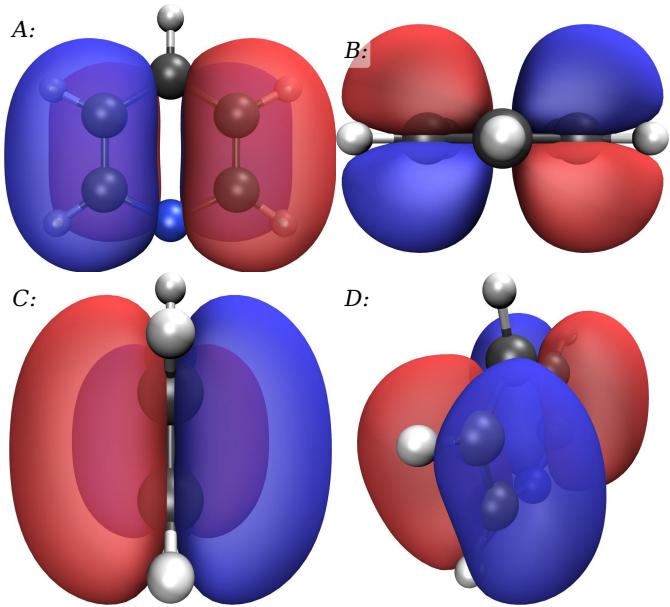


Figure 8: Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

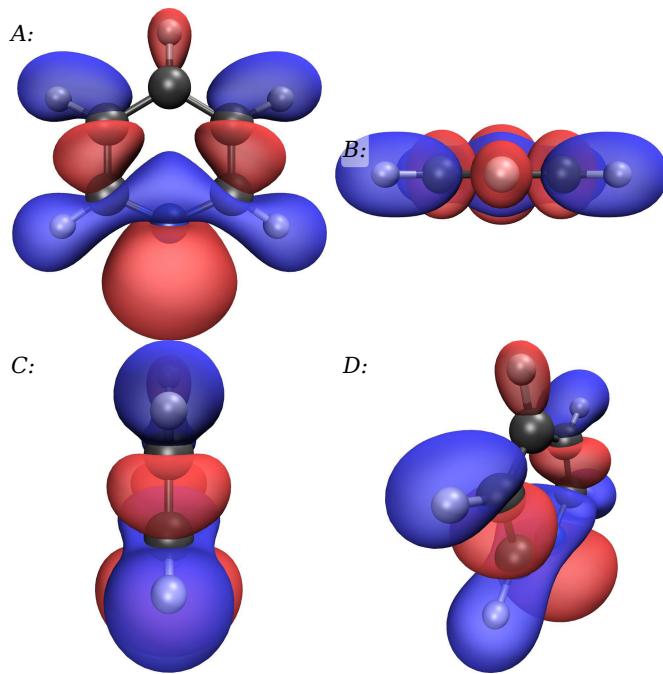


Figure 9: Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

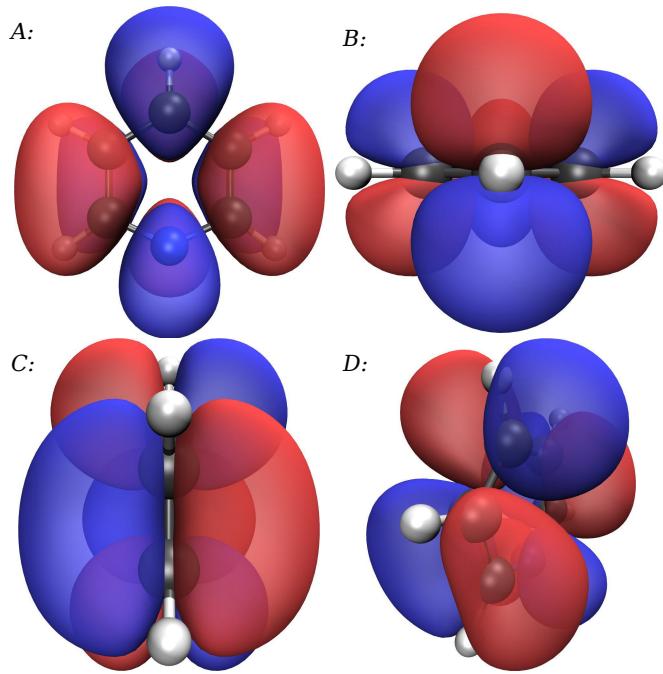


Figure 10: Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

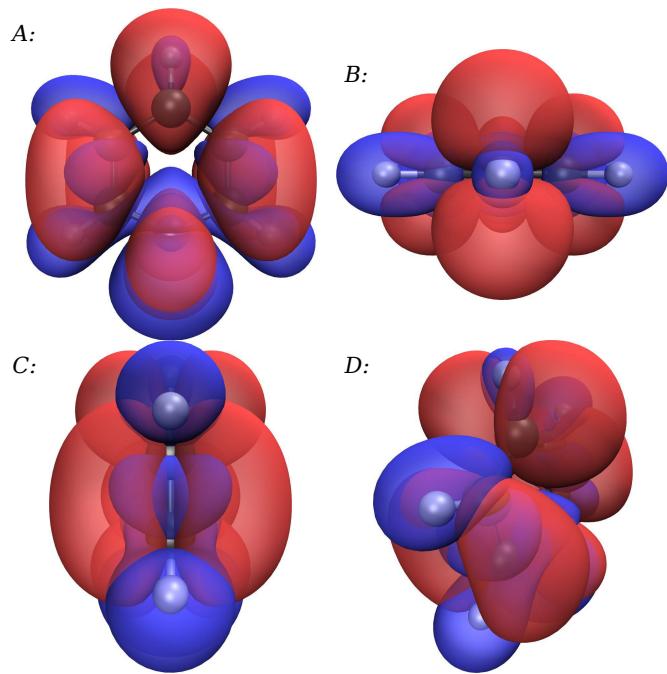


