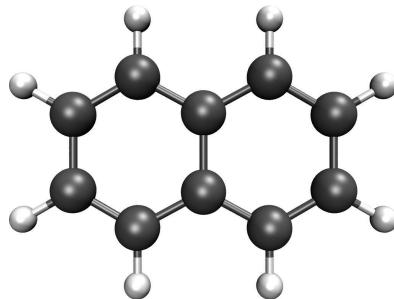




A Report On The Calculation Of The Optimised Structure And Excited States Of Naphthalene At The PBE1PBE/6-31G(d,p) Level

osl - 07th June 2022



Abstract

The calculation of optimised structure and excited states for the system 'Naphthalene' 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 -10488.88 eV after 4 steps. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -6.05 and -1.07 eV respectively, corresponding to a HOMO-LUMO band gap of 4.98 eV. The permanent dipole moment (PDM) was calculated to be 0.00 D. In total, 10 excited states were calculated with singlet multiplicity. The most intense absorption peaks were calculated to be at 198 and 271 nm. The lowest energy singlet excited state (S_1) was calculated to be 4.44 eV (279 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
07/06/2022 17:37:23	6 m, 49 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	4
Final energy	-10488.8835 eV
Final energy	-1,012,023 kJ·mol ⁻¹

Geometry

Table 3: Summary of geometry properties.

Formula	C ₁₀ H ₈
Exact mass	128.0626 g·mol ⁻¹
Molar mass	128.1705 g·mol ⁻¹
Alignment method	Minimal
X extension	6.78 Å
Y extension	5.00 Å
Z extension	0.00 Å
Linearity ratio	0.26
Planarity ratio	1.00

Molecular Orbitals

Table 4: Summary of HOMO & LUMO properties.

E _{HOMO,LUMO}	4.98 eV
E _{HOMO}	-6.05 eV
E _{LUMO}	-1.07 eV

Permanent Dipole Moment

Table 5: Summary of the permanent dipole moment properties.

Total	0.00 D
X axis angle	0.00 °

XY plane angle

0.00 °

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	0.04 D
$\theta_{\mu,x}$	0.00 °
$\theta_{\mu,xy}$	0.00 °
$m^{[d]}$	0.00 a.u.
$\theta_{m,x}$	0.00 °
$\theta_{m,xy}$	0.00 °
μ (Gaussian-CGS)	4.02e-20 esu·cm
m (Gaussian-CGS)	0.00e+00 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}	4.44 eV
λ_{S_1} (colour, CIE)	279 nm (Ultraviolet (■, (0.00, 0.00)))

f_{S_1}	0.00
Simulated Absorption Peaks	198 and 271 nm

Vertical S_1 Emission

Table 8: Summary of the vertical emission from the S_1 state.

Excited energy	-10484.45 eV
Excited multiplicity	Singlet
Ground energy	-10488.88 eV
Ground multiplicity	Singlet
Emission type	Fluorescence
S_1 energy	4.44 eV
S_1 wavelength (colour, CIE)	279 nm (Ultraviolet ■ (0.00, 0.00))
S_1 oscillator strength	0.00
S_1 rate	2.91e+05 /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 **07th June 2022** after a total duration of **6 m, 49 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 four steps, the results of which are displayed in figure 1. The energy calculated by the final step was -10488.88 eV, corresponding to -1,012,023 KJmol⁻¹. A plot of the total SCF electron density is shown in figure 2.

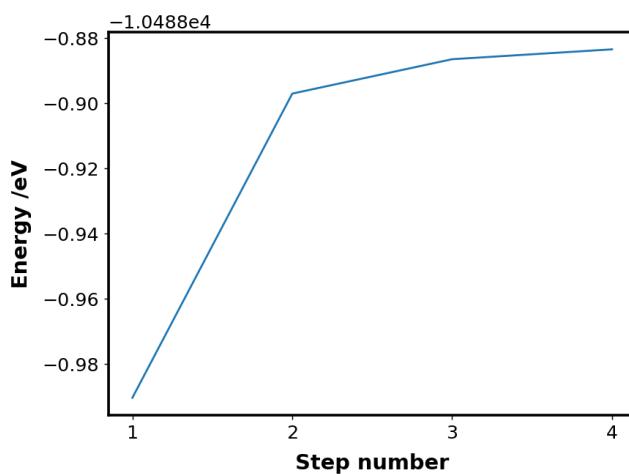


Figure 1: Graph of calculated energies at the self-consistent field (SCF) level.

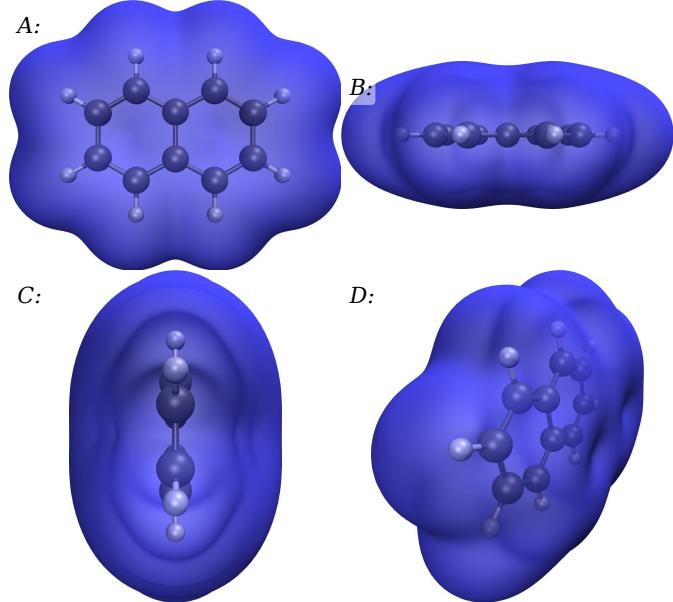


Figure 2: Plot of the total SCF electron density, plotted with an isovalue of 0.0004. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Geometry

The **empirical formula** of the studied system was $C_{10}H_8$, corresponding to a **molecular mass** of 128.17 gmol⁻¹ and an **exact mass**, considering only specific atomic isotopes, of 128.06 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 6.78, 5.00 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 0.26 and 1.00 respectively.

