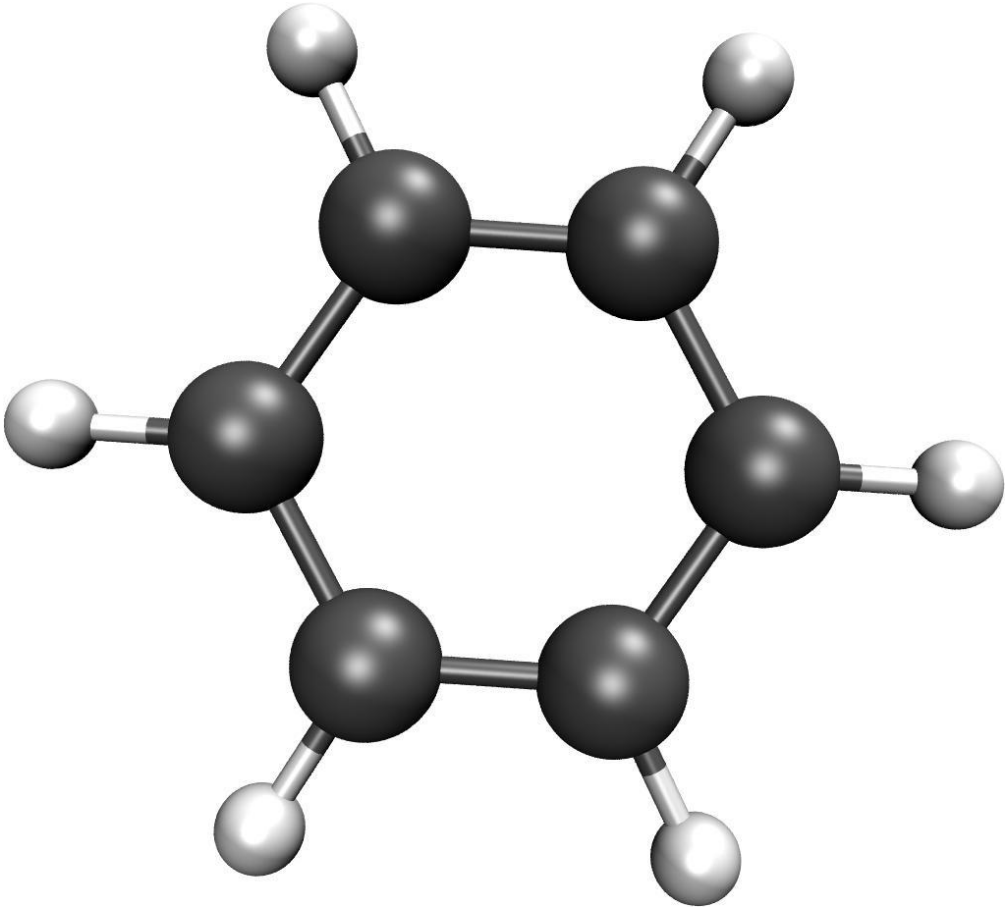
THE Zysman-Colman GROUP

Calculation Report

Benzene

Optimisation, Frequencies (Doublet)



Summary of Results

Metadata

Username:	osl
Date:	20/06/2022 17:16:54
Duration:	2 m, 13 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:	unrestricted
Multiplicity:	2 (doublet)
Calc temperature:	298.15 K
Calc pressure:	1.0 atm

SCF Energies

No. of steps:	5
Final energy:	-6310.5381 eV
Final energy:	-608,874 $kJmol^{-1}$

Geometry

Formula:	$C_6H_6^-$
Exact mass:	78.0469 $gmol^{-1}$
Molar mass:	78.1118 $gmol^{-1}$
Alignment method:	Minimal
X extension:	5.04 Å
Y extension:	4.51 Å
Z extension:	0.00 Å
Linearity ratio:	0.11
Planarity ratio:	1.00

HOMO & LUMO (alpha)

$E_{HOMO,LUMO}$:	2.44 eV
E_{HOMO}:	3.83 eV
E_{LUMO}:	6.27 eV

HOMO & LUMO (beta)

