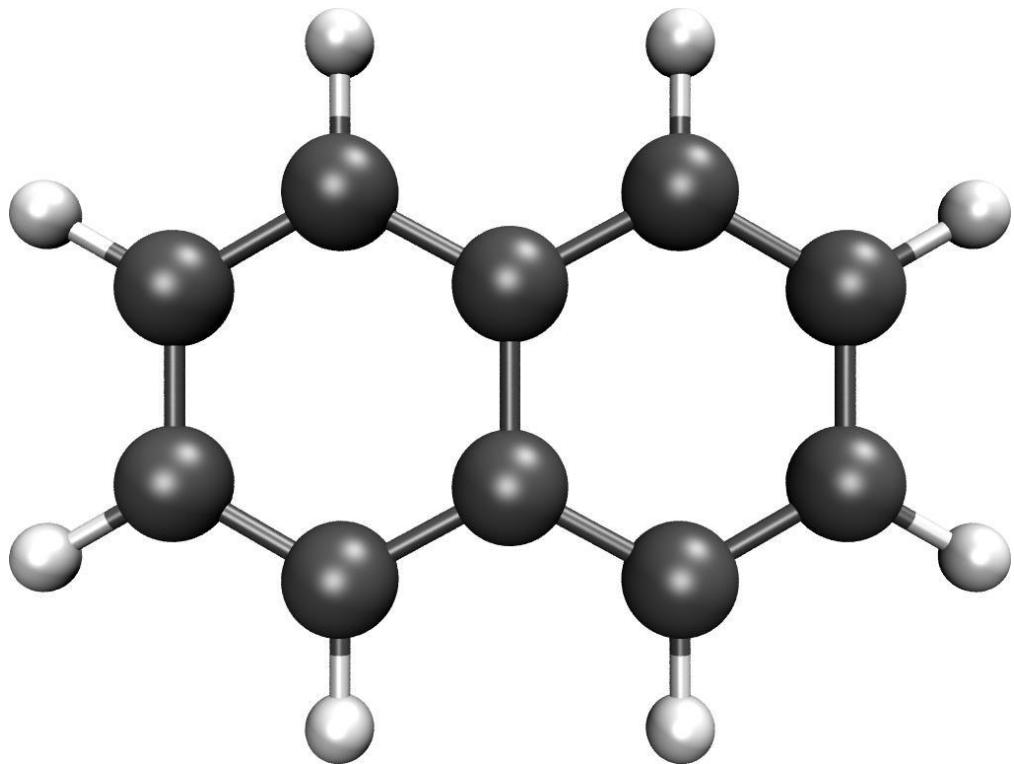


Calculation Report

Naphthalene

Optimisation, Excited States (Singlet)



Summary of Results

Metadata		SCF Energies	Geometry	
Username:	osl	No. of steps: 4	Formula:	C ₁₀ H ₈
Date:	07/06/2022 17:37:23	Final energy: -10488.8835 eV	Exact mass:	128.0626 g mol ⁻¹
Duration:	6 m, 49 s	Final energy: -1,012,023 kJ mol ⁻¹	Molar mass:	128.1705 g mol ⁻¹
Success:	True		Alignment method:	Minimal
Converged:	True		X extension:	6.78 Å
Computational package:	Gaussian (2016+C.01)		Y extension:	5.00 Å
Methods:	DFT		Z extension:	0.00 Å
Functional:	PBE1PBE		Linearity ratio:	0.26
Basis set:	6-31G(d,p)		Planarity ratio:	1.00
Calculations:	Optimisation, Excited States			
Orbital spin:	restricted			
Multiplicity:	1 (singlet)			

HOMO & LUMO

E_{HOMO,LUMO}: 4.98 eV

E_{HOMO}: -6.05 eV

E_{LUMO}: -1.07 eV

Permanent Dipole Moment

Total: 0.00 D

X axis angle: 0.00 °

XY plane angle: 0.00 °

Transition (S₁) Dipole Moment

Total: 0.04 D

X axis angle: 0.00 °

XY plane angle: 0.00 °

Vertical S₁ Emission

Excited energy: -10484.45 eV

Excited multiplicity: Singlet

Ground energy: -10488.88 eV

Ground multiplicity: Singlet

Emission type: Fluorescence

S₁ energy: 4.44 eV

S₁ wavelength: 279 nm

S₁ colour: Ultraviolet 

S₁ CIE (x,y): (0.00, 0.00)

S₁ oscillator strength: 0.00

S₁ rate /s⁻¹: 2.91e+05

Excited States

S₁ energy: 4.44 eV

S₁ wavelength: 279 nm

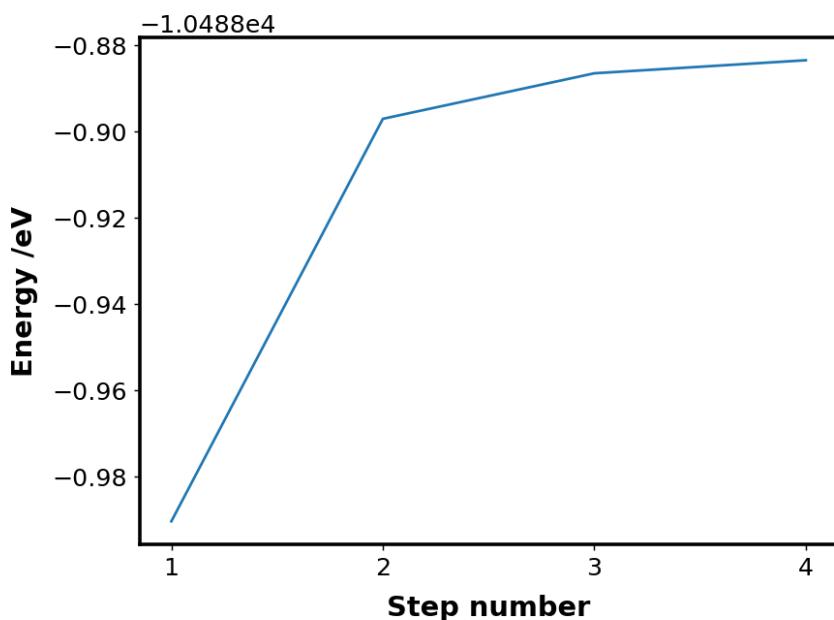
S₁ colour: Ultraviolet 

S₁ CIE (x,y): (0.00, 0.00)