Permanent Dipole Moment

The calculated **permanent dipole moment** was exactly 0 D.

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 0.04 D and 0.00 au respectively. The corresponding vector components (x,y,z) were $\mu = 0.04, -0.00, -0.00$ D and $m = 0.00, 0.00, 0.00$ au. In comparison to the molecular geometry, the angle between each dipole moment and the longest axis of the molecule (the x-axis) was $\theta_{\mu,x} = 0.00^\circ$ and $\theta_{m,x} = 0.00^\circ$, while the angle between each dipole moment and the xy-plane was $\theta_{\mu,xy} = 0.00^\circ$ 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 $\mu = 4.02e-20$ esu·cm and $m = 0.00e+00$ erg·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.

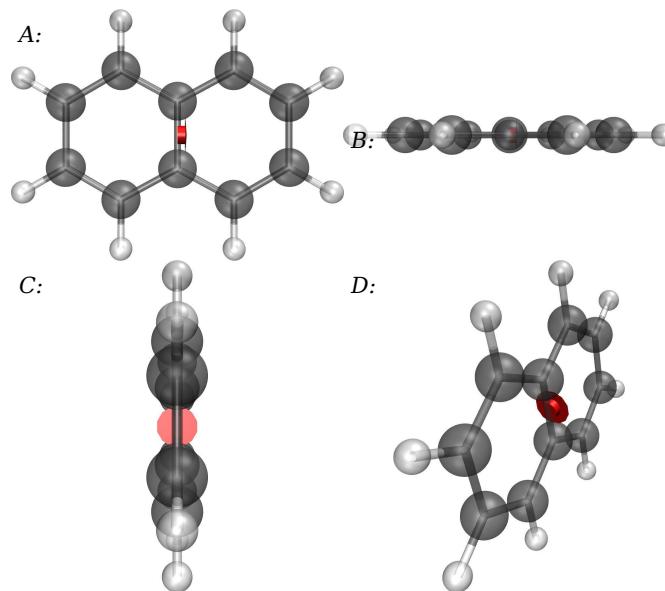


Figure 3: The electric (red arrow) and magnetic (green arrow) transition (S_1) dipole moment plotted against the aligned molecular geometry with a scale of 1 Å = 0.2 D = 0.1 au. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Molecular Orbitals

In total, 190 doubly occupied molecular orbitals were calculated, divided into 34 occupied orbitals and 156 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO** and **LUMO** were -6.05 and -1.07 eV respectively, corresponding to a **HOMO-LUMO band gap** of 4.98 eV (figure 14). Plots of the orbital density for the HOMO-5, HOMO-4, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1 and LUMO+2 are shown in figures 4-10 and 12-13 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 11.

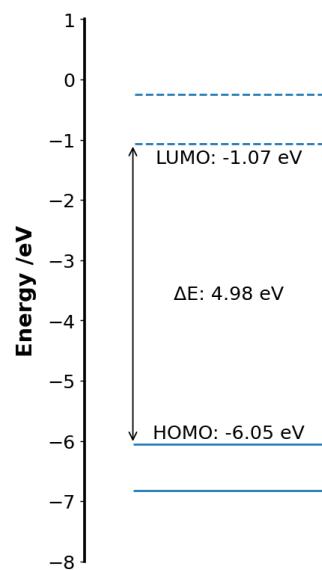


Figure 14: Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.

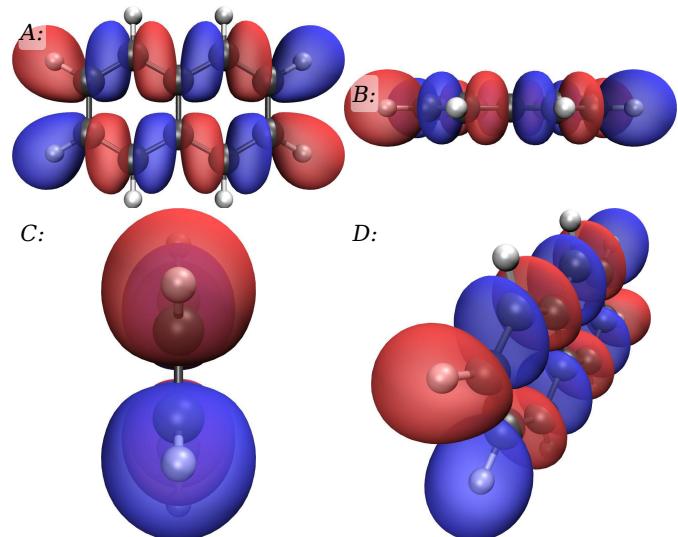


Figure 4: Orbital density plots of the HOMO-5, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

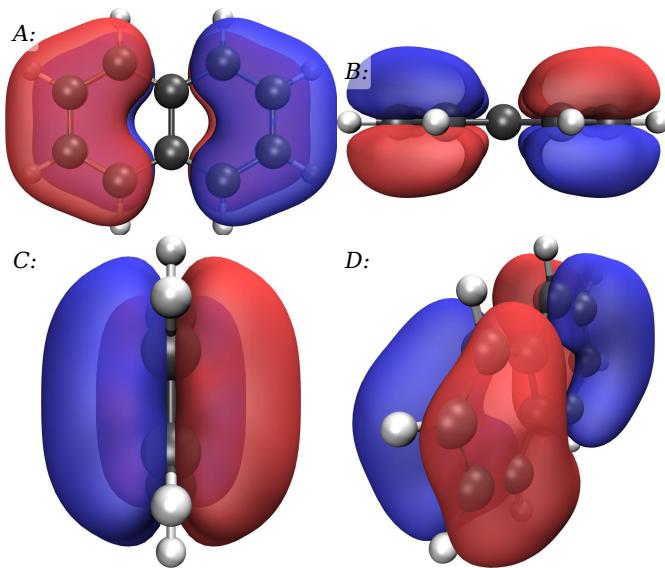


Figure 5: Orbital density plots of the HOMO-4, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

