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Transfer Of Protons Into A New Organic Compound Based On Creatinine

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Abstract:

Hydrogen bonds are of paramount importance for biological processes, they are energetically weaker than covalent bonds, and their cumulative effect strengthens the three-dimensional shape of macromolecules and maintains their structure. The weakness of these bonds is responsible for the flexibility and conformational dynamics that are necessary for the flexibility of biomolecules, which gives them their recognition capacity and therefore their very high specificity.

New compounds have been obtained by proton transfer reactions between organic compounds of type nitrogenous substance and dicarboxylic acid. These reactions present interesting aspects for the realization of molecular systems whose properties can be monitored by X-ray diffraction.

In recent literature there are many examples of organic molecules functionalized with hydrogen bond donor-acceptor groups. Carboxylic acids are a few examples which illustrate excellent model systems for the preparation of new compounds with proton transfer, hence our interest in studying new organic compounds based on creatinine and organic acids which form complexes with many organic molecules

In this study, we shed light on the structural study of a new proton transfer compound. In this crystal structure, creatinine is protonated by two hydrogens of fumaric acid, forming a new organic compound, Bis Creatinium fumarate fumaric acid, that is rich in strong hydrogen bonds.

Keywords: Proton transfer, single crystal, X-ray diffraction, H-bonds.

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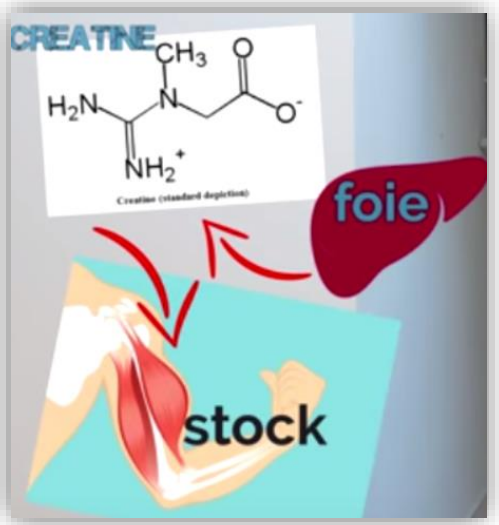
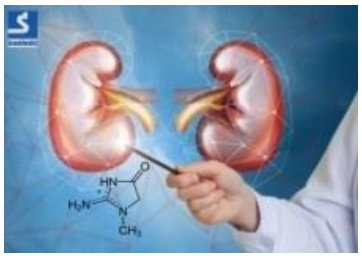
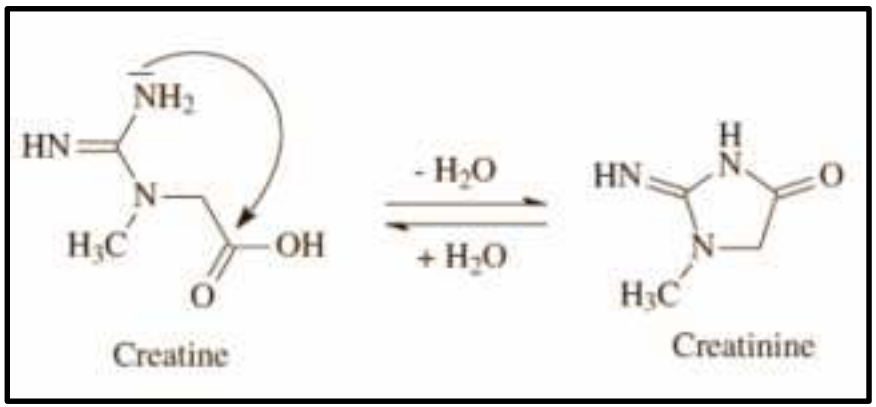
Introduction

What is creatine?