$E_{HOMO,LUMO}$:	6.36 eV
E_{HOMO}:	-0.02 eV
E_{LUMO}:	6.34 eV

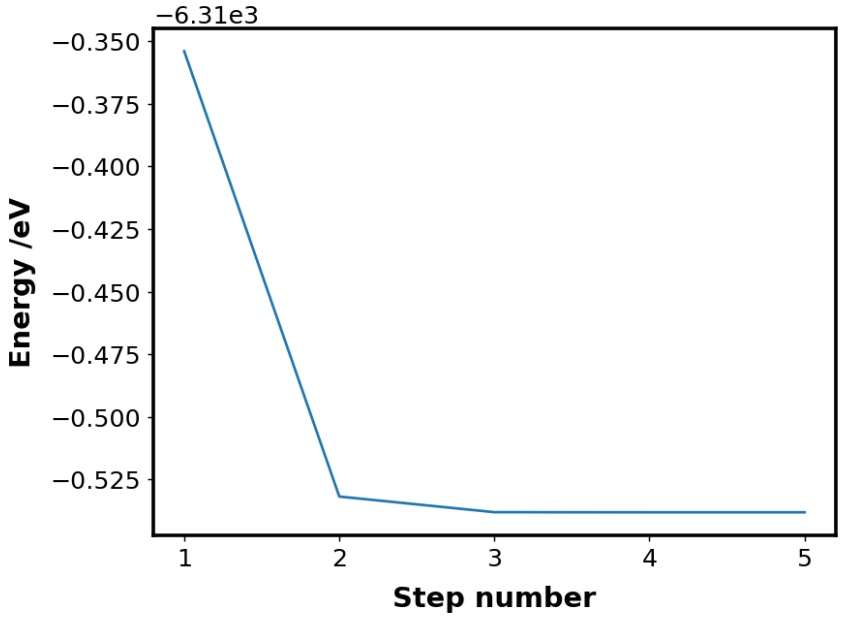
Permanent Dipole Moment

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

Vibrational Frequencies

Negative frequencies:	2
Frequency:	-299.12 cm^{-1}
Frequency:	-220.12 cm^{-1}

SCF Energies



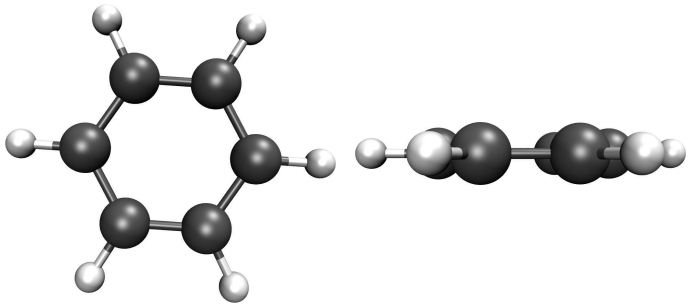
SCF Energies

No. of steps: 5

Final energy: -6310.5381 eV

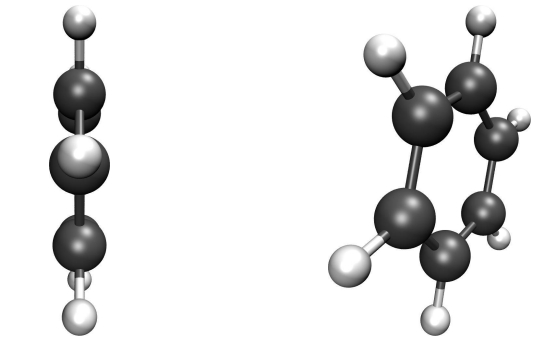
Final energy: -608,874 kJmol^{-1}

Geometry



X/Y plane

X/Z plane



Z/Y plane

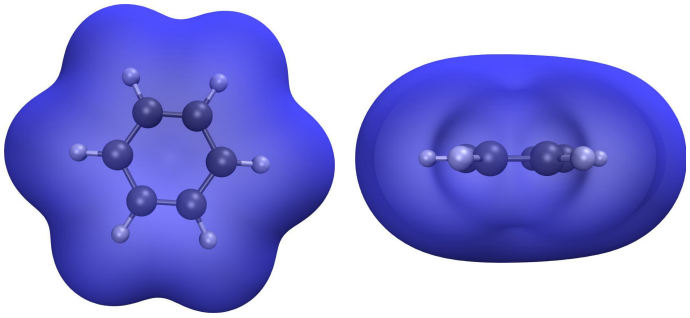
45° to axes

Aligned structure

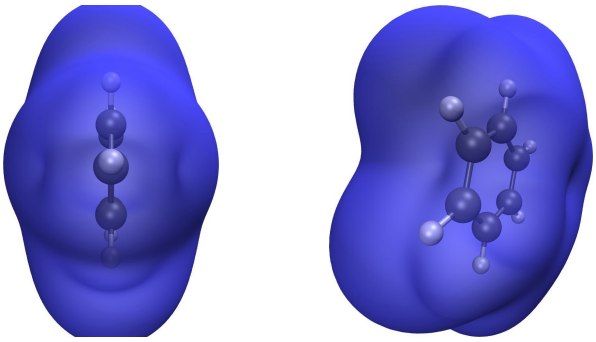
Geometry

Formula:	$C_6H_6^-$
Exact mass:	78.0469 gmol^{-1}
Molar mass:	78.1118 gmol^{-1}
Alignment method:	Minimal
X extension:	5.04 Å
Y extension:	4.51 Å
Z extension:	0.00 Å
Linearity ratio:	0.11
Planarity ratio:	1.00