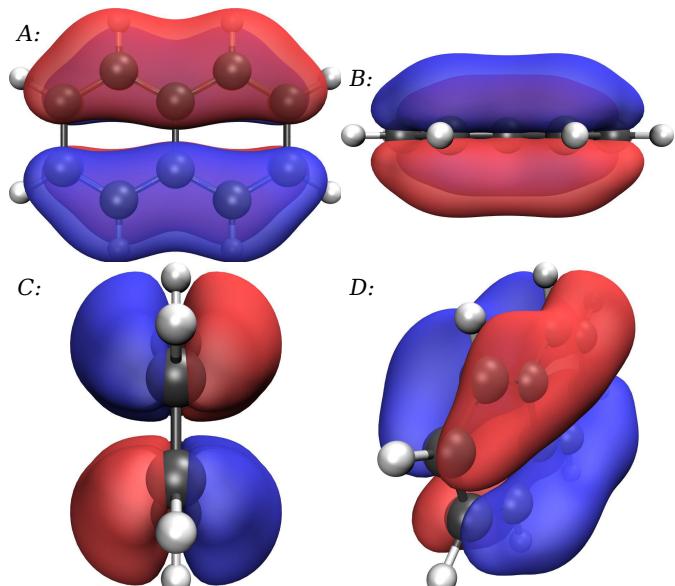


Figure 7: Orbital density plots of the HOMO-2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

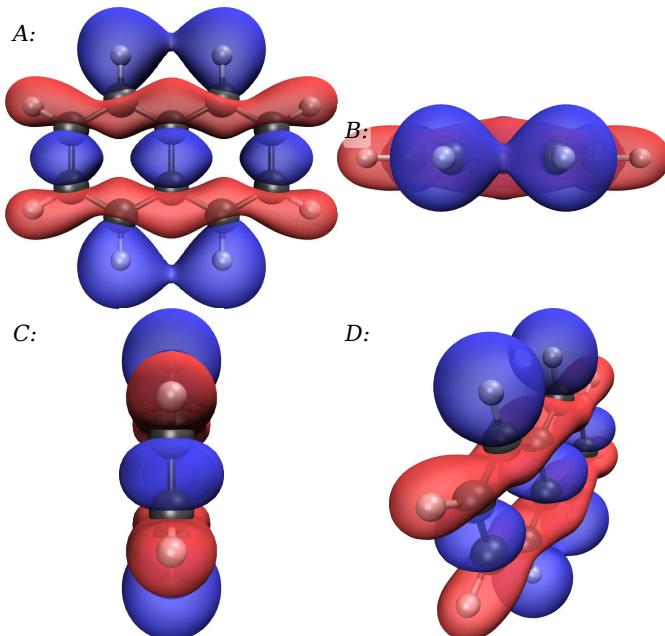


Figure 6: Orbital density plots of the HOMO-3, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

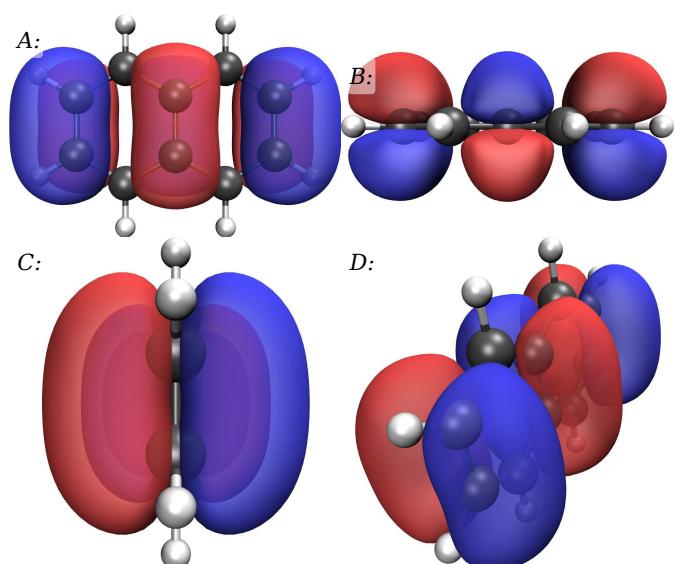


Figure 8: Orbital density plots of the HOMO-1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

