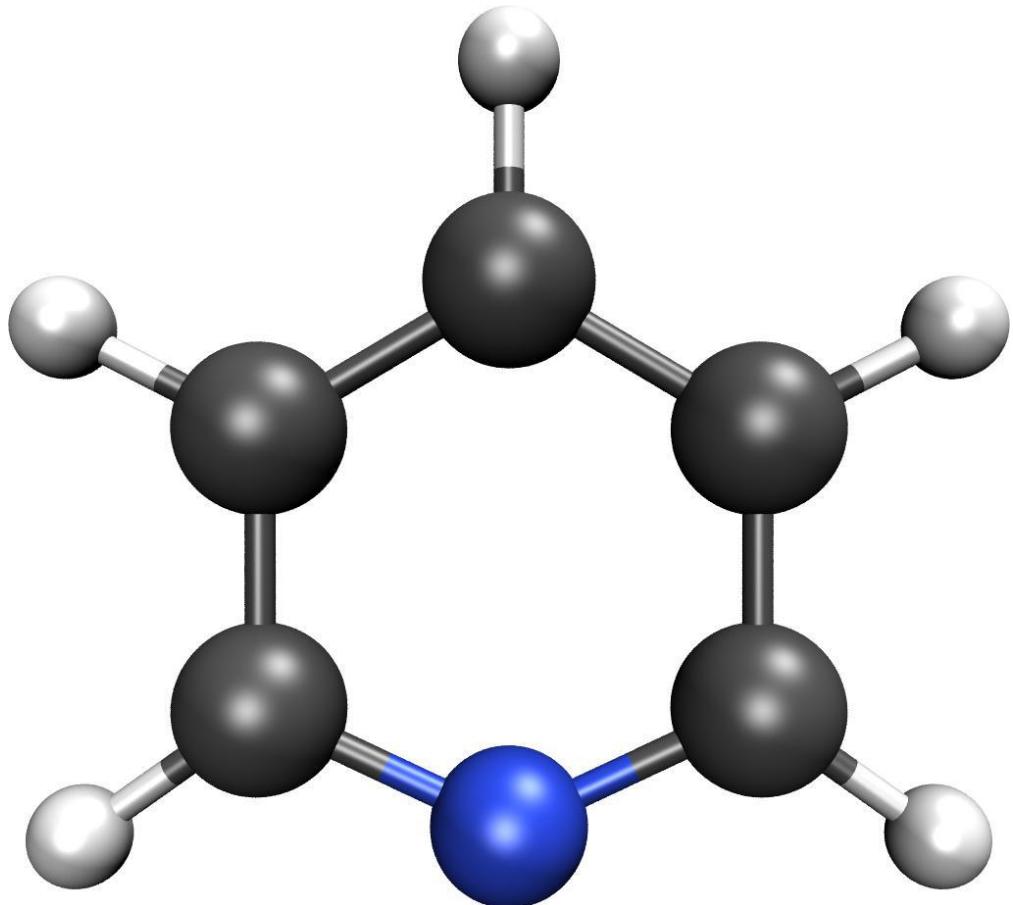


# Calculation Report

## *Pyridine*

Optimisation, Excited States (Singlet)



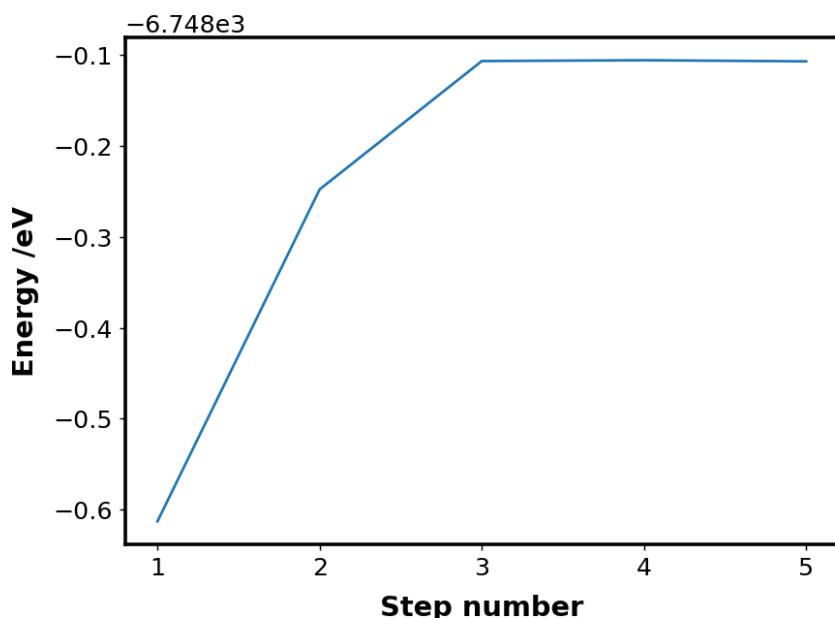
## Summary of Results

Metadata		SCF Energies	Geometry	
Username:	osl	No. of steps: 5	Formula:	C <sub>5</sub> NH <sub>5</sub>
Date:	16/06/2022 00:14:35	Final energy: -6748.1068 eV	Exact mass:	79.0422 gmol <sup>-1</sup>
Duration:	9 m, 42 s	Final energy: -651,093 kJmol <sup>-1</sup>	Molar mass:	79.0999 gmol <sup>-1</sup>
Success:	True		Alignment method:	Minimal
Converged:	True		X extension:	4.38 Å
Computational package:	Gaussian (2016+C.01)		Y extension:	3.81 Å
Methods:	DFT		Z extension:	0.00 Å
Functional:	PBE1PBE		Linearity ratio:	0.13
Basis set:	6-31G(d,p)		Planarity ratio:	1.00
Calculations:	Optimisation, Excited States			
Orbital spin:	restricted			
Multiplicity:	1 (singlet)			

HOMO & LUMO	Permanent Dipole Moment	Transition (S <sub>1</sub> ) Dipole Moment
E <sub>HOMO,LUMO</sub> : 5.90 eV		
E <sub>HOMO</sub> : -6.49 eV	Total: 0.61 D	Total: 0.50 D
E <sub>LUMO</sub> : -0.59 eV	X axis angle: 89.99 °	X axis angle: 90.00 °
	XY plane angle: 0.01 °	XY plane angle: 90.00 °

