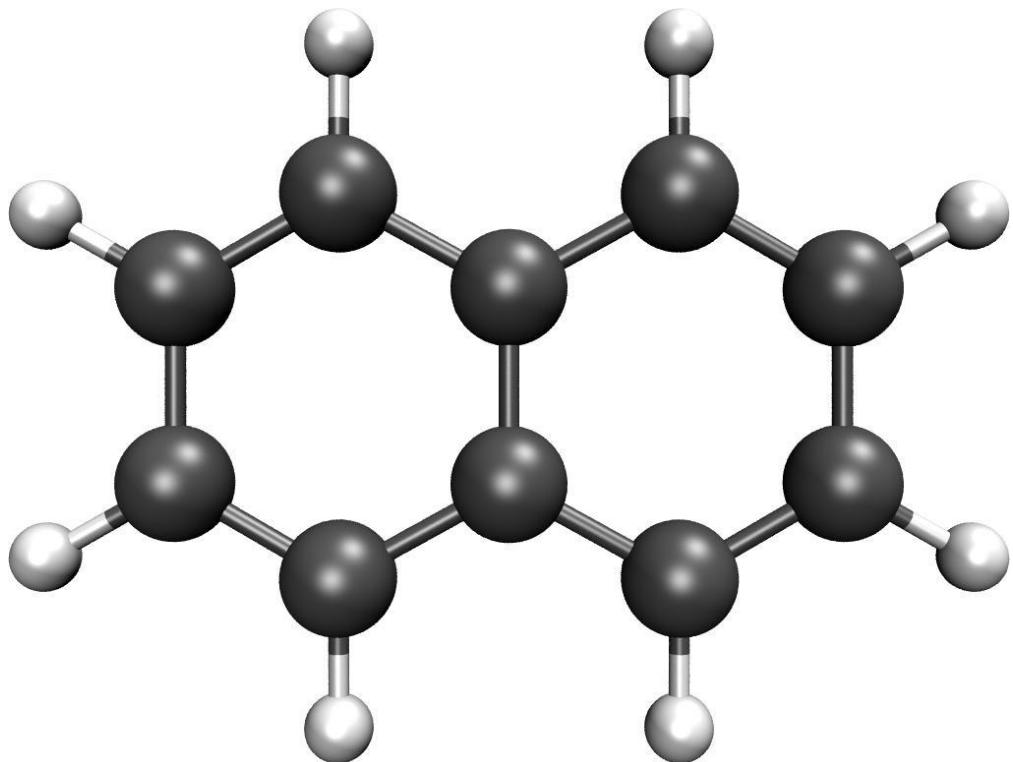


Calculation Report

Naphthalene

Optimisation, Frequencies, Excited States (Singlet, Triplet)



Summary of Results

Metadata		Calculation 1		Calculation 2	
Username:	osl	Username:	osl	Username:	osl
Date:	07/06/2022 17:37:23	Date:	07/06/2022 16:39:10	Date:	07/06/2022 16:48:19
Duration:	16 m, 7 s	Duration:	4 m, 57 s	Duration:	4 m, 21 s
Success:	True	Success:	True	Success:	True
Converged:	True	Converged:	True	Computational package:	Gaussian (2016+C.01)
Computational package:	Gaussian (2016+C.01)	Computational package:	Gaussian (2016+C.01)	Methods:	DFT
Methods:	DFT	Methods:	DFT	Functional:	PBE1PBE
Functional:	PBE1PBE	Functional:	PBE1PBE	Basis set:	6-31G(d,p)
Basis set:	6-31G(d,p)	Basis set:	6-31G(d,p)	Calculations:	Excited States
Calculations:	Optimisation, Frequencies, Excited States	Calculations:	Optimisation, Frequencies	Orbital spin:	restricted
Orbital spin:	restricted	Orbital spin:	restricted	Multiplicity:	1 (singlet)
Multiplicity:	1 (singlet)	Multiplicity:	1 (singlet)		
No. merged calculations:	3	Calc temperature:	298.15 K		
		Calc pressure:	1.0 atm		

Calculation 3

Username:	osl
Date:	07/06/2022 17:37:23
Duration:	6 m, 49 s
Success:	True
Converged:	True
Computational package:	Gaussian (2016+C.01)
Methods:	DFT
Functional:	PBE1PBE
Basis set:	6-31G(d,p)
Calculations:	Optimisation, Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	5
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 °

Vibrational Frequencies

Negative frequencies: 0

Vertical S_1 Emission

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: 279 nm

S_1 colour: Ultraviolet [REDACTED]

S_1 CIE (x,y): (0.00, 0.00)

S_1 oscillator strength: 0.00

S_1 rate /s⁻¹: 2.91e+05

Adiabatic S_1 Emission

Excited energy: -10484.45 eV

Excited multiplicity: Singlet

Ground energy: -10488.99 eV

Ground multiplicity: Singlet

Emission type: Fluorescence

S_1 energy: 4.54 eV

S_1 wavelength: 273 nm

S_1 colour: Ultraviolet [REDACTED]

S_1 CIE (x,y): (0.00, 0.00)

