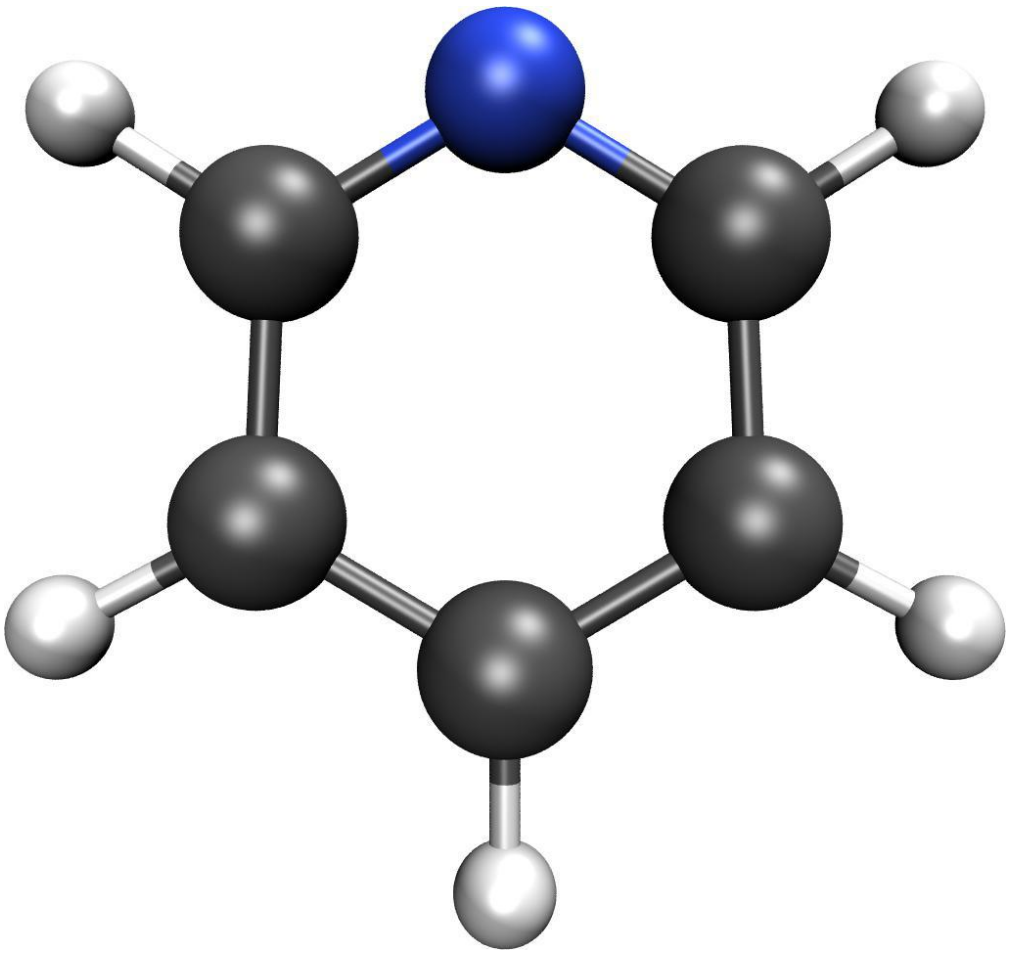
THE Zysman-Colman GROUP

Calculation Report

Pyridine

Optimisation, Frequencies (Singlet)



Summary of Results

Metadata

Username:	osl
Date:	24/06/2022 12:20:46
Duration:	33 s
Success:	True
Converged:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Optimisation, Frequencies
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	9
Final energy:	-6748.4564 eV
Final energy:	-651,127 $kJmol^{-1}$

Geometry

Formula:	C_5NH_5
Molar mass:	79.0999 $gmol^{-1}$
Alignment method:	Minimal
X extension:	4.31 Å
Y extension:	3.88 Å
Z extension:	0.00 Å
Linearity ratio:	0.10
Planarity ratio:	1.00

