



COMPUTATIONAL STUDY OF THE INFLUENCE OF THE ABILITY OF LAPACHOL AND ITS DERIVATIVES TO CHELATE IRON (II) CATION ON THEIR ANTIOXIDANT PROPERTIES

Djafarou NGOUH PAJOUORO, BIKELE MAMA Désiré*

University of Douala, Cameroon



1-ABSTRACT

The computational elucidation of the influence of the complexation of Lapachol and its derivatives with Fe^{2+} cation on their antioxidant power has been performed at B3LYP/6-311++G (d,p)//B3LYP/6-311+G(d,p) level of theory in gas phase, water, acetonitrile, benzene and toluene. Only bi-dentate and tri-dentate binding of Fe^{2+} to ligands have been taken into account. The results indicated proportionality between the metal ion affinity (MIA) values and the retained charge on Fe^{2+} cation and an inverse one between the two respectively for $k^2-(\text{O}_1, \text{O}_2)$ and $k^3-(\text{O}_2, \text{C}=\text{C})$ modes. In addition, the higher stability obtained for a tri-dentate coordination mode in which the Fe^{2+} cation is simultaneously attached to the two carbon atoms of the ethylenic bond ($\text{C}=\text{C}$) and sp^2O_3 oxygen atom. The topological analysis of complexes exhibits the localization of concentration of electron density between the oxygen atom of the ligand attached to Fe^{2+} and this metal cation for this latter mode in gas phase. Our results also indicate that the electron extraction in $\text{Fe}^{2+} \dots \text{La}_i$ complexes is more difficult than in the one in free ligand. This tight binding of electron in cationic Fe^{2+} complex system is similar to the previous computational prediction done for Fe^{2+} -caffeic acid phenethyl ester derivative complexes and Fe^{2+} -curcumin complexes