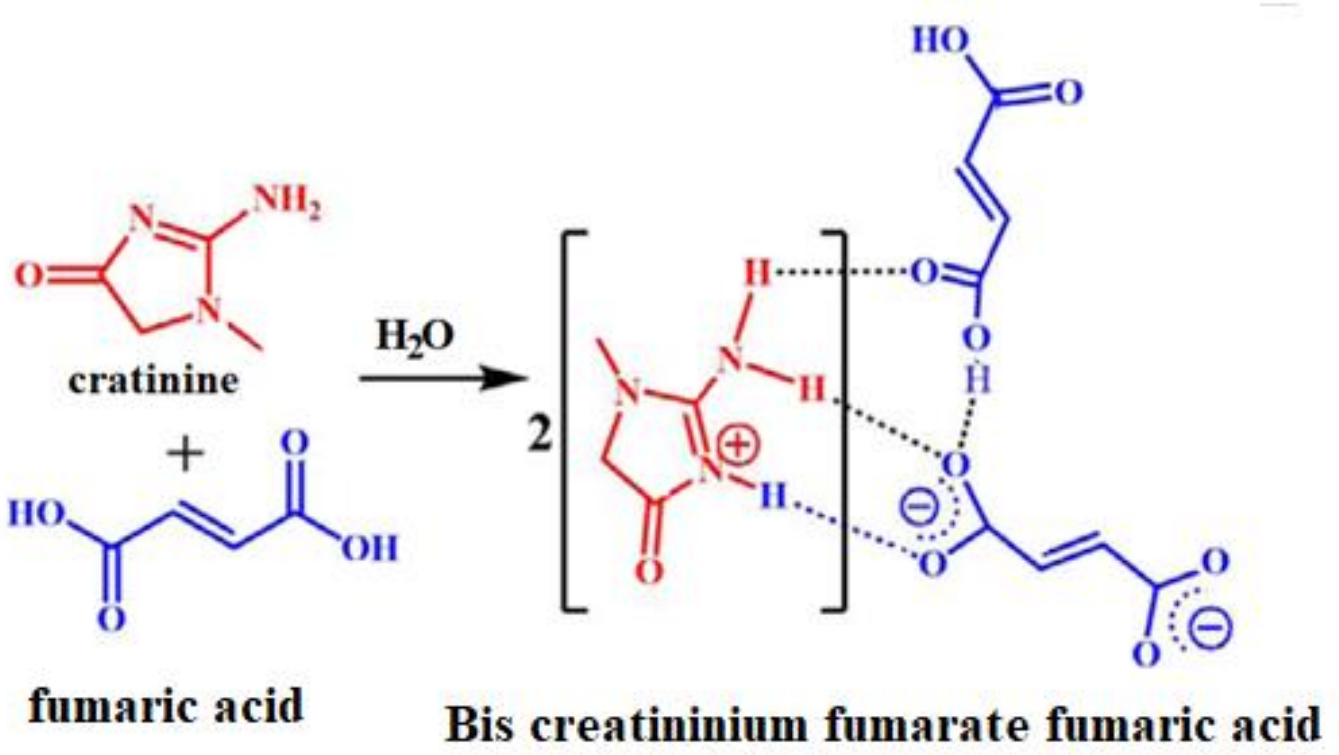






Structural analysis

Synthesis : Bis ceatininium fumarate fumaric acid (BCFF)



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Structural analysis

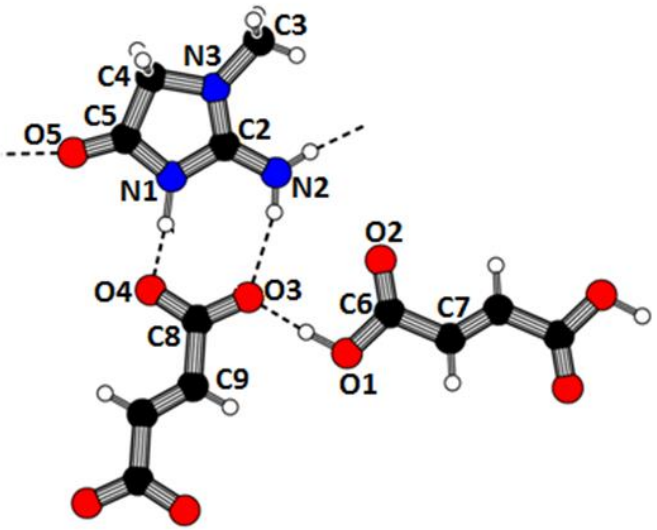
➢Resolution Structural and Refinement Of the tructure.