S_1 oscillator strength: 0.00

S_1 rate /s⁻¹: 3.13e+05

Exo

ΔE_{ST}

S_1 en

S_1 wa

S_1 co

S_1 CI

S_1 os

T_1 en

T_1 wa

T_1 co

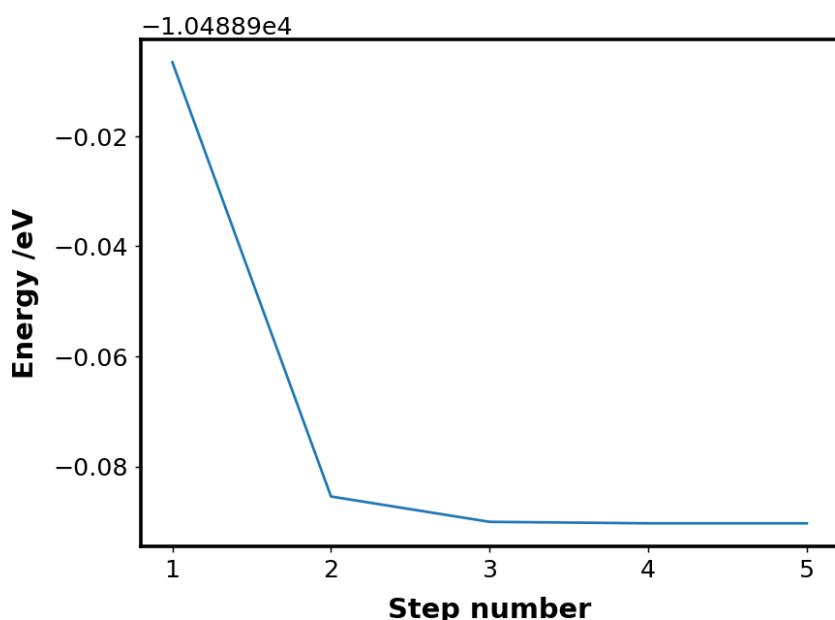
T_1 CI

T_1 os

No. c

No. c

SCF Energies



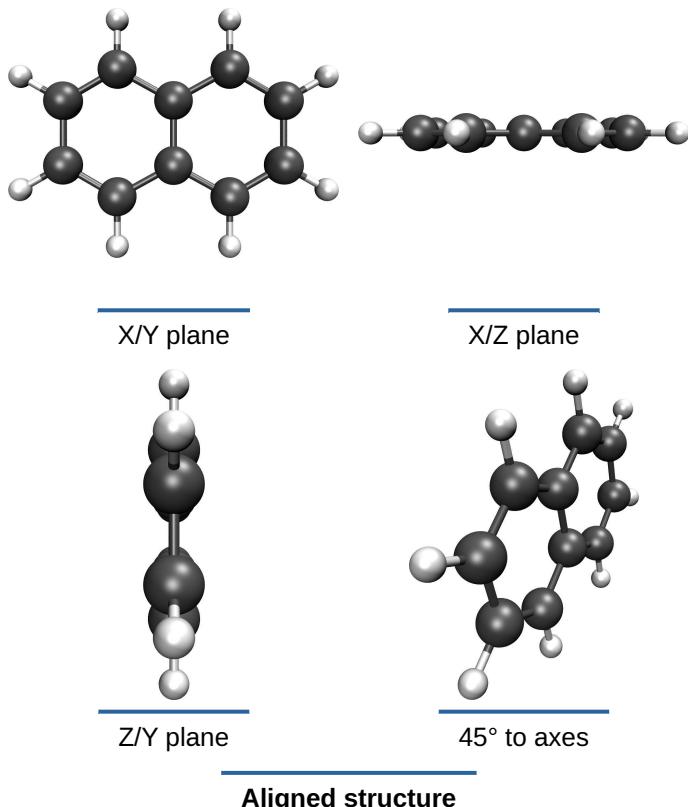
SCF Energies

No. of steps: 5

Final energy: -10488.9903 eV

Final energy: -1,012,034 kJmol⁻¹

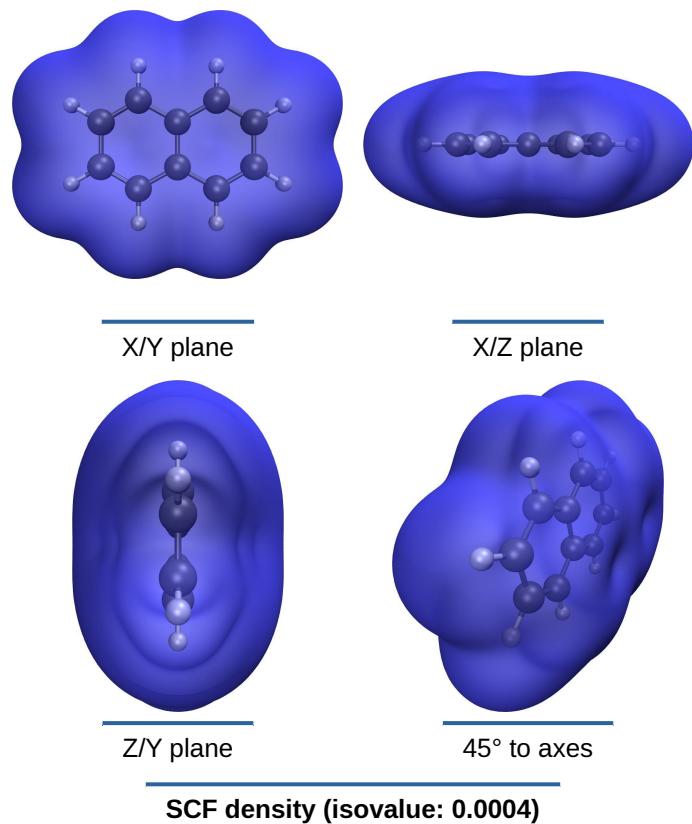
Geometry



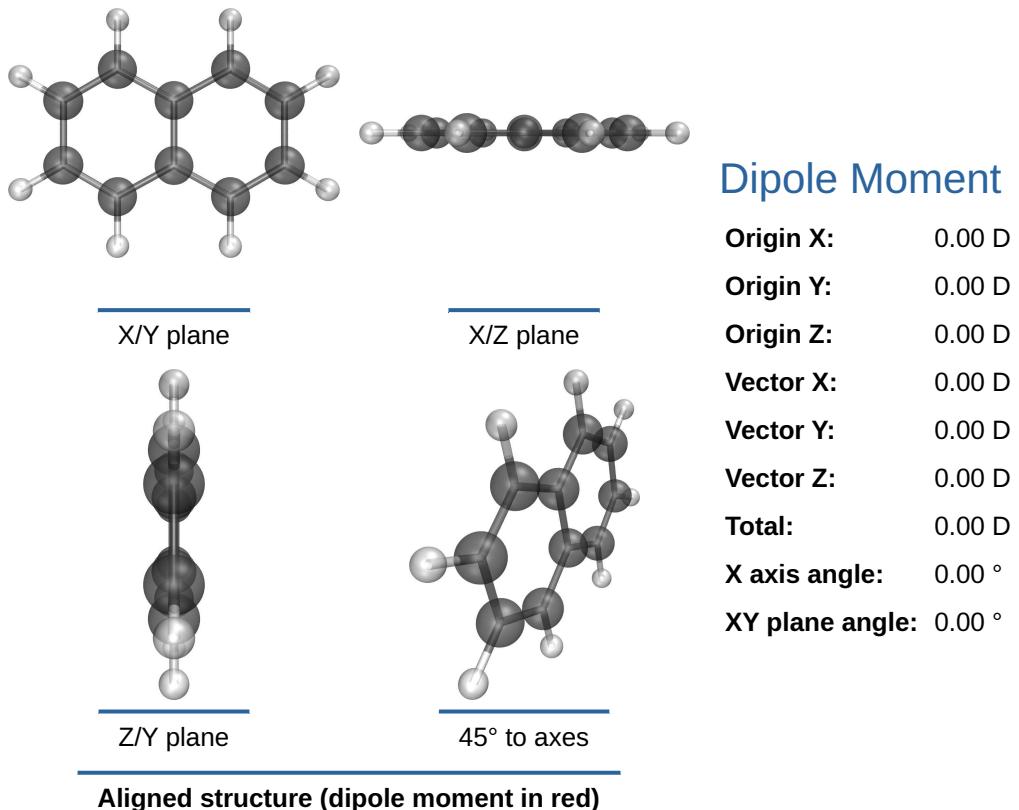
Geometry

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

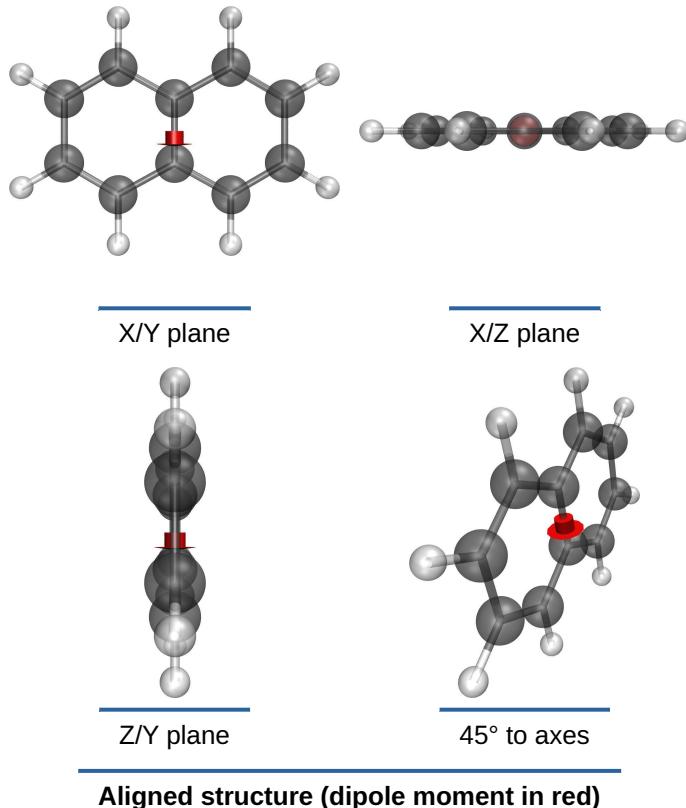
SCF Density



Permanent Dipole Moment



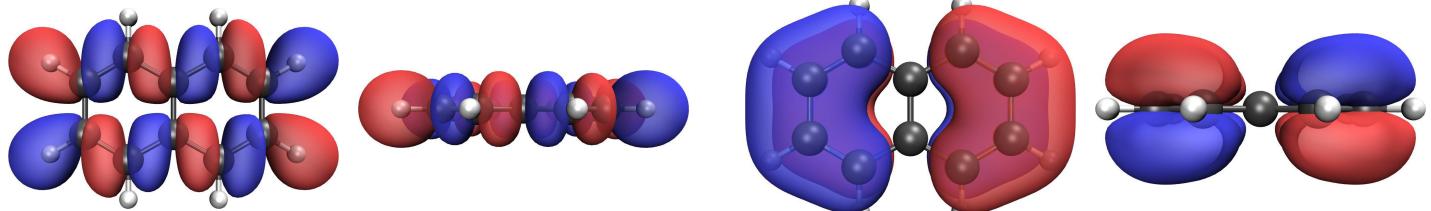
Transition (S_1) Dipole Moment



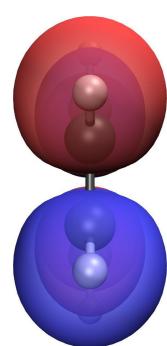
Dipole Moment

