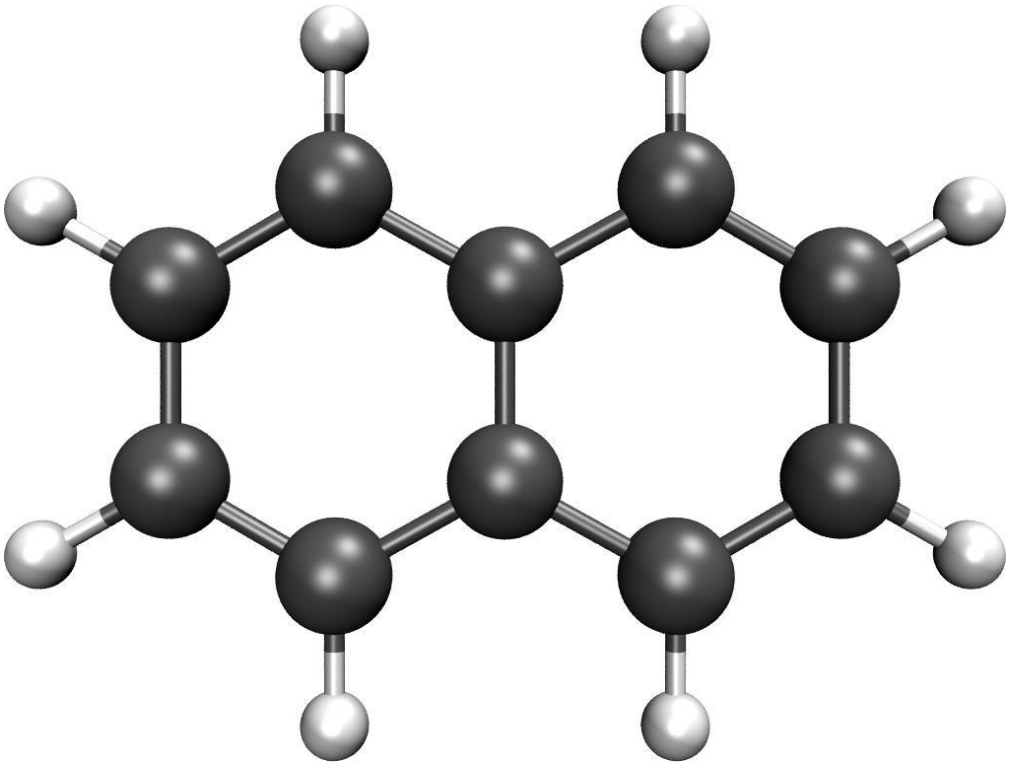
THE Zysman-Colman GROUP

Calculation Report

Naphthalene

Excited States (Singlet)



Summary of Results

Metadata

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)