Figure 11: Orbital density plots of the HOMO (blue) and LUMO (red), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

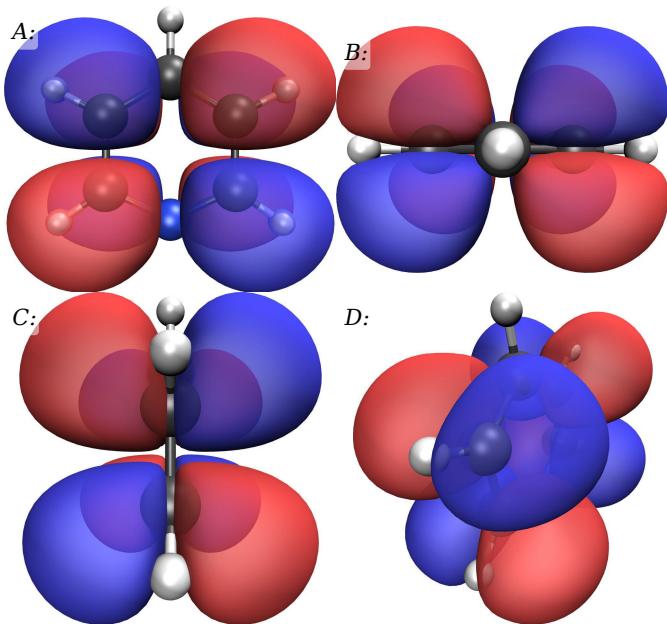


Figure 12: Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

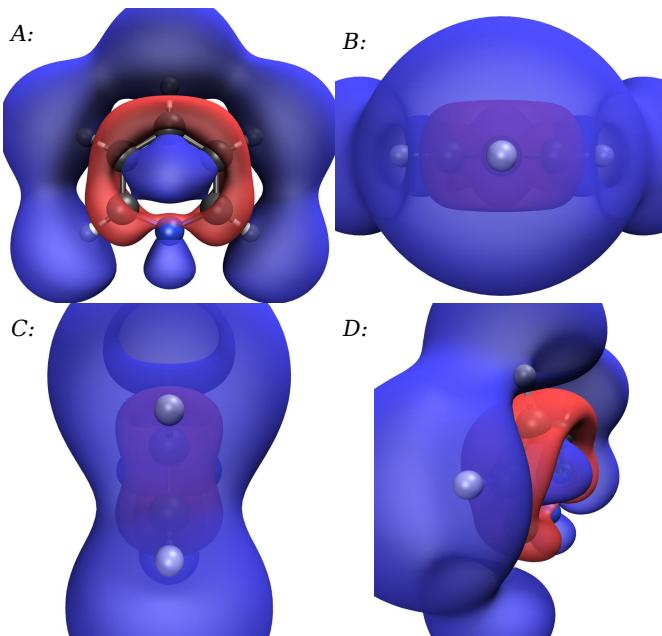


Figure 13: Orbital density plots of the LUMO+2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

