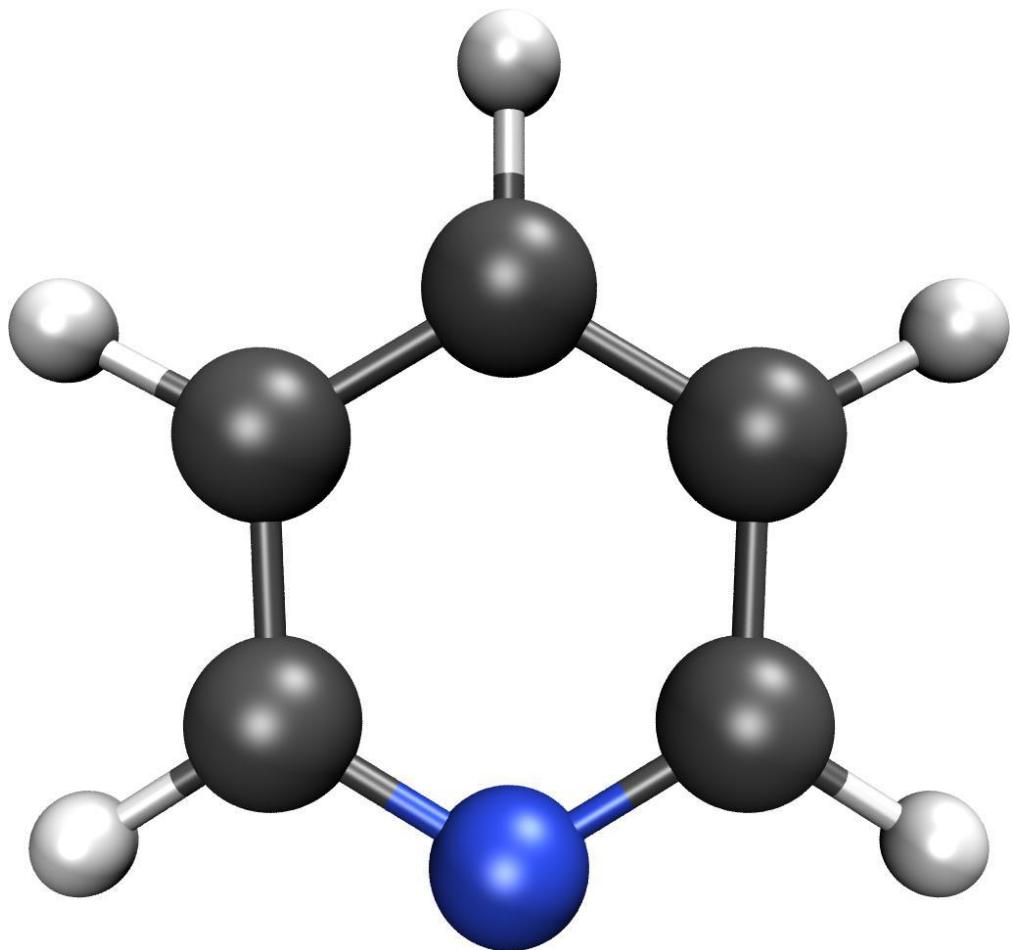


Calculation Report

Pyridine

Excited States (Singlet, Triplet)



Summary of Results

Metadata		SCF Energies	Geometry	
Username:	osl	No. of steps: 1	Formula:	C ₅ NH ₅
Date:	15/06/2022 23:33:59	Final energy: -6748.6129 eV	Exact mass:	79.0422 gmol ⁻¹
Duration:	4 m, 13 s	Final energy: -651,142 kJmol ⁻¹	Molar mass:	79.0999 gmol ⁻¹
Success:	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:	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: 0.44 D

X axis angle: 90.00 °

XY plane angle: 0.13 °

Transition (S₁) Dipole Moment

Total: 0.59 D

X axis angle: 90.00 °

XY plane angle: 89.98 °

Spin-Orbit Coupling

<S₀|H_{SO}|T₁>: 23.86 cm⁻¹

<S₀|\lambda|T₁>: 0.00

<S₁|H_{SO}|T₁>: 0.02 cm⁻¹

<S₁|\lambda|T₁>: 0.00

Excited States

ΔE_{ST}: 0.80 eV

S₁ energy: 5.07 eV

S₁ wavelength: 244 nm

S₁ colour: Ultraviolet 

S₁ CIE (x,y): (0.00, 0.00)

S₁ oscillator strength: 0.01

T₁ energy: 4.28 eV

T₁ wavelength: 290 nm

T₁ colour: Ultraviolet 

T₁ CIE (x,y): (0.00, 0.00)

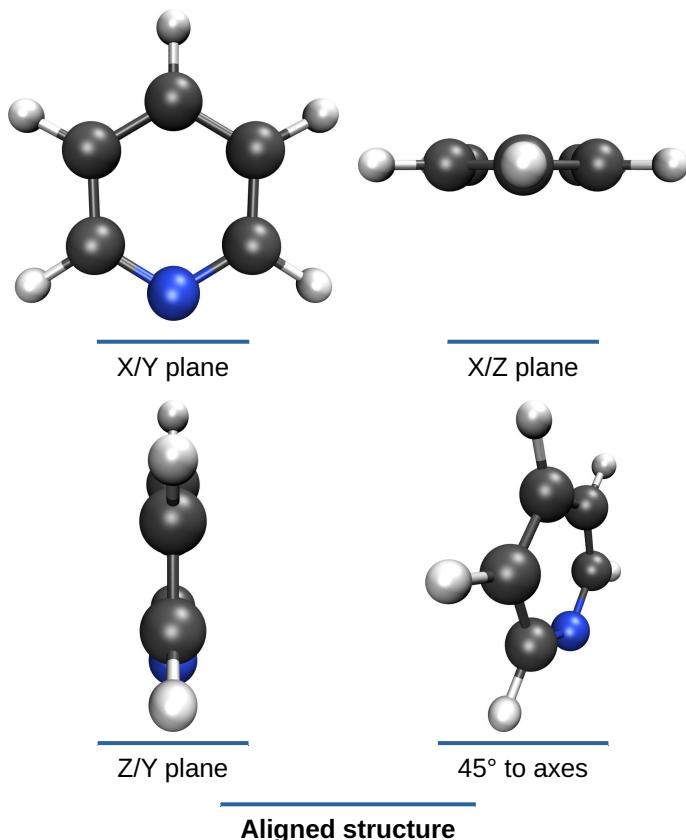
T₁ oscillator strength: 0.00

No. of singlets: 10

No. of triplets: 10

Pyridine - Excited States (Singlet, Triplet)

