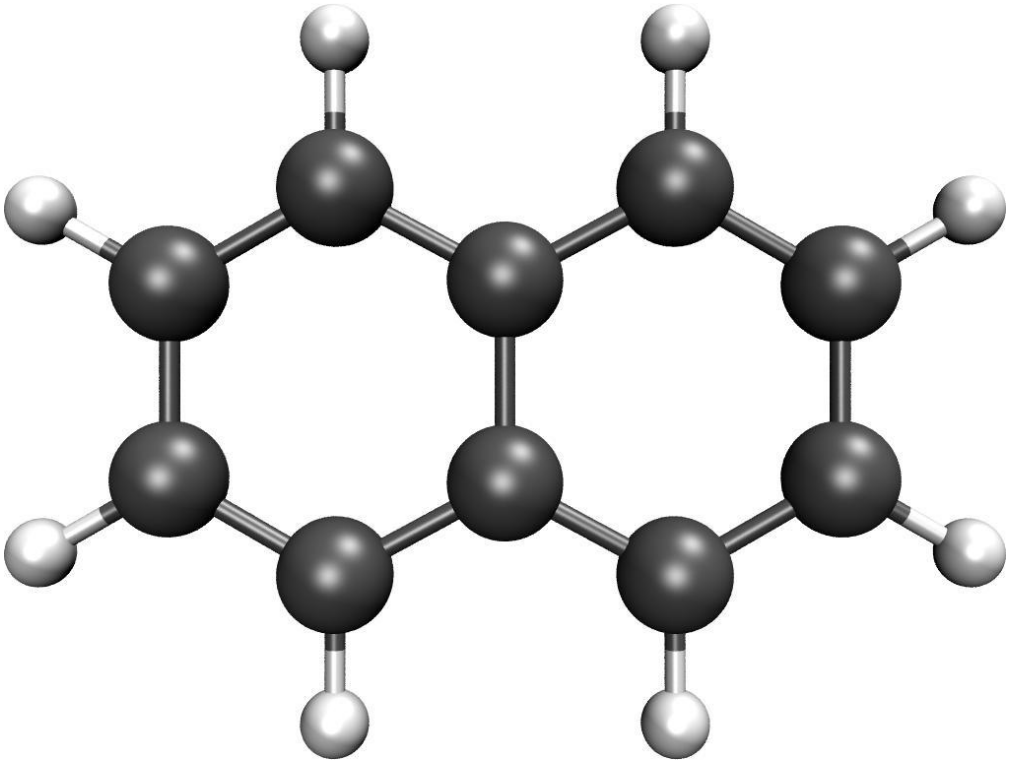
THE Zysman-Colman GROUP

# Calculation Report

## *Naphthalene*

Excited States (Singlet, Triplet)



# Summary of Results

## Metadata

| | |
|---|---|
| **Username:** | oliver |
| **Date:** | 07/06/2022 16:48:19 |
| **Duration:** | 4 m, 21 s |
| **Success:** | True |
| **Computational package:** | Gaussian (2016+C.01) |
| **Methods:** | DFT |
| **Functional:** | PBE1PBE |
| **Basis set:** | 6-31G(d,p) |
| **Calculations:** | Excited States |
| **Orbital spin:** | restricted |
| **Multiplicity:** | 1 (singlet) |

## SCF Energies

| | |
|---|---|
| **No. of steps:** | 1 |
| **Final energy:** | -10488.9903 eV |
| **Final energy:** | -1,012,034 $kJmol^{-1}$ |

## Geometry

| | |
|---|---|
| **Formula:** | $C_{10}H_8$ |
| **Exact mass:** | 128.0626 $gmol^{-1}$ |
| **Molar mass:** | 128.1705 $gmol^{-1}$ |
| **Alignment method:** | Minimal |
| **X extension:** | 6.74 Å |
| **Y extension:** | 4.97 Å |
| **Z extension:** | 0.00 Å |
| **Linearity ratio:** | 0.26 |
| **Planarity ratio:** | 1.00 |

## HOMO & LUMO

| | |
|---|---|
| **$E_{HOMO,LUMO}$:** | 5.21 eV |
| **$E_{HOMO}$:** | -6.13 eV |
| **$E_{LUMO}$:** | -0.92 eV |

## Permanent Dipole Moment

| | |
|---|---|
| **Total:** | 0.00 D |
| **X axis angle:** | 0.00 ° |
| **XY plane angle:** | 0.00 ° |

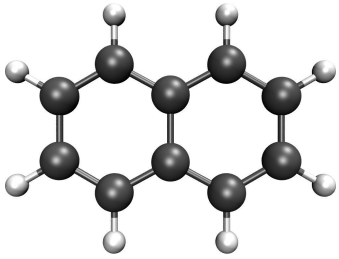
## Transition ($S_1$) Dipole Moment

| | |
|---|---|
| **Total:** | 0.07 D |
| **X axis angle:** | 0.00 ° |
| **XY plane angle:** | 0.00 ° |