SCF Density



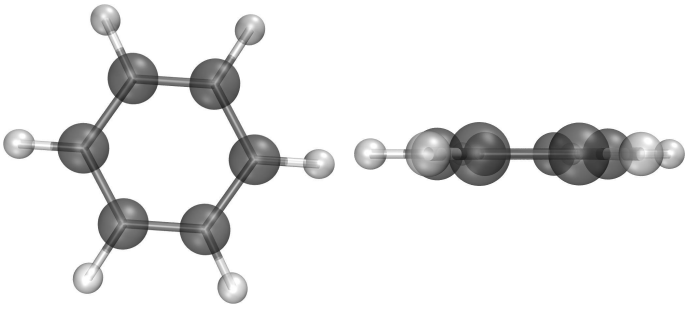
X/Y plane | X/Z plane



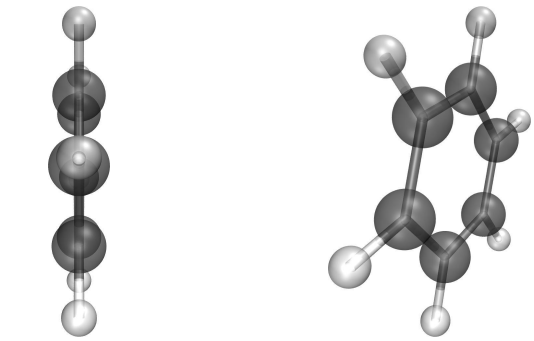
Z/Y plane | 45° to axes

SCF density (isovalue: 0.0004)

Permanent Dipole Moment



X/Y plane | X/Z plane



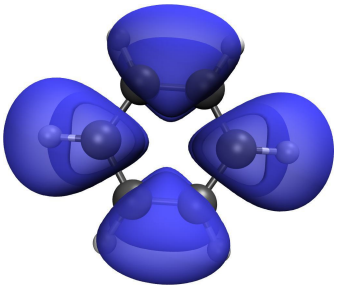
Z/Y plane | 45° to axes

Aligned structure (dipole moment in red)

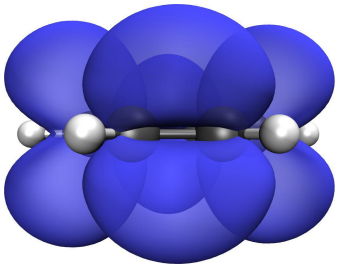
Dipole Moment

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 °

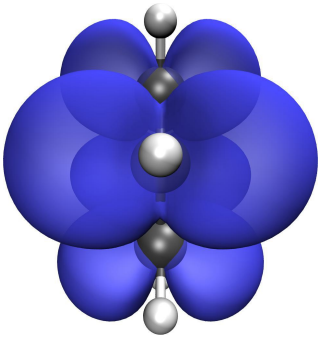
Spin Density



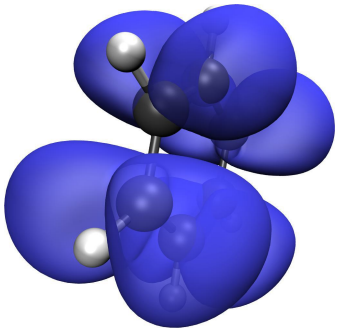
X/Y plane



X/Z plane

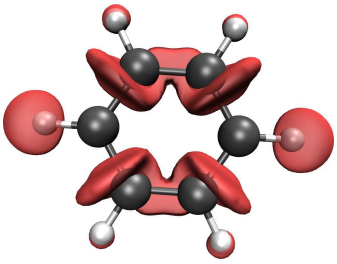


Z/Y plane

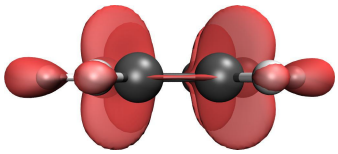


45° to axes

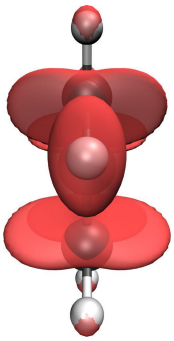
Positive spin density (electron) (isovalue: 0.0004)