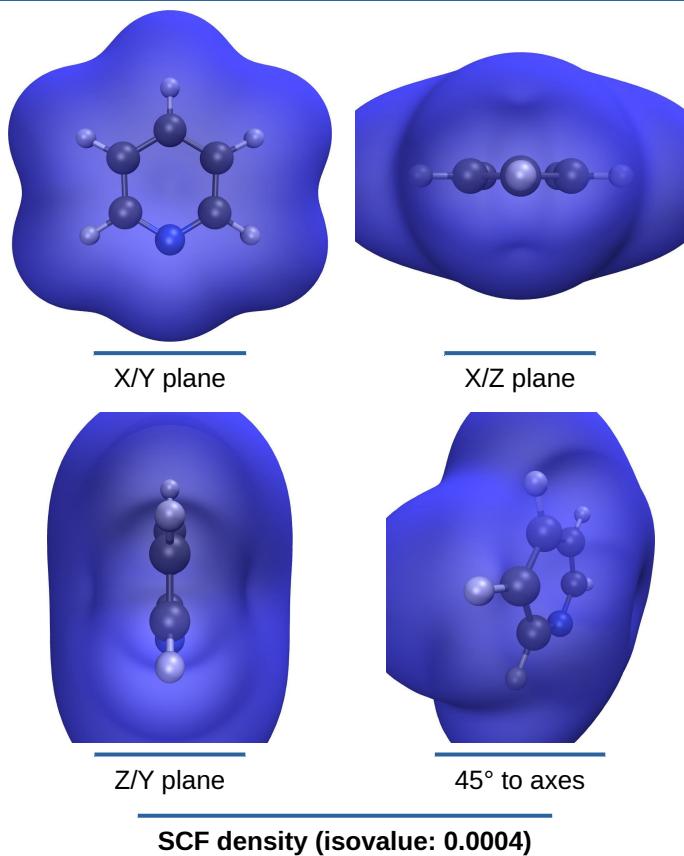
Geometry



Geometry

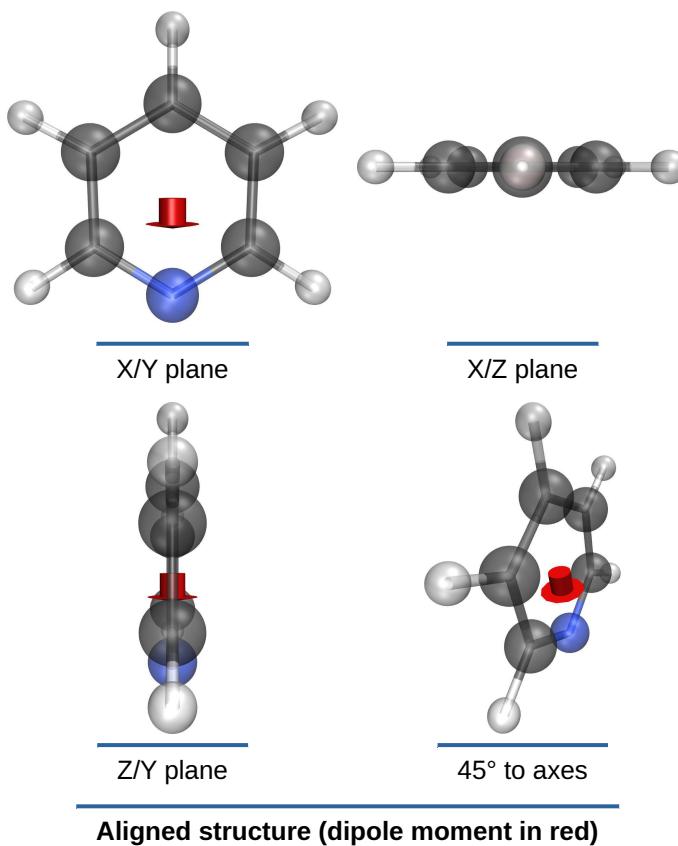
Formula:	C ₅ NH ₅
Exact mass:	79.0422 g mol ⁻¹
Molar mass:	79.0999 g mol ⁻¹
Alignment method:	Minimal
X extension:	4.31 Å
Y extension:	3.89 Å
Z extension:	0.00 Å
Linearity ratio:	0.10
Planarity ratio:	1.00

SCF Density



Pyridine - Excited States (Singlet, Triplet)

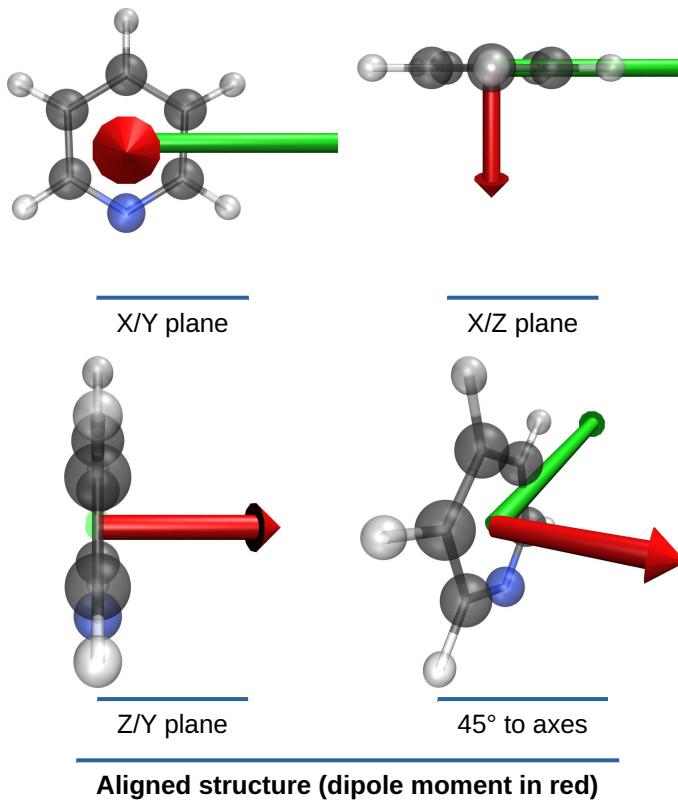
Permanent Dipole Moment



Dipole Moment

Origin X: 0.00 D
Origin Y: 0.00 D
Origin Z: 0.00 D
Vector X: 0.00 D
Vector Y: -0.44 D
Vector Z: 0.00 D
Total: 0.44 D
X axis angle: 90.00 °
XY plane angle: 0.13 °

Transition (S_1) Dipole Moment

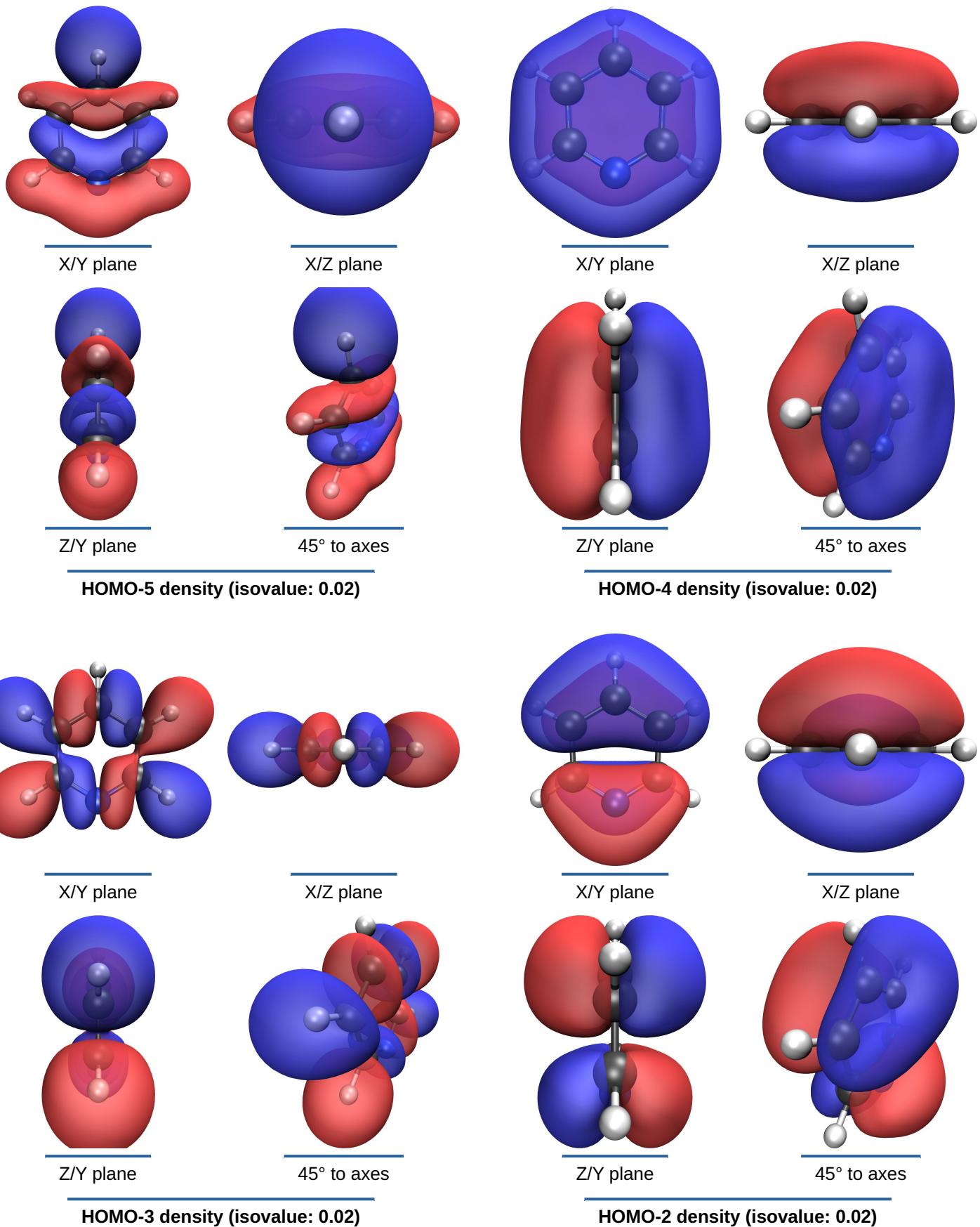


Dipole Moment

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 °

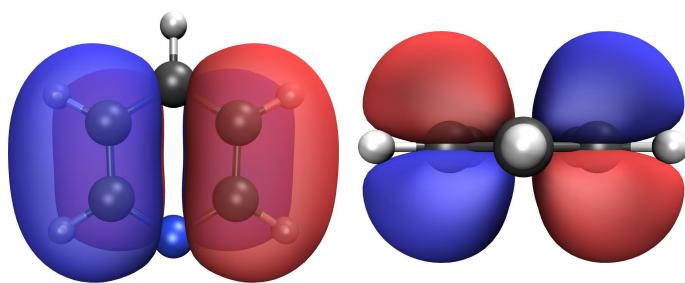
Pyridine - Excited States (Singlet, Triplet)

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

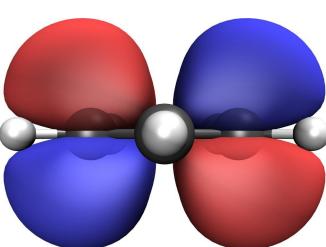


Pyridine - Excited States (Singlet, Triplet)