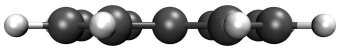
## Excited States

| | |
|---|---|
| **$\Delta E_{ST}$:** | 1.62 eV |
| **$S_1$ energy:** | 4.65 eV |
| **$S_1$ wavelength:** | 266 nm |
| **$S_1$ colour:** | Ultraviolet |
| **$S_1$ CIE (x,y):** | (0.00, 0.00) |
| **$S_1$ oscillator strength:** | 0.00 |
| **$T_1$ energy:** | 3.03 eV |
| **$T_1$ wavelength:** | 409 nm |
| **$T_1$ colour:** | Violet |
| **$T_1$ CIE (x,y):** | (0.17, 0.00) |
| **$T_1$ oscillator strength:** | 0.00 |
| **No. of singlets:** | 10 |
| **No. of triplets:** | 10 |

# Geometry

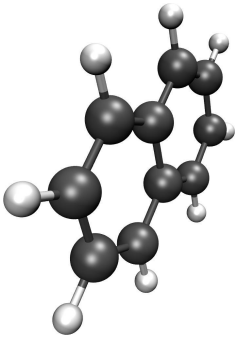


X/Y plane



X/Z plane

Z/Y plane



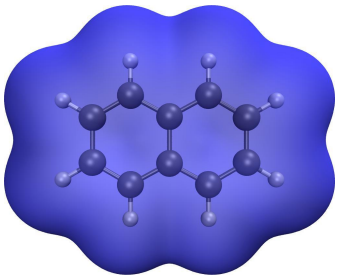
45° to axes

**Aligned structure**

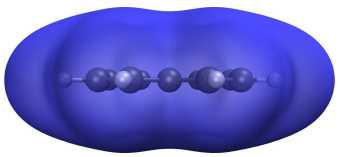
## Geometry

| | |
|---|---|
| **Formula:** | $C_{10}H_8$ |
| **Exact mass:** | 128.0626 $gmol^{-1}$ |
| **Molar mass:** | 128.1705 $gmol^{-1}$ |
| **Alignment method:** | Minimal |
| **X extension:** | 6.74 Å |
| **Y extension:** | 4.97 Å |
| **Z extension:** | 0.00 Å |
| **Linearity ratio:** | 0.26 |
| **Planarity ratio:** | 1.00 |

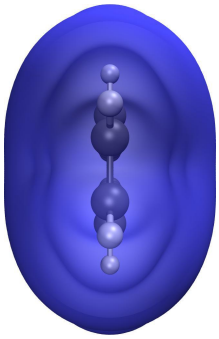
# SCF Density



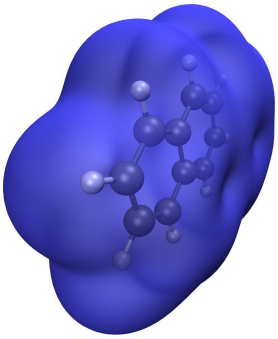
X/Y plane



X/Z plane



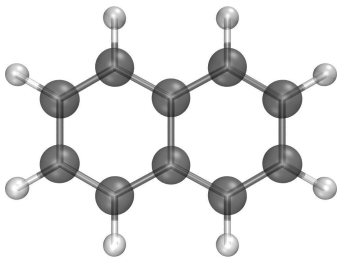
Z/Y plane



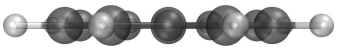
45° to axes

**SCF density (isovalue: 0.0004)**

# Permanent Dipole Moment

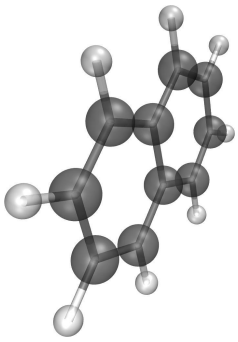


X/Y plane



X/Z plane

Z/Y plane



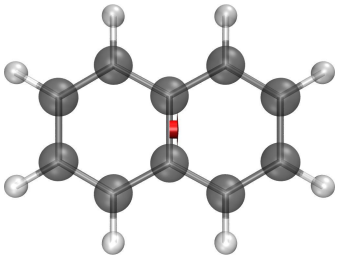
45° to axes

**Aligned structure (dipole moment in red)**

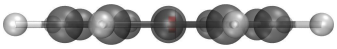
## Dipole Moment

| | |
|---|---|
| **Origin X:** | 0.00 D |
| **Origin Y:** | 0.00 D |
| **Origin Z:** | 0.00 D |
| **Vector X:** | 0.00 D |
| **Vector Y:** | 0.00 D |
| **Vector Z:** | 0.00 D |
| **Total:** | 0.00 D |
| **X axis angle:** | 0.00 ° |
| **XY plane angle:** | 0.00 ° |

