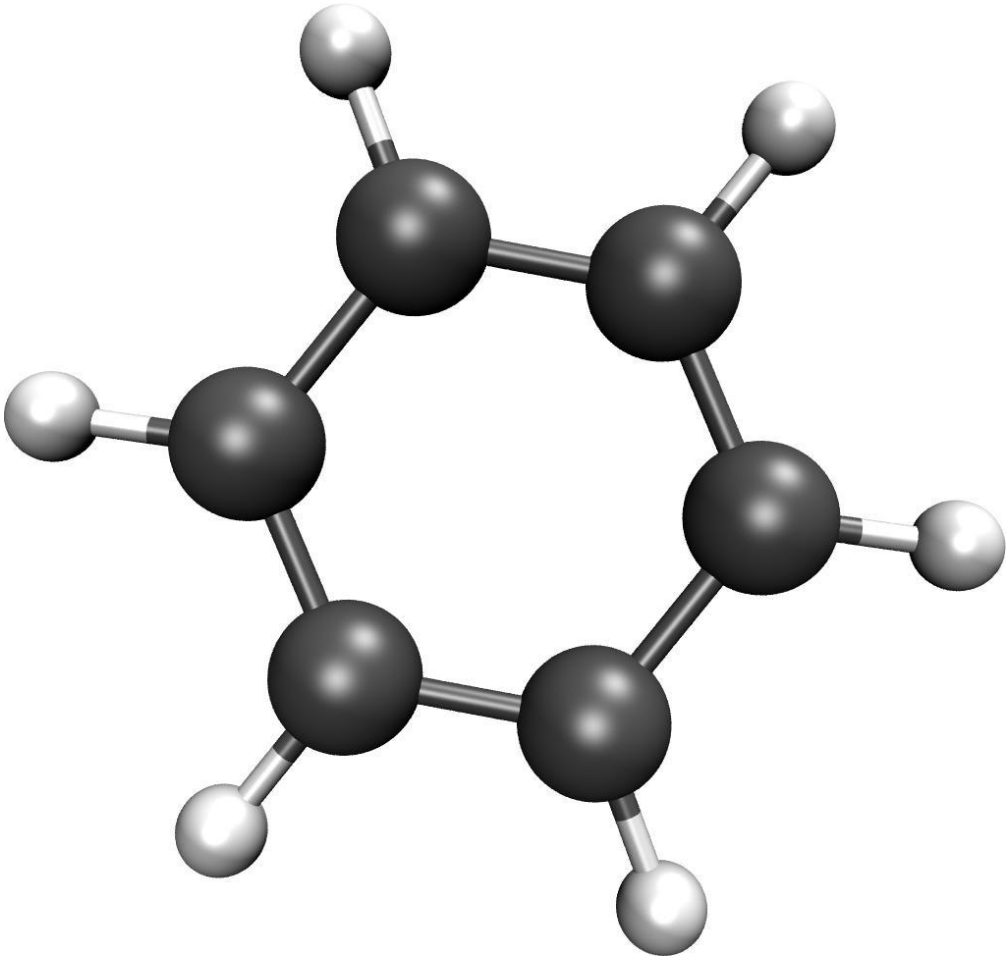
THE Zysman-Colman GROUP

Calculation Report

Benzene

Optimisation, Frequencies (Doublet)



Summary of Results

Metadata

Username:	osl
Date:	24/06/2022 12:21:56
Duration:	2 m, 12 s
Success:	True
Converged:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Optimisation, Frequencies
Orbital spin:	unrestricted
Multiplicity:	2 (doublet)

SCF Energies

No. of steps:	24
Final energy:	-6310.4572 eV
Final energy:	-608,867 $kJmol^{-1}$

Geometry

Formula:	$C_6H_6^-$
Molar mass:	78.1118 $gmol^{-1}$
Alignment method:	Minimal
X extension:	4.98 Å
Y extension:	4.72 Å
Z extension:	0.05 Å
Linearity ratio:	0.05
Planarity ratio:	0.99

HOMO & LUMO (alpha)

$E_{HOMO,LUMO}$:	2.45 eV
E_{HOMO}:	3.83 eV
E_{LUMO}:	6.28 eV

HOMO & LUMO (beta)

