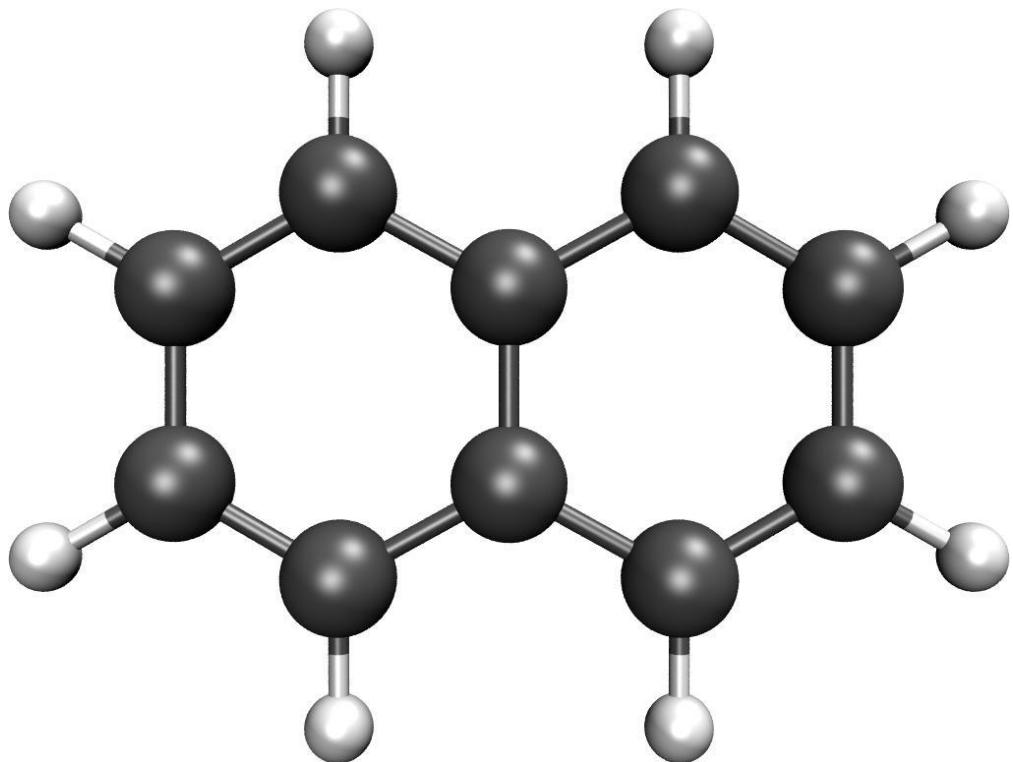


Calculation Report

Naphthalene

Excited States (Singlet, Triplet)



Summary of Results

Metadata		SCF Energies	Geometry	
Username:	osl	No. of steps: 1	Formula:	C ₁₀ H ₈
Date:	07/06/2022 16:48:19	Final energy: -10488.9903 eV	Exact mass:	128.0626 g mol ⁻¹
Duration:	4 m, 21 s	Final energy: -1,012,034 kJ mol ⁻¹	Molar mass:	128.1705 g mol ⁻¹
Success:	True		Alignment method:	Minimal
Computational package:	Gaussian (2016+C.01)		X extension:	6.74 Å
Methods:	DFT		Y extension:	4.97 Å
Functional:	PBE1PBE		Z extension:	0.00 Å
Basis set:	6-31G(d,p)		Linearity ratio:	0.26
Calculations:	Excited States		Planarity ratio:	1.00
Orbital spin:	restricted			
Multiplicity:	1 (singlet)			

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 (S₁) Dipole Moment

Total: 0.07 D

X axis angle: 0.00 °

XY plane angle: 0.00 °

Spin-Orbit Coupling

<S₀|H_{SO}|T₁>: 0.00 cm⁻¹

<S₀|\lambda|T₁>: 0.00

<S₁|H_{SO}|T₁>: 1.28 cm⁻¹

<S₁|\lambda|T₁>: 0.00

Excited States

ΔE_{ST}: 1.62 eV

S₁ energy: 4.65 eV

S₁ wavelength: 266 nm

S₁ colour: Ultraviolet 

S₁ CIE (x,y): (0.00, 0.00)

S₁ oscillator strength: 0.00

T₁ energy: 3.03 eV

T₁ wavelength: 409 nm

T₁ colour: Violet 

T₁ CIE (x,y): (0.17, 0.00)

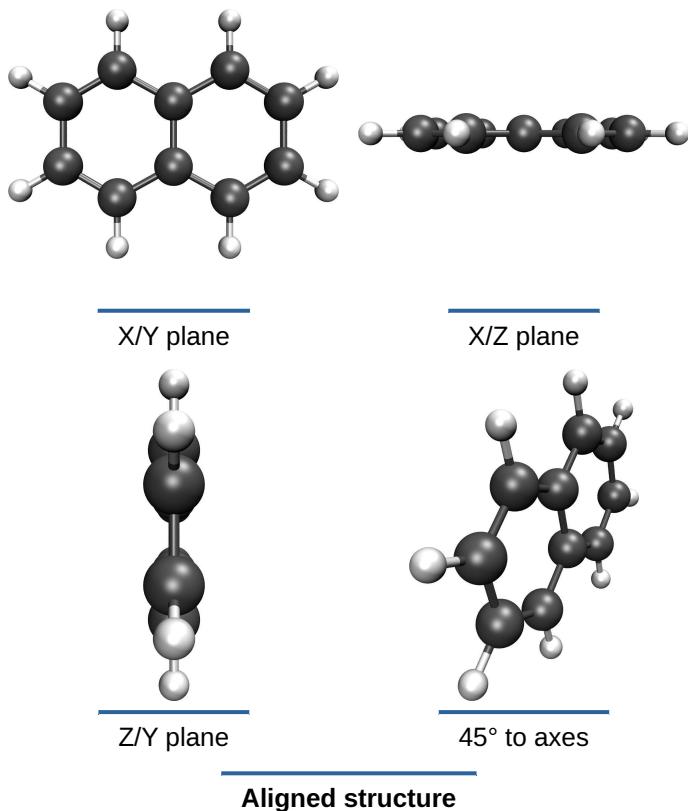
T₁ oscillator strength: 0.00

No. of singlets: 10

No. of triplets: 10

Naphthalene - Excited States (Singlet, Triplet)

