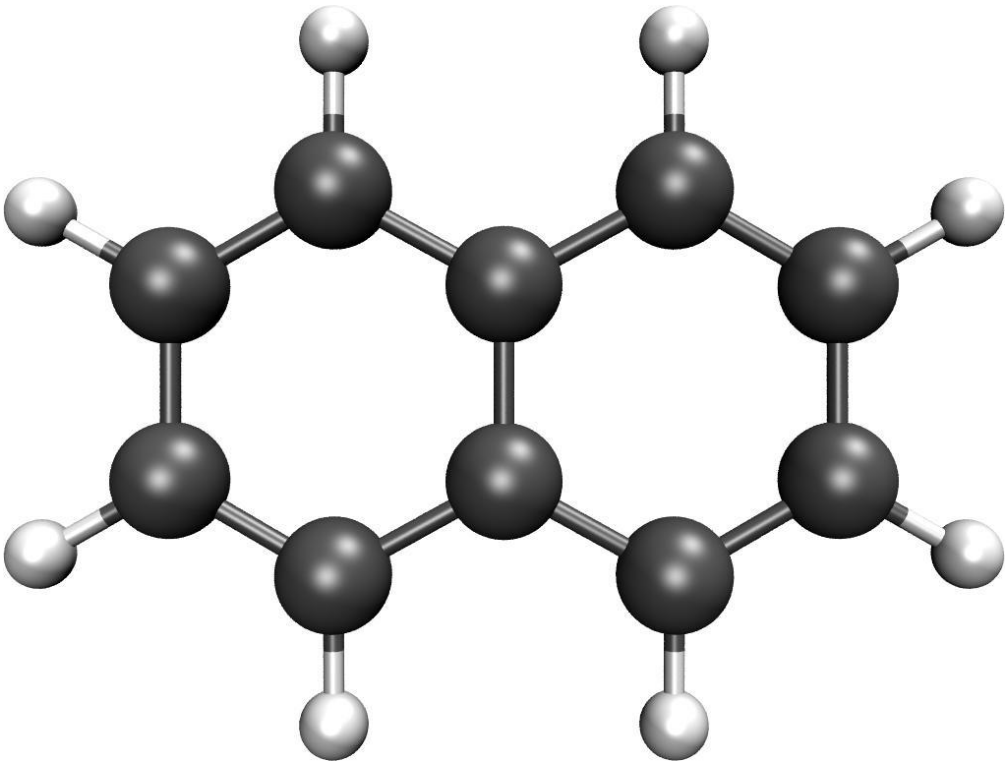
THE Zysman-Colman GROUP

Calculation Report

Naphthalene

Optimisation, Frequencies (Singlet)



Summary of Results

Metadata

Username:	osl
Date:	07/06/2022 16:39:10
Duration:	4 m, 57 s
Success:	True
Converged:	True
Computational package:	Gaussian (2016+C.01)
Methods:	DFT
Functional:	PBE1PBE
Basis set:	6-31G(d,p)
Calculations:	Optimisation, Frequencies
Orbital spin:	restricted
Multiplicity:	1 (singlet)
Calc temperature:	298.15 K
Calc pressure:	1.0 atm

