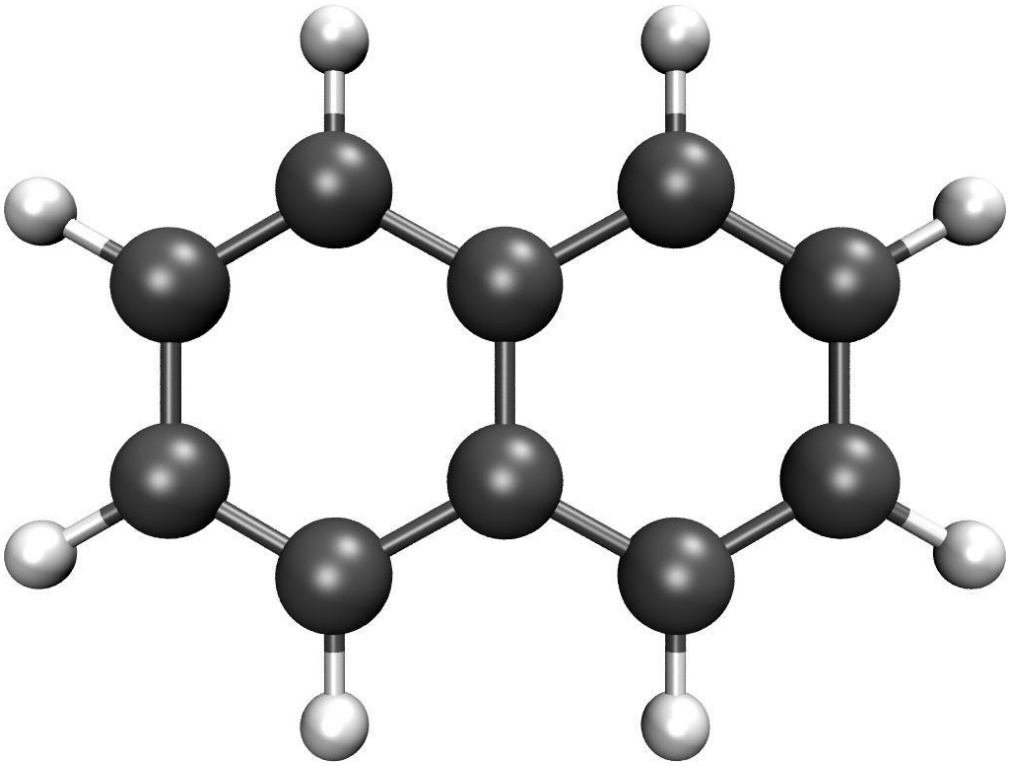
THE Zysman-Colman GROUP

Calculation Report

Naphthalene

Optimisation, Excited States (Singlet, Triplet)



Summary of Results

Metadata

Username:	osl
Date:	07/06/2022 18:50:12
Duration:	13 m, 5 s
Success:	True
Converged:	True
Computational package:	Turbomole (7.5.0)
Methods:	HF, MP2
Basis set:	cc-pVDZ
Calculations:	Optimisation, Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)
No. merged calculations:	3

Calculation 1

Username:	osl
Date:	07/06/2022 18:31:50
Duration:	4 m, 57 s
Success:	True
Converged:	True
Computational package:	Turbomole (7.5.0)
Methods:	HF, MP2
Basis set:	cc-pVDZ
Calculations:	Optimisation
Orbital spin:	restricted
Multiplicity:	1 (singlet)

Calculation 2

Username:	osl
Date:	07/06/2022 18:40:35
Duration:	4 m, 2 s
Success:	True
Computational package:	Turbomole (7.5.0)
Methods:	HF, MP2
Basis set:	cc-pVDZ
Calculations:	Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)

Calculation 3

Username:	osl
Date:	07/06/2022 18:50:12
Duration:	4 m, 5 s
Success:	True
Computational package:	Turbomole (7.5.0)
Methods:	HF, MP2
Basis set:	cc-pVDZ
Calculations:	Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	7
Final energy:	-10432.3114 eV
Final energy:	-1,006,565 kJmol^{-1}

MP Energies

No. of steps:	14
Final energy:	-10467.1582 eV
Final energy:	-1,009,927 kJmol^{-1}

