MANSOURA JOURNAL OF CHEMISTRY
Official Journal of Faculty of Science, Mansoura University, Egypt
E-mail: scimag@mans.edu.eg ISSN: 2974-4938

Some quantum chemical calculations for succinic hydrazide and its complex with copper chloride salt

Mohamed M. El-Defraway, Esam A. Gomaa, Shereen. E. Salem, Noha. M. Mohamed
Chemistry Department, Faculty of Science, Mansoura University

Received: 7/4/2021
Accepted:25/4/2021

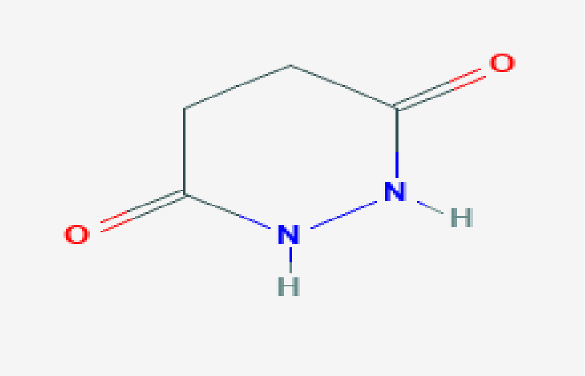
Abstract: The Gaussian 09 calculations set was applied for the calculation of vibrational modes, frequencies, force constant, normal moles and reduced mass. Vibrational analysis is carried out when the first derivatives of energy with respect to displacement of atoms is zero. In order to do that, the geometry used for vibrational analysis must be optimized while in other geometries were not valid. All the vibrations were done for succinic hydrazide and its complex with copper chloride salt. The calculated energy gap indicating better conduction of the complex than the succinic hydrazide ligand used. It was observed that the different theoretical data proved a little activity of the complex used.

keywords: MEP, Electron density, Energy gap.

1.Introduction

The Gaussian 09 calculations set was applied for the calculation of vibrational modes, frequencies, force constant, normal moles and reduced mass. Vibrational analysis is carried out when the first derivatives of energy with respect to displacement of atoms is zero. In order to do that, the geometry used for vibrational analysis must be optimized while in other geometries were not valid.

In general, the frequencies for relation and translation motions must be close to zero. The next step was to determine the moments and products of inertia for finding the matrix that diagonalized the moment of inertia. Once the vectors were known, the rest of normal modes were vibrated. So, we distinguished low frequency vibration modes from rotational and translational modes.



1-EXPERIMENTAL

Materials and Solvents

Copper chloride salt ($CuCl_2.2H_2O$) with Mol.Wt equal 170.48 g/mol, Succinic hydrazide and ethanol (EtOH) as analytical reagent grade material were used in this study and all from Merck Company.

Succinic hydrazide	
Formula	$C_4H_6N_2O_2$
Mol. Wt.	114.104 g/mol

Preparation of copper complex

A traditional method was used to prepare the copper complex by refluxing 1 mmol of $CuCl_2.2H_2O$ salt under investigation with 1 mmol of Succinic hydrazide using an ethanolic solution for 2-3 h close to the boiling point of the solvent. Then, the precipitate was filtered off, washed several times with absolute ethanol and dried in vacuum desiccators over anhydrous calcium chloride. Finally, the complex was characterized by using different techniques.

Computer programs

All tabulations and the manuscript were achieved using computer programs of the type Microsoft Office 2013. The molecular modeling and computational calculations were carried out by using DS Biovia material studio 2017, software material studio 07.0, Gaussian 09 and Docking Server software.

RESULTS AND DISCUSSION

Quantum chemical calculations for succinic hydrazide

Different steps were followed by Gaussion 09 program to perform the vibrational analysis which are estimation of mass weight by Hessian [1], determination of the principle axes of inertia, generate coordinates in the rotating and translating frame.

The other three steps were transformed the Hessain to the internal coordinates, calculation of the frequencies and calculation of the reduced mass, force constants and Cartesian displacements.

It was found that the frequencies for translations were almost close to zero. Using Gaussian 09, the vibrational modes with their frequencies and force constant were evaluate by applying basis set 6-3H G+ which includes CGs and Cartesian Gaussian functions as polarization factor to improve the properties of species line forming hydrogen bonds.

Basis sets of calculation used DFT B3 lyP/6-311G method [2]. The molecules structures with bond lengths for succinic hydrazide was given in **Fig(1)** as described by Mullikan charges, **Fig(2)**. The Mullikan charges were given separately in **Table(1)** for the different atoms in the succinic hydrazide ligand. Explaining the calculation type, calculation method B3LYP, basis set 6-311-G(D,P) and spin singlet the electronic energy was -416.1066 HZ and small dipole moment 0.42636 Debye, **Table(2)**.

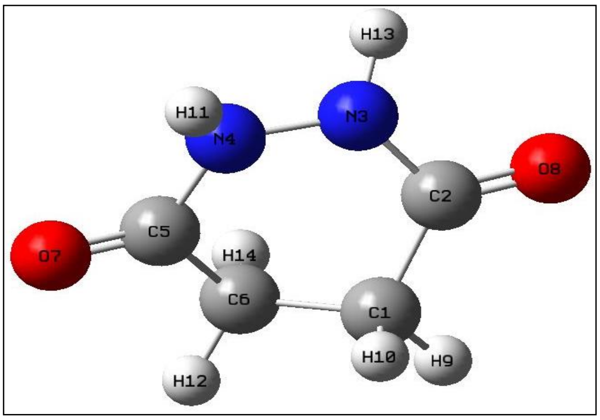


Fig.1: Optimized structure for succinic hydrazide ligand.