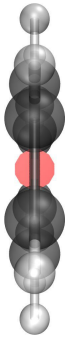
# Transition ($S_1$) Dipole Moment



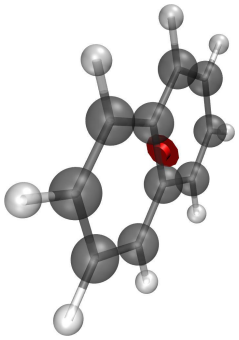
X/Y plane



X/Z plane



Z/Y plane



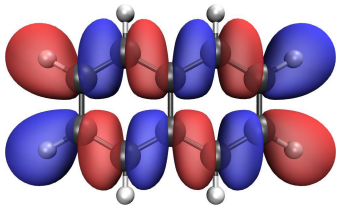
45° to axes

**Aligned structure (dipole moment in red)**

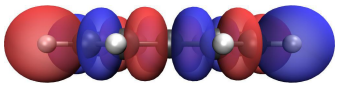
## Dipole Moment

| | |
|---|---|
| **Origin X:** | 0.00 D |
| **Origin Y:** | 0.00 D |
| **Origin Z:** | 0.00 D |
| **Vector X:** | 0.07 D |
| **Vector Y:** | -0.00 D |
| **Vector Z:** | -0.00 D |
| **Total:** | 0.07 D |
| **X axis angle:** | 0.00 ° |
| **XY plane angle:** | 0.00 ° |