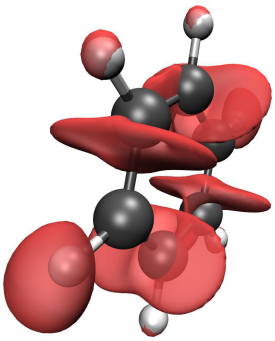
X/Y plane



X/Z plane

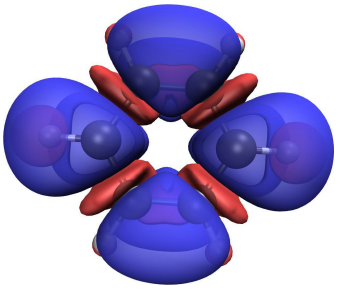


Z/Y plane

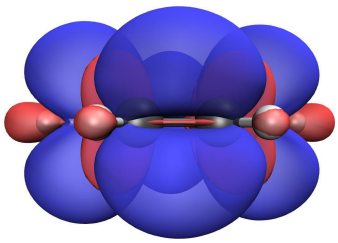


45° to axes

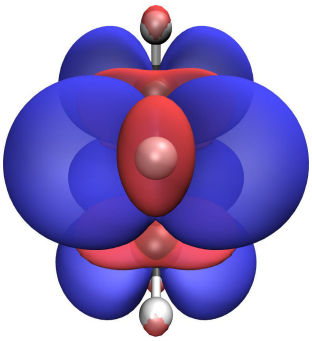
Negative spin density (hole) (isovalue: 0.0004)



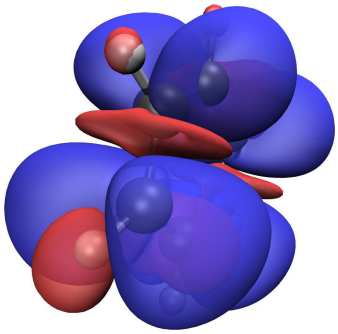
X/Y plane



X/Z plane



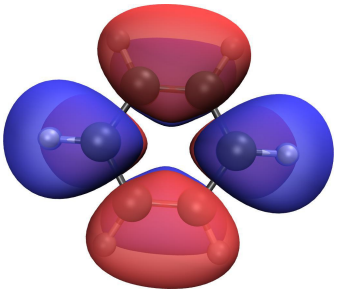
Z/Y plane



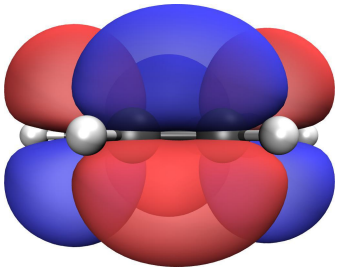
45° to axes

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

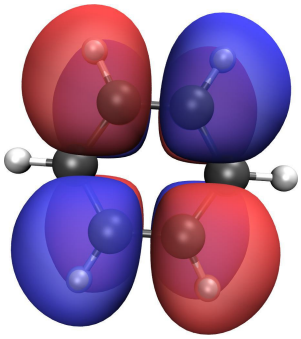
HOMO & LUMO (Alpha)