HOMO & LUMO

$E_{HOMO,LUMO}$:	6.71 eV
E_{HOMO}:	-7.17 eV
E_{LUMO}:	-0.47 eV

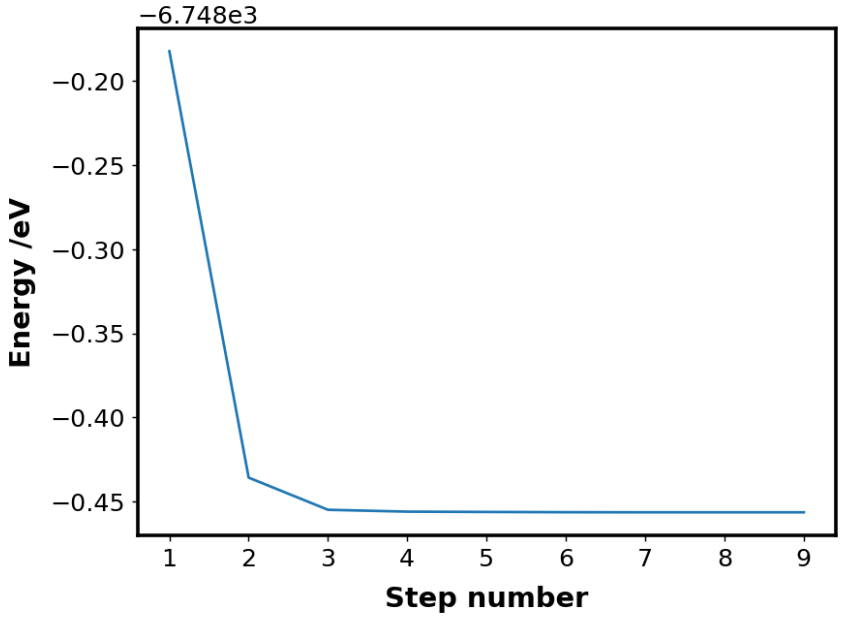
Permanent Dipole Moment

Total:	2.20 D
X axis angle:	89.98 °
XY plane angle:	0.01 °

Vibrational Frequencies

Negative frequencies:	0

SCF Energies



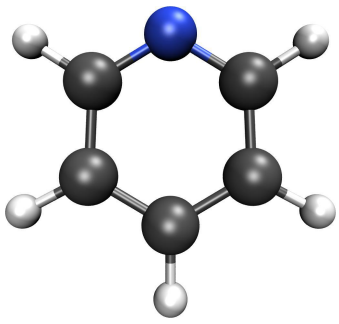
SCF Energies

No. of steps: 9

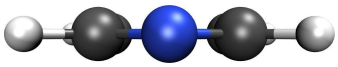
Final energy: -6748.4564 eV

Final energy: -651,127 kJmol^{-1}

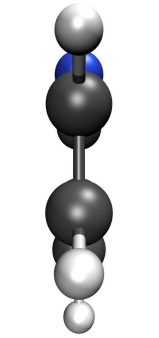
Geometry



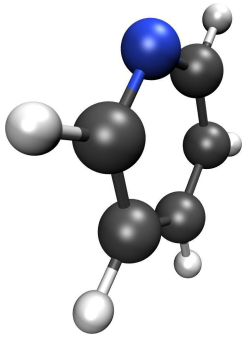
X/Y plane



X/Z plane



Z/Y plane



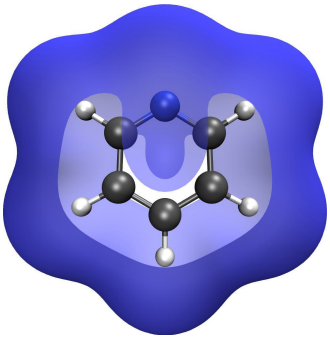
45° to axes

Aligned structure

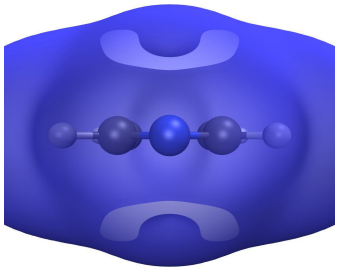
Geometry

Formula:	C_5NH_5
Molar mass:	79.0999 gmol^{-1}
Alignment method:	Minimal
X extension:	4.31 Å
Y extension:	3.88 Å
Z extension:	0.00 Å
Linearity ratio:	0.10
Planarity ratio:	1.00

