



BONDING PROPERTIES OF HALIDE TRANSITION METAL (II) COMPLEXES OF GLYOXIME LIGAND:DFT; QTAIM; EDA and CDA STUDIES.

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1-INTRODUCTION

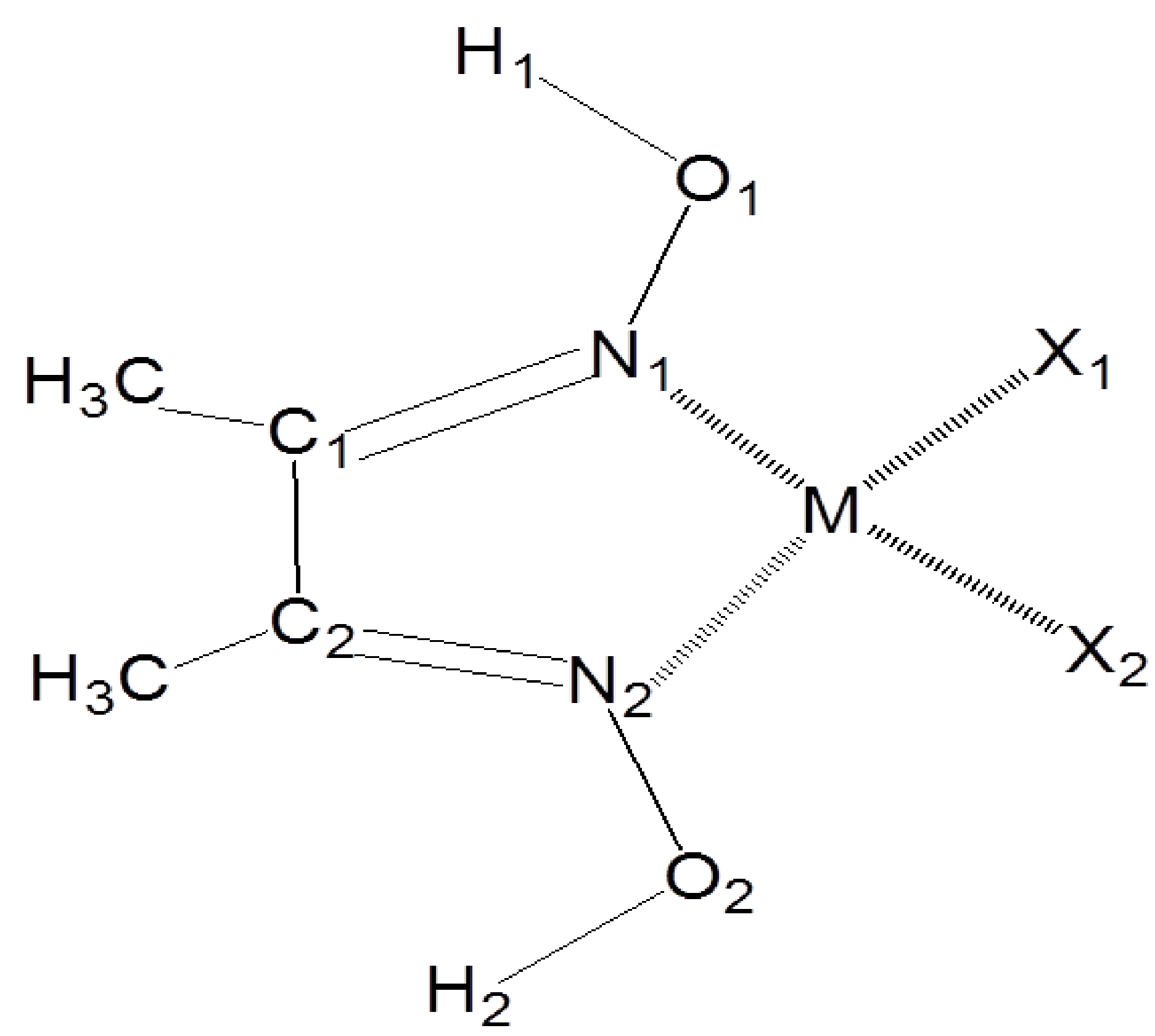
Globally, over 80% of all wastewater from our homes, industries flows back to nature without being treated or reused-polluting the environment. The wastewater from industries without being treated is sent to the environment . In the environment the wastewater discarded enter the water cycle which contains heavy metal, used for consummation and others thus causing sickness like cancer . This leads to the need of removal using dimethylglyoxime ligand



