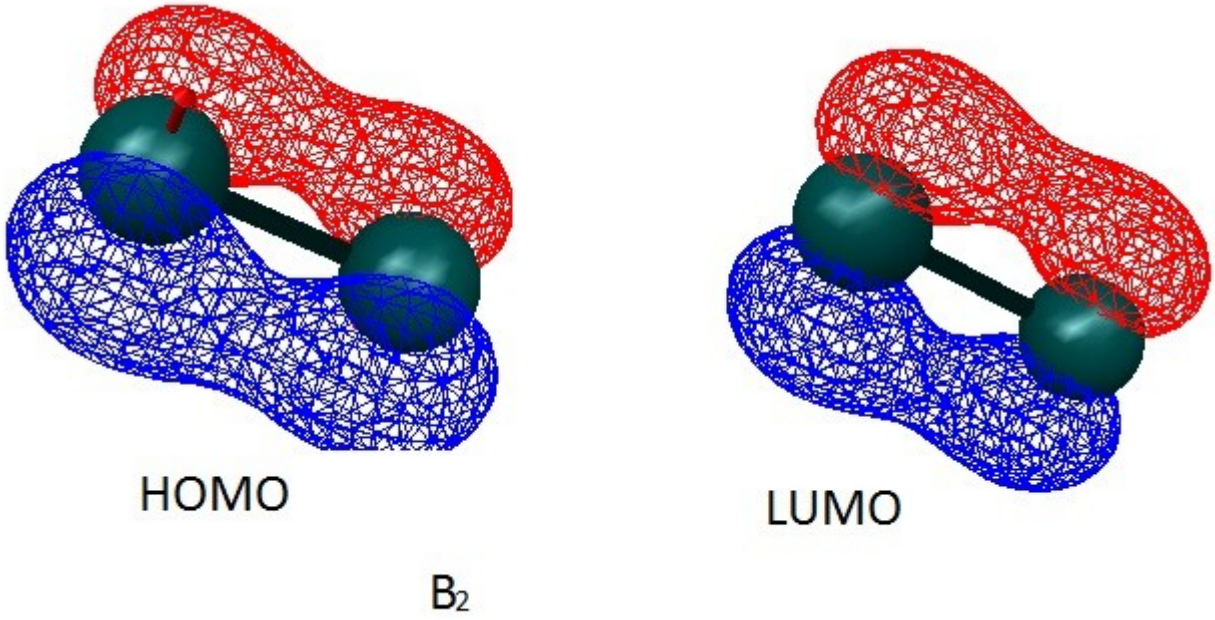
TANUJ GUPTA **Homework 2**

Ans:1

Molecule : B_2

Quantity	Simulation	Experimental
Bond Length(Angs)	1.63	1.625
Dipole Moment(Debye)	0	0

Vibration Frefquency is 971.46Hz from simulation and experimental vibrational frequency is 937.4Hz.
Bond order for B_2 is 2.
Triplet is more stable in Boron and hence it exists in Paramagnetic form.

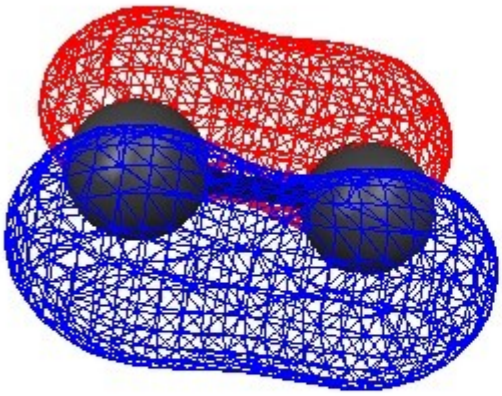


B_2

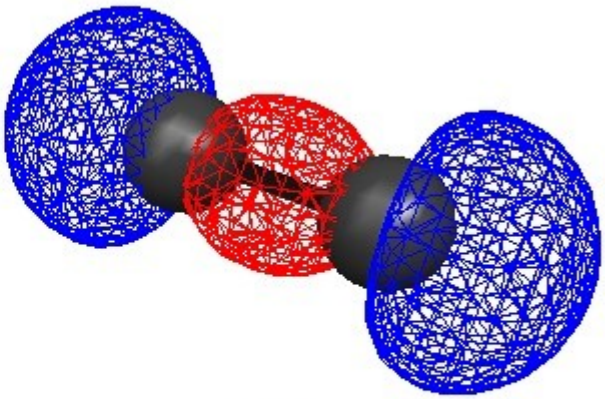
Molecule : C_2

Quantity	Simulation	Experimental
Bond Length(Angs)	1.321	1.307
Dipole Moment(Debye)	0.0000005	0.0000006

