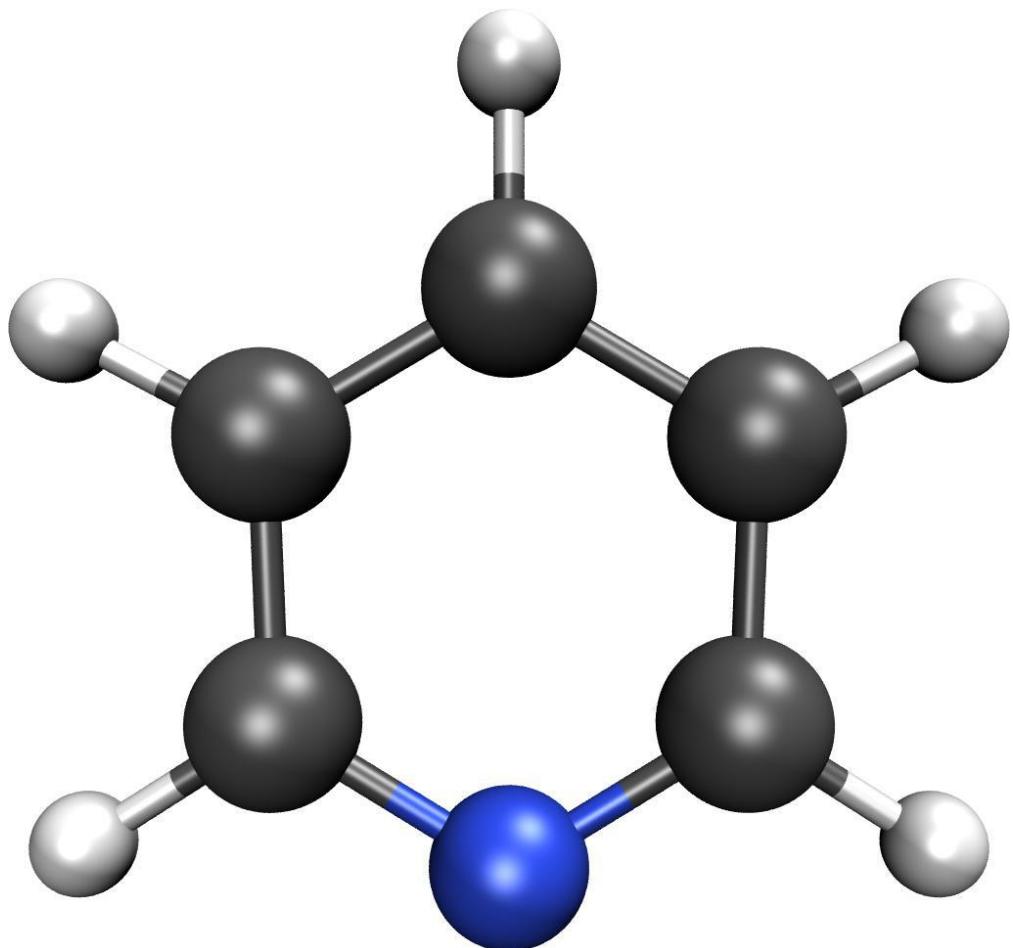


Calculation Report

Pyridine

Optimisation, Frequencies, Excited States (Singlet, Triplet)



Summary of Results

Metadata		Calculation 1		Calculation 2	
Username:	osl	Username:	osl	Username:	osl
Date:	16/06/2022 00:14:35	Date:	15/06/2022 23:24:49	Date:	15/06/2022 23:33:59
Duration:	15 m, 20 s	Duration:	1 m, 23 s	Duration:	4 m, 13 s
Success:	True	Success:	True	Success:	True
Converged:	True	Converged:	True	Computational package:	Gaussian (2016+C.01)
Computational package:	Gaussian (2016+C.01)	Computational package:	Gaussian (2016+C.01)	Methods:	DFT
Methods:	DFT	Methods:	DFT	Functional:	PBE1PBE
Functional:	PBE1PBE	Functional:	PBE1PBE	Basis set:	6-31G(d,p)
Basis set:	6-31G(d,p)	Basis set:	6-31G(d,p)	Calculations:	Excited States
Calculations:	Optimisation, Frequencies, Excited States	Calculations:	Optimisation, Frequencies	Orbital spin:	restricted
Orbital spin:	restricted	Orbital spin:	restricted	Multiplicity:	1 (singlet)
Multiplicity:	1 (singlet)	Multiplicity:	1 (singlet)	Calc temperature:	298.15 K
No. merged calculations:	3	Calc pressure:	1.0 atm	Calculation 3	SCF Energies
Username:	osl	No. of steps:	5	Geometry	
Date:	16/06/2022 00:14:35	Final energy:	-6748.6129 eV	Formula:	C ₅ NH ₅
Duration:	9 m, 42 s	Final energy:	-651,142 kJmol ⁻¹	Exact mass:	79.0422 gmol ⁻¹
Success:	True			Molar mass:	79.0999 gmol ⁻¹
Converged:	True			Alignment method:	Minimal
Computational package:	Gaussian (2016+C.01)			X extension:	4.31 Å
Methods:	DFT			Y extension:	3.89 Å
Functional:	PBE1PBE			Z extension:	0.00 Å
Basis set:	6-31G(d,p)			Linearity ratio:	0.10
Calculations:	Optimisation, Excited States			Planarity ratio:	1.00
Orbital spin:	restricted				
Multiplicity:	1 (singlet)				

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 °

Transition (S_1) Dipole Moment

Total: 0.59 D

X axis angle: 90.00 °

XY plane angle: 89.98 °

Vibrational Frequencies

Negative frequencies: 0

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 [REDACTED]

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

S_1 oscillator strength: 0.00

S_1 rate /s⁻¹: 3.54e+07

Adiabatic S_1 Emission

Excited energy: -6743.99 eV

Excited multiplicity: Singlet

Ground energy: -6748.61 eV

Ground multiplicity: Singlet

Emission type: Fluorescence

S_1 energy: 4.62 eV

S_1 wavelength: 268 nm

S_1 colour: Ultraviolet [REDACTED]

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

S_1 oscillator strength: 0.00

S_1 rate /s⁻¹: 5.01e+07

Excited States

ΔE_{ST}

S_1 energy

S_1 wavelength

S_1 colour

S_1 CIE (x,y)

S_1 oscillator strength

T_1 energy

T_1 wavelength

T_1 colour

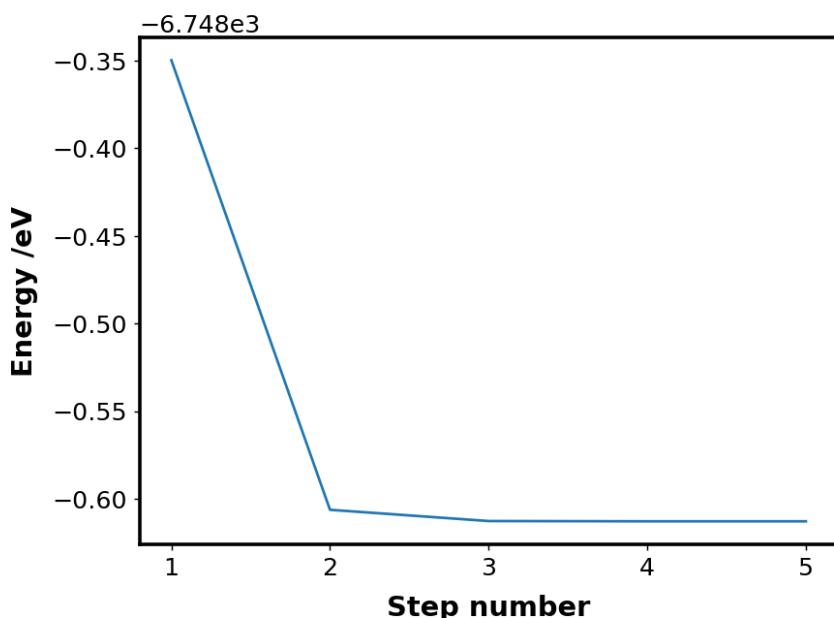
T_1 CIE (x,y)