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



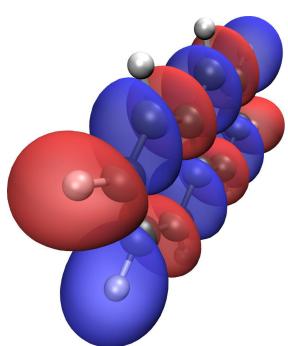
X/Y plane



Z/Y plane

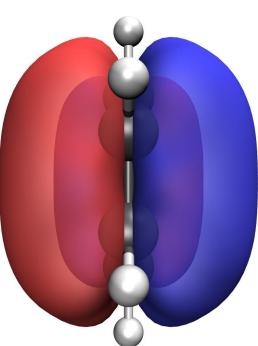
HOMO-5 density (isovalue: 0.02)

X/Z plane



45° to axes

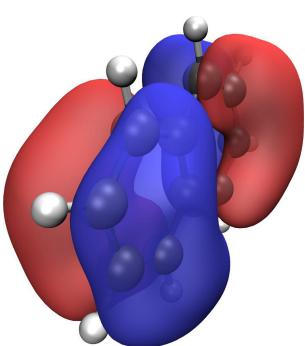
X/Y plane



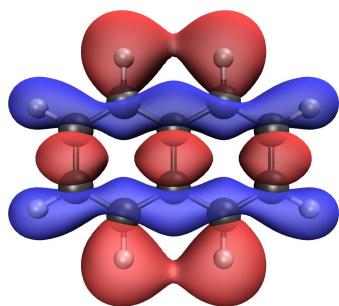
Z/Y plane

HOMO-4 density (isovalue: 0.02)

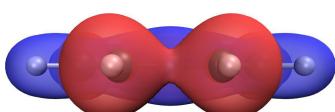
X/Z plane



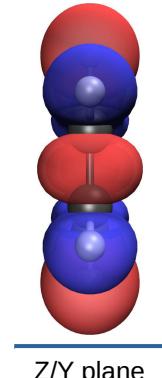
45° to axes



X/Y plane

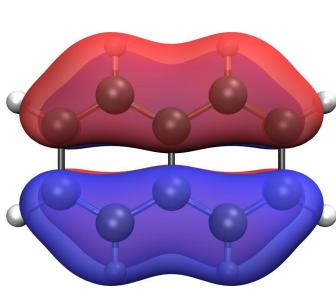


X/Z plane



Z/Y plane

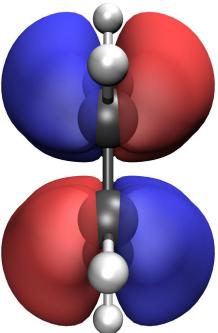
HOMO-3 density (isovalue: 0.02)



X/Y plane



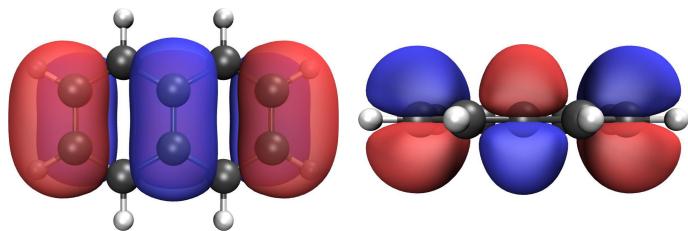
X/Z plane



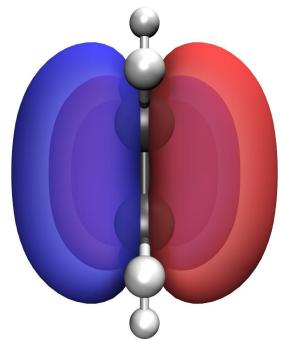
Z/Y plane

HOMO-2 density (isovalue: 0.02)