S₁ oscillator strength: 0.00

No. of singlets: 10

SCF Energies



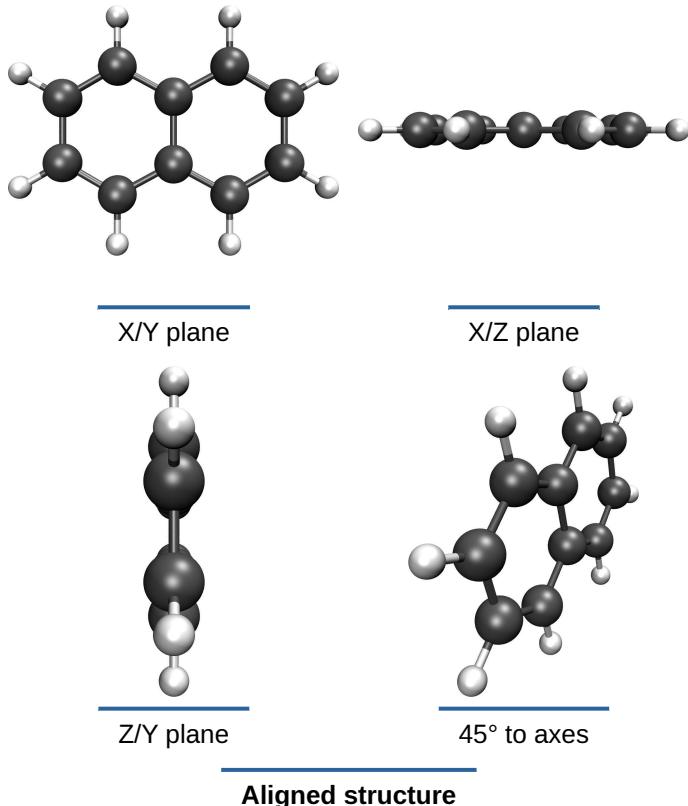
SCF Energies

No. of steps: 4

Final energy: -10488.8835 eV

Final energy: -1,012,023 kJmol⁻¹

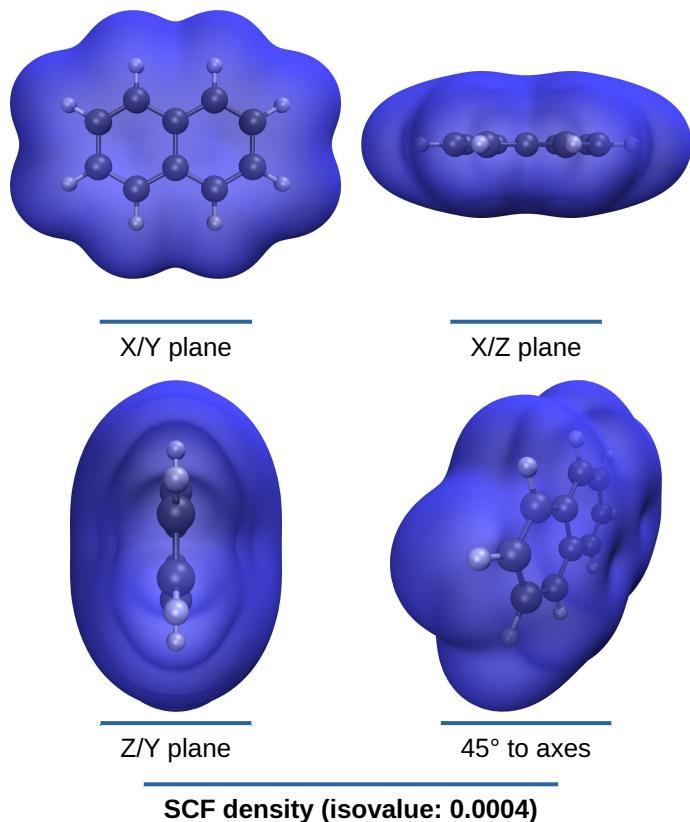
Geometry



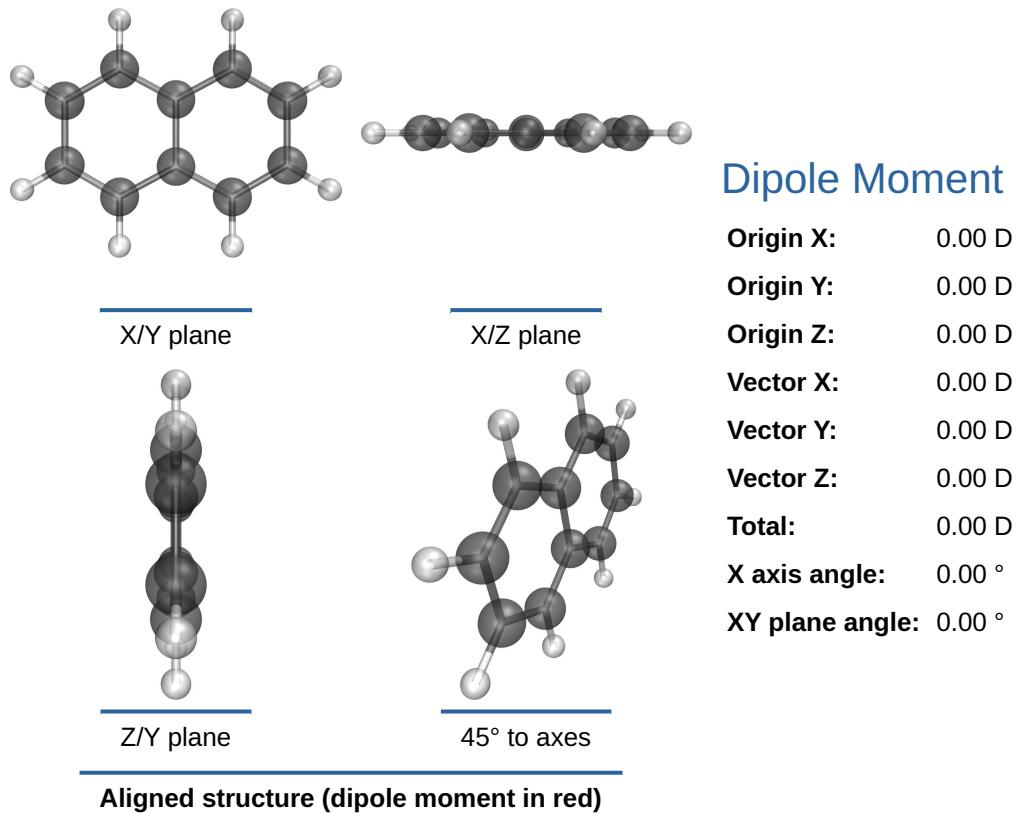
Geometry

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

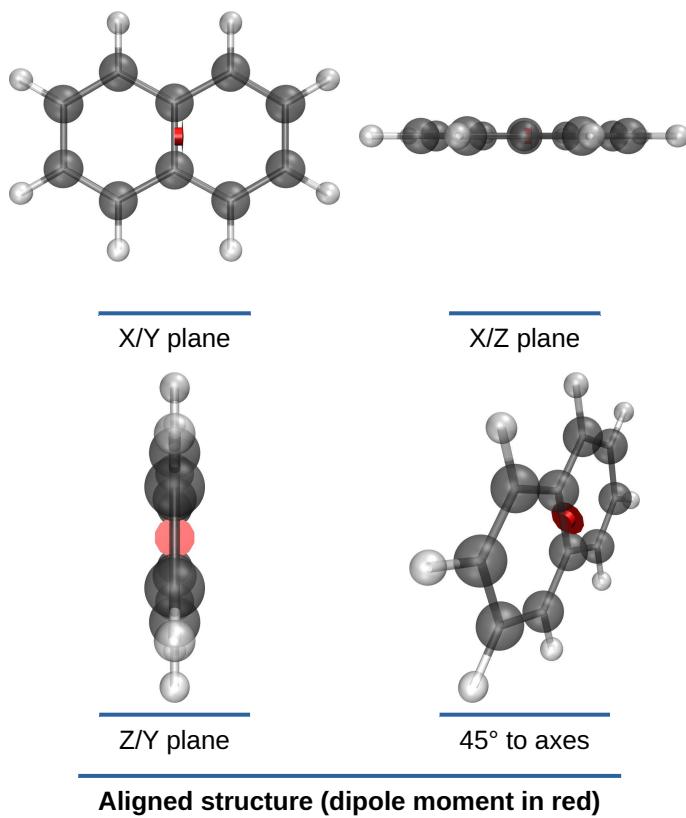
SCF Density



Permanent Dipole Moment



Transition (S_1) Dipole Moment

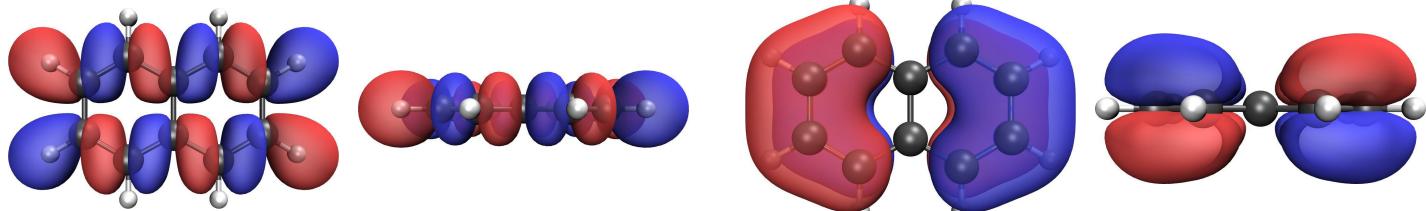


Dipole Moment

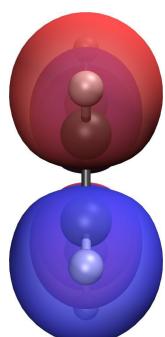
Origin X: 0.00 D
Origin Y: 0.00 D
Origin Z: 0.00 D
Vector X: 0.04 D
Vector Y: -0.00 D
Vector Z: -0.00 D
Total: 0.04 D