Vibration Frefquency is 1623.53Hz from simulation and experimental vibrational frequency is 1557.5Hz.
Expected Bond order for C_2 is 3 but simulated bond order is 2.482.
Triplet is more stable in C_2 and hence it exists in Paramagnetic form.



HOMO



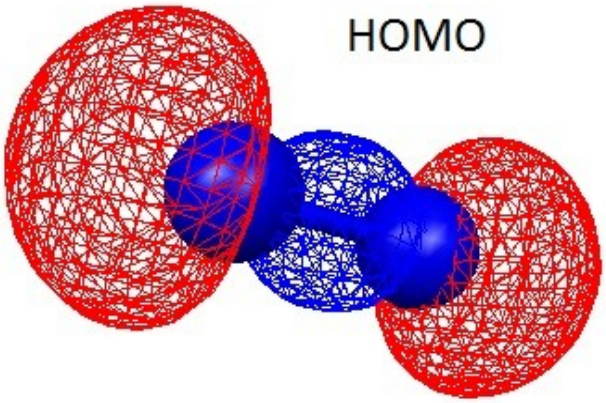
LUMO

C_2

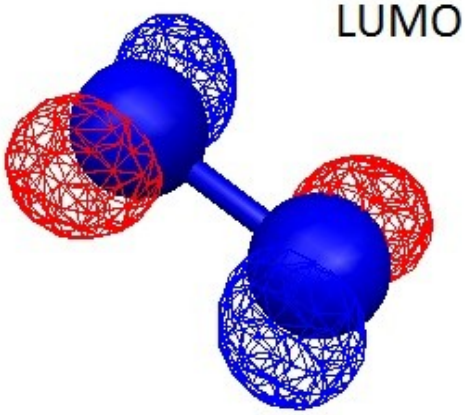
Molecule : N_2

Quantity	Simulation	Experimental
Bond Length(Angs)	1.113	1.116
Dipole Moment(Debye)	-0.0000005	0.0000006

Vibration Frefquency is 2302.53Hz from simulation and experimental vibrational frequency is 2221.5Hz.
Expected Bond order for N_2 is 3 but simulated bond order is 2.62.
Singlet is more stable in N_2 and hence it exists in Diamagnetic form.



HOMO



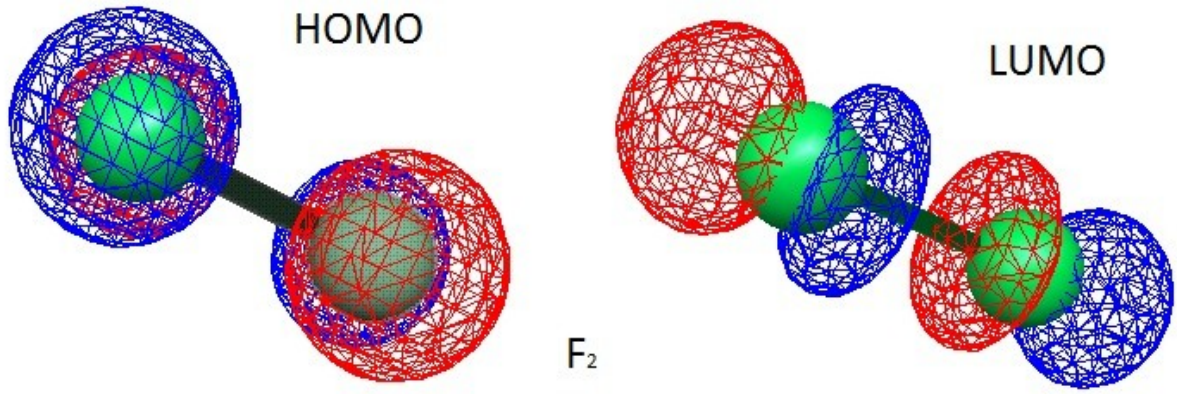
LUMO

N_2

Molecule : F_2

Quantity	Simulation	Experimental
Bond Length(Angs)	1.469	1.318
Dipole Moment(Debye)	0.000006	0.0000006

