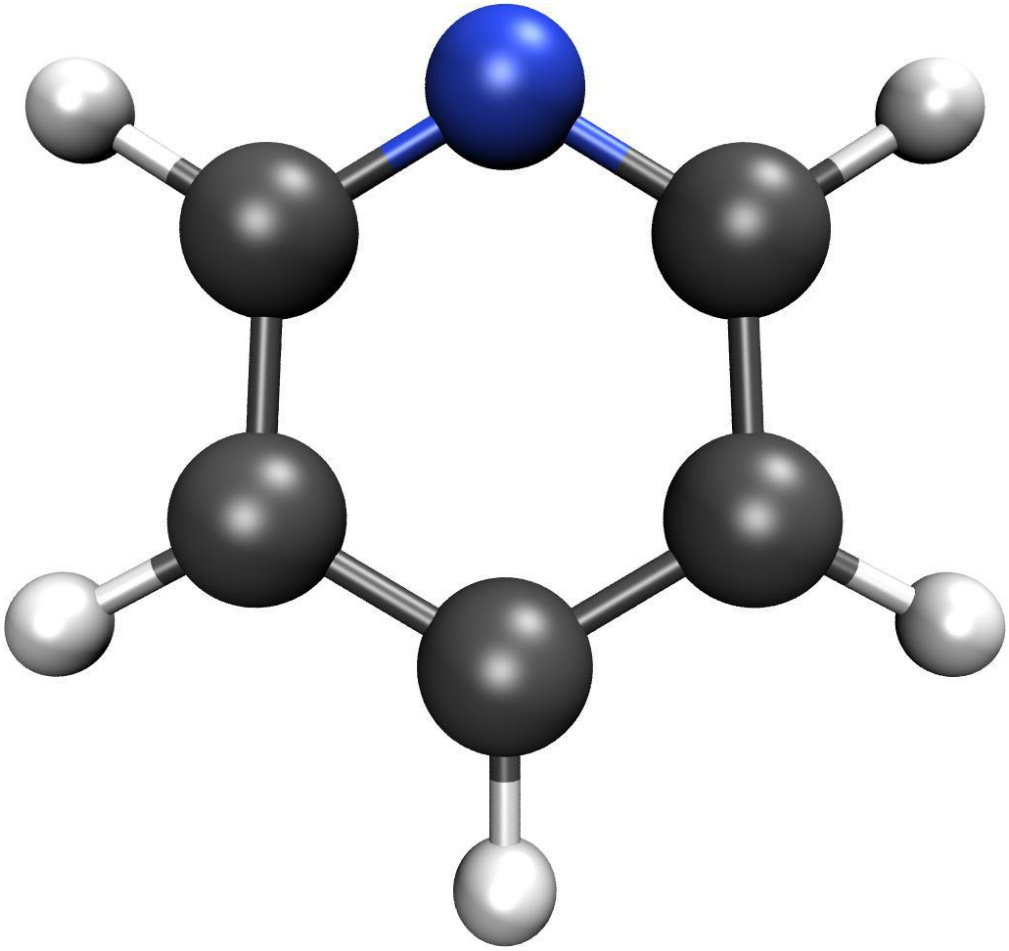
THE Zysman-Colman GROUP

Calculation Report

Pyridine

Excited States ()



Summary of Results

Metadata

Username:	osl
Date:	24/06/2022 12:24:30
Duration:	13 s
Success:	True
Computational package:	Turbomole (7.5.0)
Methods:	DFT
Functional:	PBE0
Basis set:	6-31G**
Calculations:	Excited States
Orbital spin:	restricted
Multiplicity:	1 (singlet)