2- MOLECULAR LIBRARY BUILT AROUND LAPACHOL AND ITS DERIVATIVES

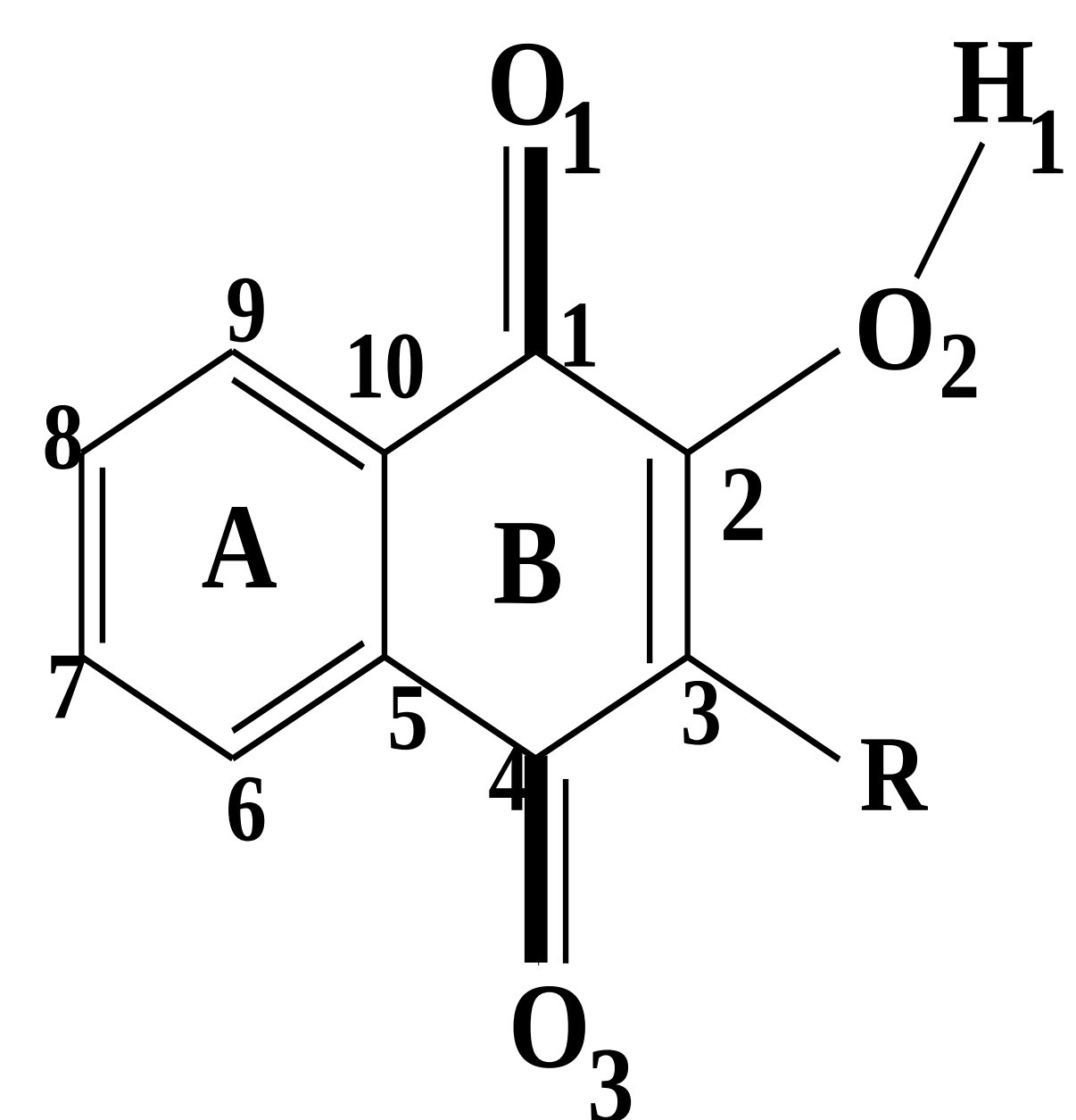