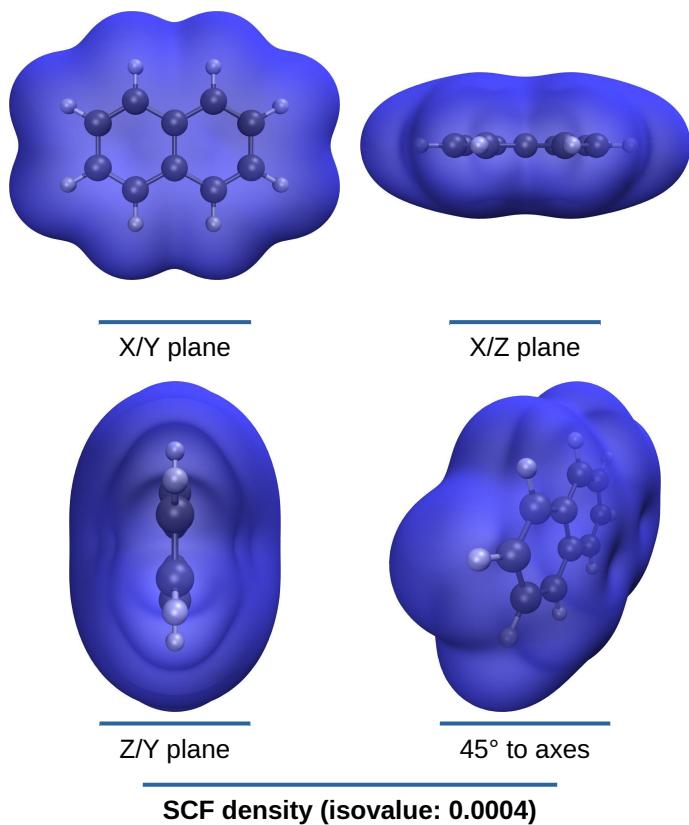
Geometry



Geometry

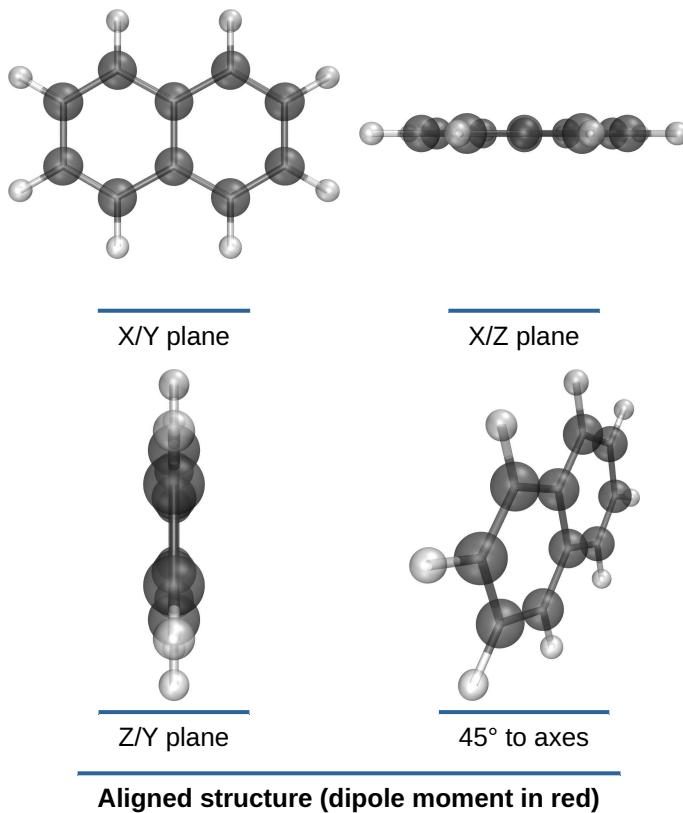
Formula: C₁₀H₈
Exact mass: 128.0626 g mol⁻¹
Molar mass: 128.1705 g mol⁻¹
Alignment method: Minimal
X extension: 6.74 Å
Y extension: 4.97 Å
Z extension: 0.00 Å
Linearity ratio: 0.26
Planarity ratio: 1.00

SCF Density



Naphthalene - Excited States (Singlet, Triplet)

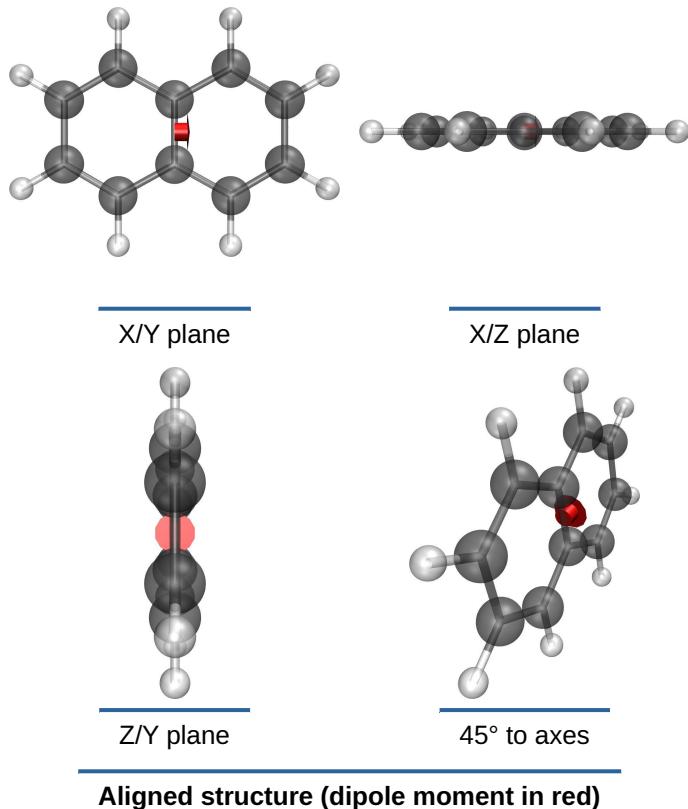
Permanent Dipole Moment



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

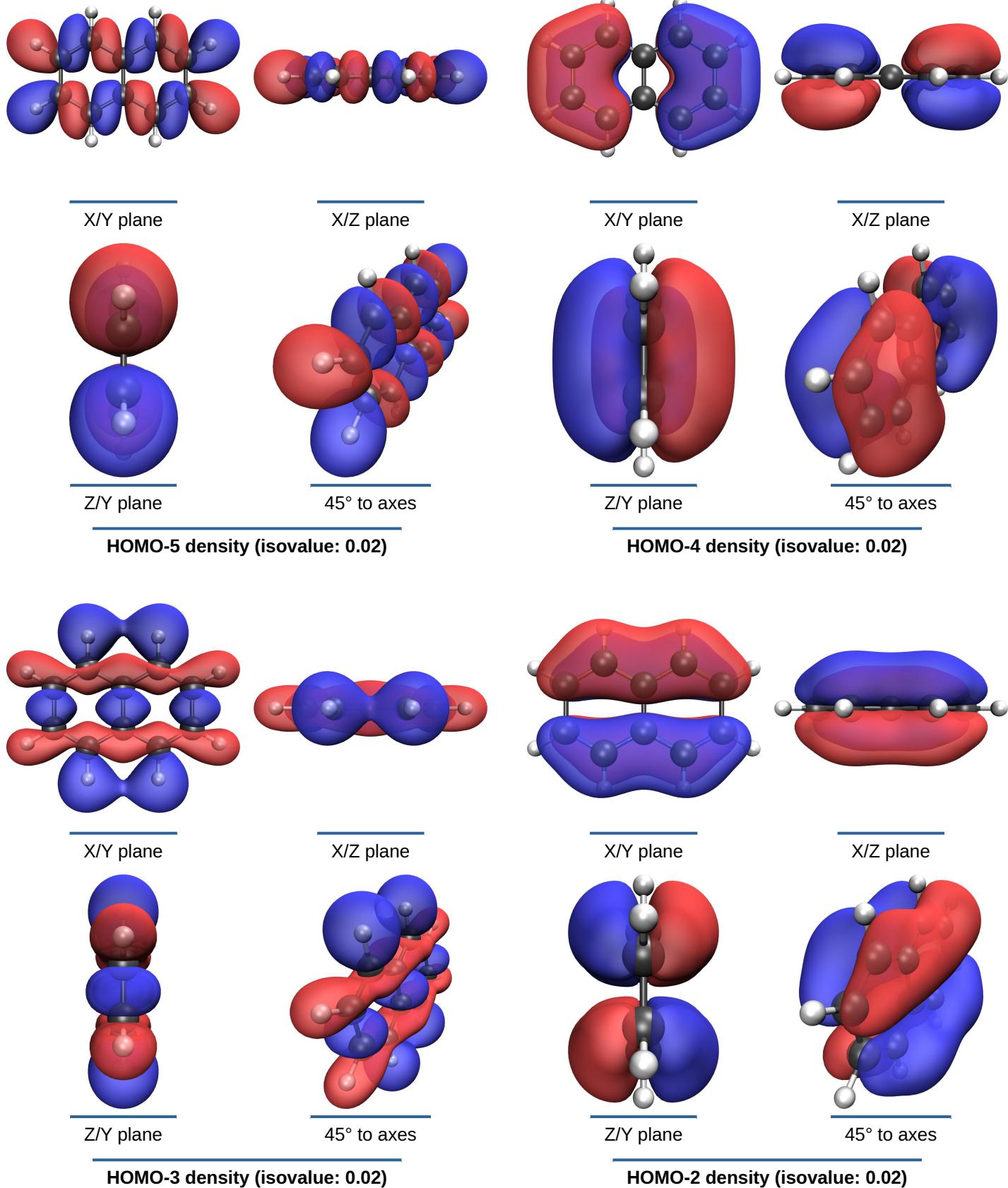


Dipole Moment

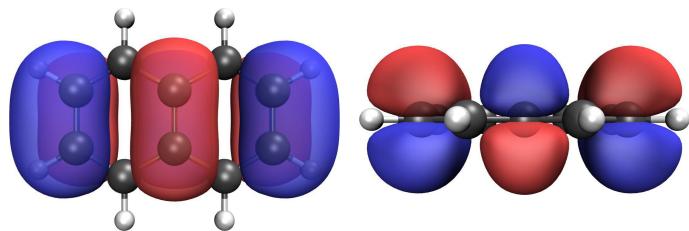
Origin X: 0.00 D
Origin Y: 0.00 D
Origin Z: 0.00 D
Vector X: 0.07 D
Vector Y: -0.00 D
Vector Z: -0.00 D
Total: 0.07 D
X axis angle: 0.00 °
XY plane angle: 0.00 °

Naphthalene - Excited States (Singlet, Triplet)