Naphthalene - Optimisation, Excited States (Singlet, Triplet)

Geometry

Formula:	$C_{10}H_8$
Molar mass:	128.1705 $gmol^{-1}$
Alignment method:	Minimal
X extension:	6.80 Å
Y extension:	5.02 Å
Z extension:	0.00 Å
Linearity ratio:	0.26
Planarity ratio:	1.00

HOMO & LUMO

$E_{HOMO,LUMO}$:	10.15 eV
E_{HOMO}:	-7.78 eV
E_{LUMO}:	2.37 eV

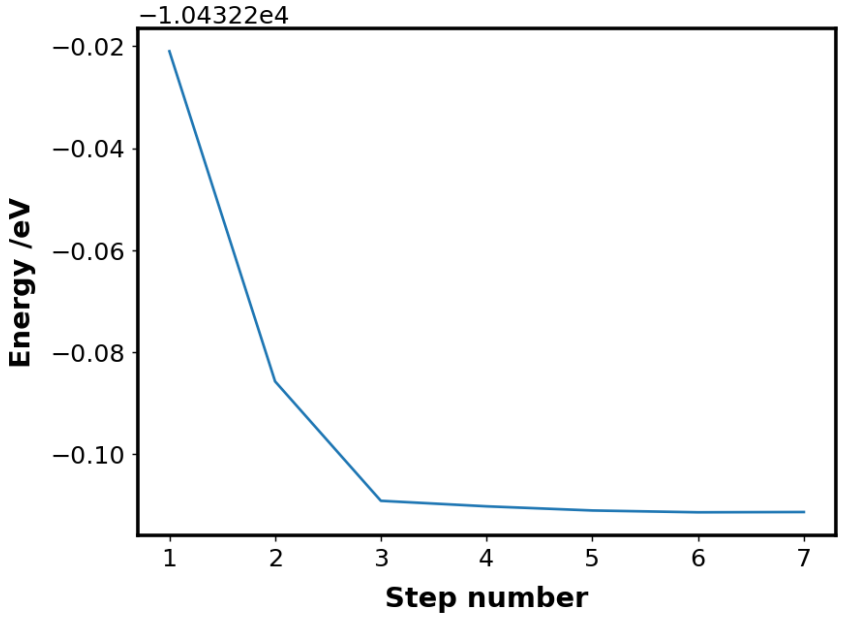
Permanent Dipole Moment

Total:	0.00 D
X axis angle:	90.00 °
XY plane angle:	84.81 °

Excited States

ΔE_{ST}:	1.10 eV
S_1 energy:	4.37 eV
S_1 wavelength:	284 nm
S_1 colour:	Ultraviolet
S_1 CIE (x,y):	(0.00, 0.00)
S_1 oscillator strength:	0.00
T_1 energy:	3.27 eV
T_1 wavelength:	379 nm
T_1 colour:	Ultraviolet
T_1 CIE (x,y):	(0.17, 0.00)
T_1 oscillator strength:	0.00
No. of singlets:	2
No. of triplets:	2