$E_{HOMO,LUMO}$:	6.38 eV
E_{HOMO}:	0.00 eV
E_{LUMO}:	6.39 eV

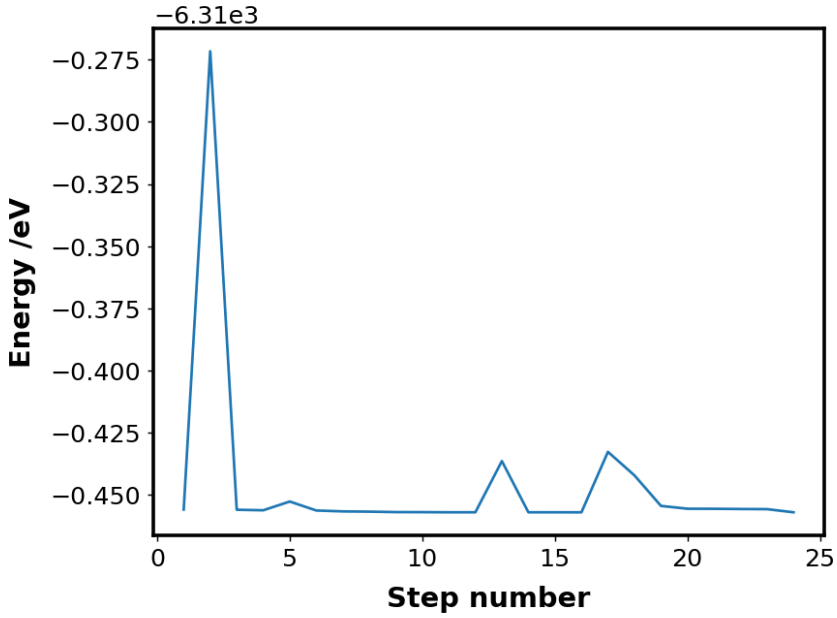
Permanent Dipole Moment

Total:	0.04 D
X axis angle:	49.10 °
XY plane angle:	4.17 °

Vibrational Frequencies

Negative frequencies:	0

SCF Energies



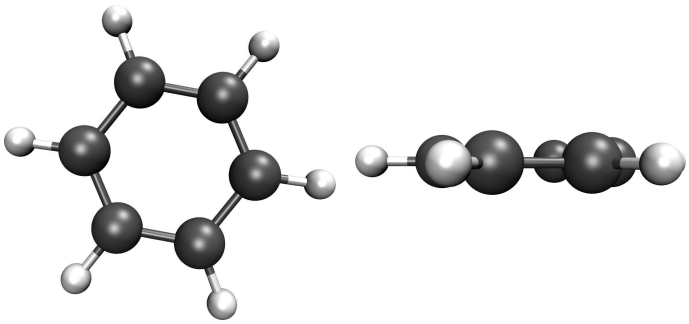
SCF Energies

No. of steps: 24

Final energy: -6310.4572 eV

Final energy: -608,867 kJmol^{-1}

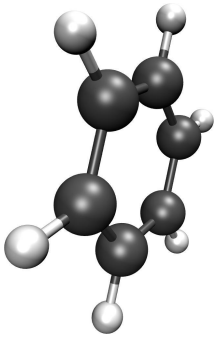
Geometry



X/Y plane

X/Z plane

Z/Y plane



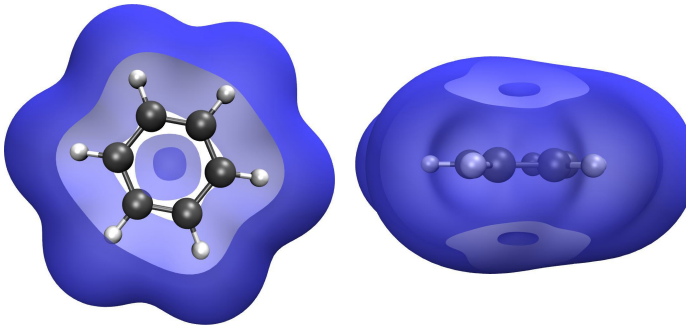
45° to axes

Aligned structure

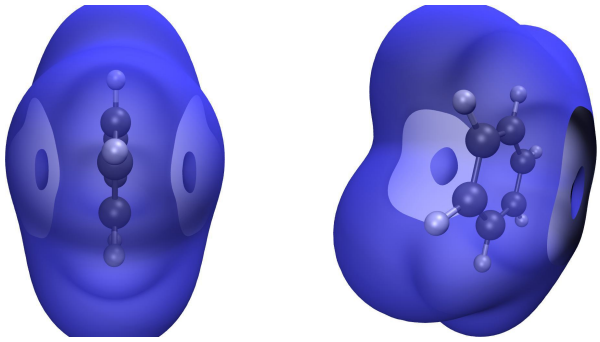
Geometry

Formula:	$C_6H_6^-$
Molar mass:	78.1118 gmol^{-1}
Alignment method:	Minimal
X extension:	4.98 Å
Y extension:	4.72 Å
Z extension:	0.05 Å
Linearity ratio:	0.05
Planarity ratio:	0.99

