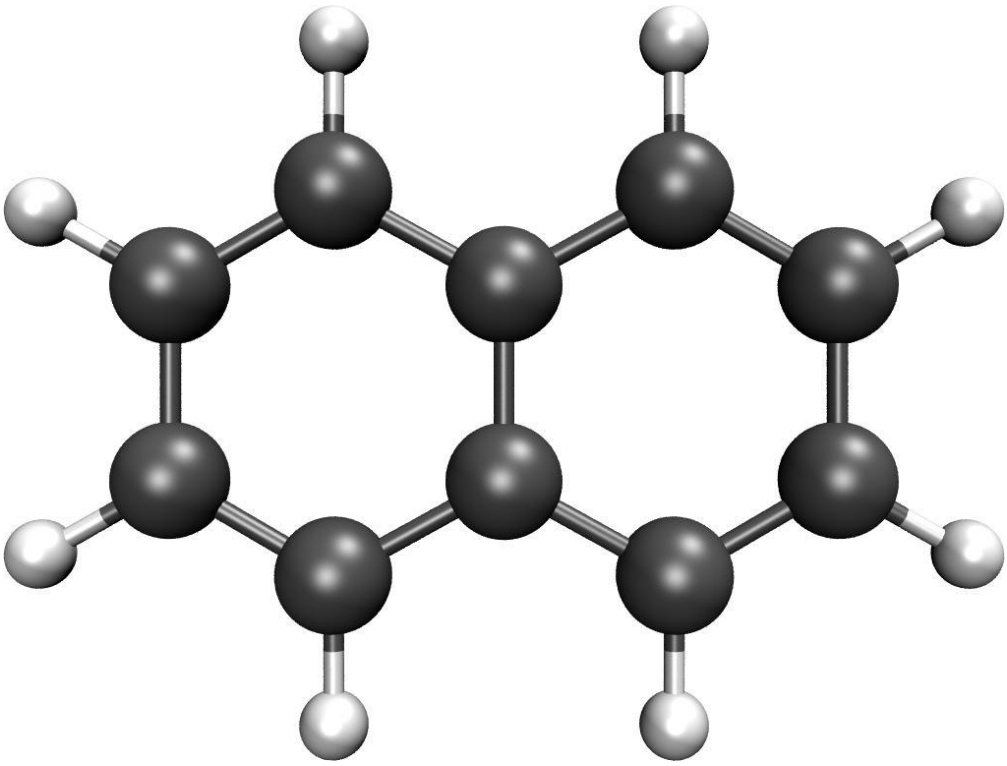
THE Zysman-Colman GROUP

Calculation Report

Naphthalene

Single Point (Singlet)



Summary of Results

Metadata

Username:	osl
Date:	21/06/2022 17:25:47
Duration:	10 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

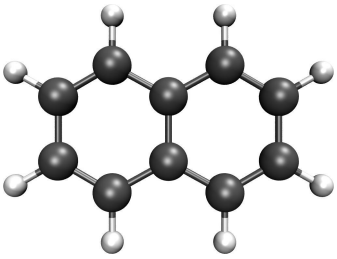
HOMO & LUMO

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

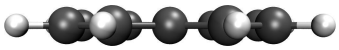
Permanent Dipole Moment

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

Geometry

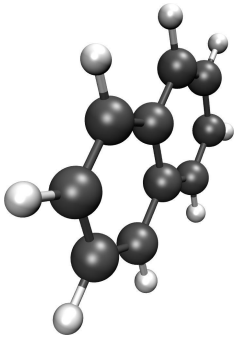


X/Y plane



X/Z plane

Z/Y plane



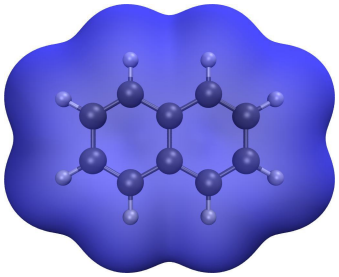
45° to axes

Aligned structure

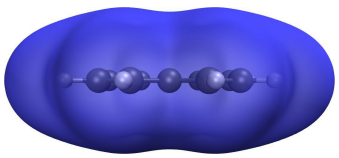
Geometry

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

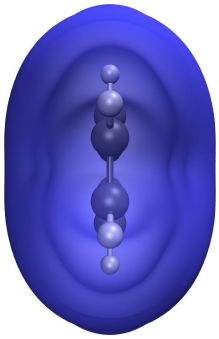
SCF Density



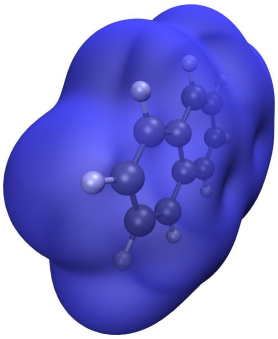
X/Y plane



X/Z plane



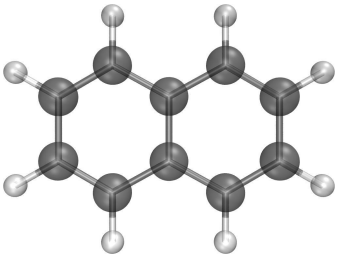
Z/Y plane



45° to axes

SCF density (isovalue: 0.0004)

