Molecular properties studies of Choline chloride, Glucose and water-based NADES

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1. Introduction:

The present work is undertaken to elucidate the structural parameters and vibrational dynamics of Choline Chloride, Glucose and water based Natural Deep Eutectic solvent(NADES) mixture. The drug-likeness properties and bioactivity score of the liquids are studied to understand their bioactivity and pharmacokinetics.

2. Materials and Methods

2.1 Computational:

Density Functional Theory is used to carry out theoretical calculation by taking B3LYP/6311+G(d,p) as level of calculation. Gauss view 6.0 is used to draw Molecular structure. The Vibrational frequency assignment is done with the help of VEDA program and Gauss view 6.0 Molecular visualization software.

2.2 Experimental Method:

Glucose and Choline chloride are purchased from sigma Aldrich and used without purification. Glucose, Choline chloride and water are mixed at the ratio of 2:1:1 to form Natural Deep Eutectic Solvent (NADES). The Raman and SERS spectra of the liquid mixtures (Chcl-Glu-W) was recorded by Horiba Xplora1 Micro-Raman system with excitation source of 785nm.

Structure of Choline Chloride-Glucose NADES

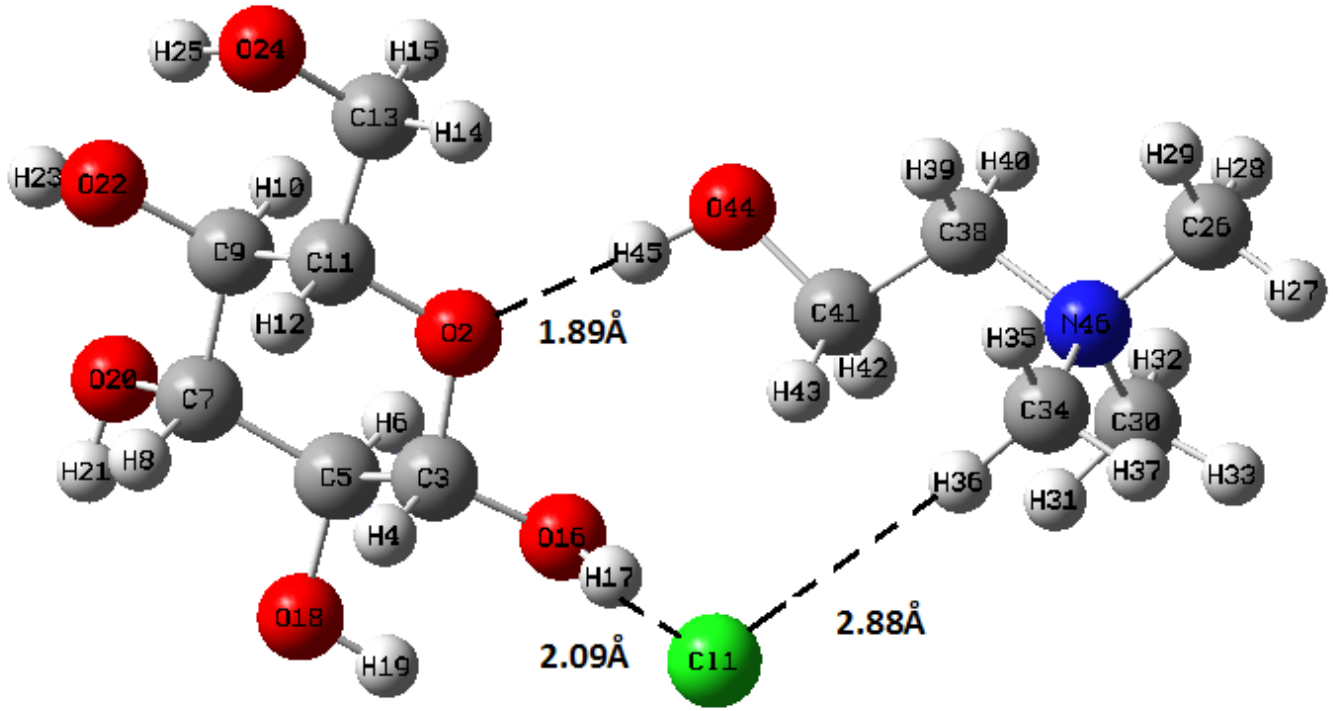
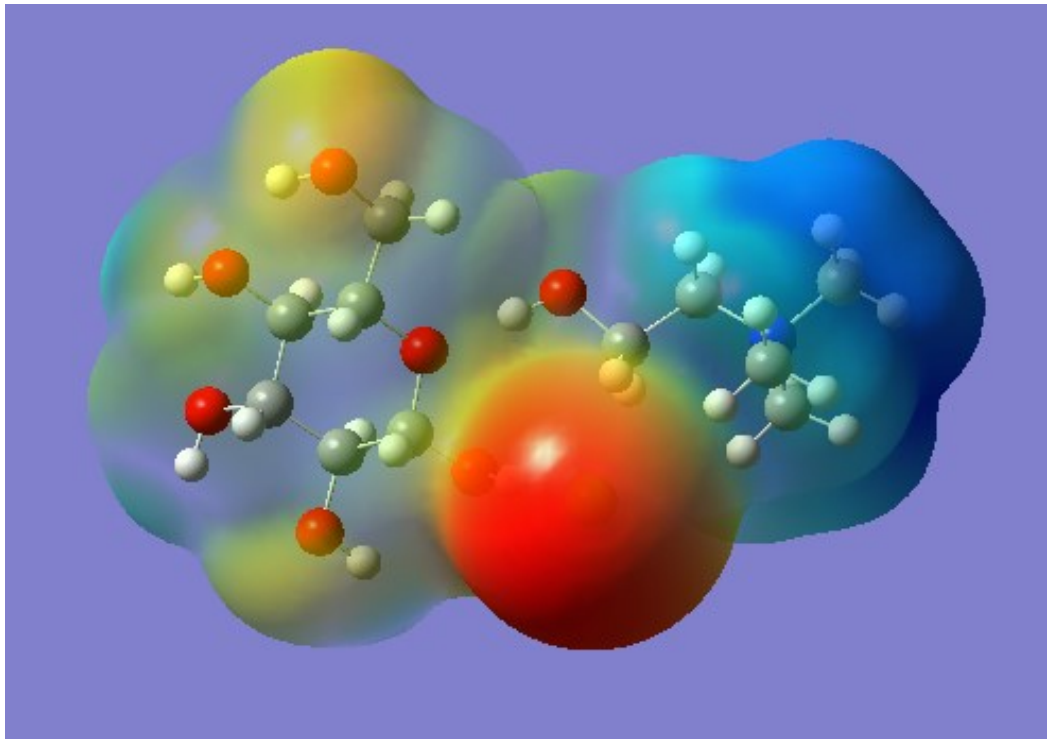