SCF Energies



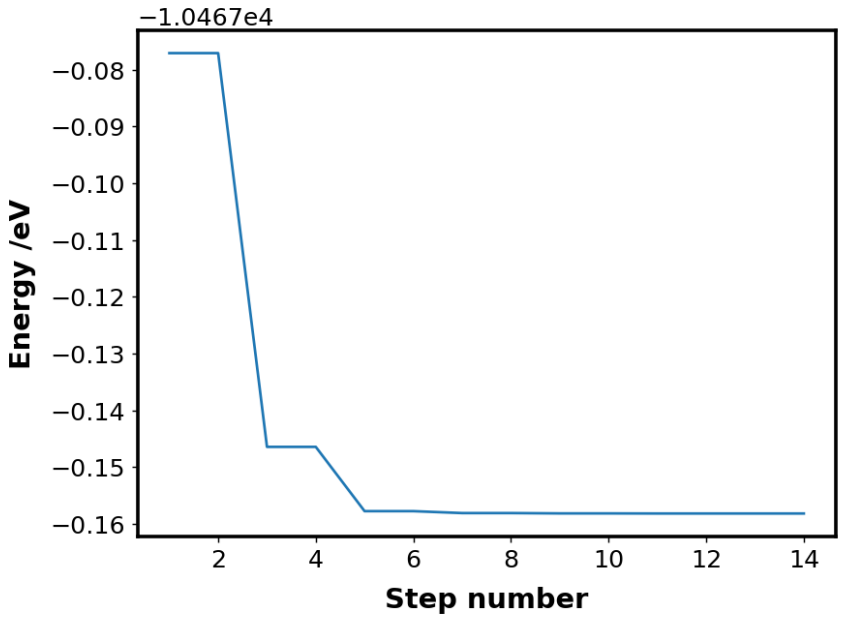
SCF Energies

No. of steps: 7

Final energy: -10432.3114 eV

Final energy: -1,006,565 kJmol^{-1}

MP Energies



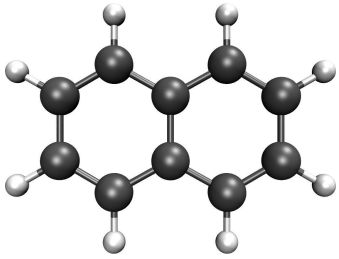
MP Energies

No. of steps: 14

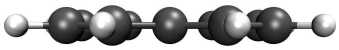
Final energy: -10467.1582 eV

Final energy: -1,009,927 kJmol^{-1}

Geometry

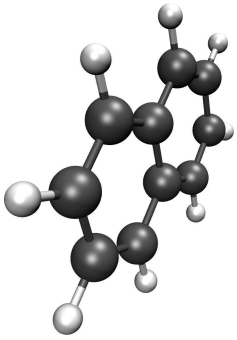


X/Y plane



X/Z plane

Z/Y plane



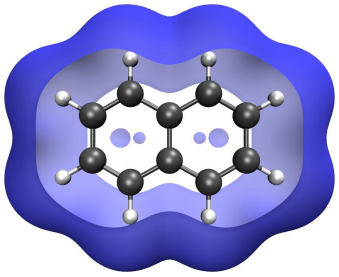
45° to axes

Aligned structure

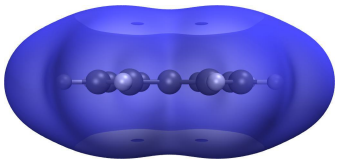
Geometry

Formula:	$C_{10}H_8$
Molar mass:	128.1705 $gmol^{-1}$
Alignment method:	Minimal
X extension:	6.80 Å
Y extension:	5.02 Å
Z extension:	0.00 Å
Linearity ratio:	0.26
Planarity ratio:	1.00

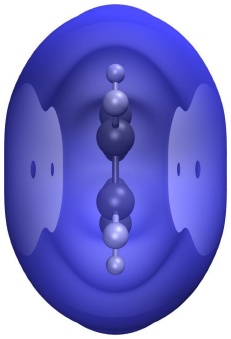
SCF Density



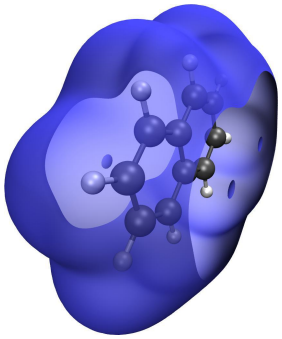
X/Y plane



X/Z plane



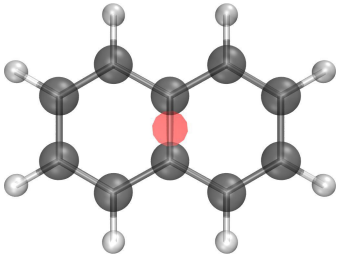
Z/Y plane



45° to axes

SCF density (isovalue: 0.0004)