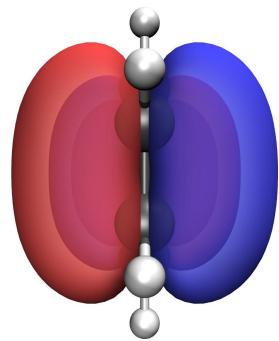
HOMO-5, HOMO-4, HOMO-3, HOMO-2



HOMO-1

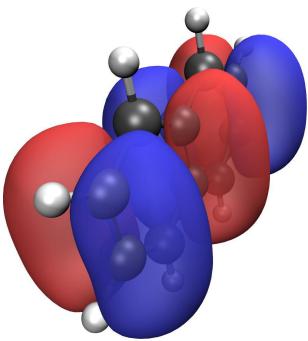


X/Y plane



Z/Y plane

X/Z plane

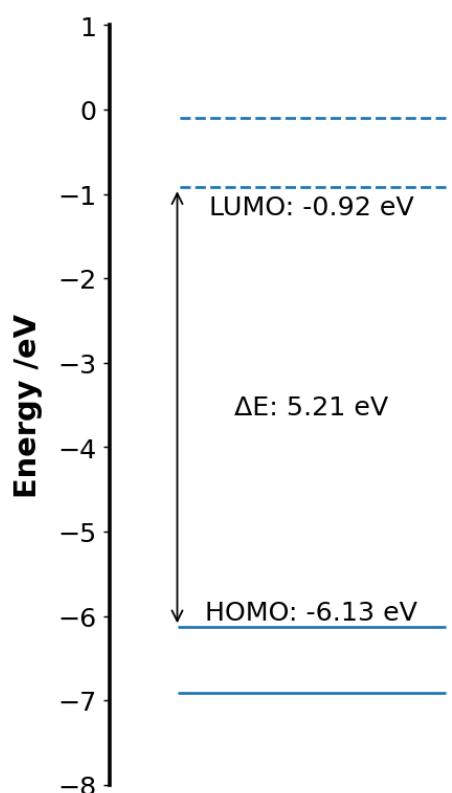
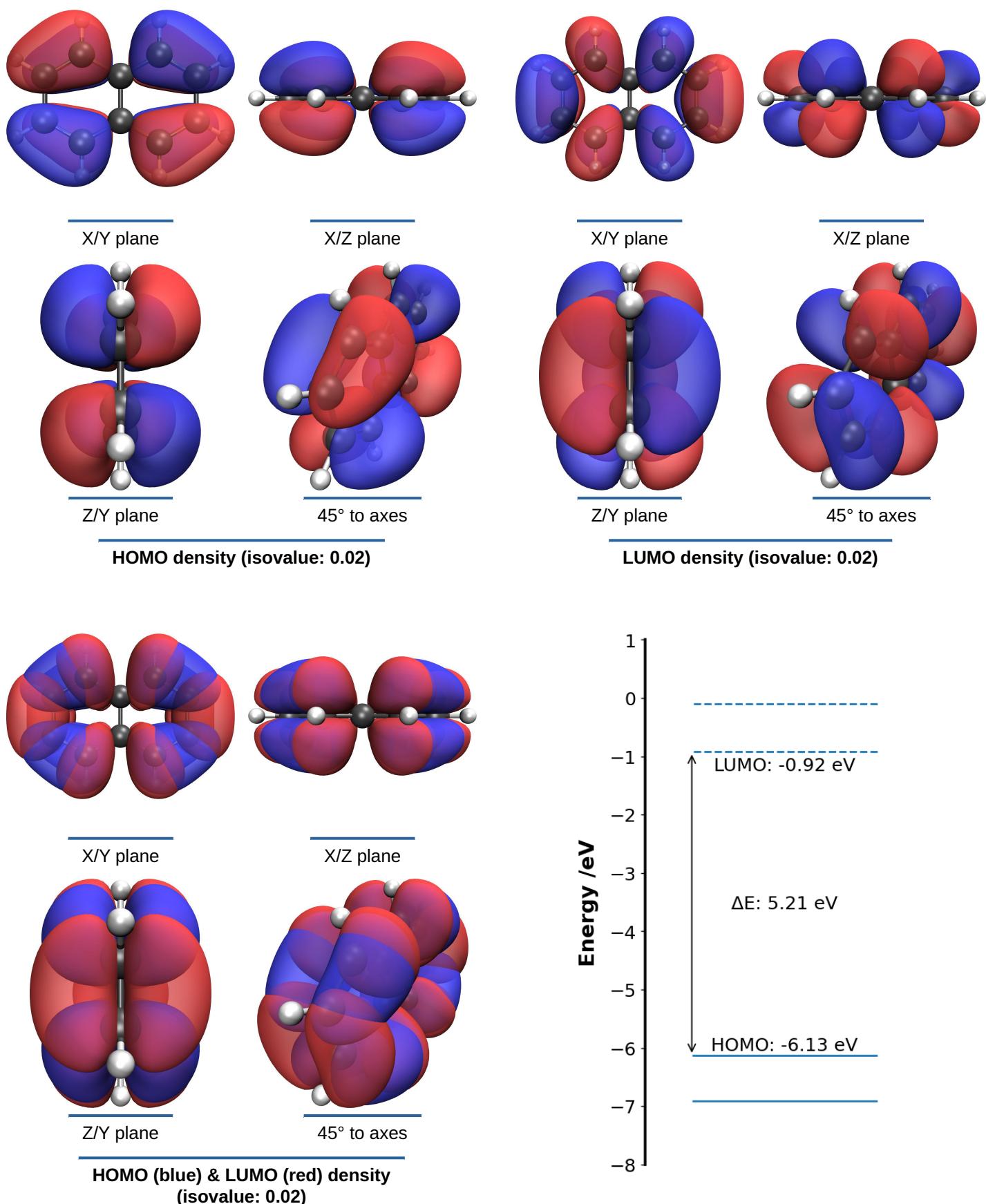


45° to axes

HOMO-1 density (isovalue: 0.02)

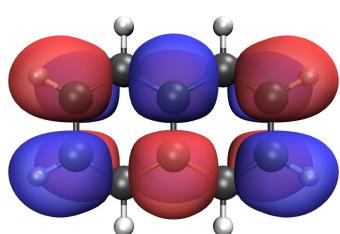
Naphthalene - Excited States (Singlet, Triplet)

HOMO & LUMO

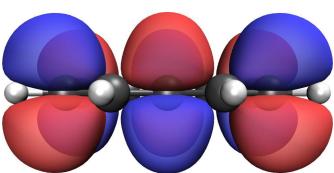


Naphthalene - Excited States (Singlet, Triplet)

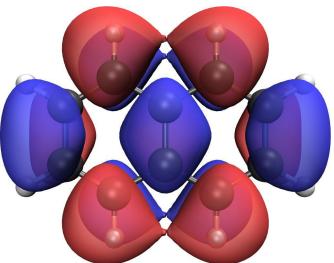
LUMO+1, LUMO+2, LUMO+4



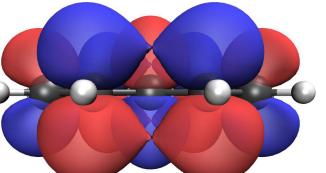
X/Y plane



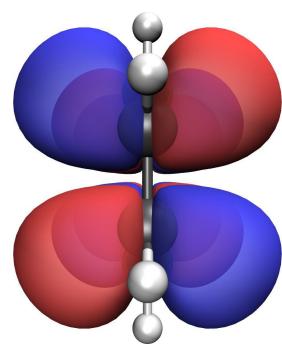
X/Z plane



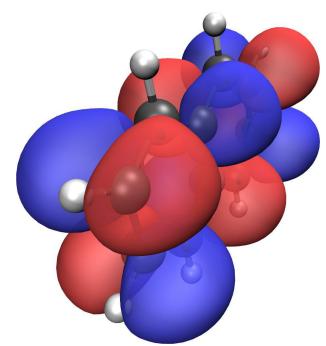
X/Y plane



X/Z plane

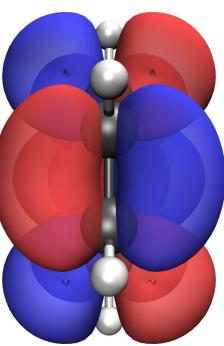


Z/Y plane

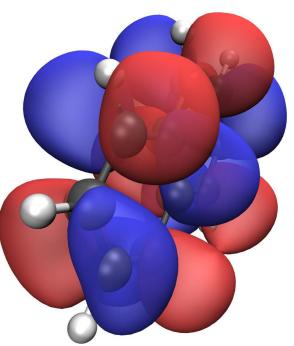


45° to axes

LUMO+1 density (isovalue: 0.02)