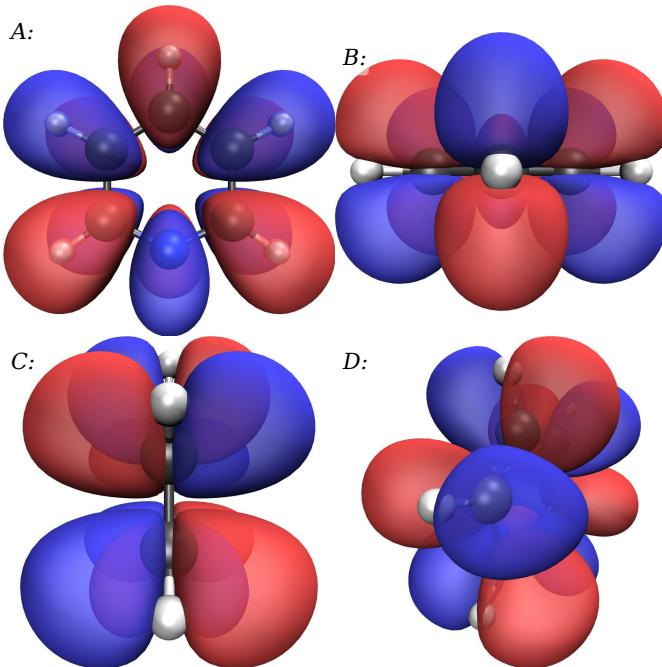


Figure 14: Orbital density plots of the LUMO+3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Excited States

In total, the energies of 10 singlet electronic excited states were calculated, which are shown in figure 16. The energy of the lowest **singlet excited state (S_1)** was 4.12 eV, corresponding to absorption by a photon with a wavelength of 301 nm, an ultraviolet 'color' ■ and CIE coordinates of (0.00, 0.00). 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 **three most intense peaks** were found at 145, 157 and 215 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 18-27.

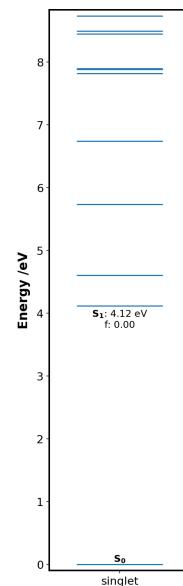


Figure 16: Graph of the calculated excited states. f: oscillator strength of the relevant ground to excited state transition.

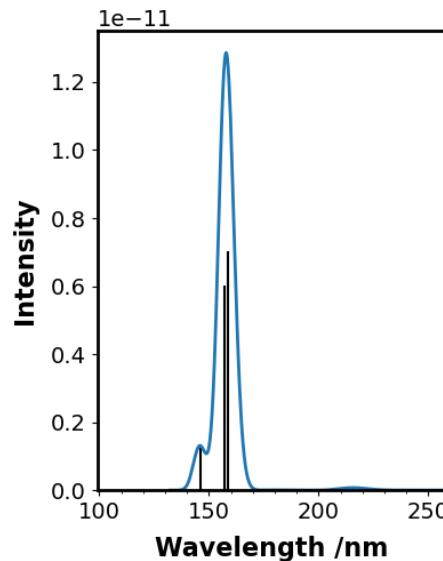


Figure 17: Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 145, 157 and 215 nm.

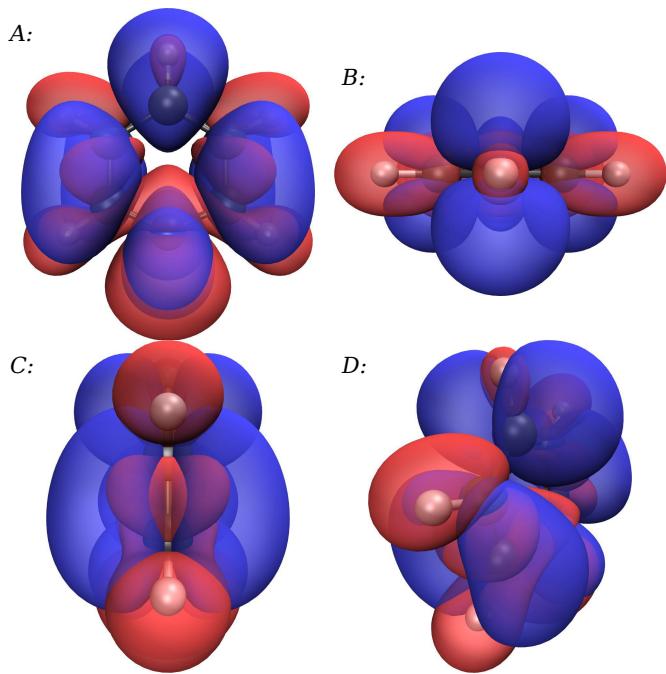


Figure 18: Density plot of the NTO hole (blue) & electron (red) of the S_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