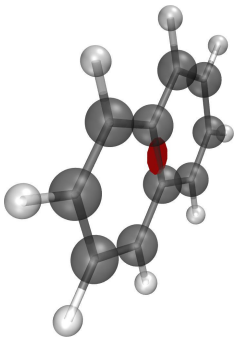
Permanent Dipole Moment



X/Y plane

X/Z plane

Z/Y plane



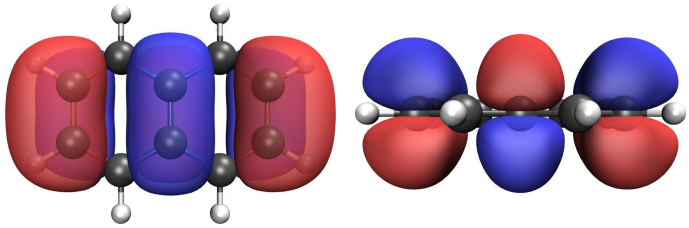
45° to axes

Aligned structure (dipole moment in red)

Dipole Moment

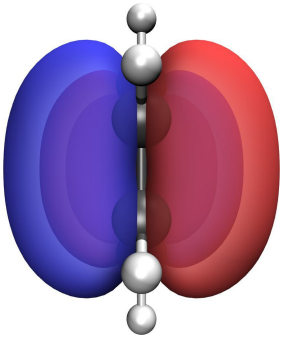
Origin X:	0.00 D
Origin Y:	0.00 D
Origin Z:	0.00 D
Vector X:	0.00 D
Vector Y:	0.00 D
Vector Z:	0.00 D
Total:	0.00 D
X axis angle:	90.00 °
XY plane angle:	84.81 °

HOMO-1

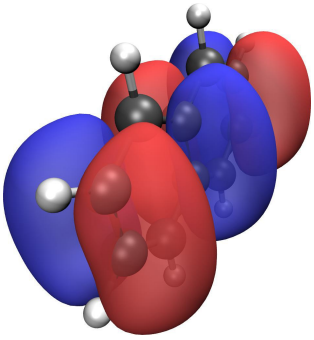


X/Y plane

X/Z plane



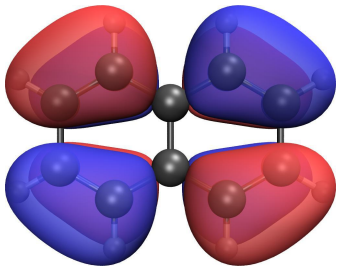
Z/Y plane



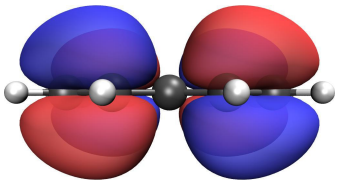
45° to axes

HOMO-1 density (isovalue: 0.02)

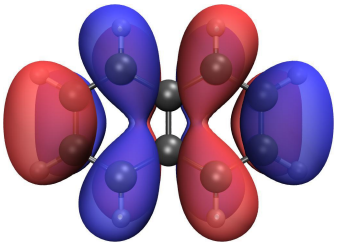
HOMO & LUMO



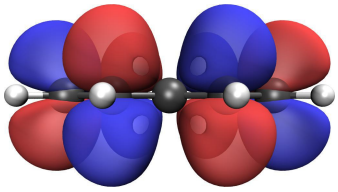
X/Y plane



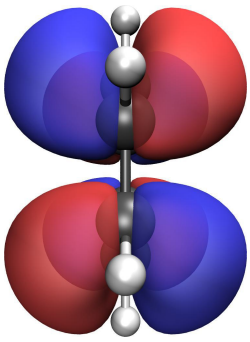
X/Z plane



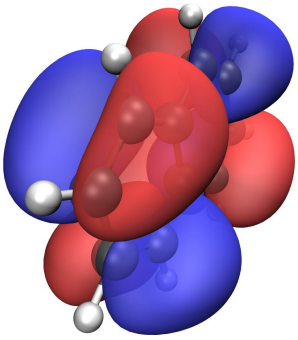
X/Y plane



X/Z plane

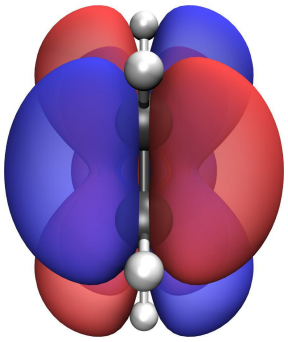


Z/Y plane

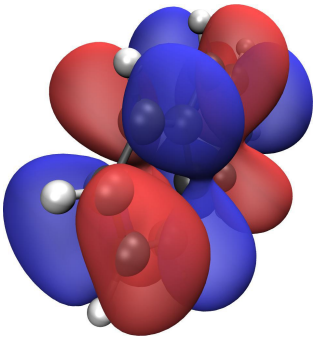


45° to axes

HOMO density (isovalue: 0.02)