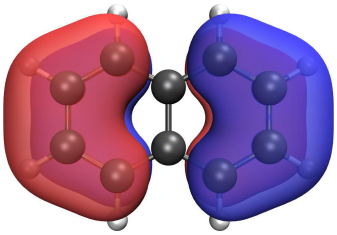
# HOMO-5, HOMO-4, HOMO-3, HOMO-2



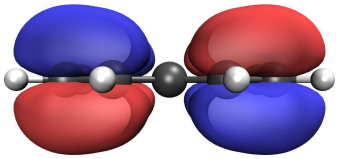
X/Y plane



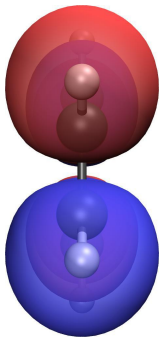
X/Z plane



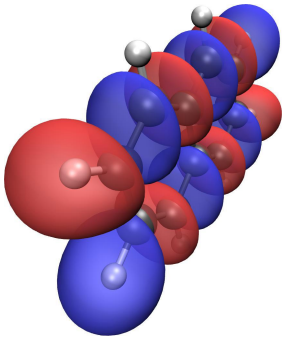
X/Y plane



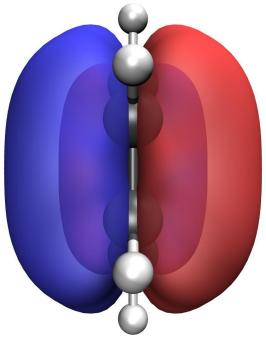
X/Z plane



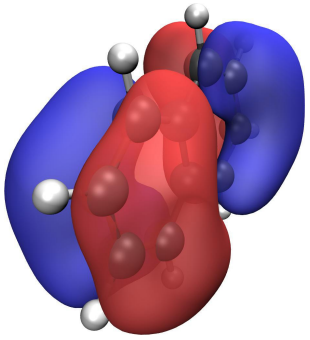
Z/Y plane



45° to axes



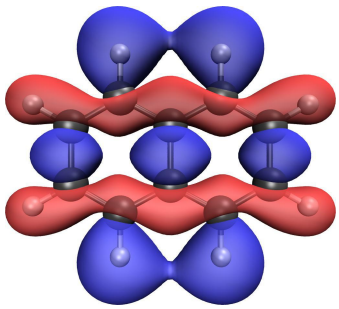
Z/Y plane



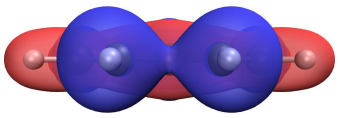
45° to axes

**HOMO-5 density (isovalue: 0.02)**

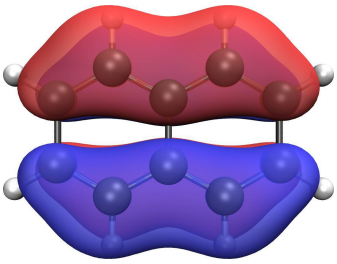
**HOMO-4 density (isovalue: 0.02)**



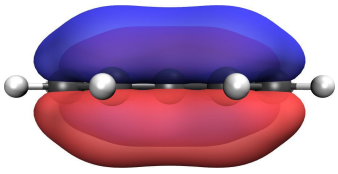
X/Y plane



X/Z plane

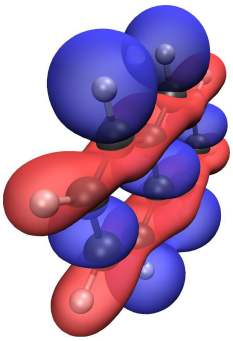


X/Y plane

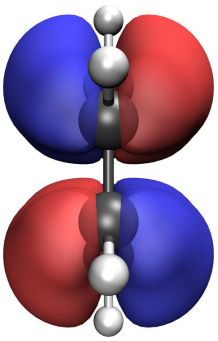


X/Z plane

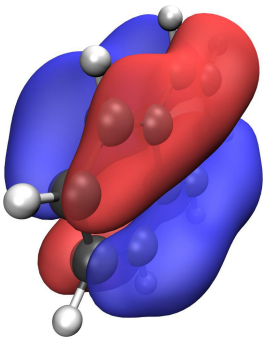
Z/Y plane



45° to axes



Z/Y plane

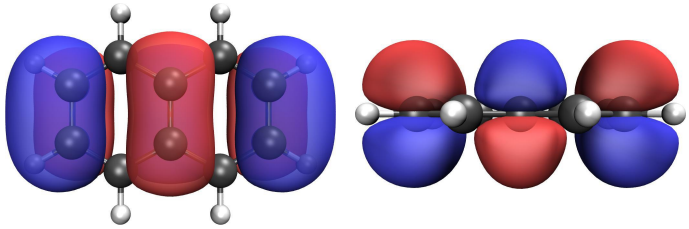


45° to axes

**HOMO-3 density (isovalue: 0.02)**

**HOMO-2 density (isovalue: 0.02)**

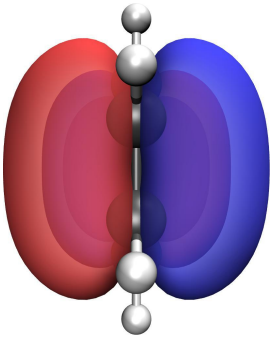