BCFF

Symmetry: Monoclinic $P2_1/c$
a = 5,8987 (7) Å
b = 21,795(5) Å
c = 7,8782(5) Å
β = 90,345(2)°
V= 1012,81 (14) $Å^3$

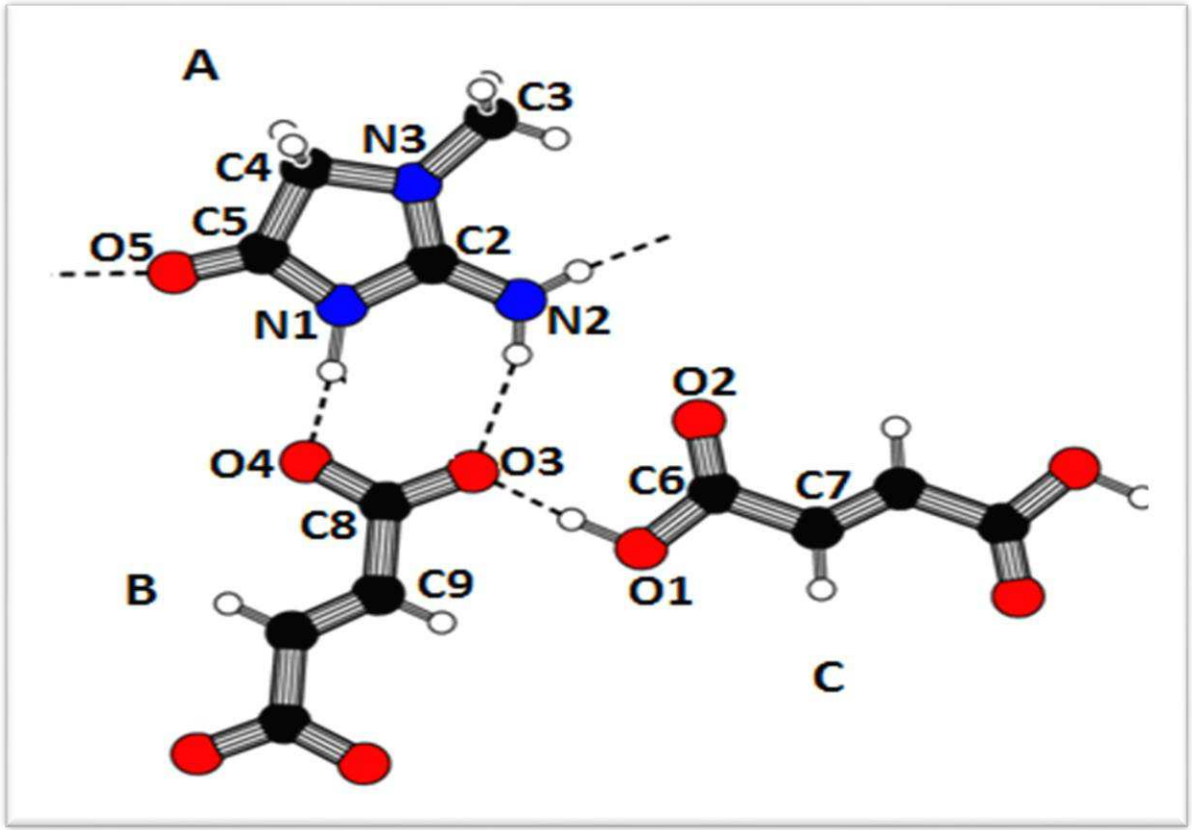
3604 Measured reflections
2105 Réflexions indépendants
Rint= 0,024