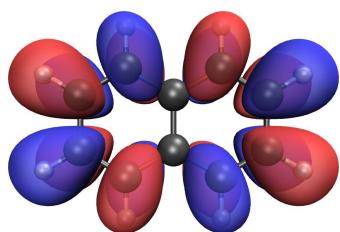


Z/Y plane

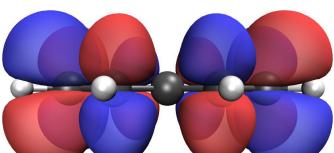


45° to axes

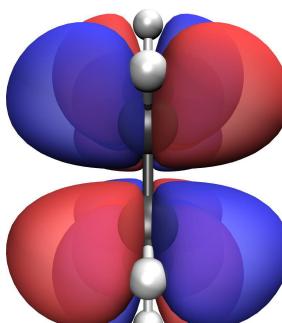
LUMO+2 density (isovalue: 0.02)



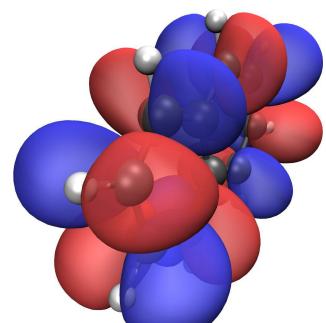
X/Y plane



X/Z plane



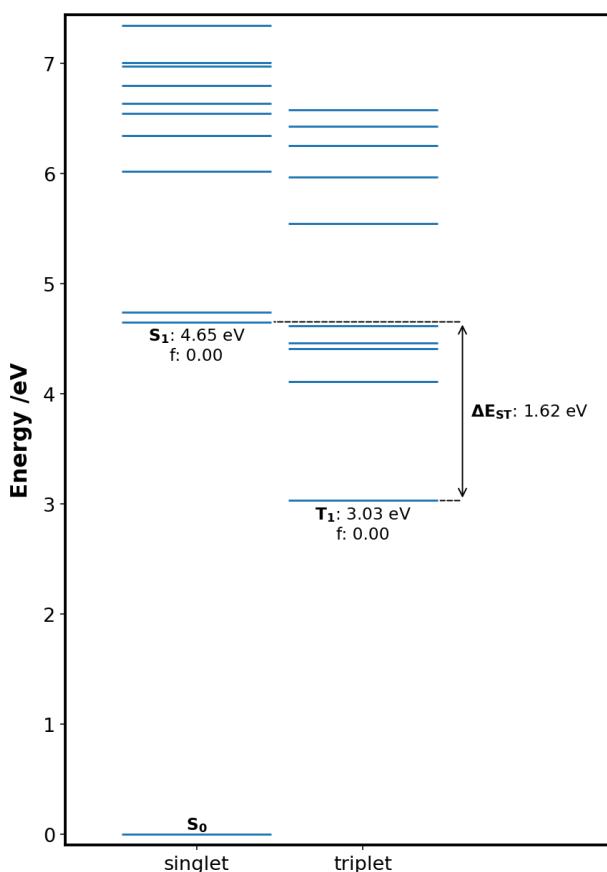
Z/Y plane



45° to axes

LUMO+4 density (isovalue: 0.02)

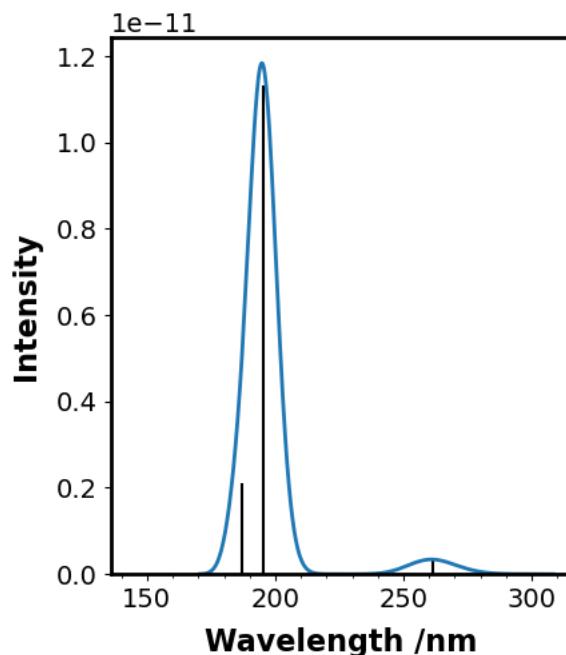
Excited States



Excited States

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.

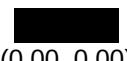
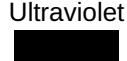
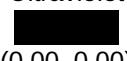
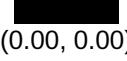
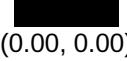
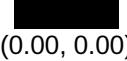
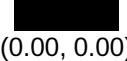
Note: high energy absorption peaks are not simulated.
For a complete absorption spectrum, use more excited states.

Naphthalene - Excited States (Singlet, Triplet)

Table of Excited States

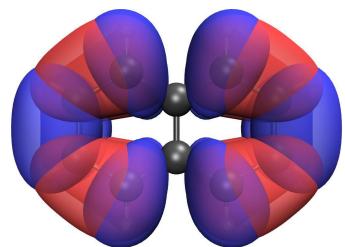
Level	Symbol	Symmetry	Energy /eV	Wavelength /nm	Colour, CIE (x,y)	Oscillator Strength	Transitions (probability)
1	T ₁	Triplet-B1U	3.0294	409.27	Violet (0.17, 0.00)	0.0000	HOMO → LUMO (0.92) HOMO-2 → LUMO+2 (0.03) HOMO-1 → LUMO+1 (0.03)
2	T ₂	Triplet-B2U	4.1078	301.83	Ultraviolet (0.00, 0.00)	0.0000	HOMO-1 → 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 - Excited States (Singlet, Triplet)

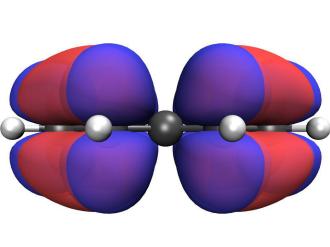
					Ultraviolet  (0.00, 0.00)		HOMO-4 → LUMO (0.04)
15	T ₁₀	Triplet-B1G	6.5767	188.52	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.98)
16	S ₆	Singlet-B1U	6.6348	186.87	Ultraviolet  (0.00, 0.00)	0.3684	HOMO-1 → LUMO+1 (0.86) HOMO-2 → LUMO+2 (0.07) HOMO → LUMO (0.04)
17	S ₇	Singlet-B1G	6.7955	182.45	Ultraviolet  (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)

Naphthalene - Excited States (Singlet, Triplet)

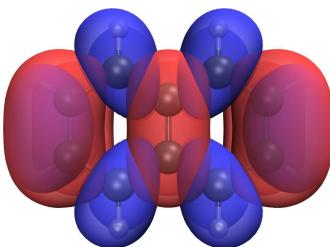
T(1), T(2), T(3), T(4) Natural Transition Orbitals



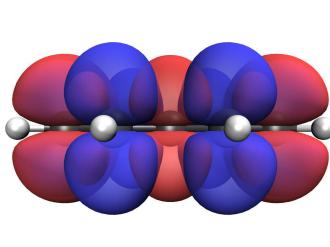
X/Y plane



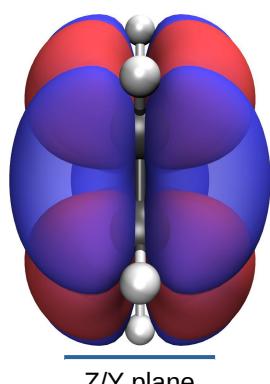
X/Z plane



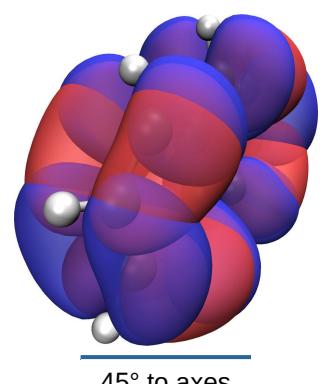
X/Y plane



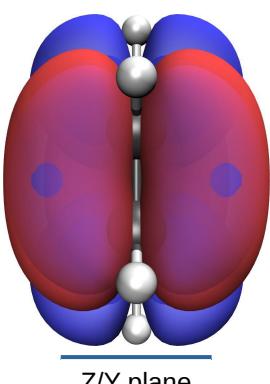
X/Z plane



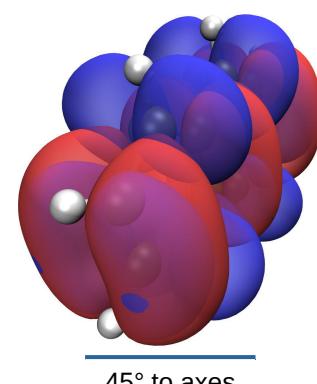
Z/Y plane



45° to axes



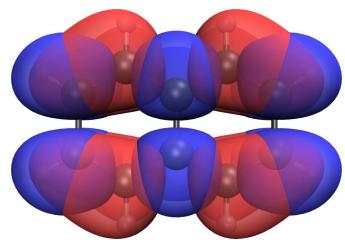
Z/Y plane



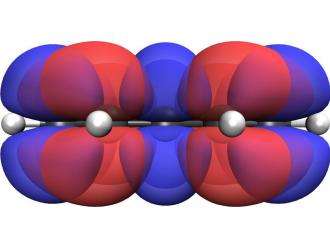
45° to axes

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

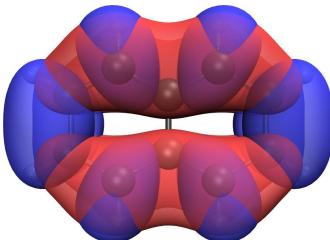
T(2) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



