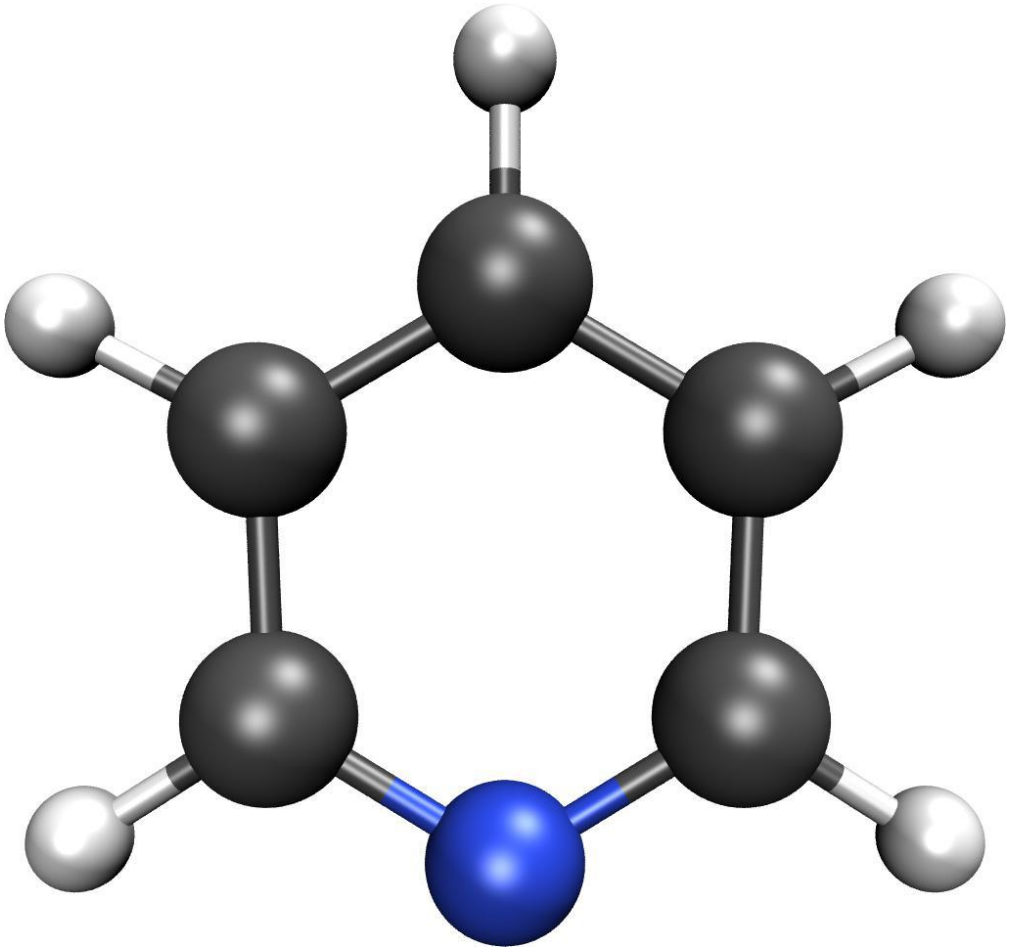
THE Zysman-Colman GROUP

Calculation Report

Pyridine

Optimisation, Frequencies (Singlet)



Summary of Results

Metadata

Username:	osl
Date:	15/06/2022 23:24:49
Duration:	1 m, 23 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:	restricted
Multiplicity:	1 (singlet)
Calc temperature:	298.15 K
Calc pressure:	1.0 atm

SCF Energies

No. of steps:	5
Final energy:	-6748.6129 eV
Final energy:	-651,142 $kJmol^{-1}$

Geometry

Formula:	C_5NH_5
Exact mass:	79.0422 $gmol^{-1}$
Molar mass:	79.0999 $gmol^{-1}$
Alignment method:	Minimal
X extension:	4.31 Å
Y extension:	3.89 Å
Z extension:	0.00 Å
Linearity ratio:	0.10
Planarity ratio:	1.00