Refinement
R1= 0,065
wR = 0,177
GOF= 1,10



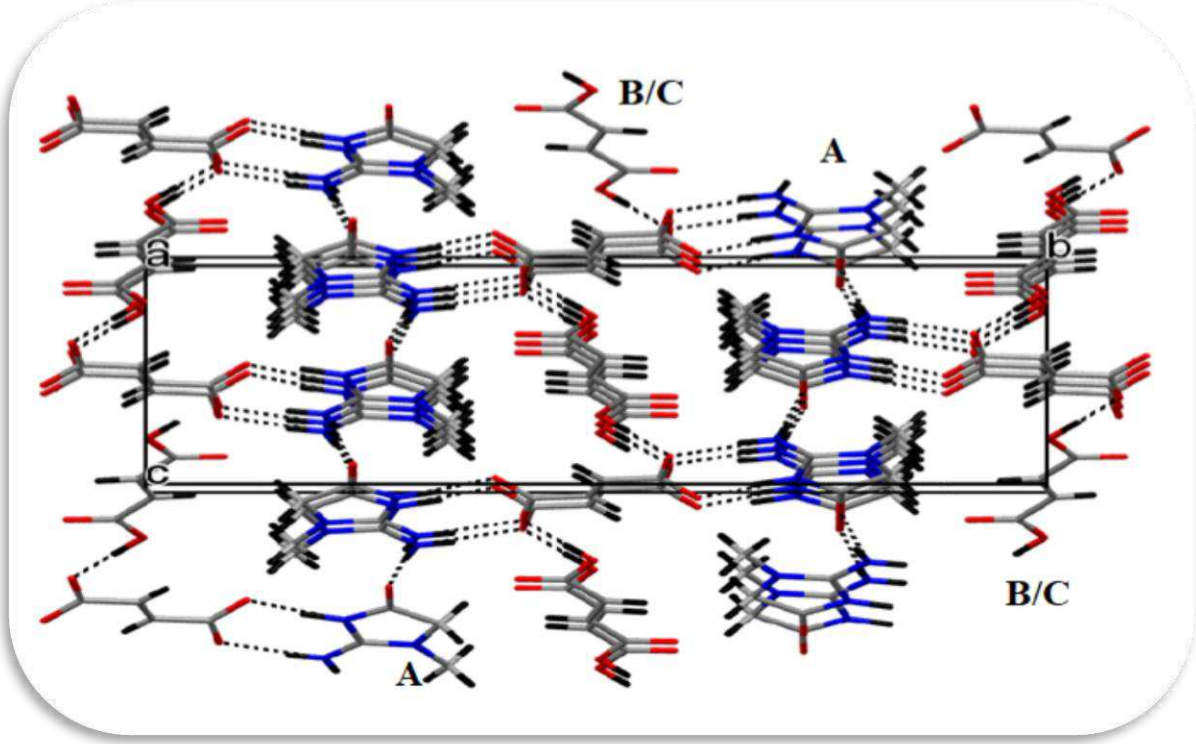
Discussion of Structure

- The asymmetric unit of the organic compound (**BCFF**).



Discussion of Structure

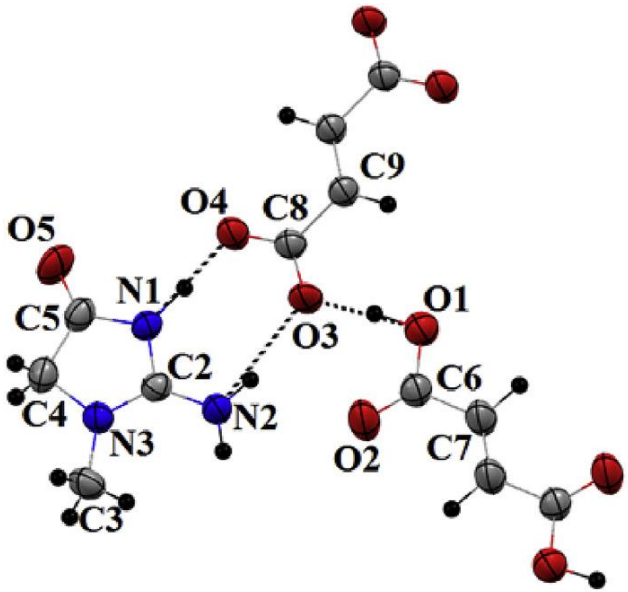
- Crystal stacking and the molecular arrangement of **(BCFF)**



