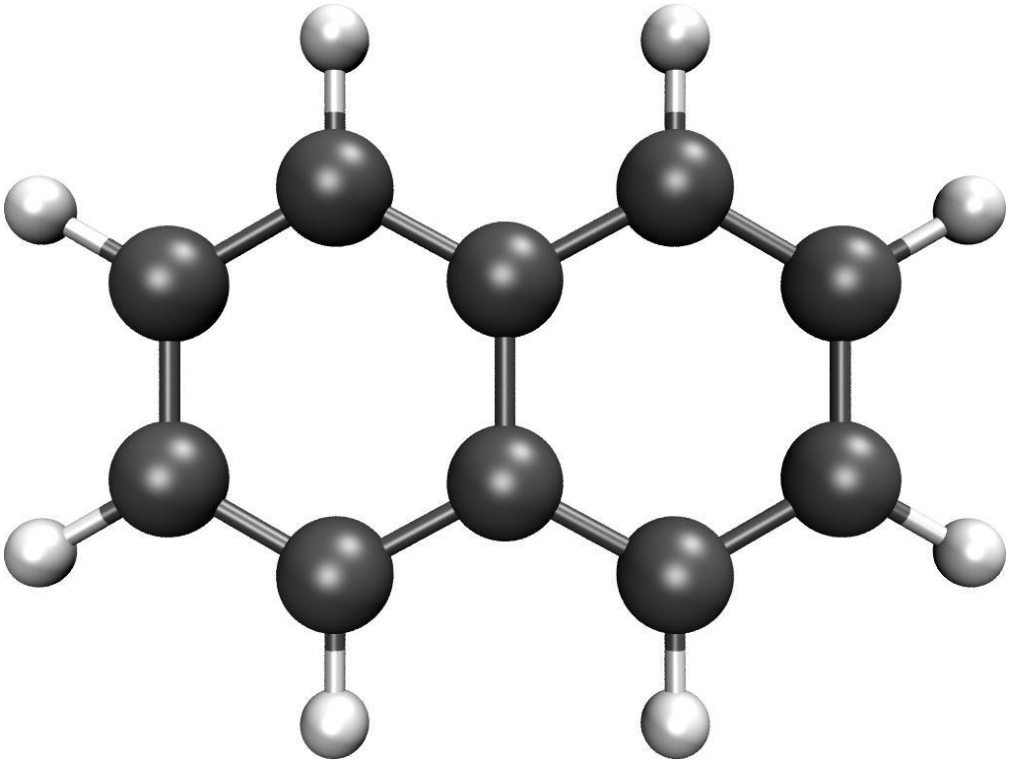
THE Zysman-Colman GROUP

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 °

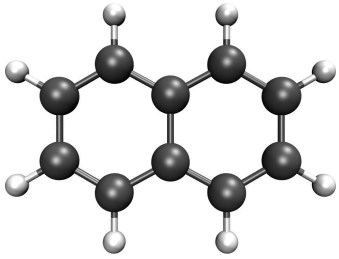
Transition (S_1) Dipole Moment

Total:	0.07 D
X axis angle:	0.00 °
XY plane angle:	0.00 °

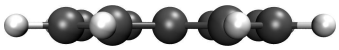
Excited States

ΔE_{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

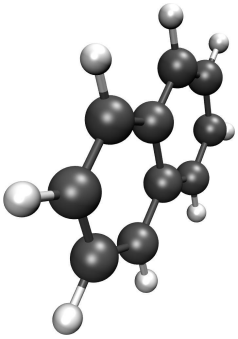


X/Y plane



X/Z plane

Z/Y plane



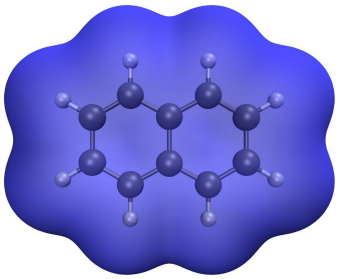
45° to axes

Aligned structure

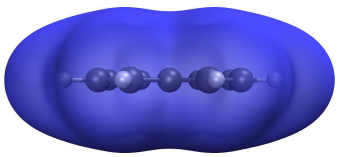
Geometry

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

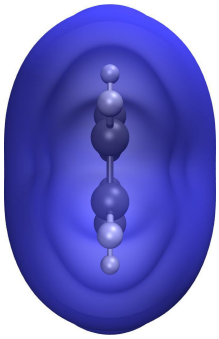
SCF Density



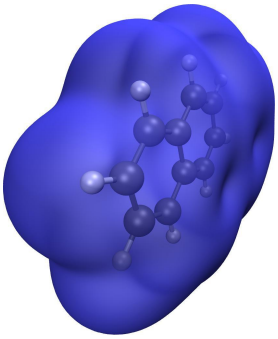
X/Y plane



X/Z plane



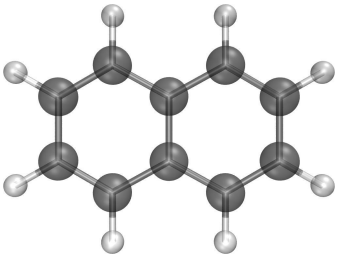
Z/Y plane



45° to axes

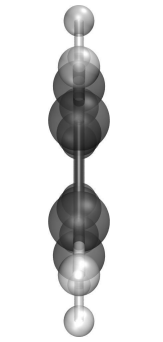
SCF density (isovalue: 0.0004)

Permanent Dipole Moment

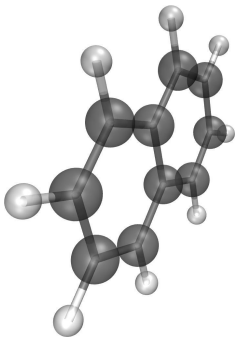