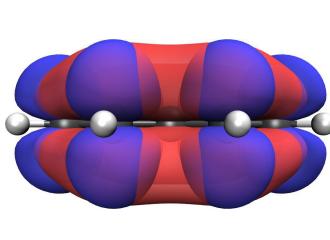
X/Y plane



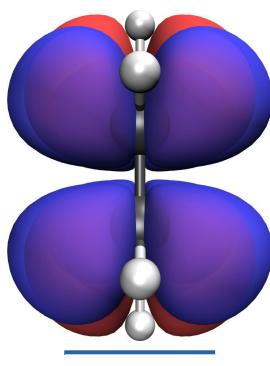
X/Z plane



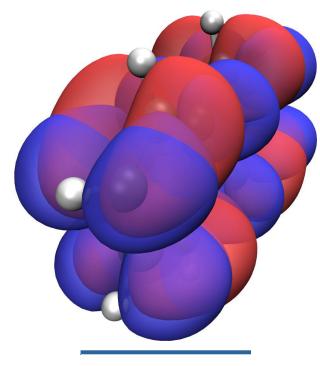
X/Y plane



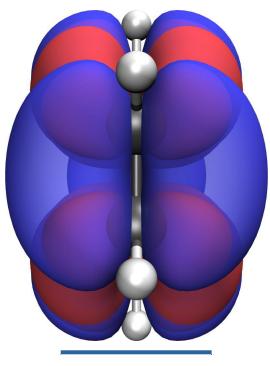
X/Z plane



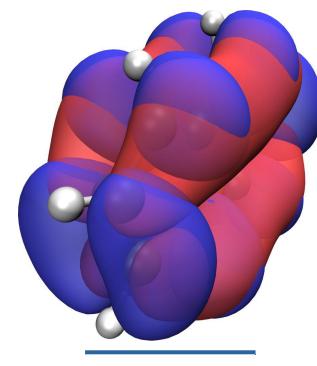
Z/Y plane



45° to axes



Z/Y plane



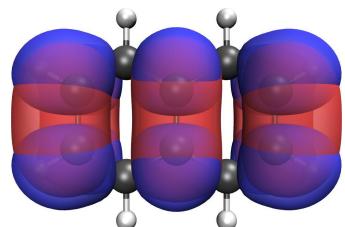
45° to axes

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

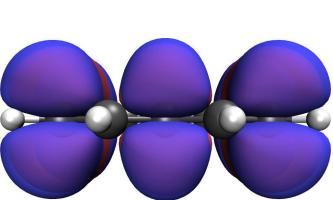
T(4) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Naphthalene - Excited States (Singlet, Triplet)

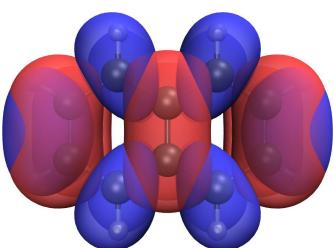
T(5), S(1), S(2), T(6) Natural Transition Orbitals



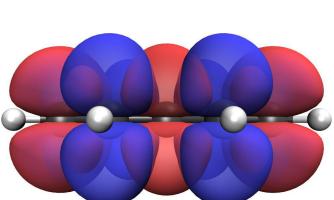
X/Y plane



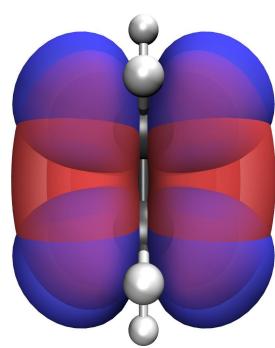
X/Z plane



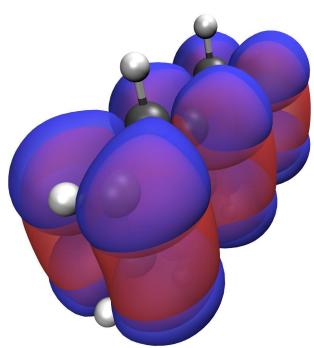
X/Y plane



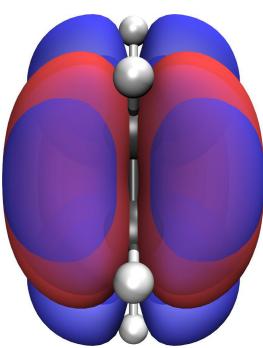
X/Z plane



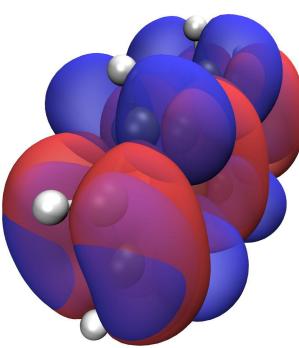
Z/Y plane



45° to axes



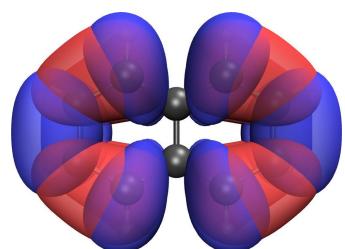
Z/Y plane



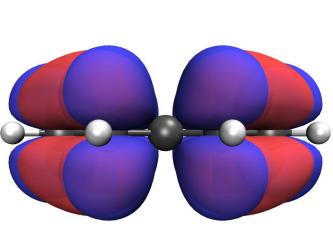
45° to axes

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

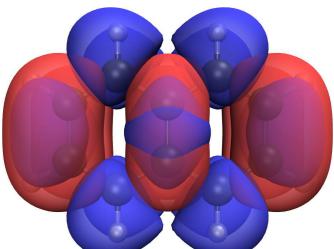
S(1) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



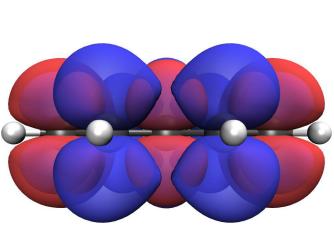
X/Y plane



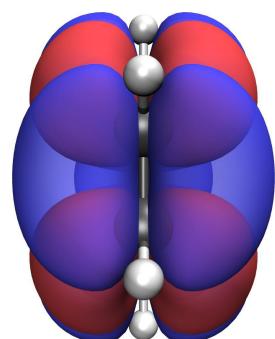
X/Z plane



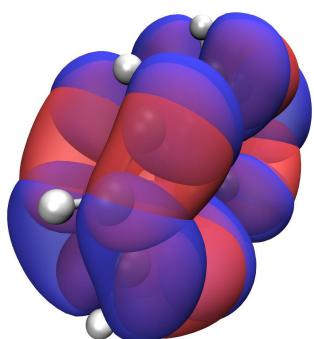
X/Y plane



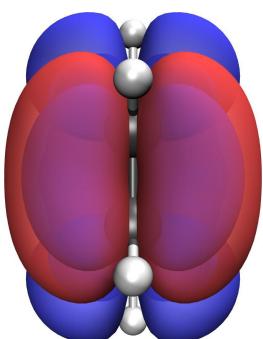
X/Z plane



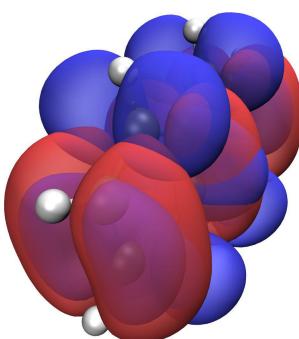
Z/Y plane



45° to axes



Z/Y plane



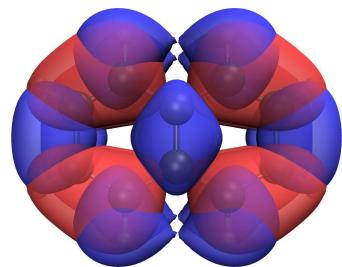
45° to axes

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

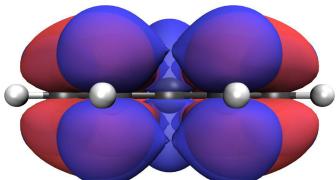
T(6) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Naphthalene - Excited States (Singlet, Triplet)