SCF Energies

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

MP Energies

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

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

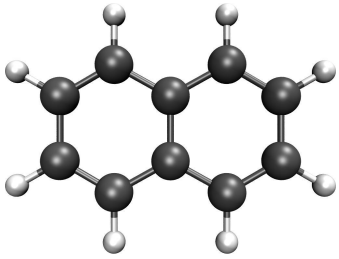
Permanent Dipole Moment

Total:	0.00 D
X axis angle:	90.00 °
XY plane angle:	75.96 °

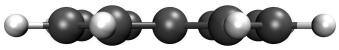
Excited States

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
No. of singlets:	2

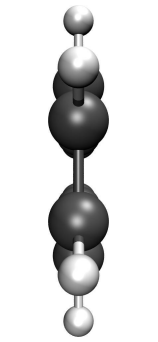
Geometry



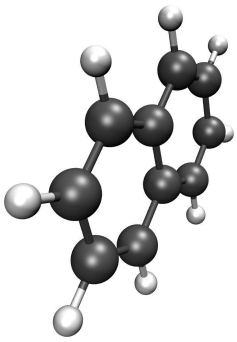
X/Y plane



X/Z plane



Z/Y plane



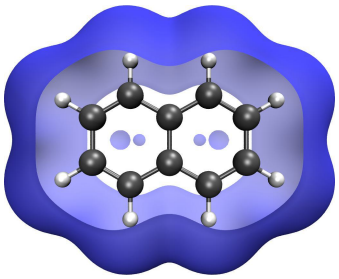
45° to axes

Aligned structure

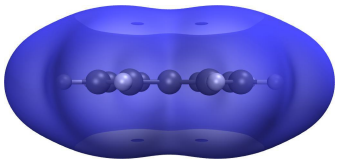
Geometry

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

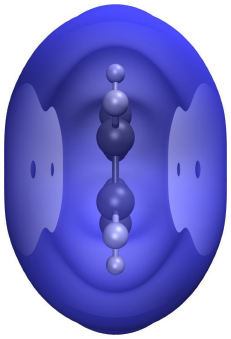
SCF Density



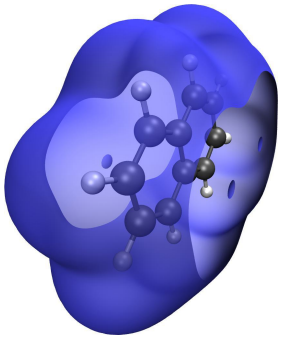
X/Y plane



X/Z plane



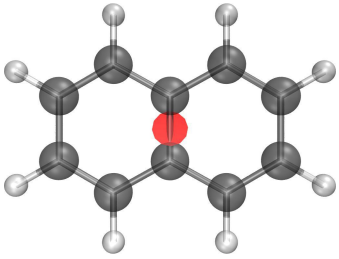
Z/Y plane



45° to axes

SCF density (isovalue: 0.0004)

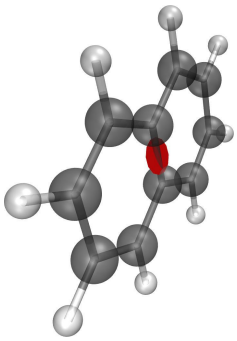
Permanent Dipole Moment



X/Y plane

X/Z plane

Z/Y plane



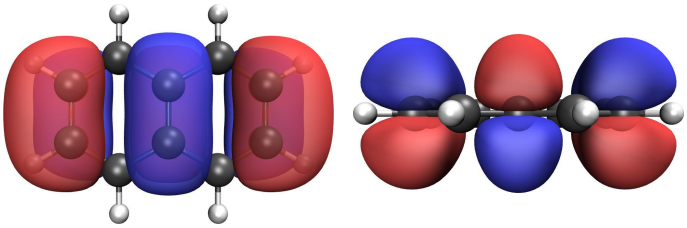
45° to axes

Aligned structure (dipole moment in red)

Dipole Moment

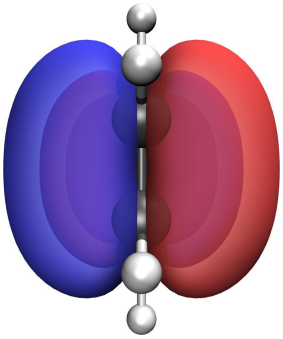
Origin X:	0.00 D
Origin Y:	0.00 D
Origin Z:	0.00 D
Vector X:	0.00 D
Vector Y:	0.00 D
Vector Z:	0.00 D
Total:	0.00 D
X axis angle:	90.00 °
XY plane angle:	75.96 °

HOMO-1

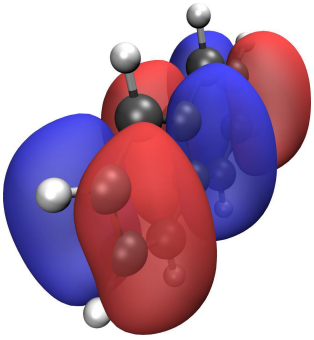


X/Y plane

X/Z plane



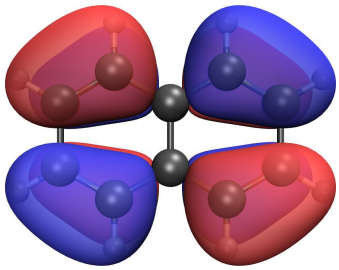
Z/Y plane



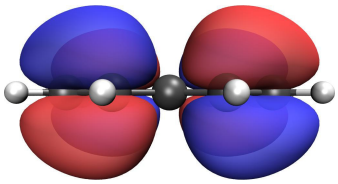
45° to axes

HOMO-1 density (isovalue: 0.02)