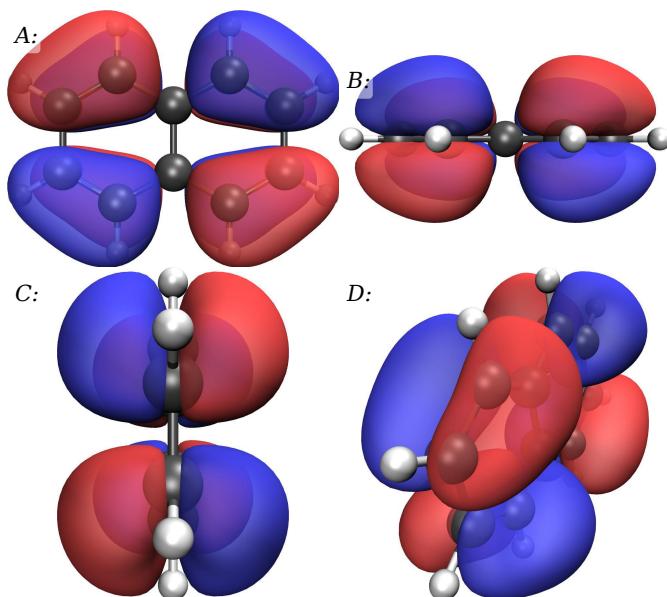


Figure 9: Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

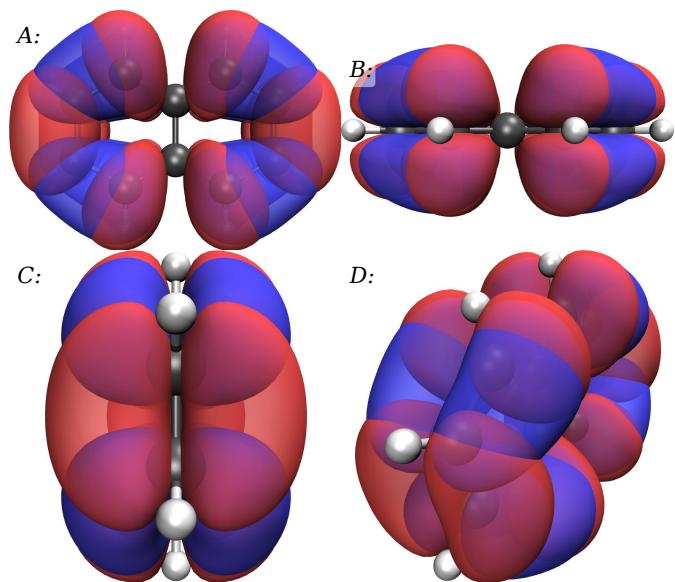


Figure 11: Orbital density plots of the HOMO (blue) and LUMO (red), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

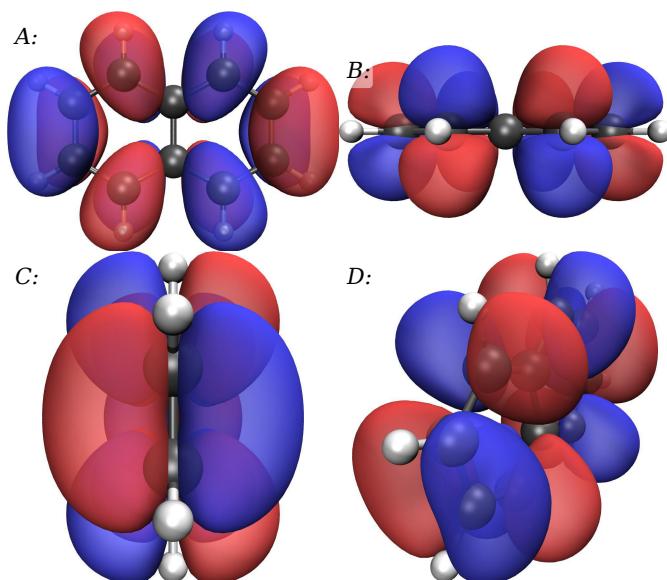


Figure 10: Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

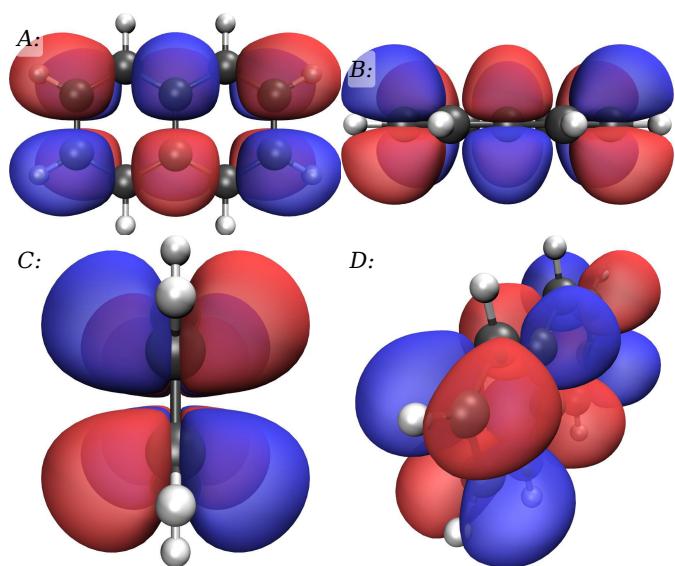


Figure 12: Orbital density plots of the LUMO+1, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

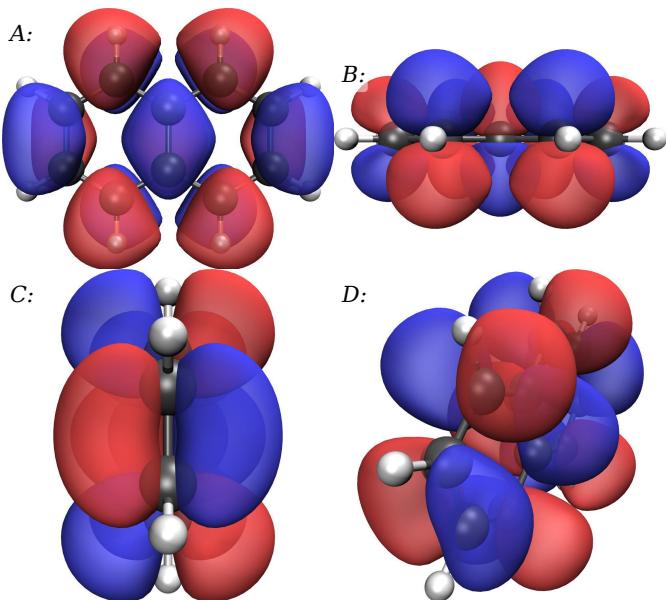


Figure 13: Orbital density plots of the LUMO+2, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Excited States

In total, the energies of 10 singlet electronic excited states were calculated, which are shown in figure 15. The energy of the lowest **singlet excited state (S_1)** was 4.44 eV, corresponding to absorption by a photon with a wavelength of 279 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 **two most intense peaks** were found at 198 and 271 nm. The full simulated absorption spectrum is shown in figure 16. Finally, **natural transition orbitals (NTOs)** were calculated for each excited state and are shown in figures 17-26.

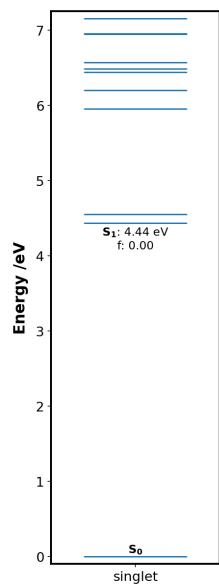


Figure 15: Graph of the calculated excited states. f : oscillator strength of the relevant ground to excited state transition.