HOMO & LUMO

$E_{HOMO,LUMO}$:	6.77 eV
E_{HOMO}:	-7.28 eV
E_{LUMO}:	-0.51 eV

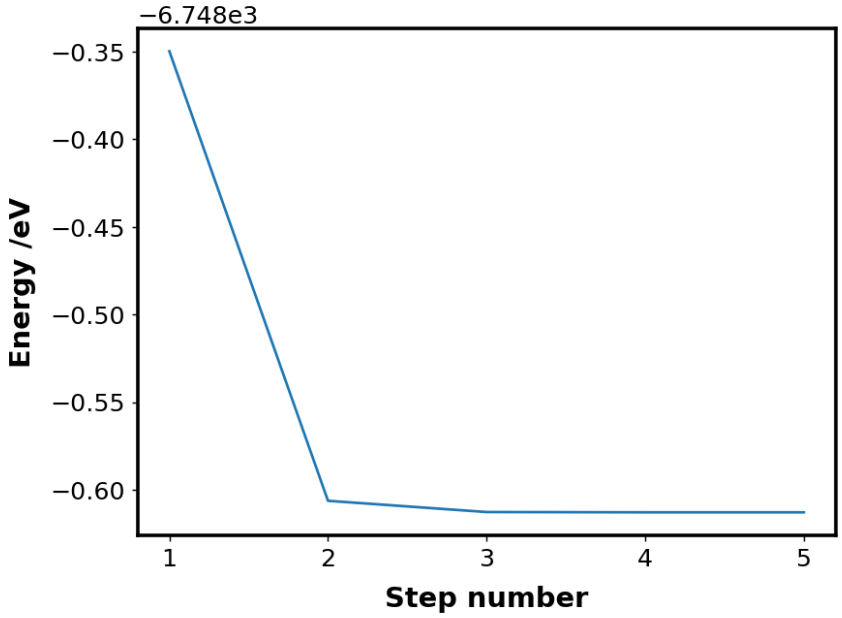
Permanent Dipole Moment

Total:	2.51 D
X axis angle:	90.00 °
XY plane angle:	0.00 °

Vibrational Frequencies

Negative frequencies:	0

SCF Energies



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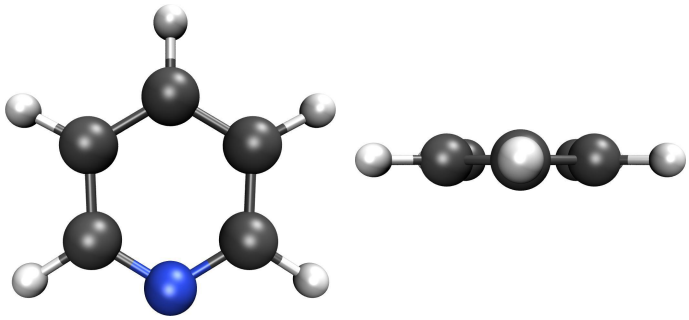
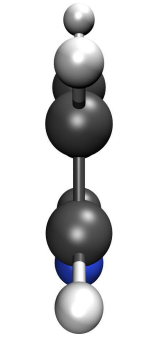
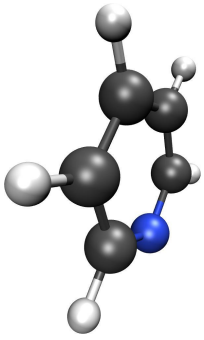