# HOMO-1



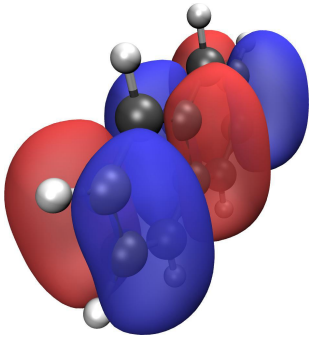
X/Y plane



X/Z plane



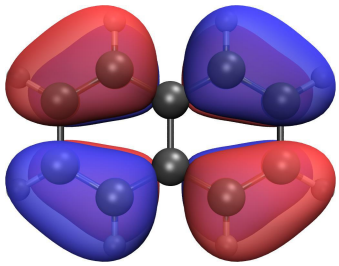
Z/Y plane



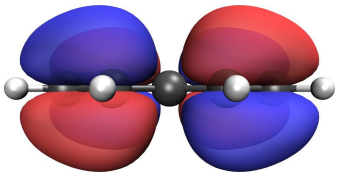
45° to axes

**HOMO-1 density (isovalue: 0.02)**

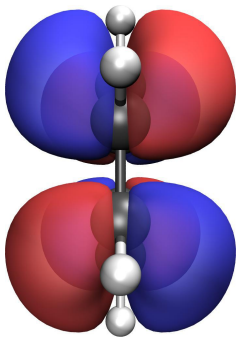
# HOMO & LUMO



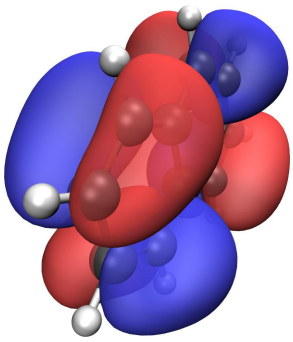
X/Y plane



X/Z plane

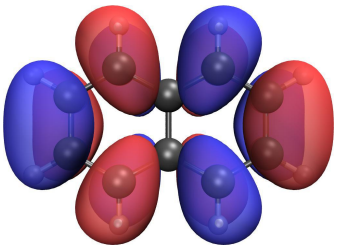


Z/Y plane

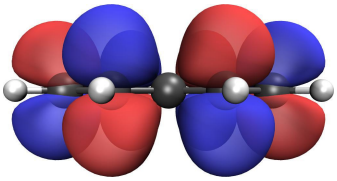


45° to axes

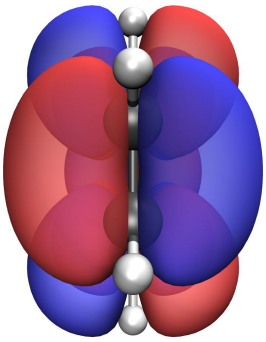
**HOMO density (isovalue: 0.02)**



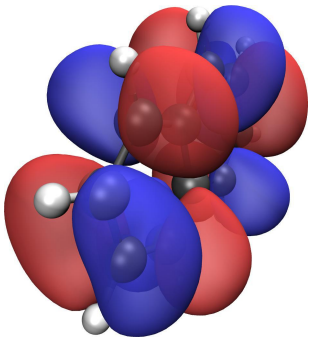
X/Y plane



X/Z plane

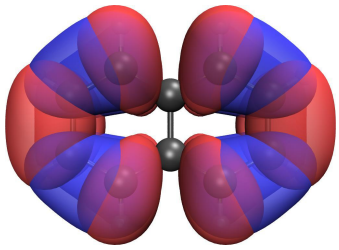


Z/Y plane

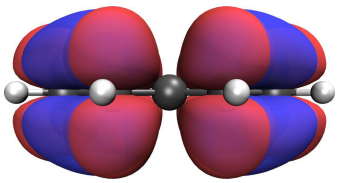


45° to axes

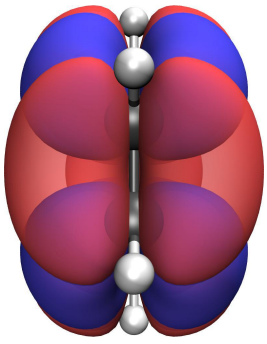
**LUMO density (isovalue: 0.02)**



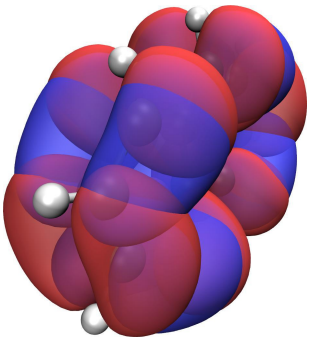
X/Y plane



X/Z plane

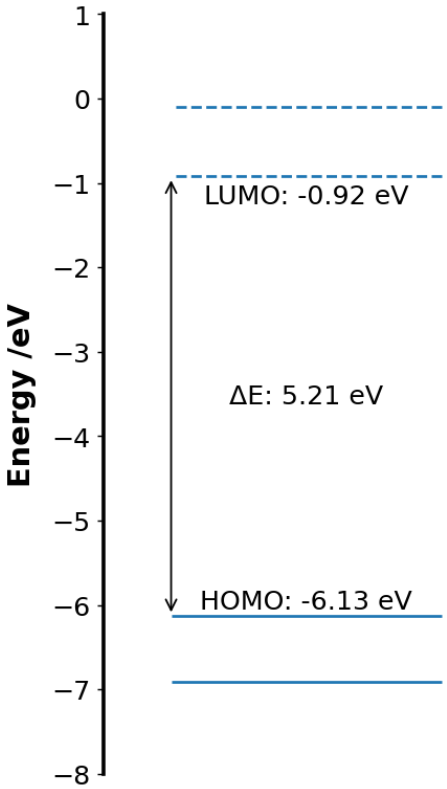


Z/Y plane

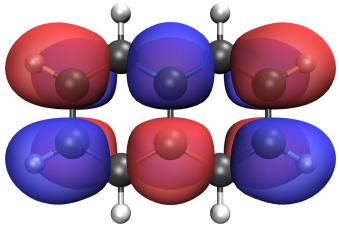


45° to axes

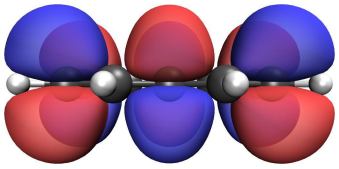
**HOMO (blue) & LUMO (red) density (isovalue: 0.02)**