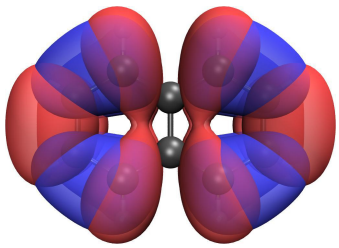


Z/Y plane

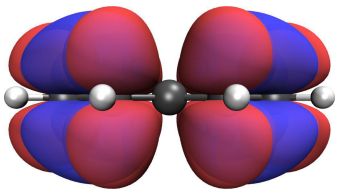


45° to axes

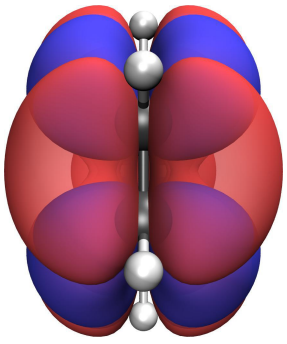
LUMO density (isovalue: 0.02)



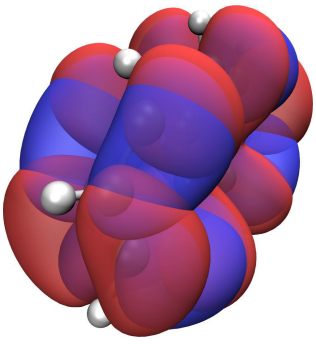
X/Y plane



X/Z plane

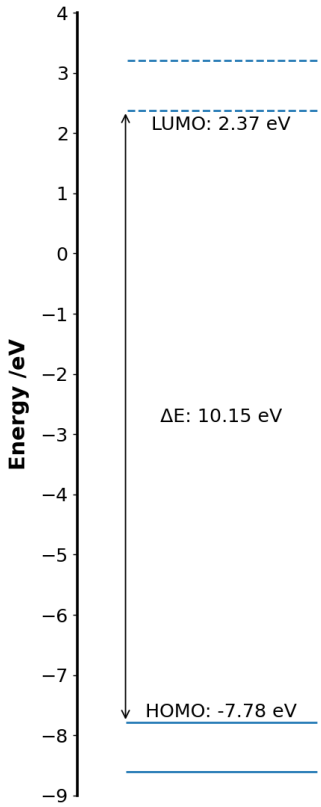


Z/Y plane

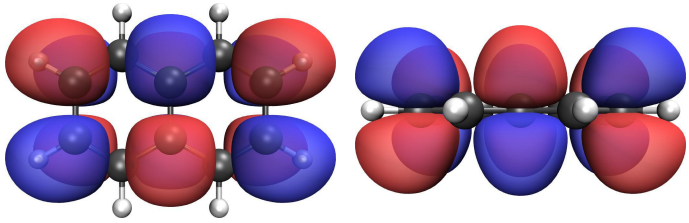


45° to axes

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

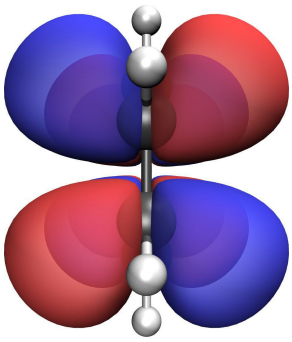


LUMO+1

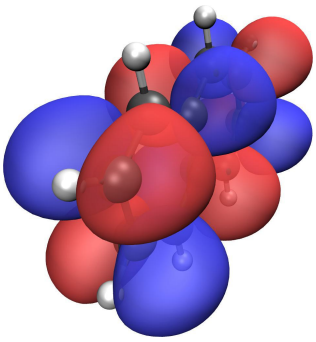


X/Y plane

X/Z plane



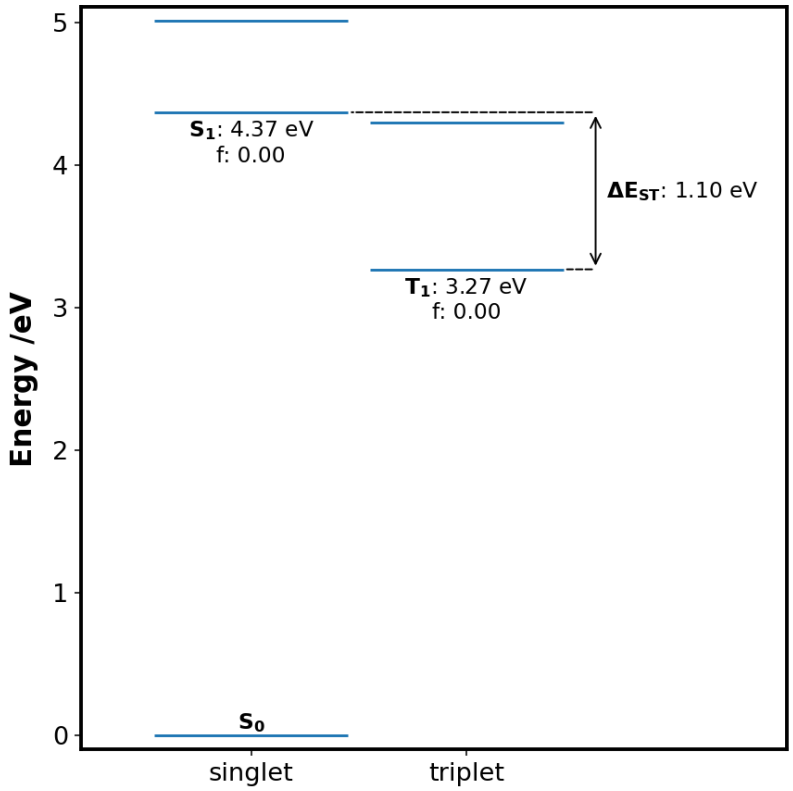
Z/Y plane



45° to axes

LUMO+1 density (isovalue: 0.02)