SCF Energies

No. of steps:	5
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

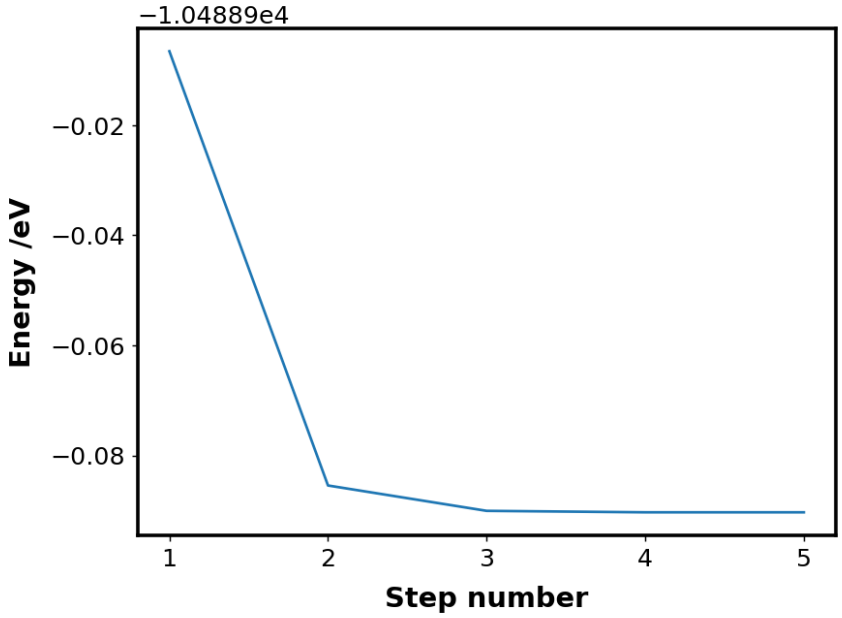
Permanent Dipole Moment

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

Vibrational Frequencies

Negative frequencies:	0

SCF Energies



SCF Energies

No. of steps: 5

Final energy: -10488.9903 eV

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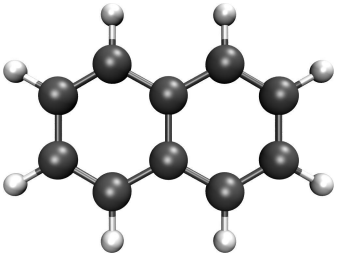
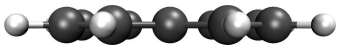
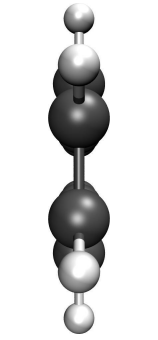
Geometry



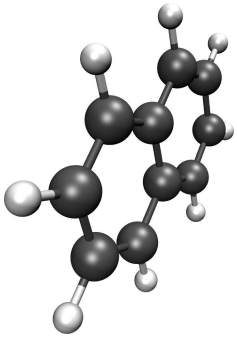
X/Y plane



X/Z plane



Z/Y plane



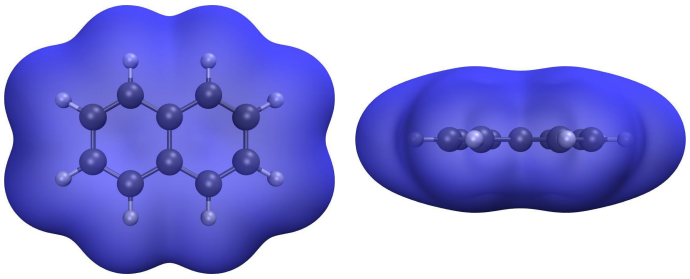
45° to axes

Aligned structure

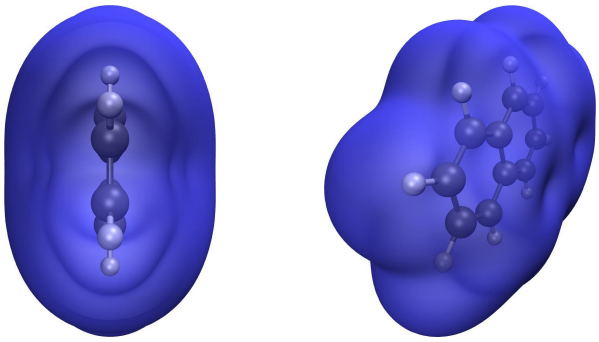
Geometry

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



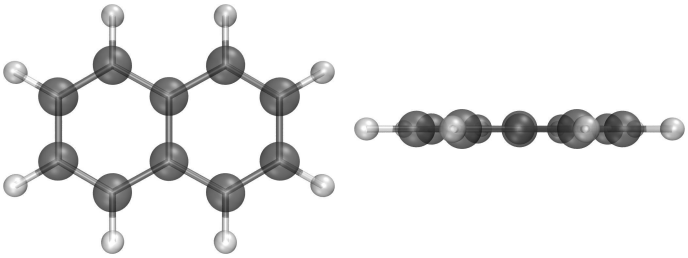
X/Y plane | X/Z plane



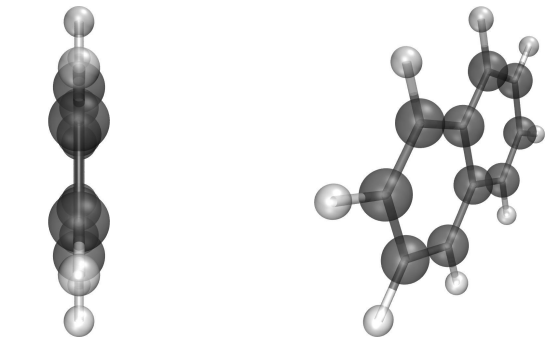
Z/Y plane | 45° to axes

SCF density (isovalue: 0.0004)