Vertical S <sub>1</sub> Emission	Excited States
Excited energy: -6743.99 eV	S <sub>1</sub> energy: 4.12 eV
Excited multiplicity: Singlet	S <sub>1</sub> wavelength: 301 nm
Ground energy: -6748.11 eV	S <sub>1</sub> colour: Ultraviolet 
Ground multiplicity: Singlet	S <sub>1</sub> CIE (x,y): (0.00, 0.00)
Emission type: Fluorescence	S <sub>1</sub> oscillator strength: 0.00
S <sub>1</sub> energy: 4.12 eV	No. of singlets: 10
S <sub>1</sub> wavelength: 301 nm	
S <sub>1</sub> colour: Ultraviolet 	
S <sub>1</sub> CIE (x,y): (0.00, 0.00)	
S <sub>1</sub> oscillator strength: 0.00	
S <sub>1</sub> rate /s <sup>-1</sup> : 3.54e+07	

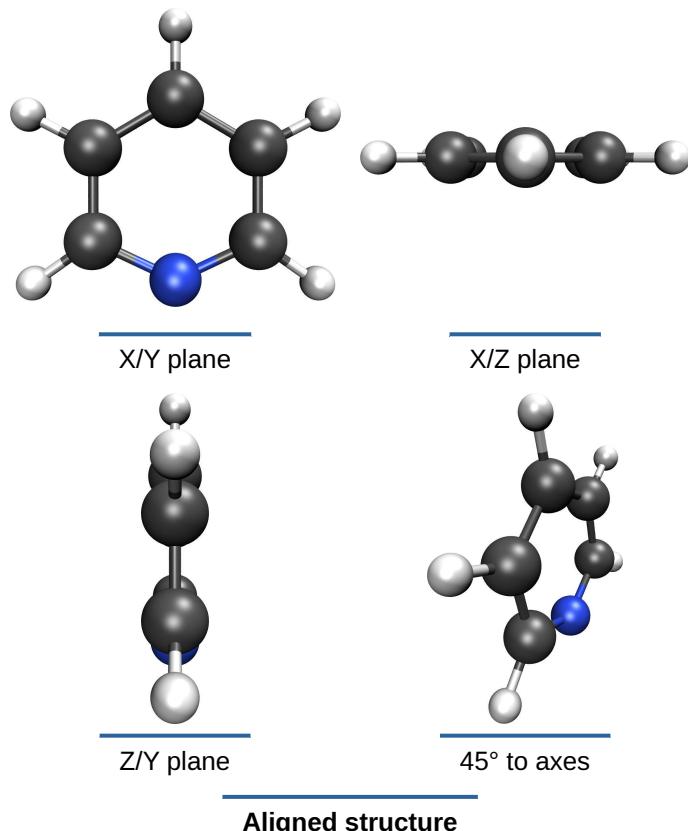
## SCF Energies



## SCF Energies

No. of steps: 5  
Final energy: -6748.1068 eV  
Final energy: -651,093 kJmol<sup>-1</sup>