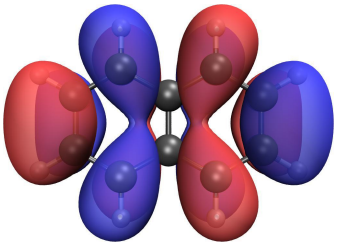
HOMO & LUMO



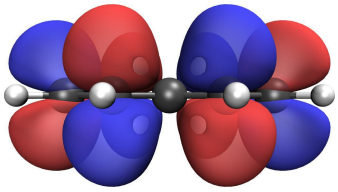
X/Y plane



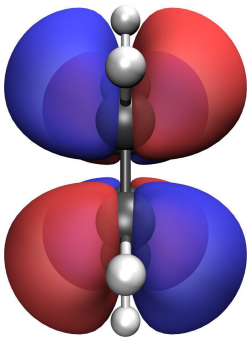
X/Z plane



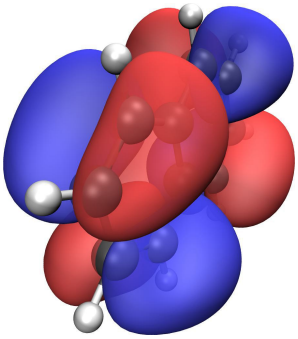
X/Y plane



X/Z plane

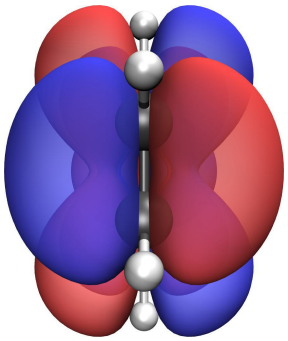


Z/Y plane

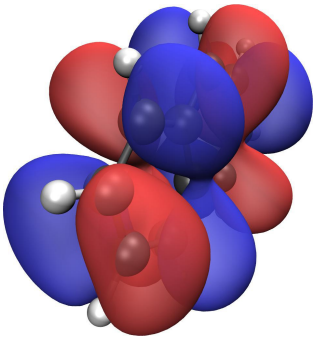


45° to axes

HOMO density (isovalue: 0.02)

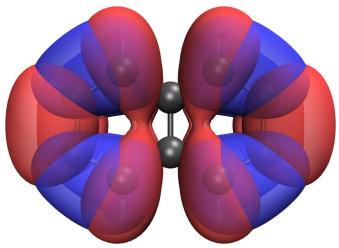


Z/Y plane

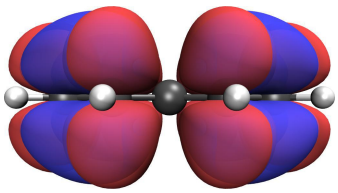


45° to axes

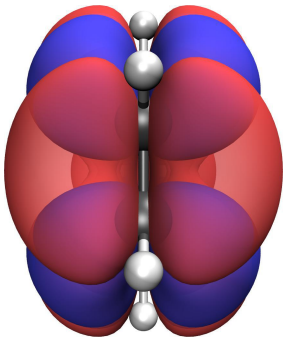
LUMO density (isovalue: 0.02)