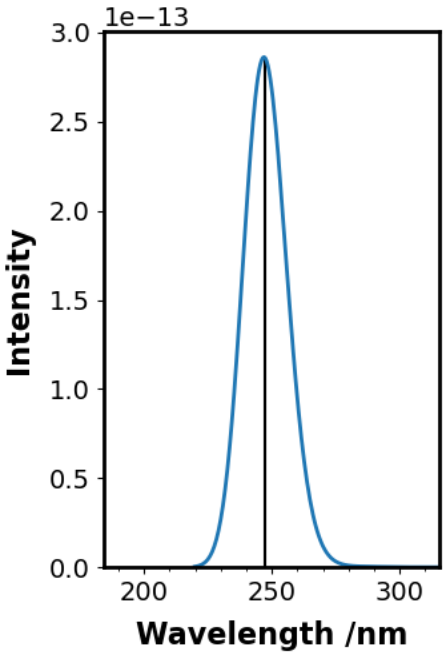
Excited States



Excited States

ΔE_{ST}:	1.10 eV
S_1 energy:	4.37 eV
S_1 wavelength:	284 nm
S_1 colour:	Ultraviolet
S_1 CIE (x,y):	(0.00, 0.00)
S_1 oscillator strength:	0.00
T_1 energy:	3.27 eV
T_1 wavelength:	379 nm
T_1 colour:	Ultraviolet
T_1 CIE (x,y):	(0.17, 0.00)
T_1 oscillator strength:	0.00
No. of singlets:	2
No. of triplets:	2

Absorptions

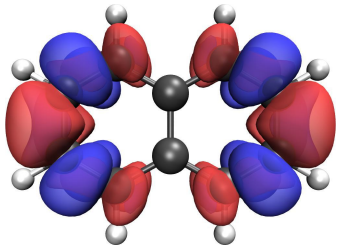


Absorption spectrum (simulated Gaussian functions with FWHM: 0.4 eV).
Peaks /nm: 246.
Note: high energy absorption peaks are not simulated.
For a complete absorption spectrum, use more excited states.