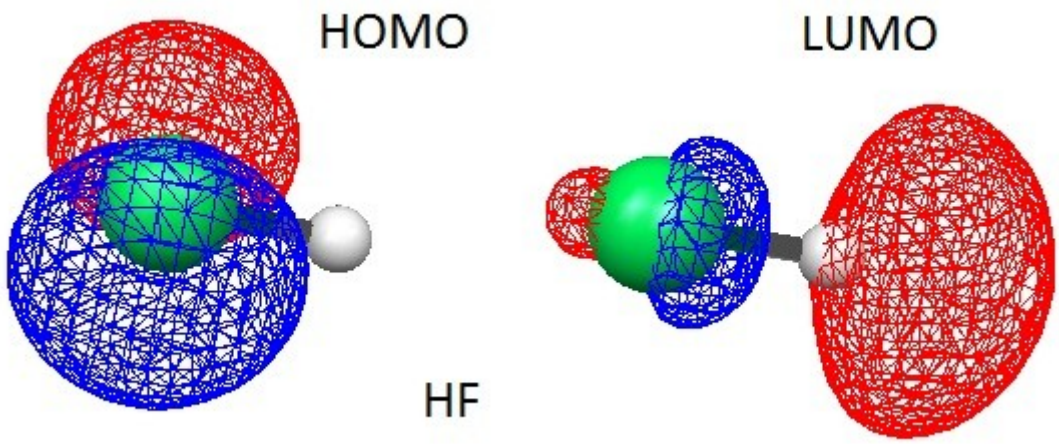
Vibration Frefquency is 952.92Hz from simulation and experimental vibrational frequency is 1088Hz.
Expected Bond order for F_2 is 1 but simulated bond order is 0.958.
Singlet is more stable in F_2 and hence it exists in Diamagnetic form.



Molecule : HF

Quantity	Simulation	Experimental
Bond Length(Angs)	0.940	1.04
Dipole Moment(Debye)	2.214910	1.932

Vibration Frefquency is 3839.37Hz from simulation and experimental vibrational frequency is 3711.1Hz.
Expected Bond order for HF is 1 but simulated bond order is 0.770.



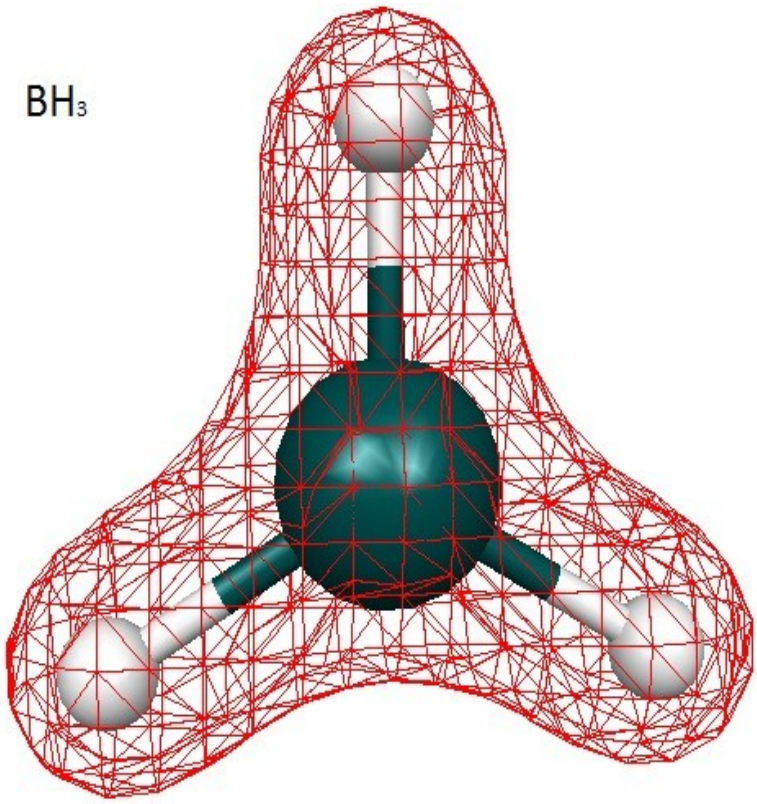
Singlet is more stable in HF and hence it exists in Diamagnetic form.

