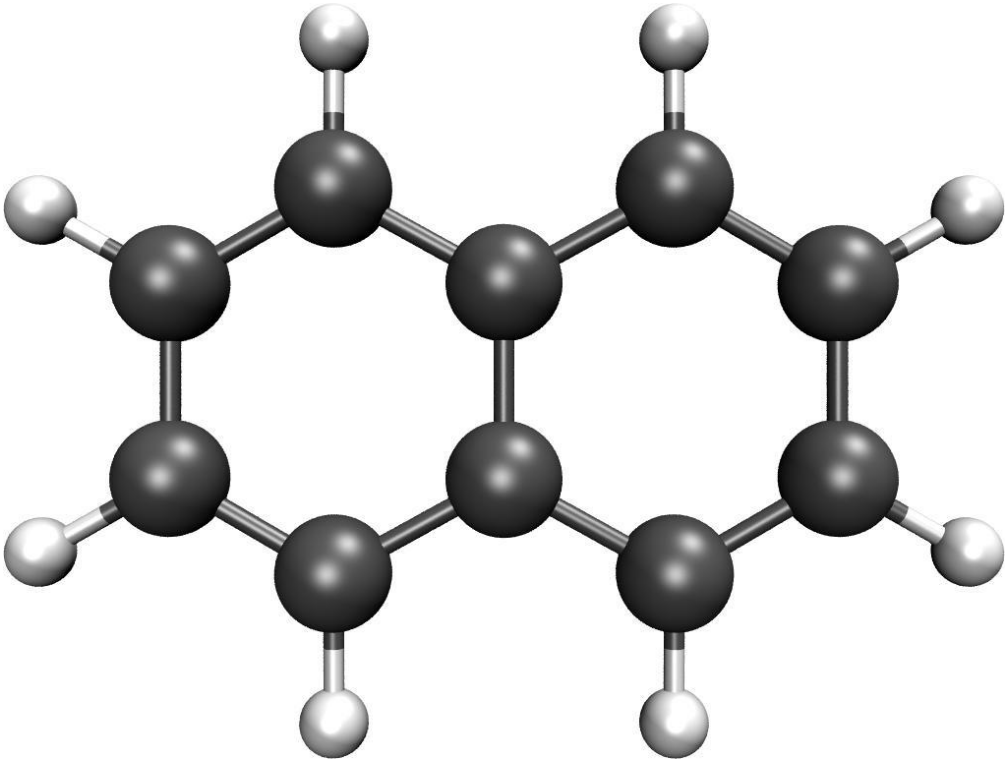
THE Zysman-Colman GROUP

Calculation Report

Naphthalene

Optimisation, Frequencies (Singlet)



Summary of Results

Metadata

Username:	osl
Date:	24/06/2022 12:43:12
Duration:	1 m, 43 s
Success:	True
Converged:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Optimisation, Frequencies
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	4
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