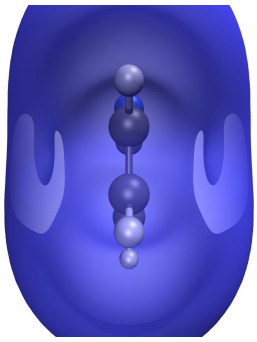
SCF Density



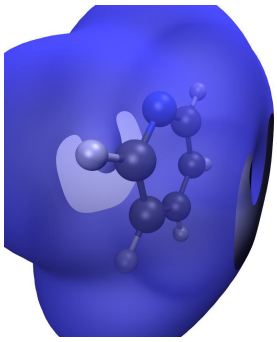
X/Y plane



X/Z plane



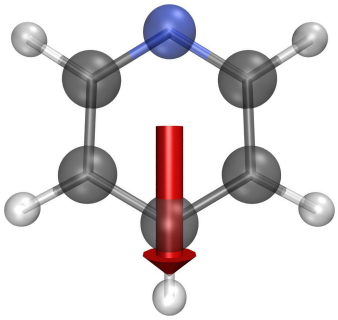
Z/Y plane



45° to axes

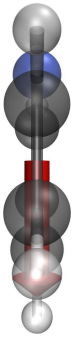
SCF density (isovalue: 0.0004)

Permanent Dipole Moment

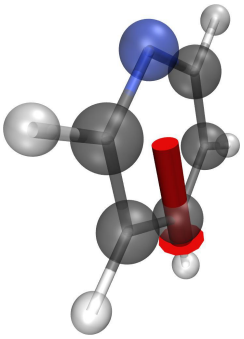


X/Y plane

X/Z plane



Z/Y plane



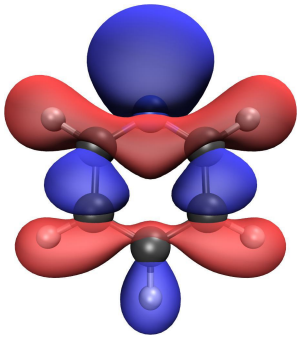
45° to axes

Aligned structure (dipole moment in red)

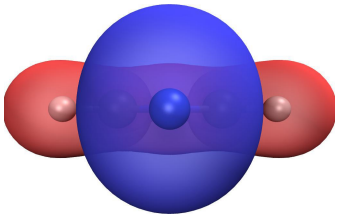
Dipole Moment

Origin X:	0.00 D
Origin Y:	0.00 D
Origin Z:	0.00 D
Vector X:	-0.00 D
Vector Y:	-2.20 D
Vector Z:	-0.00 D
Total:	2.20 D
X axis angle:	89.98 °
XY plane angle:	0.01 °