X/Y plane

X/Z plane



Z/Y plane



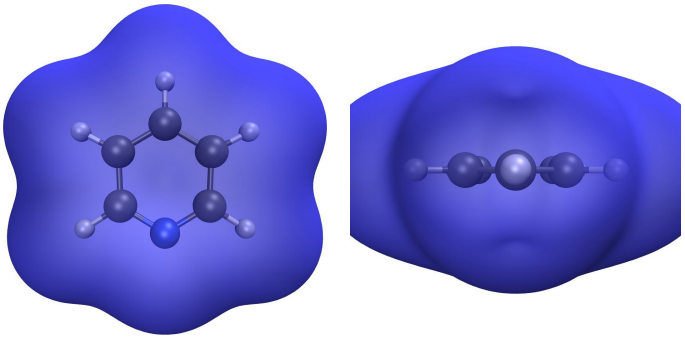
45° to axes

Aligned structure

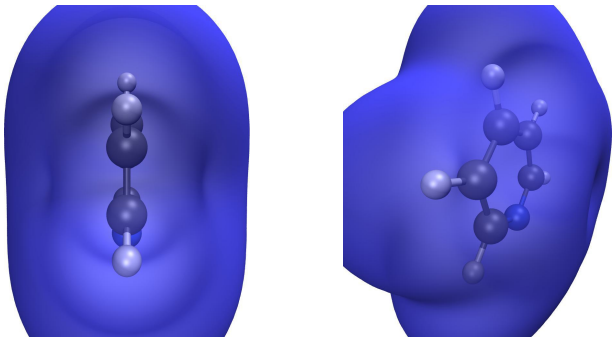
Geometry

Formula:	C_5NH_5
Exact mass:	79.0422 gmol^{-1}
Molar mass:	79.0999 gmol^{-1}
Alignment method:	Minimal
X extension:	4.31 Å
Y extension:	3.89 Å
Z extension:	0.00 Å
Linearity ratio:	0.10
Planarity ratio:	1.00

SCF Density



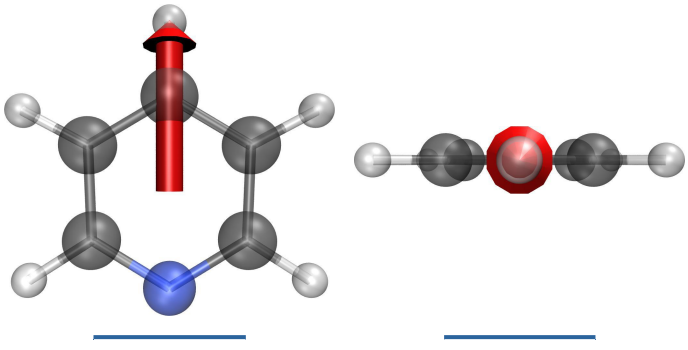
X/Y plane | X/Z plane



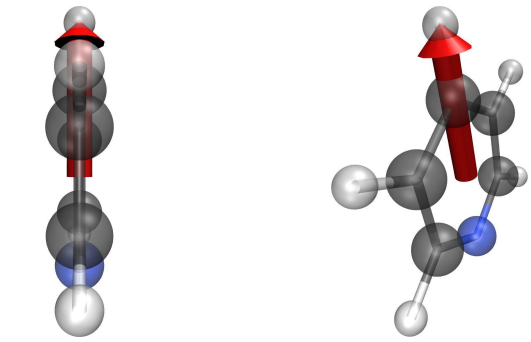
Z/Y plane | 45° to axes

SCF density (isovalue: 0.0004)

Permanent Dipole Moment



X/Y plane | X/Z plane



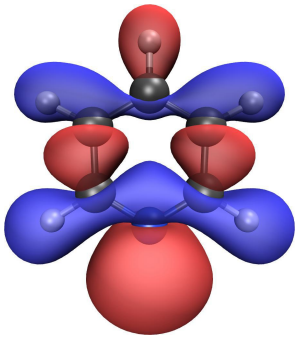
Z/Y plane | 45° to axes

Aligned structure (dipole moment in red)