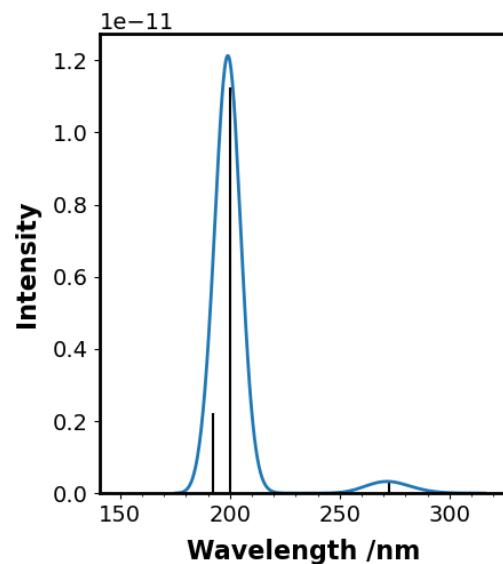


Figure 16: Graph of the simulated absorption spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.40 eV are shown as a blue line. Peaks can be found at: 198 and 271 nm.

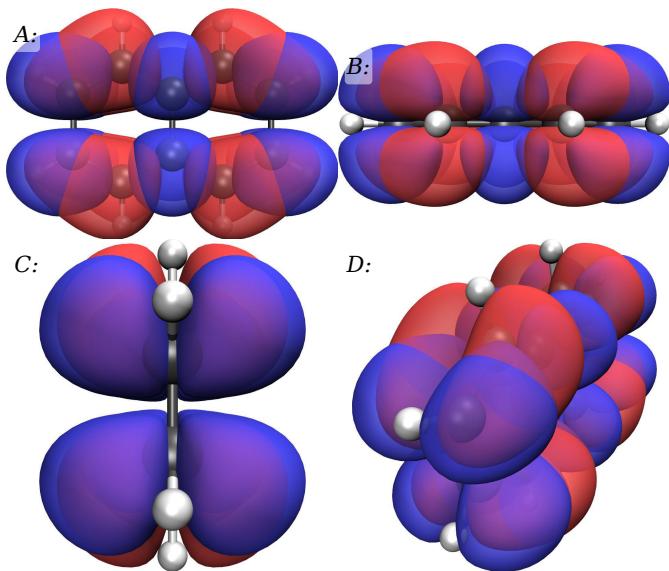


Figure 17: Density plot of the NTO hole (blue) & electron (red) of the S_1 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

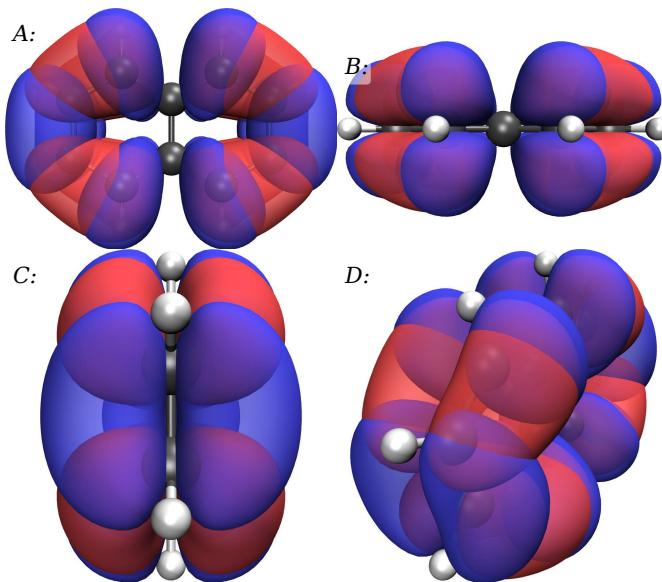


Figure 18: Density plot of the NTO hole (blue) & electron (red) of the S_2 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

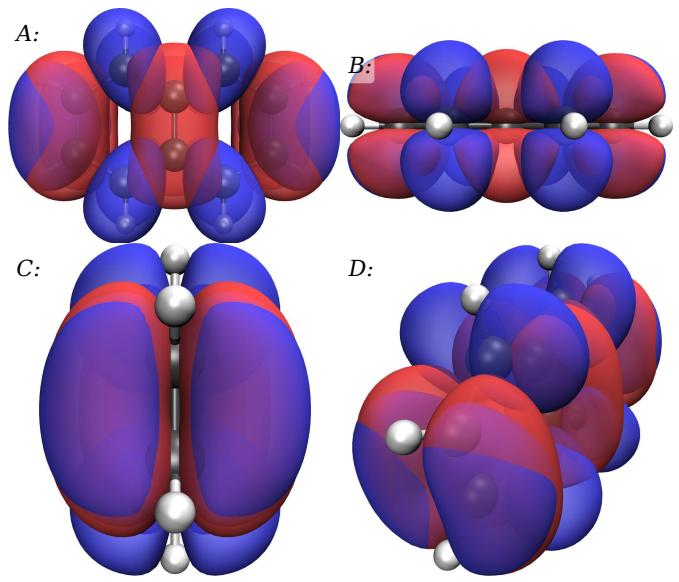


Figure 20: Density plot of the NTO hole (blue) & electron (red) of the S_4 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

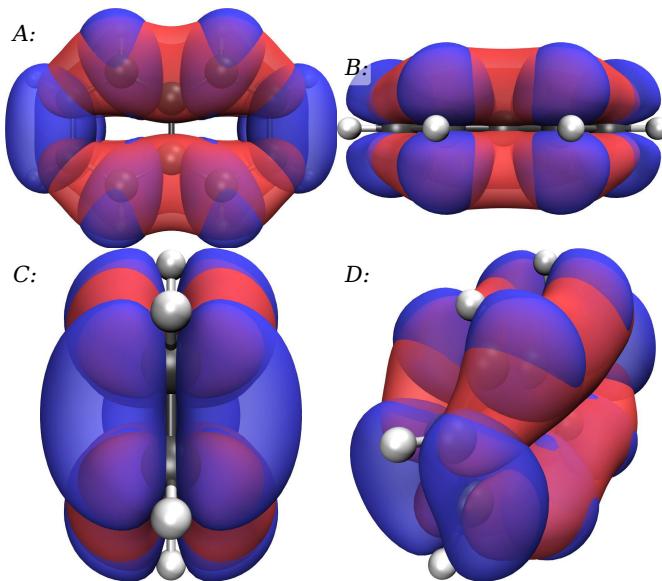


Figure 19: Density plot of the NTO hole (blue) & electron (red) of the S_3 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