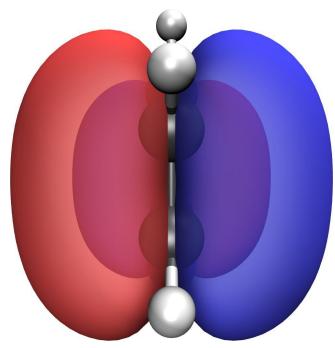
HOMO-1



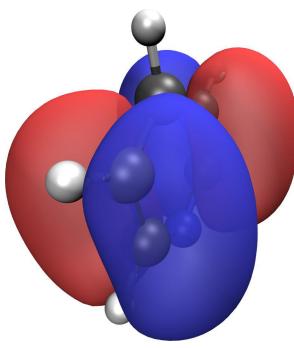
X/Y plane



X/Z plane



Z/Y plane

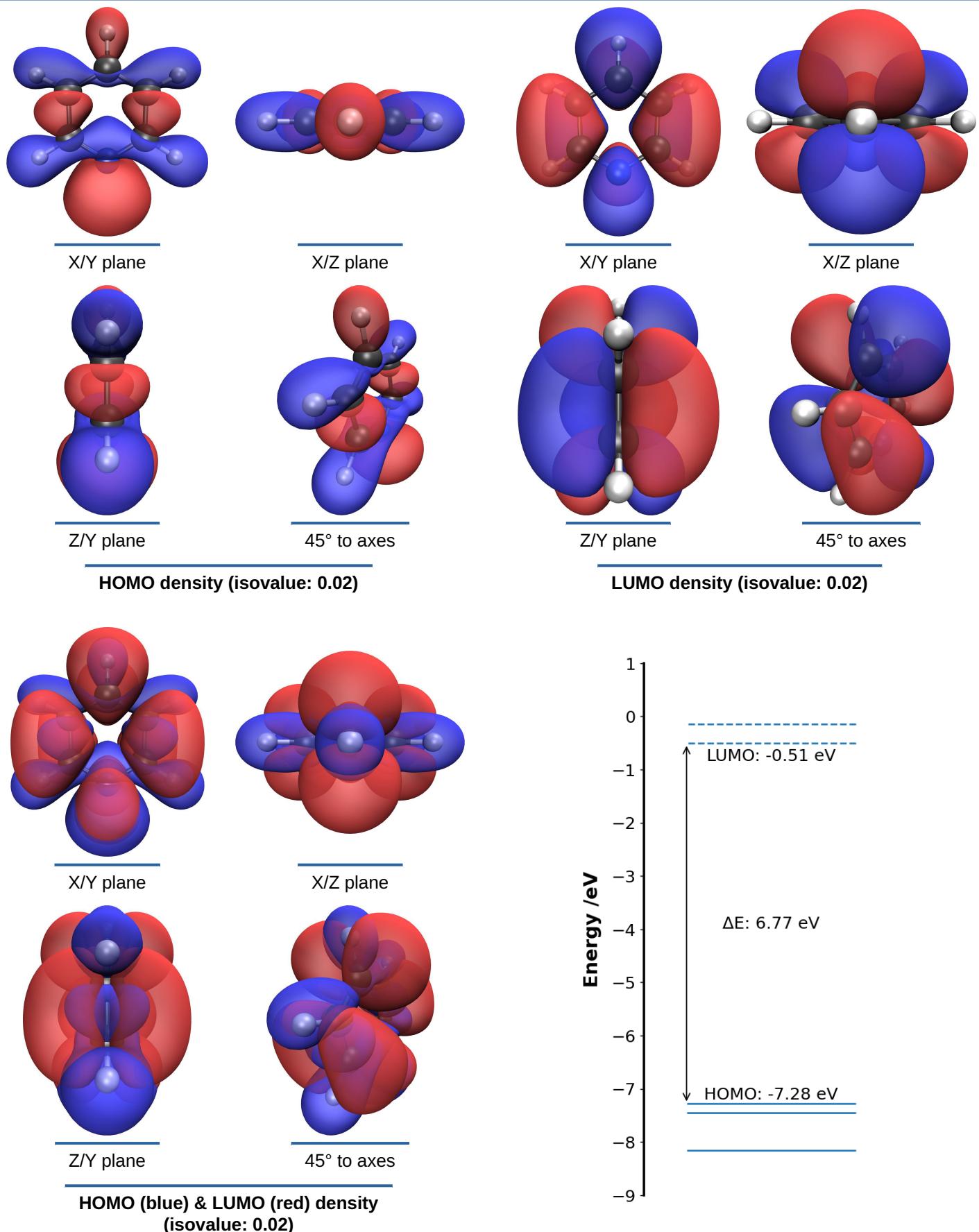


45° to axes

HOMO-1 density (isovalue: 0.02)

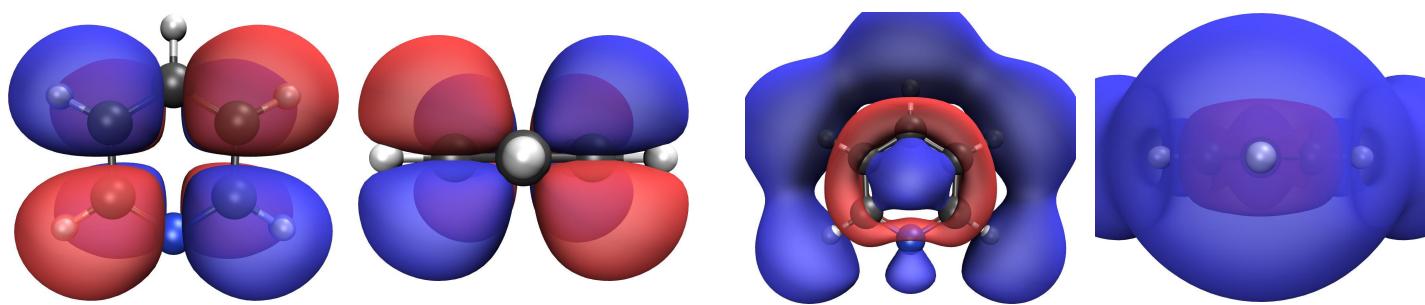
Pyridine - Excited States (Singlet, Triplet)

HOMO & LUMO



Pyridine - Excited States (Singlet, Triplet)

LUMO+1, LUMO+2, LUMO+4



X/Y plane

X/Z plane

X/Y plane

X/Z plane

Z/Y plane

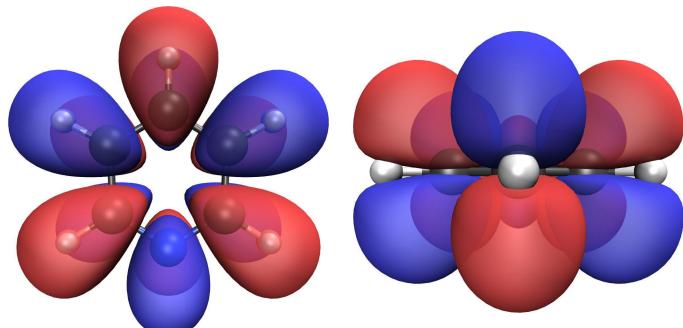
45° to axes

Z/Y plane

45° to axes

LUMO+1 density (isovalue: 0.02)

LUMO+2 density (isovalue: 0.02)