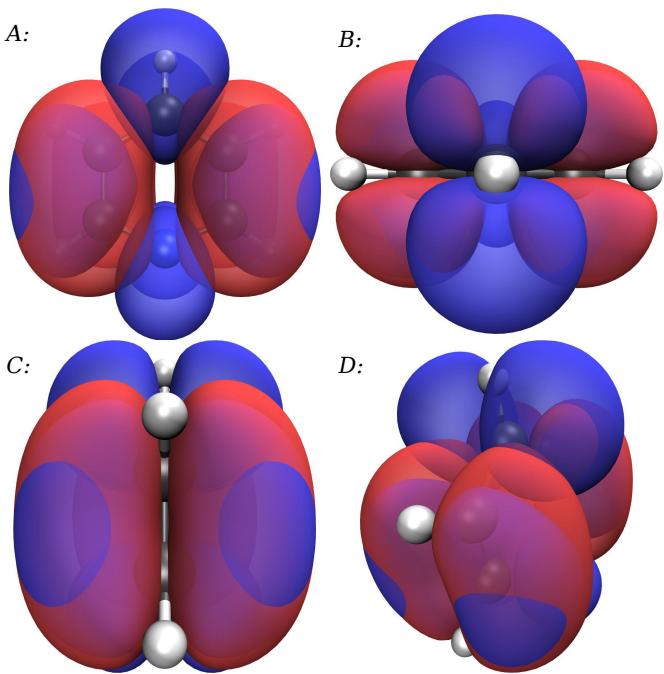


Figure 20: Density plot of the NTO hole (blue) & electron (red) of the S_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

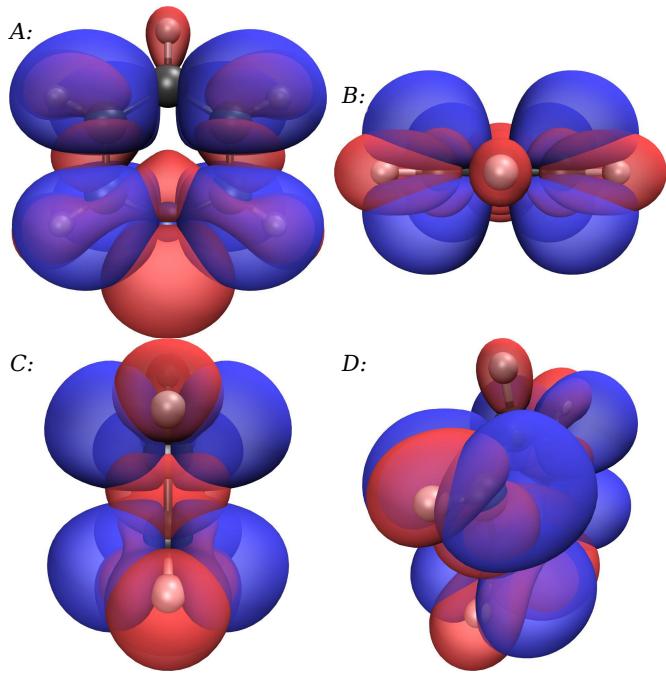


Figure 19: Density plot of the NTO hole (blue) & electron (red) of the S_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