X axis angle: 0.00 °
XY plane angle: 0.00 °

Naphthalene - Optimisation, Excited States (Singlet)

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



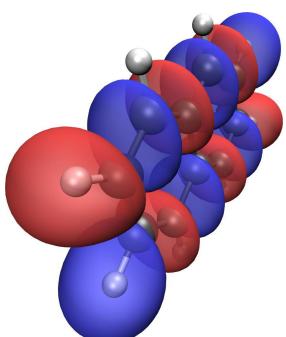
X/Y plane



Z/Y plane

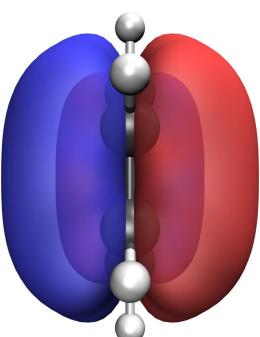
HOMO-5 density (isovalue: 0.02)

X/Z plane



45° to axes

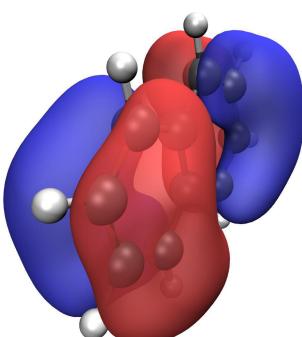
X/Y plane



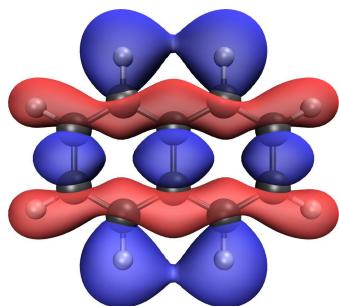
Z/Y plane

HOMO-4 density (isovalue: 0.02)

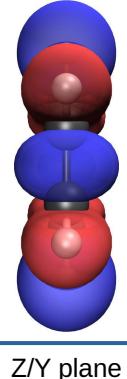
X/Z plane



45° to axes

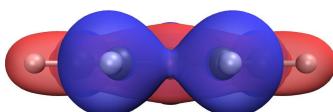


X/Y plane

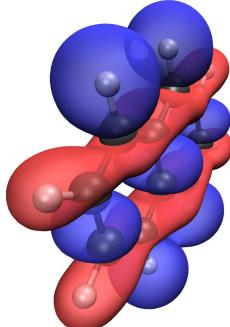


Z/Y plane

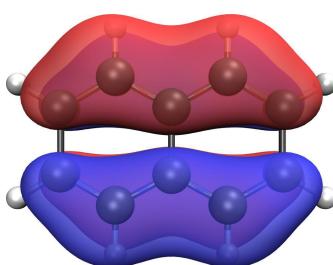
HOMO-3 density (isovalue: 0.02)