Fig.1



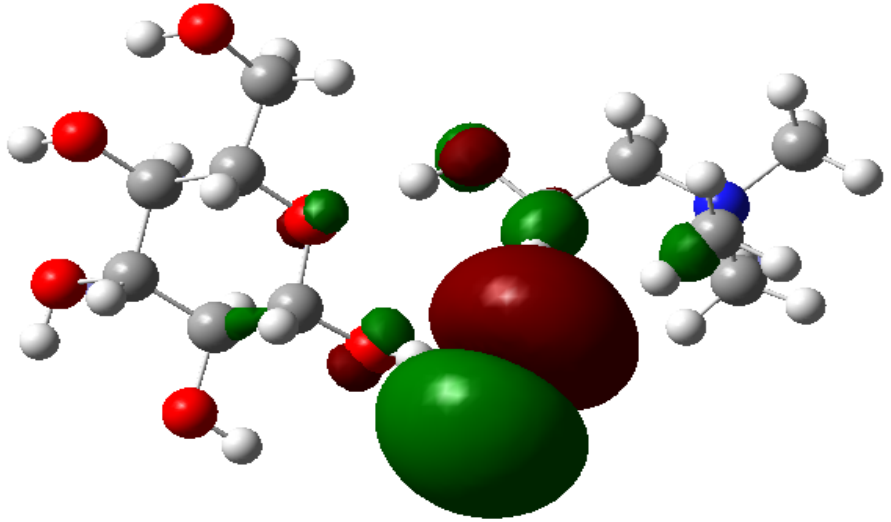
Molecular electrostatic potential surface of Choline Chloride and Glucose in medium water solvent

Table 1: Selected bond lengths and bond angles of Choline Chloride-Glucose at water solvent

Serial No	Bond	Bond Length
1	O_{16}-H_{17}	0.99
2	H_{17}-Cl_1	1.33
3	C_{30} -H_{31}	1.25
4	H_{31}-Cl_1	2.47
5	O_{44}-H_{45}	0.97
6	O_2-H_{45}	1.95
7	O_{16}-C_3	1.37
8	C_3-H_4	1.10
9	C_{11}-O_2	1.44
10	O_2-C_3	1.46
11	H_{36}-Cl_1	2.44