X/Y plane

X/Z plane

X/Y plane

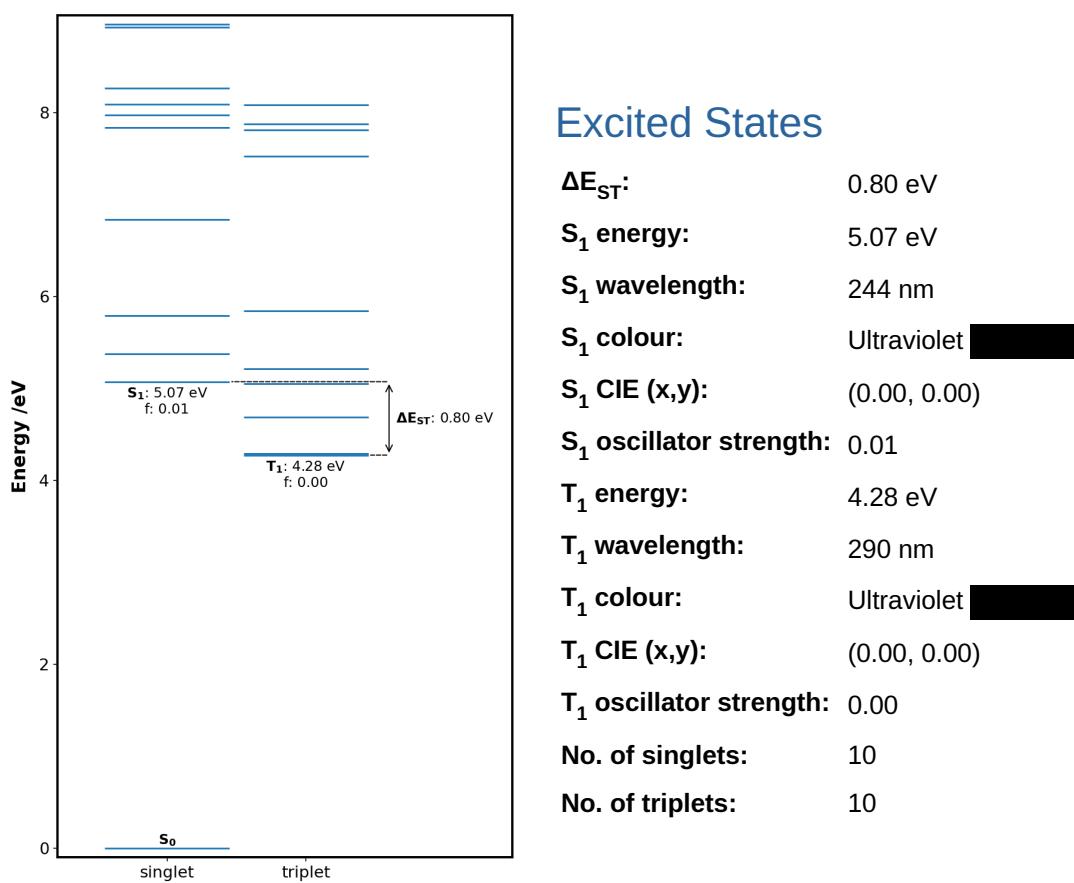
X/Z plane

Z/Y plane

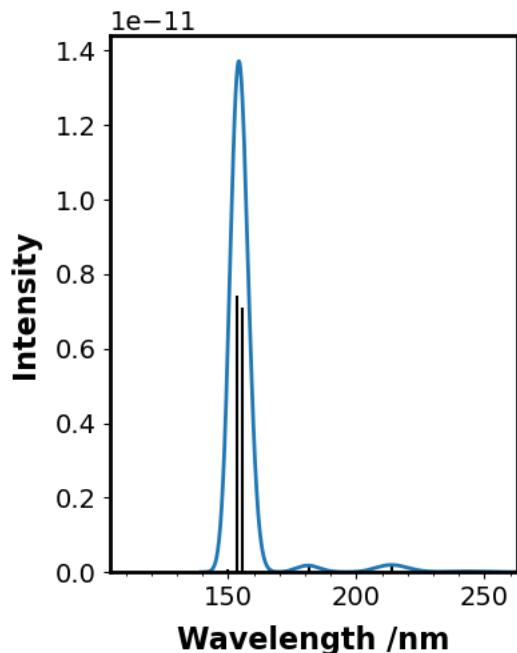
45° to axes

LUMO+4 density (isovalue: 0.02)

Excited States



Absorptions



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

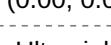
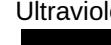
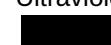
Peaks /nm: 154, 180, 213, 243.

Note: high energy absorption peaks are not simulated.

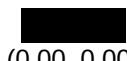
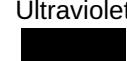
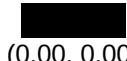
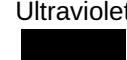
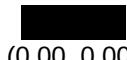
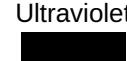
For a complete absorption spectrum, use more excited states.

Pyridine - Excited States (Singlet, Triplet)

Table of Excited States

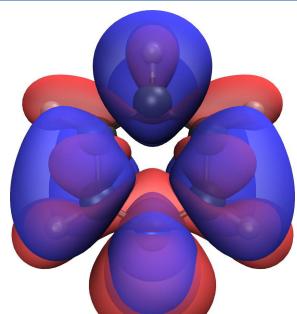
Level	Symbol	Symmetry	Energy /eV	Wavelength /nm	Colour, CIE (x,y)	Oscillator Strength	Transitions (probability)
1	T ₁	Triplet-A	4.2757	289.97	Ultraviolet  (0.00, 0.00)	0.0000	HOMO → LUMO (0.97) HOMO → LUMO+4 (0.02)
2	T ₂	Triplet-A	4.2914	288.91	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-1 → LUMO+1 (0.67) 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 - Excited States (Singlet, Triplet)

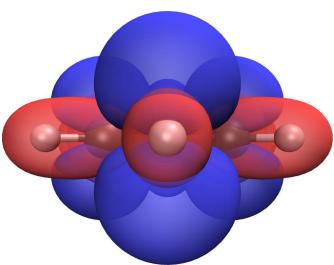
	S_6				Ultraviolet  (0.00, 0.00)		HOMO-1 → LUMO (0.27)
16	T_{10}	Triplet-A	8.0844	153.36	Ultraviolet  (0.00, 0.00)	0.0000	HOMO-4 → LUMO+1 (0.65) HOMO-1 → LUMO+4 (0.34)
17	S_7	Singlet-A	8.0937	153.19	Ultraviolet  (0.00, 0.00)	0.8783	HOMO-2 → LUMO (0.58) HOMO-1 → LUMO+1 (0.32) HOMO → LUMO+2 (0.02)
18	S_8	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)

Pyridine - Excited States (Singlet, Triplet)

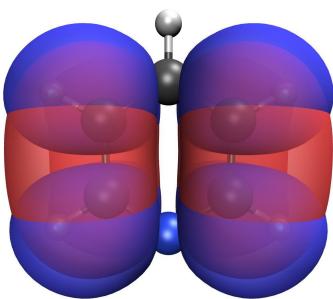
T(1), T(2), T(3), T(4) Natural Transition Orbitals



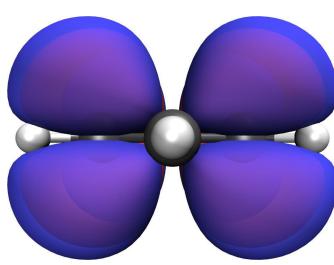
X/Y plane



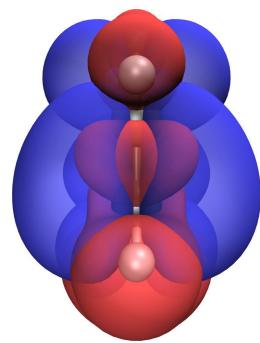
X/Z plane



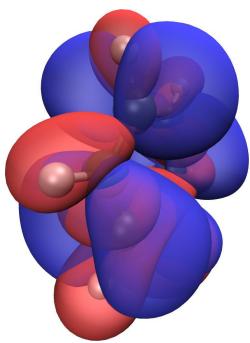
X/Y plane



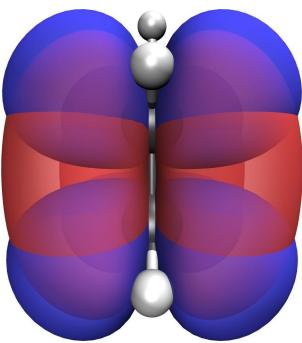
X/Z plane



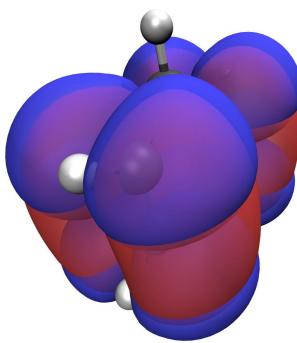
Z/Y plane



45° to axes



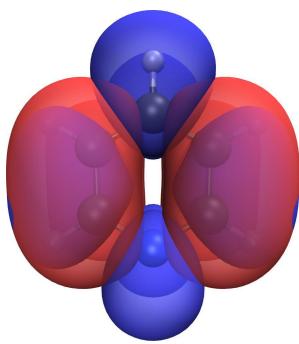
Z/Y plane



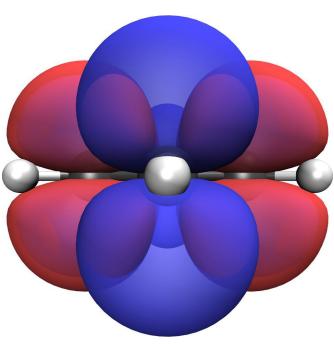
45° to axes

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

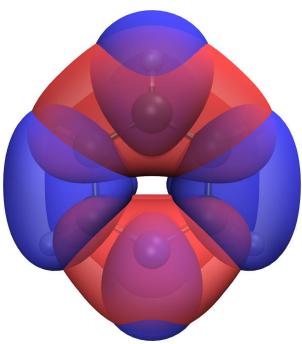
T(2) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



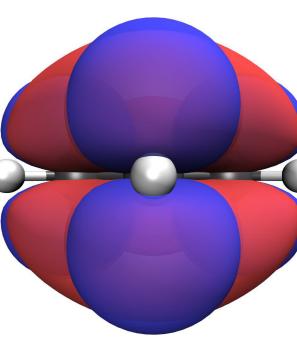
X/Y plane



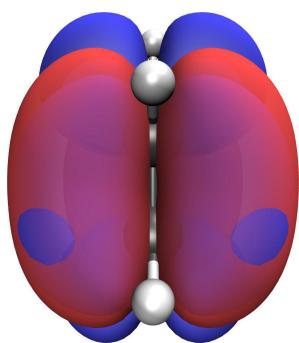
X/Z plane



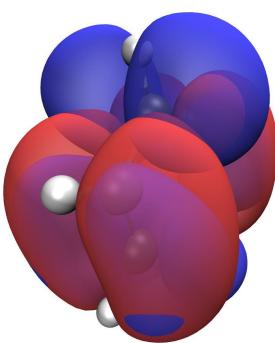
X/Y plane



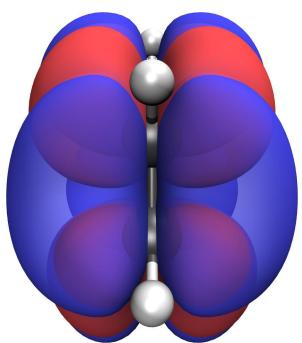
X/Z plane



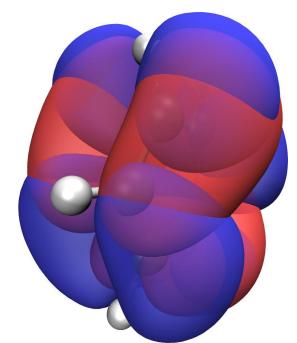
Z/Y plane



45° to axes



Z/Y plane



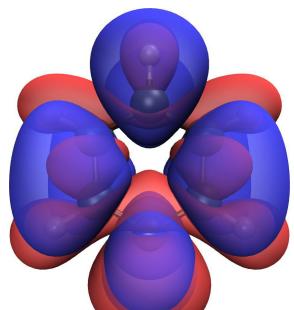
45° to axes

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

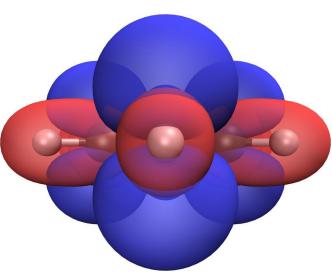
T(4) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Pyridine - Excited States (Singlet, Triplet)