Fborgenproject.org in water-quality-in-cameroon

2-NEWTON RAPHTON GEOMETRY OPTIMIZATION :

B3LYGEN: LanL2DZ for nd^x (x= 6,7 and 8) transition metals, Br and Cl and (6-311+G(d,p)) for other atoms



X ₁ =X ₂	M	
Cl	Fe	3a
	Co	3b
	Ni	3c
	Ru	4a
	Rh	4b
	Pd	4c
	Os	5a
	Ir	5b
	Pt	5c
Br	Fe	3A
	Co	3B
	Ni	3C
	Ru	4A
	Rh	4B
	Pd	4C
	Os	5A
	Ir	5B
	Pt	5C

2- RESULTS

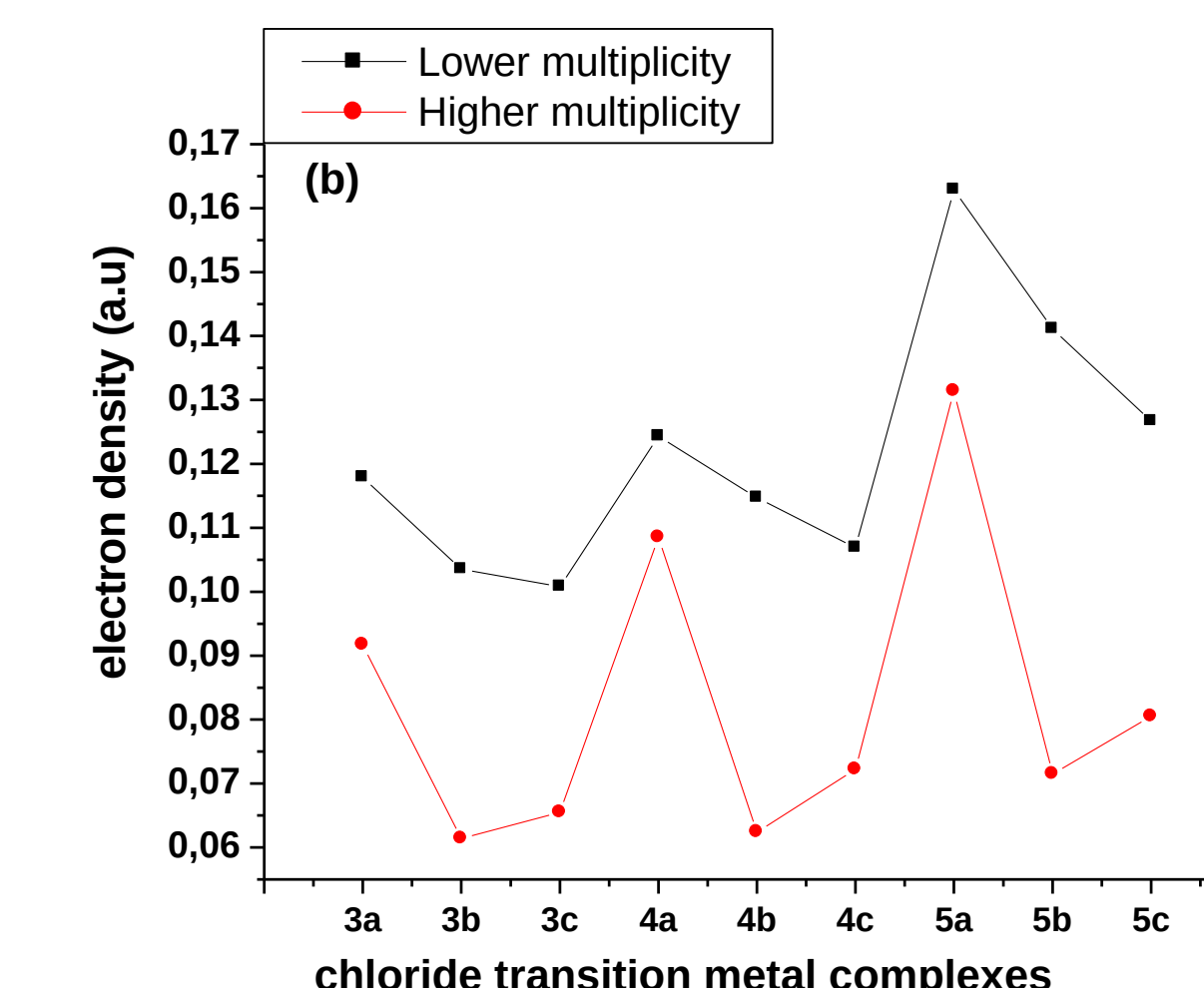
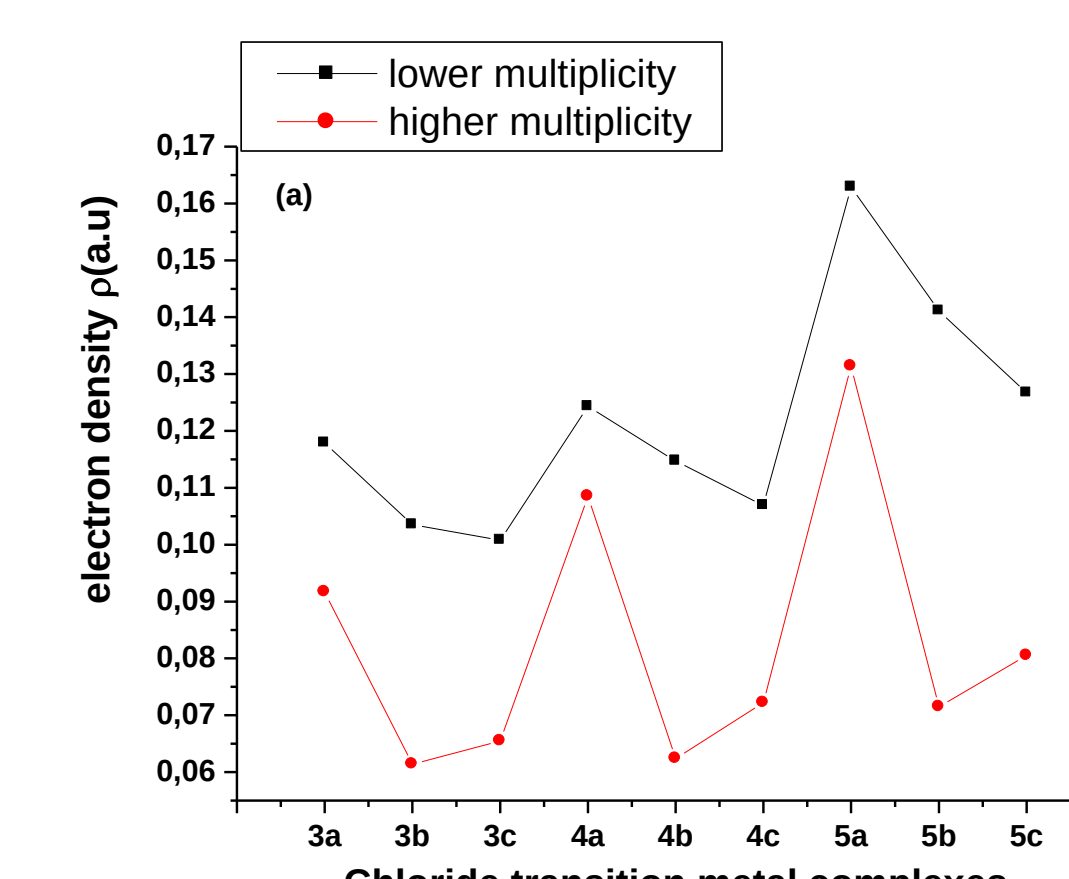