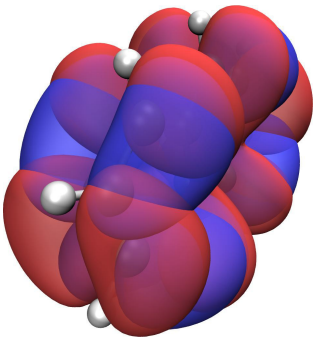
X/Y plane



X/Z plane

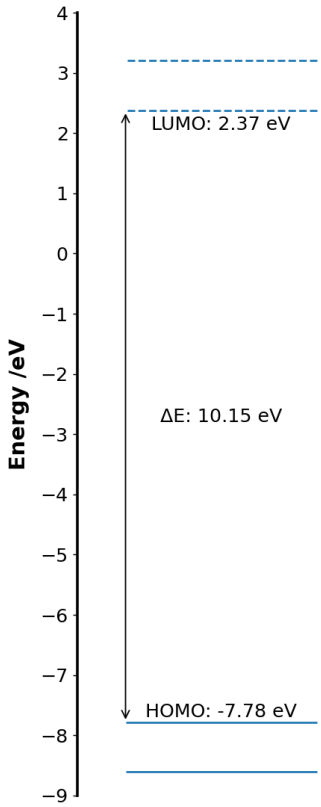


Z/Y plane

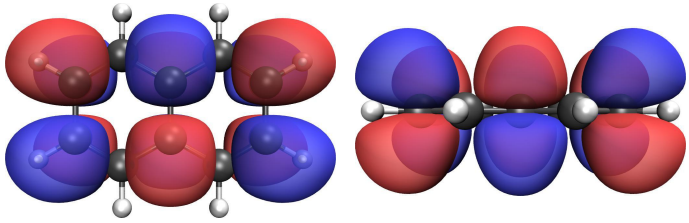


45° to axes

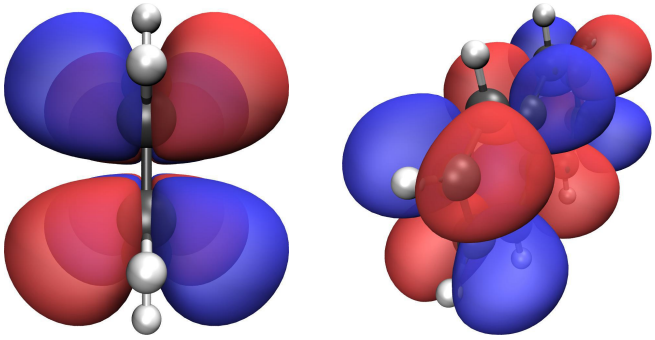
HOMO (blue) & LUMO (red) density (isovalue: 0.02)



LUMO+1



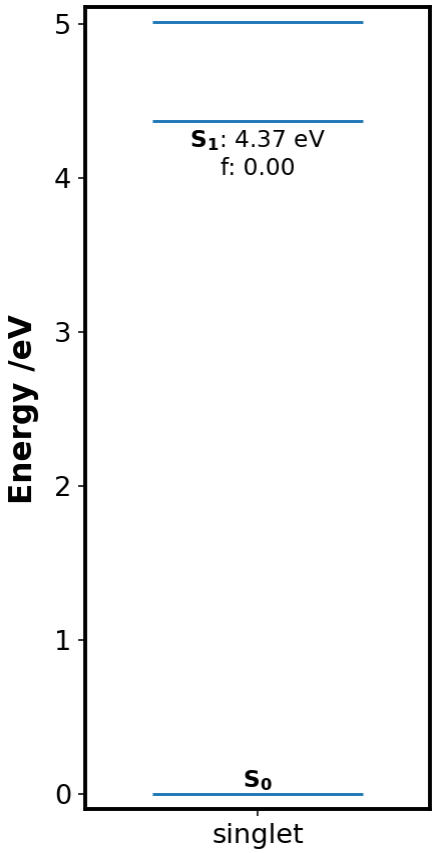
X/Y plane | X/Z plane



Z/Y plane | 45° to axes

LUMO+1 density (isovalue: 0.02)

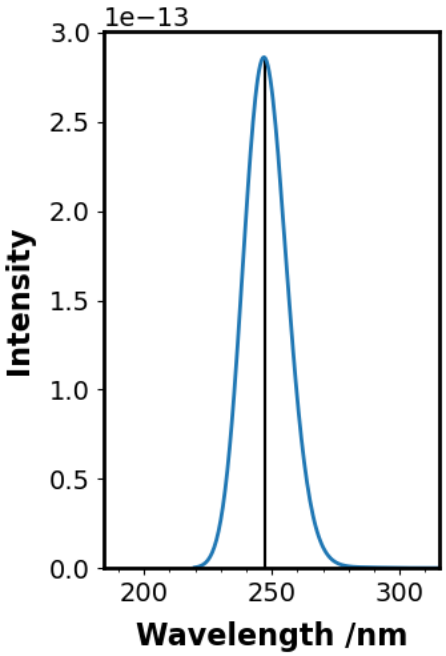
Excited States



Excited States

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
No. of singlets:	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	S_1	Singlet-A	4.3707	283.67	Ultraviolet [redacted] (0.00, 0.00)	0.0002	HOMO-1 → LUMO (0.49) HOMO → LUMO+1 (0.48)
2	S_2	Singlet-A	5.0100	247.47	Ultraviolet [redacted] (0.00, 0.00)	0.0880	HOMO → LUMO (0.90) HOMO-1 → LUMO+1 (0.08)