SCF Density



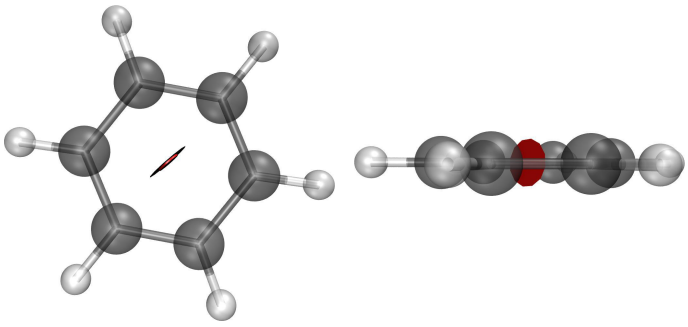
X/Y plane | X/Z plane



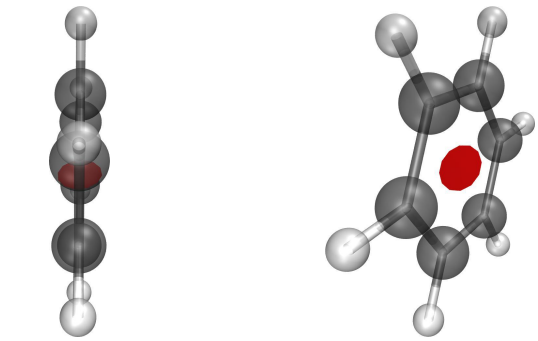
Z/Y plane | 45° to axes

SCF density (isovalue: 0.0004)

Permanent Dipole Moment



X/Y plane | X/Z plane



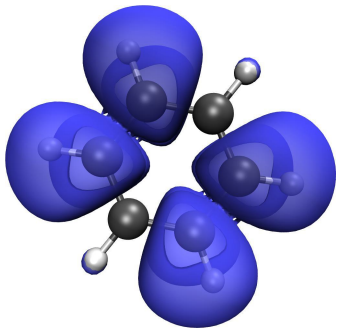
Z/Y plane | 45° to axes

Aligned structure (dipole moment in red)

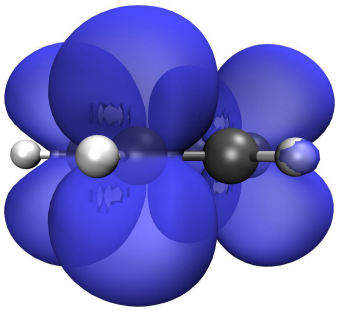
Dipole Moment

Origin X:	0.00 D
Origin Y:	0.00 D
Origin Z:	0.00 D
Vector X:	-0.02 D
Vector Y:	0.03 D
Vector Z:	-0.00 D
Total:	0.04 D
X axis angle:	49.10 °
XY plane angle:	4.17 °

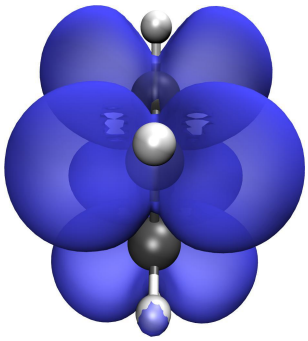
Spin Density



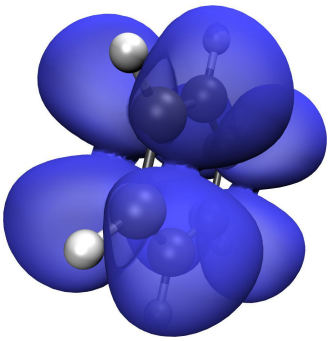
X/Y plane



X/Z plane

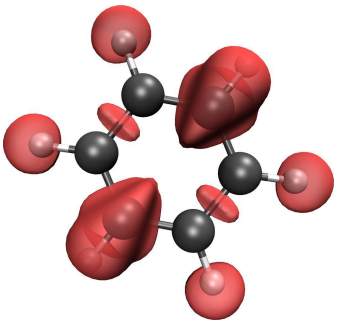


Z/Y plane

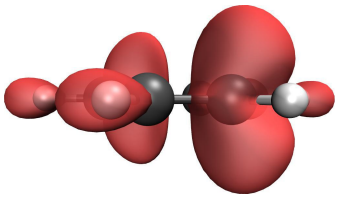


45° to axes

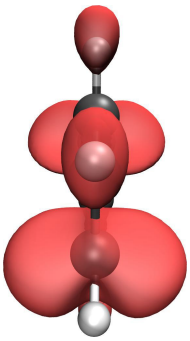
Positive spin density (electron) (isovalue: 0.0004)