HOMO-1

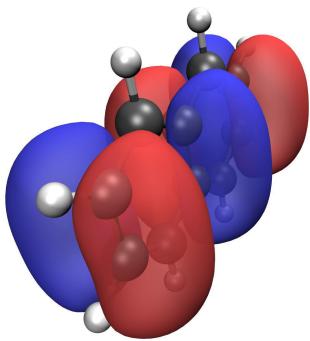


X/Y plane



Z/Y plane

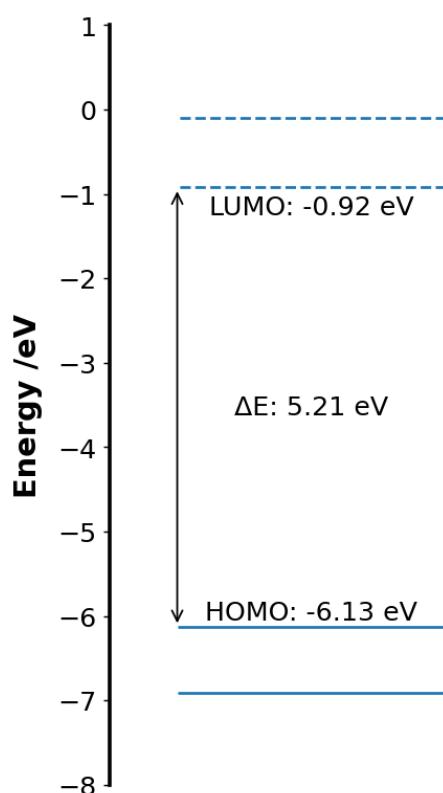
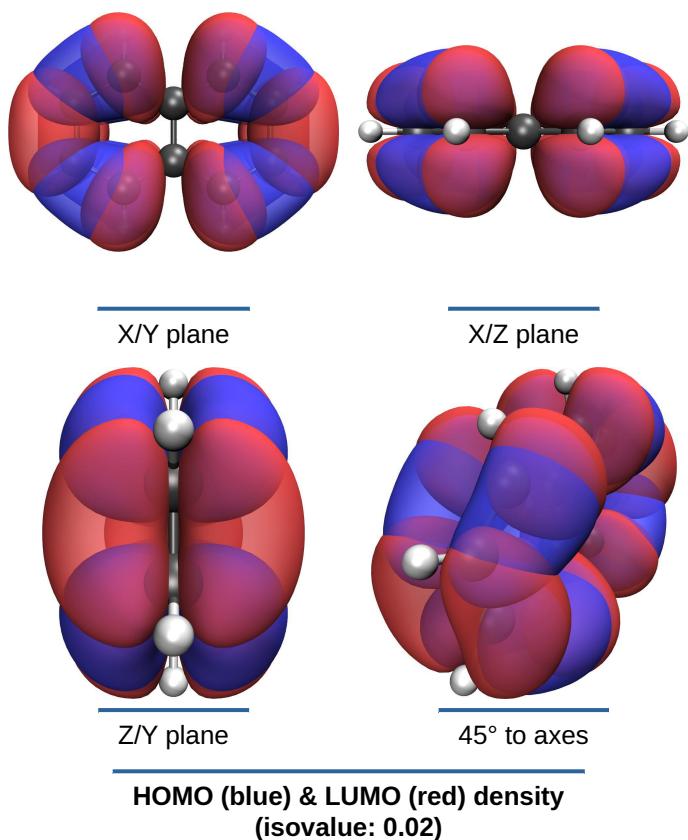
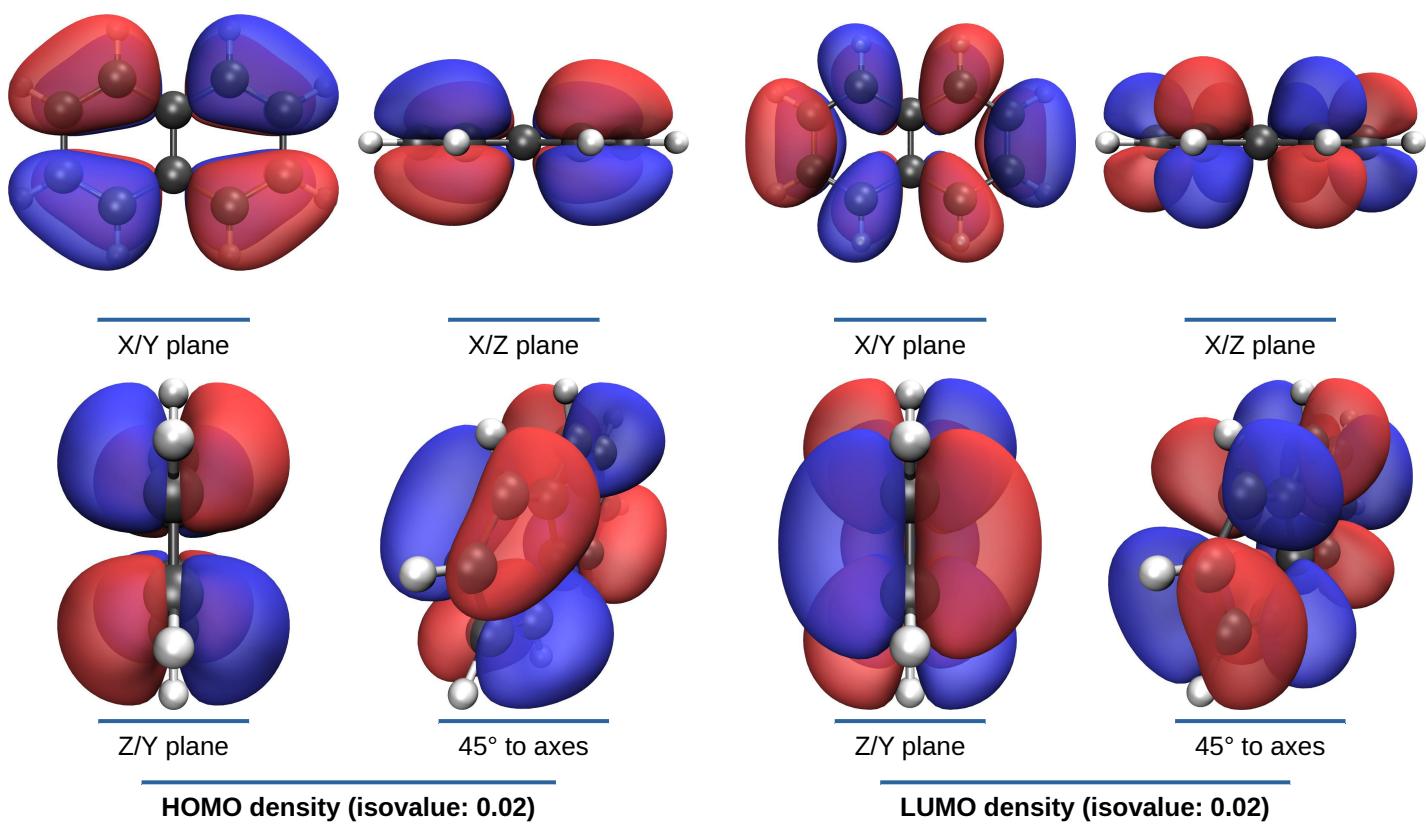
X/Z plane



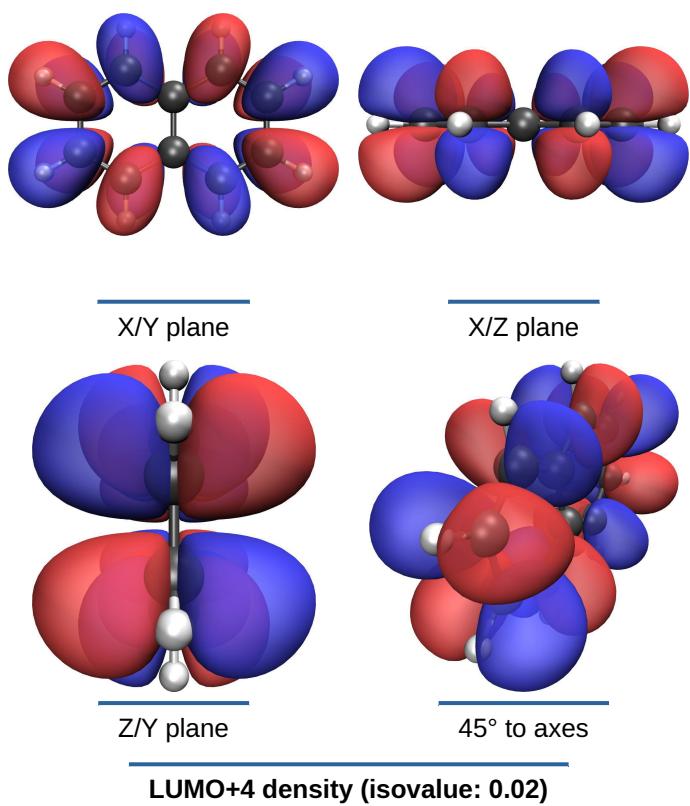
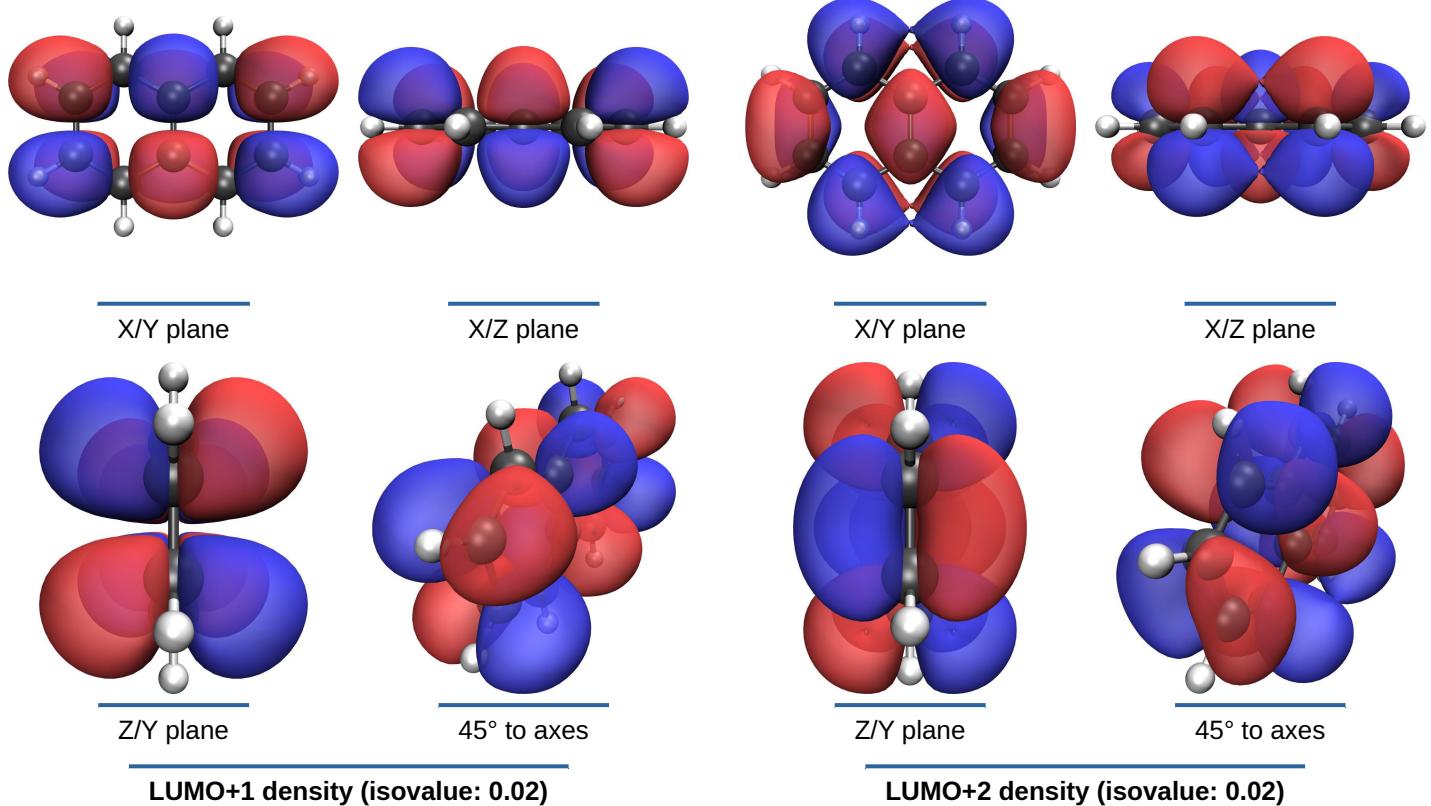
45° to axes