T_1 oscillator strength

No. of transitions

No. of excited states

SCF Energies



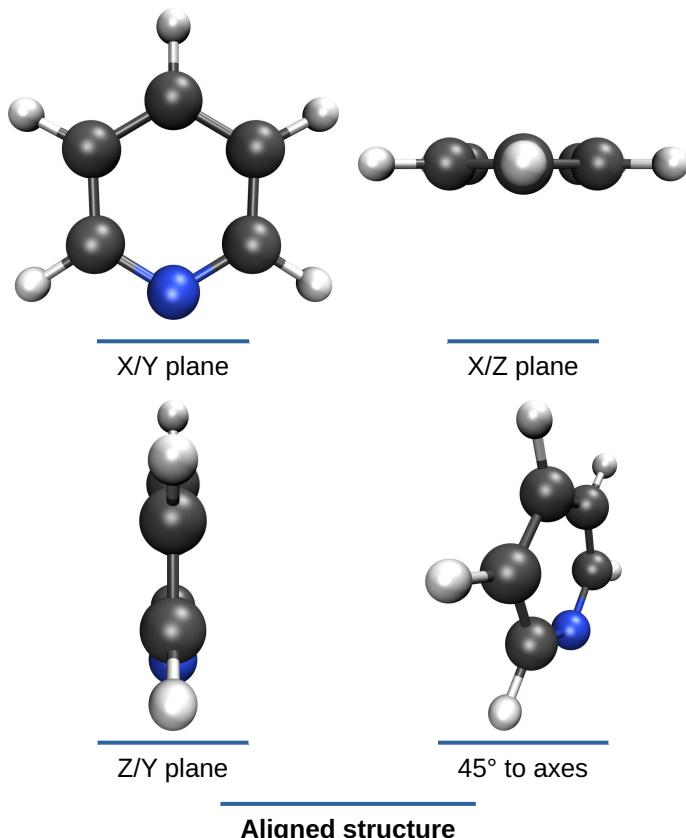
SCF Energies

No. of steps: 5

Final energy: -6748.6129 eV

Final energy: -651,142 kJmol⁻¹

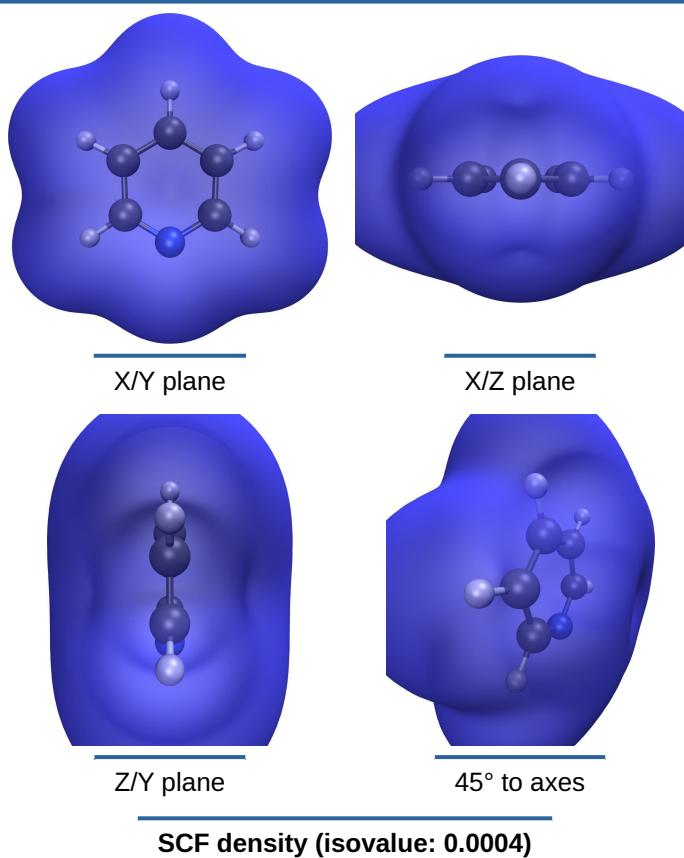
Geometry



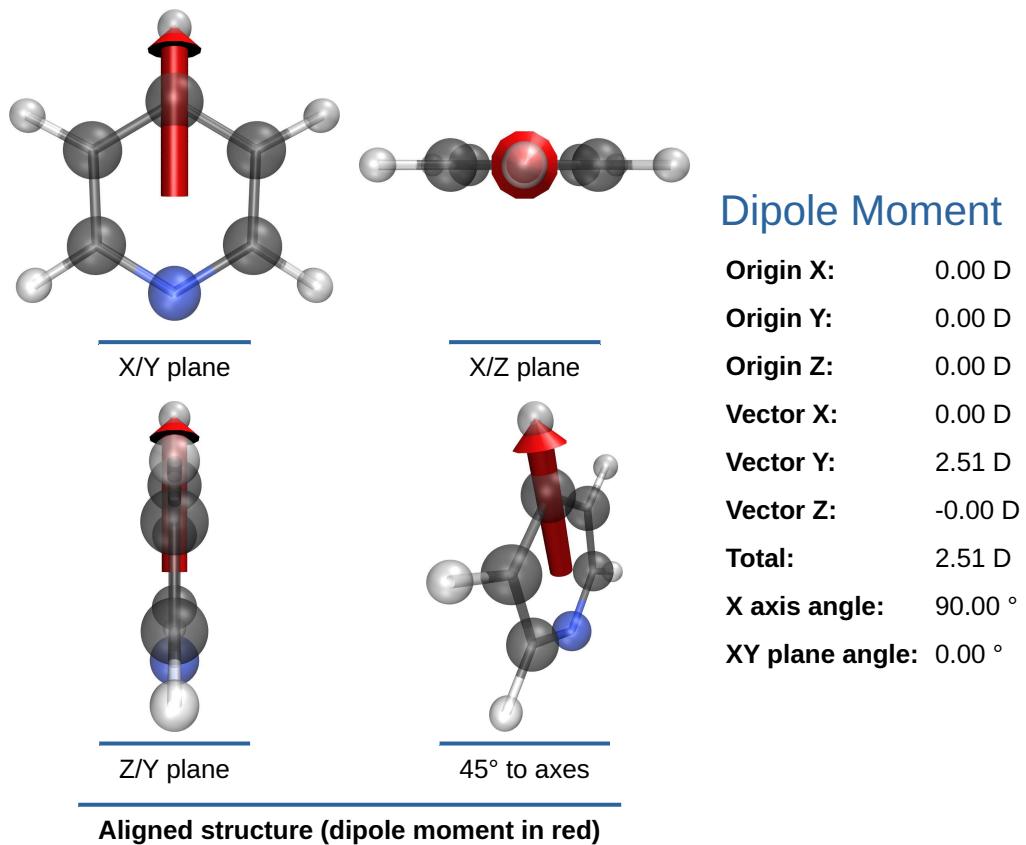
Geometry

Formula:	C ₅ NH 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