SCF Energies

No. of steps:	1
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

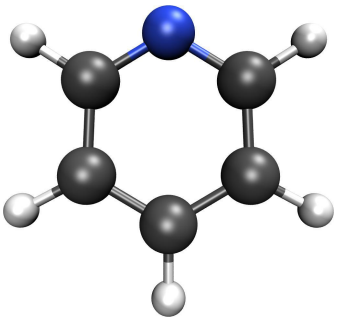
HOMO & LUMO

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

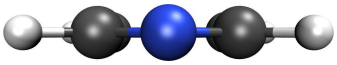
Permanent Dipole Moment

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

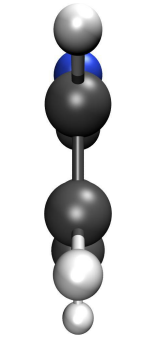
Geometry



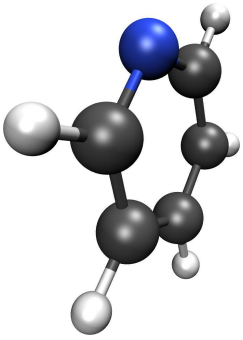
X/Y plane



X/Z plane



Z/Y plane



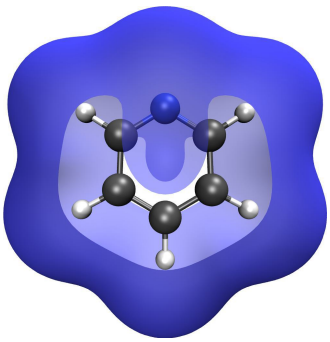
45° to axes

Aligned structure

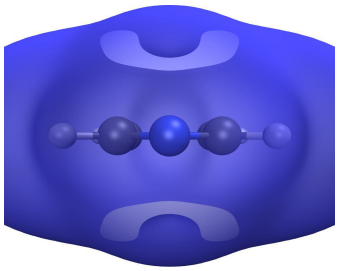
Geometry

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

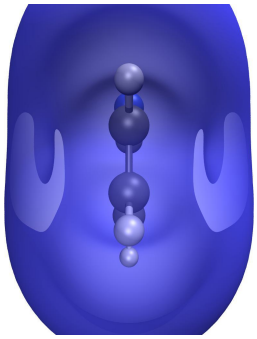
SCF Density



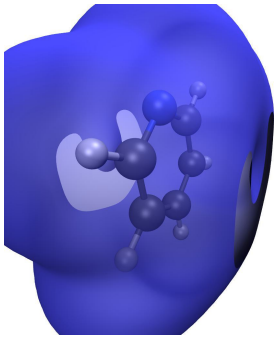
X/Y plane



X/Z plane



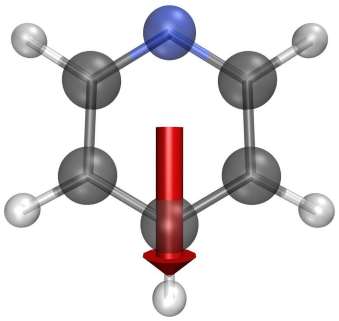
Z/Y plane



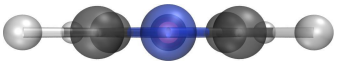
45° to axes

SCF density (isovalue: 0.0004)

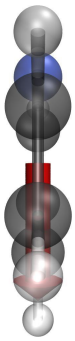
Permanent Dipole Moment



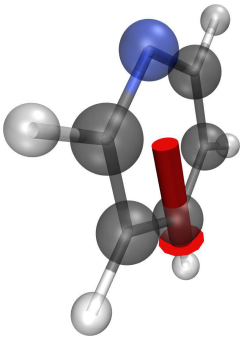
X/Y plane



X/Z plane



Z/Y plane



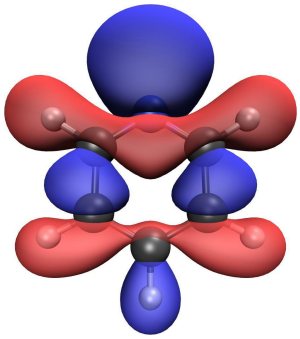
45° to axes

Aligned structure (dipole moment in red)

