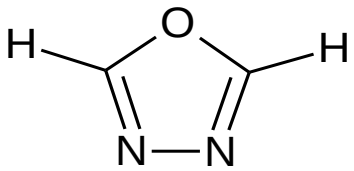
TP N° :02

Détermination des propriétés spectroscopiques.

Oxadiazole attracted a wide attention in research for therapeutic molecules. Compounds containing 1,3,4-oxadiazole cores have a broad biological activity including antibacterial, antifungal, analgesic and anticancer



Structure de 1,3,4-oxadiazole

Using your knowledge, build the 3D model in GaussView, by setting the following settings:

DFT/B3LYP method, 6-31G basis, in solvation section choose default model and water as the solvent.

-optimize the molecular structure (the first file should be named mol_opt)

Using the outputted result file (.log) we will determine some spectral data

1- open the obtained .log file, make a new calculation and choose IR in the job type (change name for the new intput file (example: name it mol_IR)

After calculation, open the new output file with GaussView, in results section, choose vibrations, fill the following table.

Functional groups	frequency
C-O	
C=N	
C-H	

2- open the .log file(mol_opt), make a new calculation and choose NMR in the job type (change name for the new input file (example: name it mol_NMR)

After calculation, open the new output file with GaussView, in results section, choose NMR

In element, choose H with the 1st reference, same step for C element.

Draw the 1H and 13C NMR spectra in your answer sheet.

3- Open the .log file (mol_opt), make a new calculation, choose energy in the job type, in method section choose the TD-SCF method, DFT/B3LYP with basis 6-31G, the remaining parameters must be unchanged (change name for the new input (example: name it mol_UV)

After calculation, open the new output file with GaussView, in results section, choose UV-VIS, fill the following table.

	λ_{max}(nm)	ν_{max}(cm^{-1})
Values		

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