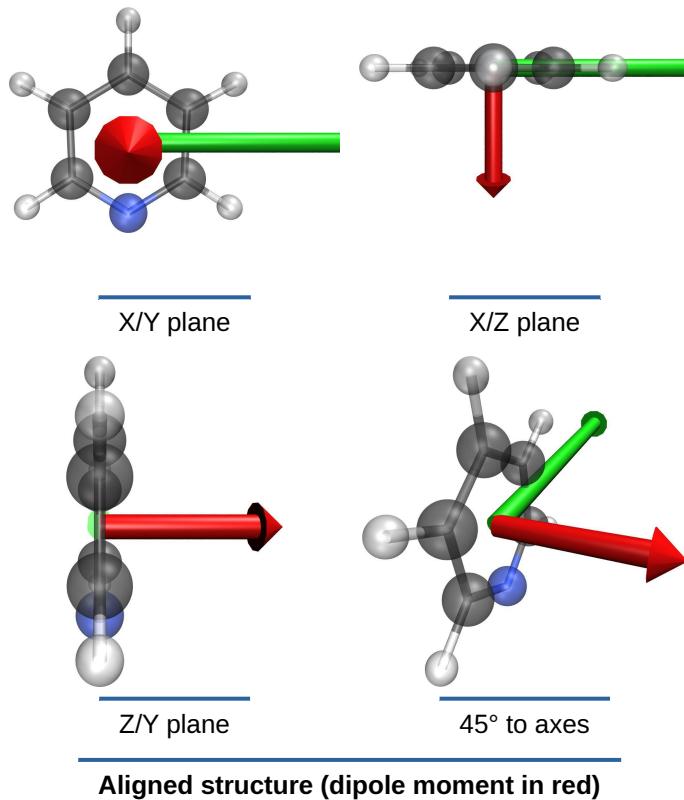
SCF Density



Permanent Dipole Moment



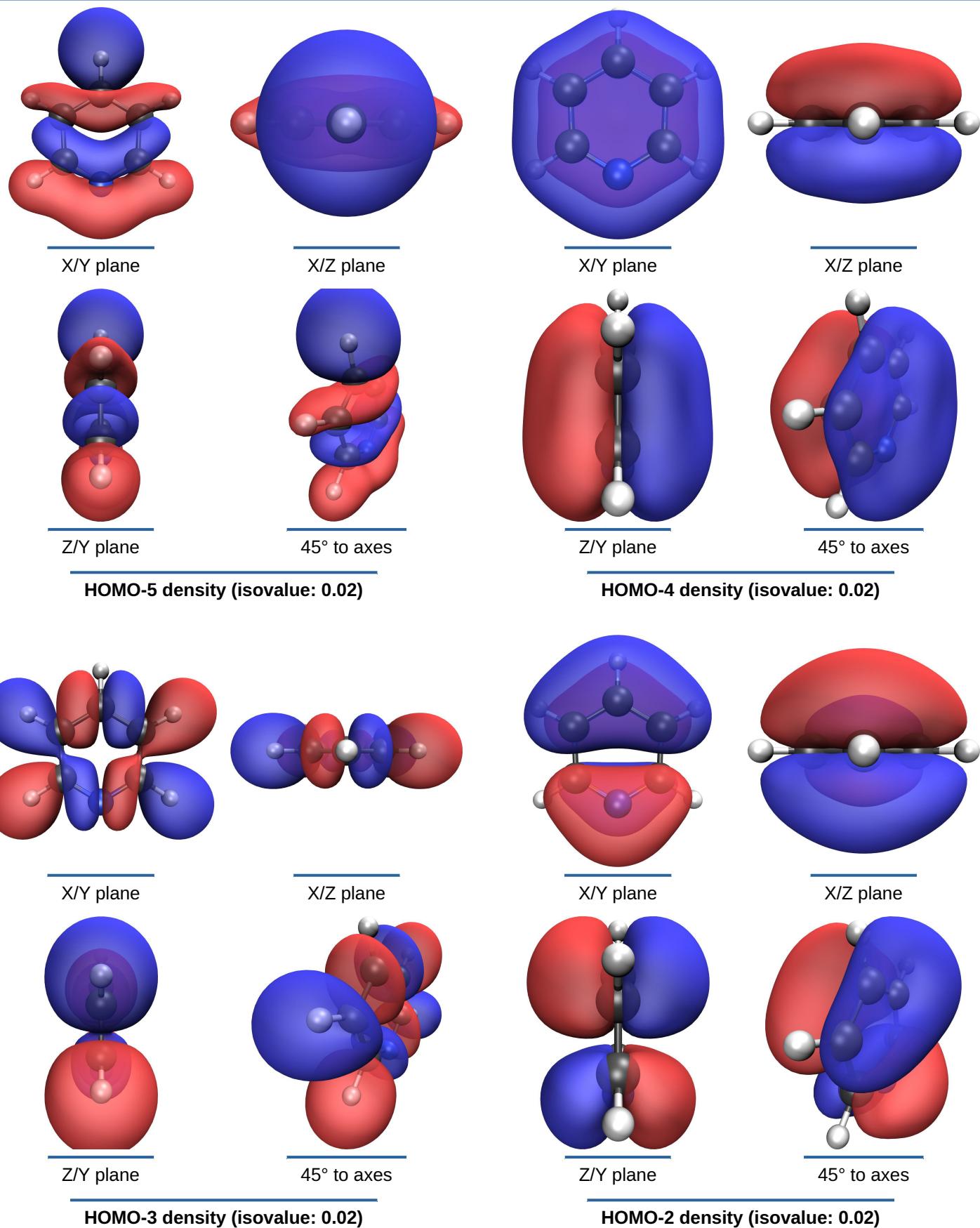
Transition (S_1) Dipole Moment



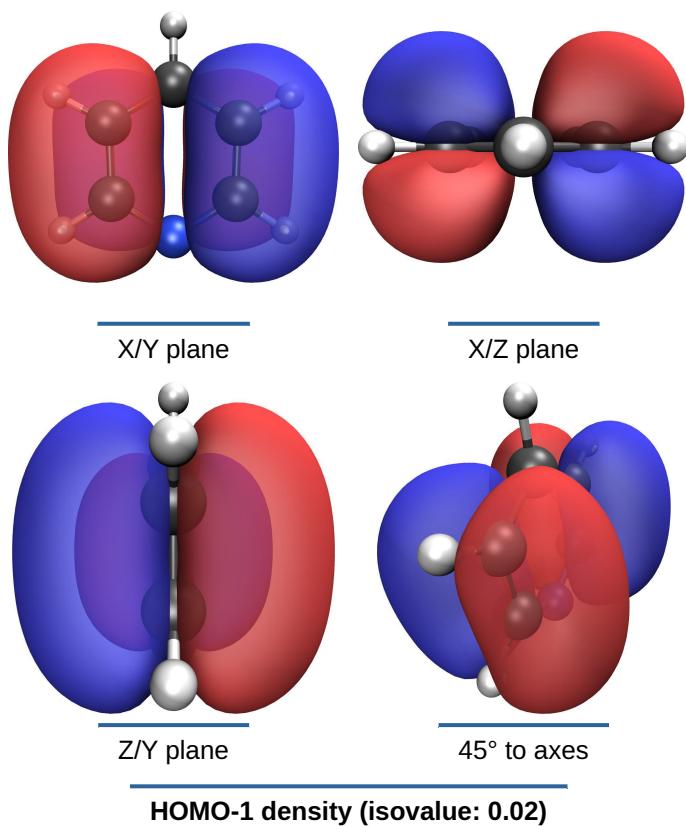
Dipole Moment

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: 0.59 D
Total: 0.59 D
X axis angle: 90.00 °
XY plane angle: 89.98 °