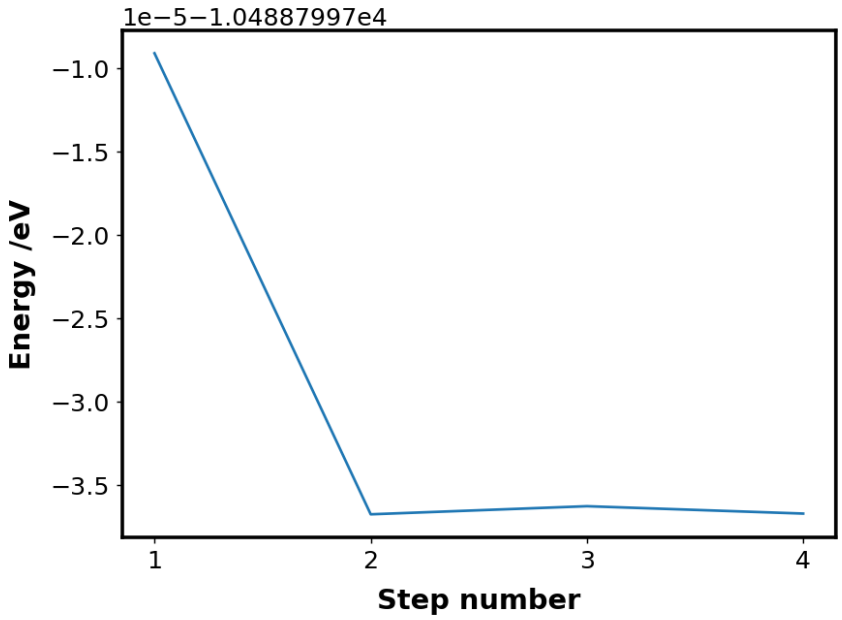
Permanent Dipole Moment

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

Vibrational Frequencies

Negative frequencies:	0

SCF Energies



SCF Energies

No. of steps: 4

Final energy: -10488.7997 eV

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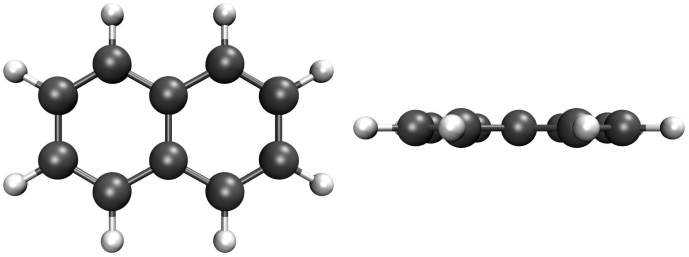
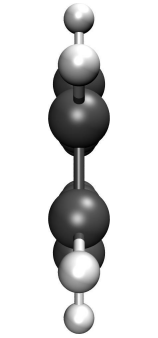
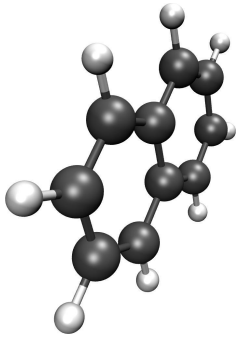


X/Y plane

X/Z plane



Z/Y plane



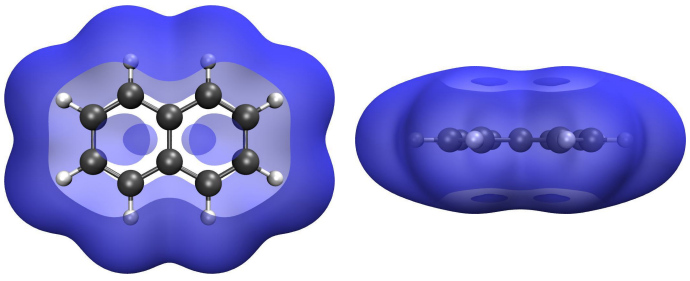
45° to axes

Aligned structure

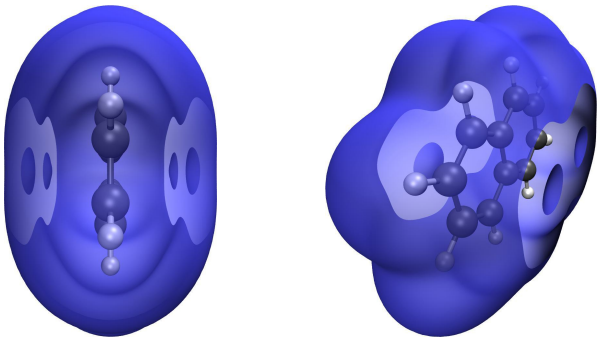
Geometry

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



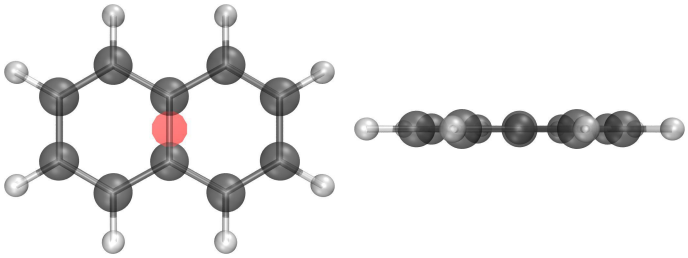
X/Y plane | X/Z plane



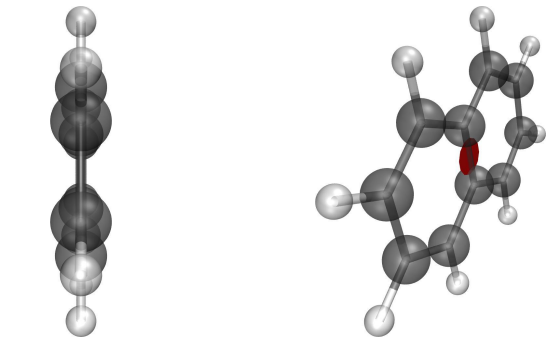
Z/Y plane | 45° to axes

SCF density (isovalue: 0.0004)