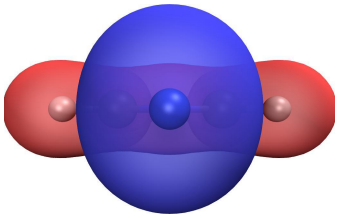
Dipole Moment

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 °

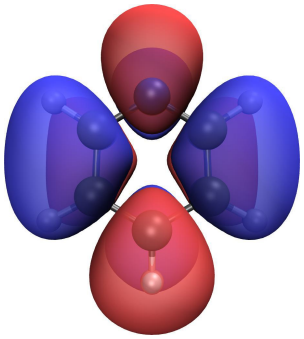
HOMO & LUMO



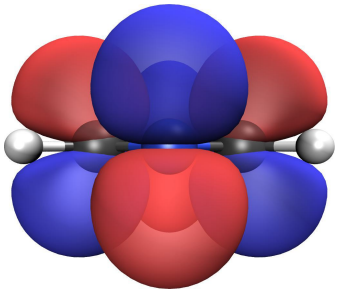
X/Y plane



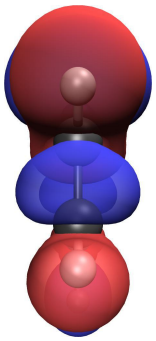
X/Z plane



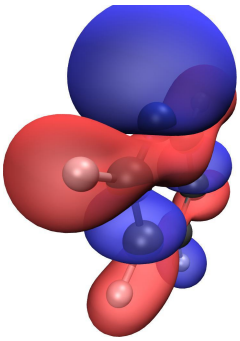
X/Y plane



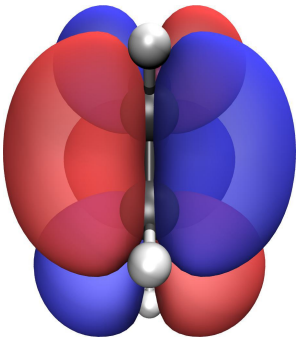
X/Z plane



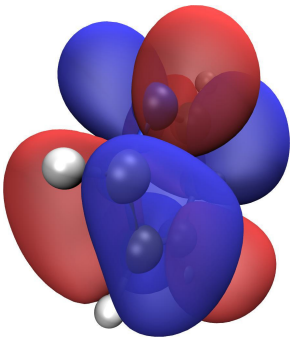
Z/Y plane



45° to axes



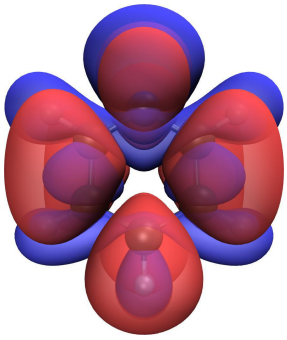
Z/Y plane



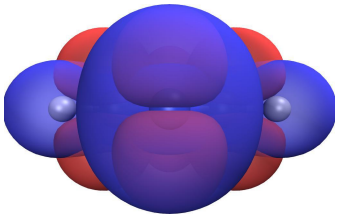
45° to axes

HOMO density (isovalue: 0.02)

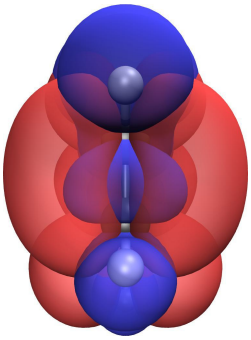
LUMO density (isovalue: 0.02)



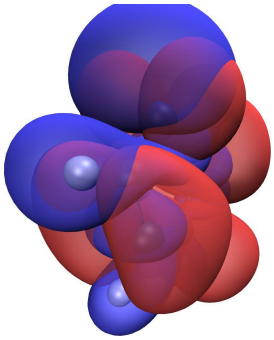
X/Y plane



X/Z plane



Z/Y plane



45° to axes

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

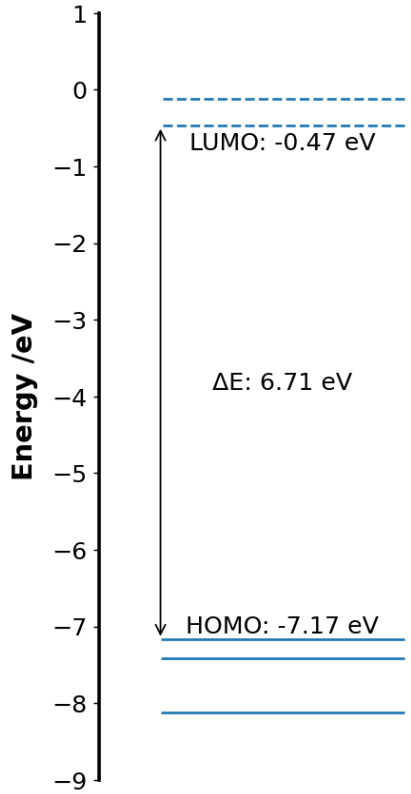


Table of Selected Molecular Orbitals

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	5.1992
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	-0.1197
22	**LUMO**	**A**	**-0.4663**
21	**HOMO**	**A**	**-7.1728**
20	HOMO-1	A	-7.4191
19	HOMO-2	A	-8.1231
18	HOMO-3	A	-10.1396
17	HOMO-4	A	-11.1929
16	HOMO-5	A	-11.2837
15	HOMO-6	A	-11.9543
14	HOMO-7	A	-13.1334
13	HOMO-8	A	-13.4086
12	HOMO-9	A	-14.7906
11	HOMO-10	A	-17.5660
10	HOMO-11	A	-17.6203
9	HOMO-12	A	-21.3179
8	HOMO-13	A	-22.5351
7	HOMO-14	A	-26.3511
6	HOMO-15	A	-278.7370

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.1374900	0.6846500	-0.0000200
C	-1.1954400	-0.7066400	0.0000700
C	-0.0004700	-1.4179200	0.0000700
C	1.1949700	-0.7074400	-0.0001500
C	1.1379500	0.6838900	0.0000900
N	0.0004600	1.3802200	0.0002000
H	-2.0551200	1.2706900	-0.0006000
H	-2.1544700	-1.2150500	0.0001500
H	-0.0008300	-2.5041600	0.0003500
H	2.1536600	-1.2164900	-0.0006400
H	2.0559700	1.2693200	0.0003000

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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