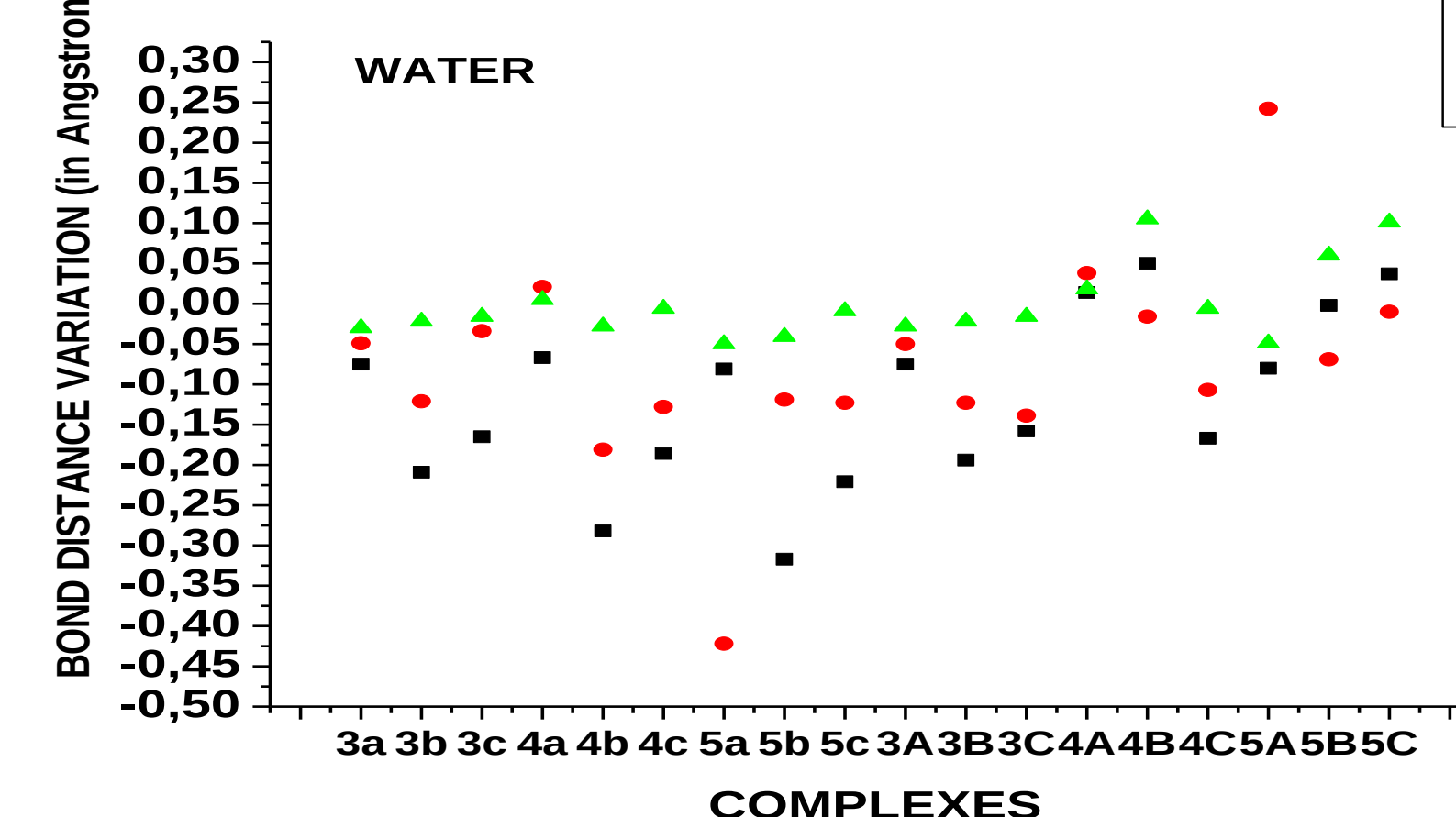
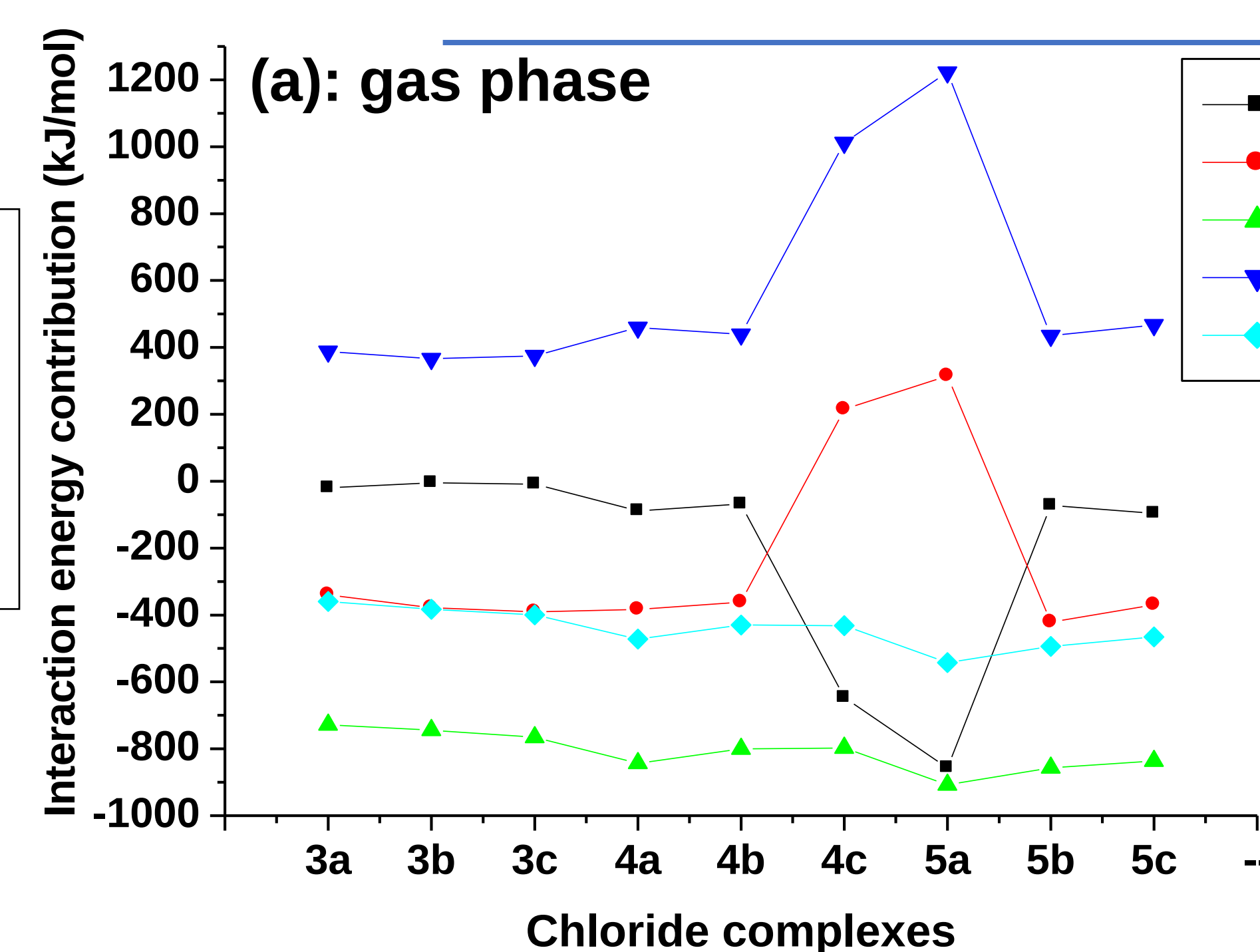
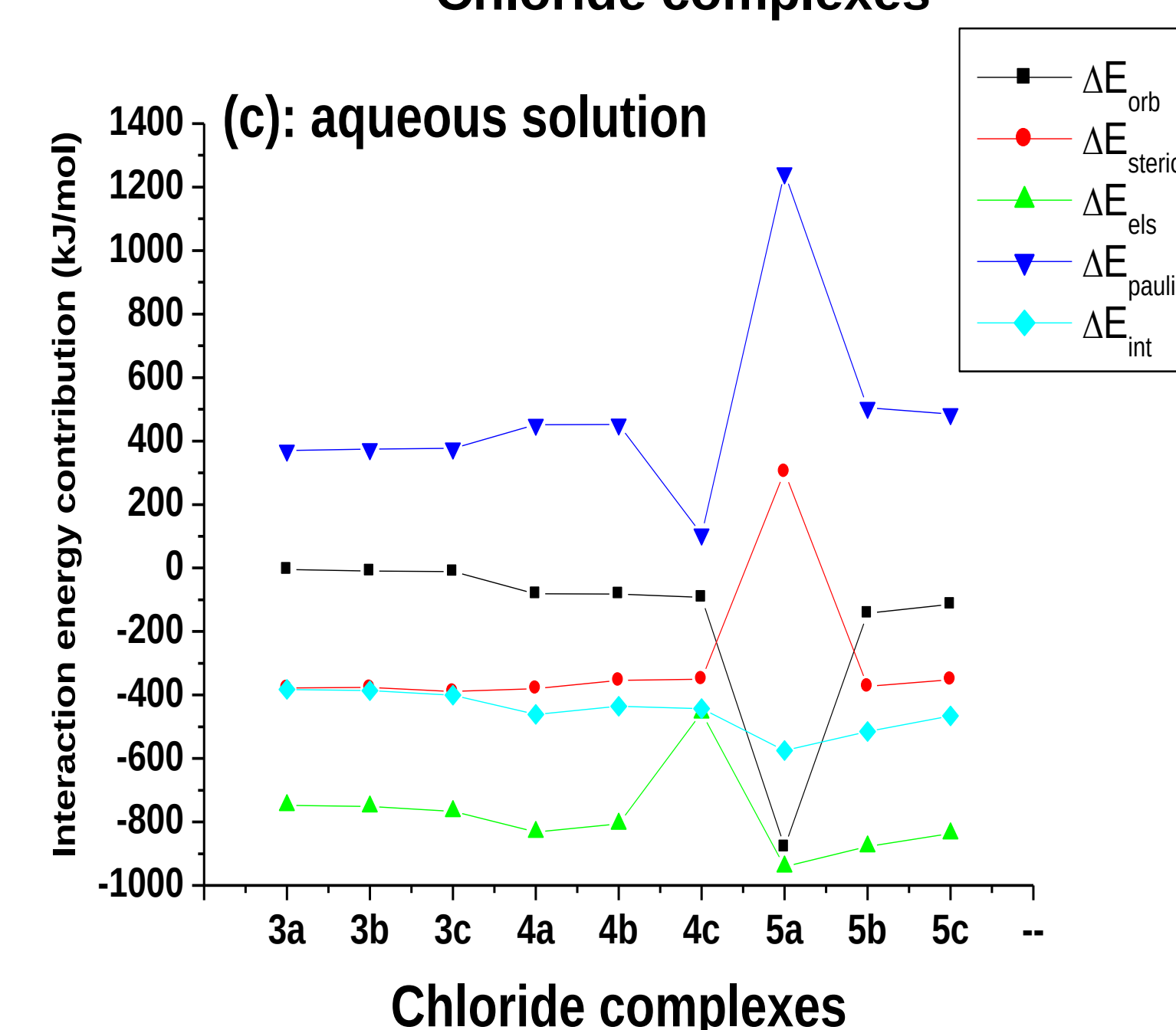