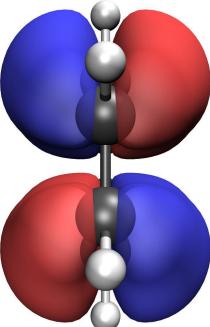
X/Z plane



45° to axes

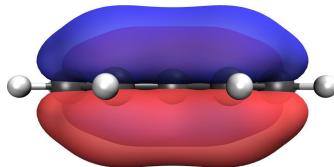


X/Y plane

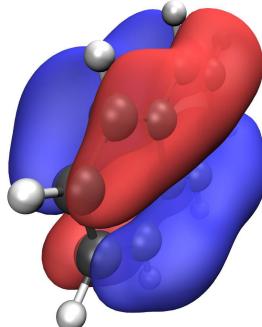


Z/Y plane

HOMO-2 density (isovalue: 0.02)

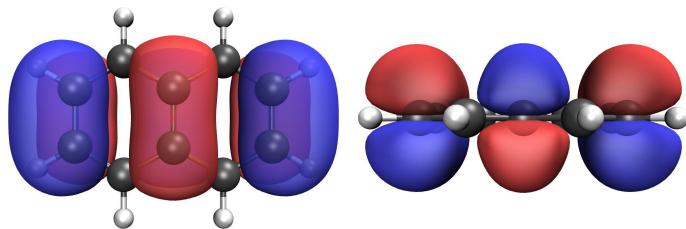


X/Z plane

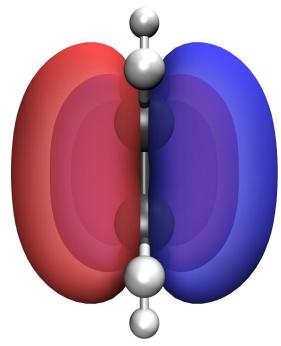


45° to axes

HOMO-1

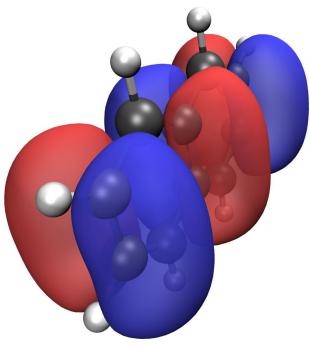


X/Y plane



Z/Y plane

X/Z plane

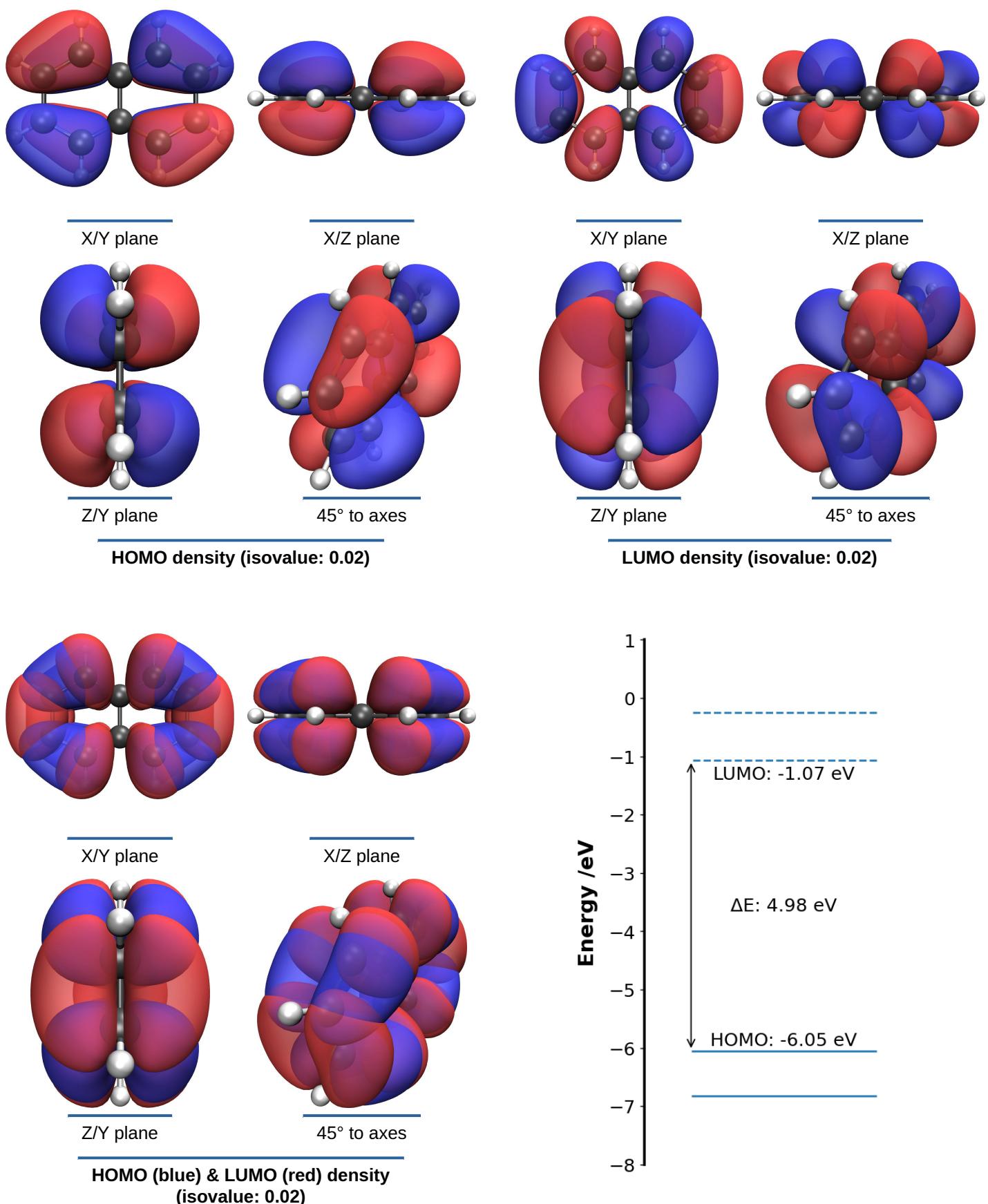


45° to axes

HOMO-1 density (isovalue: 0.02)