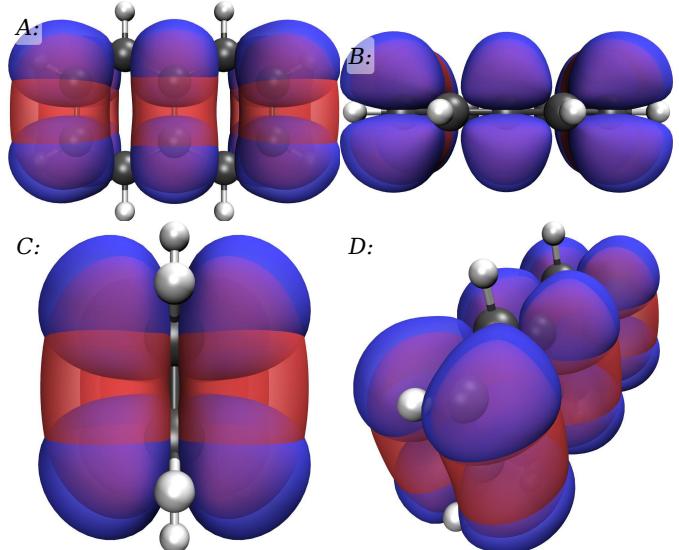


Figure 21: Density plot of the NTO hole (blue) & electron (red) of the S_5 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

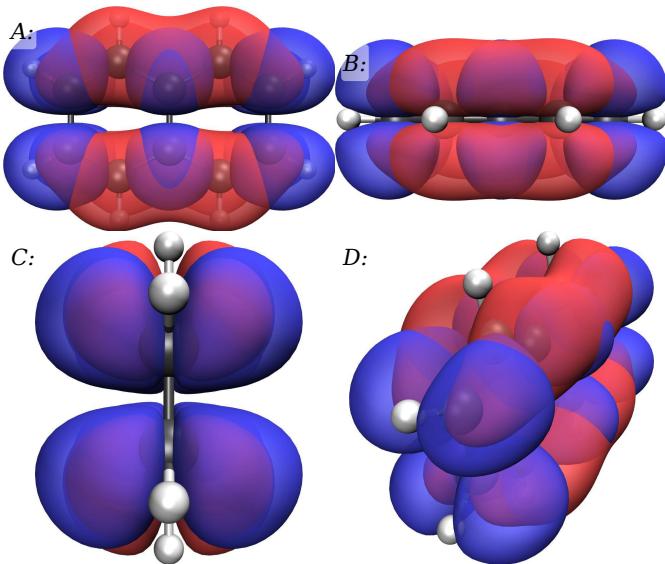


Figure 22: Density plot of the NTO hole (blue) & electron (red) of the S_6 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

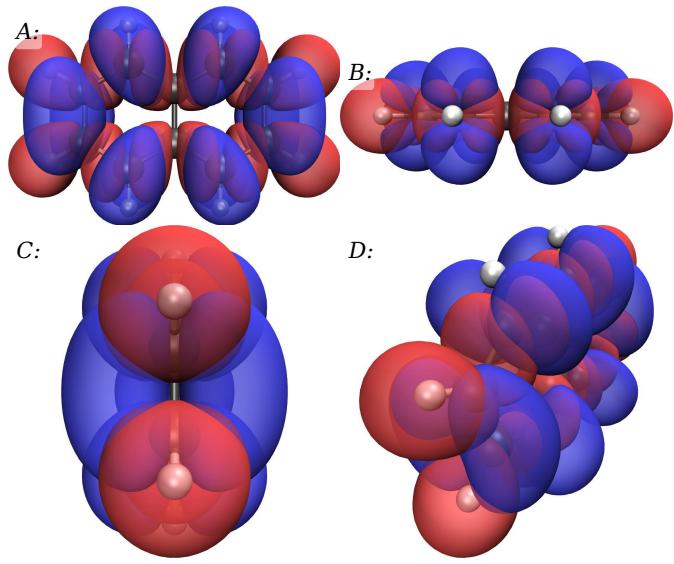


Figure 24: Density plot of the NTO hole (blue) & electron (red) of the S_8 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

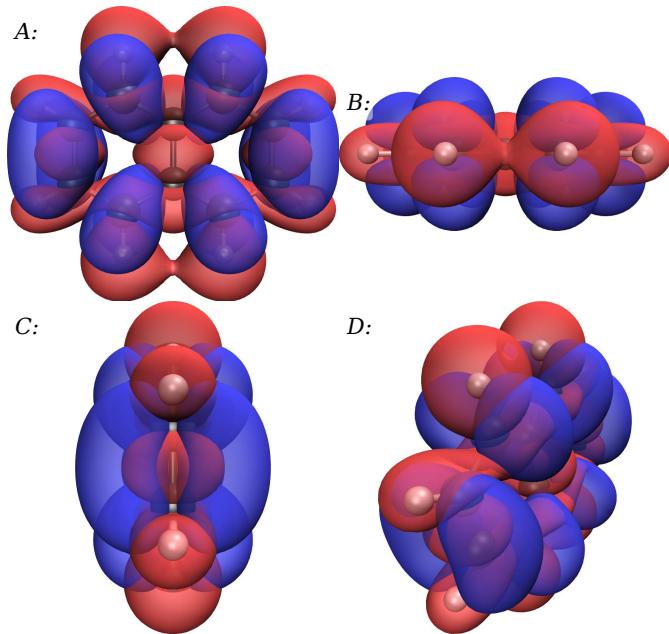


Figure 23: Density plot of the NTO hole (blue) & electron (red) of the S_7 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