Figure 1: B3LYP/Gen selected bond distances of optimized structures of complexes (a) , Electron density ρ (r) of metal-nitrogen bond (lower multiplicity and higher multiplicity) in gas phase (b) and aqueous solution (c). NBO retained charge on transition metal atom.



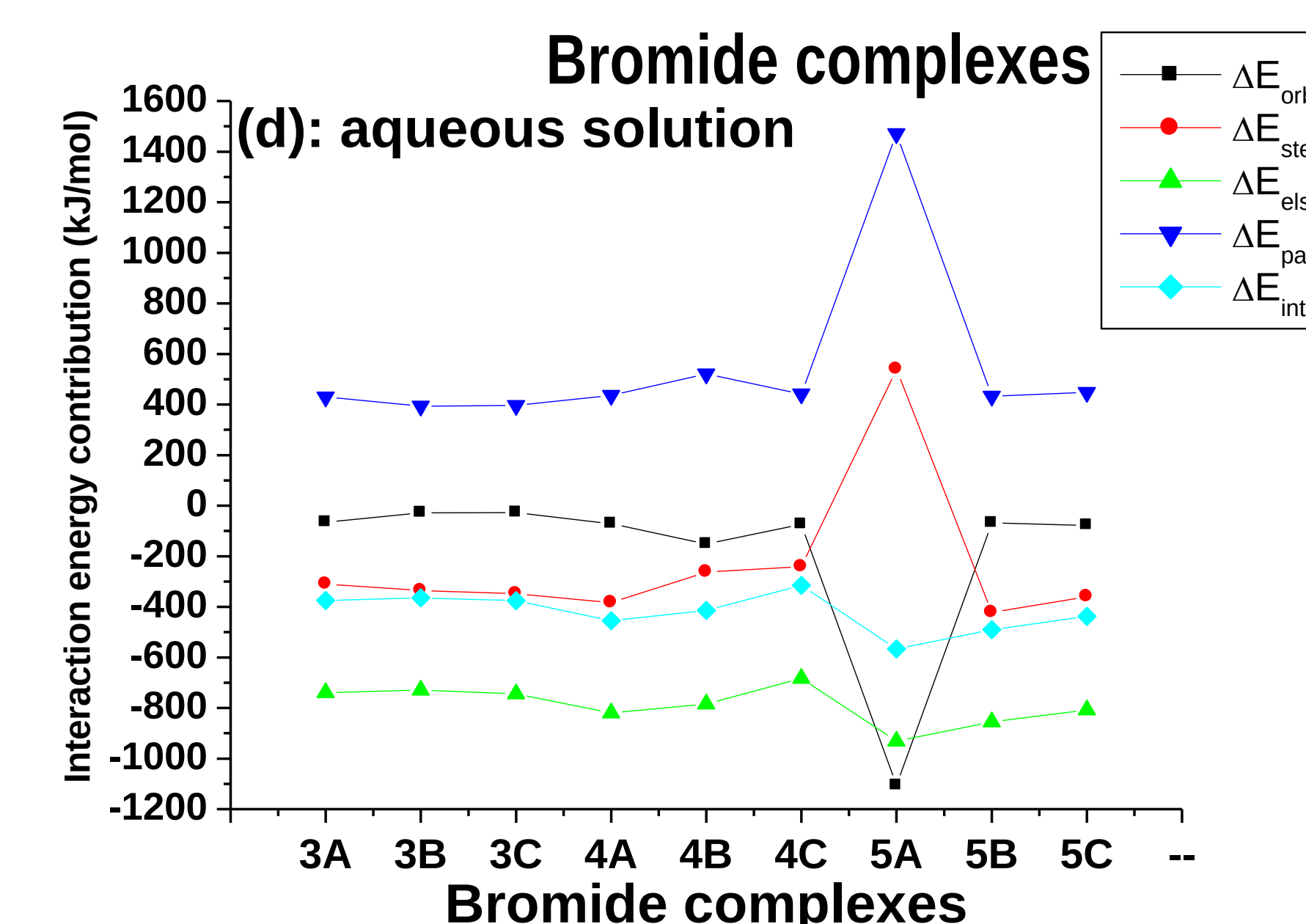
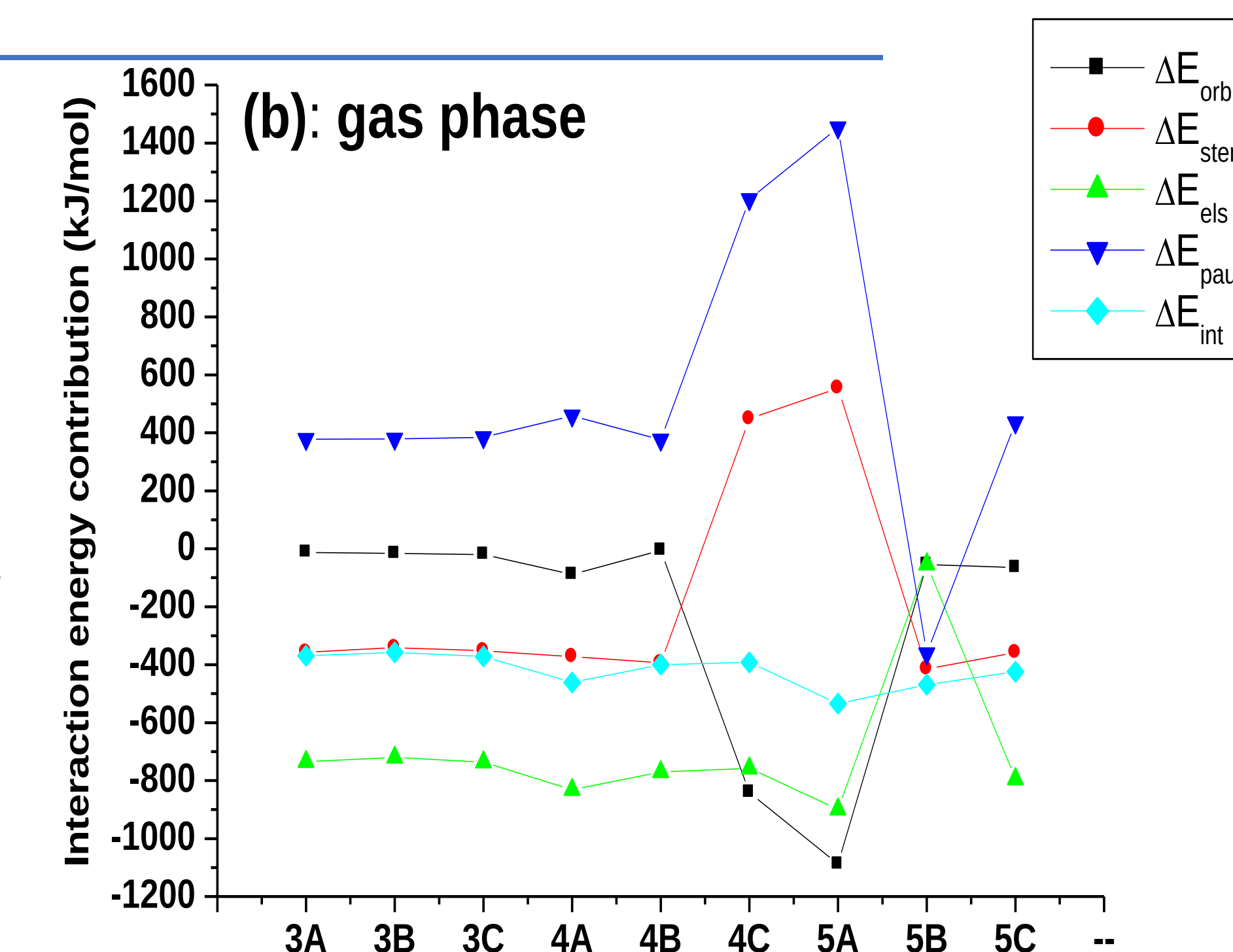
General observation
percentage contribution
of Orbital Energy
in the formation of **M-L**
[58 % ; 64 %]

**Partially covalent
interaction**



Electrostatics Interaction

Fig.2: Graphical comparative interaction energy contribution of chloride and complexes in both media of EDA



4-Conclusion

Quantum theory of atom in molecule (QTAIM) method shows that the M.....N and M....X interactions of all the complexes are partially covalent

Energy decomposition analysis (EDA) method shows that metal-ligand bond have a pronounced ionic character in all the complexes

Charge decomposition analysis (CDA) shows that there is actually a backdonation from metal towards the ligand

5- References

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6-Aknowledgements

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