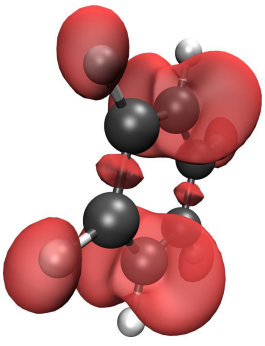
X/Y plane



X/Z plane

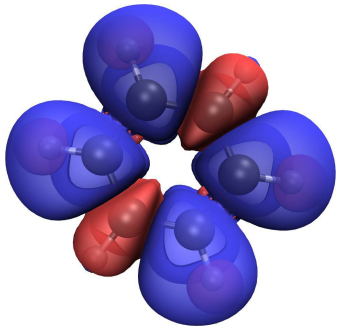


Z/Y plane

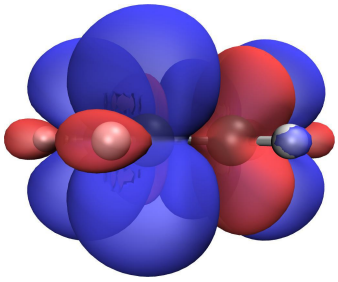


45° to axes

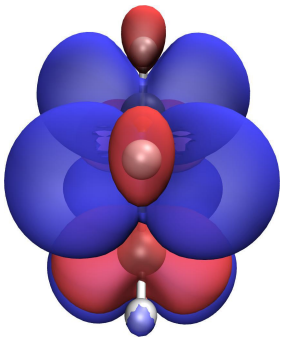
Negative spin density (hole) (isovalue: 0.0004)



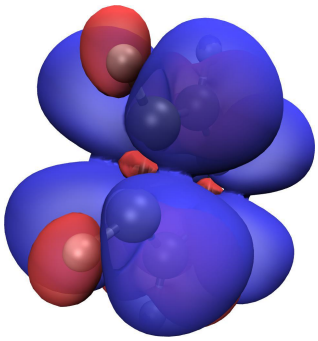
X/Y plane



X/Z plane



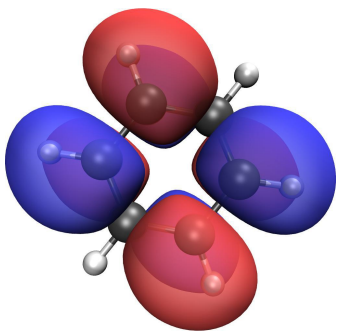
Z/Y plane



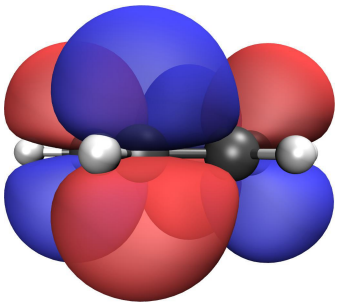
45° to axes

Positive (electron) (blue) & negative (hole) (red) spin density (isovalue: 0.0004)

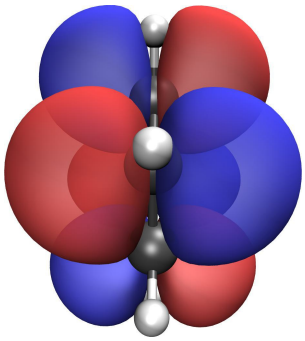
HOMO & LUMO (Alpha)



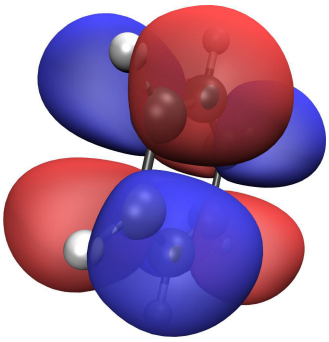
X/Y plane



X/Z plane

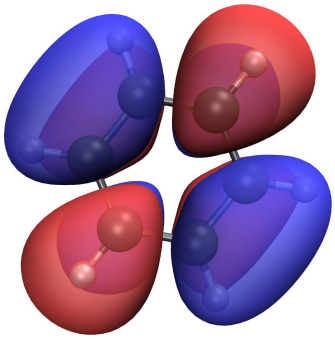


Z/Y plane

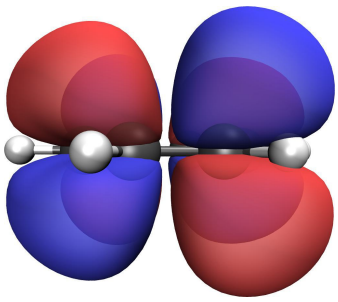


45° to axes

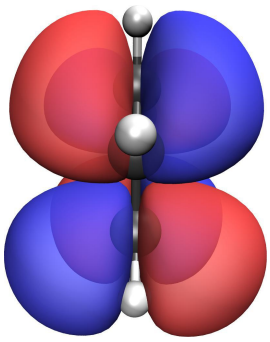
HOMO density (isovalue: 0.02)