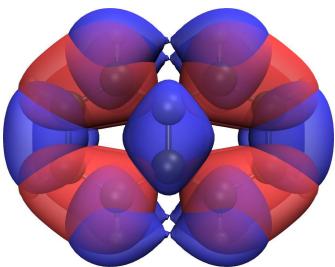
T(7), S(3), T(8), S(4) Natural Transition Orbitals



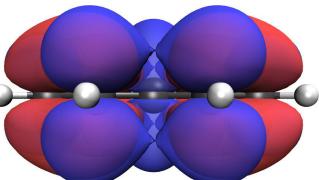
X/Y plane



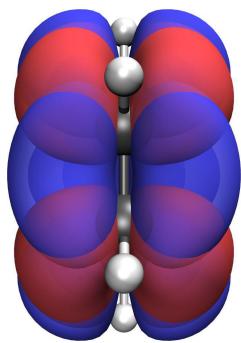
X/Z plane



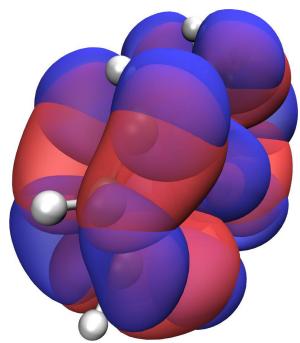
X/Y plane



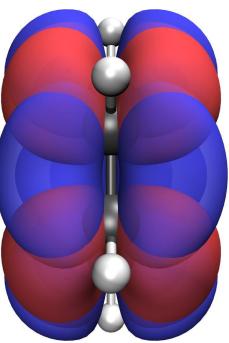
X/Z plane



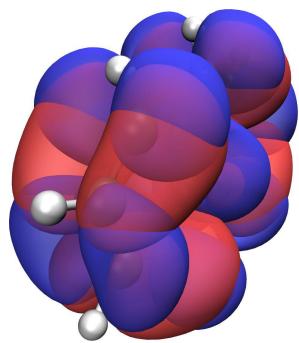
Z/Y plane



45° to axes



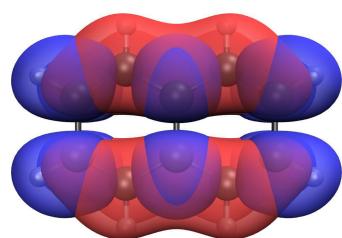
Z/Y plane



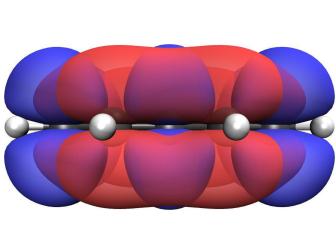
45° to axes

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

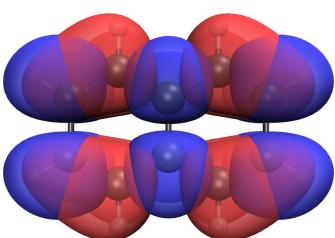
S(3) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



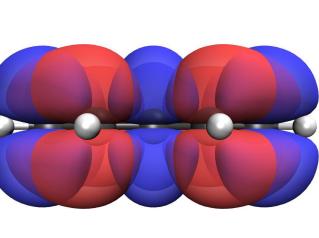
X/Y plane



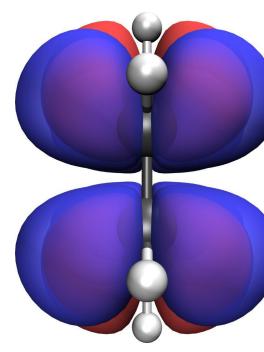
X/Z plane



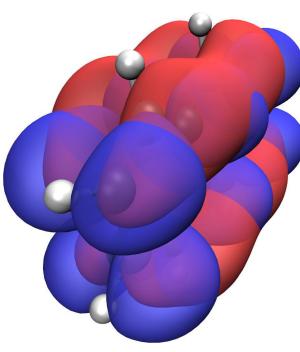
X/Y plane



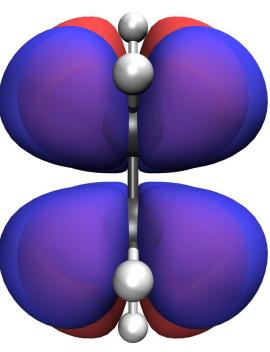
X/Z plane



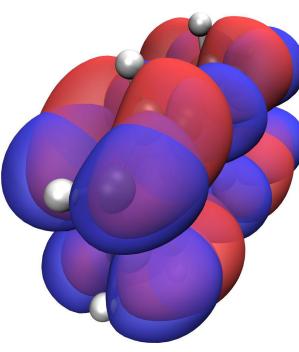
Z/Y plane



45° to axes



Z/Y plane



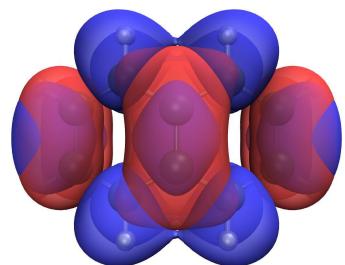
45° to axes

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

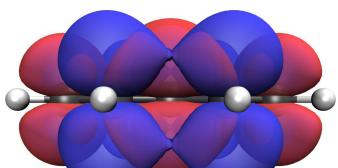
S(4) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Naphthalene - Excited States (Singlet, Triplet)

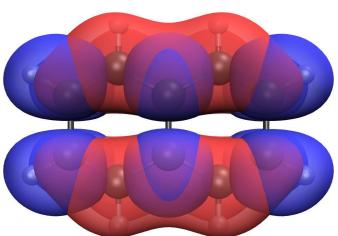
T(9), S(5), T(10), S(6) Natural Transition Orbitals



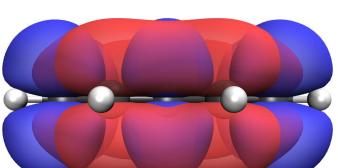
X/Y plane



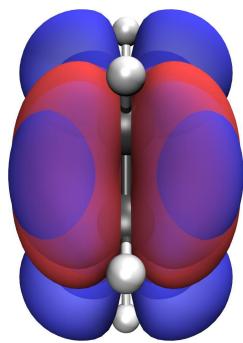
X/Z plane



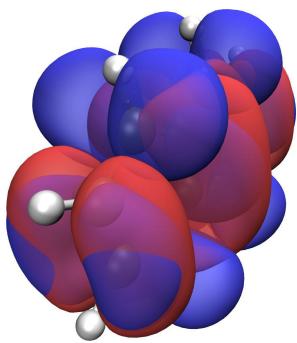
X/Y plane



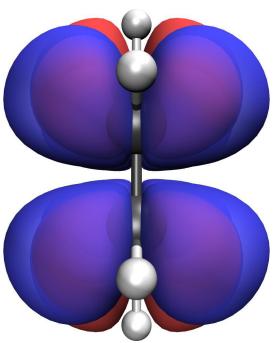
X/Z plane



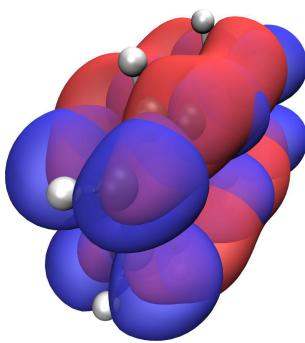
Z/Y plane



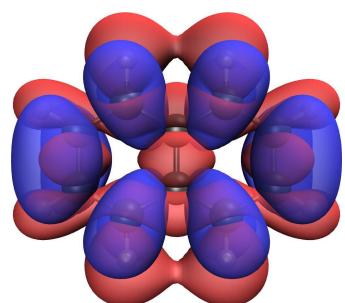
45° to axes



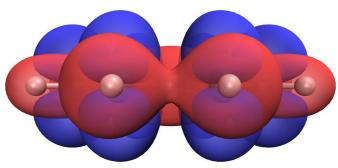
Z/Y plane



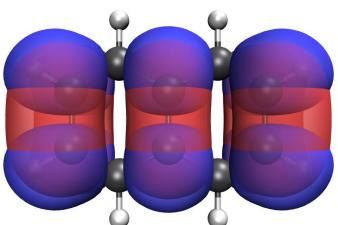
45° to axes

T(9) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)**S(5) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)**