X/Y plane

X/Z plane



Z/Y plane



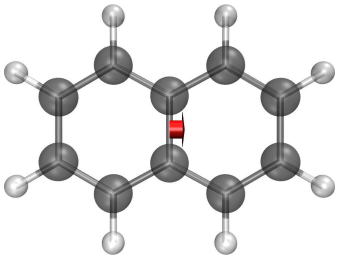
45° to axes

Aligned structure (dipole moment in red)

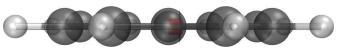
Dipole Moment

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 °

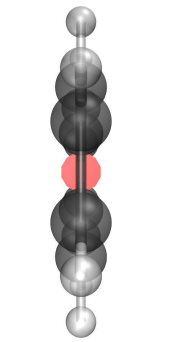
Transition (S_1) Dipole Moment



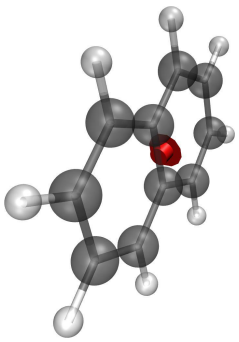
X/Y plane



X/Z plane



Z/Y plane



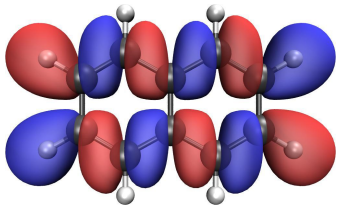
45° to axes

Aligned structure (dipole moment in red)

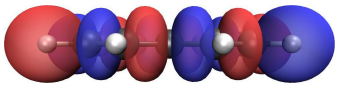
Dipole Moment

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 °

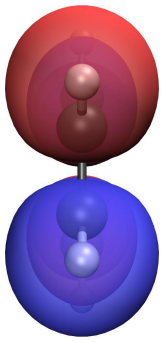
HOMO-5, HOMO-4, HOMO-3, HOMO-2



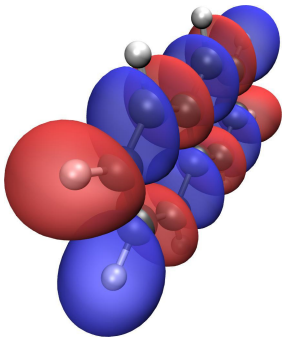
X/Y plane



X/Z plane

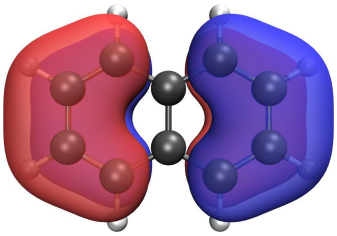


Z/Y plane

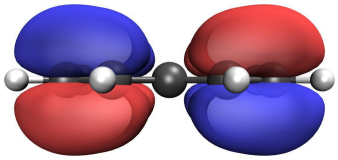


45° to axes

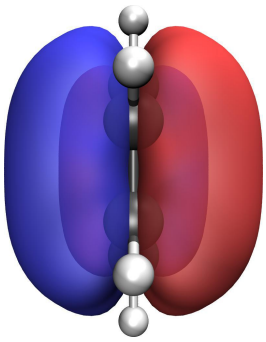
HOMO-5 density (isovalue: 0.02)