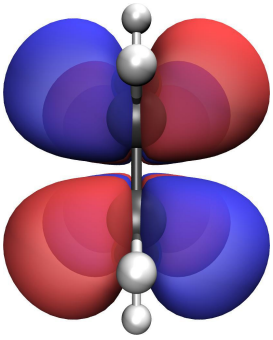
## LUMO+1, LUMO+2, LUMO+4



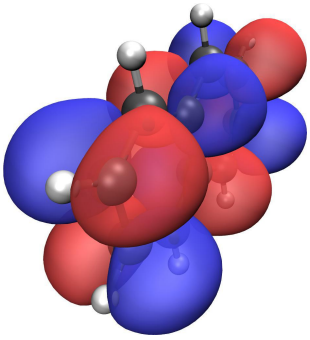
X/Y plane



X/Z plane

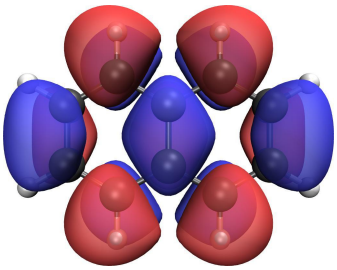


Z/Y plane

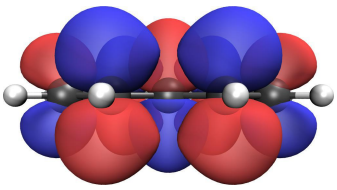


45° to axes

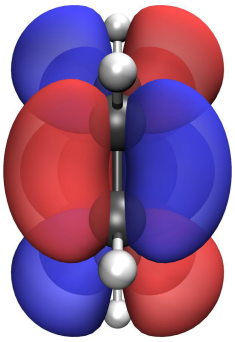
**LUMO+1 density (isovalue: 0.02)**



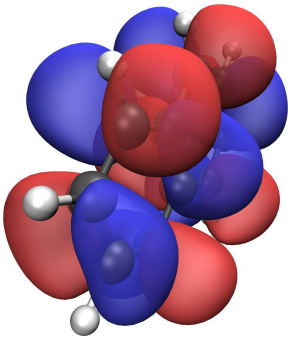
X/Y plane



X/Z plane

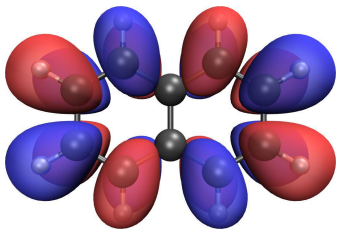


Z/Y plane

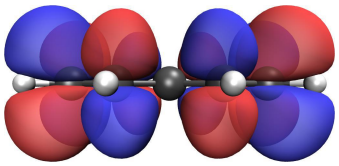


45° to axes

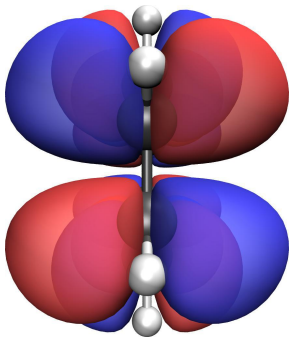
**LUMO+2 density (isovalue: 0.02)**



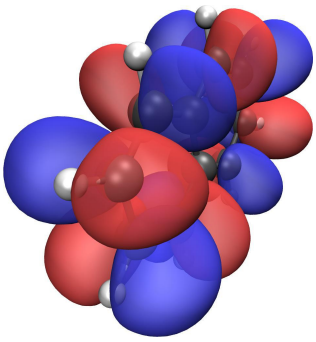
X/Y plane



X/Z plane



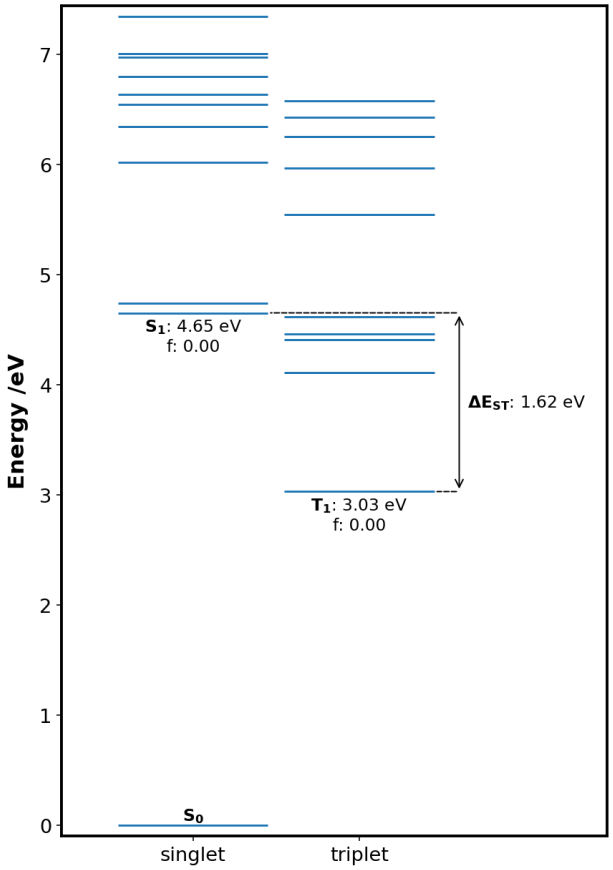
Z/Y plane



45° to axes

**LUMO+4 density (isovalue: 0.02)**

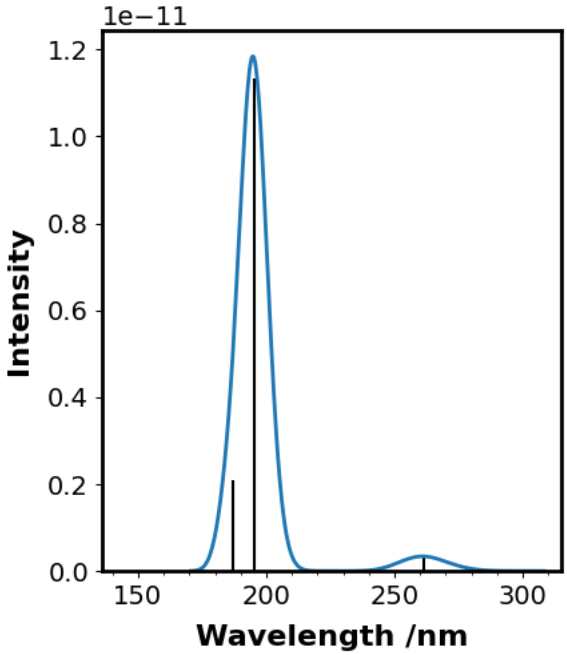
# Excited States




## Excited States

| | |
|---|---|
| **$\Delta E_{ST}$:** | 1.62 eV |
| **$S_1$ energy:** | 4.65 eV |
| **$S_1$ wavelength:** | 266 nm |
| **$S_1$ colour:** | Ultraviolet |
| **$S_1$ CIE (x,y):** | (0.00, 0.00) |
| **$S_1$ oscillator strength:** | 0.00 |
| **$T_1$ energy:** | 3.03 eV |
| **$T_1$ wavelength:** | 409 nm |
| **$T_1$ colour:** | Violet |
| **$T_1$ CIE (x,y):** | (0.17, 0.00) |
| **$T_1$ oscillator strength:** | 0.00 |
| **No. of singlets:** | 10 |
| **No. of triplets:** | 10 |