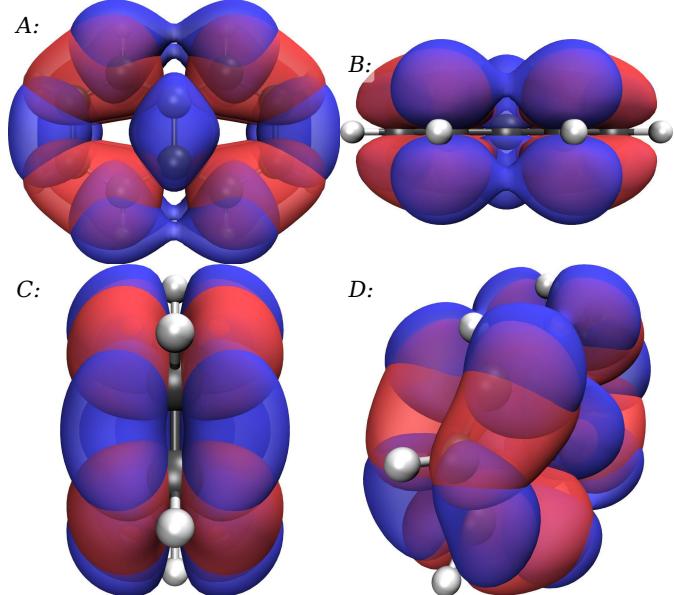


Figure 25: Density plot of the NTO hole (blue) & electron (red) of the S_9 state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

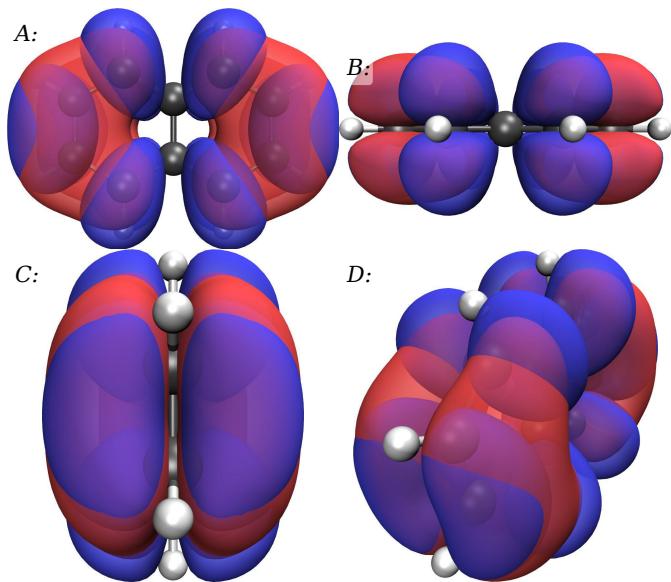


Figure 26: Density plot of the NTO hole (blue) & electron (red) of the S_{10} state, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

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 4.44 eV. This energy is equivalent to emission of a photon with a wavelength of 279 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 -10484.45 eV and a multiplicity of one, while the ground state had a total energy of -10488.88 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 $2.91 \times 10^5 \text{ s}^{-1}$

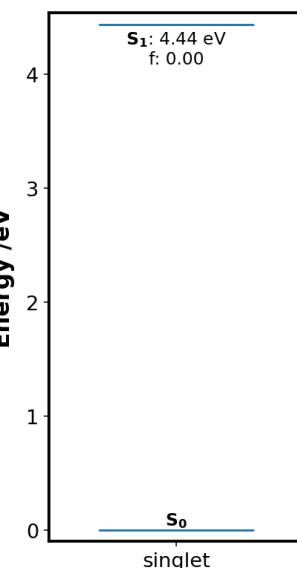


Figure 27: Graph of the calculated vertical S_1 emission energy.

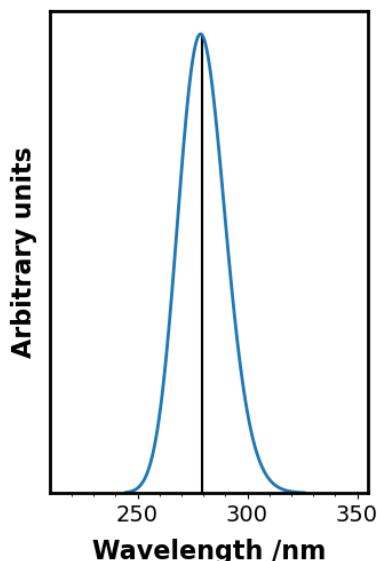


Figure 28: Graph of the simulated vertical S_1 emission spectrum. Excited states are shown as vertical black lines, while peaks simulated with a gaussian function with FWHM: 0.4 eV are shown as a blue line. The oscillator strength of each excited state has arbitrarily been set to 1 because all oscillator strengths were 0. Peaks can be found at: 278 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	-1.2400390	-1.4125330	0.0000000	42	LUMO+7	Ag	4.8912
C	-2.4491680	-0.7114860	0.0000000	41	LUMO+6	B1u	3.6510
C	-2.4491680	0.7114860	0.0000000	40	LUMO+5	B2u	3.4316
C	-1.2400390	1.4125330	-0.0000000	39	LUMO+4	Au	2.9611
C	0.0000000	0.7408730	-0.0000000	38	LUMO+3	Ag	2.7511
C	0.0000000	-0.7408730	0.0000000	37	LUMO+2	B3u	1.1233
C	1.2400390	-1.4125330	0.0000000	36	LUMO+1	B2g	-0.2495
C	1.2400390	1.4125330	-0.0000000	35	LUMO	B1g	-1.0705
C	2.4491680	0.7114860	-0.0000000	34	HOMO	Au	-6.0510
C	2.4491680	-0.7114860	-0.0000000	33	HOMO-1	B3u	-6.8303
H	-1.2436630	-2.4992410	0.0000000	32	HOMO-2	B2g	-8.1286
H	-3.3898840	-1.2513480	0.0000000	31	HOMO-3	Ag	-9.1077
H	-3.3898840	1.2513480	0.0000000	30	HOMO-4	B1g	-9.1332
H	-1.2436630	2.4992410	-0.0000000	29	HOMO-5	B3g	-9.5185
H	1.2436630	-2.4992410	0.0000000	28	HOMO-6	B2u	-10.2990
H	1.2436630	2.4992410	-0.0000000	27	HOMO-7	B3u	-10.8971
H	3.3898840	1.2513480	-0.0000000	26	HOMO-8	B1u	-11.1471
H	3.3898840	-1.2513480	-0.0000000	25	HOMO-9	B2u	-11.5760
				24	HOMO-10	B3g	-11.6334