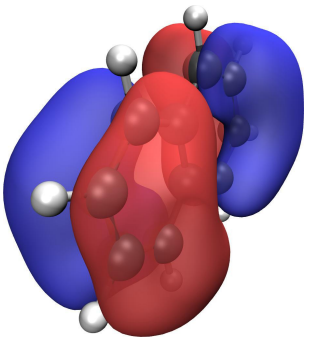
X/Y plane



X/Z plane

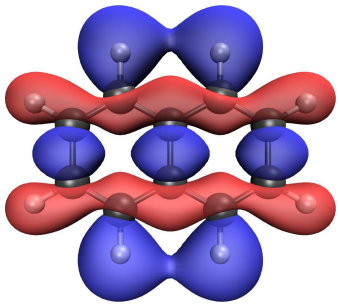


Z/Y plane

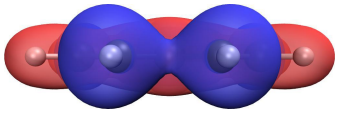


45° to axes

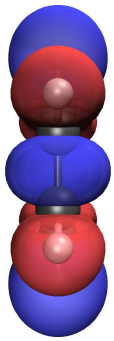
HOMO-4 density (isovalue: 0.02)



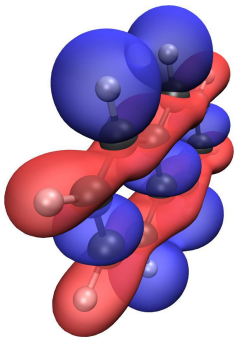
X/Y plane



X/Z plane

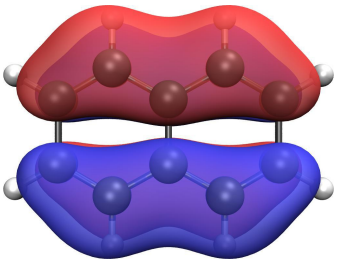


Z/Y plane

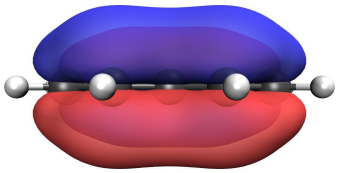


45° to axes

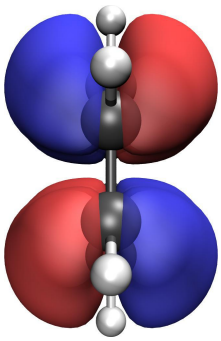
HOMO-3 density (isovalue: 0.02)



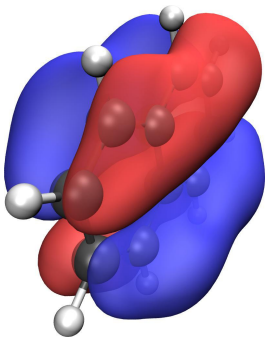
X/Y plane



X/Z plane



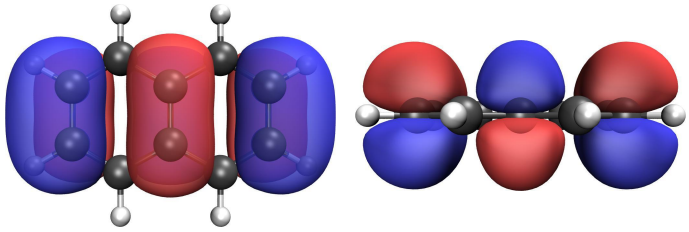
Z/Y plane



45° to axes

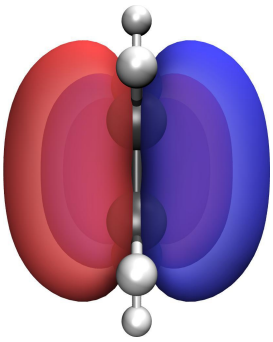
HOMO-2 density (isovalue: 0.02)