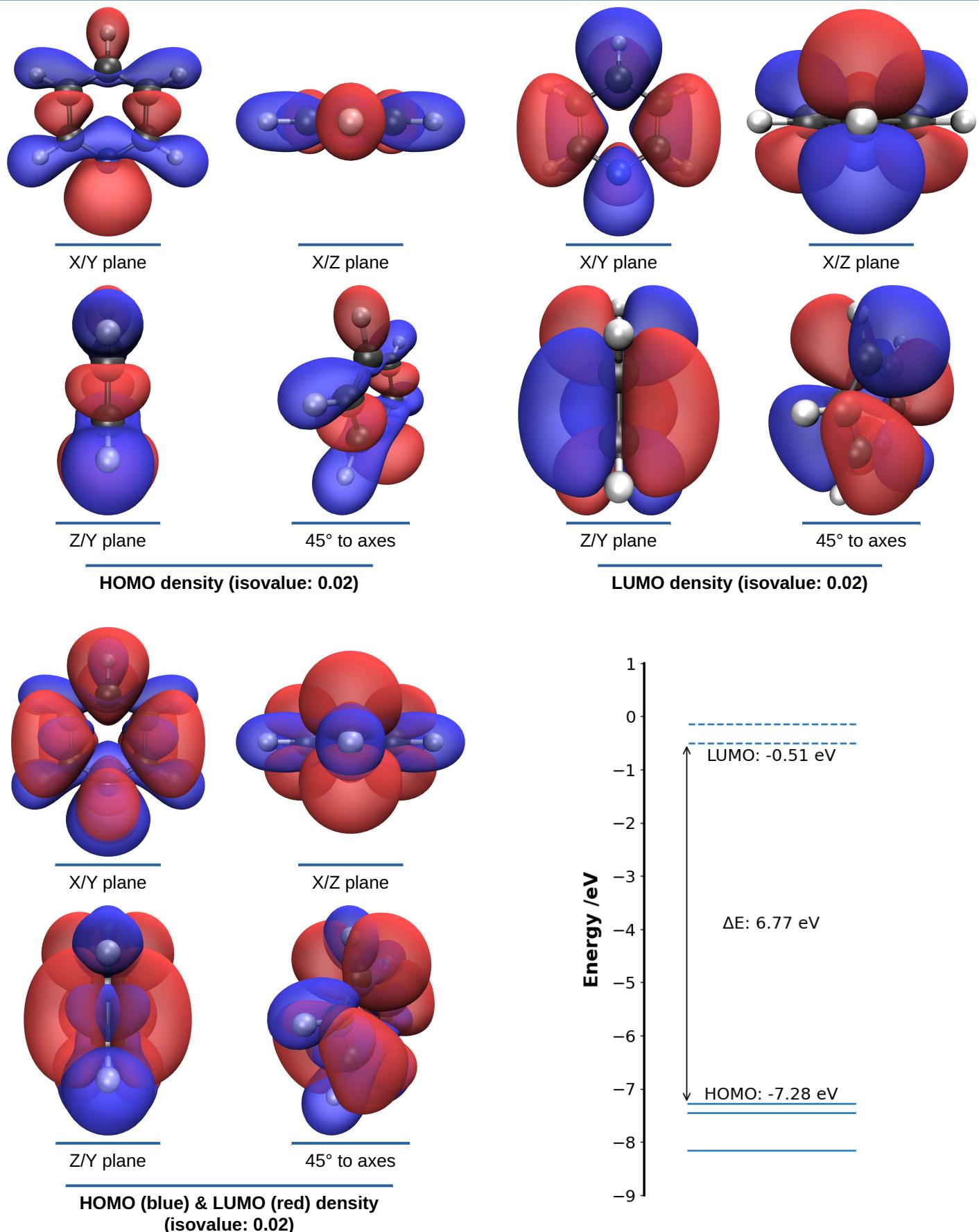
HOMO-5, HOMO-4, HOMO-3, HOMO-2



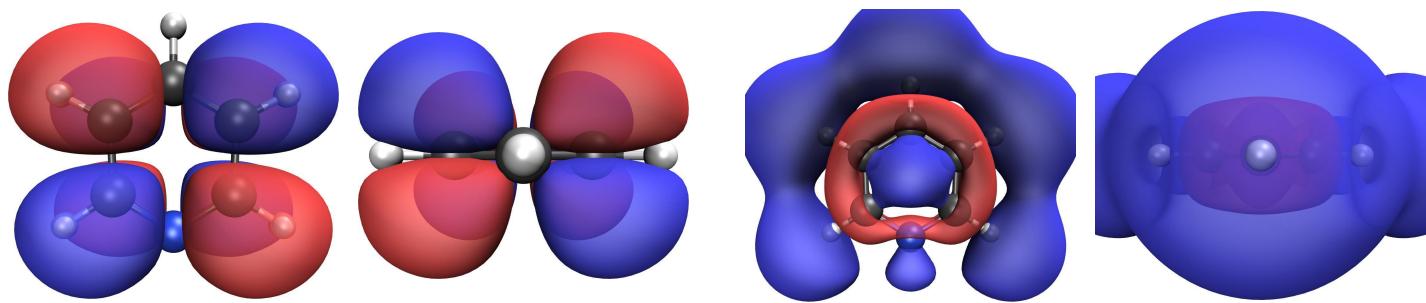
HOMO-1



HOMO & LUMO



LUMO+1, LUMO+2, LUMO+4



X/Y plane

X/Z plane

X/Y plane

X/Z plane

Z/Y plane

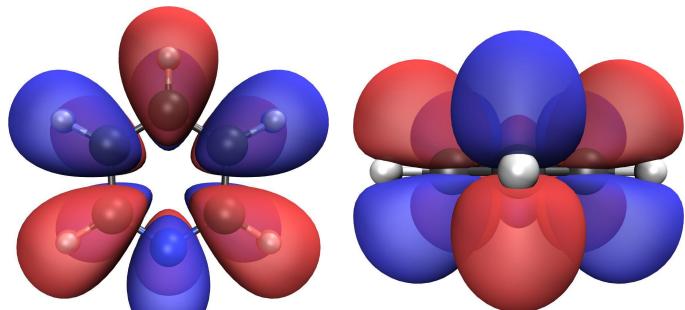
45° to axes

Z/Y plane

45° to axes

LUMO+1 density (isovalue: 0.02)

LUMO+2 density (isovalue: 0.02)

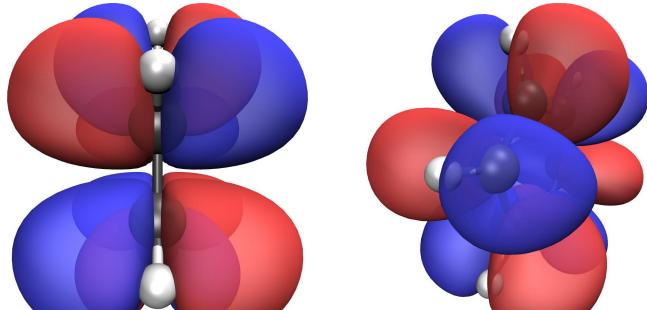


X/Y plane

X/Z plane

Z/Y plane

45° to axes



X/Y plane

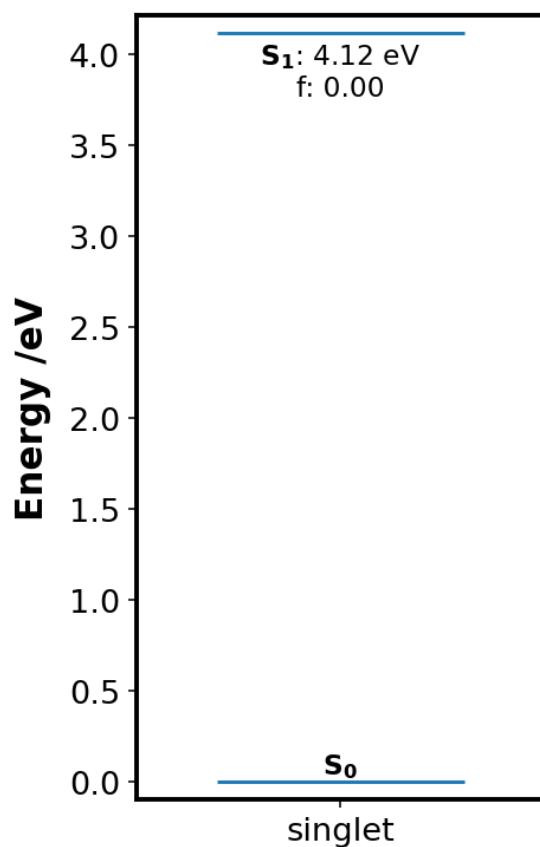
X/Z plane

Z/Y plane

45° to axes

LUMO+4 density (isovalue: 0.02)