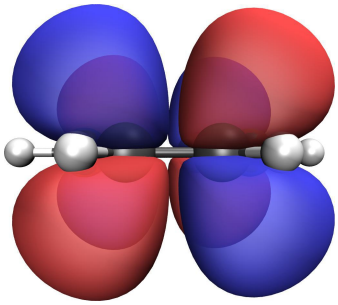
X/Y plane



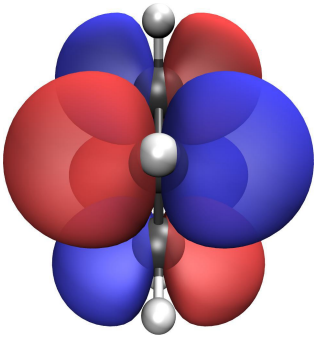
X/Z plane



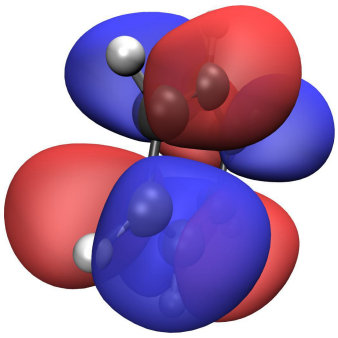
X/Y plane



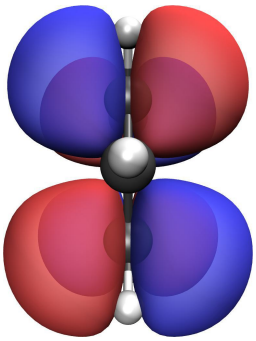
X/Z plane



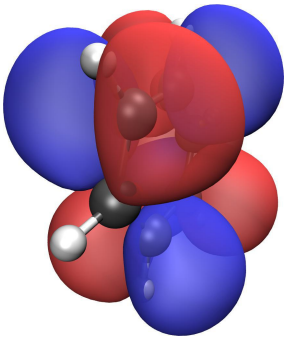
Z/Y plane



45° to axes



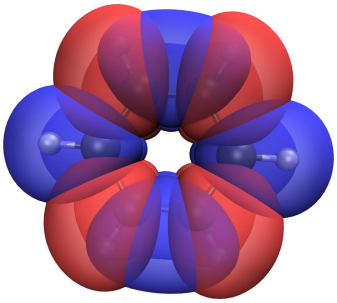
Z/Y plane



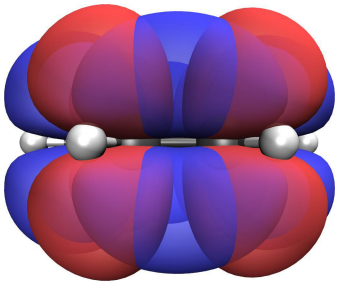
45° to axes

HOMO density (isovalue: 0.02)

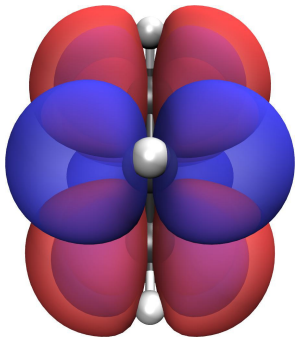
LUMO density (isovalue: 0.02)