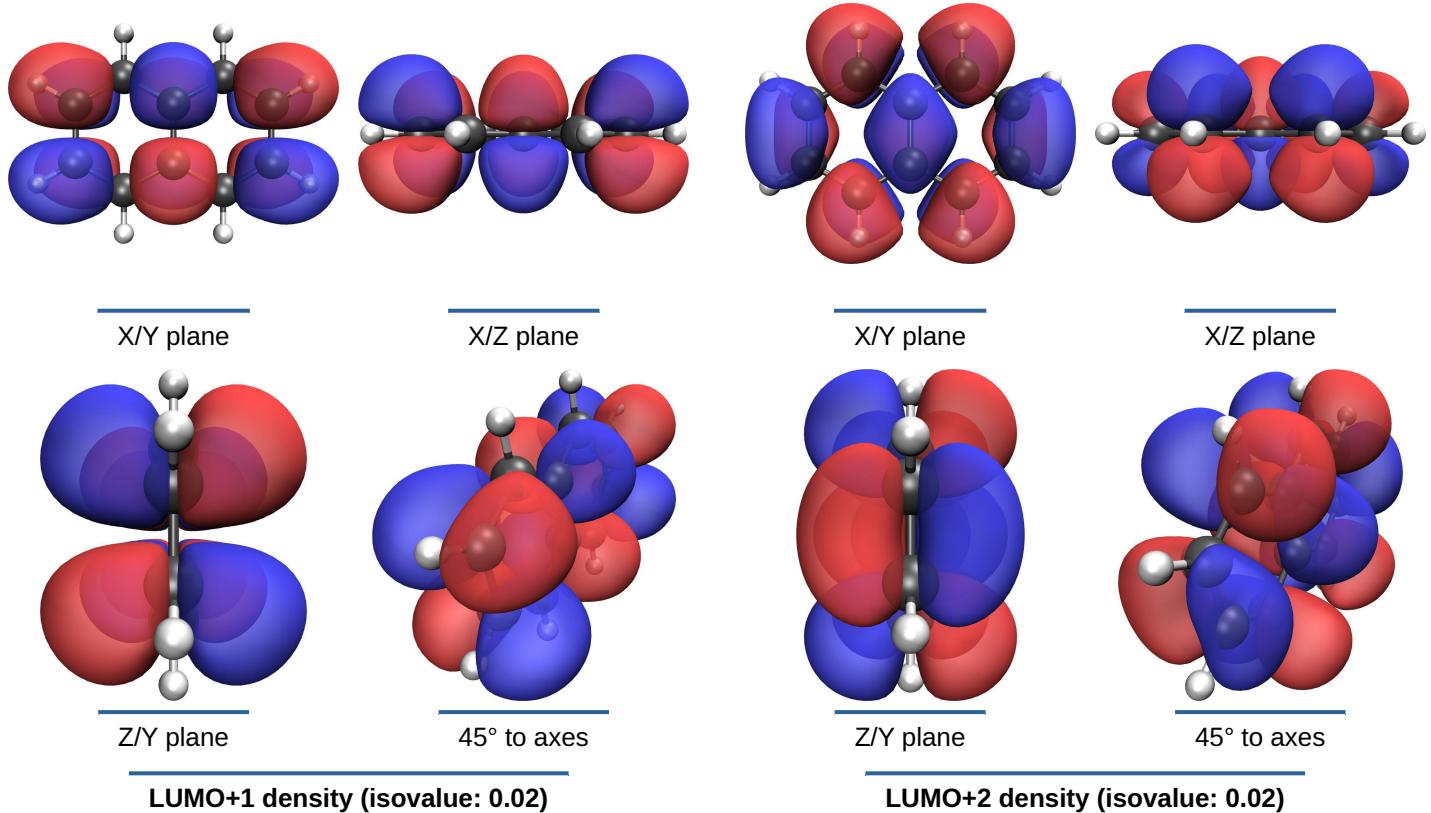
Naphthalene - Optimisation, Excited States (Singlet)

HOMO & LUMO

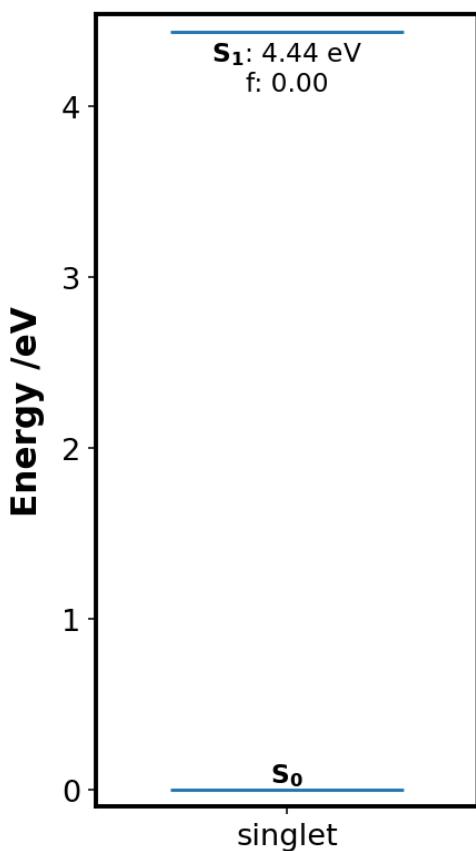


Naphthalene - Optimisation, Excited States (Singlet)

LUMO+1, LUMO+2



Vertical S_1 Emission

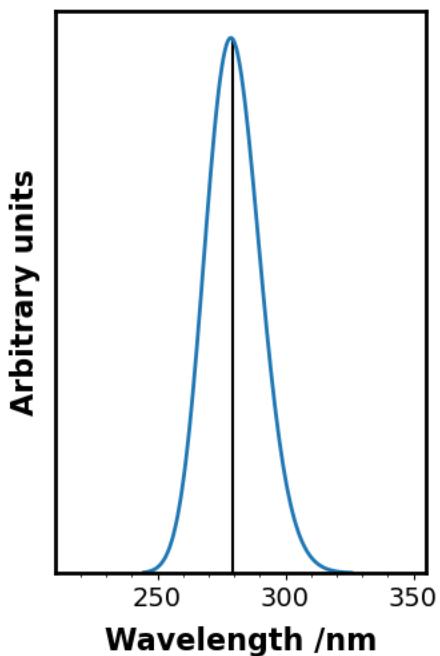


Vertical S_1 Emission

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

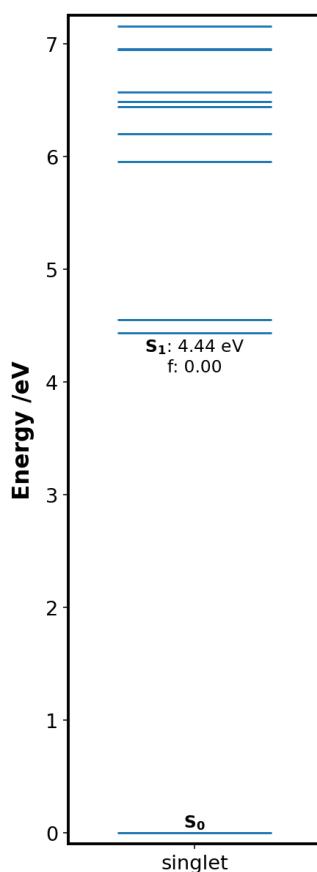
S_1 CIE (x,y): (0.00, 0.00)
 S_1 oscillator strength: 0.00
 S_1 rate /s⁻¹: 2.91e+05