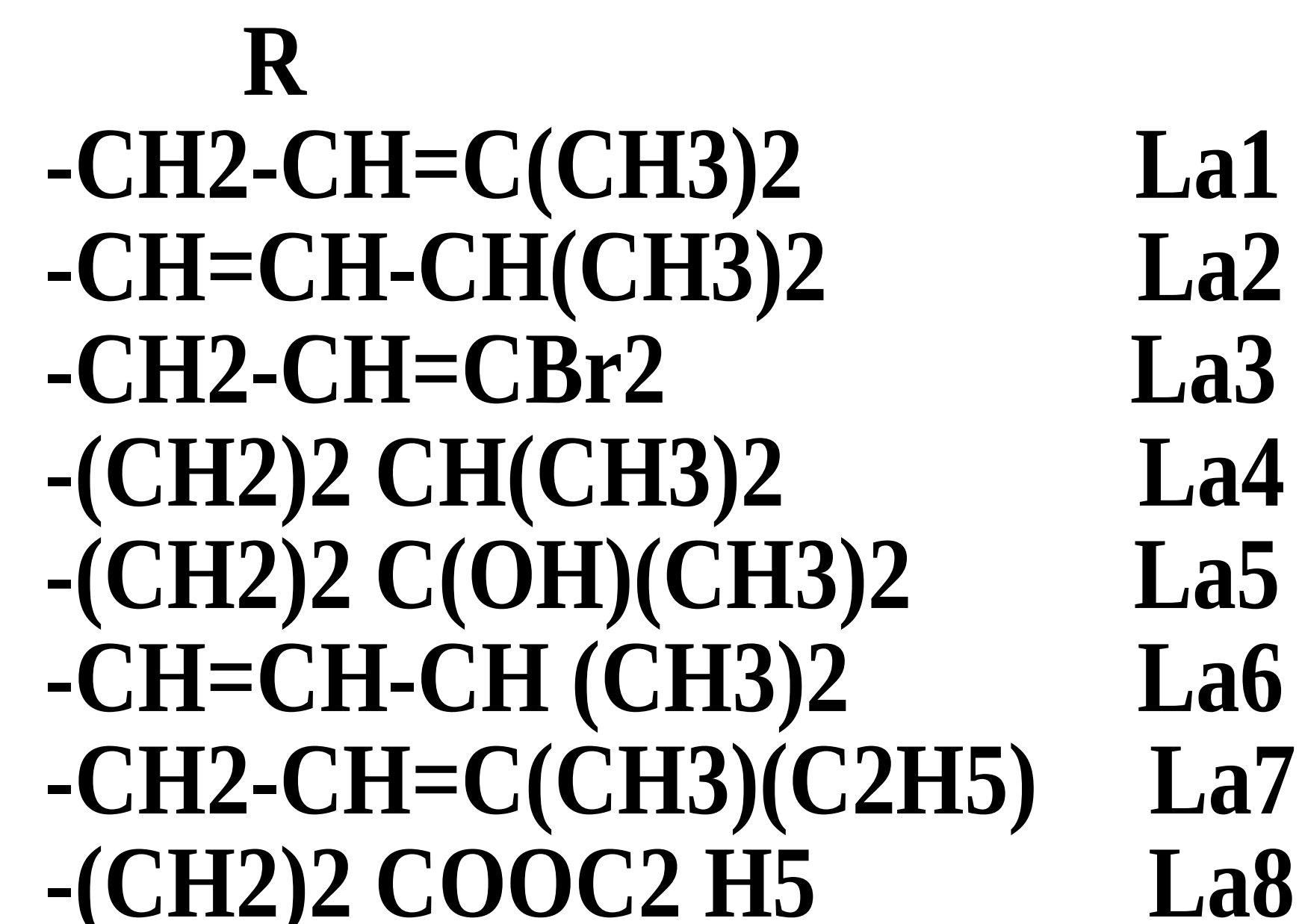
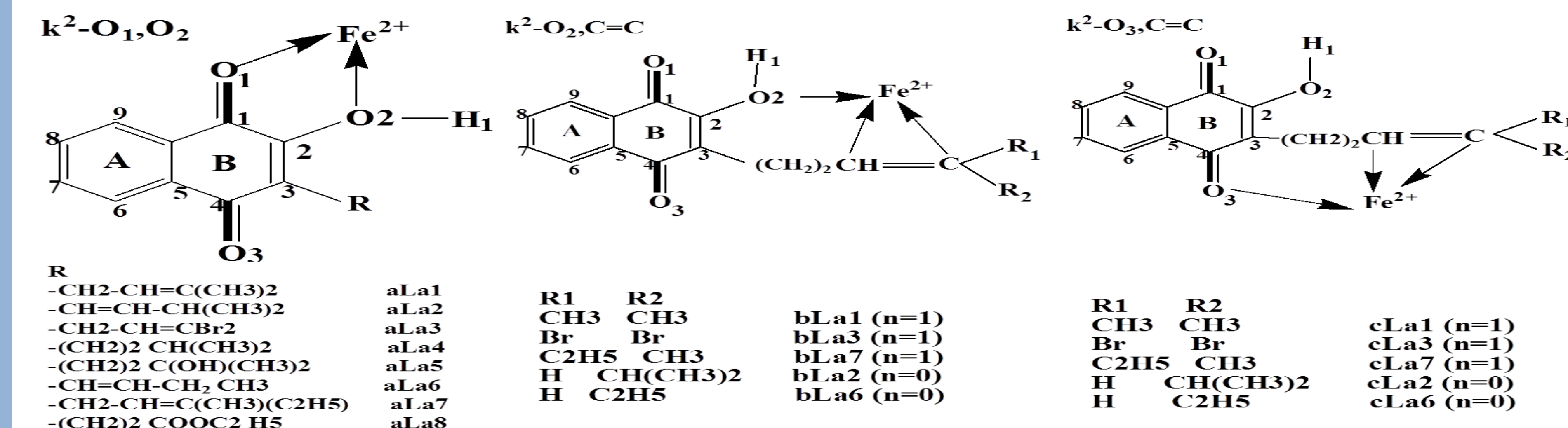