# Absorptions




**Absorption spectrum (simulated Gaussian functions with FWHM: 0.4 eV).**
**Peaks /nm: 194, 261.**
**Note: high energy absorption peaks are not simulated.**
**For a complete absorption spectrum, use more excited states.**

# Table of Excited States

| Level | Symbol | Symmetry | Energy /eV | Wavelength /nm | Colour, CIE (x,y) | Oscillator Strength | Transitions (probability) |
|---|---|---|---|---|---|---|---|
| 1 | $T_1$ | Triplet-B1U | 3.0294 | 409.27 | Violet (0.17, 0.00) | 0.0000 | HOMO → LUMO (0.92)<br>HOMO-2 → LUMO+2 (0.03)<br>HOMO-1 → LUMO+1 (0.03) |
| 2 | $T_2$ | Triplet-B2U | 4.1078 | 301.83 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-1 → LUMO (0.58)<br>HOMO → LUMO+1 (0.40) |
| 3 | $T_3$ | Triplet-B2U | 4.4060 | 281.40 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO → LUMO+1 (0.59)<br>HOMO-1 → LUMO (0.41) |
| 4 | $T_4$ | Triplet-B3G | 4.4608 | 277.94 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-2 → LUMO (0.51)<br>HOMO → LUMO+2 (0.46) |
| 5 | $T_5$ | Triplet-B1U | 4.6180 | 268.48 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-1 → LUMO+1 (0.94)<br>HOMO → LUMO (0.04) |
| 6 | $S_1$ | Singlet-B2U | 4.6525 | 266.49 | Ultraviolet (0.00, 0.00) | 0.0001 | HOMO-1 → LUMO (0.50)<br>HOMO → LUMO+1 (0.49) |
| 7 | $S_2$ | Singlet-B1U | 4.7387 | 261.64 | Ultraviolet (0.00, 0.00) | 0.1168 | HOMO → LUMO (0.90)<br>HOMO-1 → LUMO+1 (0.07) |
| 8 | $T_6$ | Triplet-AG | 5.5459 | 223.56 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-1 → LUMO+2 (0.31)<br>HOMO-4 → LUMO (0.30)<br>HOMO-2 → LUMO+1 (0.26)<br>HOMO → LUMO+4 (0.13) |
| 9 | $T_7$ | Triplet-B3G | 5.9643 | 207.88 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO → LUMO+2 (0.53)<br>HOMO-2 → LUMO (0.47) |
| 10 | $S_3$ | Singlet-B3G | 6.0185 | 206.01 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO → LUMO+2 (0.51)<br>HOMO-2 → LUMO (0.49) |
| 11 | $T_8$ | Triplet-AG | 6.2558 | 198.19 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-2 → LUMO+1 (0.62)<br>HOMO-1 → LUMO+2 (0.30)<br>HOMO-4 → LUMO (0.06) |
| 12 | $S_4$ | Singlet-B2U | 6.3419 | 195.50 | Ultraviolet (0.00, 0.00) | 2.1780 | HOMO → LUMO+1 (0.48)<br>HOMO-1 → LUMO (0.47) |
| 13 | $T_9$ | Triplet-AG | 6.4283 | 192.87 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-4 → LUMO (0.38)<br>HOMO-1 → LUMO+2 (0.36)<br>HOMO → LUMO+4 (0.12)<br>HOMO-2 → LUMO+1 (0.07)<br>HOMO-7 → LUMO+2 (0.04) |
| 14 | $S_5$ | Singlet-AG | 6.5463 | 189.40 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-2 → LUMO+1 (0.49)<br>HOMO-1 → LUMO+2 (0.46)<br>HOMO-4 → LUMO (0.04) |
| 15 | $T_{10}$ | Triplet-B1G | 6.5767 | 188.52 | Ultraviolet (0.00, 0.00) | 0.0000 | HOMO-3 → LUMO (0.98) |
| | | | | | | | HOMO-1 → LUMO+1 (0.86) |