Discussion of Structure

The characteristic hydrogen bonds of this compound are reported in the following Table :

D—H…A	D—H (Å)	H…A (Å)	D…A (Å)	D—H…A (°)
O1— H1… O3	0.96(2)	1.59(2)	2.555(4)	175(5)
N1— H1N… O3	0.98(2)	2.58(4)	3.207(3)	122(3)
N1— H1N… O4	0.98(2)	1.63(2)	2.605(3)	173(4)
N2—H2N… O3	0.92(1)	1.96(1)	2.863(4)	167(4)
N2—H3N... O5 (i)	0.92(1)	1.96(2)	2.863(4)	166(6)



Symmetry codes: (i) $x+1, -y+1/2, z+1/2$.

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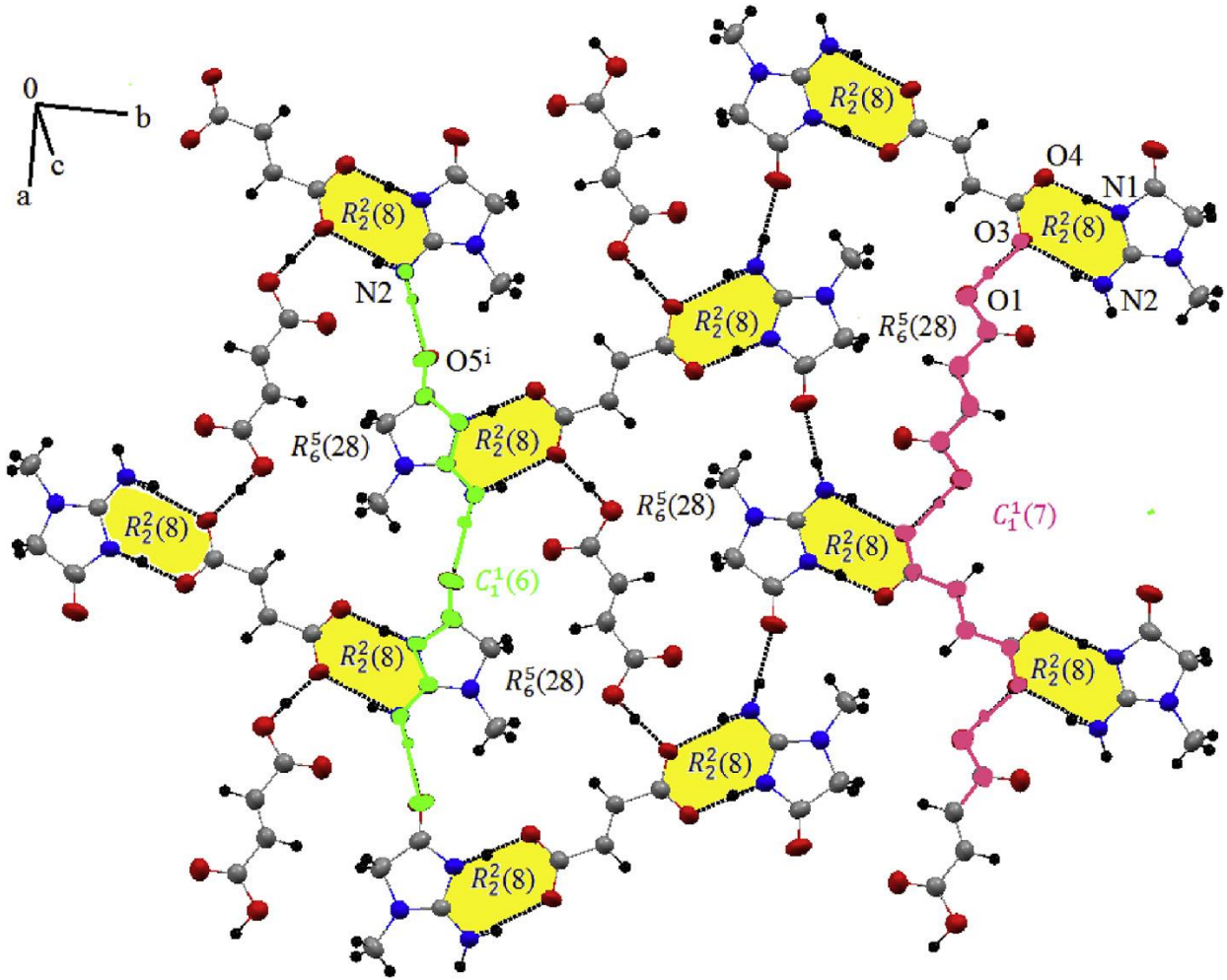
Discussion of Structure