HOMO-1 density (isovalue: 0.02)

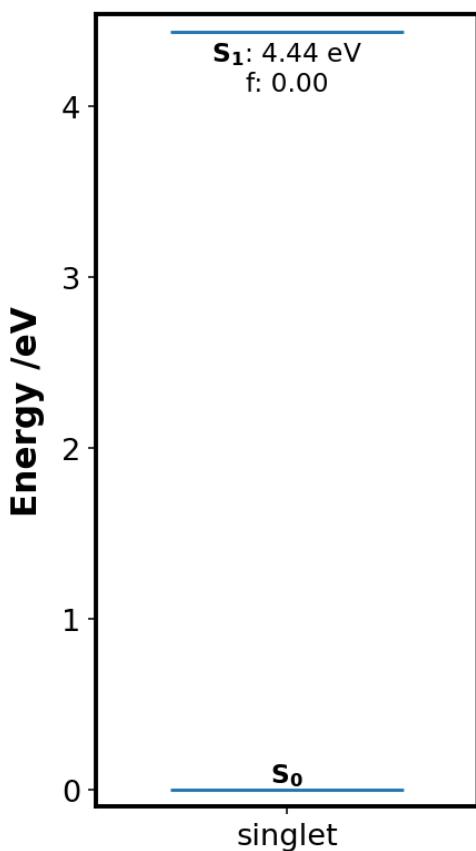
HOMO & LUMO



LUMO+1, LUMO+2, LUMO+4



Vertical S_1 Emission

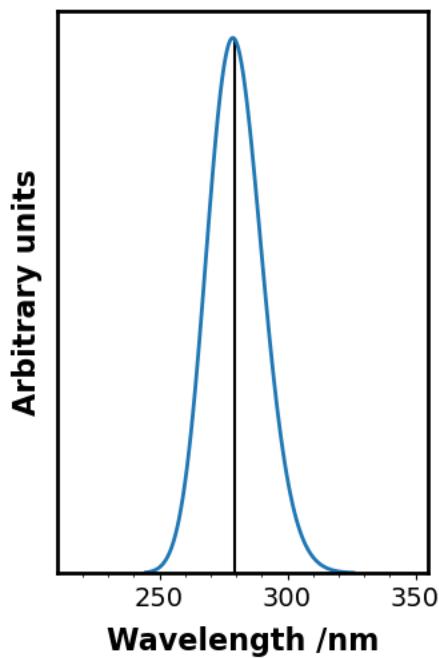


Vertical S_1 Emission

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: 279 nm
 S_1 colour: Ultraviolet

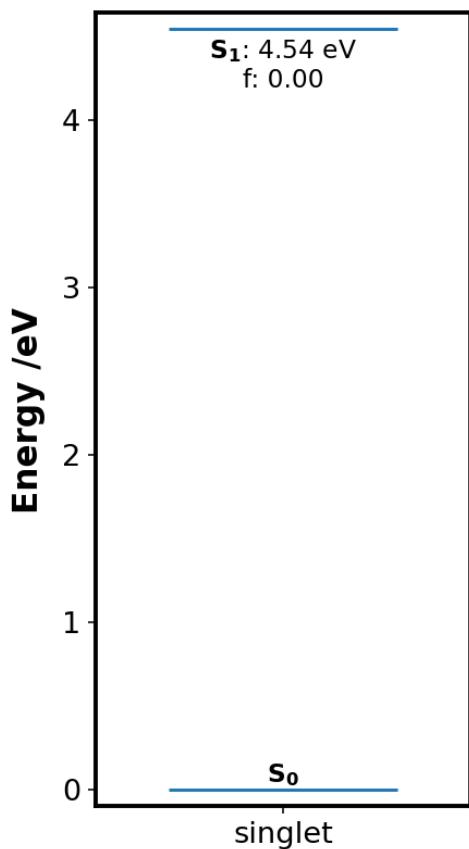
S_1 CIE (x,y): (0.00, 0.00)
 S_1 oscillator strength: 0.00
 S_1 rate /s⁻¹: 2.91e+05

Vertical S_1 Emission Spectrum



Emission spectrum (simulated Gaussian functions with FWHM: 0.4 eV)
Peaks /nm: 278.

Adiabatic S₁ Emission

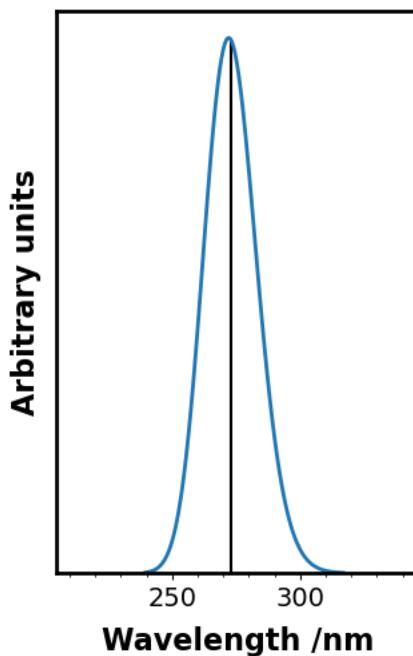


Adiabatic S₁ Emission

Excited energy: -10484.45 eV
Excited multiplicity: Singlet
Ground energy: -10488.99 eV
Ground multiplicity: Singlet
Emission type: Fluorescence
S₁ energy: 4.54 eV
S₁ wavelength: 273 nm
S₁ colour: Ultraviolet

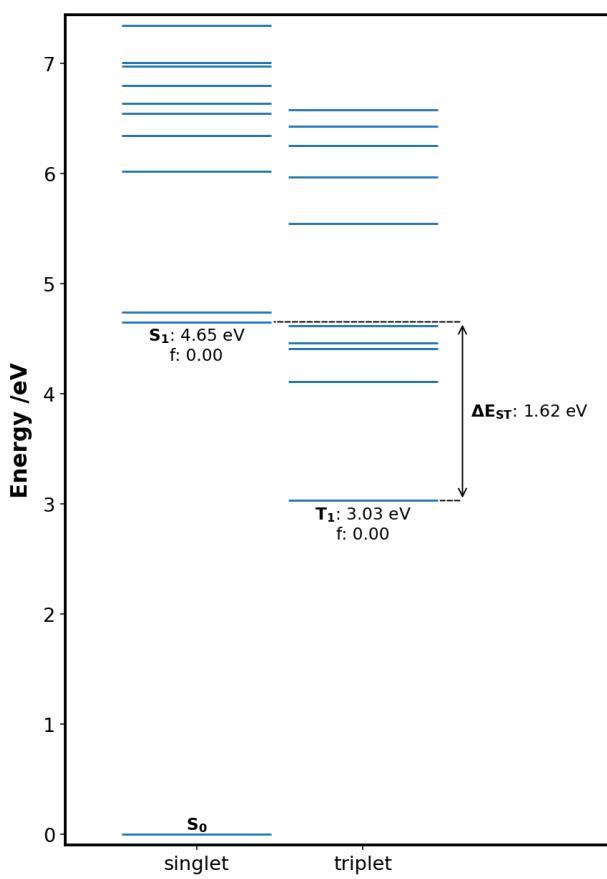
S₁ CIE (x,y): (0.00, 0.00)
S₁ oscillator strength: 0.00
S₁ rate /s⁻¹: 3.13e+05

Adiabatic S₁ Emission Spectrum



Emission spectrum (simulated Gaussian functions with FWHM: 0.4 eV)
Peaks /nm: 272.