Figure 1: numbering system used for La_i free ligand in their various coordination modes



3- RESULTS I- VARIOUS COORDINATION MODES OF $\text{Fe}^{2+} \dots \text{La}_i$ COMPLEXES



II-INTRAMOLECULAR INTERACTIONS

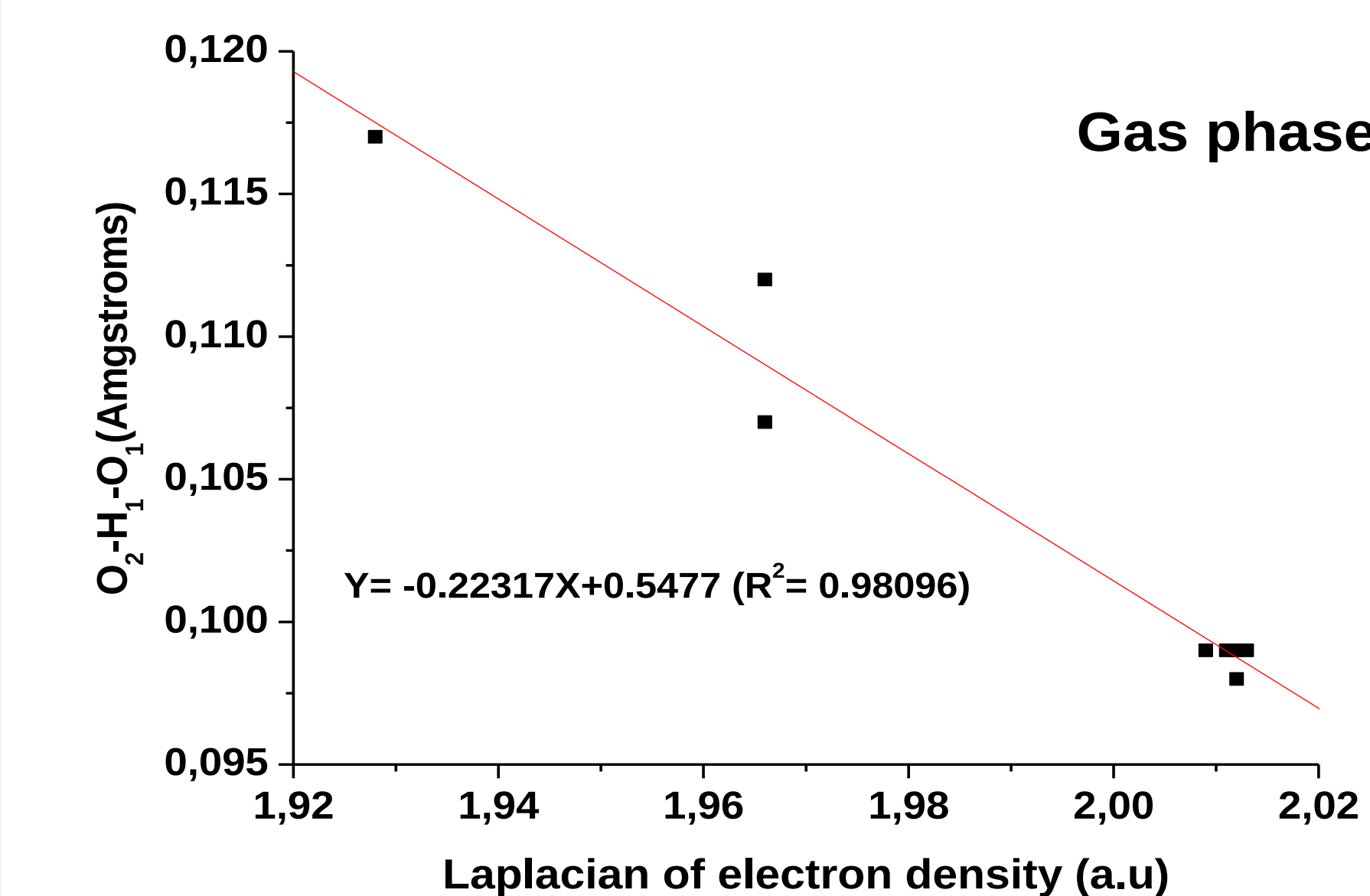
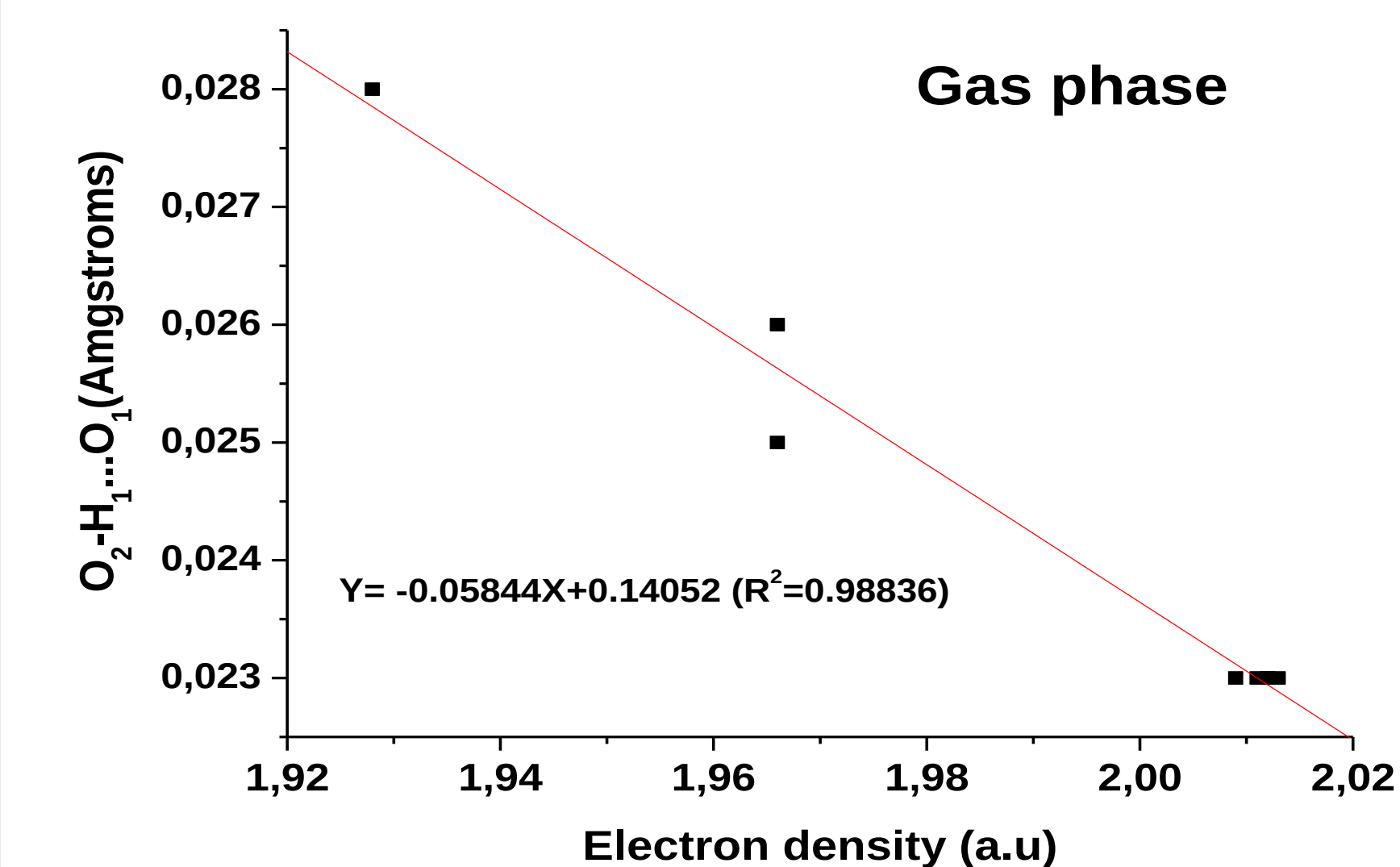