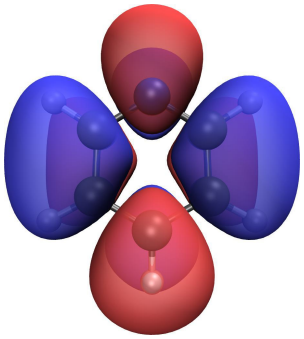
HOMO & LUMO



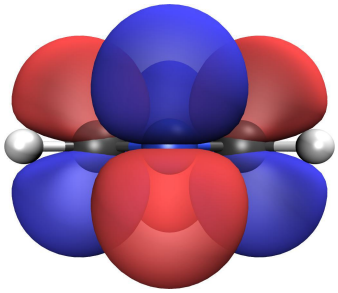
X/Y plane



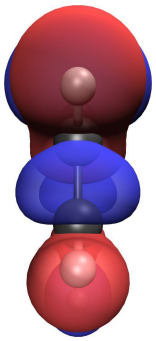
X/Z plane



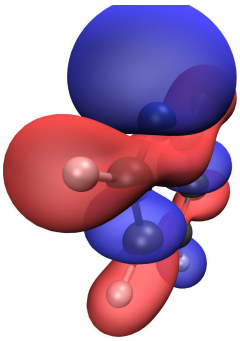
X/Y plane



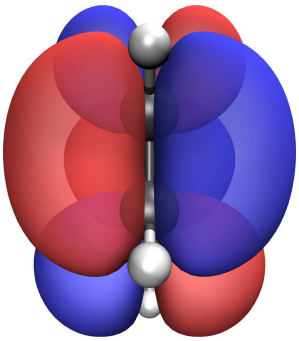
X/Z plane



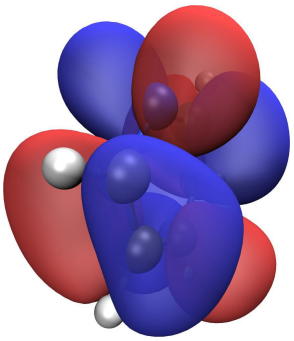
Z/Y plane



45° to axes



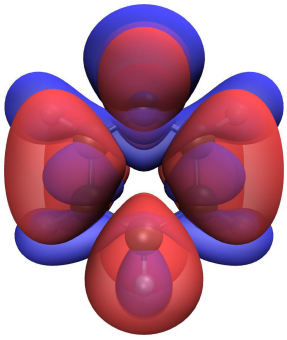
Z/Y plane



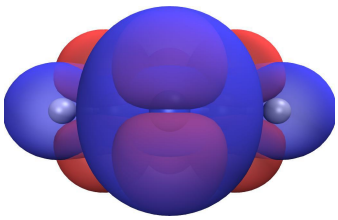
45° to axes

HOMO density (isovalue: 0.02)

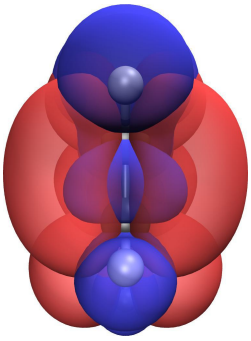
LUMO density (isovalue: 0.02)