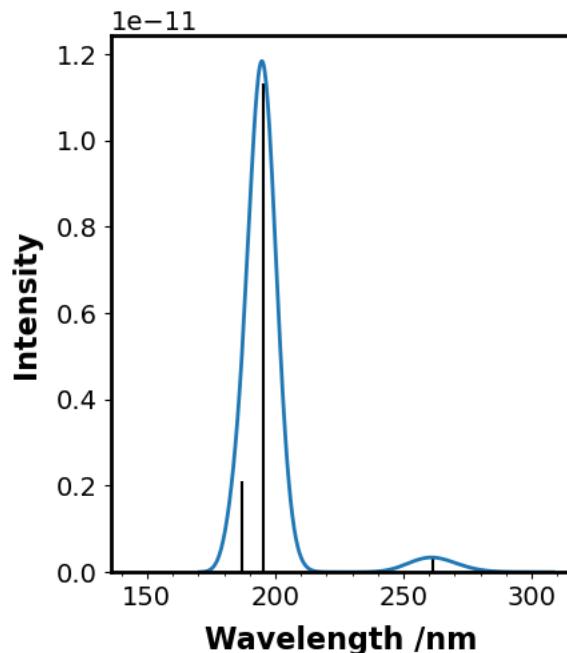
Excited States



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).

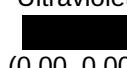
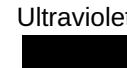
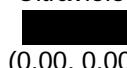
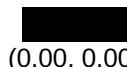
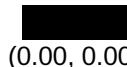
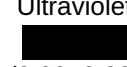
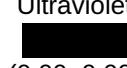
Peaks /nm: 194, 261.

Note: high energy absorption peaks are not simulated.
For a complete absorption spectrum, use more excited states.

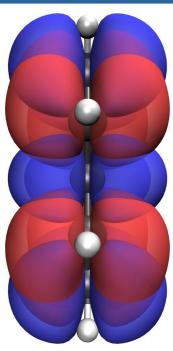
Table of Excited States

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		0.0000	HOMO-2 → LUMO+1 (0.49) HOMO-1 → LUMO+2 (0.46)

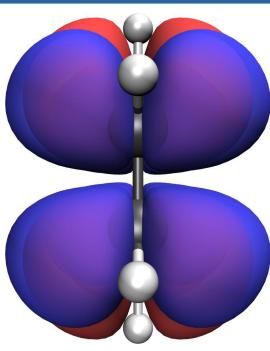
Naphthalene - Optimisation, Frequencies, Excited States (Singlet,...)

					Ultraviolet  (0.00, 0.00)		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)
16	S ₆	Singlet-B1U	6.6348	186.87	Ultraviolet  (0.00, 0.00)	0.3684	HOMO-1 → LUMO+1 (0.86) HOMO-2 → LUMO+2 (0.07) HOMO → LUMO (0.04)
17	S ₇	Singlet-B1G	6.7955	182.45	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.99)
18	S ₈	Singlet-B2G	6.9759	177.73	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-5 → LUMO (0.98)
19	S ₉	Singlet-B3G	7.0061	176.97	Ultraviolet  (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  (0.00, 0.00)	0.0000	HOMO-4 → LUMO (0.63) HOMO-1 → LUMO+2 (0.27) HOMO-2 → LUMO+1 (0.07)

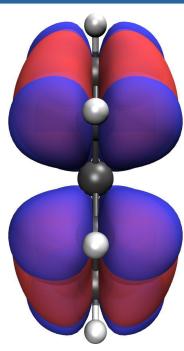
S(1), S(2), S(3), S(4) Natural Transition Orbitals



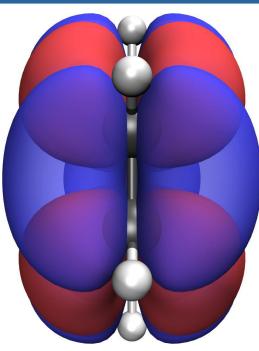
X/Y plane



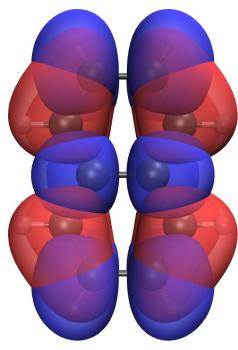
X/Z plane



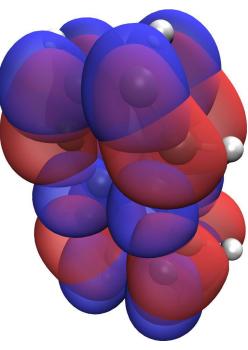
X/Y plane



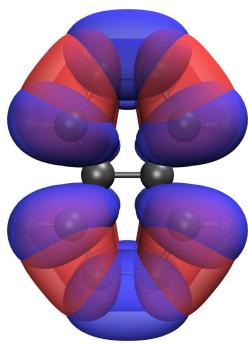
X/Z plane



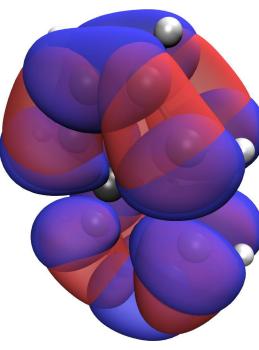
Z/Y plane



45° to axes



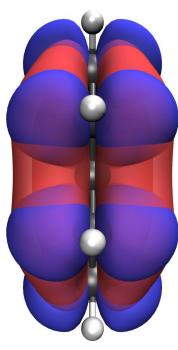
Z/Y plane



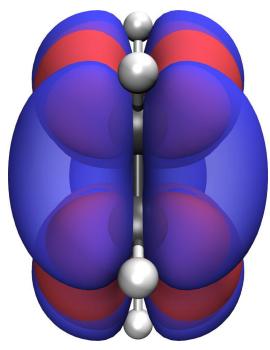
45° to axes

S(1) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

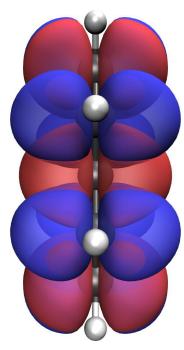
S(2) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



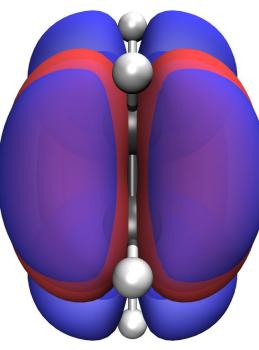
X/Y plane



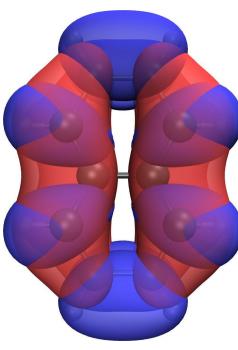
X/Z plane



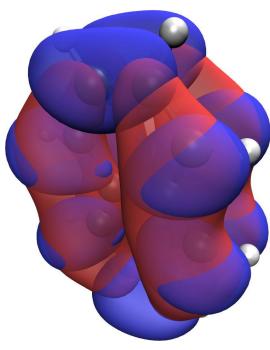
X/Y plane



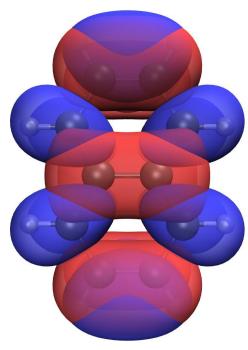
X/Z plane



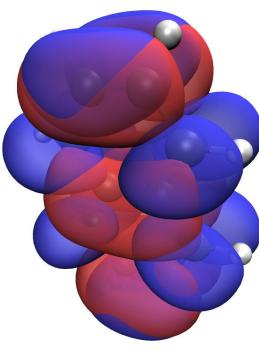
Z/Y plane



45° to axes



Z/Y plane

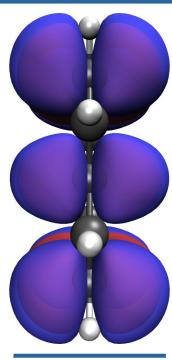


45° to axes

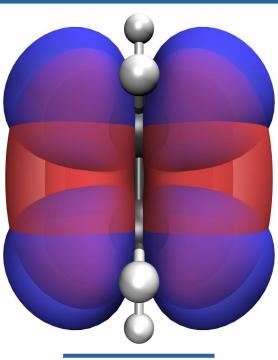
S(3) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