Permanent Dipole Moment



X/Y plane | X/Z plane



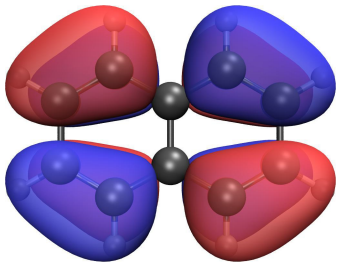
Z/Y plane | 45° to axes

Aligned structure (dipole moment in red)

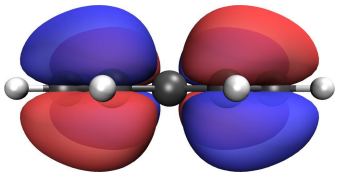
Dipole Moment

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 °

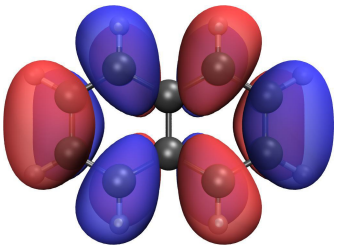
HOMO & LUMO



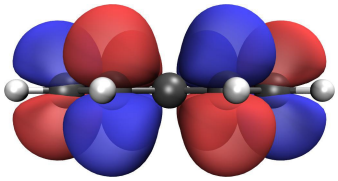
X/Y plane



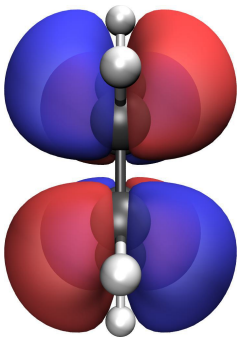
X/Z plane



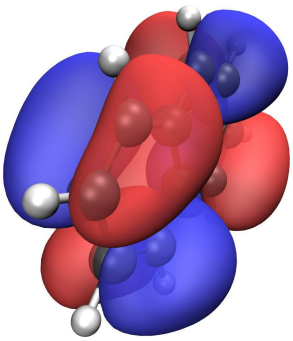
X/Y plane



X/Z plane

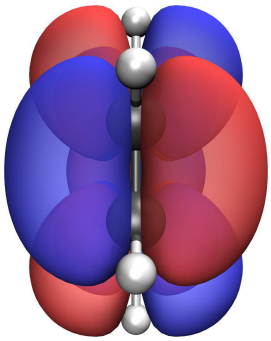


Z/Y plane

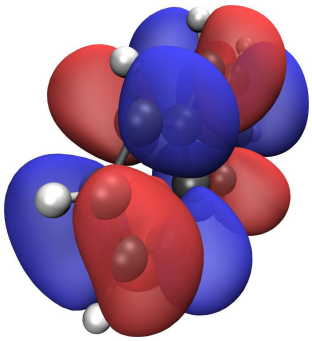


45° to axes

HOMO density (isovalue: 0.02)

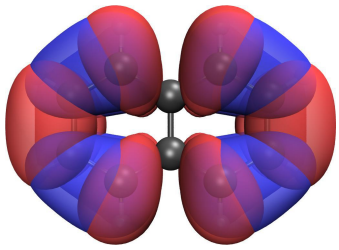


Z/Y plane

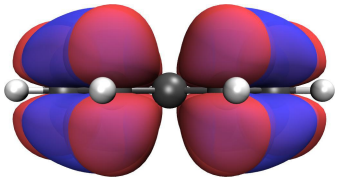


45° to axes

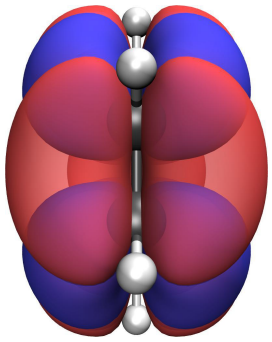
LUMO density (isovalue: 0.02)