Vertical S_1 Emission Spectrum



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

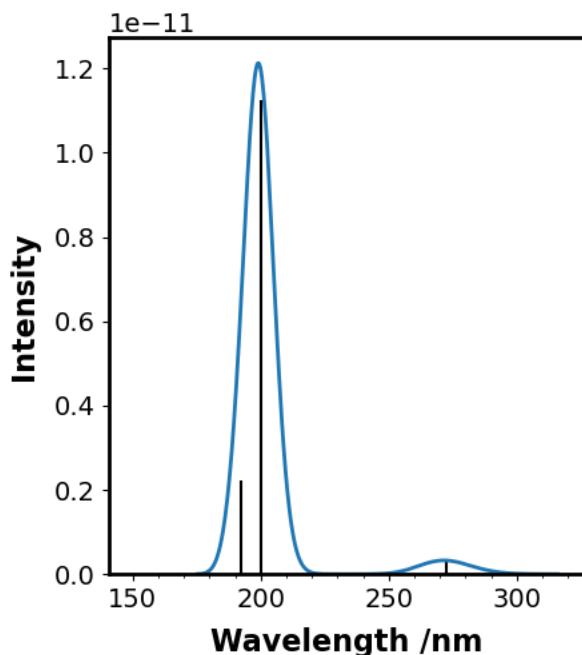
Excited States



Excited States

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
No. of singlets: 10

Absorptions



Absorption spectrum (simulated Gaussian functions with FWHM: 0.4 eV).

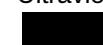
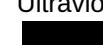
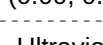
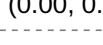
Peaks /nm: 198, 271.

Note: high energy absorption peaks are not simulated.

For a complete absorption spectrum, use more excited states.

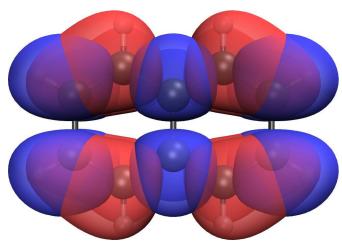
Naphthalene - Optimisation, Excited States (Singlet)

Table of Excited States

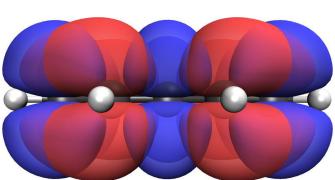
Level	Symbol	Symmetry	Energy /eV	Wavelength /nm	Colour, CIE (x,y)	Oscillator Strength	Transitions (probability)
1	S ₁	Singlet-B2U	4.4360	279.50	Ultraviolet  (0.00, 0.00)	0.0000	HOMO → LUMO+1 (0.50) HOMO-1 → LUMO (0.50)
2	S ₂	Singlet-B1U	4.5530	272.31	Ultraviolet  (0.00, 0.00)	0.1213	HOMO → LUMO (0.89) 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)

Naphthalene - Optimisation, Excited States (Singlet)

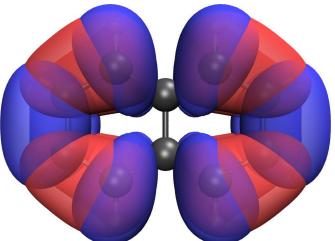
S(1), S(2), S(3), S(4) Natural Transition Orbitals



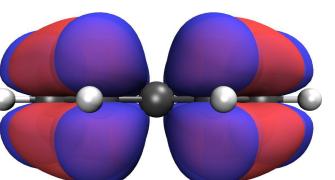
X/Y plane



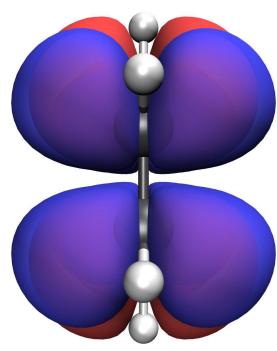
X/Z plane



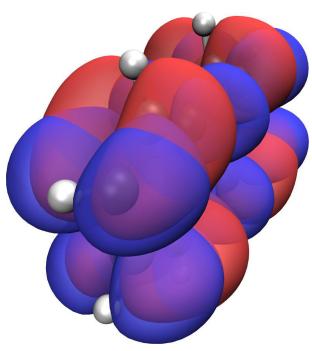
X/Y plane



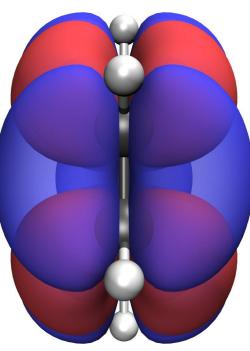
X/Z plane



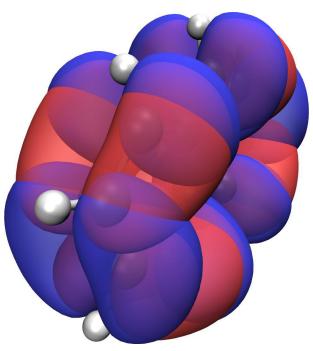
Z/Y plane



45° to axes



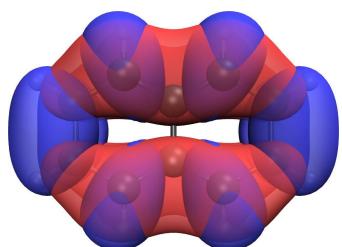
Z/Y plane



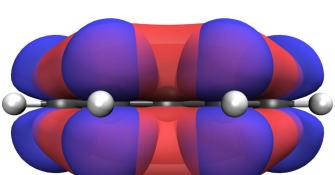
45° to axes

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

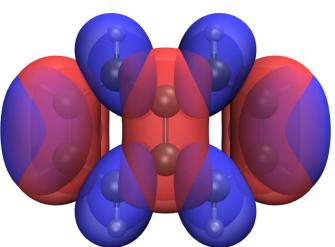
S(2) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