Ans 2

BH_3

HOMO – LUMO energy gap = -(0.3568-0.0798)
= -0.277 eV

B-H simulated bond length is 1.191 Angs each.

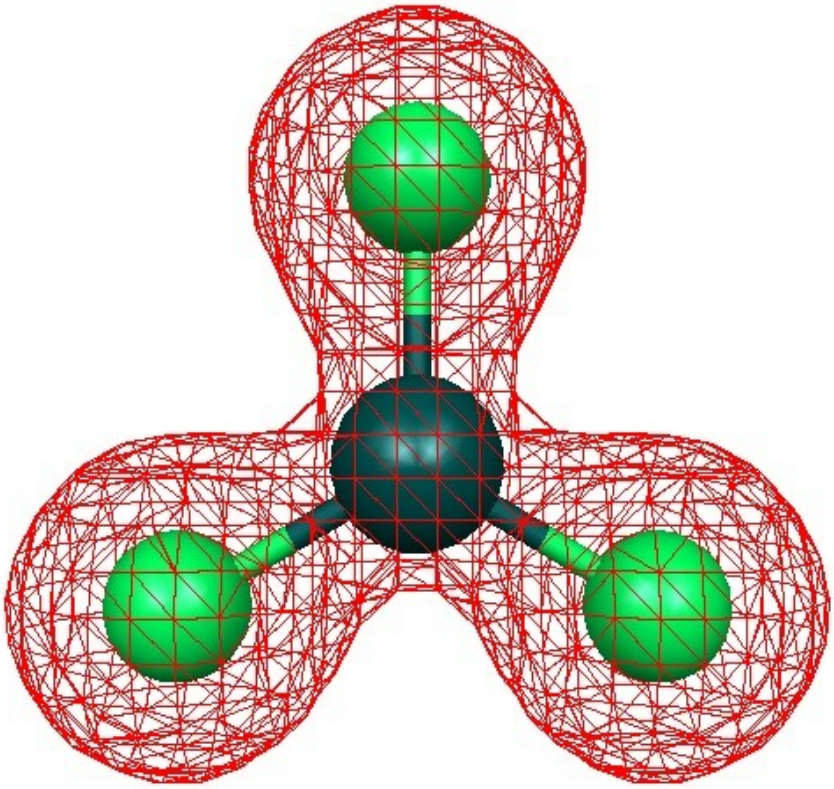


BF_3

HOMO – LUMO energy gap = -(0.4454-0.0238)
= -0.4216 eV

B-F simulated bond length is 1.341 Angs each.