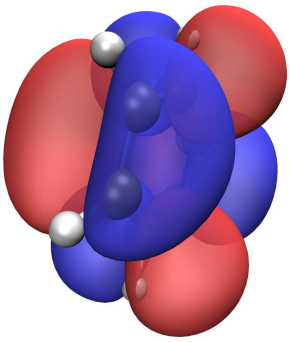
X/Y plane



X/Z plane

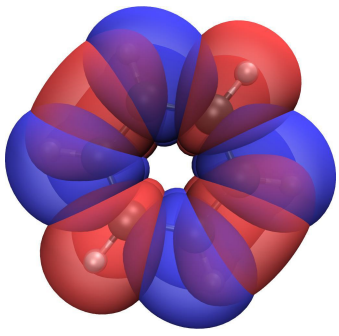


Z/Y plane

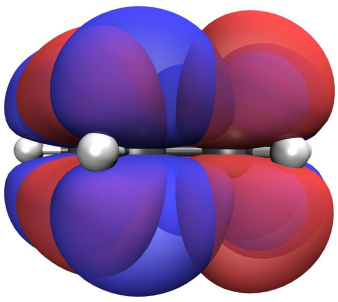


45° to axes

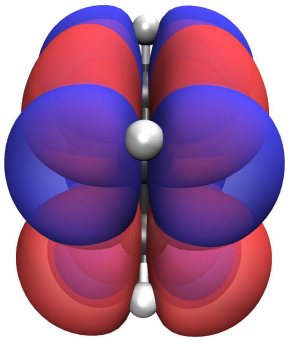
LUMO density (isovalue: 0.02)



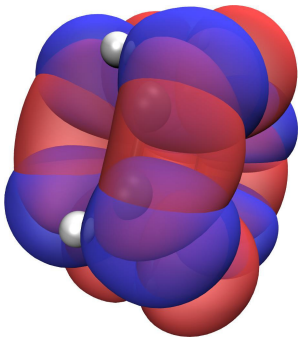
X/Y plane



X/Z plane

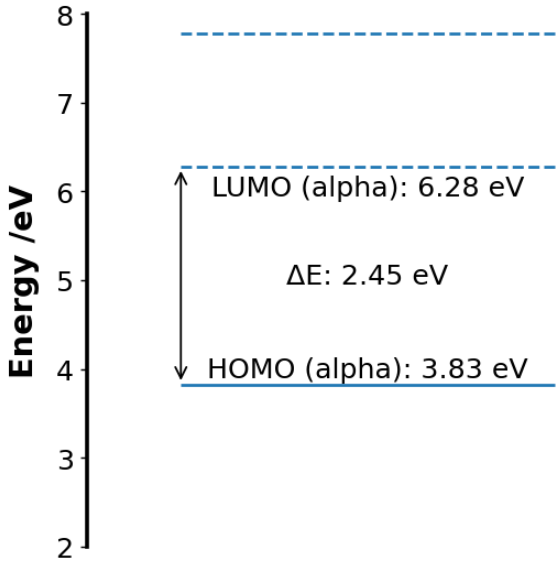


Z/Y plane

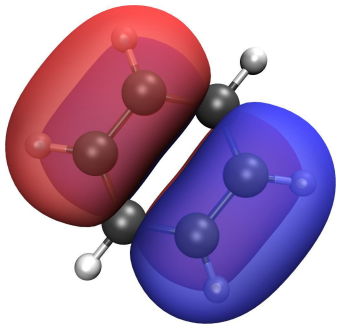


45° to axes

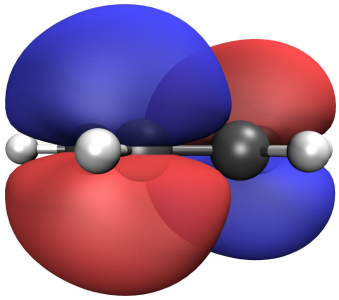
HOMO (blue) & LUMO (red) density (isovalue: 0.02)