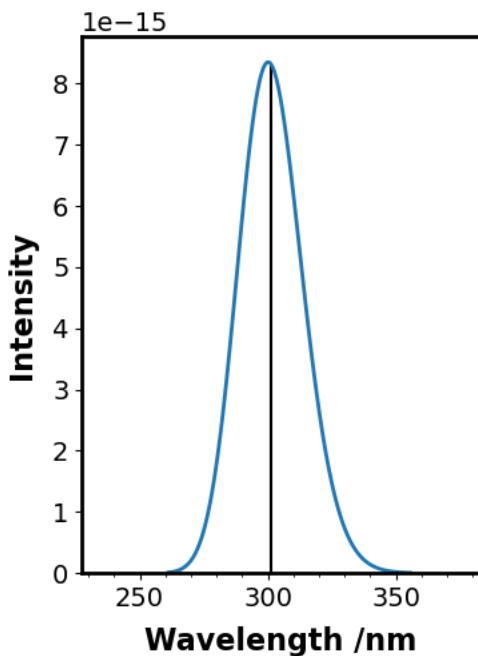
Vertical S_1 Emission



Vertical S_1 Emission

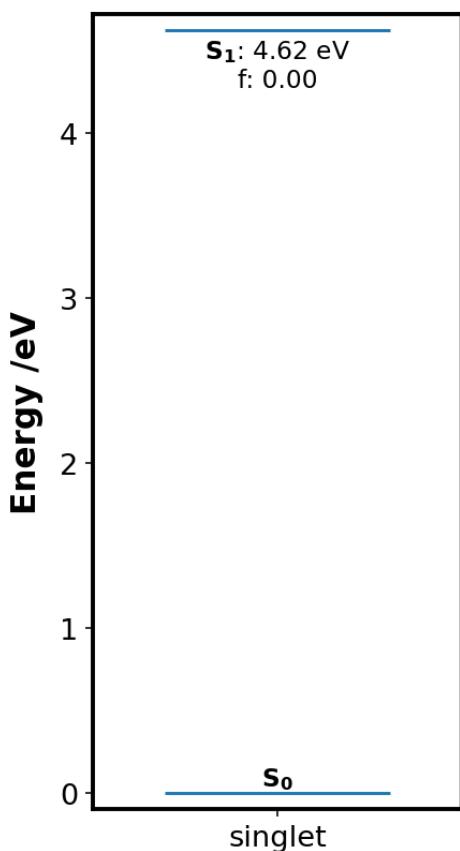
Excited energy: -6743.99 eV
Excited multiplicity: Singlet
Ground energy: -6748.11 eV
Ground multiplicity: Singlet
Emission type: Fluorescence
 S_1 energy: 4.12 eV
 S_1 wavelength: 301 nm
 S_1 colour: Ultraviolet 
 S_1 CIE (x,y): (0.00, 0.00)
 S_1 oscillator strength: 0.00
 S_1 rate /s⁻¹: 3.54e+07

Vertical S_1 Emission Spectrum



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

Adiabatic S₁ Emission



Adiabatic S₁ Emission

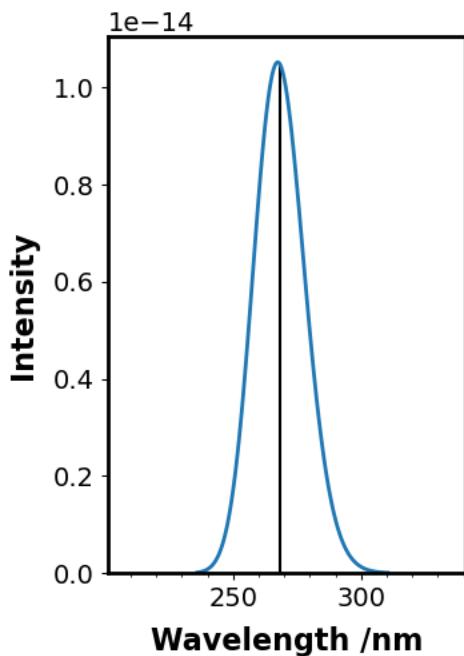
Excited energy: -6743.99 eV
Excited multiplicity: Singlet
Ground energy: -6748.61 eV
Ground multiplicity: Singlet
Emission type: Fluorescence
S₁ energy: 4.62 eV
S₁ wavelength: 268 nm
S₁ colour: Ultraviolet

S₁ CIE (x,y): (0.00, 0.00)

S₁ oscillator strength: 0.00

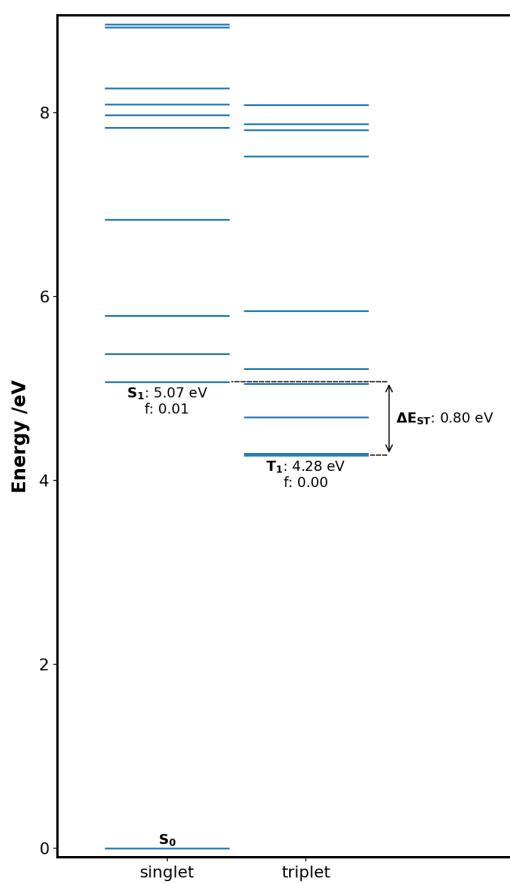
S₁ rate /s⁻¹: 5.01e+07

Adiabatic S₁ Emission Spectrum



Emission spectrum (simulated Gaussian functions with FWHM: 0.4 eV)
Peaks /nm: 267.

