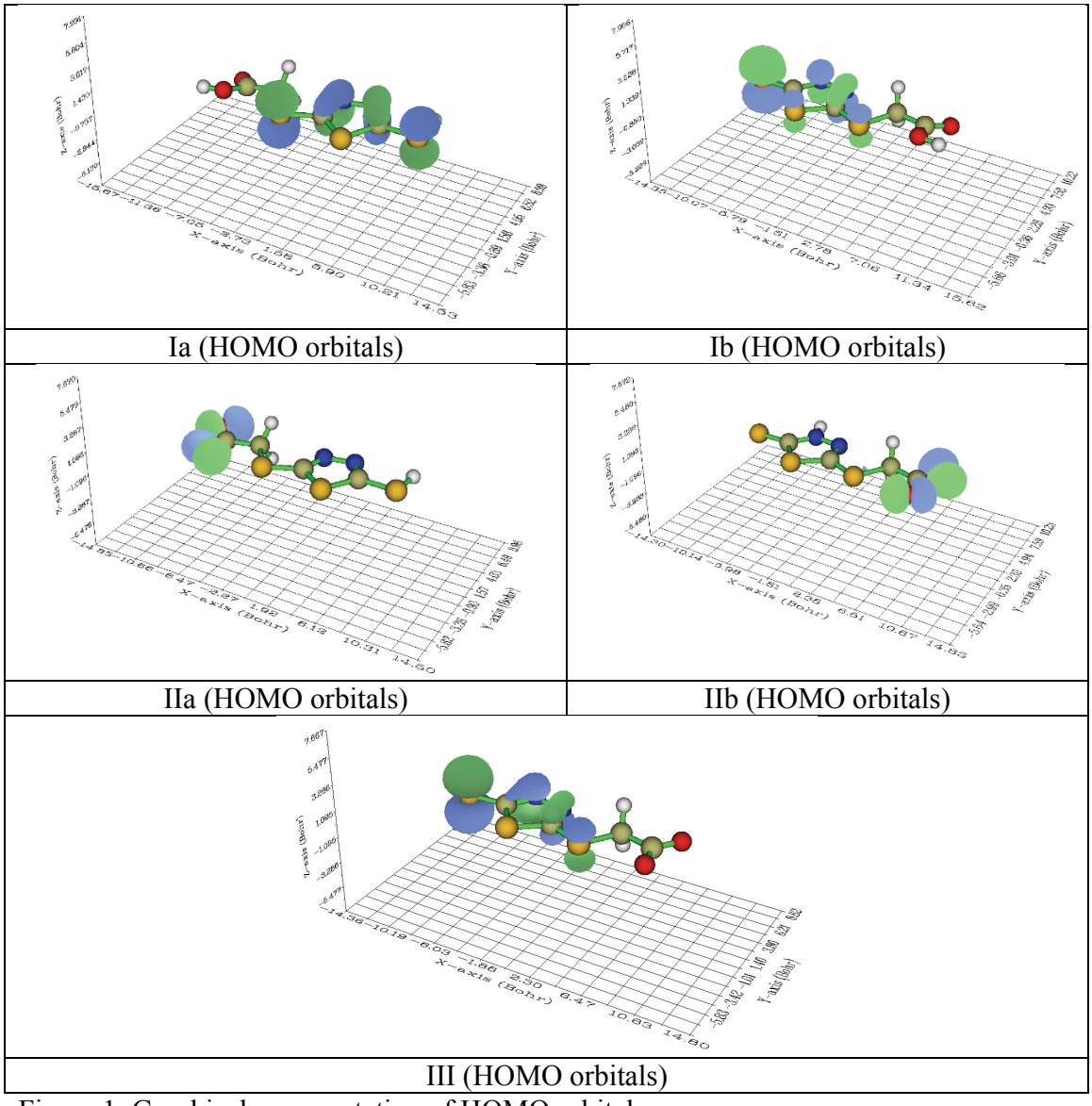
Theoretical considerations regarding the thione-thiol tautomerism in 2-mercapto-1,3,4-thiadiazol-5-yl thioacetic acid