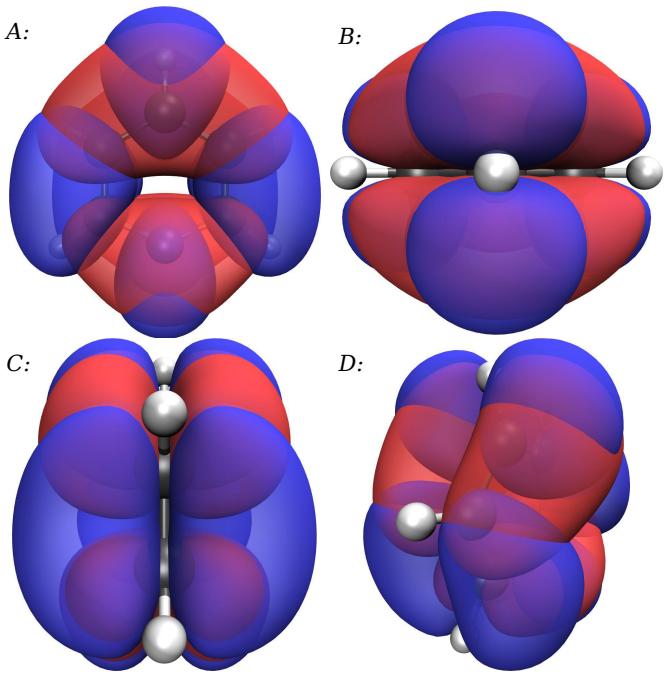


Figure 21: Density plot of the NTO hole (blue) & electron (red) of the S_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

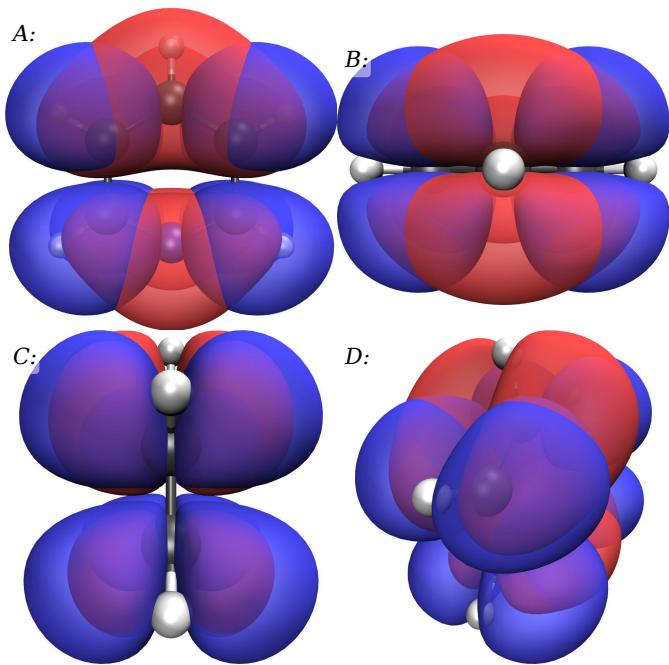


Figure 22: Density plot of the NTO hole (blue) & electron (red) of the S_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

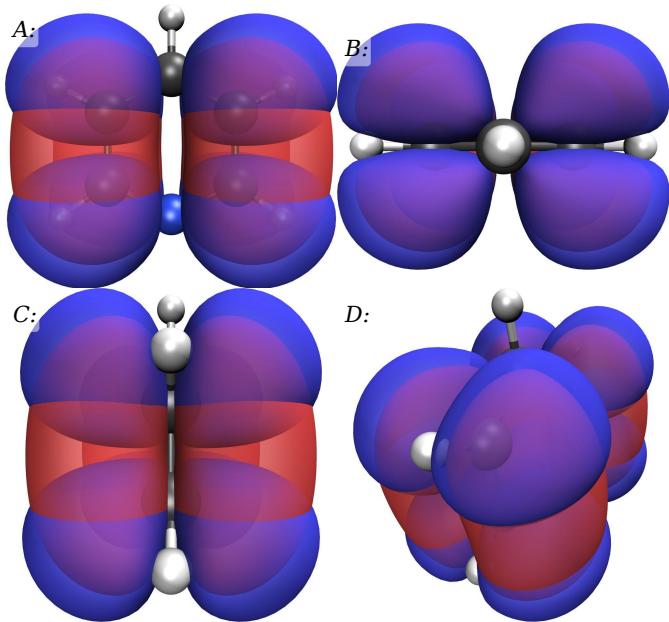


Figure 23: Density plot of the NTO hole (blue) & electron (red) of the S_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