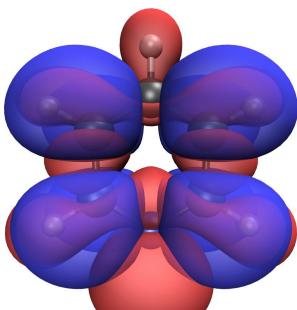
S(1), T(5), S(2), S(3) Natural Transition Orbitals



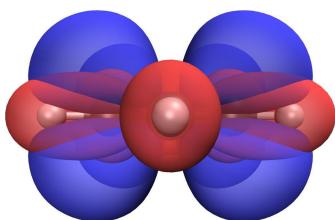
X/Y plane



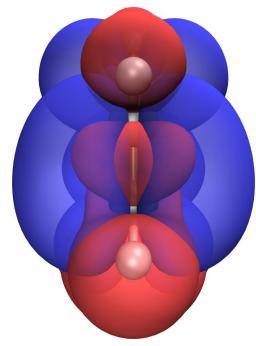
X/Z plane



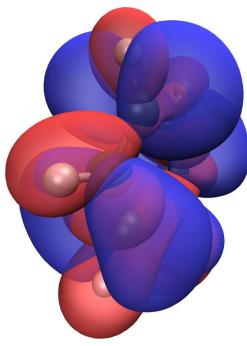
X/Y plane



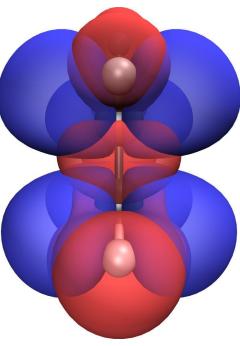
X/Z plane



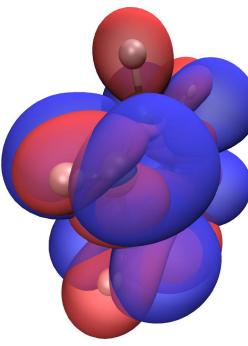
Z/Y plane



45° to axes



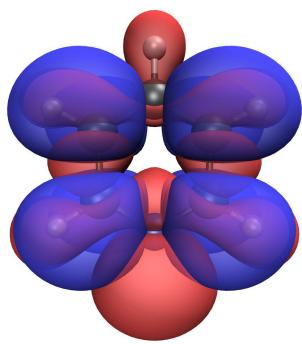
Z/Y plane



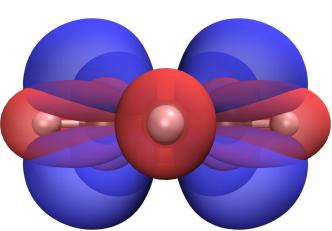
45° to axes

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

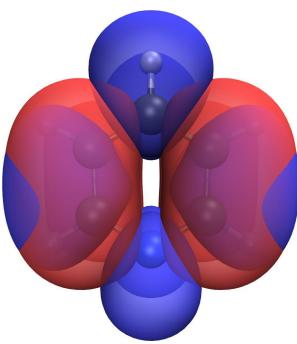
T(5) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



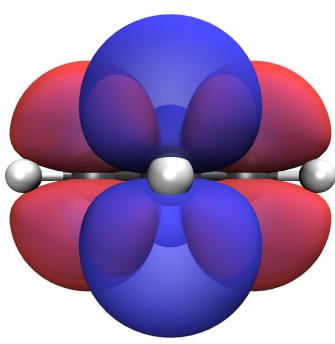
X/Y plane



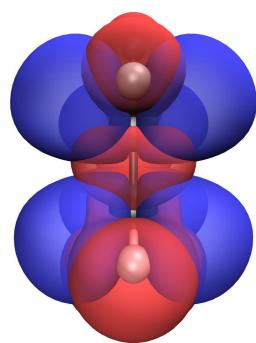
X/Z plane



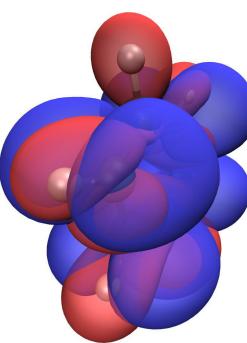
X/Y plane



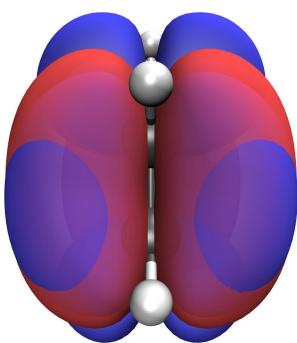
X/Z plane



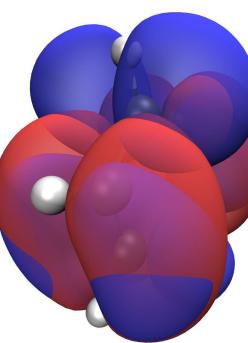
Z/Y plane



45° to axes



Z/Y plane



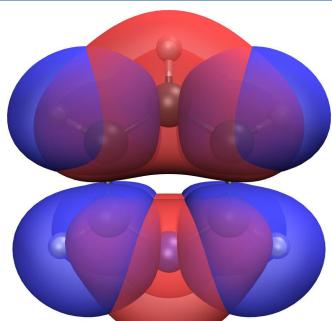
45° to axes

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

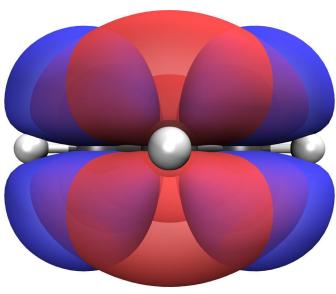
S(3) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Pyridine - Excited States (Singlet, Triplet)

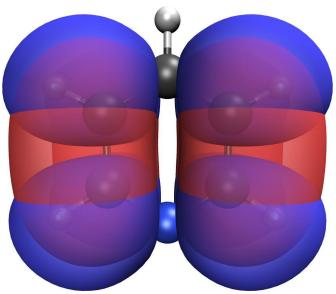
$T(6)$, $S(4)$, $T(7)$, $T(8)$ Natural Transition Orbitals



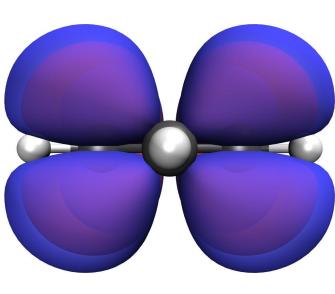
X/Y plane



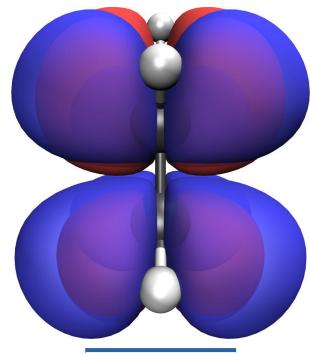
X/Z plane



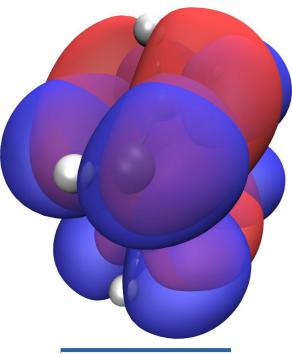
X/Y plane



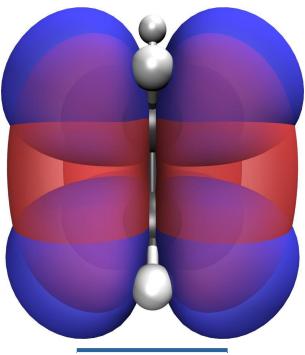
X/Z plane



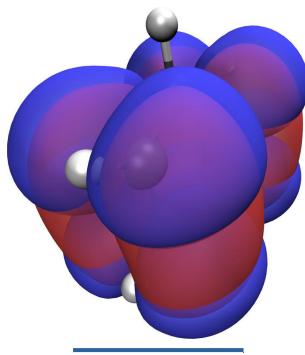
Z/Y plane



45° to axes



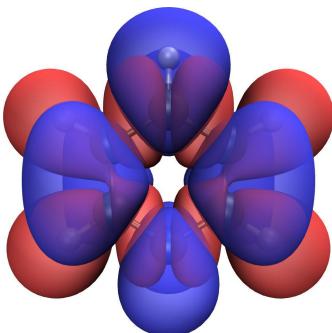
Z/Y plane



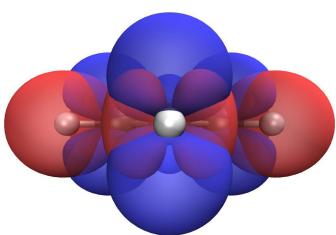
45° to axes

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

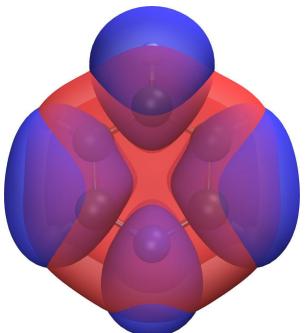
$S(4)$ unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