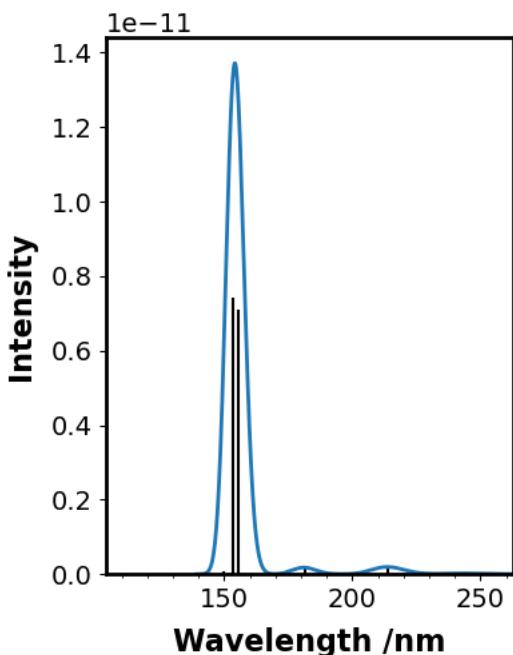
Excited States



Excited States

ΔE_{ST} :	0.80 eV
S_1 energy:	5.07 eV
S_1 wavelength:	244 nm
S_1 colour:	Ultraviolet
S_1 CIE (x,y):	(0.00, 0.00)
S_1 oscillator strength:	0.01
T_1 energy:	4.28 eV
T_1 wavelength:	290 nm
T_1 colour:	Ultraviolet
T_1 CIE (x,y):	(0.00, 0.00)
T_1 oscillator strength:	0.00
No. of singlets:	10
No. of triplets:	10

Absorptions



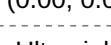
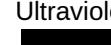
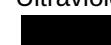
Absorption spectrum (simulated Gaussian functions with FWHM: 0.4 eV).

Peaks /nm: 154, 180, 213, 243.

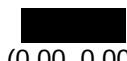
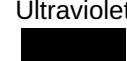
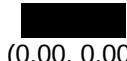
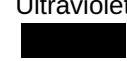
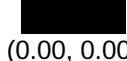
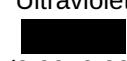
Note: high energy absorption peaks are not simulated.

For a complete absorption spectrum, use more excited states.

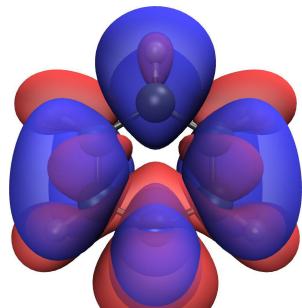
Table of Excited States

Level	Symbol	Symmetry	Energy /eV	Wavelength /nm	Colour, CIE (x,y)	Oscillator Strength	Transitions (probability)
1	T ₁	Triplet-A	4.2757	289.97	Ultraviolet  (0.00, 0.00)	0.0000	HOMO → LUMO (0.97) HOMO → LUMO+4 (0.02)
2	T ₂	Triplet-A	4.2914	288.91	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-1 → LUMO+1 (0.67) HOMO-2 → LUMO (0.30) HOMO-4 → LUMO+4 (0.02)
3	T ₃	Triplet-A	4.6850	264.64	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-1 → LUMO (0.97) HOMO-2 → LUMO+1 (0.03)
4	T ₄	Triplet-A	5.0511	245.46	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-2 → LUMO (0.68) HOMO-1 → LUMO+1 (0.32)
5	S ₁	Singlet-A	5.0737	244.37	Ultraviolet  (0.00, 0.00)	0.0066	HOMO → LUMO (0.99)
6	T ₅	Triplet-A	5.2125	237.86	Ultraviolet  (0.00, 0.00)	0.0000	HOMO → LUMO+1 (1.00)
7	S ₂	Singlet-A	5.3747	230.68	Ultraviolet  (0.00, 0.00)	0.0000	HOMO → LUMO+1 (1.00)
8	S ₃	Singlet-A	5.7931	214.02	Ultraviolet  (0.00, 0.00)	0.0445	HOMO-1 → LUMO (0.69) HOMO-2 → LUMO+1 (0.30)
9	T ₆	Triplet-A	5.8469	212.05	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-2 → LUMO+1 (0.96) HOMO-1 → LUMO (0.03)
10	S ₄	Singlet-A	6.8391	181.29	Ultraviolet  (0.00, 0.00)	0.0294	HOMO-1 → LUMO+1 (0.62) HOMO-2 → LUMO (0.35)
11	T ₇	Triplet-A	7.5290	164.68	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.98)
12	T ₈	Triplet-A	7.8093	158.76	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-4 → LUMO (0.83) HOMO-2 → LUMO+4 (0.16)
13	S ₅	Singlet-A	7.8387	158.17	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-3 → LUMO (0.99)
14	T ₉	Triplet-A	7.8738	157.46	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-3 → LUMO+1 (0.98)
15		Singlet-A	7.9756	155.45		0.8636	HOMO-2 → LUMO+1 (0.66)

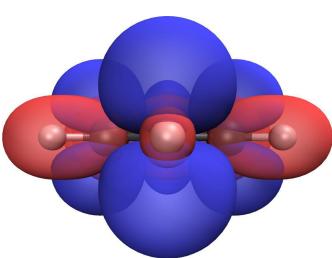
Pyridine - Optimisation, Frequencies, Excited States (Singlet, Trip...

	S_6				Ultraviolet  (0.00, 0.00)		HOMO-1 → LUMO (0.27)
16	T_{10}	Triplet-A	8.0844	153.36	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-4 → LUMO+1 (0.65) HOMO-1 → LUMO+4 (0.34)
17	S_7	Singlet-A	8.0937	153.19	Ultraviolet  (0.00, 0.00)	0.8783	HOMO-2 → LUMO (0.58) HOMO-1 → LUMO+1 (0.32) HOMO → LUMO+2 (0.02)
18	S_8	Singlet-A	8.2671	149.97	Ultraviolet  (0.00, 0.00)	0.0069	HOMO-3 → LUMO+1 (0.99)
19	S_9	Singlet-A	8.9279	138.87	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-5 → LUMO (0.96) HOMO → LUMO+4 (0.03)
20	S_{10}	Singlet-A	8.9578	138.41	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-1 → LUMO+2 (0.99)

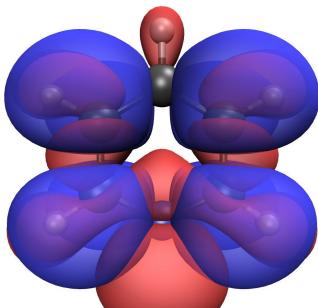
S(1), S(2), S(3), S(4) Natural Transition Orbitals



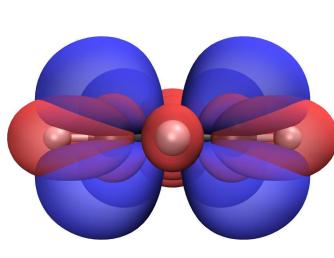
X/Y plane



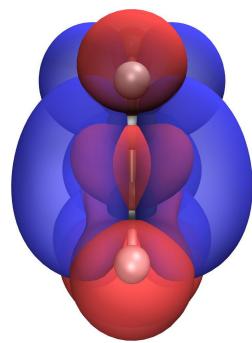
X/Z plane



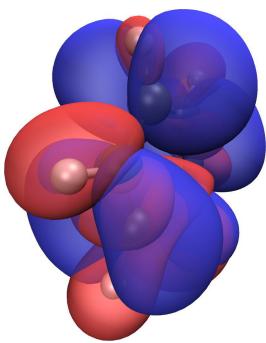
X/Y plane



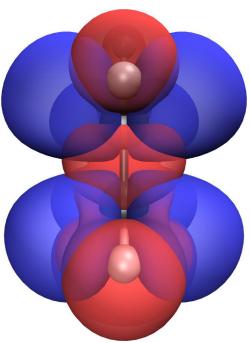
X/Z plane



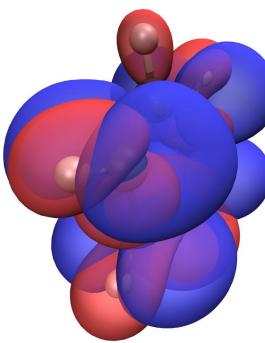
Z/Y plane



45° to axes



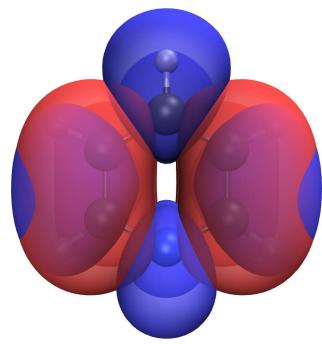
Z/Y plane



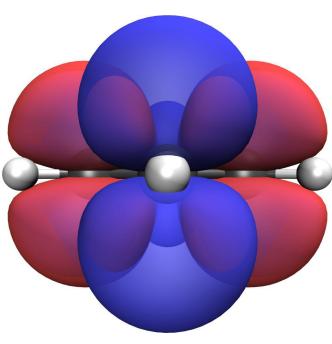
45° to axes

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

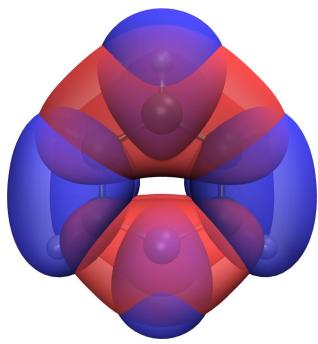
S(2) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