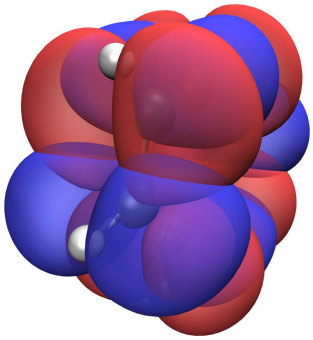
X/Y plane



X/Z plane

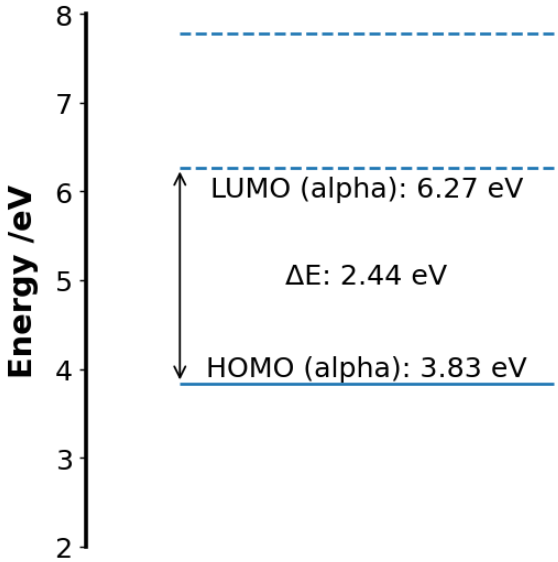


Z/Y plane

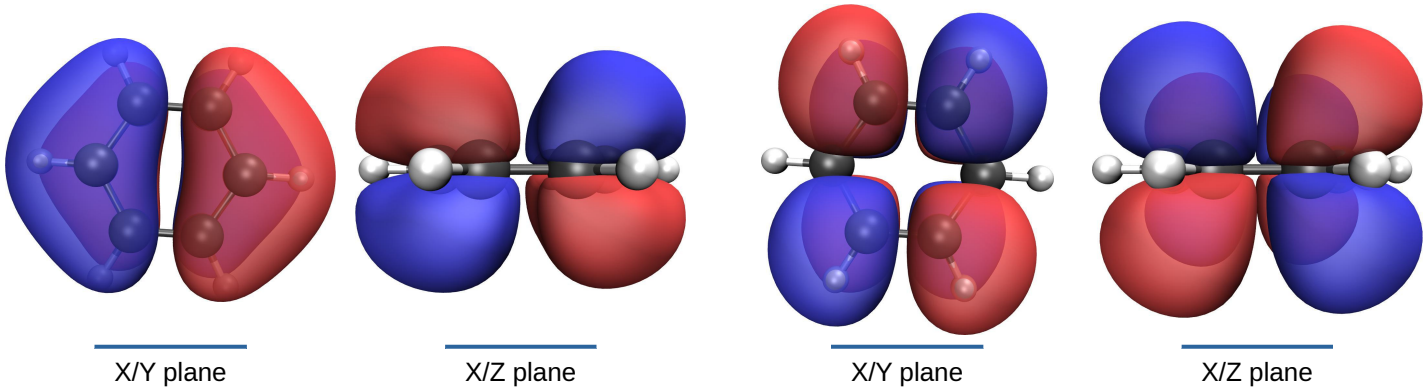


45° to axes

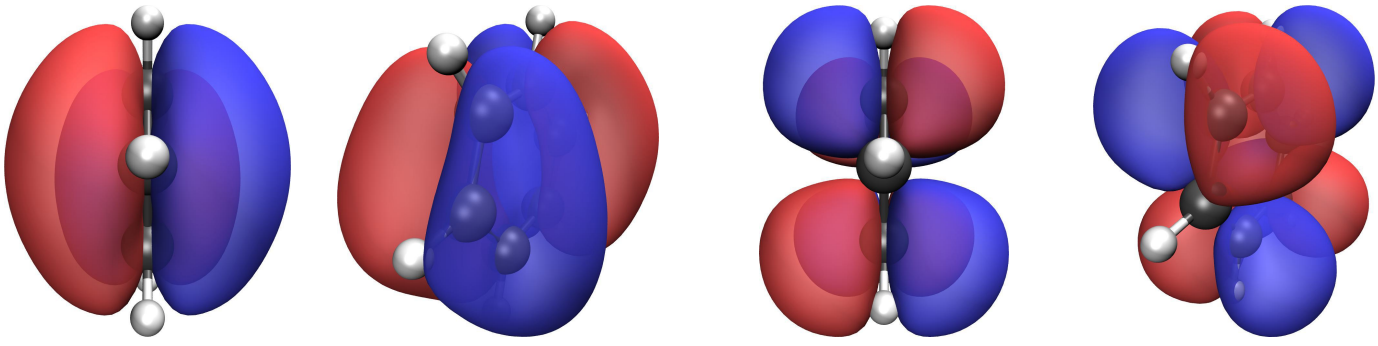
HOMO (blue) & LUMO (red) density (isovalue: 0.02)



HOMO & LUMO (Beta)