Permanent Dipole Moment



X/Y plane | X/Z plane



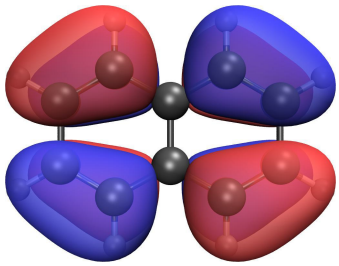
Z/Y plane | 45° to axes

Aligned structure (dipole moment in red)

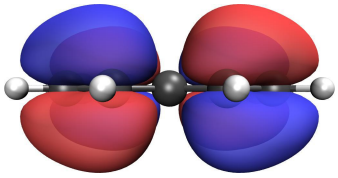
Dipole Moment

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 °

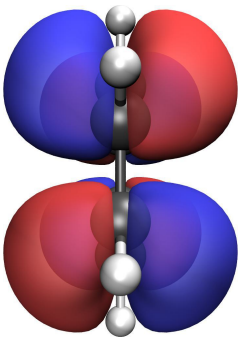
HOMO & LUMO



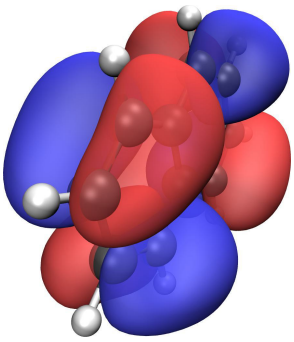
X/Y plane



X/Z plane

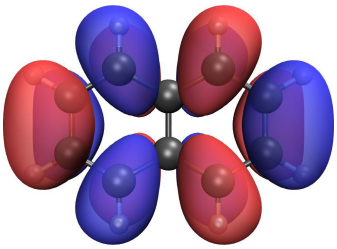


Z/Y plane

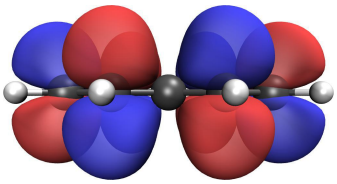


45° to axes

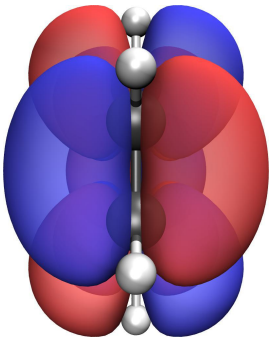
HOMO density (isovalue: 0.02)



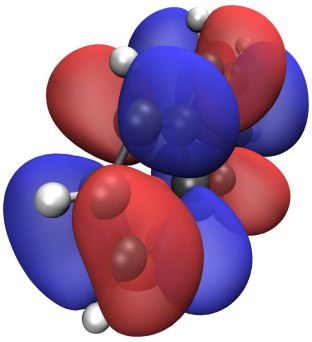
X/Y plane



X/Z plane

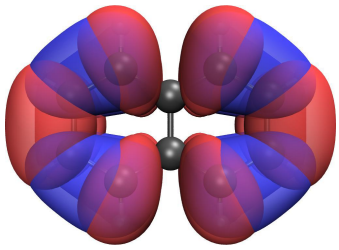


Z/Y plane

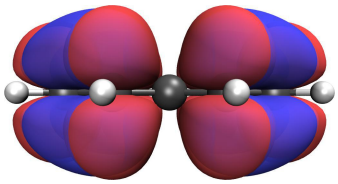


45° to axes

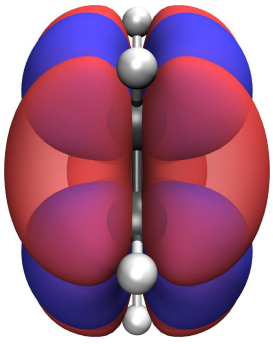
LUMO density (isovalue: 0.02)