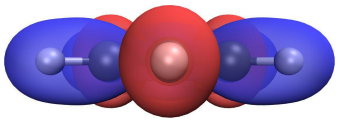
Dipole Moment

Origin X:	0.00 D
Origin Y:	0.00 D
Origin Z:	0.00 D
Vector X:	0.00 D
Vector Y:	2.51 D
Vector Z:	-0.00 D
Total:	2.51 D
X axis angle:	90.00 °
XY plane angle:	0.00 °

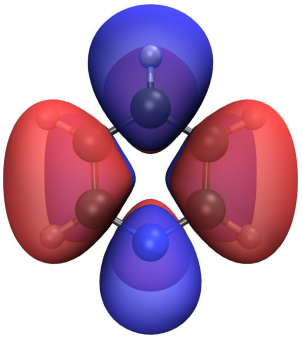
HOMO & LUMO



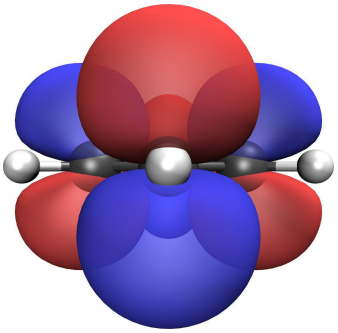
X/Y plane



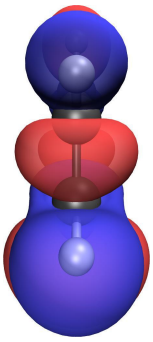
X/Z plane



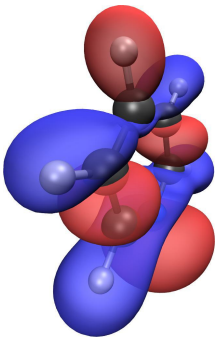
X/Y plane



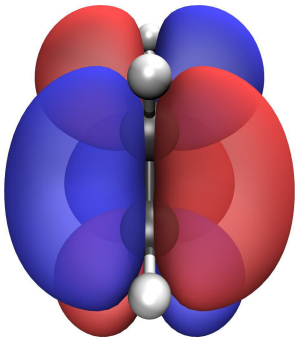
X/Z plane



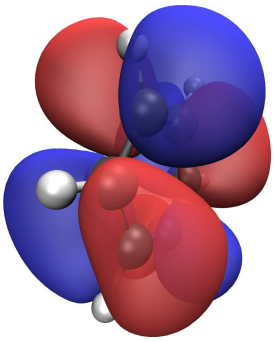
Z/Y plane



45° to axes



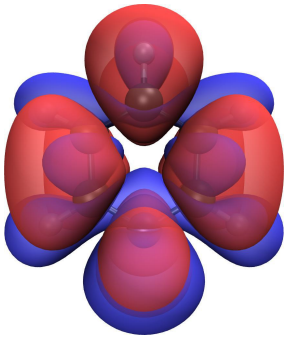
Z/Y plane



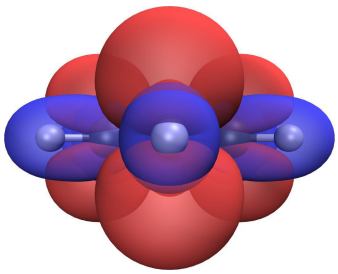
45° to axes

HOMO density (isovalue: 0.02)

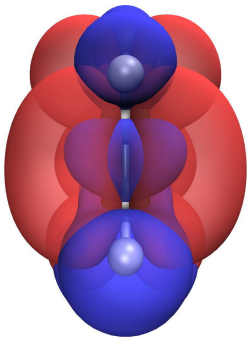
LUMO density (isovalue: 0.02)