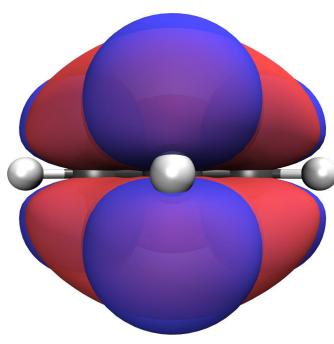
X/Y plane



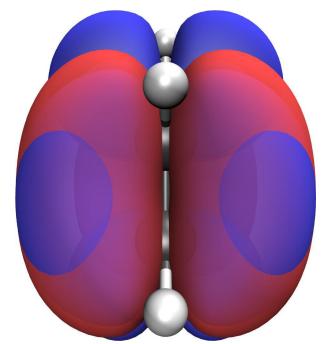
X/Z plane



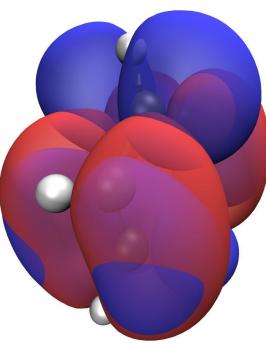
X/Y plane



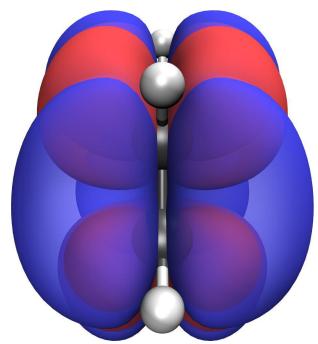
X/Z plane



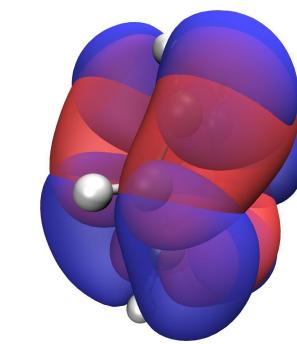
Z/Y plane



45° to axes



Z/Y plane

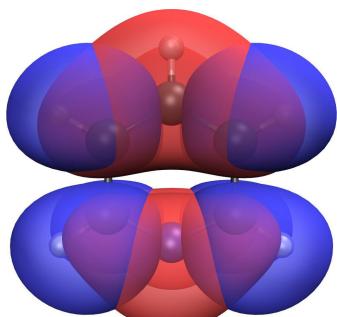


45° to axes

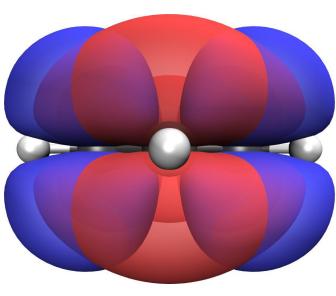
S(3) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

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

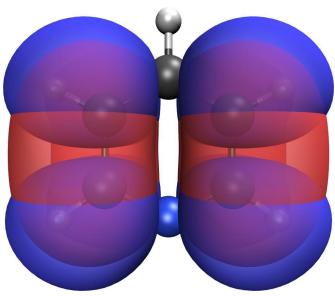
S(5), S(6), S(7), S(8) Natural Transition Orbitals



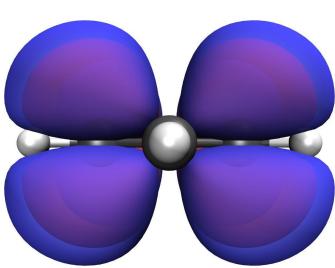
X/Y plane



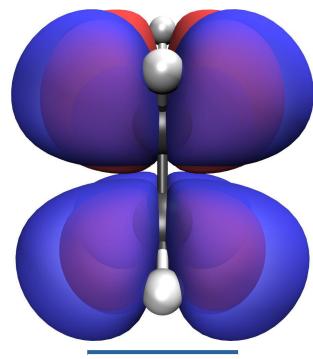
X/Z plane



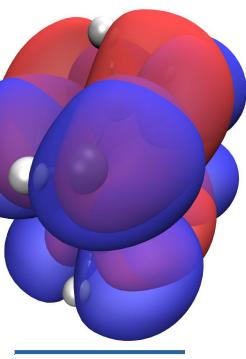
X/Y plane



X/Z plane

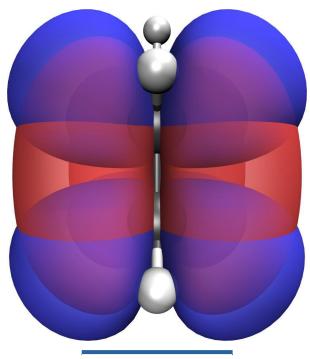


Z/Y plane

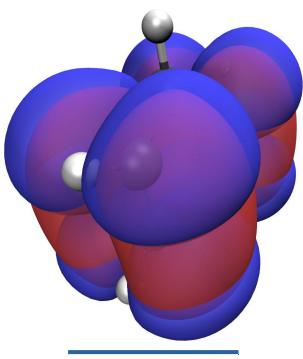


45° to axes

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

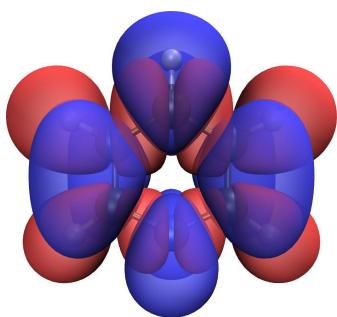


X/Y plane

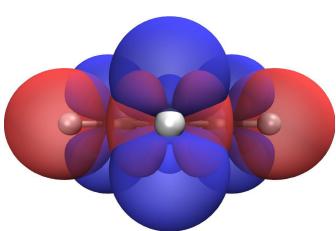


45° to axes

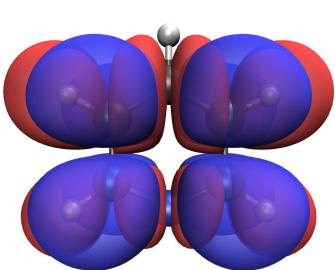
S(6) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