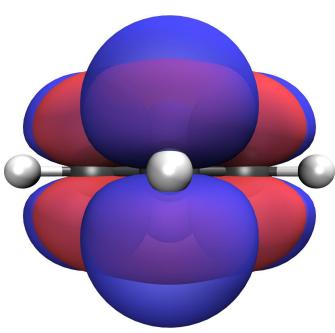
X/Y plane



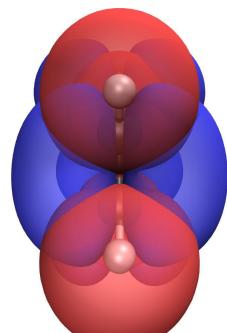
X/Z plane



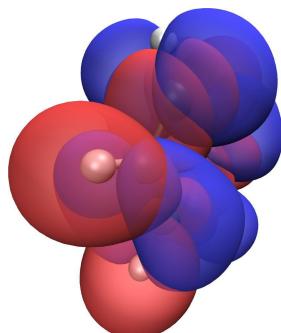
X/Y plane



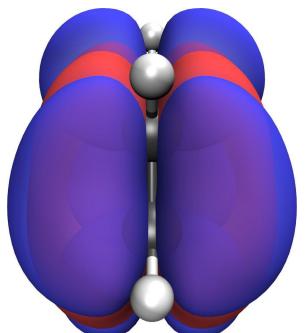
X/Z plane



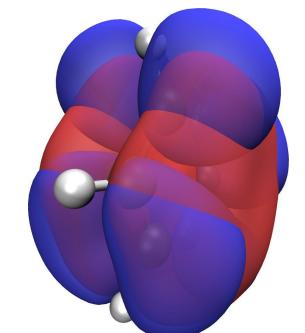
Z/Y plane



45° to axes



Z/Y plane



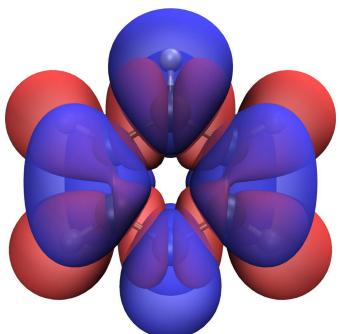
45° to axes

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

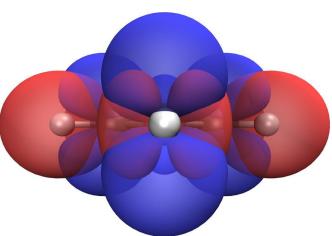
$T(8)$ unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Pyridine - Excited States (Singlet, Triplet)

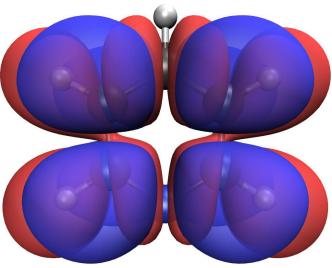
S(5), T(9), S(6), T(10) Natural Transition Orbitals



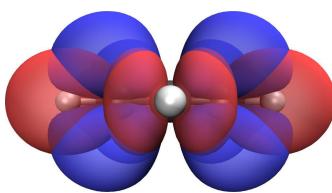
X/Y plane



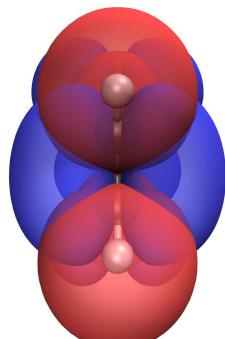
X/Z plane



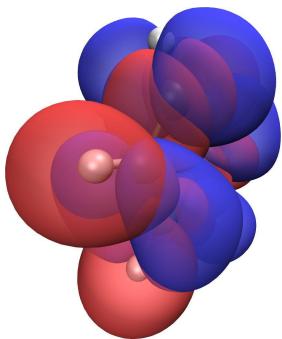
X/Y plane



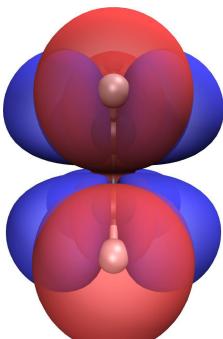
X/Z plane



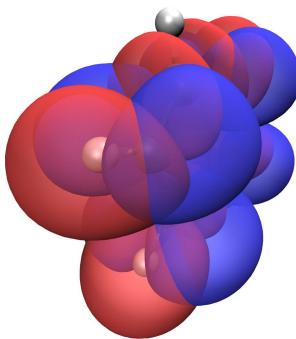
Z/Y plane



45° to axes



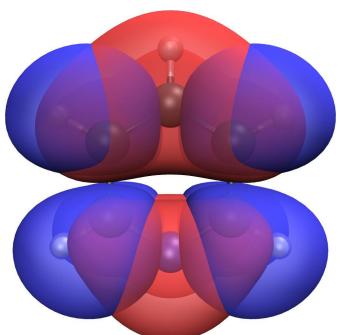
Z/Y plane



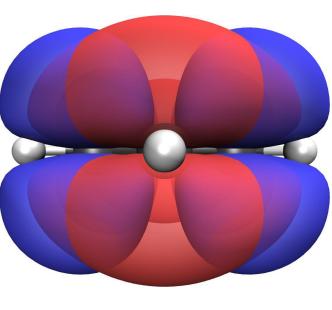
45° to axes

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

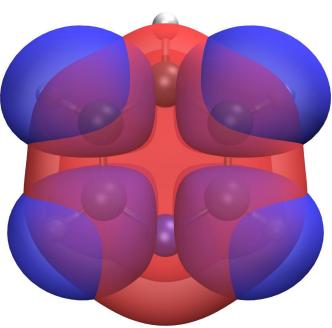
T(9) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



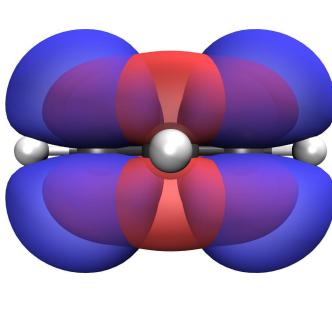
X/Y plane



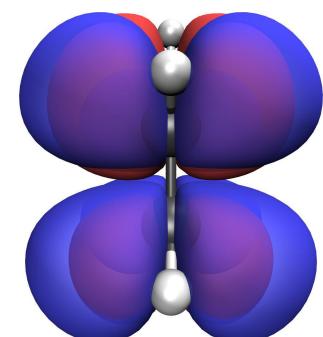
X/Z plane



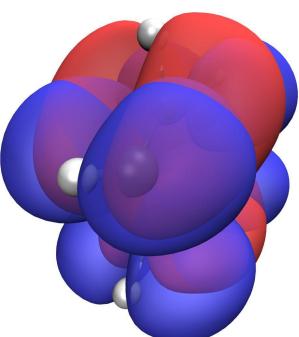
X/Y plane



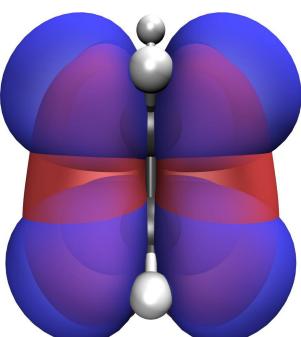
X/Z plane



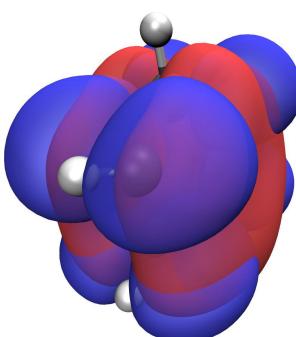
Z/Y plane



45° to axes



Z/Y plane



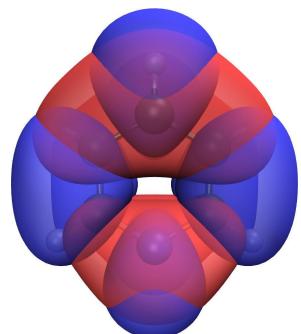
45° to axes

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

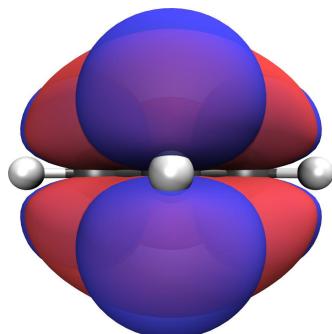
T(10) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)