- A fragment of the (BCFF) structure showing the graph set describing the hydrogen bonding.



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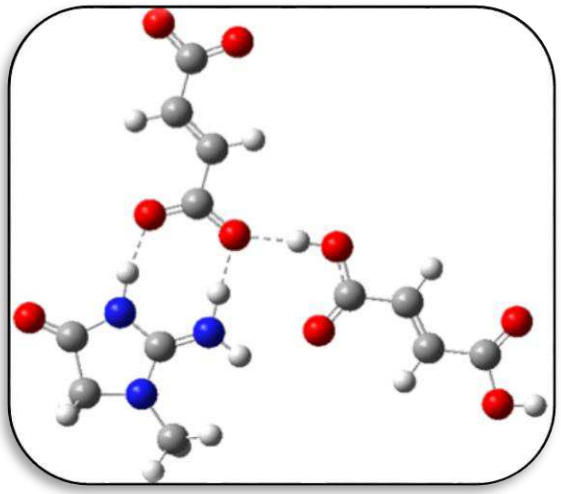
DFT quantum chemical calculations

➢Geometric parameters determined by X-rays and theoretical DFT calculations using B3LYP/6-311+G(d,p) for (**BCFF**) compound.

BCFF	Bond lengths Å Ray-X	Bond lengths Å DFT
Longueurs de liaison Å		
O4—C8	1.252(4)	1.249
O3—C8	1.256(4)	1.274
C9—C8	1.489(4)	1.451
C9—C9	1.301(7)	1.331
C9—H9	0.959(10)	1.081

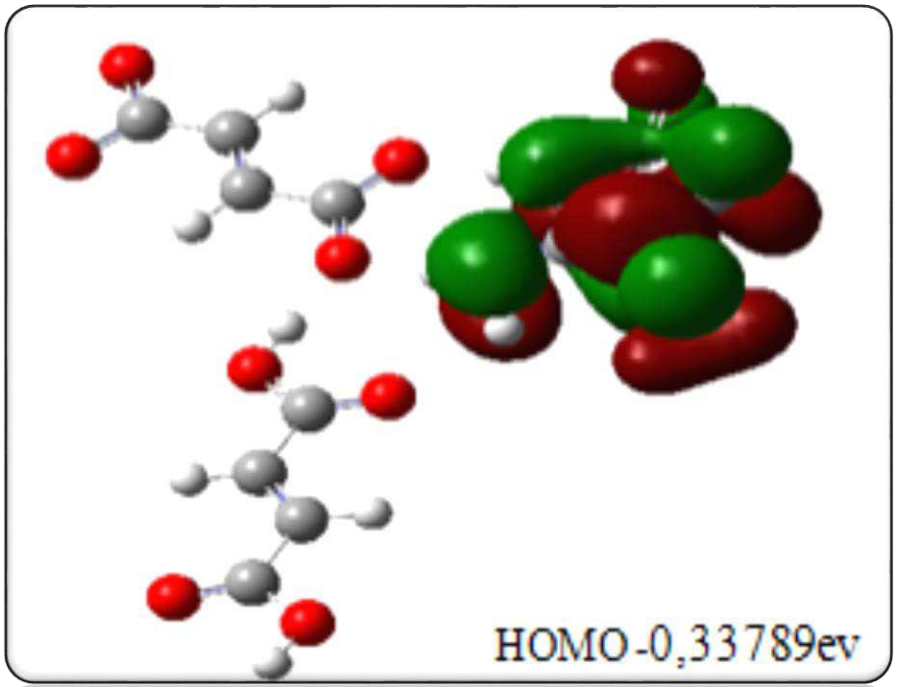
Bond angles (°)		
O4—C8—O3		125.31
C8—C9—C9	122.7(3)	121.86
C8—C9—H9	123.2(4)	117.14
C9—C9—H9	116(2)	120.78
C9—C8—O3	121(2)	123.21
C9—C8—O4	117.7(3)	120.25
O2—O6—O1	119.6(3)	125.51
C6—C7—C7	125.9(4)	123.26
C6—O1—H1	106(4)	113.49
C6—C7—H7	116(3)	117.38
C7—C7—H7	117(4)	120.89