Supplementary data

1. Computational part



Ia (HOMO orbitals) | Ib (HOMO orbitals)

IIa (HOMO orbitals) | IIb (HOMO orbitals)

III (HOMO orbitals)

Figure 1. Graphical representation of HOMO orbitals

Free energies of solvation, computed at B3LYP/6-311+G(d,p), are presented in table below:

	ΔGsolv (kcal/mol)	
Compound	**IEFPCM**	**CPCM**
Ia	-9.194	-9.270
IIa	-58.119	-58.192
IIIa	-158.131	-158.158
Ib	-9.740	-9.810
IIb	-55.228	-55.300
IIIb	-158.143	-158.159
Thioglycolic acid	-5.962	-6.021
Thioglycolate	-58.523	-58.420

Table 1. ΔGsolv (kcal/mol) (B3LYP/6-311+G(d,p) level of theory)

2. Experimental part

The acid-base titration data that have been used to determine the equivalence volume and pH and to calculate the acidity constants Ka_1 and Ka_2 by means of software applications (Visual Basic) developed by the authors (I. Julean and C. Muntean):

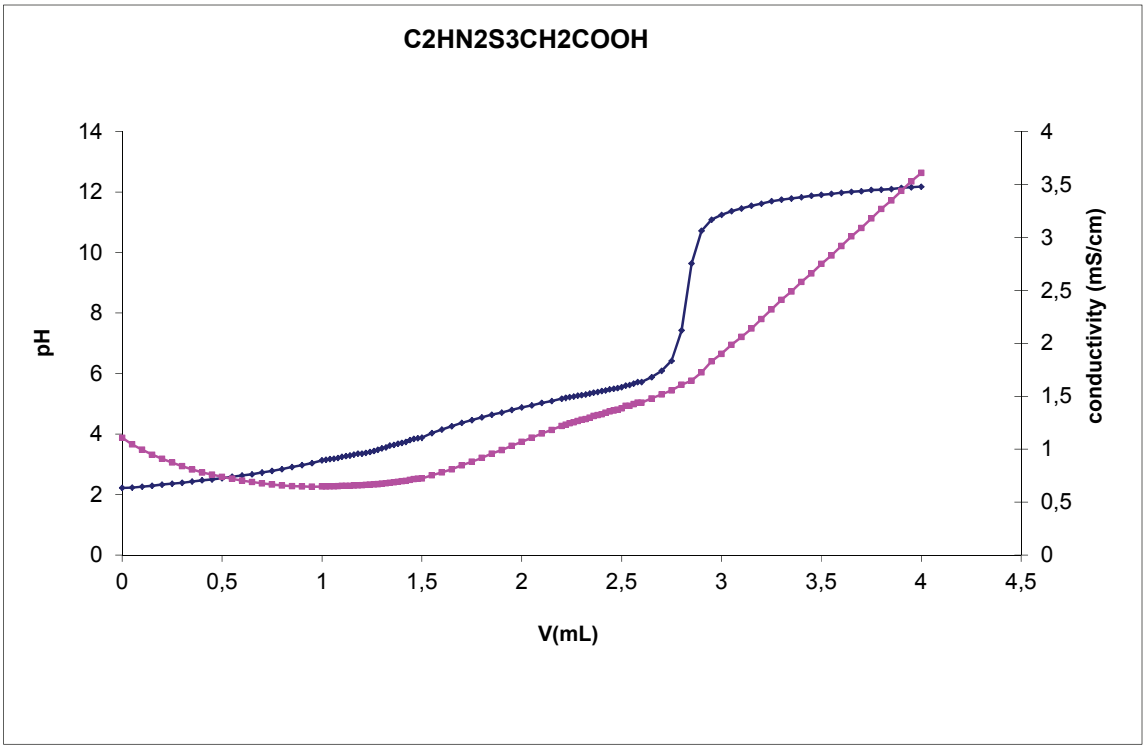


Figure 2. Conductometric (*) and acid-base titration (*) of 0.01M $C_4H_4S_3N_2O_2$ with 1M NaOH