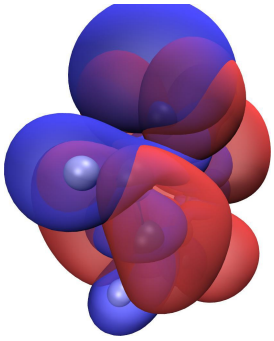
X/Y plane



X/Z plane

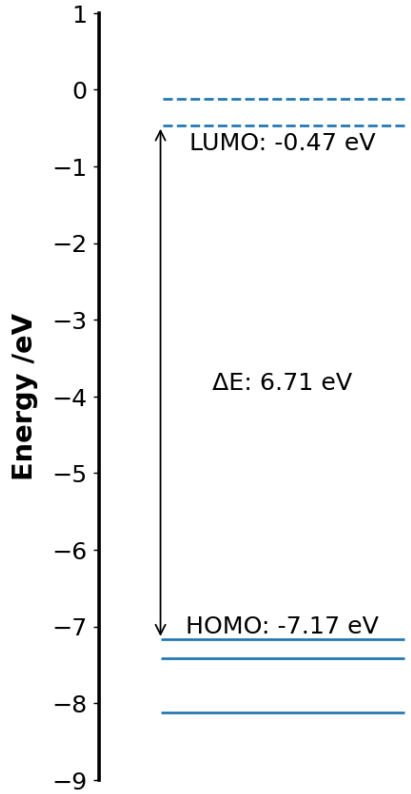


Z/Y plane

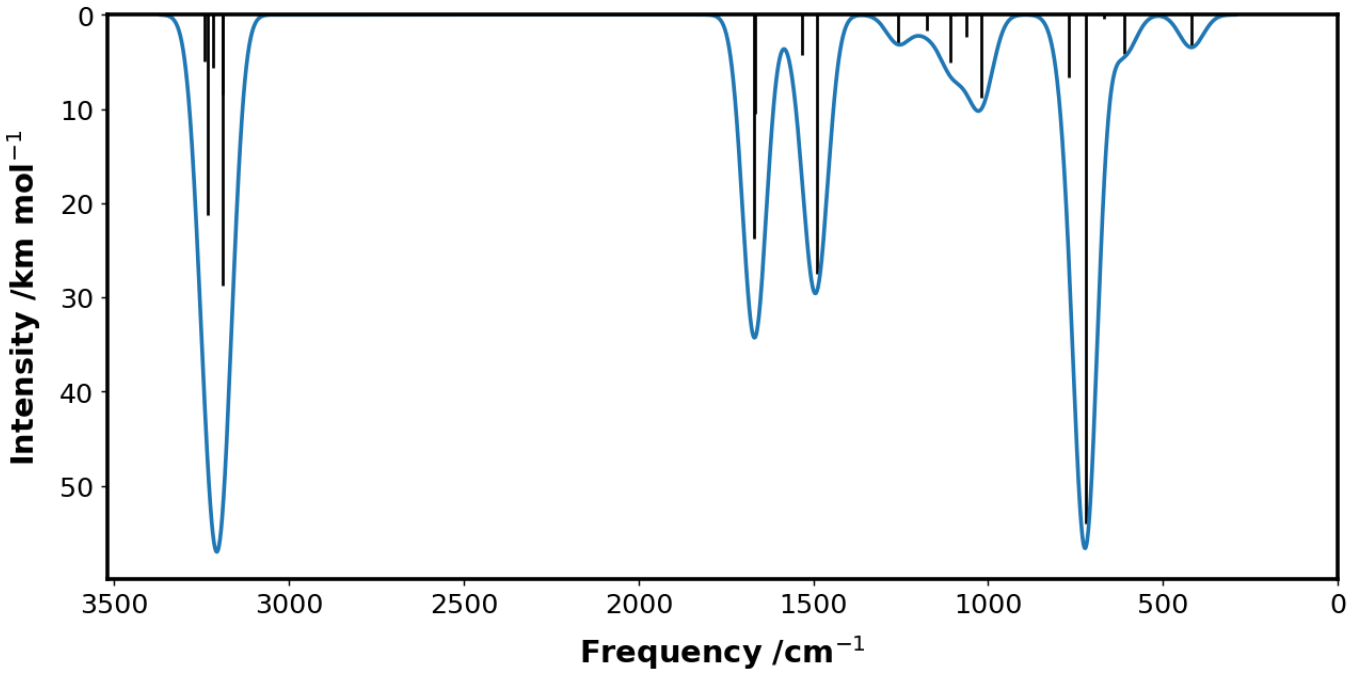


45° to axes

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



Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm^{-1})
Peaks /cm^{-1}: 418, 722, 1028, 1253, 1494, 1668, 3206.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm^{-1}	Intensity /km mol^{-1}
1	A	383.7300	0.0000
2	A	418.8300	3.4700
3	A	610.8100	4.1300
4	A	669.5500	0.4300
5	A	720.8700	53.9400
6	A	769.0500	6.6100
7	A	903.1900	0.0000
8	A	964.8600	0.0000
9	A	1006.5300	0.0000
10	A	1019.4400	8.7800
11	A	1019.6600	0.0100
12	A	1063.0900	2.3400
13	A	1094.9400	0.0300
14	A	1107.3800	5.0600
15	A	1176.8300	1.7100
16	A	1256.6600	3.0700
17	A	1347.6300	0.0200
18	A	1387.9500	0.0000
19	A	1491.3400	27.4400
20	A	1533.3700	4.3300
21	A	1666.2100	10.5600
22	A	1669.7000	23.7500
23	A	3189.0900	28.7200
24	A	3191.5700	8.4800
25	A	3216.3200	5.6200
26	A	3232.9100	21.2400
27	A	3240.5600	4.9800

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
37	LUMO+15	A	15.0342
36	LUMO+14	A	14.5841
35	LUMO+13	A	12.7701
34	LUMO+12	A	12.6778
33	LUMO+11	A	9.0193
32	LUMO+10	A	8.9991
31	LUMO+9	A	8.2736
30	LUMO+8	A	6.8258
29	LUMO+7	A	5.1991
28	LUMO+6	A	5.1849
27	LUMO+5	A	4.5869
26	LUMO+4	A	4.2866
25	LUMO+3	A	4.1186
24	LUMO+2	A	2.8373
23	LUMO+1	A	-0.1198
22	**LUMO**	**A**	**-0.4664**
21	**HOMO**	**A**	**-7.1729**
20	HOMO-1	A	-7.4192
19	HOMO-2	A	-8.1232
18	HOMO-3	A	-10.1396
17	HOMO-4	A	-11.1930
16	HOMO-5	A	-11.2837
15	HOMO-6	A	-11.9543
14	HOMO-7	A	-13.1334
13	HOMO-8	A	-13.4087
12	HOMO-9	A	-14.7906
11	HOMO-10	A	-17.5660
10	HOMO-11	A	-17.6204
9	HOMO-12	A	-21.3179
8	HOMO-13	A	-22.5352
7	HOMO-14	A	-26.3512
6	HOMO-15	A	-278.7372

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.1374880	0.6846500	-0.0000203
C	-1.1954410	-0.7066373	0.0000749
C	-0.0004716	-1.4179164	0.0000717
C	1.1949723	-0.7074353	-0.0001501
C	1.1379485	0.6838900	0.0000885
N	0.0004626	1.3802168	0.0001982
H	-2.0551243	1.2706886	-0.0005978
H	-2.1544681	-1.2150527	0.0001467
H	-0.0008321	-2.5041577	0.0003545
H	2.1536570	-1.2164949	-0.0006432
H	2.0559747	1.2693189	0.0002970

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

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