Fig.3: Linear dependence between H-bond

III-METAL ION AFFINITY AND RETAINED CHARGE ON THE Fe(II) CATION

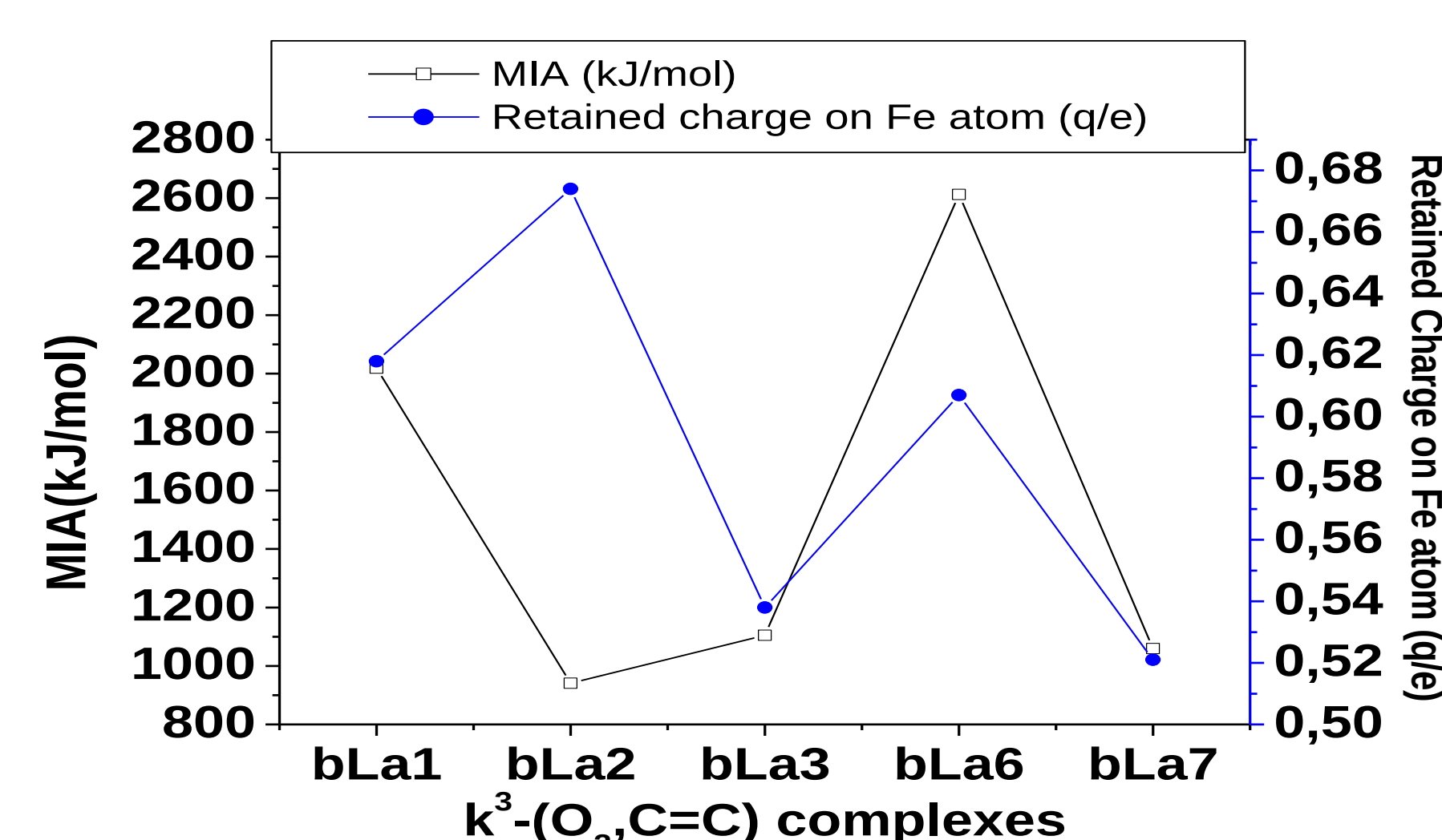
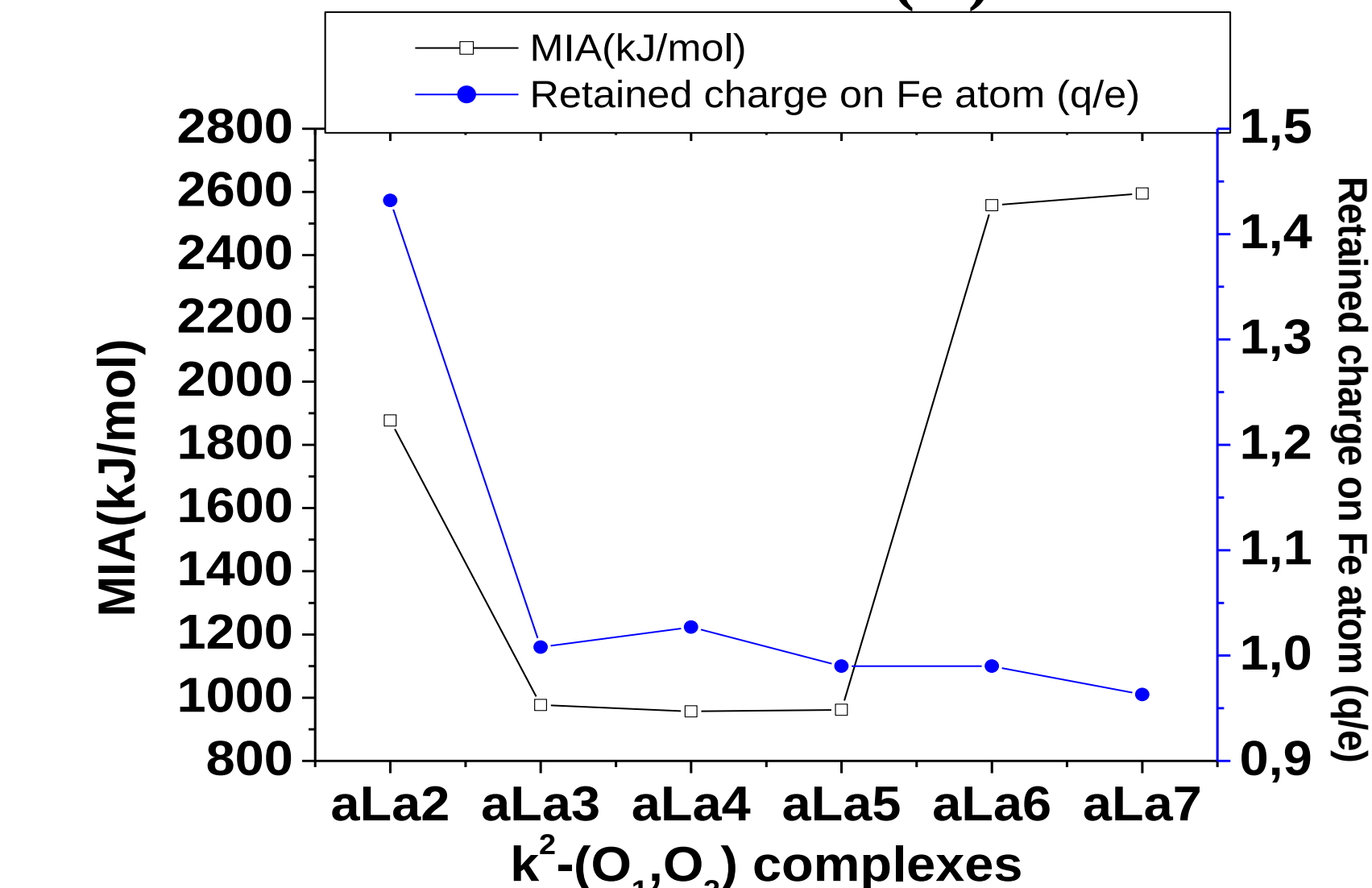


