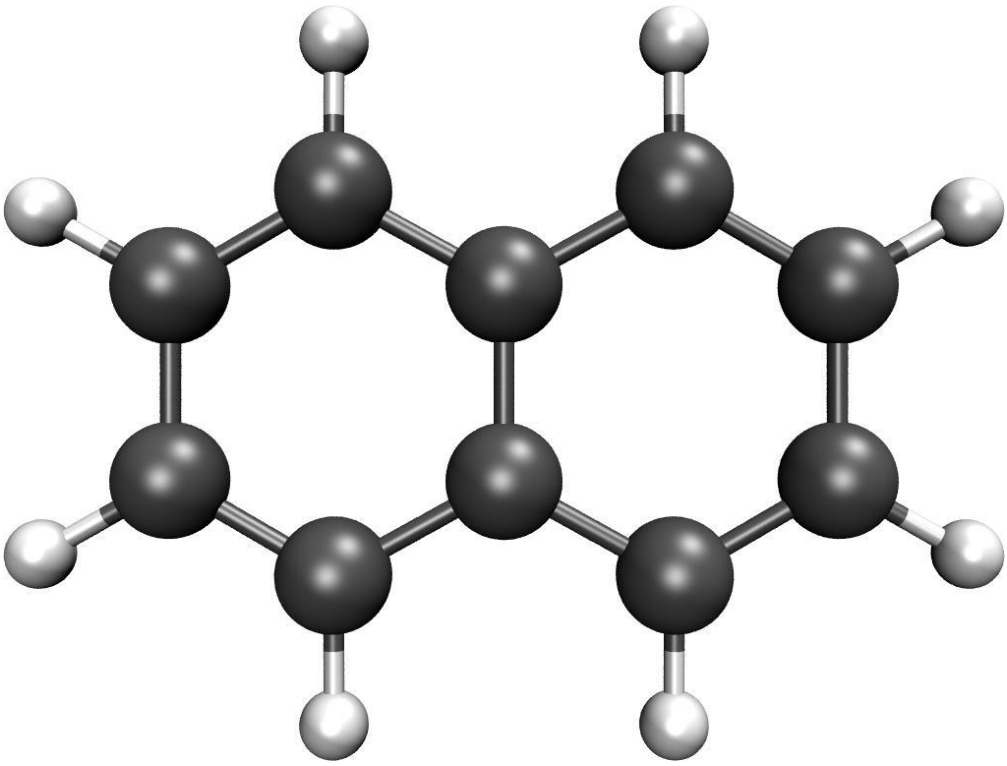
THE Zysman-Colman GROUP

Calculation Report

Naphthalene

Excited States ()



Summary of Results

Metadata

Username:	osl
Date:	24/06/2022 12:47:40
Duration:	33 s
Success:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	1
Final energy:	-10488.7997 eV
Final energy:	-1,012,015 $kJmol^{-1}$