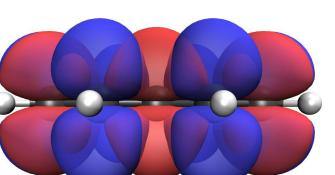
X/Y plane



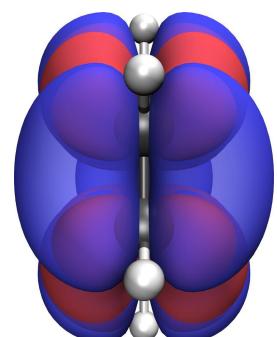
X/Z plane



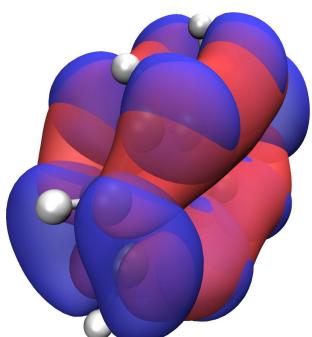
X/Y plane



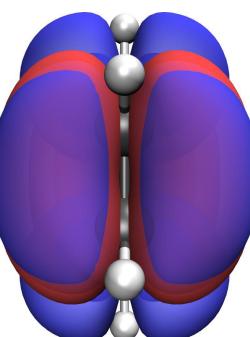
X/Z plane



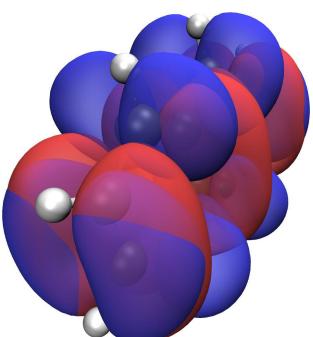
Z/Y plane



45° to axes



Z/Y plane



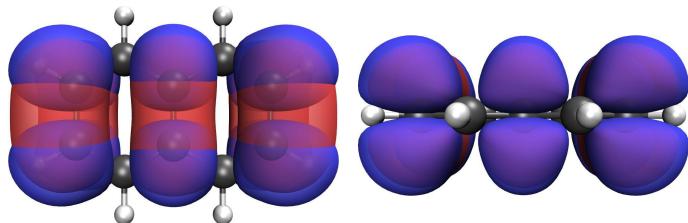
45° to axes

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

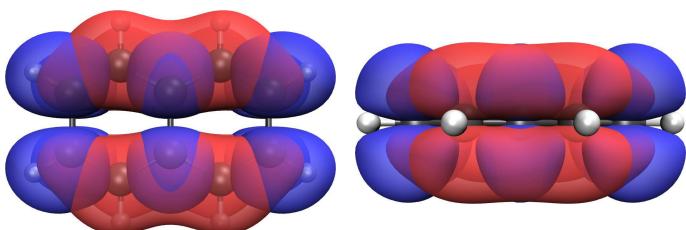
S(4) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Naphthalene - Optimisation, Excited States (Singlet)

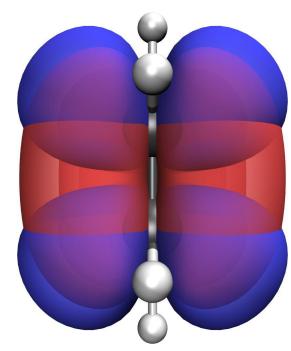
S(5), S(6), S(7), S(8) Natural Transition Orbitals



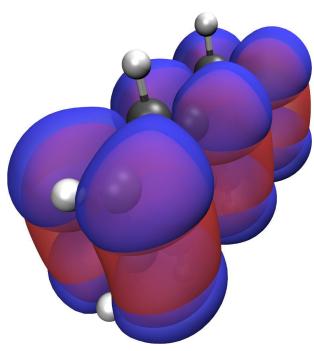
X/Y plane



X/Y plane

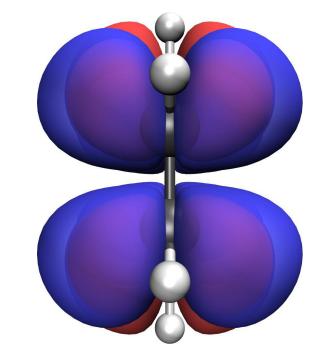


Z/Y plane

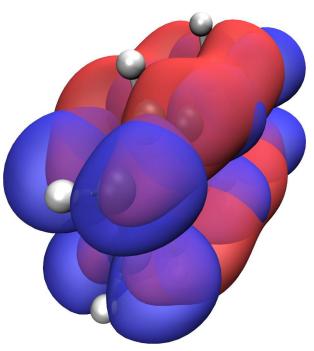


45° to axes

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

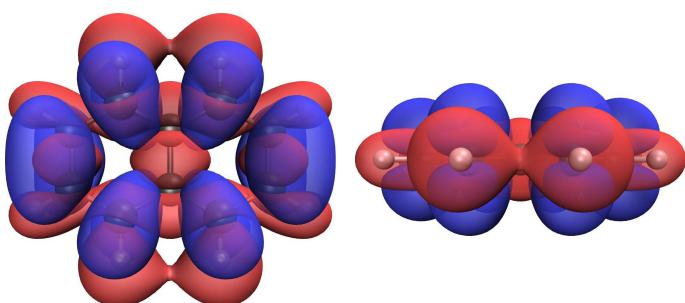


Z/Y plane

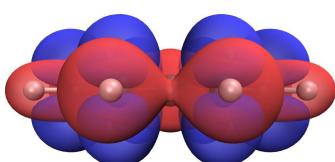


45° to axes

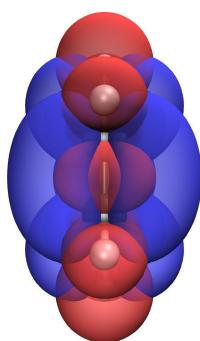
S(6) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