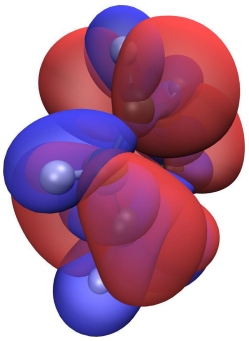
X/Y plane



X/Z plane

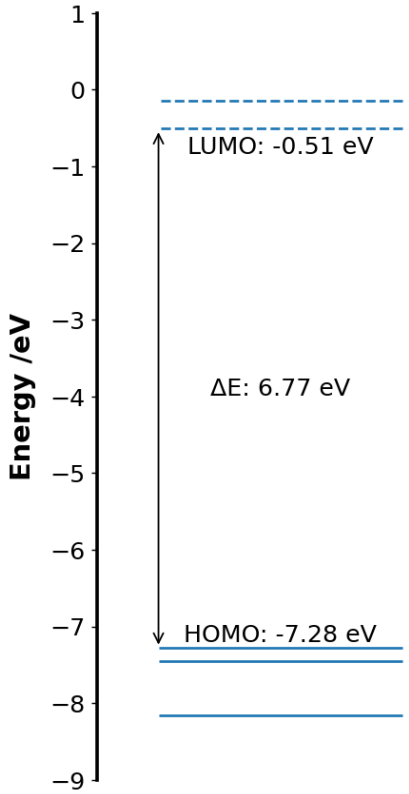


Z/Y plane

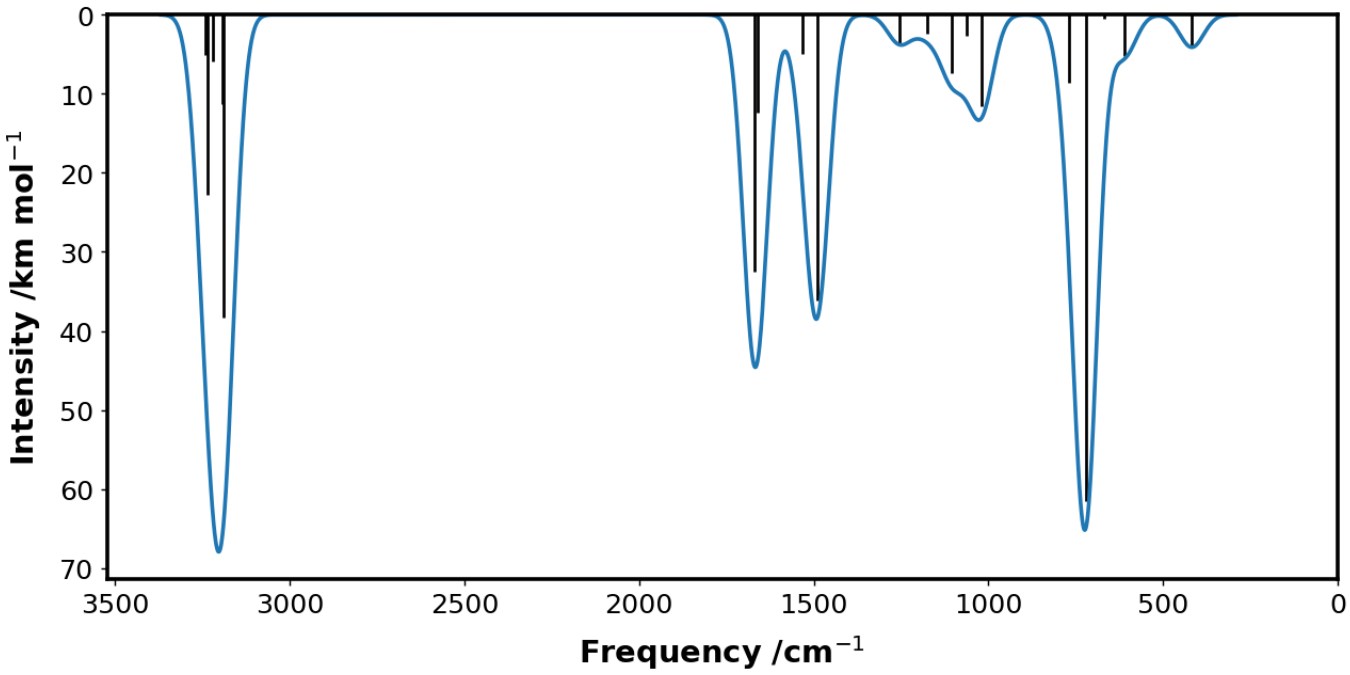


45° to axes

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



Vibrations



IR spectrum (simulated Gaussian functions with FWHM: 80 cm^{-1})
Peaks /cm^{-1}: 417, 724, 1028, 1249, 1493, 1667, 3203.

Table of Vibrational Frequencies

Level	Symmetry	Frequency /cm^{-1}	Intensity /km mol^{-1}
1	A	384.2445	0.0000
2	A	417.5700	4.1187
3	A	611.7278	5.2079
4	A	668.2642	0.4647
5	A	721.5500	61.5866
6	A	768.8726	8.6373
7	A	904.9758	0.0000
8	A	966.8891	0.0014
9	A	1007.7254	0.0000
10	A	1019.4319	11.5446
11	A	1023.1818	0.0001
12	A	1061.1575	2.6424
13	A	1094.9181	0.0005
14	A	1106.3118	7.3922
15	A	1176.6064	2.3938
16	A	1254.2108	3.6314
17	A	1342.5154	0.0027
18	A	1388.6405	0.0269
19	A	1490.0899	36.1488
20	A	1532.7236	4.9241
21	A	1661.7273	12.3410
22	A	1669.3960	32.4724
23	A	3188.5029	38.3142
24	A	3191.5774	11.3414
25	A	3219.0592	5.9386
26	A	3235.6160	22.7306
27	A	3242.8238	5.1354

Table of Selected Molecular Orbitals

Level	Label	Symmetry	Energy /eV
37	LUMO+15	A	14.9940
36	LUMO+14	A	14.5273
35	LUMO+13	A	12.7428
34	LUMO+12	A	12.6081