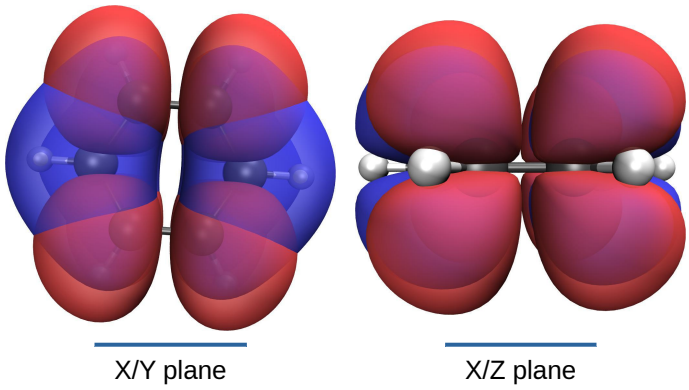


X/Y plane | X/Z plane | X/Y plane | X/Z plane

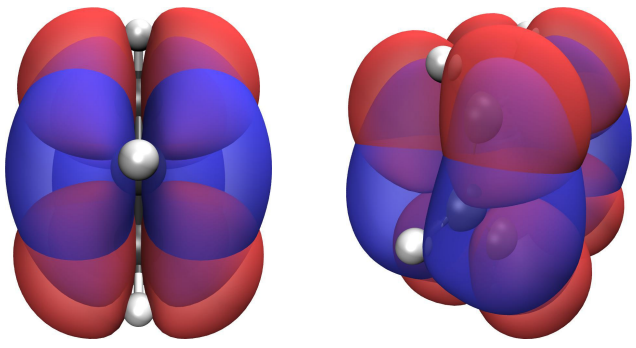


Z/Y plane | 45° to axes | Z/Y plane | 45° to axes

HOMO density (isovalue: 0.02) | **LUMO density (isovalue: 0.02)**

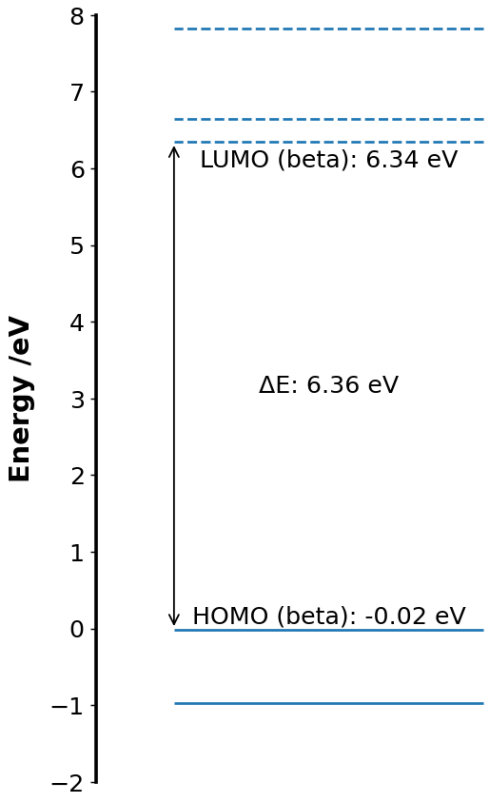


X/Y plane | X/Z plane

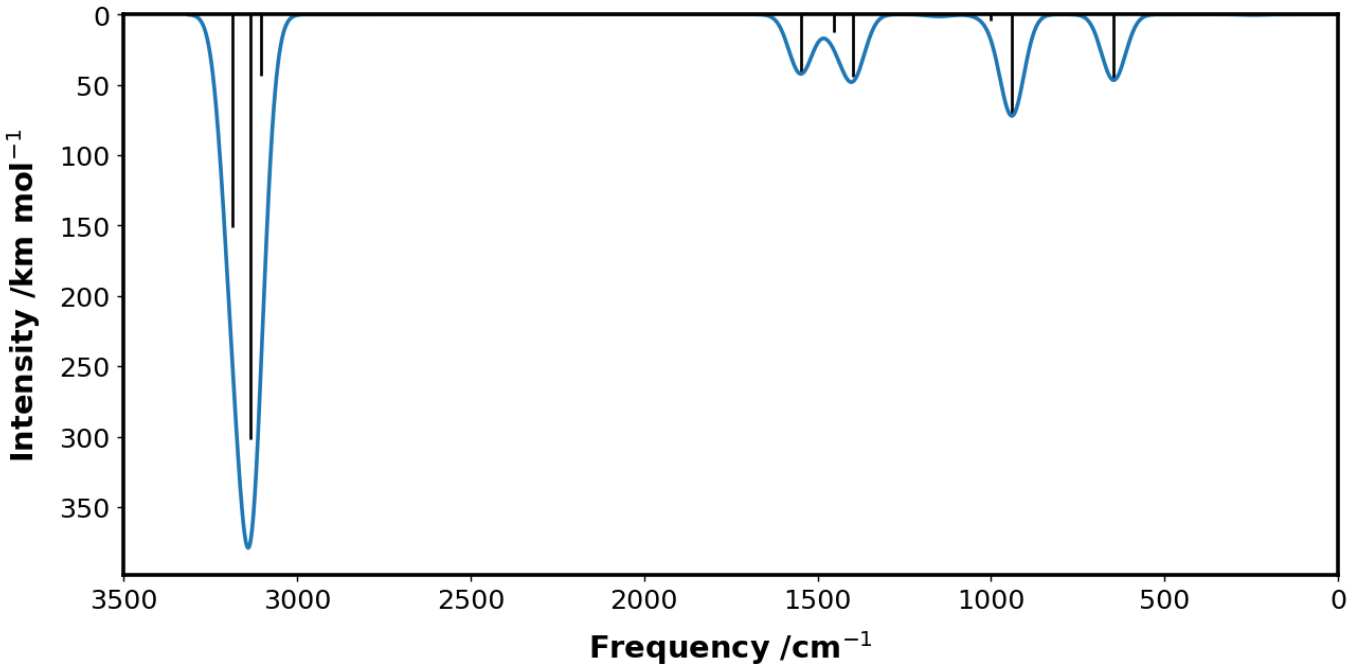


Z/Y plane | 45° to axes

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



Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm^{-1})
Peaks /cm^{-1}: -220, 242, 646, 940, 1149, 1402, 1548, 3141.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm^{-1}	Intensity /km mol^{-1}
1	A	-299.1199	0.0006
2	A	-220.1211	64.4413
3	A	157.4867	0.0000
4	A	242.2175	0.4047
5	A	444.8093	0.0072
6	A	565.2478	0.0000
7	A	622.3455	0.0000
8	A	646.6220	46.6961
9	A	651.6166	0.0010
10	A	717.1228	0.0000
11	A	863.0493	0.0000
12	A	863.6642	0.0006
13	A	939.5250	71.2484
14	A	985.5880	0.0000
15	A	1000.6886	4.1103
16	A	1042.7355	0.0149
17	A	1149.3141	1.3956
18	A	1190.9143	0.0000
19	A	1268.9169	0.0000
20	A	1340.3245	0.0000
21	A	1398.2403	44.4296
22	A	1453.7231	12.4799
23	A	1548.7904	41.9984
24	A	1685.9705	0.0000
25	A	3098.0460	0.0000
26	A	3104.1485	43.6269
27	A	3133.5420	0.0000
28	A	3135.3627	301.9398
29	A	3188.4116	150.9304
30	A	3197.2484	0.0000