Geometry

Formula:	$C_{10}H_8$
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

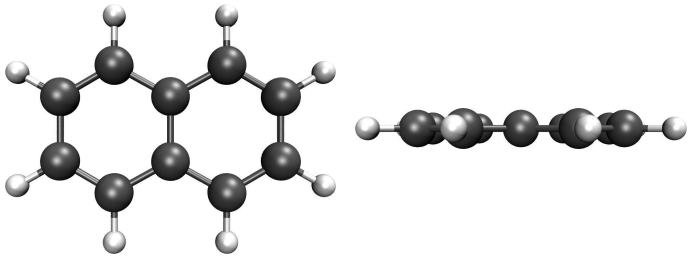
HOMO & LUMO

$E_{HOMO,LUMO}$:	5.20 eV
E_{HOMO}:	-6.07 eV
E_{LUMO}:	-0.87 eV

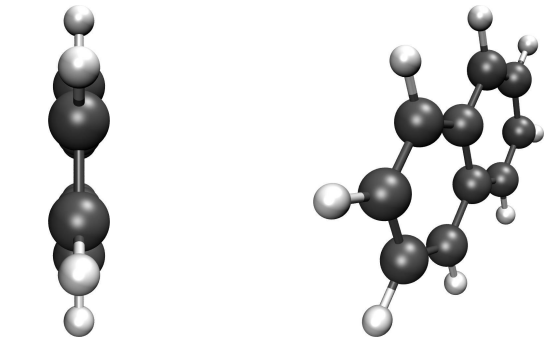
Permanent Dipole Moment

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

Geometry



X/Y plane | X/Z plane



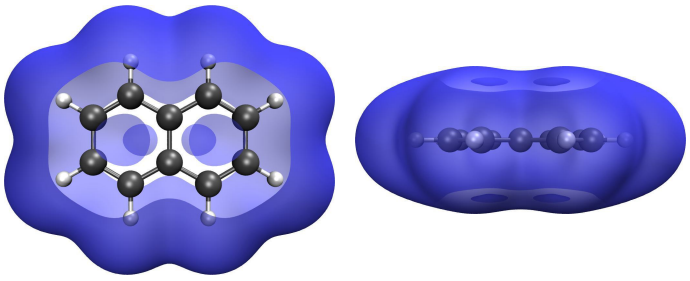
Z/Y plane | 45° to axes

Aligned structure

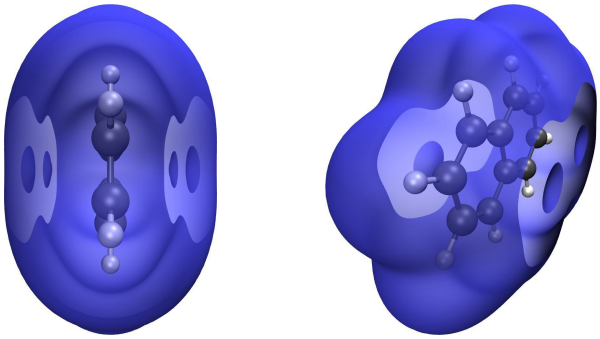
Geometry

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

SCF Density



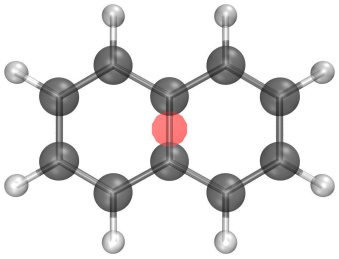
X/Y plane | X/Z plane



Z/Y plane | 45° to axes

SCF density (isovalue: 0.0004)

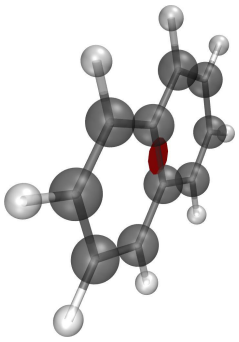
Permanent Dipole Moment



X/Y plane

X/Z plane

Z/Y plane



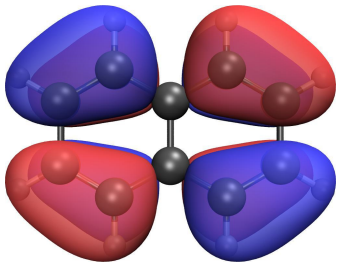
45° to axes

Aligned structure (dipole moment in red)

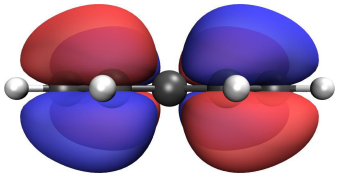
Dipole Moment

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:	90.00 °
XY plane angle:	90.00 °

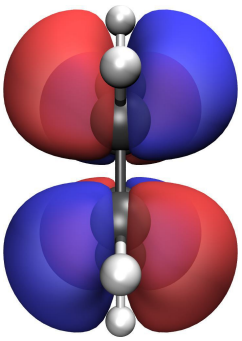
HOMO & LUMO



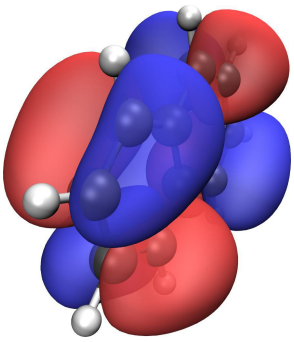
X/Y plane



X/Z plane

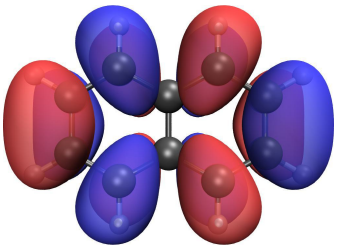


Z/Y plane

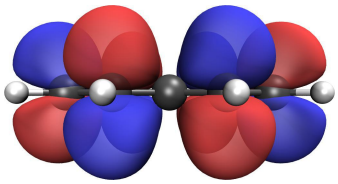


45° to axes

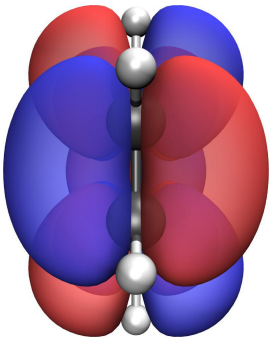
HOMO density (isovalue: 0.02)