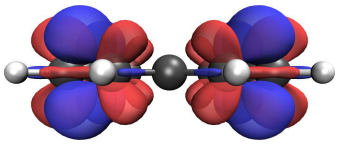
Table of Excited States

Level	Symbol	Symmetry	Energy /eV	Wavelength /nm	Colour, CIE (x,y)	Oscillator Strength	Transitions (probability)
1	T_1	Triplet-A	3.2689	379.29	Ultraviolet  (0.17, 0.00)	0.0000	HOMO → LUMO (0.85) HOMO-2 → LUMO+2 (0.06) HOMO-1 → LUMO+1 (0.05)
2	T_2	Triplet-A	4.2983	288.45	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-1 → LUMO (0.49) HOMO → LUMO+1 (0.46) HOMO-3 → LUMO+2 (0.02)
3	S_1	Singlet-A	4.3707	283.67	Ultraviolet  (0.00, 0.00)	0.0002	HOMO-1 → LUMO (0.49) HOMO → LUMO+1 (0.48)
4	S_2	Singlet-A	5.0100	247.47	Ultraviolet  (0.00, 0.00)	0.0880	HOMO → LUMO (0.90) HOMO-1 → LUMO+1 (0.08)

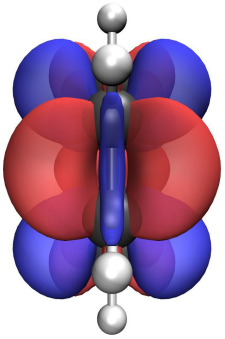
T(1), T(2), S(1), S(2) Difference Densities



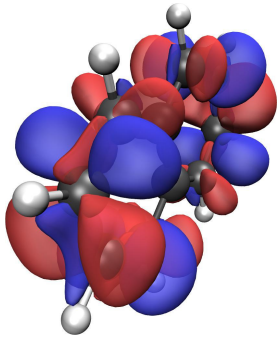
X/Y plane



X/Z plane

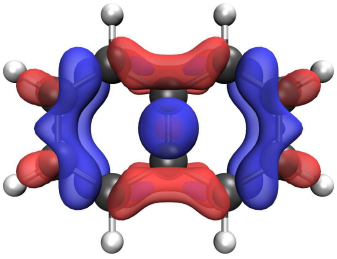


Z/Y plane

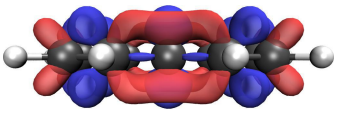


45° to axes

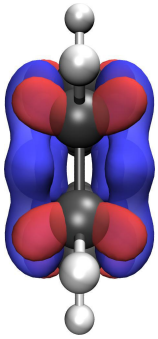
T(1) positive (hole) (blue) & negative (electron) (red) difference density (isovalue: 0.001)



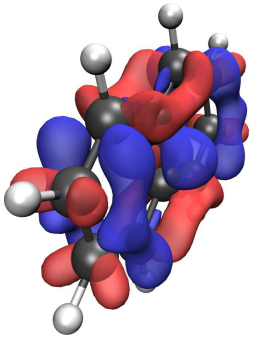
X/Y plane



X/Z plane

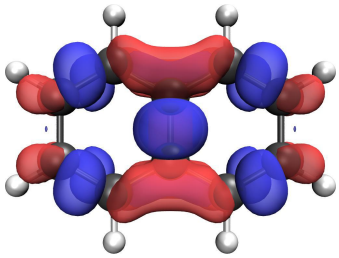


Z/Y plane

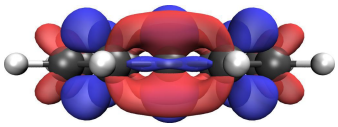


45° to axes

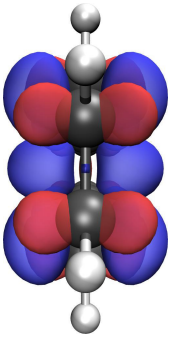
T(2) positive (hole) (blue) & negative (electron) (red) difference density (isovalue: 0.001)