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV	Label	Symmetry	Energy /eV
38	LUMO+15 (alpha)	A	20.8573	LUMO+16 (beta)	A	20.9495
37	LUMO+14 (alpha)	A	20.6385	LUMO+15 (beta)	A	20.9473
36	LUMO+13 (alpha)	A	20.4352	LUMO+14 (beta)	A	20.7661
35	LUMO+12 (alpha)	A	18.8390	LUMO+13 (beta)	A	18.9111
34	LUMO+11 (alpha)	A	14.6035	LUMO+12 (beta)	A	14.6601
33	LUMO+10 (alpha)	A	14.0237	LUMO+11 (beta)	A	14.1611
32	LUMO+9 (alpha)	A	13.9929	LUMO+10 (beta)	A	14.0343
31	LUMO+8 (alpha)	A	13.6315	LUMO+9 (beta)	A	13.8076
30	LUMO+7 (alpha)	A	10.1686	LUMO+8 (beta)	A	10.7997
29	LUMO+6 (alpha)	A	10.1605	LUMO+7 (beta)	A	10.2669
28	LUMO+5 (alpha)	A	10.0720	LUMO+6 (beta)	A	10.2473
27	LUMO+4 (alpha)	A	9.8935	LUMO+5 (beta)	A	10.2149
26	LUMO+3 (alpha)	A	9.3822	LUMO+4 (beta)	A	9.4530
25	LUMO+2 (alpha)	A	9.0628	LUMO+3 (beta)	A	9.0747
24	LUMO+1 (alpha)	A	7.7748	LUMO+2 (beta)	A	7.8181
23	**LUMO (alpha)**	**A**	**6.2681**	LUMO+1 (beta)	A	6.6480
22	**HOMO (alpha)**	**A**	**3.8325**	**LUMO (beta)**	**A**	**6.3427**
21	HOMO-1 (alpha)	A	-1.1374	**HOMO (beta)**	**A**	**-0.0158**
20	HOMO-2 (alpha)	A	-1.3600	HOMO-1 (beta)	A	-0.9791
19	HOMO-3 (alpha)	A	-3.2548	HOMO-2 (beta)	A	-3.1897
18	HOMO-4 (alpha)	A	-3.7837	HOMO-3 (beta)	A	-3.6115
17	HOMO-5 (alpha)	A	-4.1682	HOMO-4 (beta)	A	-3.7103
16	HOMO-6 (alpha)	A	-5.4964	HOMO-5 (beta)	A	-5.4034
15	HOMO-7 (alpha)	A	-5.6777	HOMO-6 (beta)	A	-5.6268
14	HOMO-8 (alpha)	A	-6.0235	HOMO-7 (beta)	A	-5.9549
13	HOMO-9 (alpha)	A	-7.1770	HOMO-8 (beta)	A	-7.0140
12	HOMO-10 (alpha)	A	-8.4516	HOMO-9 (beta)	A	-8.3768
11	HOMO-11 (alpha)	A	-10.4867	HOMO-10 (beta)	A	-10.4541
10	HOMO-12 (alpha)	A	-10.9207	HOMO-11 (beta)	A	-10.5300
9	HOMO-13 (alpha)	A	-14.2971	HOMO-12 (beta)	A	-13.9548
8	HOMO-14 (alpha)	A	-14.7608	HOMO-13 (beta)	A	-14.6269
7	HOMO-15 (alpha)	A	-17.2893	HOMO-14 (beta)	A	-17.0904
6	HOMO-16 (alpha)	A	-271.8910	HOMO-15 (beta)	A	-271.7030

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.4360800	0.0964170	-0.0000050
C	-0.7678990	-1.1729720	-0.0000330
C	0.6034130	-1.2662280	0.0000420
C	1.4360800	-0.0964130	-0.0000160
C	0.7679010	1.1729710	-0.0000340
C	-0.6034150	1.2662260	0.0000430
H	-2.5203110	0.1691460	-0.0001060
H	-1.3622100	-2.0901160	-0.0000400
H	1.0688330	-2.2548880	0.0001390
H	2.5203100	-0.1691580	-0.0000640
H	1.3622030	2.0901200	-0.0000390
H	-1.0688250	2.2548910	0.0001390

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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