BF_3

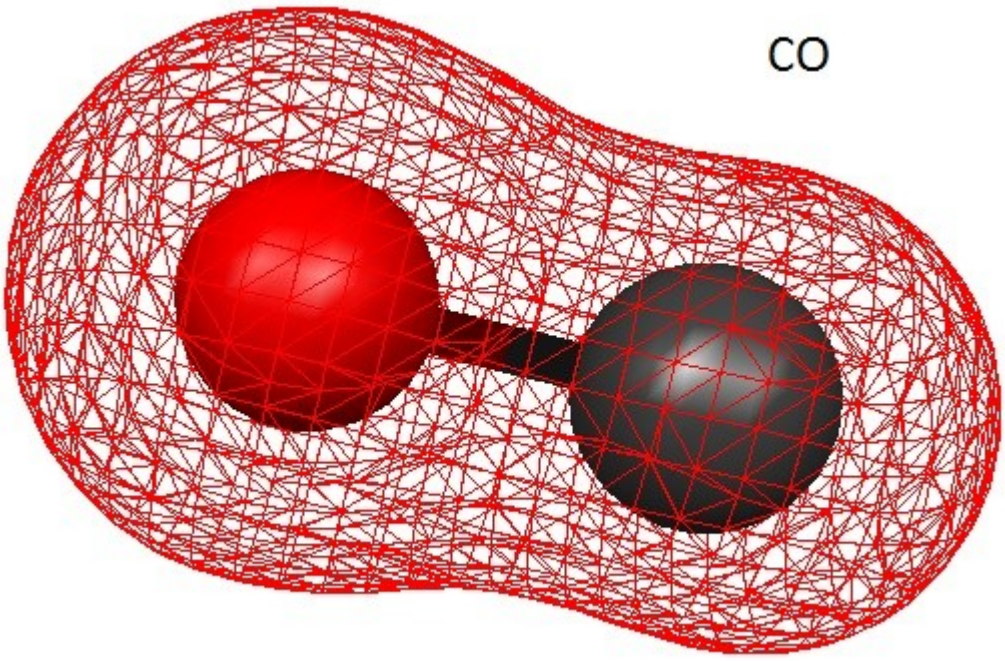


CO

HOMO – LUMO energy gap = -(0.3846-0.0526)

= -0.332 eV

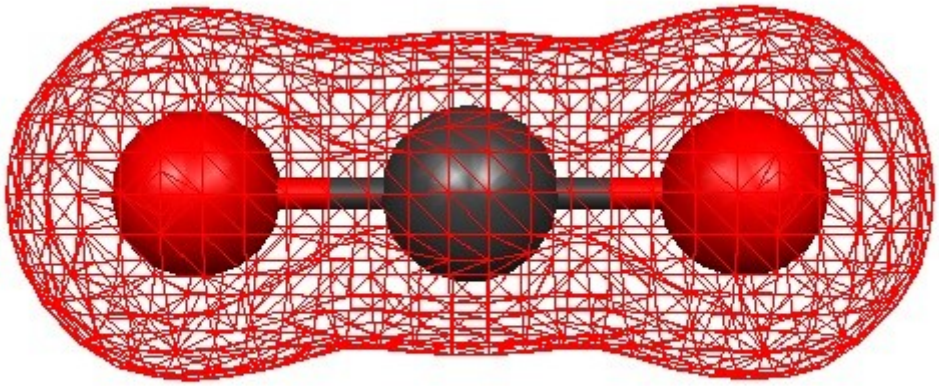
C=O simulated bond length is 1.148 Angs.