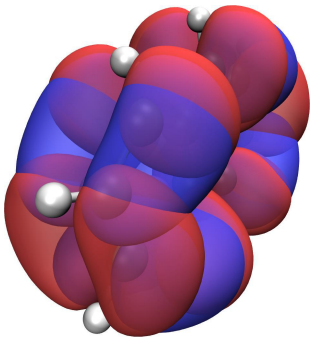
X/Y plane



X/Z plane

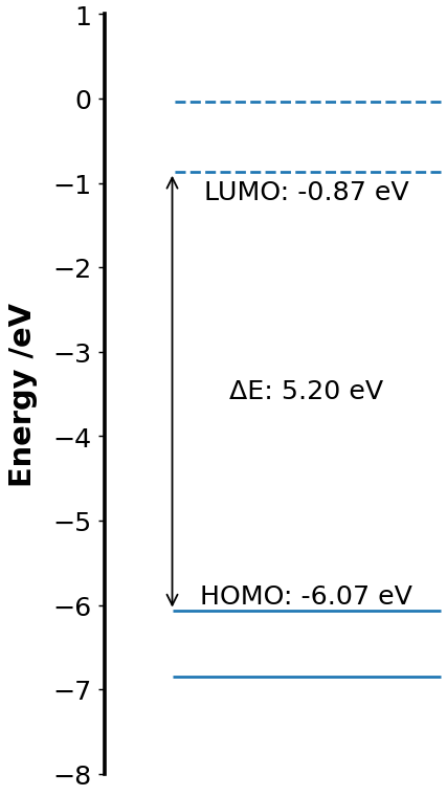


Z/Y plane

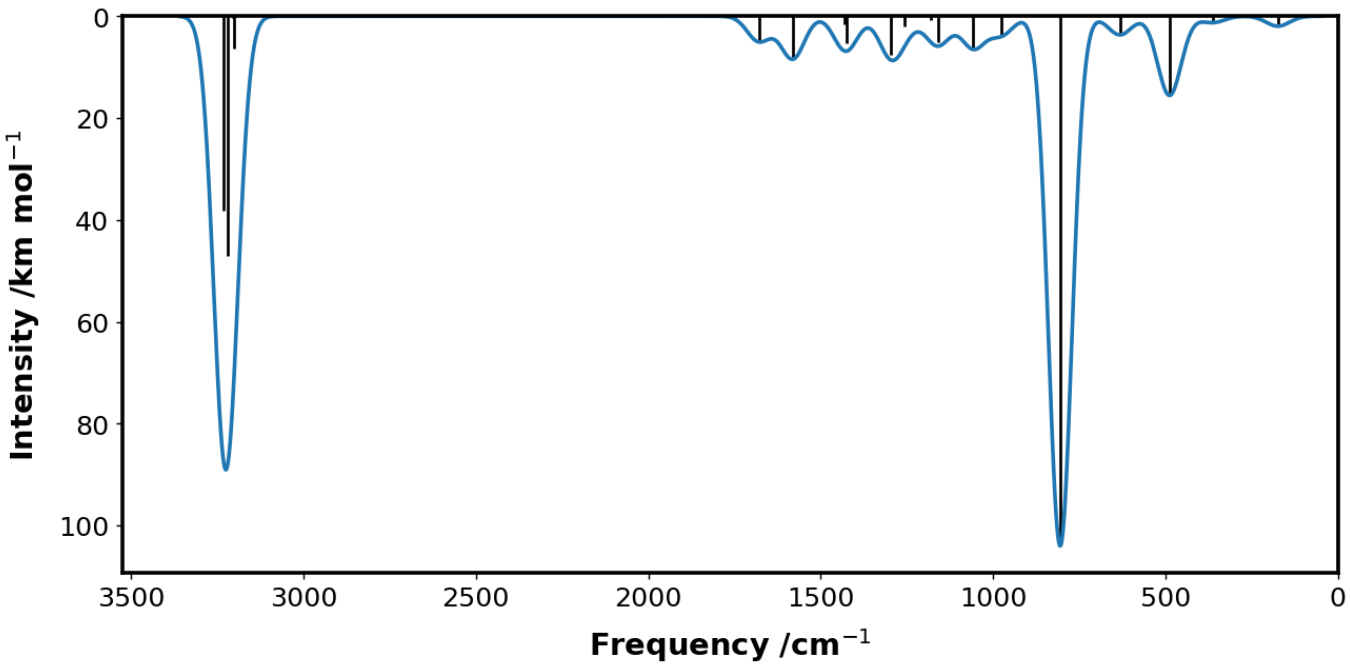


45° to axes

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



Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm^{-1})
Peaks /cm^{-1}: 173, 365, 488, 631, 805, 1054, 1160, 1291, 1426, 1582, 1675, 3224.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm^{-1}	Intensity /km mol^{-1}
1	A	173.8900	1.9600
2	A	188.7600	0.0000
3	A	363.1000	1.2600
4	A	395.4100	0.0000
5	A	478.4100	0.0000
6	A	488.2700	15.5600
7	A	517.1100	0.0000
8	A	523.4600	0.0000
9	A	632.0700	3.6700
10	A	636.9300	0.0000
11	A	733.3100	0.0000
12	A	783.2300	0.0000
13	A	789.1200	0.0000
14	A	805.2800	103.7700
15	A	809.9100	0.2400
16	A	854.7500	0.0000
17	A	900.3200	0.0000
18	A	948.3000	0.0000
19	A	958.2500	0.0000
20	A	975.8600	3.6500
21	A	995.7800	0.0000
22	A	1003.4600	0.0000
23	A	1057.1100	6.2700
24	A	1066.1500	0.0000
25	A	1157.9100	5.0900
26	A	1179.0900	0.8300
27	A	1179.9300	0.0000
28	A	1188.1900	0.0000
29	A	1256.2900	2.0900
30	A	1273.3900	0.0000
31	A	1296.9100	7.5700
32	A	1425.3000	5.2900
33	A	1432.3300	1.6100
34	A	1455.0500	0.0000

35	A	1507.0400	0.0000
36	A	1511.4100	0.0000
37	A	1581.5300	8.3900
38	A	1658.1900	0.0000
39	A	1678.9300	4.9400
40	A	1716.7200	0.0000
41	A	3201.6100	0.0000
42	A	3202.4800	6.2700