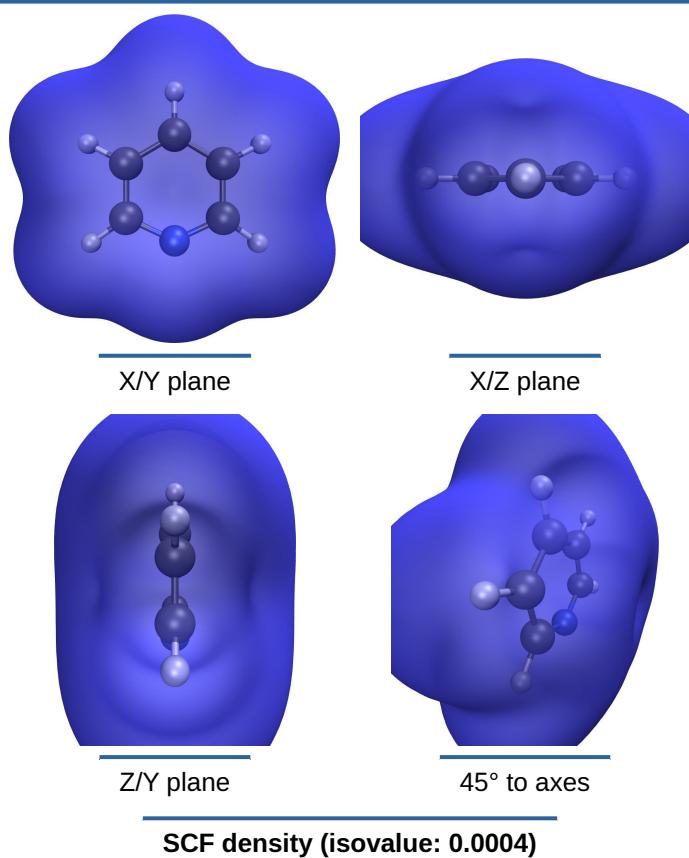
## Geometry



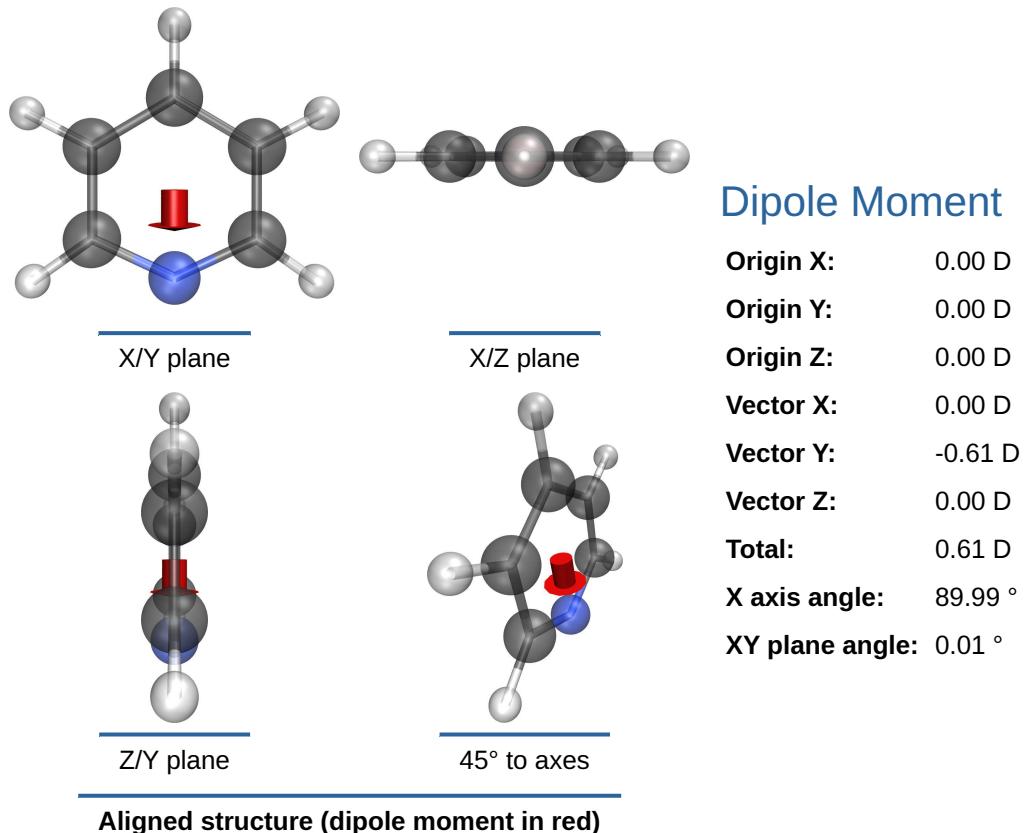
## Geometry

Formula: C<sub>5</sub>NH<sub>5</sub>  
Exact mass: 79.0422 gmol<sup>-1</sup>  
Molar mass: 79.0999 gmol<sup>-1</sup>  
Alignment method: Minimal  
X extension: 4.38 Å  
Y extension: 3.81 Å  
Z extension: 0.00 Å  
Linearity ratio: 0.13  
Planarity ratio: 1.00

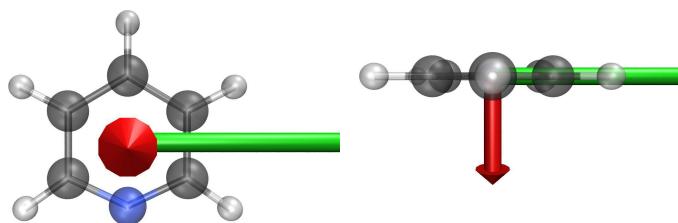
### SCF Density



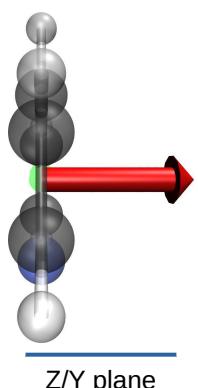
### Permanent Dipole Moment



## *Transition ( $S_1$ ) Dipole Moment*

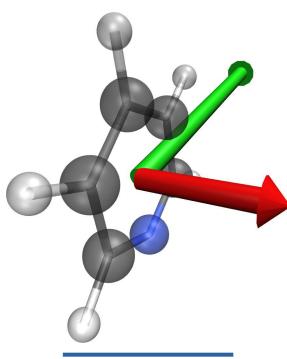


X/Y plane



Z/Y plane

X/Z plane



45° to axes

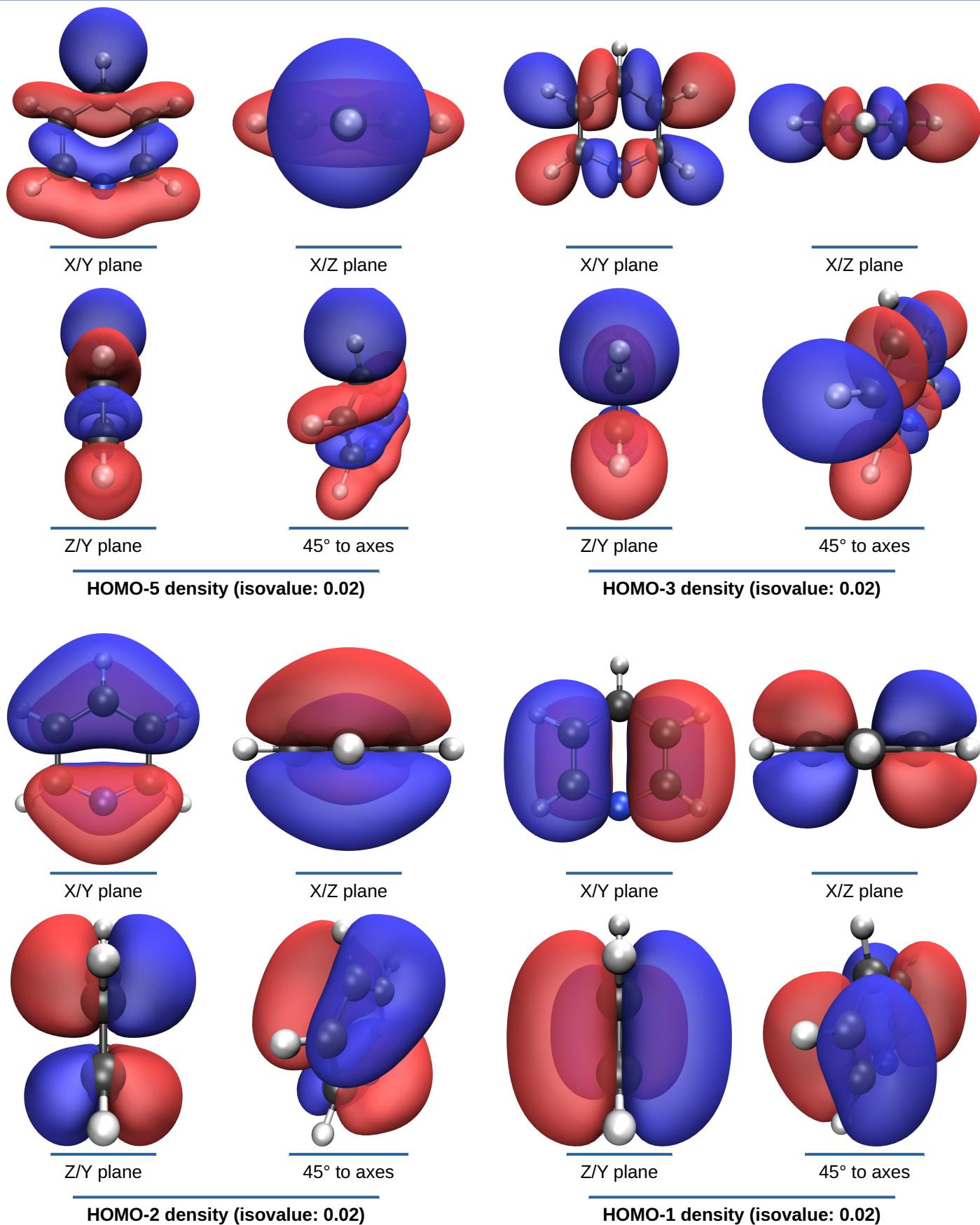
**Aligned structure (dipole moment in red)**

### Dipole Moment

<b>Origin X:</b>	0.00 D
<b>Origin Y:</b>	0.00 D
<b>Origin Z:</b>	0.00 D
<b>Vector X:</b>	0.00 D
<b>Vector Y:</b>	0.00 D
<b>Vector Z:</b>	0.50 D
<b>Total:</b>	0.50 D
<b>X axis angle:</b>	90.00 °
<b>XY plane angle:</b>	90.00 °