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
50	LUMO+15	A	11.9600
49	LUMO+14	A	11.7353
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	-15.7422
24	HOMO-10	A	-15.7464
23	HOMO-11	A	-16.4964
22	HOMO-12	A	-16.8787
21	HOMO-13	A	-18.2419
20	HOMO-14	A	-18.8268
19	HOMO-15	A	-19.1551

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.2509100	-1.4118100	-0.0000100
C	-2.4487500	-0.7132700	0.0000100
C	-2.4487500	0.7132700	0.0000100
C	-1.2509100	1.4118100	-0.0000100
C	-0.0000000	0.7179300	-0.0000200
C	-0.0000000	-0.7179400	-0.0000200
C	1.2509100	-1.4118100	-0.0000100
C	1.2509100	1.4118100	-0.0000100
C	2.4487500	0.7132700	0.0000100
C	2.4487500	-0.7132700	0.0000100
H	-1.2480900	-2.5080700	-0.0000100
H	-3.4000100	-1.2561900	0.0000200
H	-3.4000100	1.2561900	0.0000300
H	-1.2480900	2.5080700	-0.0000100
H	1.2480900	-2.5080700	-0.0000100
H	1.2480900	2.5080700	-0.0000200
H	3.4000100	1.2561900	0.0000300
H	3.4000100	-1.2561900	0.0000200

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

[1] N. M. O'boyle, A. L. Tenderholt and K. M. Langner, *Journal of Computational Chemistry,* 2008, **29,** 839--845

[2] W. Humphrey, A. Dalke and K. Schulten, *Journal of Molecular Graphics,* 1996, **14,** 33--38

[3] J. Stone, Masters Thesis, Computer Science Department, University of Missouri-Rolla, 1998

[4] J. D. Hunter, *Computing in Science & Engineering,* 2007, **9,** 90--95

[5] T. Mansencal, M. Mauderer, M. Parsons, N. Shaw, K. Wheatley, S. Cooper, J. D. Vandenberg, L. Canavan, K. Crowson, O. Lev, K. Leinweber, S. Sharma, T. J. Sobotka, D. Moritz, M. Pppp, C. Rane, P. Eswaramoorthy, J. Mertic, B. Pearlstine, M. Leonhardt, O. Niemitalo, M. Szymanski and M. Schambach, Colour 0.3.15, Zenodo, 2020

[6] M. Bayer, https://www.makotemplates.org, (accessed May 2020)

[7] K. Community, https://weasyprint.org, (accessed May 2020)

[8] P. Virtanen, R. Gommers, T. E. Oliphant, M. Haberland, T. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, K. Jarrod Millman, N. Mayorov, A. R. J. Nelson, E. Jones, R. Kern, E. Larson, C. Carey, İ. Polat, Y. Feng, E. W. Moore, J. Vand erPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt and S. 1. 0. Contributors, *Nature Methods,* 2020, **17,** 261--272

[9] N. M. O'Boyle, C. Morley and G. R. Hutchison, *Chemistry Central Journal,* 2008, **2,** 5

[10] N. M. O'Boyle, M. Banck, C. A. James, C. Morley, T. Vandermeersch and G. R. Hutchison, *Journal of Cheminformatics,* 2011, **3,** 33

[11] X. Gao, S. Bai, D. Fazzi, T. Niehaus, M. Barbatti and W. Thiel, *Journal of Chemical Theory and Computation,* 2017, **13,** 515--524

[12] G. Landrum, https://www.rdkit.org/, (accessed February 2022)

[13] M. McKerns, L. Strand, T. Sullivan, A. Fang and M. Aivazis, *Proceedings of the 10th Python in Science Conference,* 2011,

[14] M. McKerns and M. Aivazis, https://uqfoundation.github.io/project/pathos, (accessed February 2022)

[15] K. Shizu and H. Kaji, *The Journal of Physical Chemistry A,* 2021, **125,** 9000--9010