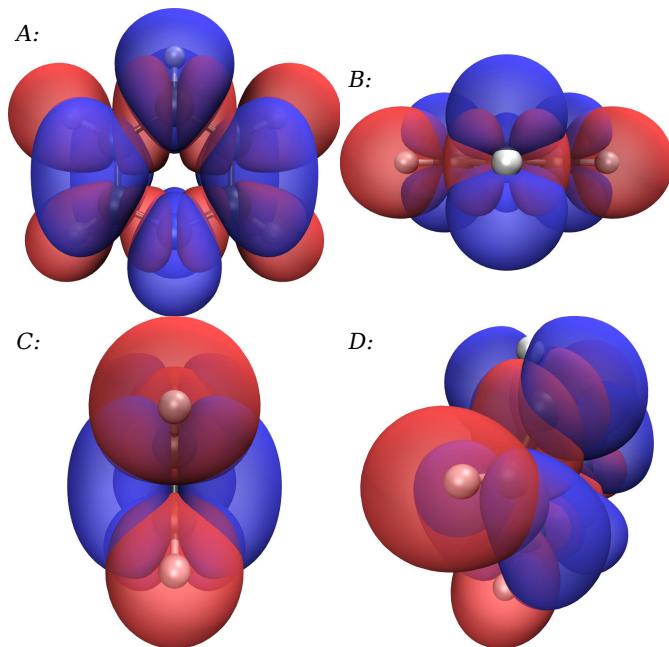


Figure 24: Density plot of the NTO hole (blue) & electron (red) of the S_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

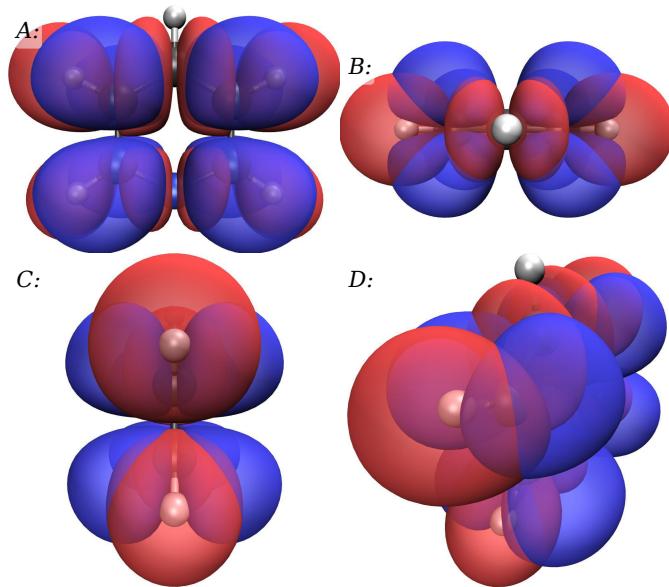


Figure 25: Density plot of the NTO hole (blue) & electron (red) of the S_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

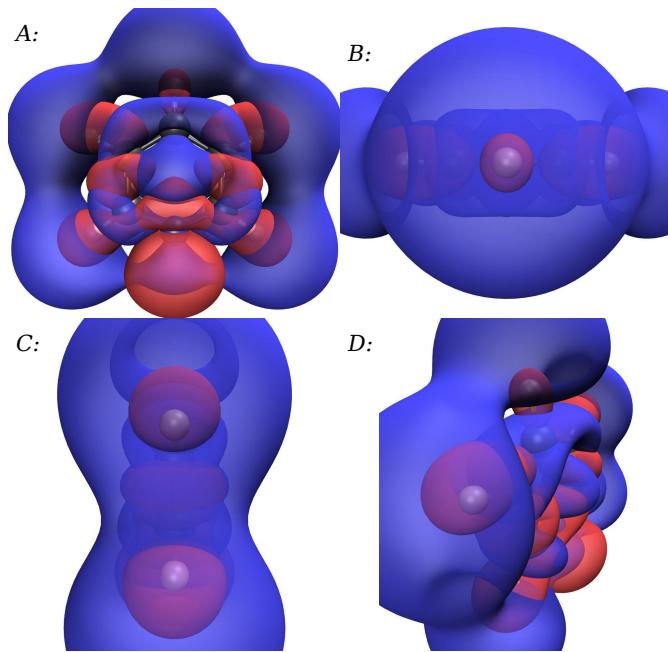


Figure 26: Density plot of the NTO hole (blue) & electron (red) of the S_g state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