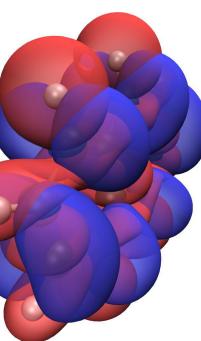
X/Y plane



X/Z plane

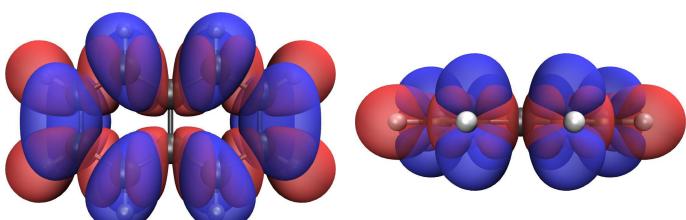


Z/Y plane

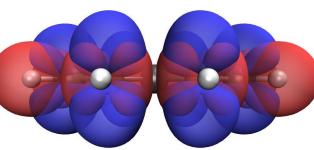


45° to axes

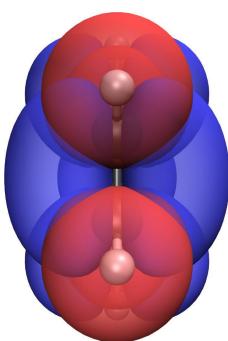
S(7) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



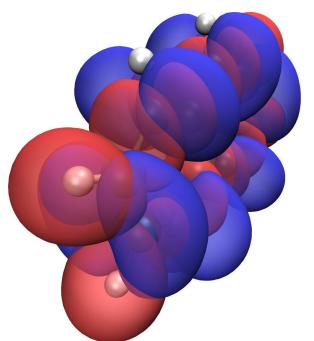
X/Y plane



X/Z plane



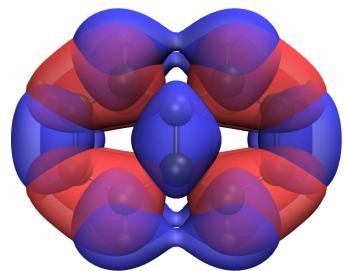
Z/Y plane



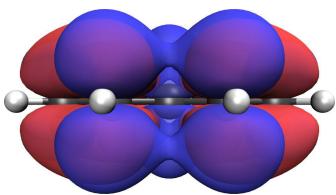
45° to axes

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

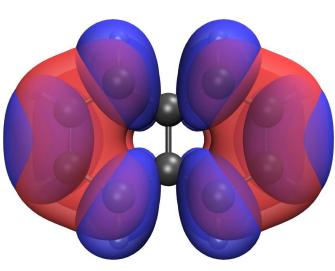
S(9), S(10) Natural Transition Orbitals



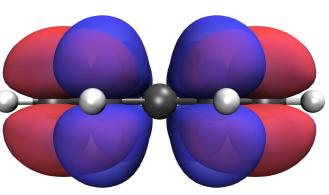
X/Y plane



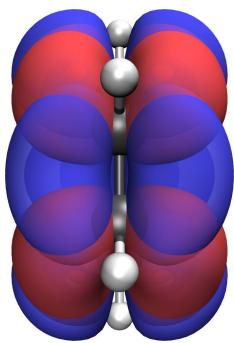
X/Z plane



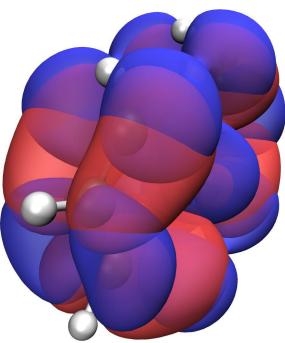
X/Y plane



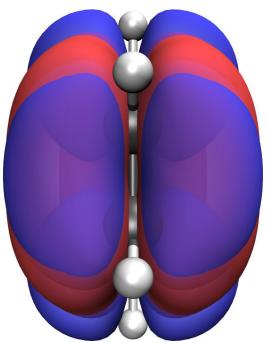
X/Z plane



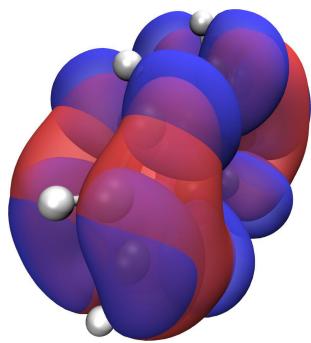
Z/Y plane



45° to axes



Z/Y plane



45° to axes

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

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

Naphthalene - Optimisation, Excited States (Singlet)

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
50	LUMO+15	B1u	8.1699
49	LUMO+14	Ag	7.5952
48	LUMO+13	B1u	6.7778
47	LUMO+12	B3g	5.9990
46	LUMO+11	B2g	5.5762
45	LUMO+10	B2u	5.3781
44	LUMO+9	B1u	5.0300
43	LUMO+8	B3g	4.9791
42	LUMO+7	Ag	4.8912
41	LUMO+6	B1u	3.6510
40	LUMO+5	B2u	3.4316
39	LUMO+4	Au	2.9611
38	LUMO+3	Ag	2.7511
37	LUMO+2	B3u	1.1233
36	LUMO+1	B2g	-0.2495
35	LUMO	B1g	-1.0705
34	HOMO	Au	-6.0510
33	HOMO-1	B3u	-6.8303
32	HOMO-2	B2g	-8.1286
31	HOMO-3	Ag	-9.1077
30	HOMO-4	B1g	-9.1332
29	HOMO-5	B3g	-9.5185
28	HOMO-6	B2u	-10.2990
27	HOMO-7	B3u	-10.8971
26	HOMO-8	B1u	-11.1471
25	HOMO-9	B2u	-11.5760
24	HOMO-10	B3g	-11.6334
23	HOMO-11	Ag	-12.1597
22	HOMO-12	B1u	-12.5284
21	HOMO-13	Ag	-13.7186
20	HOMO-14	B3g	-14.2688
19	HOMO-15	B2u	-14.3711

Naphthalene - Optimisation, Excited States (Singlet)

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2400390	-1.4125330	0.0000000
C	-2.4491680	-0.7114860	0.0000000
C	-2.4491680	0.7114860	0.0000000
C	-1.2400390	1.4125330	-0.0000000
C	0.0000000	0.7408730	-0.0000000
C	0.0000000	-0.7408730	0.0000000
C	1.2400390	-1.4125330	0.0000000
C	1.2400390	1.4125330	-0.0000000
C	2.4491680	0.7114860	-0.0000000
C	2.4491680	-0.7114860	-0.0000000
H	-1.2436630	-2.4992410	0.0000000
H	-3.3898840	-1.2513480	0.0000000
H	-3.3898840	1.2513480	0.0000000
H	-1.2436630	2.4992410	-0.0000000
H	1.2436630	-2.4992410	0.0000000
H	1.2436630	2.4992410	-0.0000000
H	3.3898840	1.2513480	-0.0000000
H	3.3898840	-1.2513480	-0.0000000

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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