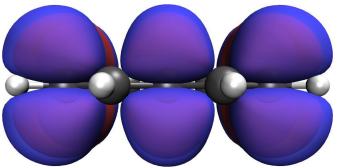
X/Y plane



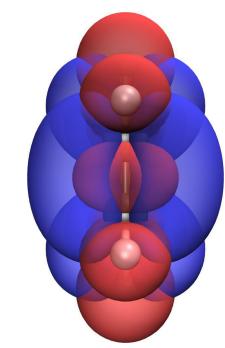
X/Z plane



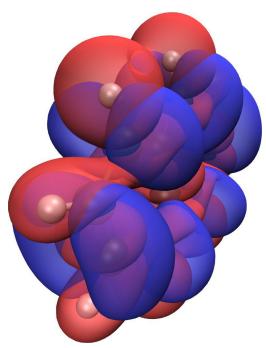
X/Y plane



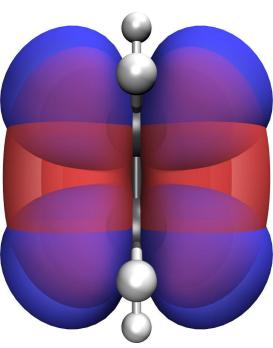
X/Z plane



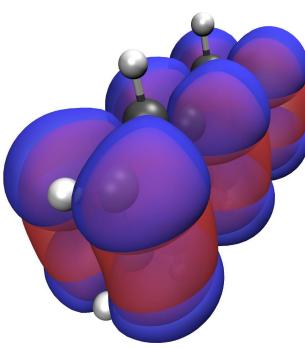
Z/Y plane



45° to axes



Z/Y plane

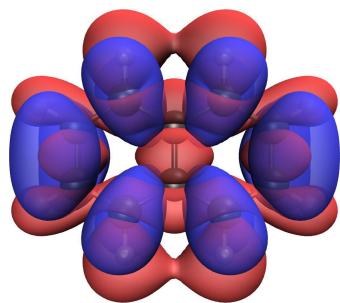


45° to axes

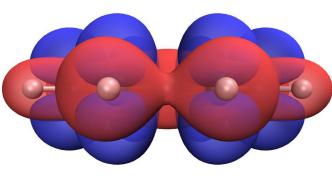
T(10) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)**S(6) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)**

Naphthalene - Excited States (Singlet, Triplet)

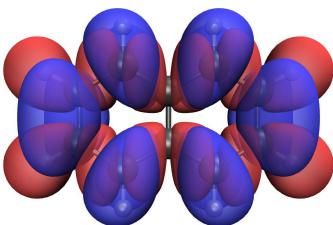
S(7), S(8), S(9), S(10) Natural Transition Orbitals



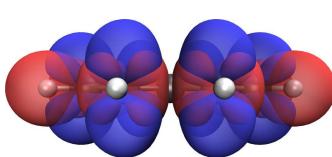
X/Y plane



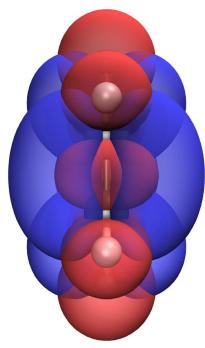
X/Z plane



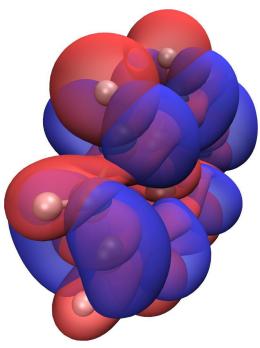
X/Y plane



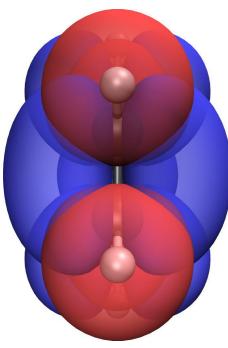
X/Z plane



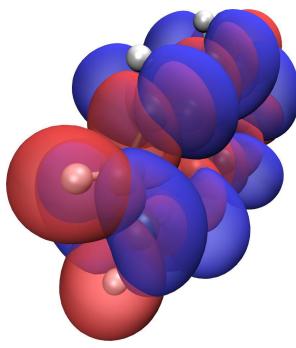
Z/Y plane



45° to axes



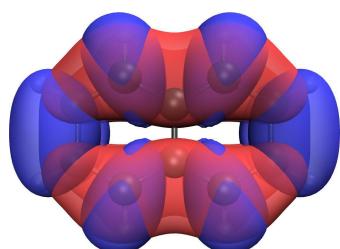
Z/Y plane



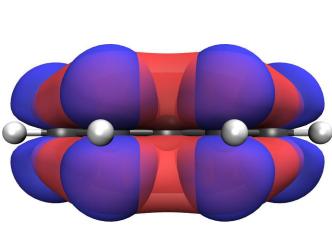
45° to axes

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

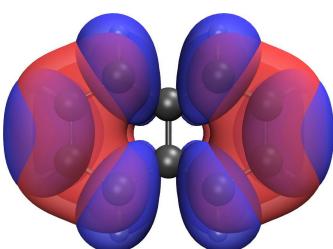
S(8) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



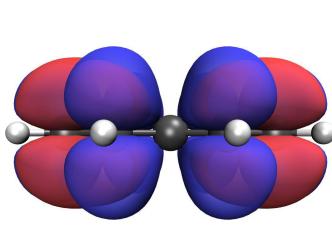
X/Y plane



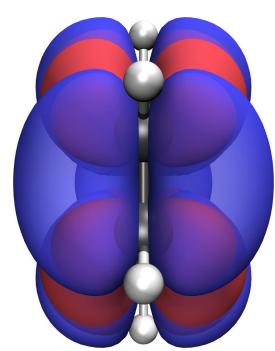
X/Z plane



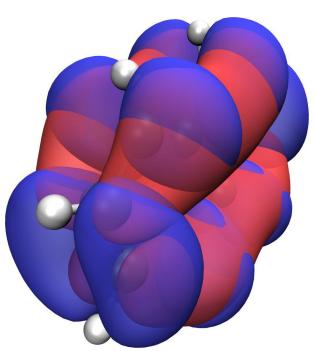
X/Y plane



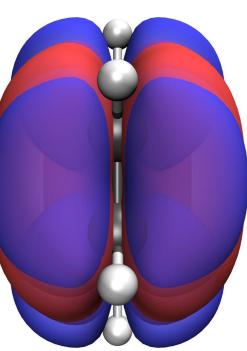
X/Z plane



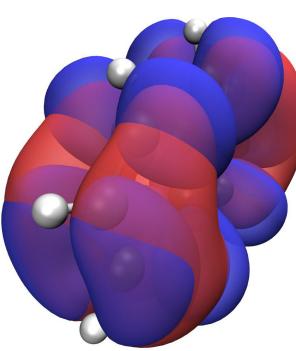
Z/Y plane



45° to axes



Z/Y plane



45° to axes

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

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

Naphthalene - Excited States (Singlet, Triplet)

Table of Spin-Orbit Coupling

Singlet	Triplet	SOC +1 /cm ⁻¹	SOC 0 /cm ⁻¹	SOC -1 /cm ⁻¹	SOC Root		First Order
					Sum Square /cm ⁻¹	H _{SO} /eV	Mixing Coefficient
S ₀	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	3.0294 0.0000
S ₀	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	4.1078 0.0000
S ₀	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	4.4060 0.0000
S ₀	T ₄	0.4874	0.0000	0.4874	0.6892	0.0001	4.4608 0.0000
S ₀	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	4.6180 0.0000
S ₀	T ₆	0.0000	0.0000	0.0000	0.0000	0.0000	5.5459 0.0000
S ₀	T ₇	0.2331	0.0000	0.2331	0.3297	0.0000	5.9643 0.0000
S ₀	T ₈	0.0000	0.0000	0.0000	0.0000	0.0000	6.2558 0.0000
S ₀	T ₉	0.0000	0.0000	0.0000	0.0000	0.0000	6.4283 0.0000
S ₀	T ₁₀	0.0000	2.3162	0.0000	2.3162	0.0003	6.5767 0.0000
S ₁	T ₁	0.9053	0.0000	0.9053	1.2803	0.0002	1.6231 0.0001
S ₁	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	0.5447 0.0000
S ₁	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	0.2465 0.0000
S ₁	T ₄	0.0000	0.0000	0.0000	0.0000	0.0000	0.1917 0.0000
S ₁	T ₅	0.6095	0.0000	0.6095	0.8620	0.0001	0.0345 0.0031
S ₁	T ₆	0.0000	0.0000	0.0000	0.0000	0.0000	0.8934 0.0000
S ₁	T ₇	0.0000	0.0000	0.0000	0.0000	0.0000	1.3118 0.0000
S ₁	T ₈	0.0000	0.0000	0.0000	0.0000	0.0000	1.6033 0.0000
S ₁	T ₉	0.0000	0.0000	0.0000	0.0000	0.0000	1.7758 0.0000
S ₁	T ₁₀	0.0000	0.0000	0.0000	0.0000	0.0000	1.9242 0.0000
S ₂	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	1.7093 0.0000
S ₂	T ₂	0.0688	0.0000	0.0688	0.0972	0.0000	0.6309 0.0000
S ₂	T ₃	0.9798	0.0000	0.9798	1.3857	0.0002	0.3327 0.0005
S ₂	T ₄	0.0000	0.0000	0.0000	0.0000	0.0000	0.2779 0.0000
S ₂	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	0.1207 0.0000
S ₂	T ₆	0.0000	0.0000	0.0000	0.0000	0.0000	0.8072 0.0000
S ₂	T ₇	0.0000	0.0000	0.0000	0.0000	0.0000	1.2256 0.0000
S ₂	T ₈	0.0000	0.0000	0.0000	0.0000	0.0000	1.5171 0.0000
S ₂	T ₉	0.0000	0.0000	0.0000	0.0000	0.0000	1.6896 0.0000