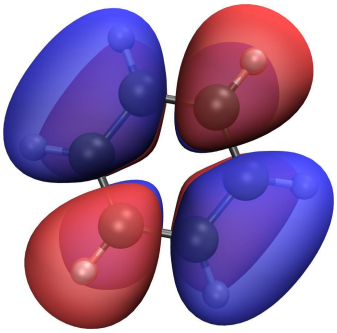
HOMO & LUMO (Beta)



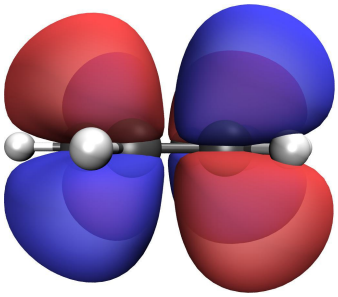
X/Y plane



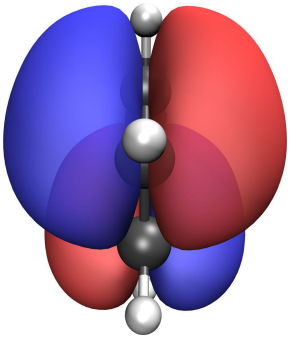
X/Z plane



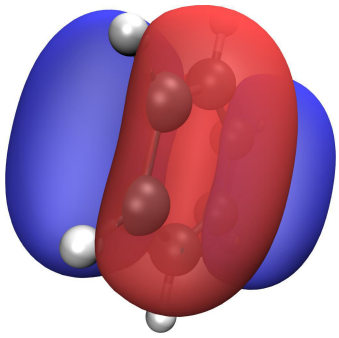
X/Y plane



X/Z plane

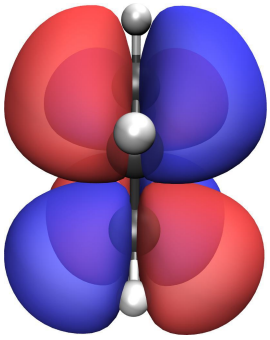


Z/Y plane

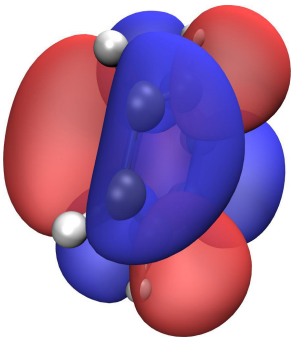


45° to axes

HOMO density (isovalue: 0.02)

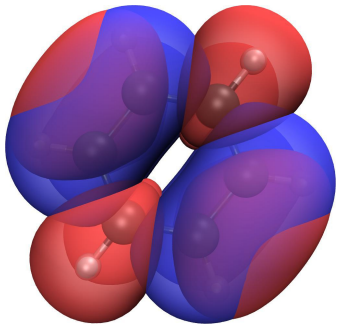


Z/Y plane

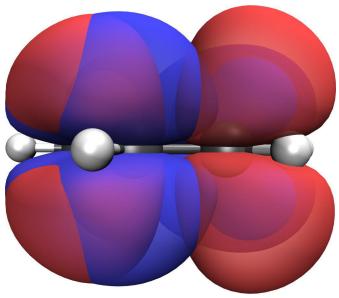


45° to axes

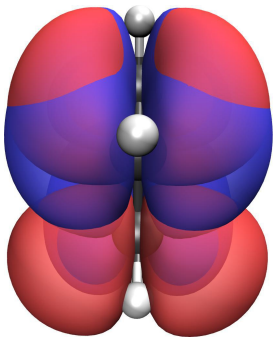
LUMO density (isovalue: 0.02)