Pyridine - Excited States (Singlet, Triplet)

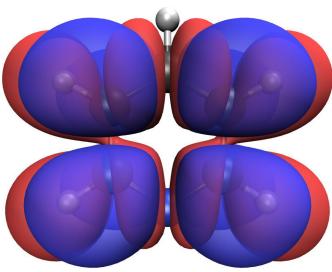
S(7), S(8), S(9), S(10) Natural Transition Orbitals



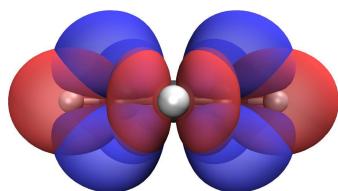
X/Y plane



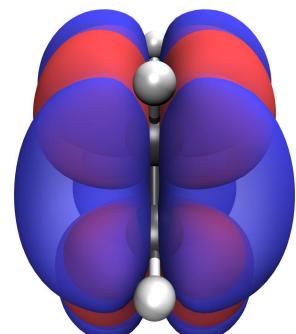
X/Z plane



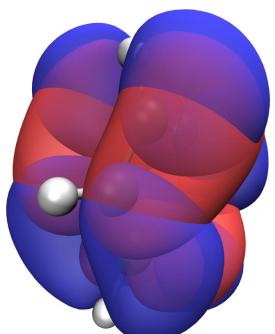
X/Y plane



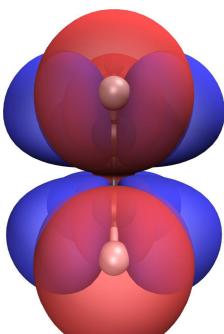
X/Z plane



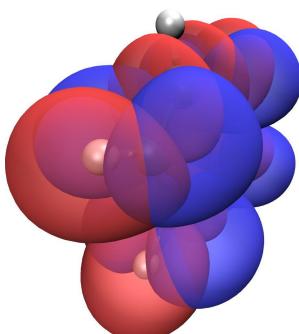
Z/Y plane



45° to axes



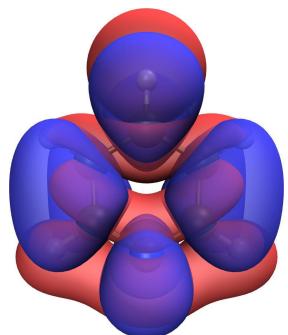
Z/Y plane



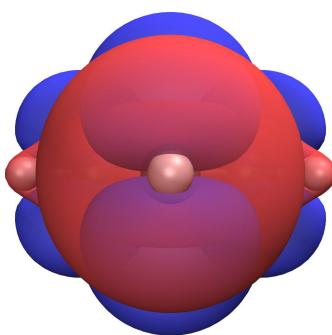
45° to axes

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

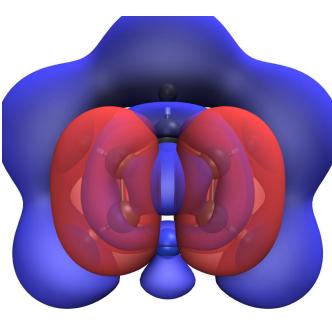
S(8) unoccupied (hole) (blue) & occupied (electron) (red) NTOs (isovalue: 0.02)



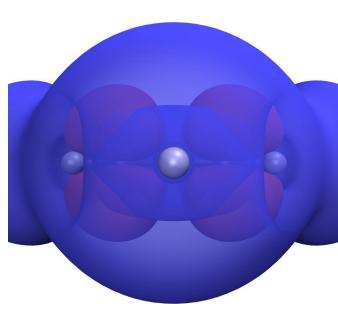
X/Y plane



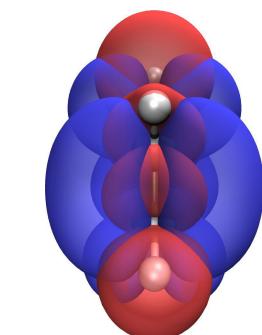
X/Z plane



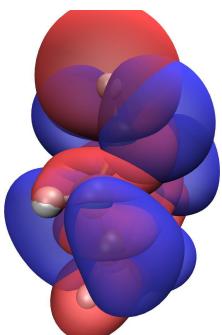
X/Y plane



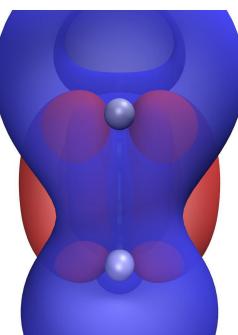
X/Z plane



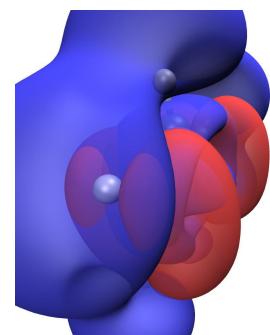
Z/Y plane



45° to axes



Z/Y plane



45° to axes

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

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

Pyridine - Excited States (Singlet, Triplet)

Table of Spin-Orbit Coupling

Singlet	Triplet	SOC +1 /cm ⁻¹	SOC 0 /cm ⁻¹	SOC -1 /cm ⁻¹	SOC Root		First Order
					Sum Square /cm ⁻¹	H _{SO} /eV	Mixing Coefficient
S ₀	T ₁	16.8740	0.0004	16.8740	23.8634	0.0030	4.2757
S ₀	T ₂	0.0549	0.0000	0.0549	0.0777	0.0000	4.2914
S ₀	T ₃	0.0013	0.0020	0.0013	0.0027	0.0000	4.6850
S ₀	T ₄	0.0013	0.0000	0.0013	0.0019	0.0000	5.0511
S ₀	T ₅	1.3715	0.0004	1.3715	1.9396	0.0002	5.2125
S ₀	T ₆	0.0002	0.2194	0.0002	0.2194	0.0000	5.8469
S ₀	T ₇	2.6921	0.0007	2.6921	3.8071	0.0005	7.5290
S ₀	T ₈	0.0013	0.0002	0.0013	0.0018	0.0000	7.8093
S ₀	T ₉	2.4312	0.0001	2.4312	3.4383	0.0004	7.8738
S ₀	T ₁₀	0.0008	0.1435	0.0008	0.1435	0.0000	8.0844
S ₁	T ₁	0.0134	0.0001	0.0134	0.0190	0.0000	0.7980
S ₁	T ₂	4.0883	0.0003	4.0883	5.7818	0.0007	0.7823
S ₁	T ₃	1.0593	0.0000	1.0593	1.4980	0.0002	0.3887
S ₁	T ₄	5.5698	0.0007	5.5698	7.8770	0.0010	0.0226
S ₁	T ₅	0.0008	1.4694	0.0008	1.4694	0.0002	0.1388
S ₁	T ₆	0.0284	0.0001	0.0284	0.0402	0.0000	0.7732
S ₁	T ₇	0.0005	14.9524	0.0005	14.9524	0.0019	2.4553
S ₁	T ₈	7.0308	0.0009	7.0308	9.9431	0.0012	2.7356
S ₁	T ₉	0.0005	0.0001	0.0005	0.0007	0.0000	2.8001
S ₁	T ₁₀	0.2621	0.0000	0.2621	0.3706	0.0000	3.0107
S ₂	T ₁	0.0027	1.1667	0.0027	1.1667	0.0001	1.0990
S ₂	T ₂	0.7498	0.0035	0.7498	1.0604	0.0001	1.0833
S ₂	T ₃	1.3330	0.0000	1.3330	1.8851	0.0002	0.6897
S ₂	T ₄	0.5194	0.0001	0.5194	0.7346	0.0001	0.3236
S ₂	T ₅	0.0001	0.0001	0.0001	0.0002	0.0000	0.1622
S ₂	T ₆	6.2743	0.0006	6.2743	8.8732	0.0011	0.4722
S ₂	T ₇	0.0001	0.0001	0.0001	0.0001	0.0000	2.1543
S ₂	T ₈	0.0155	0.0007	0.0155	0.0220	0.0000	2.4346
S ₂	T ₉	0.0007	14.5661	0.0007	14.5661	0.0018	2.4991

Pyridine - Excited States (Singlet, Triplet)