HOMO-1

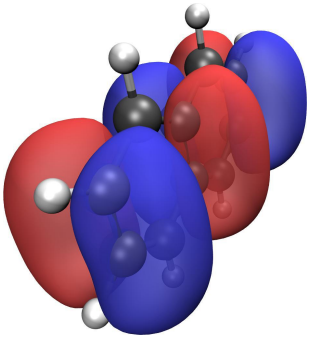


X/Y plane

X/Z plane



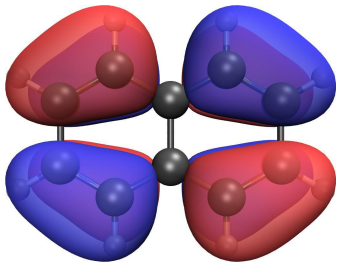
Z/Y plane



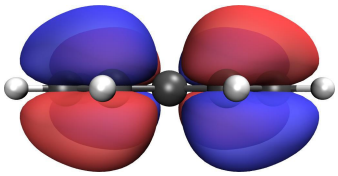
45° to axes

HOMO-1 density (isovalue: 0.02)

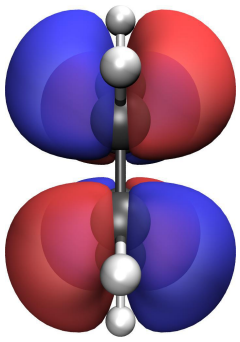
HOMO & LUMO



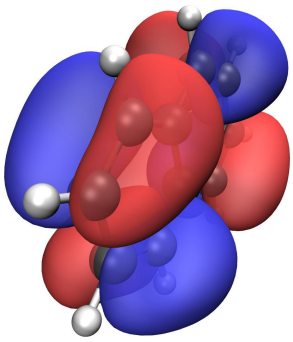
X/Y plane



X/Z plane

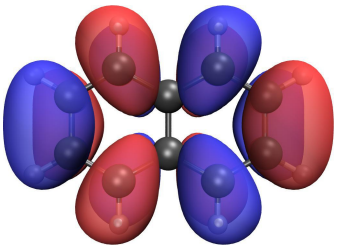


Z/Y plane

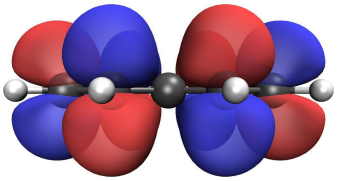


45° to axes

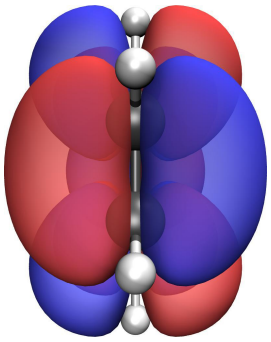
HOMO density (isovalue: 0.02)



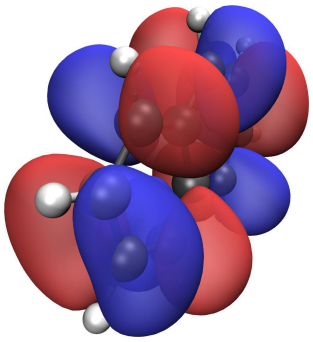
X/Y plane



X/Z plane

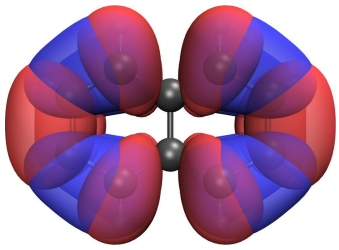


Z/Y plane

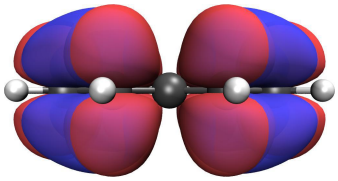


45° to axes

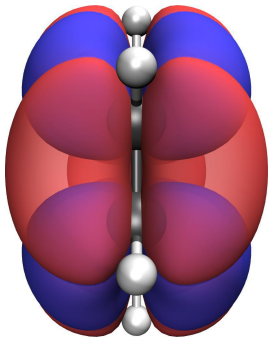
LUMO density (isovalue: 0.02)