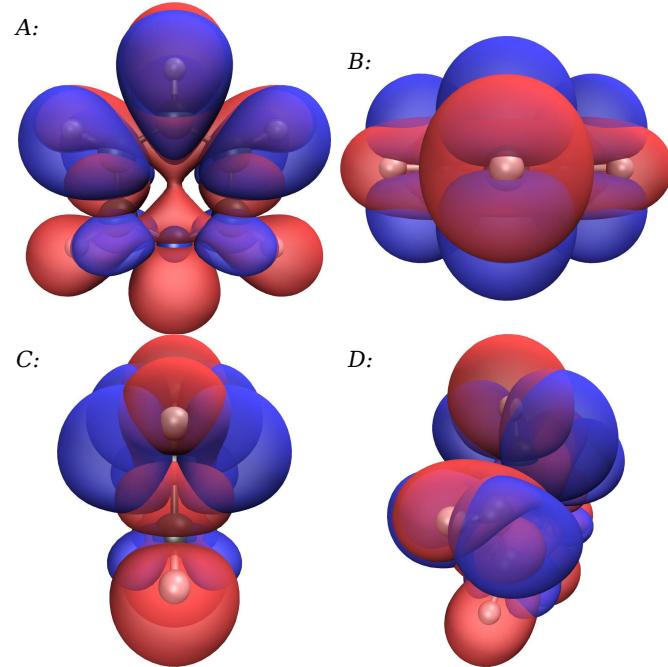


Figure 27: Density plot of the NTO hole (blue) & electron (red) of the S_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Vertical Emission Energy

The vertical emission energy, corresponding to the difference in energy between an excited state at an excited state geometry, and the ground state at the ground state geometry, from the S_1 state to the ground state was calculated and found to be 4.12 eV.

This energy is equivalent to emission of a photon with a wavelength of 301 nm, corresponding to a colour of Ultraviolet ■ and CIE coordinates (x,y) of (0.00, 0.00). The excited state had a total energy of -6743.99 eV and a multiplicity of one, while the ground state had a total energy of -6748.11 eV and a multiplicity of one. This emission is therefore a fluorescence type process, because both the ground and excited state have the same multiplicity. Finally, the rate constant of the emission was calculated to be $3.54 \times 10^7 \text{ s}^{-1}$

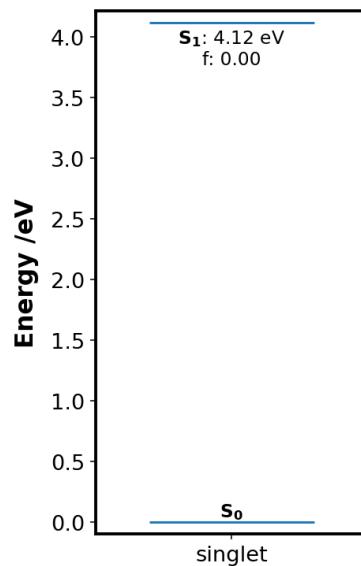


Figure 28: Graph of the calculated vertical S_1 emission energy.

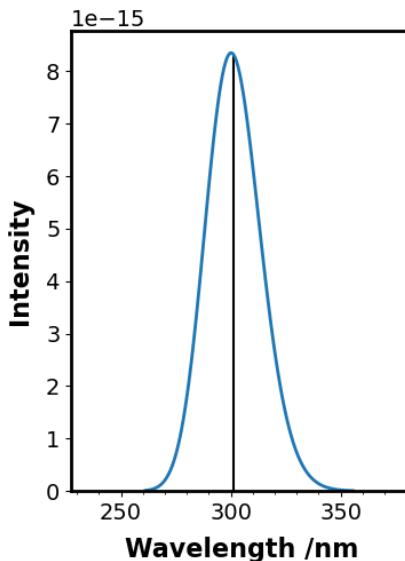


Figure 29: Graph of the simulated vertical S_1 emission spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.4 eV are shown as a blue line. Peaks can be found at: 300 nm.

Tables Of Results**Atom Coordinates****Table 10:** 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	1.2223280	-0.7327140	-0.0000160	26	LUMO+4	A	4.1282
C	1.2236890	0.6422610	0.0000110	25	LUMO+3	A	4.1062
C	0.0000010	1.3694790	0.0000280	24	LUMO+2	A	3.0885
C	-1.2236670	0.6422750	0.0000240	23	LUMO+1	A	-0.1135
C	-1.2223510	-0.7327070	-0.0000170	22	LUMO	A	-0.5872
N	-0.0000010	-1.3065420	-0.0000430	21	HOMO	A	-6.4894
H	2.1060240	-1.3583370	-0.0000070	20	HOMO-1	A	-7.6132
H	2.1890680	1.1397590	0.0000350	19	HOMO-2	A	-7.7732
H	0.0000010	2.4513310	0.0000610	18	HOMO-3	A	-10.2780
H	-2.1890380	1.1397920	0.0000510	17	HOMO-4	A	-11.0663
H	-2.1060520	-1.3583170	-0.0000210	16	HOMO-5	A	-11.2557
				15	HOMO-6	A	-12.3368

Molecular Orbitals**Table 11:** Energies of the calculated molecular orbitals.