CO_2

HOMO – LUMO energy gap = -(0.3807-0.0098)
= -0.3709 eV

C=O simulated bond length is 1.183 Angs. each

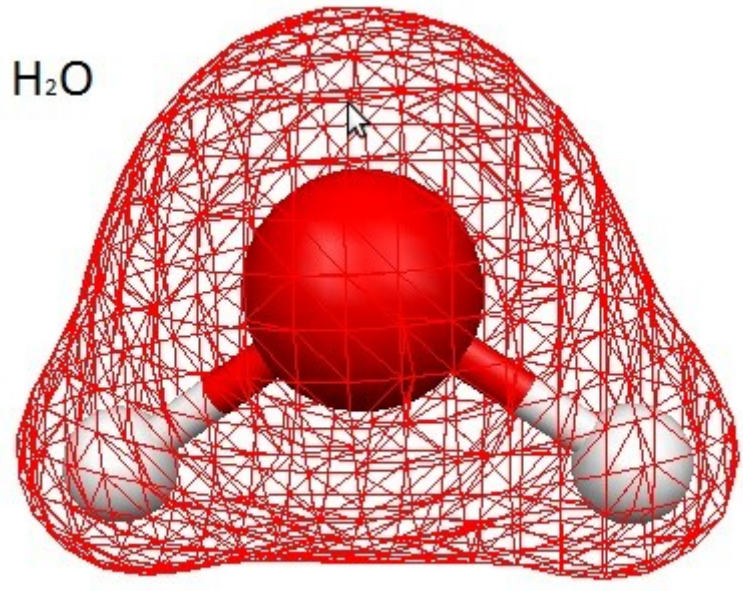


CO_2

H_2O

HOMO – LUMO energy gap = -(0.3103+0.0132)
= -0.3235 eV

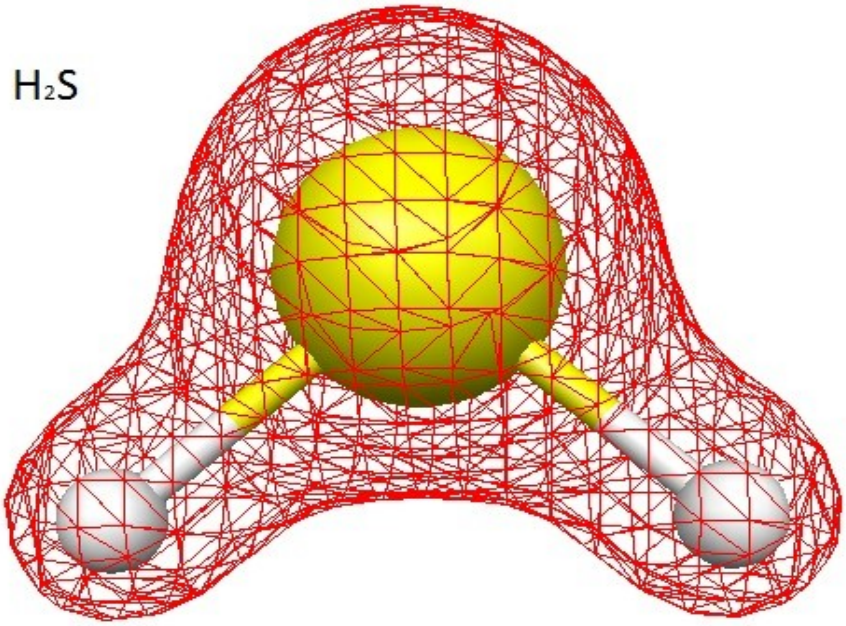
O-H simulated bond length is 0.974 Angs. each



H_2S

HOMO – LUMO energy gap = -(0.2644-0.0006)
= -0.2638 eV

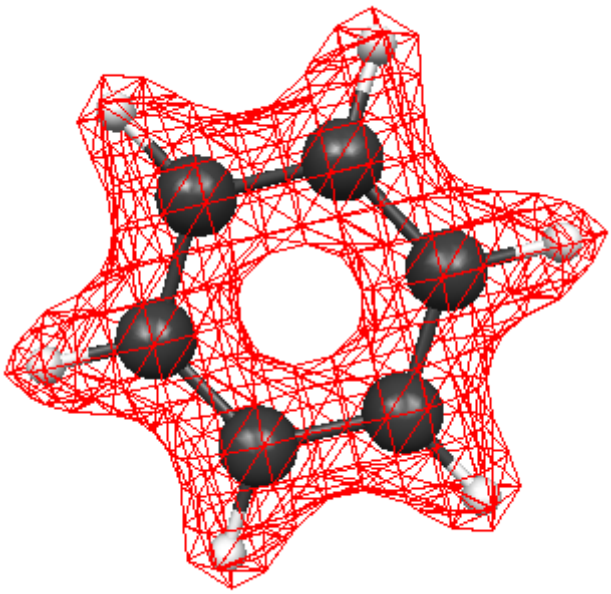
S-H simulated bond length is 1.383 Angs. each.



Benzene

HOMO – LUMO energy gap = -(0.2561-0.0087)
= -0.2474 eV

C-H simulated bond length is 1.083 Angs. each.
C-C simulated bond length is 2.795 Angs. each.
C=C simulated bond length is 1.397 Angs. each.

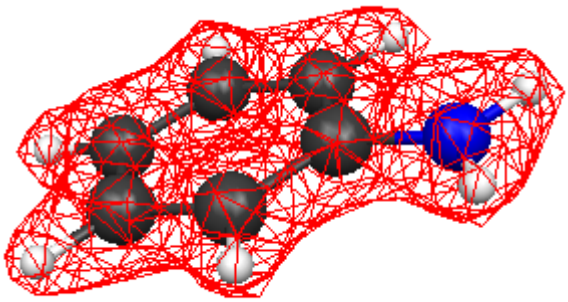


Benzene

Aniline

HOMO – LUMO energy gap = -(0.2461-0.0034)
= -0.2427 eV

C-H simulated bond length is 1.070 Angs. each.
C=C simulated bond length is 1.38 Angs. each.
C-C simulated bond length is 1.39 Angs. each.
C-C simulated bond length(near the carbon-carbon bond next to Nitrogen) is 1.4 Angs. each.
C-N simulated bond length is 1.38 Angs.
N-H simulated bond length is 0.99 Angs.



Aniline