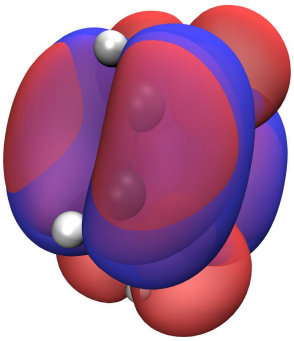
X/Y plane



X/Z plane

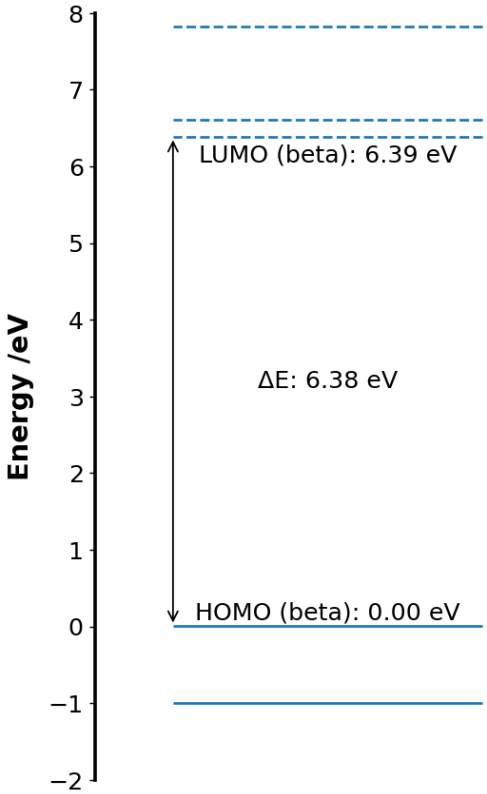


Z/Y plane

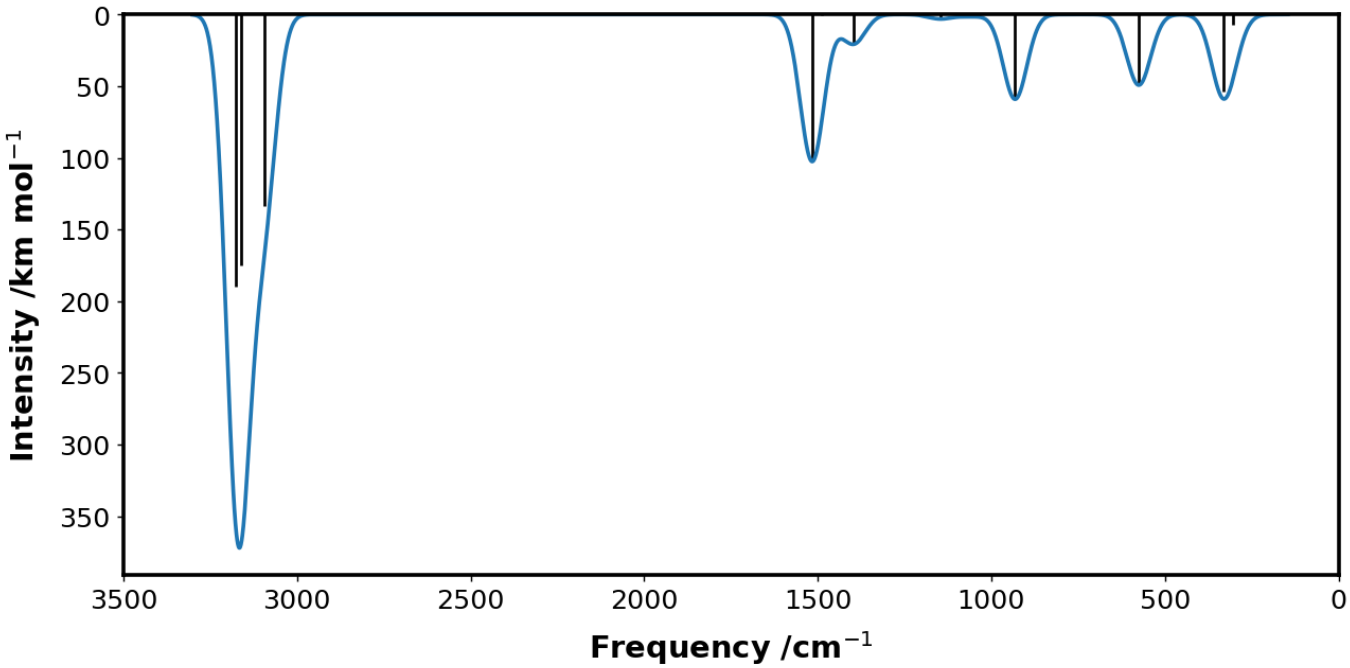


45° to axes

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



Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm^{-1})
Peaks /cm^{-1}: 329, 575, 931, 1060, 1145, 1399, 1516, 3165.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm^{-1}	Intensity /km mol^{-1}
1	A	263.6800	0.0000
2	A	271.7900	0.0200
3	A	302.7500	7.5100
4	A	332.2100	53.6200
5	A	457.5000	0.0000
6	A	489.4700	0.0000
7	A	575.0600	49.2700
8	A	613.8100	0.0000
9	A	639.2500	0.0000
10	A	692.3400	0.0000
11	A	880.0000	0.1400
12	A	905.0800	0.0000
13	A	931.3800	59.0500
14	A	984.1200	0.0000
15	A	995.8600	0.1300
16	A	1057.9600	1.4800
17	A	1146.9700	3.1400
18	A	1150.1900	0.0000
19	A	1290.4800	0.0000
20	A	1340.5200	0.0000
21	A	1397.2500	20.6200
22	A	1489.6200	0.6200
23	A	1516.0100	102.0900
24	A	1568.0200	0.0000
25	A	3094.2700	133.9900
26	A	3097.0400	0.0000
27	A	3145.4900	0.0000
28	A	3162.1900	174.8000
29	A	3174.7500	190.1700
30	A	3189.1200	0.0000