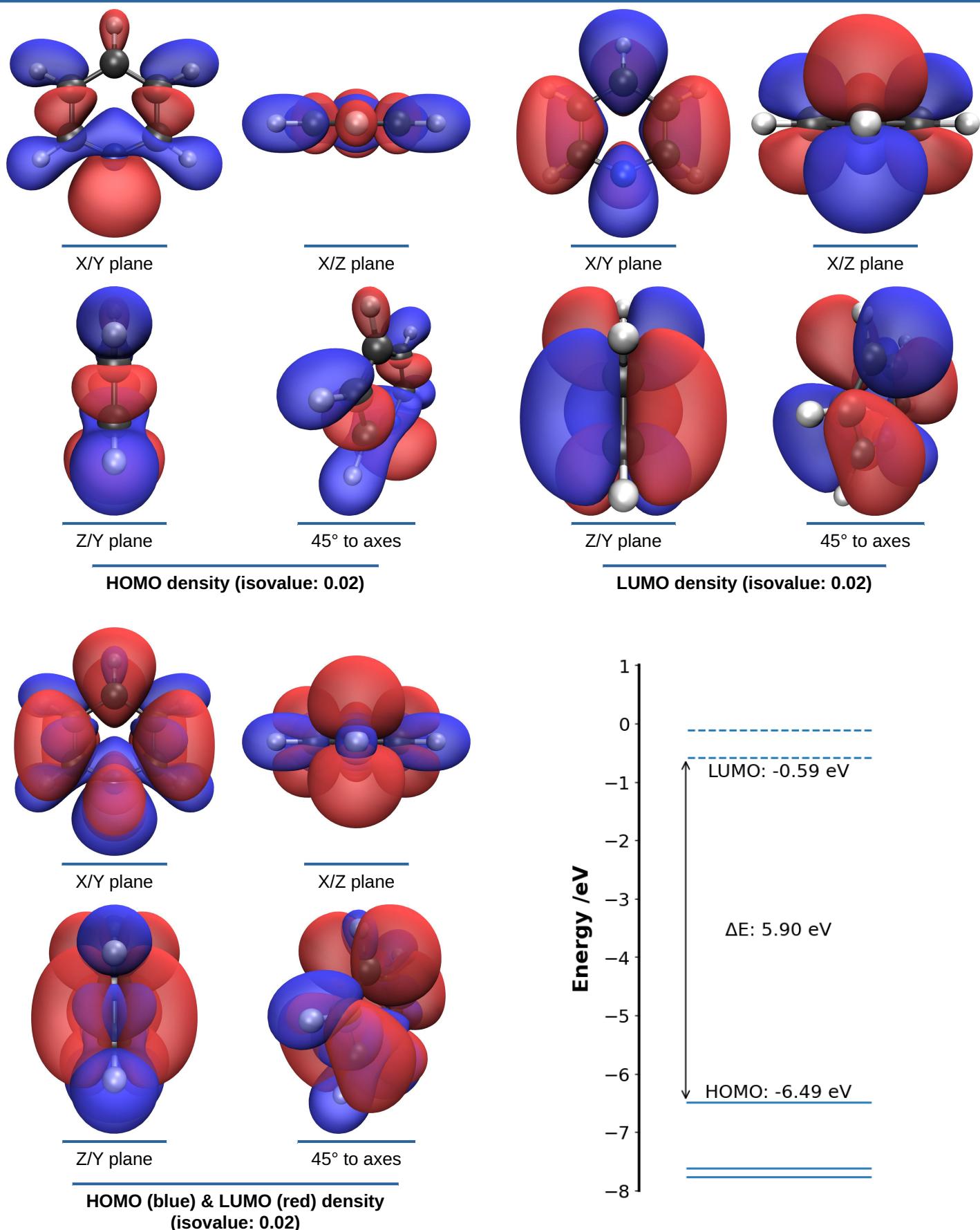
## Pyridine - Optimisation, Excited States (Singlet)

### HOMO-5, HOMO-3, HOMO-2, HOMO-1



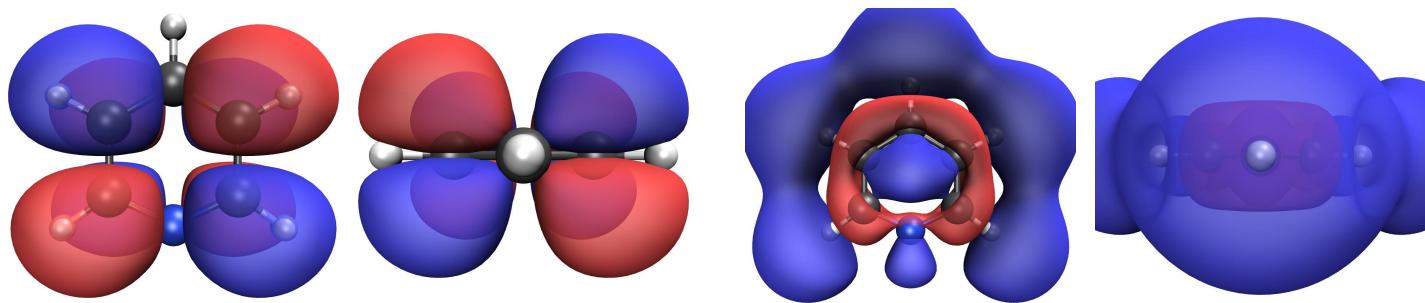
## Pyridine - Optimisation, Excited States (Singlet)

### HOMO & LUMO



## Pyridine - Optimisation, Excited States (Singlet)

### LUMO+1, LUMO+2, LUMO+3



X/Y plane

X/Z plane

X/Y plane

X/Z plane

Z/Y plane

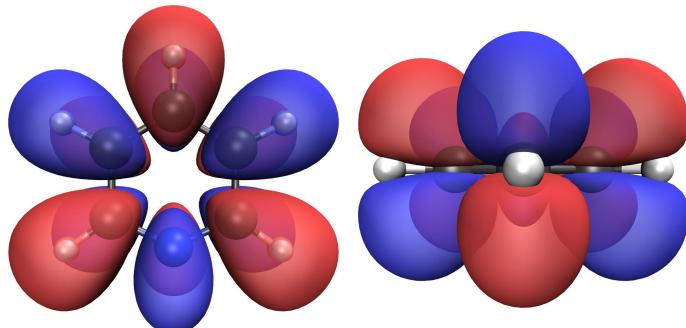
45° to axes

Z/Y plane

45° to axes

LUMO+1 density (isovalue: 0.02)