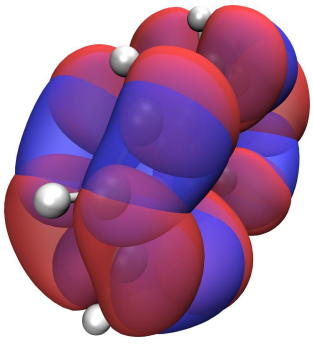
X/Y plane



X/Z plane

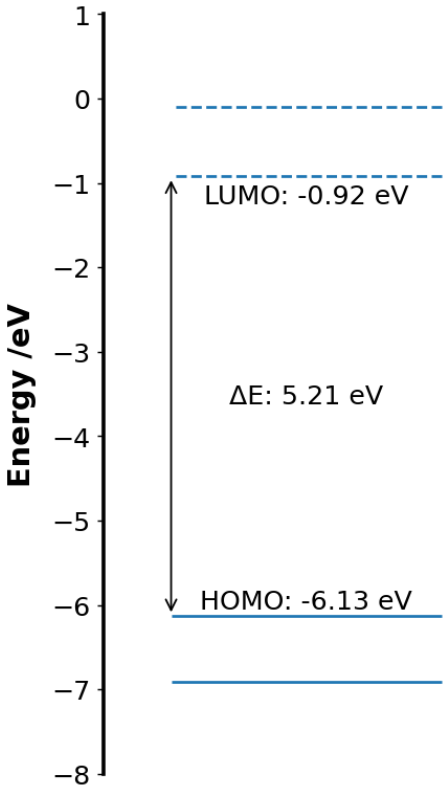


Z/Y plane

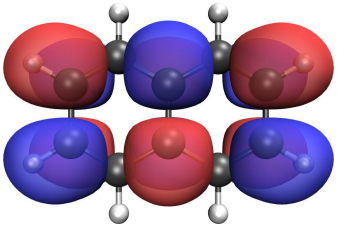


45° to axes

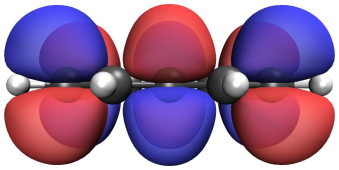
HOMO (blue) & LUMO (red) density (isovalue: 0.02)



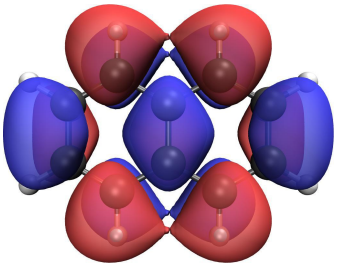
LUMO+1, LUMO+2, LUMO+4



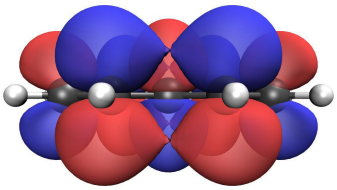
X/Y plane



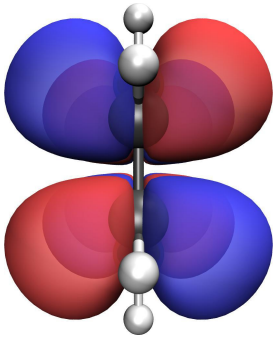
X/Z plane



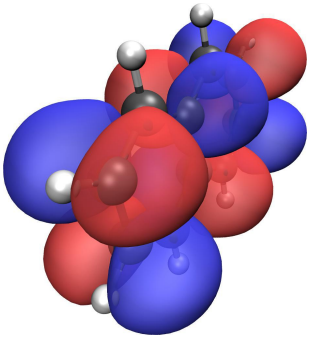
X/Y plane



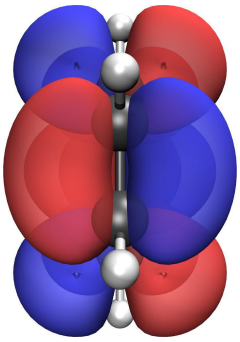
X/Z plane



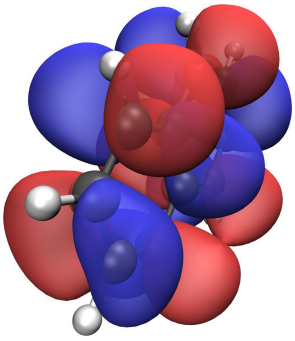
Z/Y plane



45° to axes



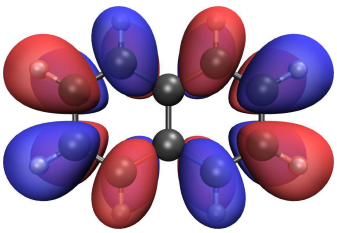
Z/Y plane



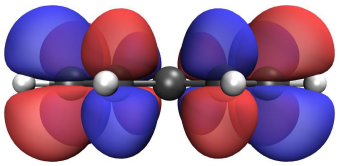
45° to axes

LUMO+1 density (isovalue: 0.02)