Naphthalene - Excited States (Singlet, Triplet)

S ₂	T ₁₀	0.0000	0.0000	0.0000	0.0000	0.0000	1.8380	0.0000
S ₃	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	2.9891	0.0000
S ₃	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	1.9107	0.0000
S ₃	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	1.6125	0.0000
S ₃	T ₄	0.0000	0.0000	0.0000	0.0000	0.0000	1.5577	0.0000
S ₃	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	1.4005	0.0000
S ₃	T ₆	0.1916	0.0000	0.1916	0.2709	0.0000	0.4726	0.0001
S ₃	T ₇	0.0000	0.0000	0.0000	0.0000	0.0000	0.0542	0.0000
S ₃	T ₈	0.2373	0.0000	0.2373	0.3356	0.0000	0.2373	0.0002
S ₃	T ₉	0.5620	0.0000	0.5620	0.7948	0.0001	0.4098	0.0002
S ₃	T ₁₀	0.5588	0.0000	0.5588	0.7903	0.0001	0.5582	0.0002
S ₄	T ₁	0.1830	0.0000	0.1830	0.2587	0.0000	3.3125	0.0000
S ₄	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	2.2341	0.0000
S ₄	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	1.9359	0.0000
S ₄	T ₄	0.0000	0.0000	0.0000	0.0000	0.0000	1.8811	0.0000
S ₄	T ₅	0.2596	0.0000	0.2596	0.3672	0.0000	1.7239	0.0000
S ₄	T ₆	0.0000	0.0000	0.0000	0.0000	0.0000	0.7960	0.0000
S ₄	T ₇	0.0000	0.0000	0.0000	0.0000	0.0000	0.3776	0.0000
S ₄	T ₈	0.0000	0.0000	0.0000	0.0000	0.0000	0.0861	0.0000
S ₄	T ₉	0.0000	0.0000	0.0000	0.0000	0.0000	0.0864	0.0000
S ₄	T ₁₀	0.0000	0.0000	0.0000	0.0000	0.0000	0.2348	0.0000
S ₅	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	3.5169	0.0000
S ₅	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	2.4385	0.0000
S ₅	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	2.1403	0.0000
S ₅	T ₄	0.6743	0.0000	0.6743	0.9535	0.0001	2.0855	0.0001
S ₅	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	1.9283	0.0000
S ₅	T ₆	0.0000	0.0000	0.0000	0.0000	0.0000	1.0004	0.0000
S ₅	T ₇	0.1548	0.0000	0.1548	0.2190	0.0000	0.5820	0.0000
S ₅	T ₈	0.0000	0.0000	0.0000	0.0000	0.0000	0.2905	0.0000
S ₅	T ₉	0.0000	0.0000	0.0000	0.0000	0.0000	0.1180	0.0000
S ₅	T ₁₀	0.0000	0.4049	0.0000	0.4049	0.0001	0.0304	0.0017
S ₆	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	3.6054	0.0000

Naphthalene - Excited States (Singlet, Triplet)

S ₆	T ₂	0.3120	0.0000	0.3120	0.4413	0.0001	2.5270	0.0000
S ₆	T ₃	0.5747	0.0000	0.5747	0.8127	0.0001	2.2288	0.0000
S ₆	T ₄	0.0000	0.0000	0.0000	0.0000	0.0000	2.1740	0.0000
S ₆	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	2.0168	0.0000
S ₆	T ₆	0.0000	0.0000	0.0000	0.0000	0.0000	1.0889	0.0000
S ₆	T ₇	0.0000	0.0000	0.0000	0.0000	0.0000	0.6705	0.0000
S ₆	T ₈	0.0000	0.0000	0.0000	0.0000	0.0000	0.3790	0.0000
S ₆	T ₉	0.0000	0.0000	0.0000	0.0000	0.0000	0.2065	0.0000
S ₆	T ₁₀	0.0000	0.0000	0.0000	0.0000	0.0000	0.0581	0.0000
S ₇	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	3.7661	0.0000
S ₇	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	2.6877	0.0000
S ₇	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	2.3895	0.0000
S ₇	T ₄	0.5456	0.0000	0.5456	0.7716	0.0001	2.3347	0.0000
S ₇	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	2.1775	0.0000
S ₇	T ₆	0.0000	0.6770	0.0000	0.6770	0.0001	1.2496	0.0001
S ₇	T ₇	0.4784	0.0000	0.4784	0.6766	0.0001	0.8312	0.0001
S ₇	T ₈	0.0000	0.3760	0.0000	0.3760	0.0000	0.5397	0.0001
S ₇	T ₉	0.0000	0.5478	0.0000	0.5478	0.0001	0.3672	0.0002
S ₇	T ₁₀	0.0000	0.0000	0.0000	0.0000	0.0000	0.2188	0.0000
S ₈	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	3.9465	0.0000
S ₈	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	2.8681	0.0000
S ₈	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	2.5699	0.0000
S ₈	T ₄	0.0000	1.1728	0.0000	1.1728	0.0001	2.5151	0.0001
S ₈	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	2.3579	0.0000
S ₈	T ₆	0.5129	0.0000	0.5129	0.7254	0.0001	1.4300	0.0001
S ₈	T ₇	0.0000	1.0010	0.0000	1.0010	0.0001	1.0116	0.0001
S ₈	T ₈	0.1853	0.0000	0.1853	0.2620	0.0000	0.7201	0.0000
S ₈	T ₉	0.3888	0.0000	0.3888	0.5498	0.0001	0.5476	0.0001
S ₈	T ₁₀	9.6592	0.0000	9.6592	13.6602	0.0017	0.3992	0.0042
S ₉	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	3.9767	0.0000
S ₉	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	2.8983	0.0000
S ₉	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	2.6001	0.0000

Naphthalene - Excited States (Singlet, Triplet)

S ₉	T ₄	0.0000	0.0000	0.0000	0.0000	0.0000	2.5453	0.0000
S ₉	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	2.3881	0.0000
S ₉	T ₆	0.0733	0.0000	0.0733	0.1037	0.0000	1.4602	0.0000
S ₉	T ₇	0.0000	0.0000	0.0000	0.0000	0.0000	1.0418	0.0000
S ₉	T ₈	0.7368	0.0000	0.7368	1.0420	0.0001	0.7503	0.0002
S ₉	T ₉	0.0056	0.0000	0.0056	0.0079	0.0000	0.5778	0.0000
S ₉	T ₁₀	0.0629	0.0000	0.0629	0.0889	0.0000	0.4294	0.0000
S ₁₀	T ₁	0.0000	0.0000	0.0000	0.0000	0.0000	4.3144	0.0000
S ₁₀	T ₂	0.0000	0.0000	0.0000	0.0000	0.0000	3.2360	0.0000
S ₁₀	T ₃	0.0000	0.0000	0.0000	0.0000	0.0000	2.9378	0.0000
S ₁₀	T ₄	0.2396	0.0000	0.2396	0.3389	0.0000	2.8830	0.0000
S ₁₀	T ₅	0.0000	0.0000	0.0000	0.0000	0.0000	2.7258	0.0000
S ₁₀	T ₆	0.0000	0.0000	0.0000	0.0000	0.0000	1.7979	0.0000
S ₁₀	T ₇	0.4193	0.0000	0.4193	0.5930	0.0001	1.3795	0.0001
S ₁₀	T ₈	0.0000	0.0000	0.0000	0.0000	0.0000	1.0880	0.0000
S ₁₀	T ₉	0.0000	0.0000	0.0000	0.0000	0.0000	0.9155	0.0000
S ₁₀	T ₁₀	0.0000	0.8692	0.0000	0.8692	0.0001	0.7671	0.0001

Naphthalene - Excited States (Singlet, Triplet)

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

Naphthalene - Excited States (Singlet, Triplet)

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.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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