Bond	Bond Angle
C_3-O_{16}-H_{17}	110.40
O_2-C_3-O_{16}	112.94
C_{11}-O_2-C_3	103.63
O_{16}-C_3-H_4	111.44
H_{45}-O_{44}-C_{41}	105.64
O_{44}-C_{41}-C_{38}	104.98
O_{44}-C_{41}-H_{43}	111.47
H_{36}-C_{34}-H_{37}	109.16
H_{31}-C_{30}-H_{33}	109.34
H_{31}-C_{30}-N_{46}	108.77
O_2-C_3-H_4	107.77

Fig.2 :FMO of ChCl-Glucose at water solvent



HOMO-LUMO GAP=6.88 eV

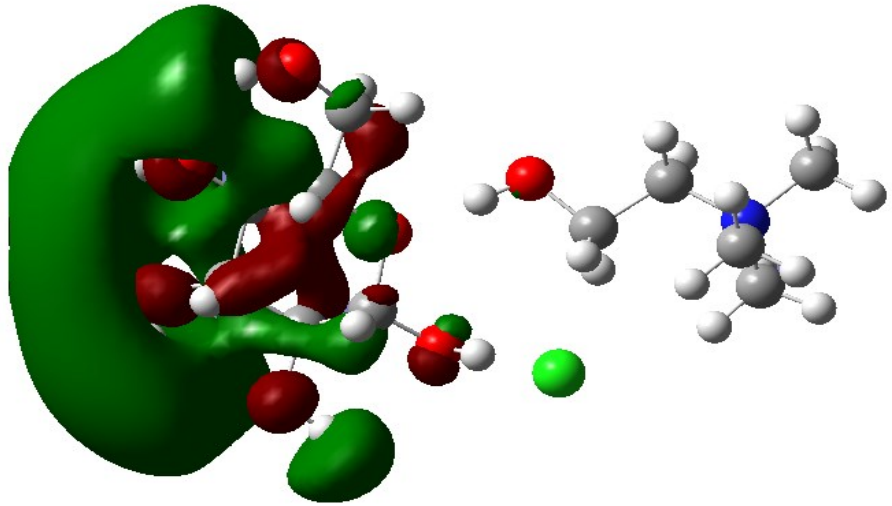
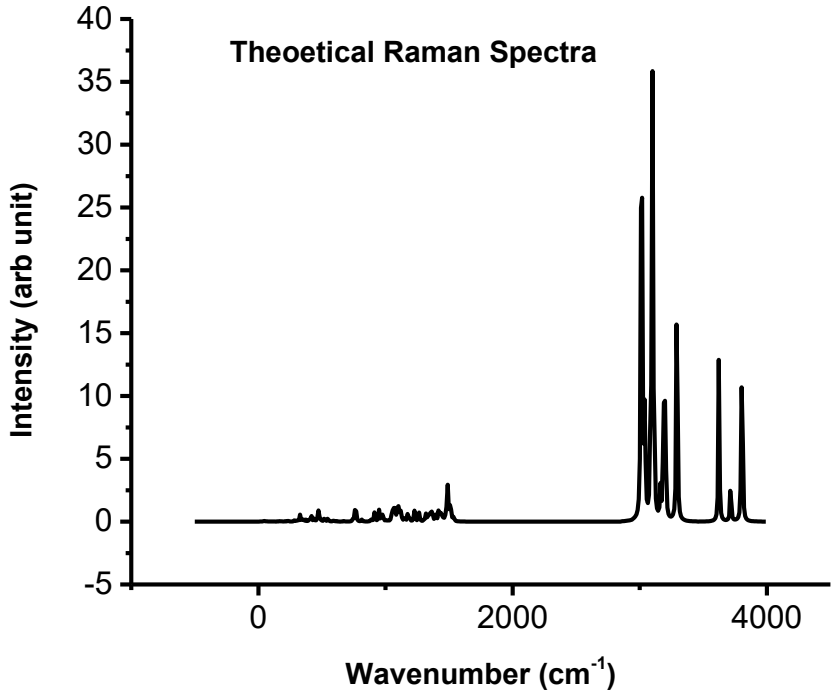


