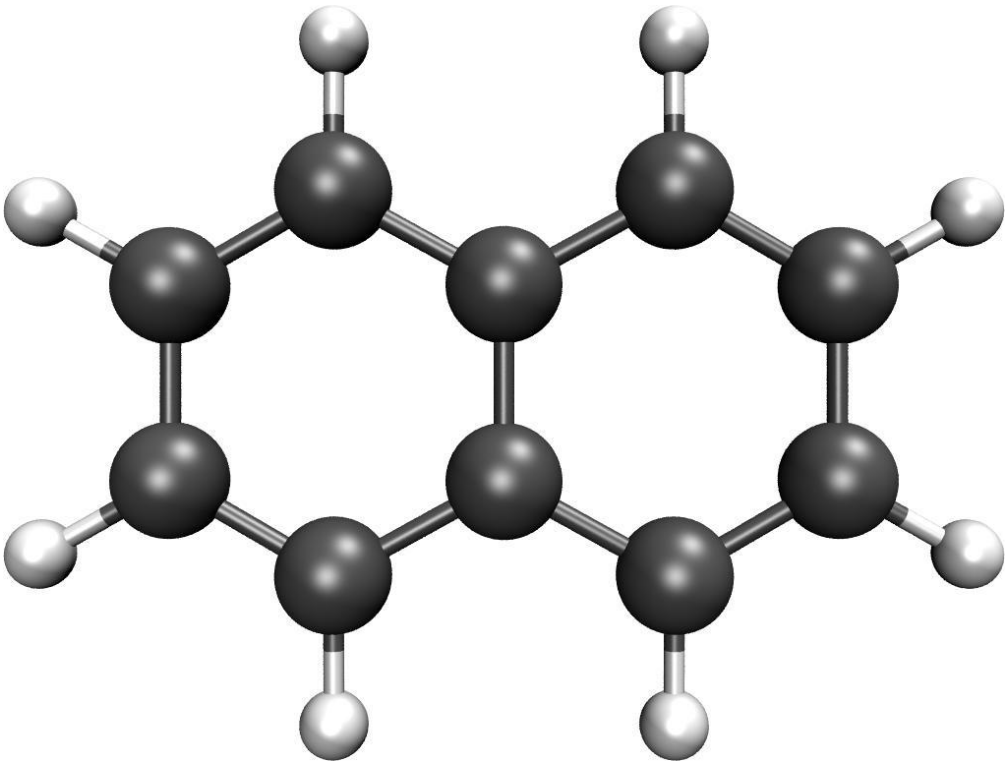
THE Zysman-Colman GROUP

Calculation Report

Naphthalene

Single Point (Singlet)



Summary of Results

Metadata

Username:	osl
Date:	15/06/2022 14:52:56
Duration:	24 s
Success:	True
Computational package:	Gaussian (2016+C.01)
Methods:	DFT
Functional:	PBE1PBE
Basis set:	6-31G(d,p)
Calculations:	Single Point
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	1
Final energy:	-10488.9903 eV
Final energy:	-1,012,034 $kJmol^{-1}$

Geometry

Formula:	$C_{10}H_8$
Exact mass:	128.0626 $gmol^{-1}$
Molar mass:	128.1705 $gmol^{-1}$
Alignment method:	Minimal
X extension:	6.74 Å
Y extension:	4.97 Å
Z extension:	0.00 Å
Linearity ratio:	0.26
Planarity ratio:	1.00

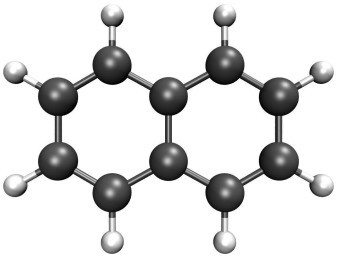
HOMO & LUMO

$E_{HOMO,LUMO}$:	5.21 eV
E_{HOMO}:	-6.13 eV
E_{LUMO}:	-0.92 eV

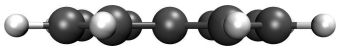
Permanent Dipole Moment

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

Geometry

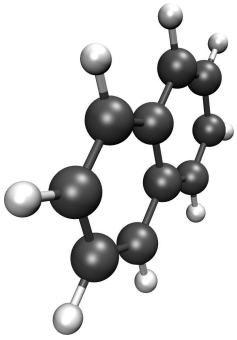


X/Y plane



X/Z plane

Z/Y plane



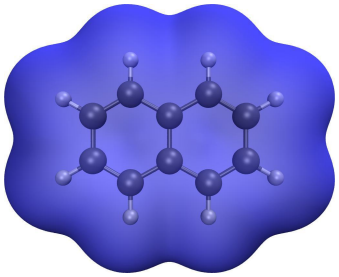
45° to axes

Aligned structure

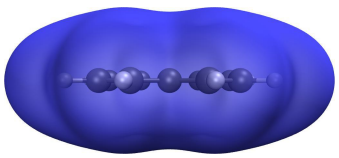
Geometry

Formula:	$C_{10}H_8$
Exact mass:	128.0626 $gmol^{-1}$
Molar mass:	128.1705 $gmol^{-1}$
Alignment method:	Minimal
X extension:	6.74 Å
Y extension:	4.97 Å
Z extension:	0.00 Å
Linearity ratio:	0.26
Planarity ratio:	1.00