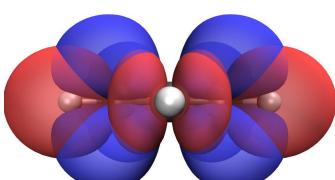
X/Y plane



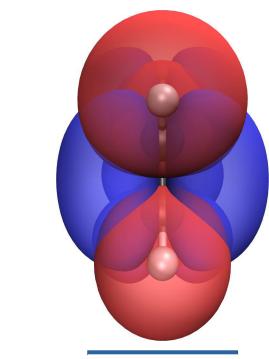
X/Z plane



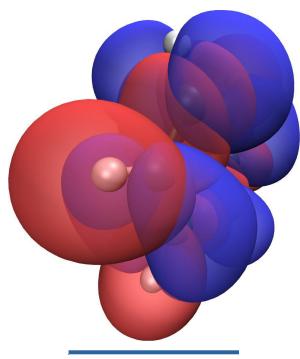
X/Y plane



X/Z plane

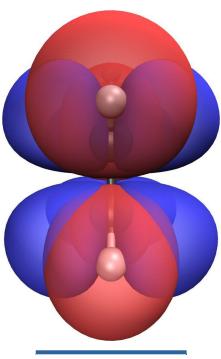


Z/Y plane

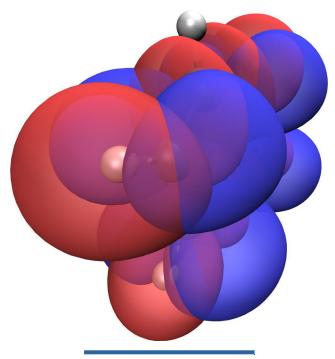


45° to axes

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



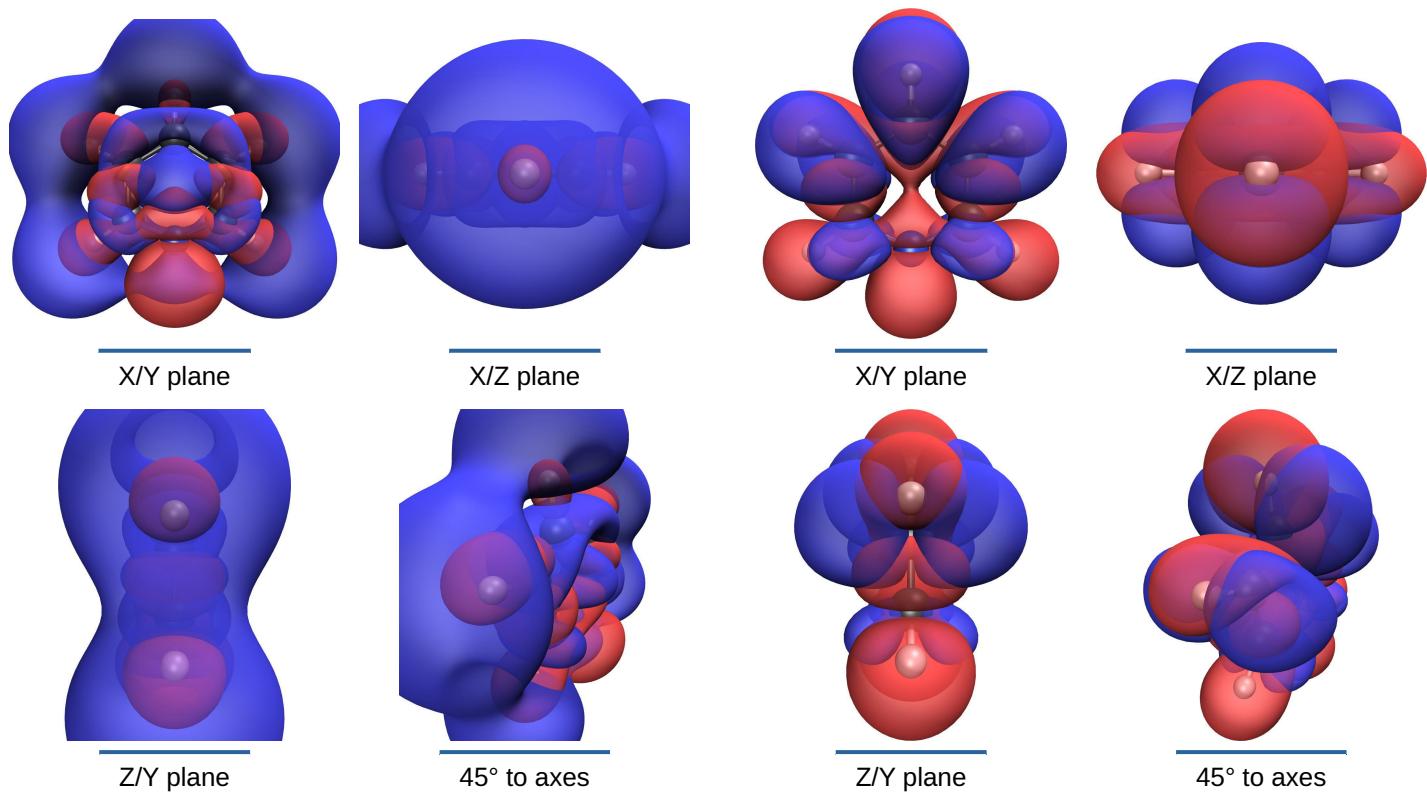
Z/Y plane



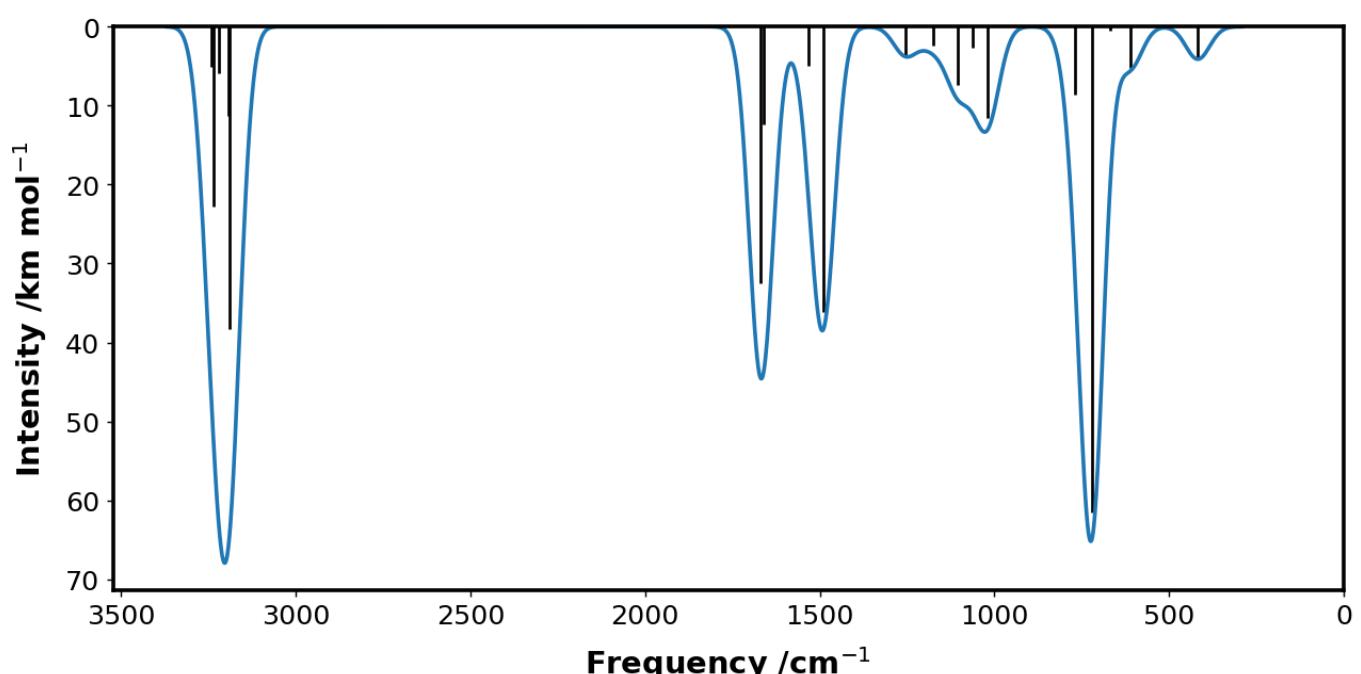
45° to axes

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

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



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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