43	A	3205.4800	0.4000
44	A	3207.6900	0.0000
45	A	3220.3300	0.0000
46	A	3220.9700	47.0100
47	A	3233.1600	38.0800
48	A	3234.0200	0.0000

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	5.8556
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	3.6416
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	-6.8459
32	HOMO-2	A	-8.0113
31	HOMO-3	A	-9.1658
30	HOMO-4	A	-9.1940
29	HOMO-5	A	-9.3747
28	HOMO-6	A	-10.2483
27	HOMO-7	A	-10.9559
26	HOMO-8	A	-11.1181
25	HOMO-9	A	-11.5629
24	HOMO-10	A	-11.5950
23	HOMO-11	A	-12.2691
22	HOMO-12	A	-12.4566
21	HOMO-13	A	-13.7514
20	HOMO-14	A	-14.2144
19	HOMO-15	A	-14.3454

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2401190	-1.3986652	0.0000236
C	-2.4257456	-0.7064589	-0.0000163
C	-2.4257455	0.7064589	-0.0000245
C	-1.2401189	1.3986651	0.0000155
C	0.0000000	0.7136890	0.0000487
C	0.0000000	-0.7136891	0.0000482
C	1.2401190	-1.3986652	0.0000162
C	1.2401189	1.3986651	0.0000249
C	2.4257455	0.7064589	-0.0000165
C	2.4257456	-0.7064589	-0.0000247
H	-1.2360956	-2.4857078	0.0000366
H	-3.3697021	-1.2435414	-0.0000442
H	-3.3697019	1.2435415	-0.0000637
H	-1.2360954	2.4857078	0.0000215
H	1.2360956	-2.4857078	0.0000257
H	1.2360954	2.4857078	0.0000403
H	3.3697019	1.2435415	-0.0000460
H	3.3697021	-1.2435414	-0.0000653

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]

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