LUMO+2 density (isovalue: 0.02)



X/Y plane

X/Z plane

X/Y plane

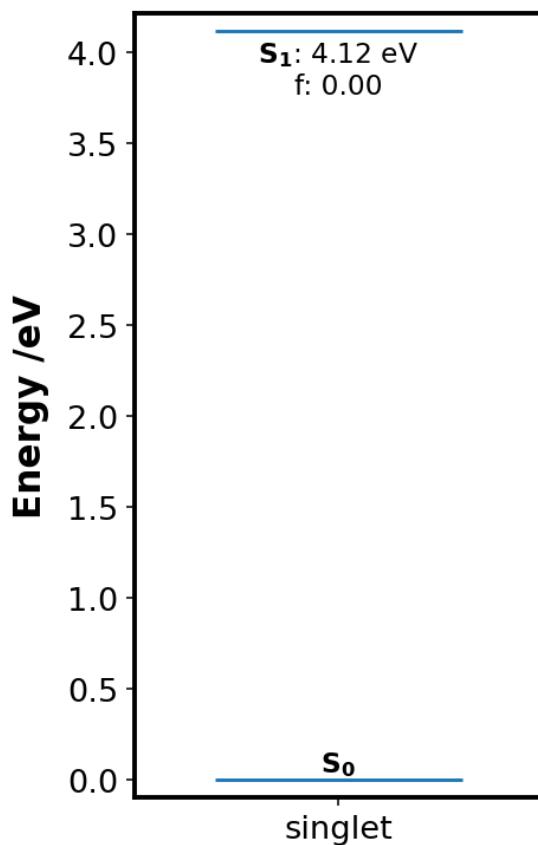
X/Z plane

Z/Y plane

45° to axes

LUMO+3 density (isovalue: 0.02)

## Vertical $S_1$ Emission



### Vertical $S_1$ Emission

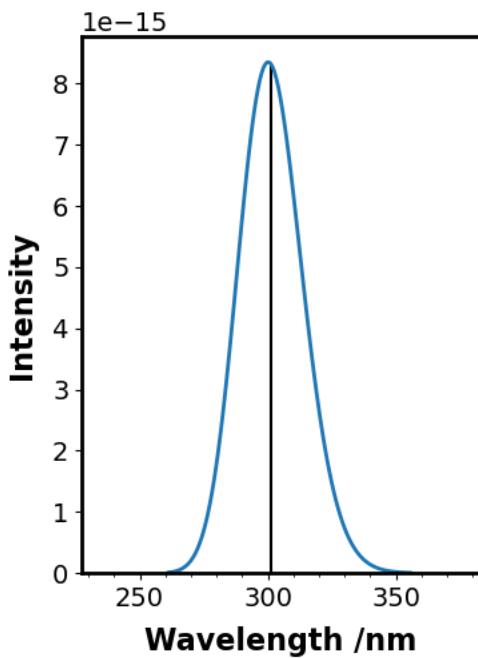
**Excited energy:** -6743.99 eV  
**Excited multiplicity:** Singlet  
**Ground energy:** -6748.11 eV  
**Ground multiplicity:** Singlet  
**Emission type:** Fluorescence  
 **$S_1$  energy:** 4.12 eV  
 **$S_1$  wavelength:** 301 nm  
 **$S_1$  colour:** Ultraviolet

**$S_1$  CIE (x,y):** (0.00, 0.00)

**$S_1$  oscillator strength:** 0.00

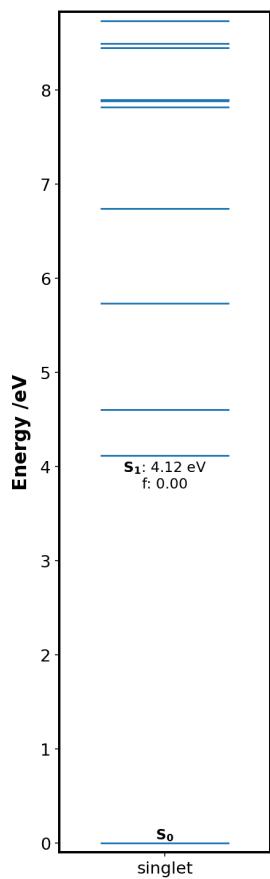
**$S_1$  rate /s<sup>-1</sup>:** 3.54e+07

## Vertical $S_1$ Emission Spectrum



**Emission spectrum (simulated Gaussian functions with FWHM: 0.4 eV)**  
**Peaks /nm: 300.**

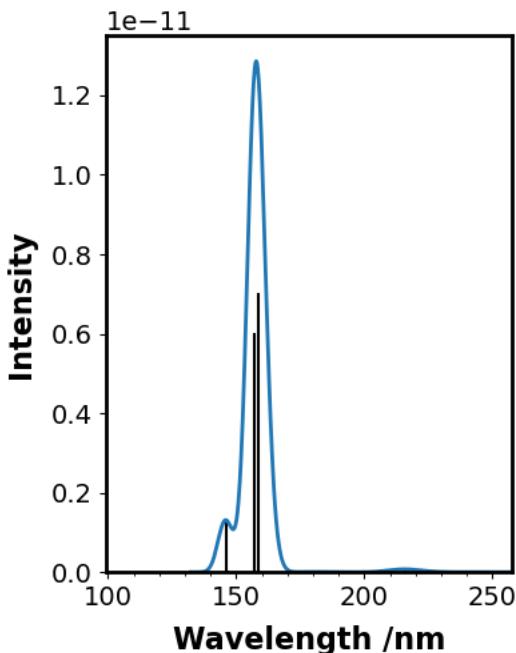
### Excited States



### Excited States

**$S_1$  energy:** 4.12 eV  
 **$S_1$  wavelength:** 301 nm  
 **$S_1$  colour:** Ultraviolet   
 **$S_1$  CIE (x,y):** (0.00, 0.00)  
 **$S_1$  oscillator strength:** 0.00  
**No. of singlets:** 10

### Absorptions



Absorption spectrum (simulated Gaussian functions with FWHM: 0.4 eV).

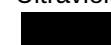
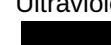
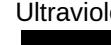
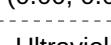
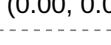
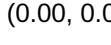
Peaks /nm: 145, 157, 215.

Note: high energy absorption peaks are not simulated.

For a complete absorption spectrum, use more excited states.