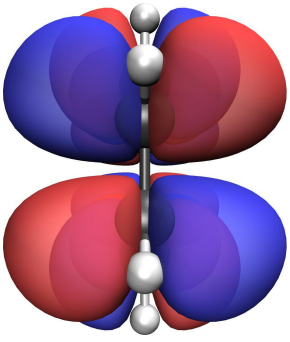
LUMO+2 density (isovalue: 0.02)



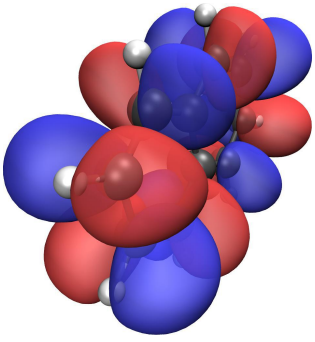
X/Y plane



X/Z plane



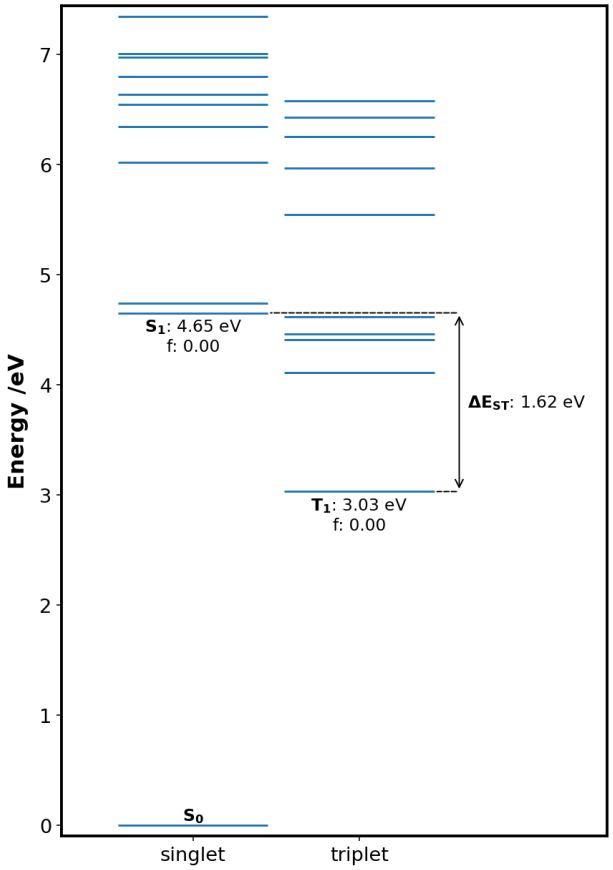
Z/Y plane



45° to axes

LUMO+4 density (isovalue: 0.02)

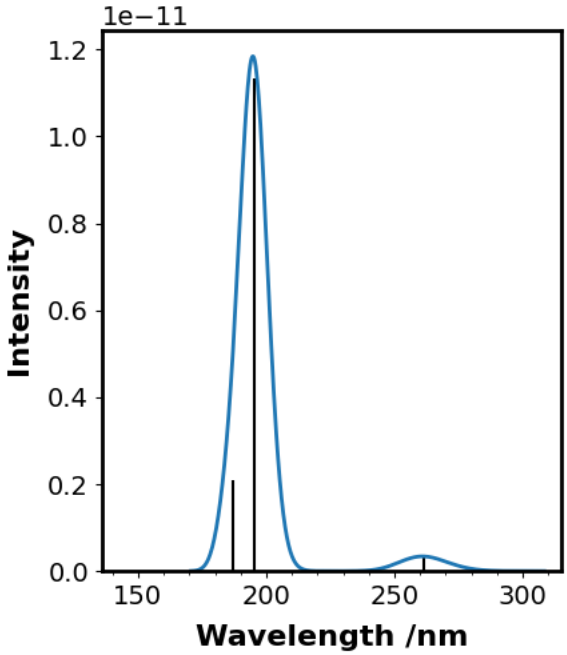
Excited States



Excited States

ΔE_{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) HOMO-2 → LUMO+2 (0.03) 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) 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) 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) 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) 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) 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) 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) HOMO-4 → LUMO (0.30) HOMO-2 → LUMO+1 (0.26) 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) 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) 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) HOMO-1 → LUMO+2 (0.30) 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) 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) HOMO-1 → LUMO+2 (0.36) HOMO → LUMO+4 (0.12) HOMO-2 → LUMO+1 (0.07) 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) HOMO-1 → LUMO+2 (0.46) 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) 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) 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) HOMO-1 → LUMO+2 (0.27) 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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