S(4) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

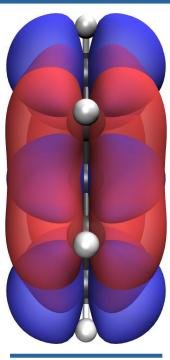
S(5), S(6), S(7), S(8) Natural Transition Orbitals



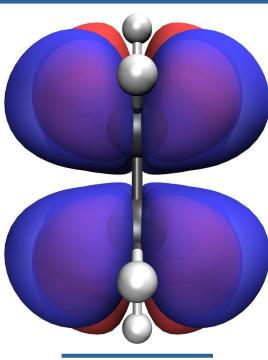
X/Y plane



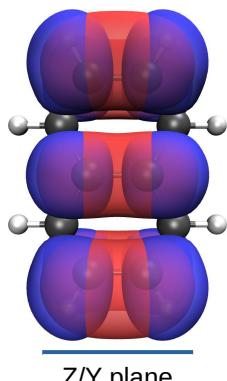
X/Z plane



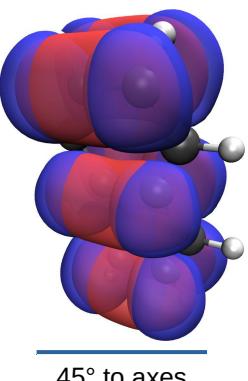
X/Y plane



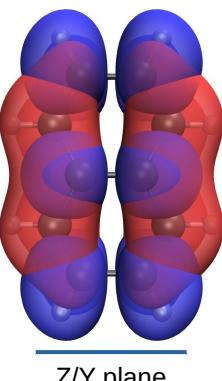
X/Z plane



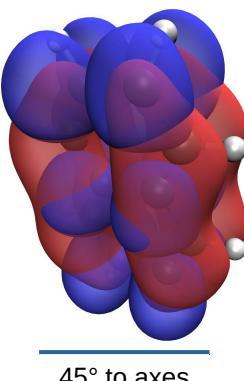
Z/Y plane



45° to axes



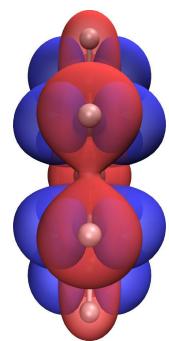
Z/Y plane



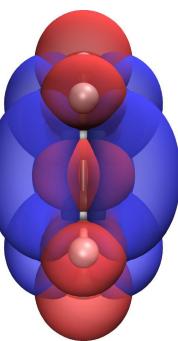
45° to axes

S(5) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

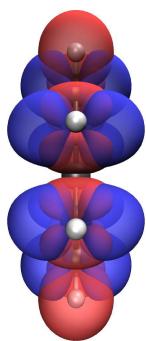
S(6) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