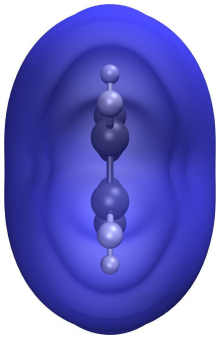
SCF Density



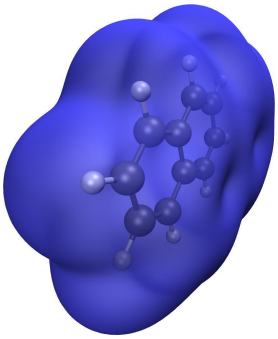
X/Y plane



X/Z plane



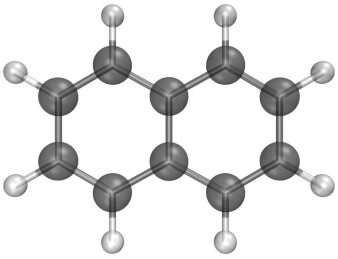
Z/Y plane



45° to axes

SCF density (isovalue: 0.0004)

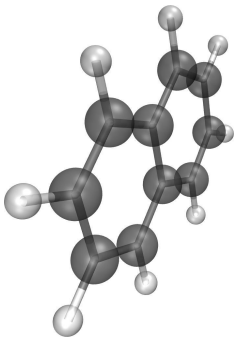
Permanent Dipole Moment



X/Y plane

X/Z plane

Z/Y plane



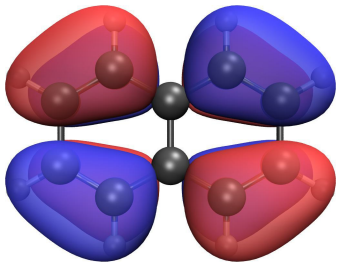
45° to axes

Aligned structure (dipole moment in red)

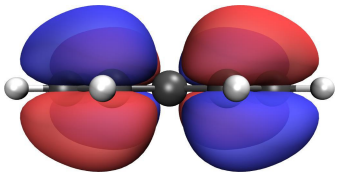
Dipole Moment

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

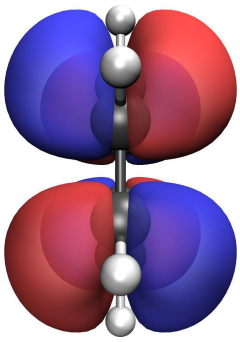
HOMO & LUMO



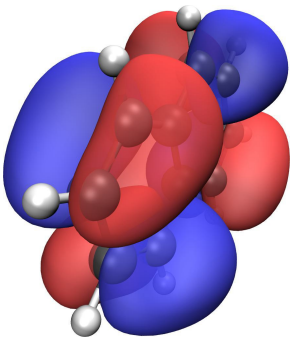
X/Y plane



X/Z plane

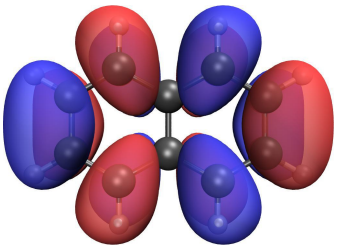


Z/Y plane

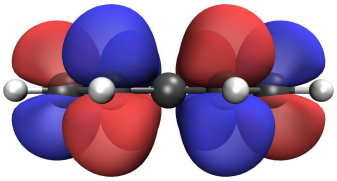


45° to axes

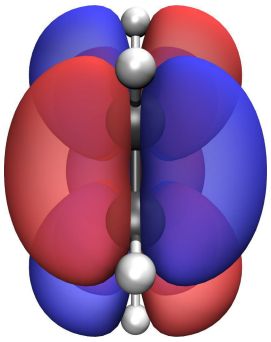
HOMO density (isovalue: 0.02)



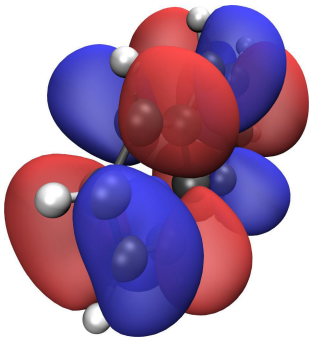
X/Y plane



X/Z plane

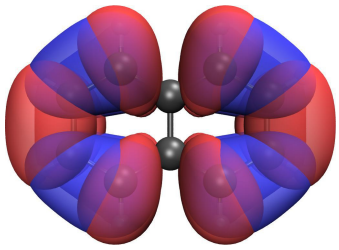


Z/Y plane

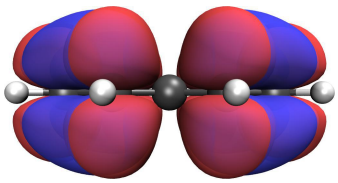


45° to axes

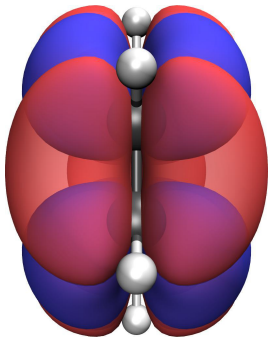
LUMO density (isovalue: 0.02)