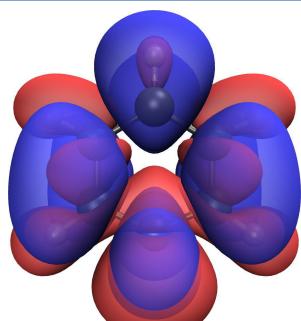
## Pyridine - Optimisation, Excited States (Singlet)

### Table of Excited States

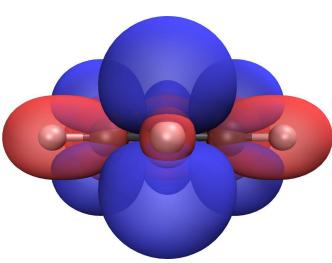
Level	Symbol	Symmetry	Energy /eV	Wavelength /nm	Colour, CIE (x,y)	Oscillator Strength	Transitions (probability)
1	S <sub>1</sub>	Singlet-A	4.1172	301.14	Ultraviolet  (0.00, 0.00)	0.0038	HOMO → LUMO (0.99)
2	S <sub>2</sub>	Singlet-A	4.6017	269.43	Ultraviolet  (0.00, 0.00)	0.0000	HOMO → LUMO+1 (1.00)
3	S <sub>3</sub>	Singlet-A	5.7361	216.15	Ultraviolet  (0.00, 0.00)	0.0173	HOMO-1 → LUMO (0.60) HOMO-2 → LUMO+1 (0.40)
4	S <sub>4</sub>	Singlet-A	6.7431	183.87	Ultraviolet  (0.00, 0.00)	0.0013	HOMO-2 → LUMO (0.58) HOMO-1 → LUMO+1 (0.39)
5	S <sub>5</sub>	Singlet-A	7.8174	158.60	Ultraviolet  (0.00, 0.00)	0.8914	HOMO-2 → LUMO+1 (0.56) HOMO-1 → LUMO (0.36)
6	S <sub>6</sub>	Singlet-A	7.8802	157.34	Ultraviolet  (0.00, 0.00)	0.7514	HOMO-1 → LUMO+1 (0.53) HOMO-2 → LUMO (0.31) HOMO → LUMO+2 (0.09)
7	S <sub>7</sub>	Singlet-A	7.8952	157.04	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.99)
8	S <sub>8</sub>	Singlet-A	8.4452	146.81	Ultraviolet  (0.00, 0.00)	0.0051	HOMO-3 → LUMO+1 (0.99)
9	S <sub>9</sub>	Singlet-A	8.4945	145.96	Ultraviolet  (0.00, 0.00)	0.1342	HOMO → LUMO+2 (0.85) HOMO-2 → LUMO (0.05) HOMO-4 → LUMO (0.04) HOMO-1 → LUMO+1 (0.03)
10	S <sub>10</sub>	Singlet-A	8.7332	141.97	Ultraviolet  (0.00, 0.00)	0.0006	HOMO → LUMO+3 (0.50) HOMO-5 → LUMO (0.48)

## Pyridine - Optimisation, Excited States (Singlet)

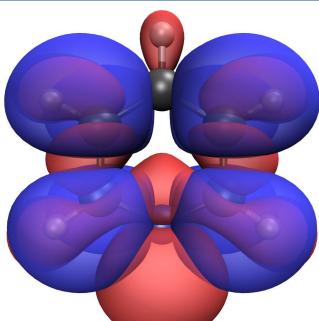
### S(1), S(2), S(3), S(4) Natural Transition Orbitals



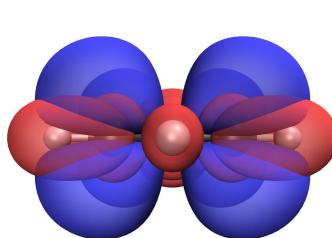
X/Y plane



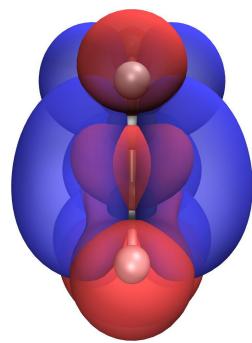
X/Z plane



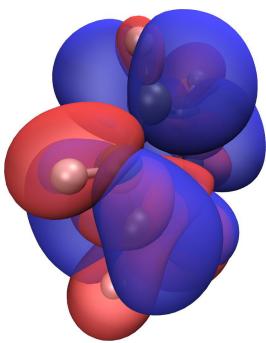
X/Y plane



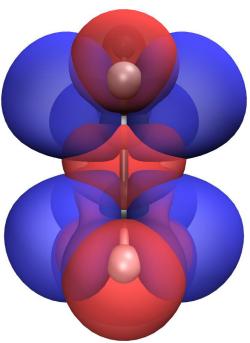
X/Z plane



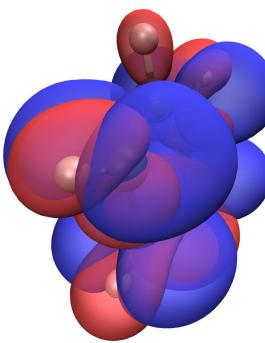
Z/Y plane



45° to axes



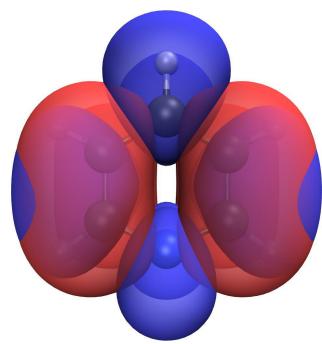
Z/Y plane



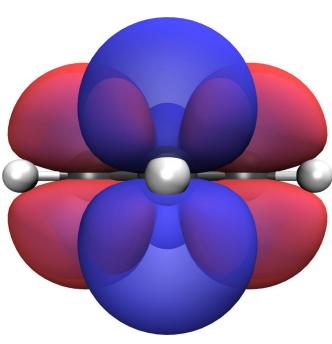
45° to axes

S(1) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

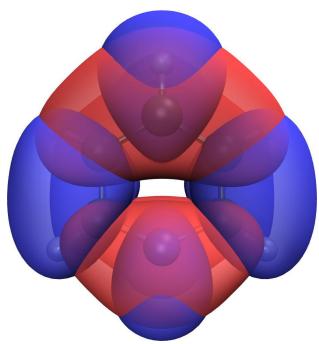
S(2) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