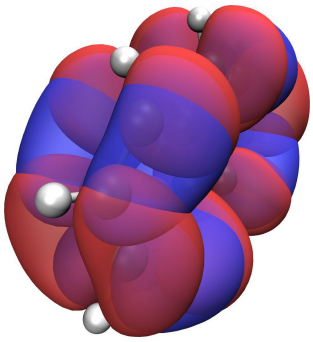
X/Y plane



X/Z plane

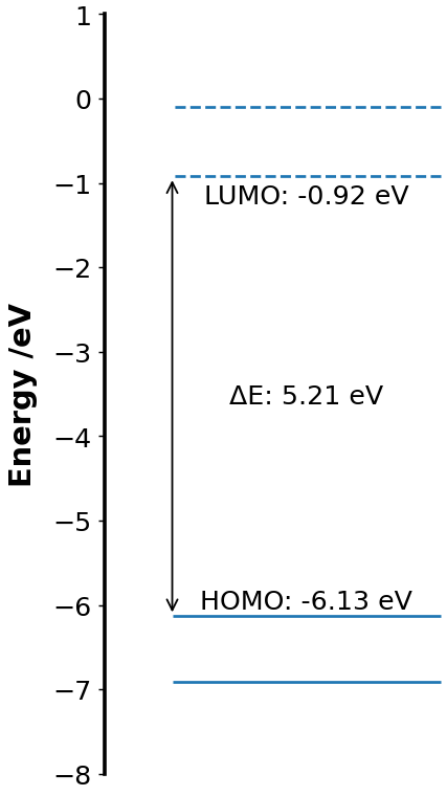


Z/Y plane

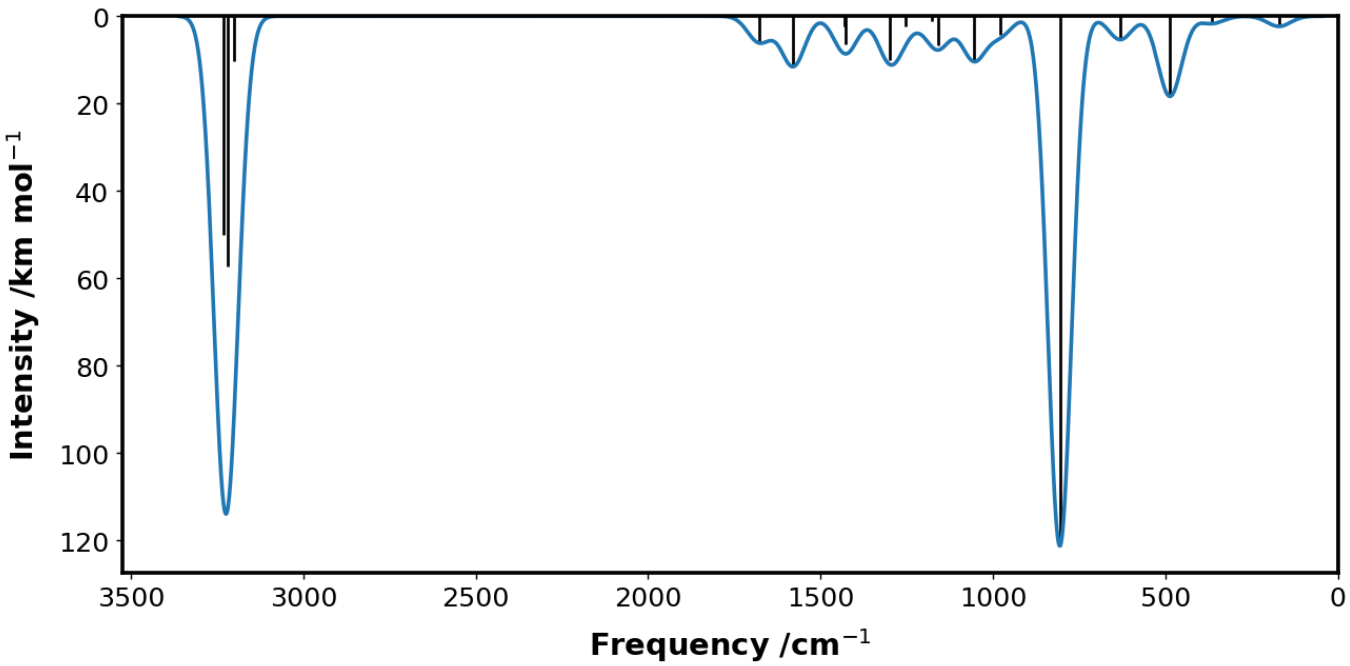


45° to axes

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



Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm^{-1})
Peaks /cm^{-1}: 170, 368, 487, 631, 806, 1053, 1160, 1294, 1427, 1580, 1673, 3224.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm^{-1}	Intensity /km mol^{-1}
1	A	170.6603	2.3323
2	A	186.3677	0.0000
3	A	365.1609	1.6874
4	A	393.2304	0.0000
5	A	477.4391	0.0000
6	A	486.8646	18.3491
7	A	516.9575	0.0000
8	A	522.9547	0.0000
9	A	631.0734	5.3597
10	A	636.2303	0.0000
11	A	734.4453	0.0000
12	A	783.2293	0.0000
13	A	787.4275	0.0000
14	A	806.2853	121.0015
15	A	809.4087	0.2244
16	A	856.6594	0.0000
17	A	901.2132	0.0000
18	A	947.6833	0.0000
19	A	961.3577	0.0000
20	A	978.7553	4.2681
21	A	999.1135	0.0000
22	A	1006.5492	0.0000
23	A	1055.4957	10.0015
24	A	1066.4428	0.0000
25	A	1158.3757	6.7028
26	A	1178.7603	1.0658
27	A	1179.8776	0.0000
28	A	1188.4321	0.0000
29	A	1254.2980	2.4273
30	A	1274.8273	0.0000
31	A	1299.2065	10.0549
32	A	1426.1623	6.3760
33	A	1430.5870	2.2480
34	A	1451.2573	0.0000

35	A	1508.0715	0.0000
36	A	1510.3663	0.0000
37	A	1579.8388	11.4633
38	A	1655.4851	0.0000
39	A	1677.4730	5.9807
40	A	1714.4767	0.0000
41	A	3201.3483	0.0000
42	A	3202.4466	10.2646
43	A	3204.6890	0.2493
44	A	3207.0173	0.0000
45	A	3220.0583	0.0000
46	A	3220.5827	57.2959
47	A	3232.8358	49.9545
48	A	3233.8528	0.0000