Fig. 4:Correlation between the MIA (kJ/mol) and retained charge (Q/e) of Fe in $k^3-(\text{O}_2, \text{C}=\text{C})$ coordination

IV-INFLUENCE ON Fe^{2+} CHELATION ON ANTIOXIDANT POWER

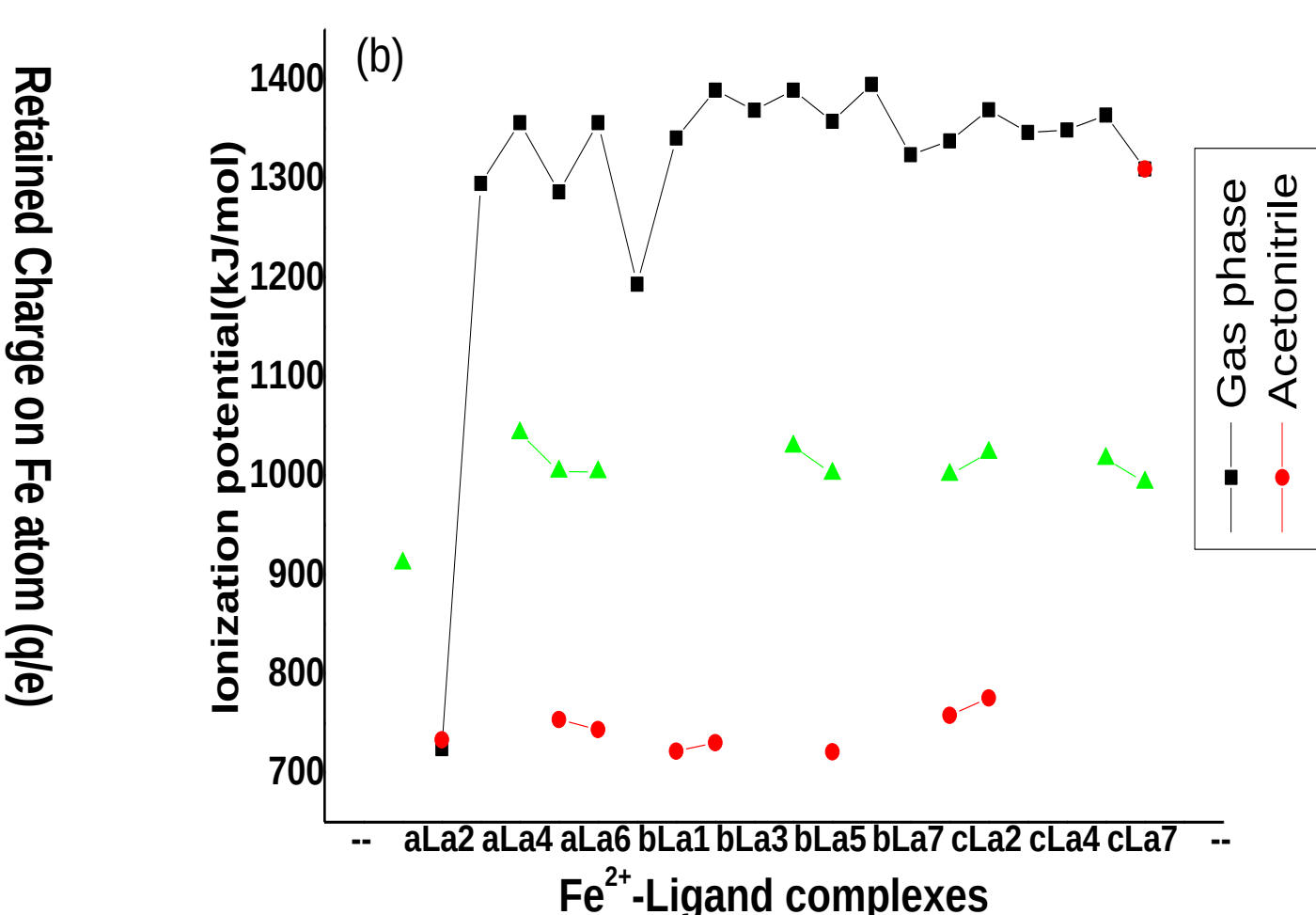
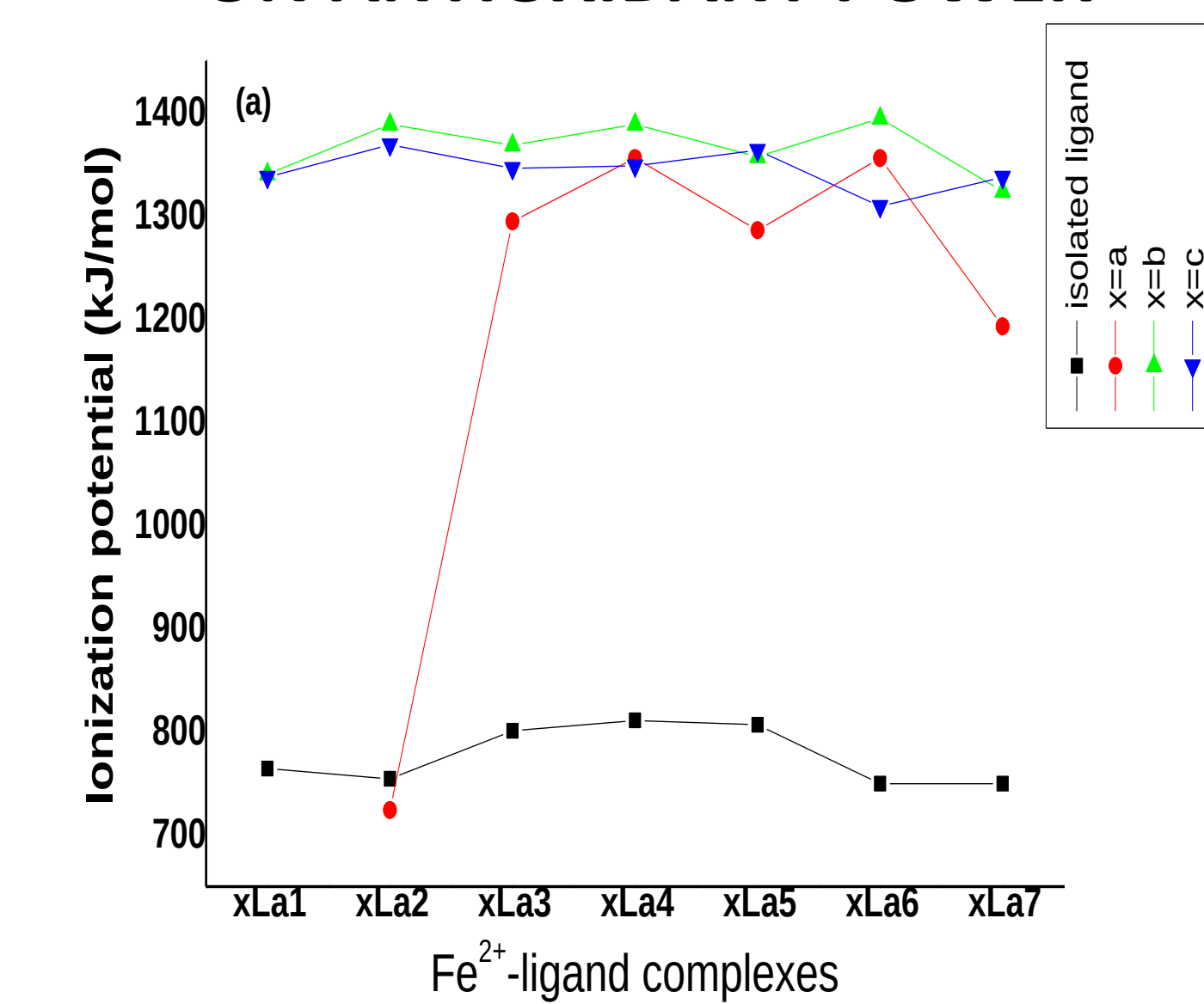


Fig.5: Ionization potential (kJ/mol) of Fe^{2+} -ligand complexes

4-Conclusion

This work is focused on the impact of the complexation of Lapachol and its derivatives to Fe^{2+} cation on their antioxidant powers by the means of computational tools. Our results have indicated that the electron extraction from $\text{Fe}^{2+} \dots \text{La}_i$ complexes is more difficult compared to that from free ligands.

5-Aknowledgements

This work was supported by the Ministry of Higher Education of Cameroon
Autor courriel: bikelemama@yahoo.f

5- References

- [1] S.G.C. Fonseca, R.M.C Braga, D.P Santana. The Revista Brasileira de Ciências Farmacéuticas 2003, 84, 9-16.
- [2] Lei C. Journal of Food Microbiol. 2018, 2(1), 4-6.
- [3] Sun J, Huang Y, Sun G, Sun X, Qin M, Zhao D. 2012, 37(13), 1958-62..
- [4] Y. Chen, H. Xiao, J. Zheng, and G. Liang, PLoS ONE, 2015, 10, 3.
- [5] O. Holtomo, M. Nsangou, J. J. Fifen, and O. Motapon, Computational and Theoretical Chemistry 2015.