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV	Label	Symmetry	Energy /eV
38	LUMO+15 (alpha)	A	20.8419	LUMO+16 (beta)	A	20.9823
37	LUMO+14 (alpha)	A	20.6414	LUMO+15 (beta)	A	20.9339
36	LUMO+13 (alpha)	A	20.4394	LUMO+14 (beta)	A	20.7688
35	LUMO+12 (alpha)	A	18.8435	LUMO+13 (beta)	A	18.9156
34	LUMO+11 (alpha)	A	14.5989	LUMO+12 (beta)	A	14.6539
33	LUMO+10 (alpha)	A	14.0413	LUMO+11 (beta)	A	14.1639
32	LUMO+9 (alpha)	A	14.0251	LUMO+10 (beta)	A	14.0768
31	LUMO+8 (alpha)	A	13.5835	LUMO+9 (beta)	A	13.7651
30	LUMO+7 (alpha)	A	10.1823	LUMO+8 (beta)	A	10.7969
29	LUMO+6 (alpha)	A	10.1712	LUMO+7 (beta)	A	10.2684
28	LUMO+5 (alpha)	A	10.0530	LUMO+6 (beta)	A	10.2415
27	LUMO+4 (alpha)	A	9.8948	LUMO+5 (beta)	A	10.2233
26	LUMO+3 (alpha)	A	9.3798	LUMO+4 (beta)	A	9.4586
25	LUMO+2 (alpha)	A	9.0680	LUMO+3 (beta)	A	9.0742
24	LUMO+1 (alpha)	A	7.7818	LUMO+2 (beta)	A	7.8245
23	**LUMO (alpha)**	**A**	**6.2757**	LUMO+1 (beta)	A	6.6032
22	**HOMO (alpha)**	**A**	**3.8253**	**LUMO (beta)**	**A**	**6.3875**
21	HOMO-1 (alpha)	A	-1.1278	**HOMO (beta)**	**A**	**0.0035**
20	HOMO-2 (alpha)	A	-1.3676	HOMO-1 (beta)	A	-0.9948
19	HOMO-3 (alpha)	A	-3.2454	HOMO-2 (beta)	A	-3.1799
18	HOMO-4 (alpha)	A	-3.7915	HOMO-3 (beta)	A	-3.6112
17	HOMO-5 (alpha)	A	-4.1658	HOMO-4 (beta)	A	-3.7183
16	HOMO-6 (alpha)	A	-5.4369	HOMO-5 (beta)	A	-5.3397
15	HOMO-7 (alpha)	A	-5.7879	HOMO-6 (beta)	A	-5.7684
14	HOMO-8 (alpha)	A	-5.9674	HOMO-7 (beta)	A	-5.8700
13	HOMO-9 (alpha)	A	-7.1742	HOMO-8 (beta)	A	-7.0124
12	HOMO-10 (alpha)	A	-8.4458	HOMO-9 (beta)	A	-8.3708
11	HOMO-11 (alpha)	A	-10.4704	HOMO-10 (beta)	A	-10.4269
10	HOMO-12 (alpha)	A	-10.9305	HOMO-11 (beta)	A	-10.5491
9	HOMO-13 (alpha)	A	-14.3088	HOMO-12 (beta)	A	-13.9481
8	HOMO-14 (alpha)	A	-14.7385	HOMO-13 (beta)	A	-14.6226
7	HOMO-15 (alpha)	A	-17.2797	HOMO-14 (beta)	A	-17.0821
6	HOMO-16 (alpha)	A	-271.9499	HOMO-15 (beta)	A	-271.8150

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	1.4169241	-0.2092420	0.0058053
C	0.5002493	-1.3420930	-0.0092482
C	-0.8696348	-1.0889060	-0.0138056
C	-1.4073637	0.1982578	-0.0046956
C	-0.4906871	1.3311115	0.0101902
C	0.8791979	1.0779217	0.0148167
H	2.4949251	-0.3614925	0.0095117
H	0.8751772	-2.3642463	-0.0163120
H	-1.5571891	-1.9411002	-0.0250246
H	-2.4853611	0.3505124	-0.0092797
H	-0.8656171	2.3532591	0.0179698
H	1.5667493	1.9301175	0.0261019

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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