S ₂	T ₁₀	6.7335	0.0017	6.7335	9.5226	0.0012	2.7097	0.0004
S ₃	T ₁	0.7876	0.0048	0.7876	1.1139	0.0001	1.5174	0.0001
S ₃	T ₂	0.0026	1.5192	0.0026	1.5192	0.0002	1.5017	0.0001
S ₃	T ₃	0.0003	0.0001	0.0003	0.0005	0.0000	1.1081	0.0000
S ₃	T ₄	0.0009	0.1772	0.0009	0.1772	0.0000	0.7420	0.0000
S ₃	T ₅	4.0364	0.0004	4.0364	5.7083	0.0007	0.5806	0.0012
S ₃	T ₆	0.0002	0.0000	0.0002	0.0003	0.0000	0.0538	0.0000
S ₃	T ₇	0.6281	0.0005	0.6281	0.8882	0.0001	1.7359	0.0001
S ₃	T ₈	0.0003	0.0509	0.0003	0.0509	0.0000	2.0162	0.0000
S ₃	T ₉	2.1150	0.0016	2.1150	2.9911	0.0004	2.0807	0.0002
S ₃	T ₁₀	0.0010	0.0000	0.0010	0.0014	0.0000	2.2913	0.0000
S ₄	T ₁	4.0865	0.0003	4.0865	5.7791	0.0007	2.5634	0.0003
S ₄	T ₂	0.0129	0.0001	0.0129	0.0183	0.0000	2.5477	0.0000
S ₄	T ₃	0.0005	0.9851	0.0005	0.9851	0.0001	2.1541	0.0001
S ₄	T ₄	0.0002	0.0000	0.0002	0.0003	0.0000	1.7880	0.0000
S ₄	T ₅	0.8023	0.0002	0.8023	1.1346	0.0001	1.6266	0.0001
S ₄	T ₆	0.0002	1.2640	0.0002	1.2640	0.0002	0.9922	0.0002
S ₄	T ₇	1.7093	0.0002	1.7093	2.4173	0.0003	0.6899	0.0004
S ₄	T ₈	0.0002	0.0000	0.0002	0.0003	0.0000	0.9702	0.0000
S ₄	T ₉	0.0024	0.0001	0.0024	0.0035	0.0000	1.0347	0.0000
S ₄	T ₁₀	0.0001	0.1615	0.0001	0.1615	0.0000	1.2453	0.0000
S ₅	T ₁	0.0053	14.3557	0.0053	14.3557	0.0018	3.5630	0.0005
S ₅	T ₂	1.6926	0.0459	1.6926	2.3941	0.0003	3.5473	0.0001
S ₅	T ₃	0.4370	0.0012	0.4370	0.6180	0.0001	3.1537	0.0000
S ₅	T ₄	2.4429	0.0011	2.4429	3.4548	0.0004	2.7876	0.0002
S ₅	T ₅	0.0008	0.0006	0.0008	0.0013	0.0000	2.6262	0.0000
S ₅	T ₆	0.0207	0.0001	0.0207	0.0293	0.0000	1.9918	0.0000
S ₅	T ₇	0.0001	0.0000	0.0001	0.0002	0.0000	0.3097	0.0000
S ₅	T ₈	1.9123	0.0004	1.9123	2.7044	0.0003	0.0294	0.0114
S ₅	T ₉	0.0003	1.2561	0.0003	1.2561	0.0002	0.0351	0.0044
S ₅	T ₁₀	0.1062	0.0005	0.1062	0.1502	0.0000	0.2457	0.0001
S ₆	T ₁	0.1908	0.0026	0.1908	0.2698	0.0000	3.6999	0.0000

Pyridine - Excited States (Singlet, Triplet)

S ₆	T ₂	0.0009	0.2299	0.0009	0.2299	0.0000	3.6842	0.0000
S ₆	T ₃	0.0003	0.0000	0.0003	0.0004	0.0000	3.2906	0.0000
S ₆	T ₄	0.0006	0.5807	0.0006	0.5808	0.0001	2.9245	0.0000
S ₆	T ₅	4.4927	0.0018	4.4927	6.3536	0.0008	2.7631	0.0003
S ₆	T ₆	0.0005	0.0000	0.0005	0.0007	0.0000	2.1287	0.0000
S ₆	T ₇	0.0075	0.0001	0.0075	0.0106	0.0000	0.4466	0.0000
S ₆	T ₈	0.0001	0.0707	0.0001	0.0707	0.0000	0.1663	0.0001
S ₆	T ₉	1.1001	0.0001	1.1001	1.5558	0.0002	0.1018	0.0019
S ₆	T ₁₀	0.0005	0.0000	0.0005	0.0008	0.0000	0.1088	0.0000
S ₇	T ₁	6.9229	0.0010	6.9229	9.7905	0.0012	3.8180	0.0003
S ₇	T ₂	0.0218	0.0000	0.0218	0.0308	0.0000	3.8023	0.0000
S ₇	T ₃	0.0004	0.2867	0.0004	0.2867	0.0000	3.4087	0.0000
S ₇	T ₄	0.0004	0.0000	0.0004	0.0005	0.0000	3.0426	0.0000
S ₇	T ₅	0.6701	0.0008	0.6701	0.9477	0.0001	2.8812	0.0000
S ₇	T ₆	0.0003	0.4886	0.0003	0.4886	0.0001	2.2468	0.0000
S ₇	T ₇	3.6241	0.0001	3.6241	5.1253	0.0006	0.5647	0.0011
S ₇	T ₈	0.0004	0.0000	0.0004	0.0006	0.0000	0.2844	0.0000
S ₇	T ₉	0.1942	0.0002	0.1942	0.2747	0.0000	0.2199	0.0002
S ₇	T ₁₀	0.0003	0.0652	0.0003	0.0652	0.0000	0.0093	0.0009
S ₈	T ₁	0.0009	0.0005	0.0009	0.0014	0.0000	3.9914	0.0000
S ₈	T ₂	0.3708	0.0007	0.3708	0.5244	0.0001	3.9757	0.0000
S ₈	T ₃	0.5478	0.0006	0.5478	0.7747	0.0001	3.5821	0.0000
S ₈	T ₄	0.3810	0.0022	0.3810	0.5389	0.0001	3.2160	0.0000
S ₈	T ₅	0.0004	14.7811	0.0004	14.7811	0.0018	3.0546	0.0006
S ₈	T ₆	2.7755	0.0015	2.7755	3.9252	0.0005	2.4202	0.0002
S ₈	T ₇	0.0001	0.9296	0.0001	0.9296	0.0001	0.7381	0.0002
S ₈	T ₈	0.0761	0.0001	0.0761	0.1077	0.0000	0.4578	0.0000
S ₈	T ₉	0.0004	0.0000	0.0004	0.0005	0.0000	0.3933	0.0000
S ₈	T ₁₀	1.8787	0.0002	1.8787	2.6570	0.0003	0.1827	0.0018
S ₉	T ₁	0.0066	0.0001	0.0066	0.0094	0.0000	4.6522	0.0000
S ₉	T ₂	2.1664	0.0001	2.1664	3.0638	0.0004	4.6365	0.0001
S ₉	T ₃	0.0986	0.0001	0.0986	0.1395	0.0000	4.2429	0.0000

Pyridine - Excited States (Singlet, Triplet)

S ₉	T ₄	2.6693	0.0000	2.6693	3.7749	0.0005	3.8768	0.0001
S ₉	T ₅	0.0003	0.0118	0.0003	0.0118	0.0000	3.7154	0.0000
S ₉	T ₆	0.0442	0.0000	0.0442	0.0625	0.0000	3.0810	0.0000
S ₉	T ₇	0.0004	4.8880	0.0004	4.8880	0.0006	1.3989	0.0004
S ₉	T ₈	5.3454	0.0008	5.3454	7.5596	0.0009	1.1186	0.0008
S ₉	T ₉	0.0004	0.0001	0.0004	0.0006	0.0000	1.0541	0.0000
S ₉	T ₁₀	0.4233	0.0001	0.4233	0.5986	0.0001	0.8435	0.0001
S ₁₀	T ₁	0.0020	0.6367	0.0020	0.6367	0.0001	4.6821	0.0000
S ₁₀	T ₂	0.3465	0.0020	0.3465	0.4900	0.0001	4.6664	0.0000
S ₁₀	T ₃	2.3635	0.0000	2.3635	3.3425	0.0004	4.2728	0.0001
S ₁₀	T ₄	0.3420	0.0000	0.3420	0.4837	0.0001	3.9067	0.0000
S ₁₀	T ₅	0.0001	0.0001	0.0001	0.0002	0.0000	3.7453	0.0000
S ₁₀	T ₆	0.5086	0.0000	0.5086	0.7193	0.0001	3.1109	0.0000
S ₁₀	T ₇	0.0001	0.0003	0.0001	0.0004	0.0000	1.4288	0.0000
S ₁₀	T ₈	0.1447	0.0000	0.1447	0.2047	0.0000	1.1485	0.0000
S ₁₀	T ₉	0.0001	0.3405	0.0001	0.3405	0.0000	1.0840	0.0000
S ₁₀	T ₁₀	1.1089	0.0000	1.1089	1.5682	0.0002	0.8734	0.0002

Pyridine - Excited States (Singlet, Triplet)

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	-11.2780
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	-17.5726
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

Pyridine - Excited States (Singlet, Triplet)

Table of Atoms

Element	X Coord	Y Coord	Z Coord
C	1.1386510	-0.7199620	-0.0000210
C	1.1954040	0.6709180	0.0000190
C	0.0000400	1.3817880	0.0000190
C	-1.1953660	0.6709790	0.0000190
C	-1.1386990	-0.7199010	0.0000290
N	-0.0000350	-1.4172120	-0.0000610
H	2.0570560	-1.3046500	-0.0000410
H	2.1540580	1.1793990	0.0000390
H	0.0000600	2.4678180	0.0000490
H	-2.1539920	1.1795280	0.0000190
H	-2.0571240	-1.3045430	-0.0000410

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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