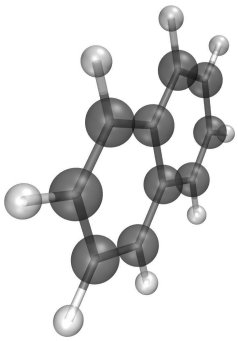
Permanent Dipole Moment



X/Y plane

X/Z plane

Z/Y plane



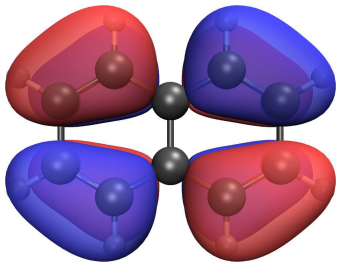
45° to axes

Aligned structure (dipole moment in red)

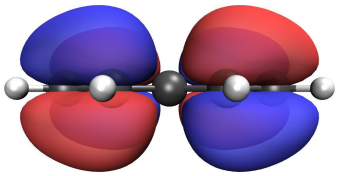
Dipole Moment

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 °

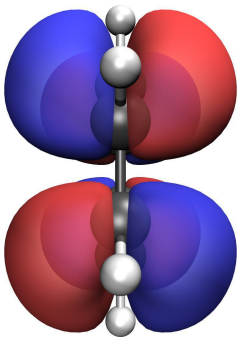
HOMO & LUMO



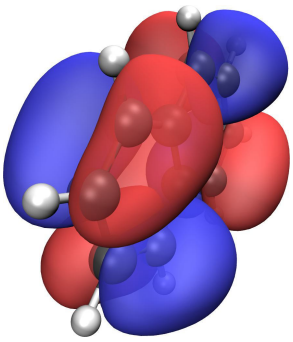
X/Y plane



X/Z plane

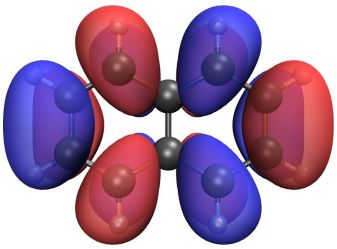


Z/Y plane

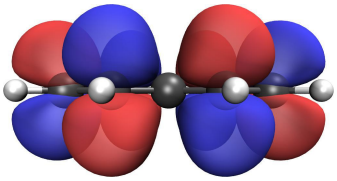


45° to axes

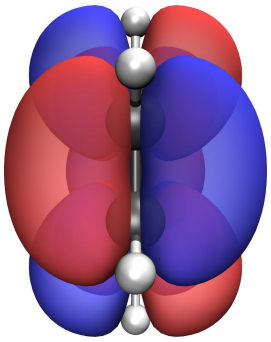
HOMO density (isovalue: 0.02)



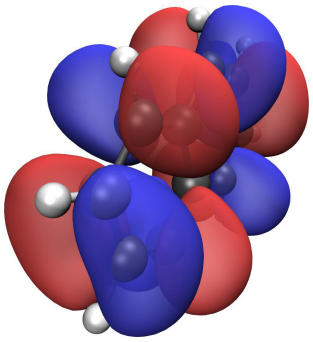
X/Y plane



X/Z plane

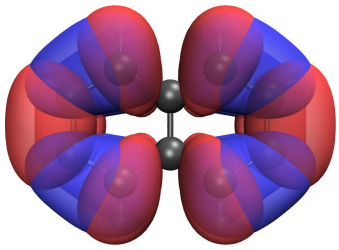


Z/Y plane

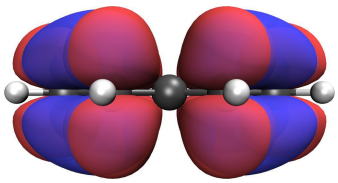


45° to axes

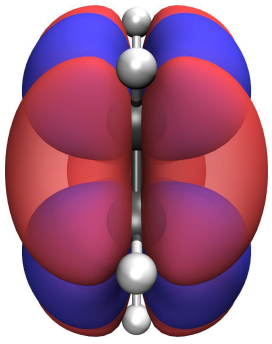
LUMO density (isovalue: 0.02)



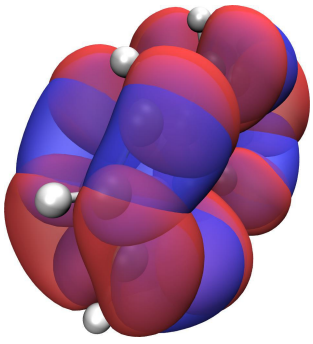
X/Y plane



X/Z plane



Z/Y plane



45° to axes

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

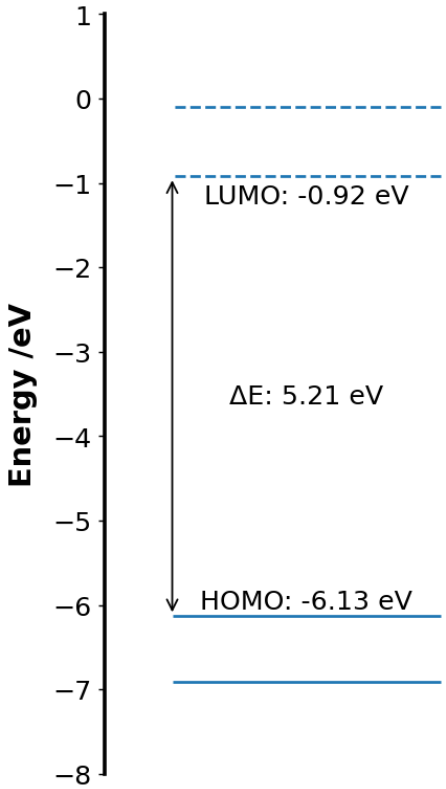


Table of Selected Molecular Orbitals

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.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

[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