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
50	LUMO+15	A	8.6396
49	LUMO+14	A	7.9114
48	LUMO+13	A	6.9152
47	LUMO+12	A	6.0692
46	LUMO+11	A	5.7949
45	LUMO+10	A	5.3487
44	LUMO+9	A	5.1506
43	LUMO+8	A	5.0034
42	LUMO+7	A	4.9519
41	LUMO+6	A	3.6912
40	LUMO+5	A	3.4207
39	LUMO+4	A	2.9674
38	LUMO+3	A	2.9127
37	LUMO+2	A	1.0612
36	LUMO+1	A	-0.1010
35	**LUMO**	**A**	**-0.9244**
34	**HOMO**	**A**	**-6.1307**
33	HOMO-1	A	-6.9087
32	HOMO-2	A	-8.0747
31	HOMO-3	A	-9.1879
30	HOMO-4	A	-9.2562
29	HOMO-5	A	-9.4032
28	HOMO-6	A	-10.2679
27	HOMO-7	A	-11.0274
26	HOMO-8	A	-11.1363
25	HOMO-9	A	-11.5961
24	HOMO-10	A	-11.6187
23	HOMO-11	A	-12.3015
22	HOMO-12	A	-12.4753
21	HOMO-13	A	-13.7777
20	HOMO-14	A	-14.2411
19	HOMO-15	A	-14.3709

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2404550	-1.3991360	-0.0000000
C	-2.4260000	-0.7066350	-0.0000000
C	-2.4260000	0.7066350	0.0000010
C	-1.2404550	1.3991360	0.0000010
C	0.0000000	0.7142260	-0.0000010
C	0.0000000	-0.7142260	-0.0000010
C	1.2404550	-1.3991360	0.0000010
C	1.2404550	1.3991360	-0.0000000
C	2.4260000	0.7066350	-0.0000000
C	2.4260000	-0.7066350	0.0000010
H	-1.2366960	-2.4861970	-0.0000030
H	-3.3696970	-1.2439660	0.0000010
H	-3.3696970	1.2439660	-0.0000010
H	-1.2366960	2.4861970	0.0000000
H	1.2366960	-2.4861970	0.0000000
H	1.2366960	2.4861970	-0.0000030
H	3.3696970	1.2439660	0.0000010
H	3.3696970	-1.2439660	-0.0000010

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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