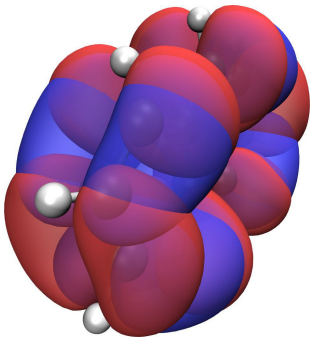
X/Y plane



X/Z plane



Z/Y plane



45° to axes

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

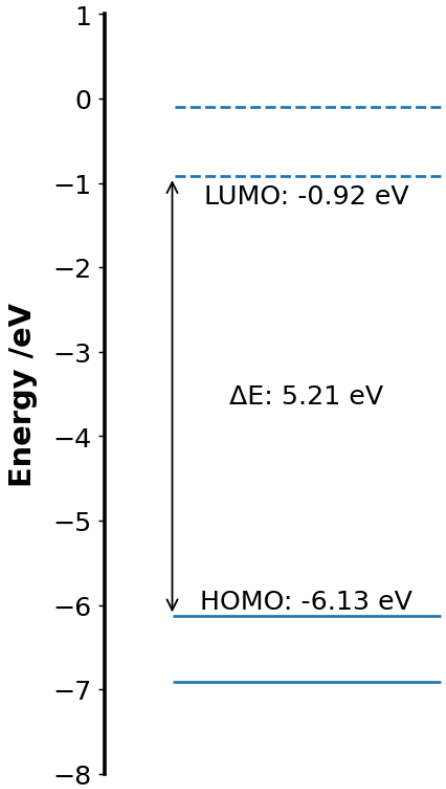


Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
50	LUMO+15	B1u	8.6396
49	LUMO+14	Ag	7.9114
48	LUMO+13	B1u	6.9150
47	LUMO+12	B3g	6.0692
46	LUMO+11	B2g	5.7949
45	LUMO+10	B2u	5.3487
44	LUMO+9	B1u	5.1506
43	LUMO+8	B3g	5.0031
42	LUMO+7	Ag	4.9519
41	LUMO+6	B1u	3.6912
40	LUMO+5	B2u	3.4207
39	LUMO+4	Au	2.9674
38	LUMO+3	Ag	2.9127
37	LUMO+2	B3u	1.0612
36	LUMO+1	B2g	-0.1010
35	**LUMO**	**B1g**	**-0.9244**
34	**HOMO**	**Au**	**-6.1307**
33	HOMO-1	B3u	-6.9084
32	HOMO-2	B2g	-8.0747
31	HOMO-3	Ag	-9.1879
30	HOMO-4	B1g	-9.2562
29	HOMO-5	B3g	-9.4032
28	HOMO-6	B2u	-10.2679
27	HOMO-7	B3u	-11.0274
26	HOMO-8	B1u	-11.1363
25	HOMO-9	B2u	-11.5961
24	HOMO-10	B3g	-11.6187
23	HOMO-11	Ag	-12.3015
22	HOMO-12	B1u	-12.4753
21	HOMO-13	Ag	-13.7777
20	HOMO-14	B3g	-14.2411
19	HOMO-15	B2u	-14.3709

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2404600	-1.3991400	0.0000000
C	-2.4260000	-0.7066400	0.0000000
C	-2.4260000	0.7066400	0.0000000
C	-1.2404600	1.3991400	-0.0000000
C	0.0000000	0.7142300	-0.0000000
C	-0.0000000	-0.7142300	0.0000000
C	1.2404600	-1.3991400	0.0000000
C	1.2404600	1.3991400	-0.0000000
C	2.4260000	0.7066400	-0.0000000
C	2.4260000	-0.7066400	-0.0000000
H	-1.2367000	-2.4862000	0.0000000
H	-3.3697000	-1.2439700	0.0000000
H	-3.3697000	1.2439700	0.0000000
H	-1.2367000	2.4862000	-0.0000000
H	1.2367000	-2.4862000	0.0000000
H	1.2367000	2.4862000	-0.0000000
H	3.3697000	1.2439700	-0.0000000
H	3.3697000	-1.2439700	-0.0000000

About

Silico Calculation Report

Part of the silico software package

Version 1.0.0-pre.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]

Bibliography

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