33	LUMO+11	A	9.0029
32	LUMO+10	A	8.9866
31	LUMO+9	A	8.3038
30	LUMO+8	A	6.7868
29	LUMO+7	A	5.2853
28	LUMO+6	A	5.2515
27	LUMO+5	A	4.6436
26	LUMO+4	A	4.2561
25	LUMO+3	A	4.2020
24	LUMO+2	A	2.9309
23	LUMO+1	A	-0.1420
22	**LUMO**	**A**	**-0.5097**
21	**HOMO**	**A**	**-7.2829**
20	HOMO-1	A	-7.4475
19	HOMO-2	A	-8.1539
18	HOMO-3	A	-10.1324
17	HOMO-4	A	-11.2402
16	HOMO-5	A	-11.2778
15	HOMO-6	A	-11.9507
14	HOMO-7	A	-13.1140
13	HOMO-8	A	-13.4217
12	HOMO-9	A	-14.7872
11	HOMO-10	A	-17.5723
10	HOMO-11	A	-17.6352
9	HOMO-12	A	-21.3397
8	HOMO-13	A	-22.5449
7	HOMO-14	A	-26.3953
6	HOMO-15	A	-278.8609

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	-1.1386600	-0.7199540	0.0000200
C	-1.1953980	0.6709320	-0.0000220
C	-0.0000260	1.3817850	-0.0000190
C	1.1953740	0.6709710	-0.0000200
C	1.1386890	-0.7199120	-0.0000270
N	0.0000240	-1.4172140	0.0000620
H	-2.0570650	-1.3046280	0.0000360
H	-2.1540460	1.1794230	-0.0000390
H	-0.0000390	2.4678210	-0.0000450
H	2.1539990	1.1795060	-0.0000200
H	2.0571100	-1.3045590	0.0000440

About

Silico Calculation Report

Part of the silico software package

Version 1.0.0-pre.30

7 June 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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