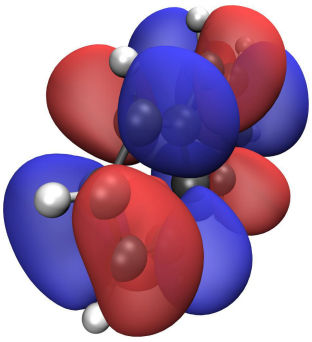
X/Y plane



X/Z plane

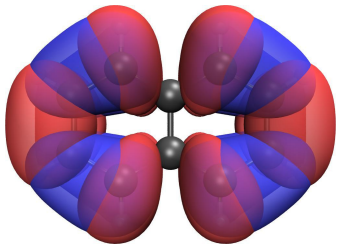


Z/Y plane

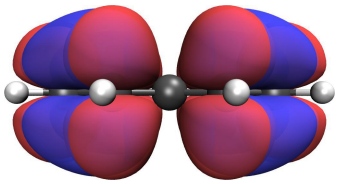


45° to axes

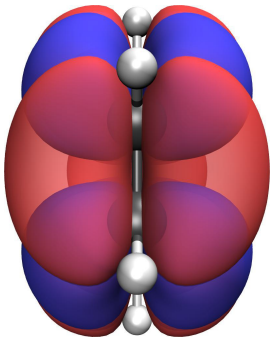
LUMO density (isovalue: 0.02)



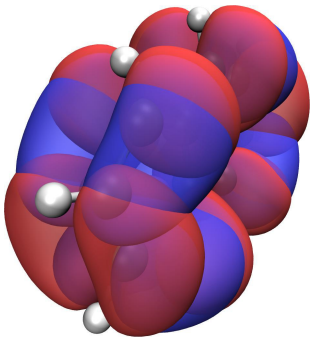
X/Y plane



X/Z plane



Z/Y plane



45° to axes

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

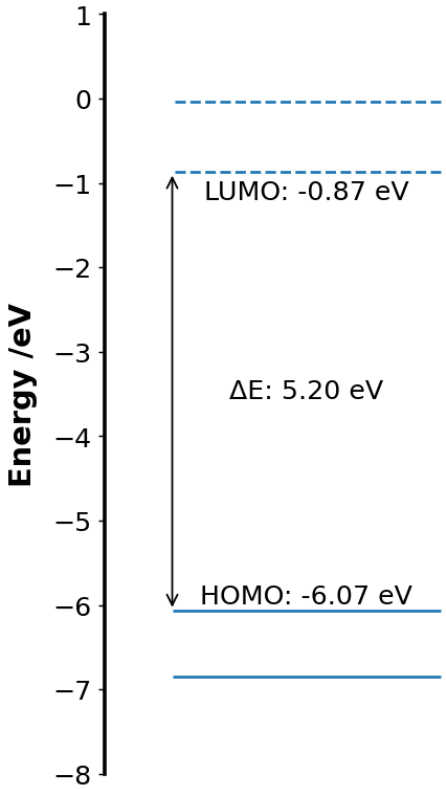


Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
50	LUMO+15	A	8.6772
49	LUMO+14	A	7.9408
48	LUMO+13	A	6.9385
47	LUMO+12	A	6.0199
46	LUMO+11	A	5.8555
45	LUMO+10	A	5.3160
44	LUMO+9	A	5.1150
43	LUMO+8	A	4.9563
42	LUMO+7	A	4.9002
41	LUMO+6	A	3.6415
40	LUMO+5	A	3.3840
39	LUMO+4	A	3.0181
38	LUMO+3	A	2.8726
37	LUMO+2	A	1.1210
36	LUMO+1	A	-0.0372
35	**LUMO**	**A**	**-0.8685**
34	**HOMO**	**A**	**-6.0723**
33	HOMO-1	A	-6.8458
32	HOMO-2	A	-8.0113
31	HOMO-3	A	-9.1659
30	HOMO-4	A	-9.1939
29	HOMO-5	A	-9.3747
28	HOMO-6	A	-10.2482
27	HOMO-7	A	-10.9559
26	HOMO-8	A	-11.1181
25	HOMO-9	A	-11.5628
24	HOMO-10	A	-11.5951
23	HOMO-11	A	-12.2690
22	HOMO-12	A	-12.4567
21	HOMO-13	A	-13.7513
20	HOMO-14	A	-14.2144
19	HOMO-15	A	-14.3454

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2401200	-1.3986700	0.0000200
C	-2.4257500	-0.7064600	-0.0000200
C	-2.4257500	0.7064600	-0.0000200
C	-1.2401200	1.3986700	0.0000200
C	0.0000000	0.7136900	0.0000500
C	0.0000000	-0.7136900	0.0000500
C	1.2401200	-1.3986700	0.0000200
C	1.2401200	1.3986700	0.0000200
C	2.4257500	0.7064600	-0.0000200
C	2.4257500	-0.7064600	-0.0000200
H	-1.2361000	-2.4857100	0.0000400
H	-3.3697000	-1.2435400	-0.0000400
H	-3.3697000	1.2435400	-0.0000600
H	-1.2361000	2.4857100	0.0000200
H	1.2361000	-2.4857100	0.0000300
H	1.2361000	2.4857100	0.0000400
H	3.3697000	1.2435400	-0.0000500
H	3.3697000	-1.2435400	-0.0000700

About

Silico Calculation Report

Part of the silico software package

Version 1.0.0-pre.32

11 February 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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