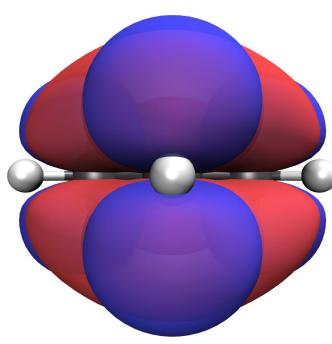
X/Y plane



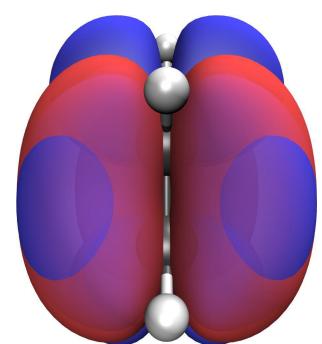
X/Z plane



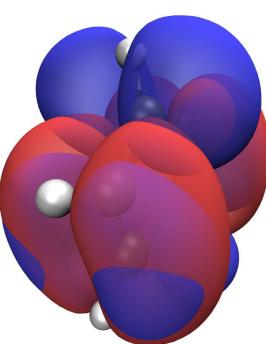
X/Y plane



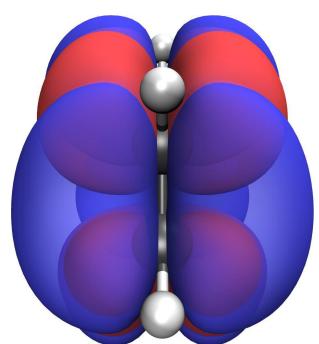
X/Z plane



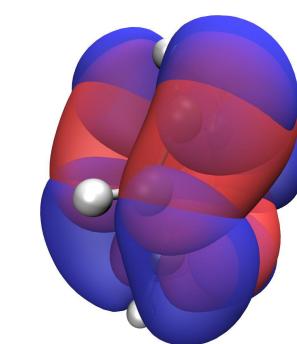
Z/Y plane



45° to axes



Z/Y plane



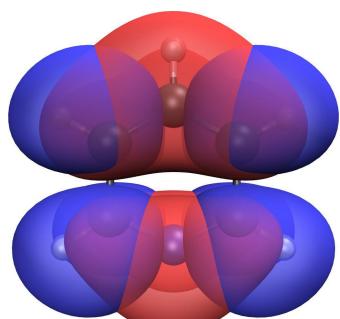
45° to axes

S(3) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

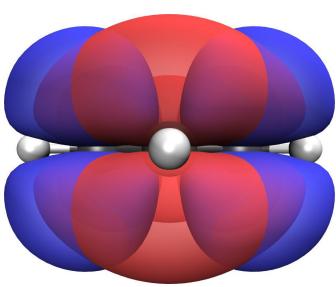
S(4) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

## Pyridine - Optimisation, Excited States (Singlet)

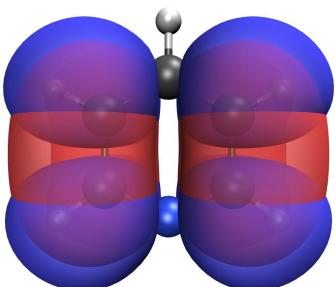
### S(5), S(6), S(7), S(8) Natural Transition Orbitals



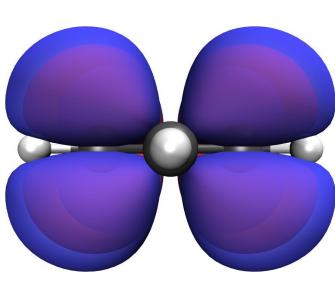
X/Y plane



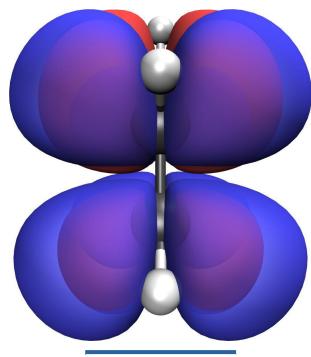
X/Z plane



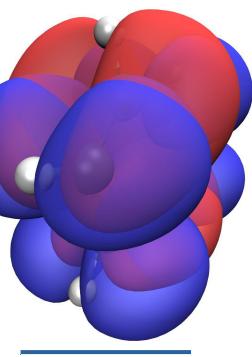
X/Y plane



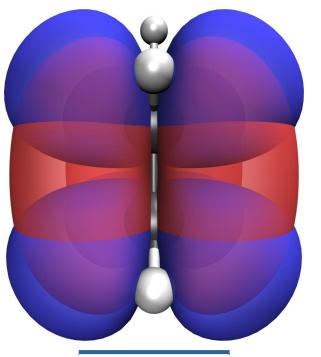
X/Z plane



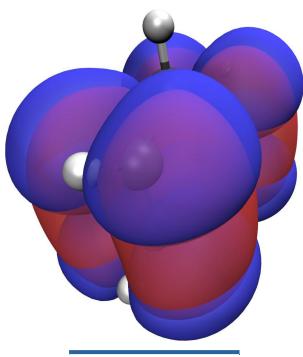
Z/Y plane



45° to axes



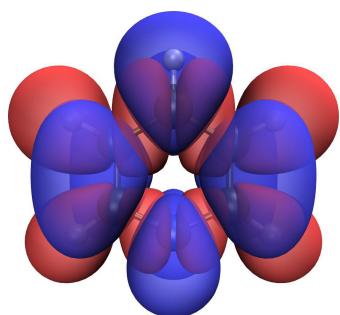
Z/Y plane



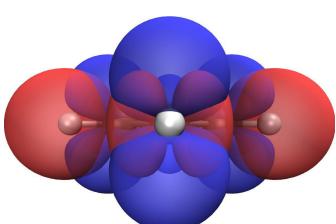
45° to axes

S(5) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

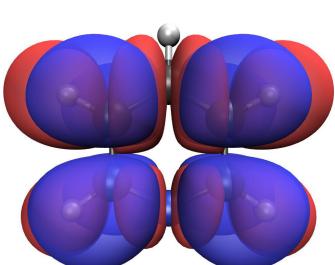
S(6) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