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

Level	Label	Symmetry	Energy /eV			
50	LUMO+15	B1u	8.1699	20	HOMO-14	B3g
49	LUMO+14	Ag	7.5952	19	HOMO-15	B2u

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-B2U	4.4360	279.50	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO → LUMO+1 (0.50) HOMO-1 → LUMO (0.50)
2	S ₂	Singlet-B1U	4.5530	272.31	Ultraviolet [■] (0.00, 0.00)	0.1213	HOMO → LUMO (0.89) HOMO-1 → LUMO+1 (0.07)
3	S ₃	Singlet-B3G	5.9542	208.23	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-2 → LUMO (0.52) HOMO → LUMO+2 (0.48)
4	S ₄	Singlet-B2U	6.2008	199.95	Ultraviolet [■] (0.00, 0.00)	2.2652	HOMO → LUMO+1 (0.47) HOMO-1 → LUMO (0.47)
5	S ₅	Singlet-B1U	6.4441	192.40	Ultraviolet [■] (0.00, 0.00)	0.4131	HOMO-1 → LUMO+1 (0.87) HOMO → LUMO (0.05) HOMO-2 → LUMO+2 (0.05)
6	S ₆	Singlet-AG	6.4872	191.12	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-2 → LUMO+1 (0.51) HOMO-1 → LUMO+2 (0.41) HOMO-4 → LUMO (0.06)
7	S ₇	Singlet-B1G	6.5682	188.76	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.99)
8	S ₈	Singlet-B2G	6.9495	178.41	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-5 → LUMO (0.97)
9	S ₉	Singlet-B3G	6.9576	178.20	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO → LUMO+2 (0.48) HOMO-2 → LUMO (0.45) HOMO-4 → LUMO+1 (0.02)
10	S ₁₀	Singlet-AG	7.1544	173.30	Ultraviolet [■] (0.00, 0.00)	0.0000	HOMO-4 → LUMO (0.69) HOMO-1 → LUMO+2 (0.24) HOMO → LUMO+3 (0.06)

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 (TMMD), in atomic units (au). [e]: Angle between the TMMD and the x-axis of the molecule. [f]: Angle between the TMMD and xy-plane of the molecule. [g]: The TEDM, in Gaussian CGS (centimetre, gram, second) units. [h]: The TMMD, 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	0.04, -0.00, -0.00	0.04	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	4.02e-20	0.00e+00	90.00	0.00	0.000
S ₂	0.00, 2.65, -0.00	2.65	90.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	2.65e-18	0.00e+00	90.00	0.00	0.000
S ₃	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 0.39	0.39	90.00	90.00	0.00e+00	3.59e-21	90.00	0.00	0.000
S ₄	9.81, -0.00, -0.00	9.81	0.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	9.81e-18	0.00e+00	90.00	0.00	0.000
S ₅	0.00, -4.11, 0.00	4.11	90.00	0.00	0.00, 0.00, 0.00	0.00	0.00	0.00	4.11e-18	0.00e+00	90.00	0.00	0.000
S 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 ₇	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.22, -0.00	0.22	90.00	0.00	0.00e+00	2.07e-21	90.00	0.00	0.000
S ₈	0.00, 0.00, 0.00	0.00	0.00	0.00	-0.03, 0.00, 0.00	0.03	0.00	0.00	0.00e+00	2.98e-22	90.00	0.00	0.000
S ₉	0.00, 0.00, 0.00	0.00	0.00	0.00	0.00, 0.00, 1.12	1.12	90.00	90.00	0.00e+00	1.04e-20	90.00	0.00	0.000
S 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

References

- N. M. O'boyle, A. L. Tenderholt and K. M. Langner, *Journal of Computational Chemistry*, 2008, **29**, 839–845
- P. Virtanen, R. Gommers, T. E. Oliphant, M. Haberland, T. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, K. Jarrod Millman, N. Mayorov, A. R. J. Nelson, E. Jones, R. Kern, E. Larson, C. Carey, I. Polat, Y. Feng, E. W. Moore, J. VanderPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt and S. 1. 0. Contributors, *Nature Methods*, 2020, **17**, 261–272
- T. Mansencal, M. Mauderer, M. Parsons, N. Shaw, K. Wheatley, S. Cooper, J. D. Vandenberg, L. Canavan, K. Crowson, O. Lev, K. Leinweber, S. Sharma, T. J. Sobotka, D. Moritz, M. Papp, C. Rane, P. Eswaramoorthy, J. Mertic, B. Pearlstine, M. Leonhardt, O. Niemitalo, M. Szymanski and M. Schambach, Colour 0.3.15, Zenodo, 2020
- K. Shizu and H. Kaji, *The Journal of Physical Chemistry A*, 2021, **125**, 9000–9010
- W. Humphrey, A. Dalke and K. Schulten, *Journal of Molecular Graphics*, 1996, **14**, 33–38
- J. Stone, Masters Thesis, Computer Science Department, University of Missouri-Rolla, 1998

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7. J. D. Hunter, *Computing in Science & Engineering*, 2007, **9**, 90–95
8. M. Bayer, <https://www.makotemplates.org>, (accessed May 2020)
9. K. Community, <https://weasyprint.org>, (accessed May 2020)