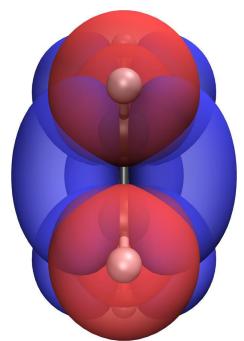
X/Y plane



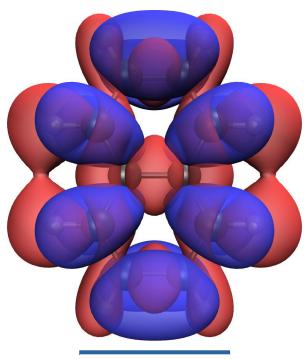
X/Z plane



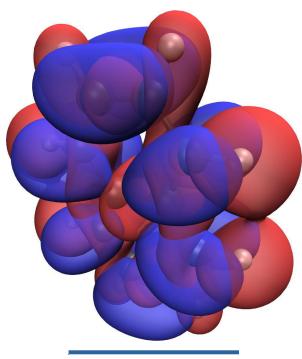
X/Y plane



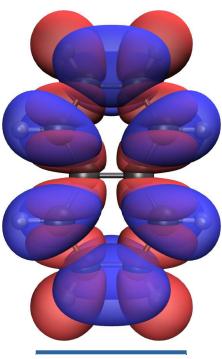
X/Z plane



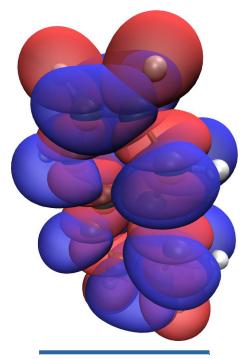
Z/Y plane



45° to axes



Z/Y plane

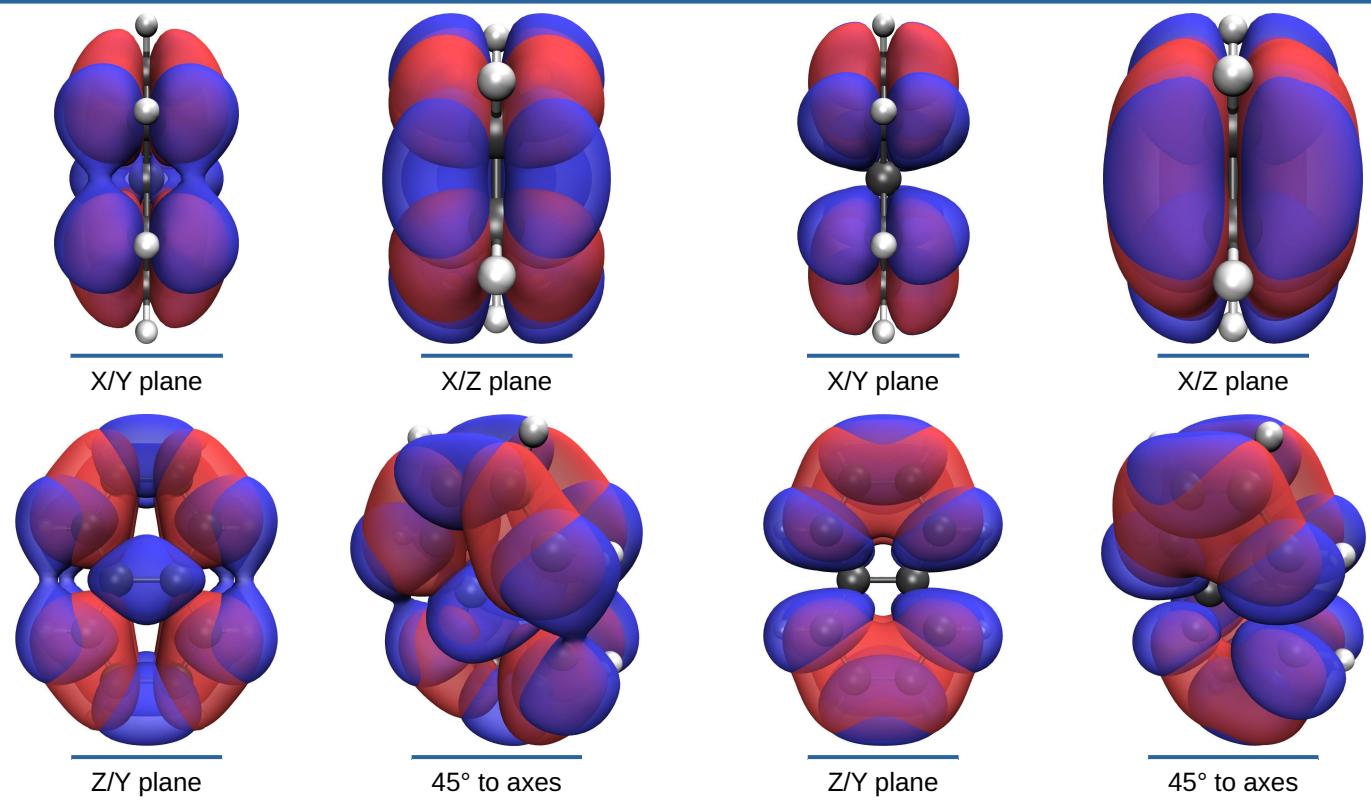


45° to axes

S(7) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

S(8) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

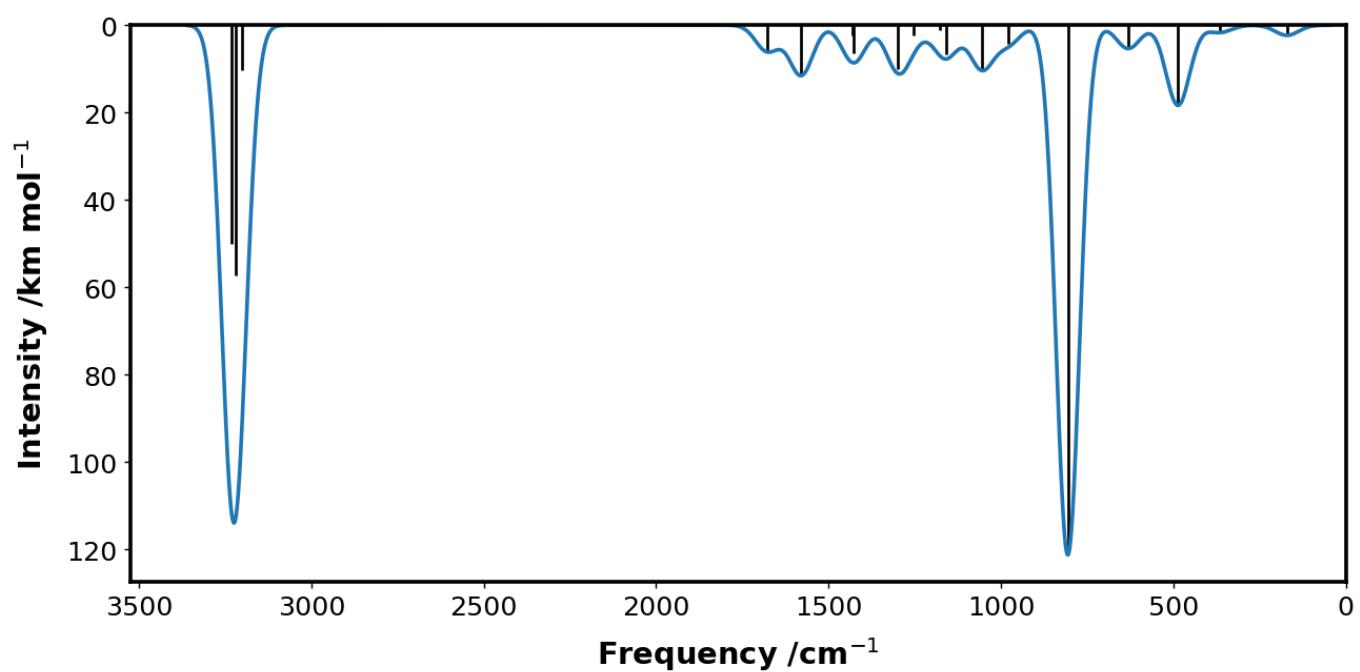
S(9), S(10) Natural Transition Orbitals



S(9) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

S(10) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm⁻¹)
Peaks /cm⁻¹: 170, 368, 487, 631, 806, 1053, 1160, 1294, 1427, 1580, 1673,
3224.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm ⁻¹	Intensity /km mol ⁻¹
1	A	170.6603	2.3323
2	A	186.3677	0.0000
3	A	365.1609	1.6874
4	A	393.2304	0.0000
5	A	477.4391	0.0000
6	A	486.8646	18.3491
7	A	516.9575	0.0000
8	A	522.9547	0.0000
9	A	631.0734	5.3597
10	A	636.2303	0.0000
11	A	734.4453	0.0000
12	A	783.2293	0.0000
13	A	787.4275	0.0000
14	A	806.2853	121.0015
15	A	809.4087	0.2244
16	A	856.6594	0.0000
17	A	901.2132	0.0000
18	A	947.6833	0.0000
19	A	961.3577	0.0000
20	A	978.7553	4.2681
21	A	999.1135	0.0000
22	A	1006.5492	0.0000
23	A	1055.4957	10.0015
24	A	1066.4428	0.0000
25	A	1158.3757	6.7028
26	A	1178.7603	1.0658
27	A	1179.8776	0.0000
28	A	1188.4321	0.0000
29	A	1254.2980	2.4273
30	A	1274.8273	0.0000
31	A	1299.2065	10.0549
32	A	1426.1623	6.3760
33	A	1430.5870	2.2480
34	A	1451.2573	0.0000

Naphthalene - Optimisation, Frequencies, Excited States (Singlet,...

35	A	1508.0715	0.0000
36	A	1510.3663	0.0000
37	A	1579.8388	11.4633
38	A	1655.4851	0.0000
39	A	1677.4730	5.9807
40	A	1714.4767	0.0000
41	A	3201.3483	0.0000
42	A	3202.4466	10.2646
43	A	3204.6890	0.2493
44	A	3207.0173	0.0000
45	A	3220.0583	0.0000
46	A	3220.5827	57.2959
47	A	3232.8358	49.9545
48	A	3233.8528	0.0000

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
50	LUMO+15	A	8.6396
49	LUMO+14	A	7.9114
48	LUMO+13	A	6.9152
47	LUMO+12	A	6.0692
46	LUMO+11	A	5.7949
45	LUMO+10	A	5.3487
44	LUMO+9	A	5.1506
43	LUMO+8	A	5.0034
42	LUMO+7	A	4.9519
41	LUMO+6	A	3.6912
40	LUMO+5	A	3.4207
39	LUMO+4	A	2.9674
38	LUMO+3	A	2.9127
37	LUMO+2	A	1.0612
36	LUMO+1	A	-0.1010
35	LUMO	A	-0.9244
34	HOMO	A	-6.1307
33	HOMO-1	A	-6.9087
32	HOMO-2	A	-8.0747
31	HOMO-3	A	-9.1879
30	HOMO-4	A	-9.2562
29	HOMO-5	A	-9.4032
28	HOMO-6	A	-10.2679
27	HOMO-7	A	-11.0274
26	HOMO-8	A	-11.1363
25	HOMO-9	A	-11.5961
24	HOMO-10	A	-11.6187
23	HOMO-11	A	-12.3015
22	HOMO-12	A	-12.4753
21	HOMO-13	A	-13.7777
20	HOMO-14	A	-14.2411
19	HOMO-15	A	-14.3709

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2404550	-1.3991360	-0.0000000
C	-2.4260000	-0.7066350	-0.0000000
C	-2.4260000	0.7066350	0.0000010
C	-1.2404550	1.3991360	0.0000010
C	0.0000000	0.7142260	-0.0000010
C	0.0000000	-0.7142260	-0.0000010
C	1.2404550	-1.3991360	0.0000010
C	1.2404550	1.3991360	-0.0000000
C	2.4260000	0.7066350	-0.0000000
C	2.4260000	-0.7066350	0.0000010
H	-1.2366960	-2.4861970	-0.0000030
H	-3.3696970	-1.2439660	0.0000010
H	-3.3696970	1.2439660	-0.0000010
H	-1.2366960	2.4861970	0.0000000
H	1.2366960	-2.4861970	0.0000000
H	1.2366960	2.4861970	-0.0000030
H	3.3696970	1.2439660	0.0000010
H	3.3696970	-1.2439660	-0.0000010

About

Silico Calculation Report

Part of the silico software package

Version 1.0.0-pre.30

7 June 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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