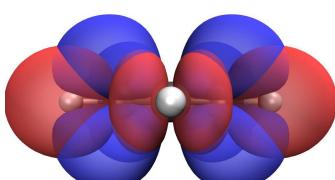
X/Y plane



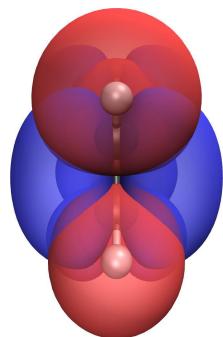
X/Z plane



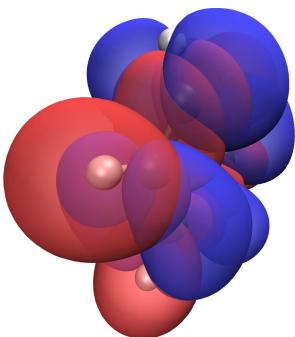
X/Y plane



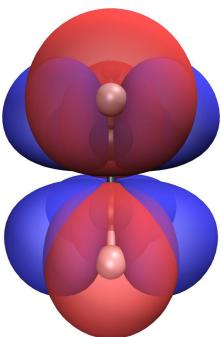
X/Z plane



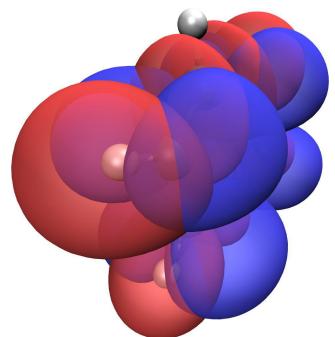
Z/Y plane



45° to axes



Z/Y plane

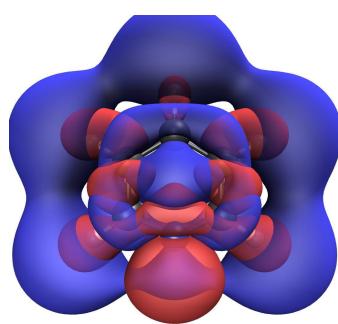


45° to axes

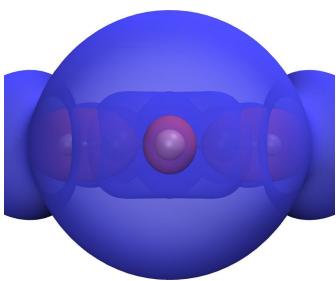
S(7) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

S(8) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

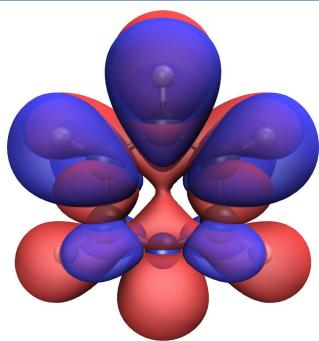
***S(9), S(10) Natural Transition Orbitals***



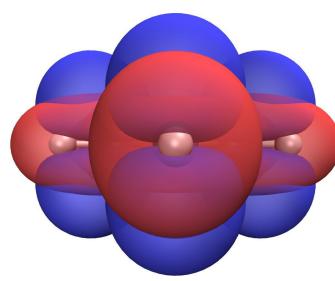
X/Y plane



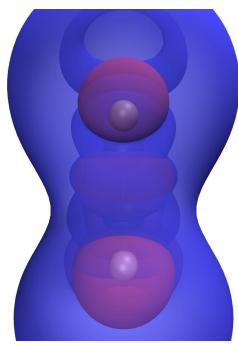
X/Z plane



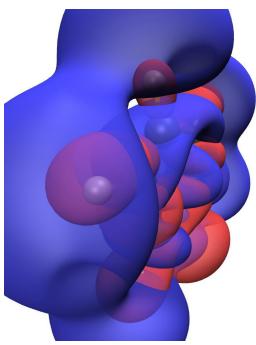
X/Y plane



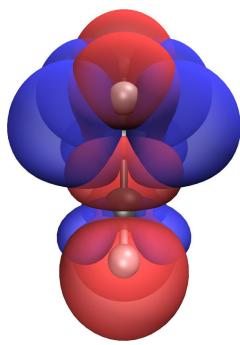
X/Z plane



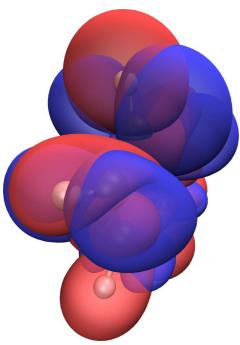
Z/Y plane



45° to axes



Z/Y plane



45° to axes

**S(9) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)**

**S(10) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)**

## Pyridine - Optimisation, Excited States (Singlet)

*Table of Selected Molecular Orbitals*

Level	Label	Symmetry	Energy /eV
37	LUMO+15	A	14.9352
36	LUMO+14	A	14.5437
35	LUMO+13	A	12.6778
34	LUMO+12	A	11.8563
33	LUMO+11	A	9.5588
32	LUMO+10	A	8.8491
31	LUMO+9	A	7.7661
30	LUMO+8	A	6.6399
29	LUMO+7	A	5.2311
28	LUMO+6	A	5.0240
27	LUMO+5	A	4.4888
26	LUMO+4	A	4.1282
25	LUMO+3	A	4.1062
24	LUMO+2	A	3.0885
23	LUMO+1	A	-0.1135
22	<b>LUMO</b>	<b>A</b>	<b>-0.5872</b>
21	<b>HOMO</b>	<b>A</b>	<b>-6.4894</b>
20	HOMO-1	A	-7.6132
19	HOMO-2	A	-7.7732
18	HOMO-3	A	-10.2780
17	HOMO-4	A	-11.0663
16	HOMO-5	A	-11.2557
15	HOMO-6	A	-12.3368
14	HOMO-7	A	-13.0998
13	HOMO-8	A	-13.3205
12	HOMO-9	A	-14.7584
11	HOMO-10	A	-17.4754
10	HOMO-11	A	-17.5821
9	HOMO-12	A	-21.5990
8	HOMO-13	A	-21.9944
7	HOMO-14	A	-26.0127
6	HOMO-15	A	-278.9110

## Pyridine - Optimisation, Excited States (Singlet)

### Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	1.2223280	-0.7327140	-0.0000160
C	1.2236890	0.6422610	0.0000110
C	0.0000010	1.3694790	0.0000280
C	-1.2236670	0.6422750	0.0000240
C	-1.2223510	-0.7327070	-0.0000170
N	-0.0000010	-1.3065420	-0.0000430
H	2.1060240	-1.3583370	-0.0000070
H	2.1890680	1.1397590	0.0000350
H	0.0000010	2.4513310	0.0000610
H	-2.1890380	1.1397920	0.0000510
H	-2.1060520	-1.3583170	-0.0000210

## About

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# 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 3<sup>rd</sup> party libraries and programs; please cite these appropriately in your works:**

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Extraction and processing of results: **cclib**<sup>[1]</sup>

Rendering of 3D images: **VMD**<sup>[2]</sup>, **Tachyon**<sup>[3]</sup>

Rendering of graphs: **Matplotlib**<sup>[4]</sup>

Calculation of CIE colour coordinates: **Colour Science**<sup>[5]</sup>

Generation of reports: **Mako**<sup>[6]</sup>, **Weasyprint**<sup>[7]</sup>

Scientific constants: **SciPy**<sup>[8]</sup>

Conversion of file formats: **Pybel**<sup>[9]</sup>, **Openbabel**<sup>[10]</sup>

Calculation of spin-orbit coupling: **PySOC**<sup>[11]</sup>

Rendering of 2D structures: **RDKit**<sup>[12]</sup>

Saving of state during submission: **Dill**<sup>[13,14]</sup>

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