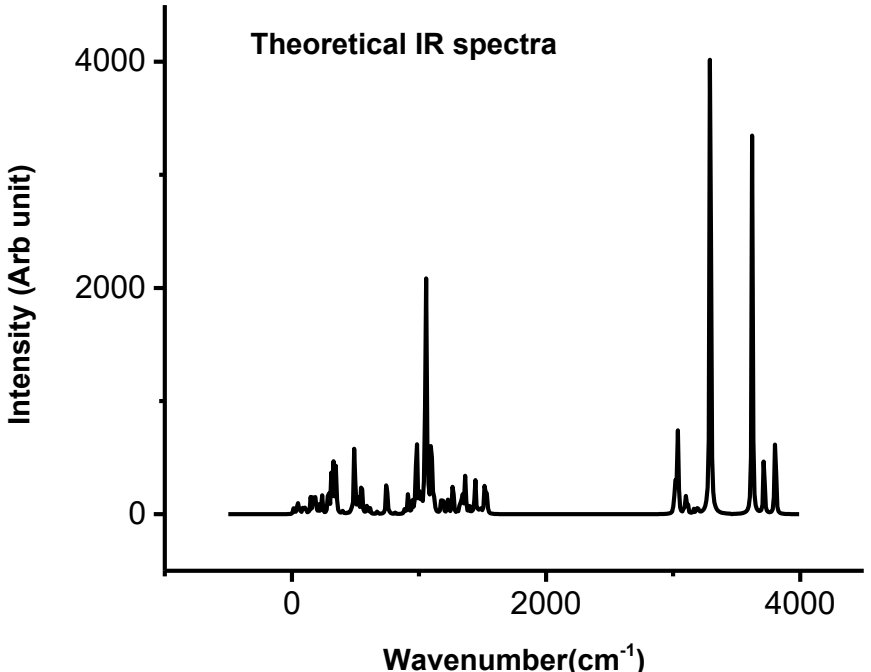
Table 2: NBO analysis of Choline chloride-glucose at water solvent

Donor	Acceptor	E^2 kcal/mol
$n_1(Cl_1)$	$\sigma^*(O_{16}- H_{17})$	25.16
$n_1(Cl_1)$	$\sigma^*(C_{34} -H_{36})$	2.17
$\sigma(O_2 - C_3)$	$\sigma^*(C_5 - O_{18})$	1.89
$\sigma(C_3 - C_5)$	$\sigma^*(C_7 - O_{20})$	2.92
$n_2(O_2)$	$\sigma^*(C_3 - C_5)$	5.34
$n_2(O_2)$	$\sigma^*(C_9 - C_{11})$	6.05
$n_2(O_{16})$	$\sigma^*(O_2 - C_3)$	18.35
$n_1(O_2)$	$\sigma^*(O_{44} - H_{45})$	11.24
$\sigma(O_{44}-H_{45})$	$\sigma^*(O_2-C_{11})$	0.09
$n_2(O_{44})$	$\sigma^*(C_{41} - H_{42})$	7.34

Table 3: Quantum chemical Parameters of Chcl-Glu-W

Parameters	Chcl-Glu-W
SCF energy (Hartree)	-1476.45
Total energy (thermal)(Kcal mol^{-1})	263.92
Zero point Vibrational energy (Kcal mol^{-1})	248.41
Dipole moment (Debye) μ	17.33
E_{LUMO}	-0.11 eV
E_{HOMO}	-6.99 eV
E_{HOMO}- E_{LUMO}	6.88 eV
Hardness(η)=1/2(E_{LUMO}- E_{HOMO})	3.44 eV
chemical potential(μ)=1/2(E_{HOMO}+E_{LUMO})	-3.50 eV
IE = -E_{HOMO}	6.99 eV
EA=-E_{LUMO}	0.11 eV
Global electro-philicity index(ω)=μ^2/2 η	1.78





Topological parameters of hydrogen bonds at the bond critical points of Choline Chloride and glucose at solvent water

Hydrogen Bond	ρ_{BCP}	$\nabla^2 \rho_{BCP}$	H_{BCP}	G (r)	V (r)
O2…H45-O44	0.00274	0.0805	-0.00014	0.0203	-0.0204
O16-H17…Cl1	0.0324	0.0658	-0.00234	0.0188	-0.0211
Cl1…H43-C41	0.00763	0.0230	0.00109	0.00465	-0.00356

Drug likeliness study parameters

TPSA (Å²)	Molecular weight (g/mol)	Milog P	Hydrogen bond donors (nOHNH))	Hydrogen bond acceptors (nON	Number of rotatable bonds	Lipinski's violation
133.85	319.78	-2.46	6	7	3	1

Conclusion:

1. The study gives information about the interacting mechanism of Choline Chloride, Glucose in water solvent using the DFT-IEFPCM model.
2. Charge transfer between the two molecules is observed in the complex.
3. The topological parameters of the Hydrogen bond indicate the non-covalent hydrogen bond taking place in the complex.
4. The biomolecular complex has the potential to be used as drug.

THANK YOU

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