Level	Label	Symmetry	Energy /eV				
37	LUMO+15	A	14.9352	11	HOMO-10	A	-17.4754
36	LUMO+14	A	14.5437	10	HOMO-11	A	-17.5821
35	LUMO+13	A	12.6778	9	HOMO-12	A	-21.5990
34	LUMO+12	A	11.8563	8	HOMO-13	A	-21.9944
33	LUMO+11	A	9.5588	7	HOMO-14	A	-26.0127
				6	HOMO-15	A	-278.9110

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	S ₁	Singlet-A	4.1172	301.14	Ultraviolet [■] (0.00, 0.00)	0.0038	HOMO → LUMO (0.99)
2	S ₂	Singlet-A	4.6017	269.43	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO → LUMO+1 (1.00)
3	S ₃	Singlet-A	5.7361	216.15	Ultraviolet [■] (0.00, 0.00)	0.0173	HOMO-1 → LUMO (0.60) HOMO-2 → LUMO+1 (0.40)
4	S ₄	Singlet-A	6.7431	183.87	Ultraviolet [■] (0.00, 0.00)	0.0013	HOMO-2 → LUMO (0.58) HOMO-1 → LUMO+1 (0.39)
5	S ₅	Singlet-A	7.8174	158.60	Ultraviolet [■] (0.00, 0.00)	0.8914	HOMO-2 → LUMO+1 (0.56) HOMO-1 → LUMO (0.36)
6	S ₆	Singlet-A	7.8802	157.34	Ultraviolet [■] (0.00, 0.00)	0.7514	HOMO-1 → LUMO+1 (0.53) HOMO-2 → LUMO (0.31) HOMO → LUMO+2 (0.09)
7	S ₇	Singlet-A	7.8952	157.04	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.99)
8	S ₈	Singlet-A	8.4452	146.81	Ultraviolet [■] (0.00, 0.00)	0.0051	HOMO-3 → LUMO+1 (0.99)
9	S ₉	Singlet-A	8.4945	145.96	Ultraviolet [■] (0.00, 0.00)	0.1342	HOMO → LUMO+2 (0.85) HOMO-2 → LUMO (0.05) HOMO-4 → LUMO (0.04) HOMO-1 → LUMO+1 (0.03)
10	S ₁₀	Singlet-A	8.7332	141.97	Ultraviolet [■] (0.00, 0.00)	0.0006	HOMO → LUMO+3 (0.50) HOMO-5 → LUMO (0.48)

Transition Dipole Moments

Table 12: 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	$\theta_{\mu,m}^{[i]}$ /°	$\cos(\theta_{\mu,m})^{[j]}$	$g_{lum}^{[k]}$
S ₁	0.00, 0.00, 0.50	0.50	90.00	90.00	0.74, 0.00, 0.00	0.74	0.00	0.00	4.95e-19	6.86e-21	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	89.60	0.00	0.00e+00	2.68e-22	90.00	0.00	0.000
S ₃	-0.89, 0.00, 0.00	0.89	0.00	0.00	0.00, 0.00, -0.07	0.07	90.00	90.00	8.93e-19	6.27e-22	90.00	0.00	0.000
S ₄	-0.00, 0.23, 0.00	0.23	89.81	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	2.27e-19	0.00e+00	90.00	0.00	0.000
S ₅	5.48, -0.00, 0.00	5.48	0.01	0.00	0.00, 0.00, 0.04	0.04	90.00	90.00	5.48e-18	3.37e-22	90.00	0.00	0.000
S ₆	-0.00, -5.01, 0.00	5.01	89.99	0.00	0.00, -0.00, 0.00	< 0.01	90.00	0.00	5.01e-18	9.27e-25	179.99	-1.00	< 0.001
S ₇	0.00, 0.00, 0.00	< 0.01	90.00	0.00	-0.00, -0.42, 0.00	0.42	89.99	0.00	7.63e-22	3.88e-21	0.01	1.00	0.756
S ₈	0.00, 0.00, -0.40	0.40	90.00	90.00	0.05, 0.00, 0.00	0.05	0.11	0.00	3.98e-19	4.95e-22	90.00	0.00	0.000
S ₉	0.00, 2.04, 0.00	2.04	90.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	2.04e-18	0.00e+00	90.00	0.00	0.000
S ₁₀	0.00, 0.00, 0.14	0.14	90.00	90.00	1.67, 0.00, 0.00	1.67	0.00	0.00	1.38e-19	1.55e-20	90.00	-0.00	-0.000

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