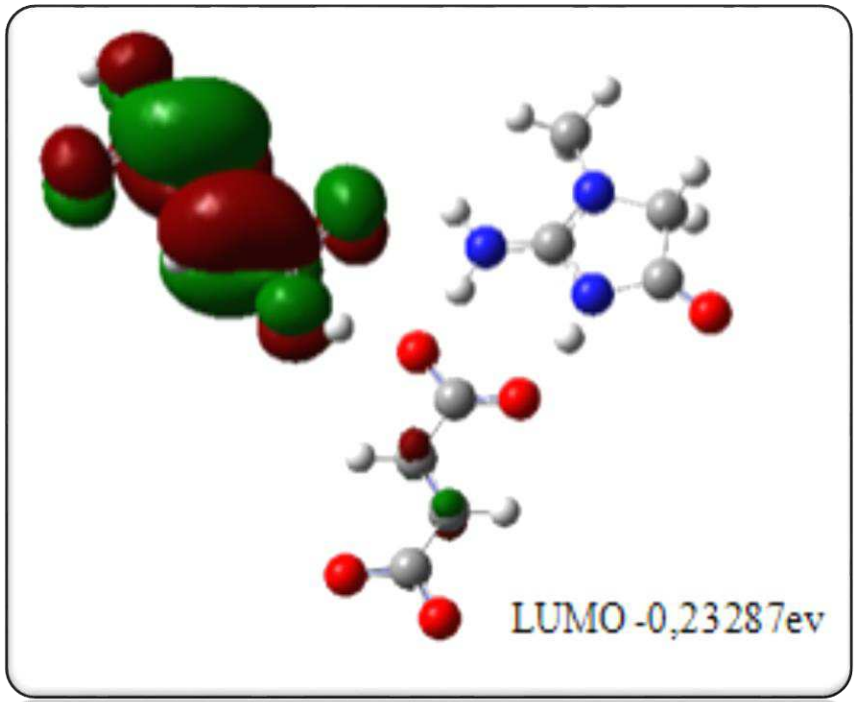
Torsion angles (°)		
O3—C8—C9—C9	-167.3(4)	-171.99
O4—C8—C9—C9	11.9(7)	11.01
O1—C6—C7—C7	-176.7(6)	-179.92
N2—C2—N3—C3	-1.0(6)	-0.27
N2—C2—N3—C4	77.91(3)	176.66
C2—N1—C5—O5	-179.3(4)	-179.69
N2—C2—N1—C5	-178.6(3)	-178.32
C3—N3—C4—C5	1.5(4)	-175.05



DFT quantum chemical calculations

➢Frontier molecular orbitals (HOMO and LUMO) of (**BCFF**).





$\Delta E_{\text{HOMO-LUMO gap}}$ (ev) =0,10502

Conclusion

Our work is more particularly interested in the protonation of creatinine, including a new compound with proton transfer, **Bis creatininium fumarate fumaric acid**, which has been synthesized and characterized mainly by X-ray diffraction techniques on single crystals, the diffraction data have been processed by direct methods using the WINGX program. The compound (**BCFF**) is very rich in strong hydrogen bonds of type **N – H… O** and **O – H… O.**

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Acknowledgments

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