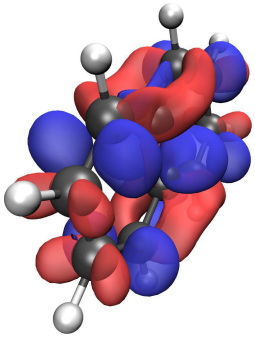
X/Y plane



X/Z plane

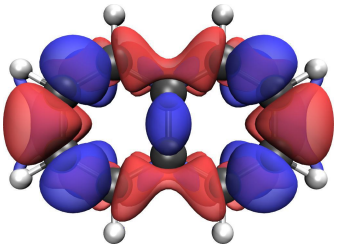


Z/Y plane

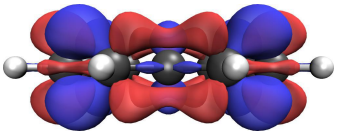


45° to axes

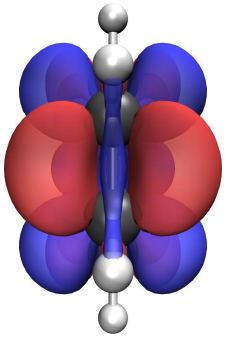
S(1) positive (hole) (blue) & negative (electron) (red) difference density (isovalue: 0.001)



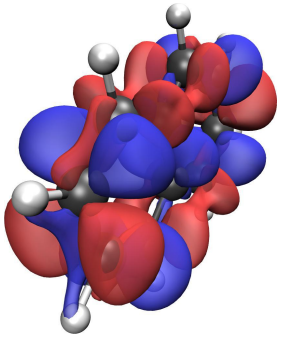
X/Y plane



X/Z plane



Z/Y plane



45° to axes

S(2) positive (hole) (blue) & negative (electron) (red) difference density (isovalue: 0.001)

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
50	LUMO+15	A	11.9600
49	LUMO+14	A	11.7352
48	LUMO+13	A	10.6261
47	LUMO+12	A	10.4351
46	LUMO+11	A	7.9455
45	LUMO+10	A	7.4055
44	LUMO+9	A	7.3699
43	LUMO+8	A	6.8297
42	LUMO+7	A	6.4869
41	LUMO+6	A	6.3480
40	LUMO+5	A	5.4144
39	LUMO+4	A	5.4053
38	LUMO+3	A	4.9896
37	LUMO+2	A	4.7431
36	LUMO+1	A	3.2023
35	**LUMO**	**A**	**2.3705**
34	**HOMO**	**A**	**-7.7835**
33	HOMO-1	A	-8.6036
32	HOMO-2	A	-10.3698
31	HOMO-3	A	-12.0540
30	HOMO-4	A	-12.9253
29	HOMO-5	A	-13.1917
28	HOMO-6	A	-14.1706
27	HOMO-7	A	-14.3301
26	HOMO-8	A	-15.2492
25	HOMO-9	A	-15.7421
24	HOMO-10	A	-15.7464
23	HOMO-11	A	-16.4964
22	HOMO-12	A	-16.8786
21	HOMO-13	A	-18.2419
20	HOMO-14	A	-18.8267
19	HOMO-15	A	-19.1551

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2509141	-1.4118092	-0.0000069
C	-2.4487537	-0.7132682	0.0000087
C	-2.4487547	0.7132694	0.0000104
C	-1.2509134	1.4118084	-0.0000068
C	-0.0000000	0.7179339	-0.0000210
C	-0.0000000	-0.7179354	-0.0000202
C	1.2509141	-1.4118092	-0.0000071
C	1.2509134	1.4118084	-0.0000084
C	2.4487547	0.7132694	0.0000099
C	2.4487537	-0.7132682	0.0000093
H	-1.2480933	-2.5080746	-0.0000131
H	-3.4000079	-1.2561870	0.0000192
H	-3.4000083	1.2561881	0.0000264
H	-1.2480915	2.5080739	-0.0000147
H	1.2480933	-2.5080746	-0.0000148
H	1.2480915	2.5080739	-0.0000190
H	3.4000083	1.2561881	0.0000266
H	3.4000079	-1.2561870	0.0000218

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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