## *Naphthalene - Excited States (Singlet, Triplet)*

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 16 | $S_6$ | Singlet-B1U | 6.6348 | 186.87 | Ultraviolet [redacted] (0.00, 0.00) | 0.3684 | HOMO-2 → LUMO+2 (0.07)<br>HOMO → LUMO (0.04) |
| 17 | $S_7$ | Singlet-B1G | 6.7955 | 182.45 | Ultraviolet [redacted] (0.00, 0.00) | 0.0000 | HOMO-3 → LUMO (0.99) |
| 18 | $S_8$ | Singlet-B2G | 6.9759 | 177.73 | Ultraviolet [redacted] (0.00, 0.00) | 0.0000 | HOMO-5 → LUMO (0.98) |
| 19 | $S_9$ | Singlet-B3G | 7.0061 | 176.97 | Ultraviolet [redacted] (0.00, 0.00) | 0.0000 | HOMO-2 → LUMO (0.48)<br>HOMO → LUMO+2 (0.45) |
| 20 | $S_{10}$ | Singlet-AG | 7.3438 | 168.83 | Ultraviolet [redacted] (0.00, 0.00) | 0.0000 | HOMO-4 → LUMO (0.63)<br>HOMO-1 → LUMO+2 (0.27)<br>HOMO-2 → LUMO+1 (0.07) |

# Table of Selected Molecular Orbitals

| Level | Label | Symmetry | Energy /eV |
|---|---|---|---|
| 50 | LUMO+15 | B1u | 8.6396 |
| 49 | LUMO+14 | Ag | 7.9114 |
| 48 | LUMO+13 | B1u | 6.9150 |
| 47 | LUMO+12 | B3g | 6.0692 |
| 46 | LUMO+11 | B2g | 5.7949 |
| 45 | LUMO+10 | B2u | 5.3487 |
| 44 | LUMO+9 | B1u | 5.1506 |
| 43 | LUMO+8 | B3g | 5.0031 |
| 42 | LUMO+7 | Ag | 4.9519 |
| 41 | LUMO+6 | B1u | 3.6912 |
| 40 | LUMO+5 | B2u | 3.4207 |
| 39 | LUMO+4 | Au | 2.9674 |
| 38 | LUMO+3 | Ag | 2.9127 |
| 37 | LUMO+2 | B3u | 1.0612 |
| 36 | LUMO+1 | B2g | -0.1010 |
| 35 | **LUMO** | **B1g** | **-0.9244** |
| 34 | **HOMO** | **Au** | **-6.1307** |
| 33 | HOMO-1 | B3u | -6.9084 |
| 32 | HOMO-2 | B2g | -8.0747 |
| 31 | HOMO-3 | Ag | -9.1879 |
| 30 | HOMO-4 | B1g | -9.2562 |
| 29 | HOMO-5 | B3g | -9.4032 |
| 28 | HOMO-6 | B2u | -10.2679 |
| 27 | HOMO-7 | B3u | -11.0274 |
| 26 | HOMO-8 | B1u | -11.1363 |
| 25 | HOMO-9 | B2u | -11.5961 |
| 24 | HOMO-10 | B3g | -11.6187 |
| 23 | HOMO-11 | Ag | -12.3015 |
| 22 | HOMO-12 | B1u | -12.4753 |
| 21 | HOMO-13 | Ag | -13.7777 |
| 20 | HOMO-14 | B3g | -14.2411 |
| 19 | HOMO-15 | B2u | -14.3709 |

# Table of Atoms

| Element | X Coord | Y Coord | Z Coord |
|---|---|---|---|
| C | -1.2404600 | -1.3991400 | 0.0000000 |
| C | -2.4260000 | -0.7066400 | 0.0000000 |
| C | -2.4260000 | 0.7066400 | 0.0000000 |
| C | -1.2404600 | 1.3991400 | -0.0000000 |
| C | -0.0000000 | 0.7142300 | -0.0000000 |
| C | -0.0000000 | -0.7142300 | 0.0000000 |
| C | 1.2404600 | -1.3991400 | 0.0000000 |
| C | 1.2404600 | 1.3991400 | -0.0000000 |
| C | 2.4260000 | 0.7066400 | -0.0000000 |
| C | 2.4260000 | -0.7066400 | -0.0000000 |
| H | -1.2367000 | -2.4862000 | 0.0000000 |
| H | -3.3697000 | -1.2439700 | 0.0000000 |
| H | -3.3697000 | 1.2439700 | 0.0000000 |
| H | -1.2367000 | 2.4862000 | -0.0000000 |
| H | 1.2367000 | -2.4862000 | 0.0000000 |
| H | 1.2367000 | 2.4862000 | -0.0000000 |
| H | 3.3697000 | 1.2439700 | -0.0000000 |
| H | 3.3697000 | -1.2439700 | -0.0000000 |

# About

## Silico Calculation Report

*Part of the silico software package*

Version 1.0.0-pre.31

11 February 2022

**Silico makes use of a number of 3rd party libraries and programs; please cite these appropriately in your works:**

Extraction and processing of results: **cclib**[1]
Rendering of 3D images: **VMD**[2], **Tachyon**[3]
Rendering of graphs: **Matplotlib**[4]
Calculation of CIE colour coordinates: **Colour Science**[5]
Generation of reports: **Mako**[6], **Weasyprint**[7]
Scientific constants: **SciPy**[8]
Conversion of file formats: **Pybel**[9], **Openbabel**[10]
Calculation of spin-orbit coupling: **PySOC**[11]
Rendering of 2D structures: **RDKit**[12]
Saving of state during submission: **Dill**[13,14]

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