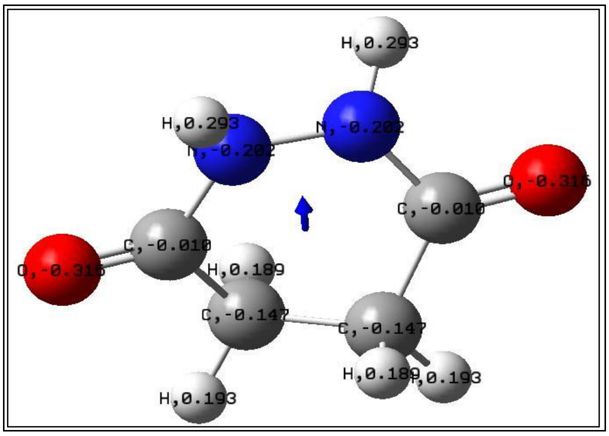


Fig.2: Mullikan charges for succinic hydrazide ligand.

Table (1): Mullikan charges for succinic hydrazide ligand.

C	-0.146983
C	-0.009806
N	-0.201775
N	-0.201775
C	-0.009806
C	-0.146983
O	-0.316286
O	-0.316286
H	0.192752
H	0.188928
H	0.293170
H	0.192752
H	0.293170
H	0.188928

Table(2): Succinic hydrazide checkout (Gaussian summary data).

Succinic hydrazide (Opt step 9of 9)		
File type	Checkout	Units
Calculation Type	FOPT	
Calculation Method	RB3LYP	
Basis Set	6-311+G(D,P)	
Charge	0	
Spin	Singlet	
Solvation	None	
Electronic Energy	-416.10661	Hartz
RMS Gradient Norm	0.000095	Hartz/Bohr
Dipole Moment	0.426632	Debye

The values indicated that succinic hydrazide is inactive ligand having stable electronic energy and low dipole moment. Quantum chemical parameters for the ligand as the energy of the highest occupied molecular orbitals for succinic hydrazide ligand (E_{Homo}) was -0.2638 ev and the energy of the lowest unoccupied molecules orbitals (E_{lumo}) was about -0.3160 ev.

Succinic hydrazide had small gap energy (E_{gap}) with value -0.2322e.v so; it can be used as a semiconductor in solid state. The shapes of molecular orbitals for succinic hydrazide [Homo, Lumo and MEP] were shown in **Figs(3-5)**. In **Fig(6)**, the electronic lowed of succinic hydrazide was small in MEP due to absence of the used color so, it indicated great electron density. The frequencies of succinic hydrazide ligand were theoretically evaluated from the theoretical IR, **Fig(7)**. Also, the dipole moment field (independent basis in Debye) was evaluated from frequency data and multiple dipole moments estimated.

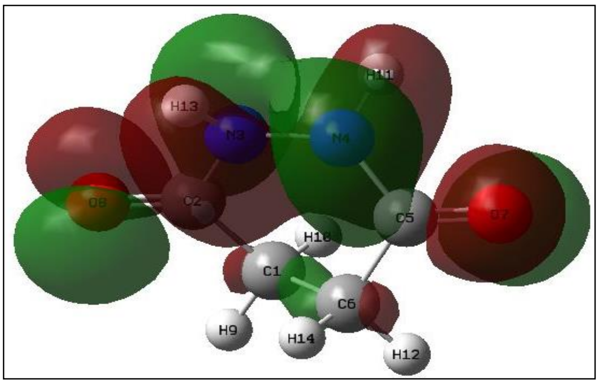


Fig.3: Homo orbital of succinic hydrazide ligand.

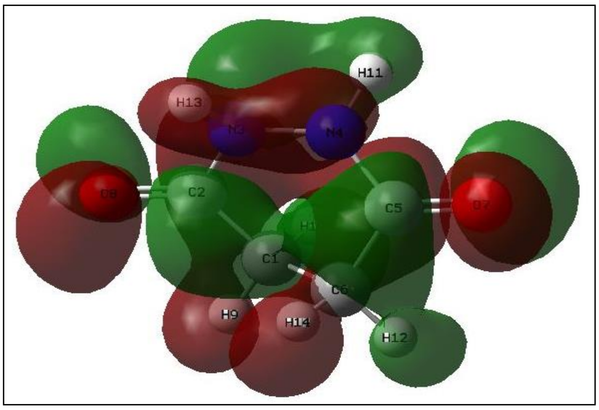


Fig.4: LOMO orbital of succinic hydrazide ligand.

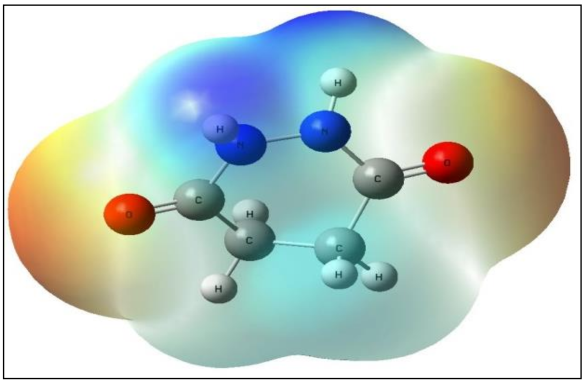


Fig.5: MEP for succinic hydrazide ligand.

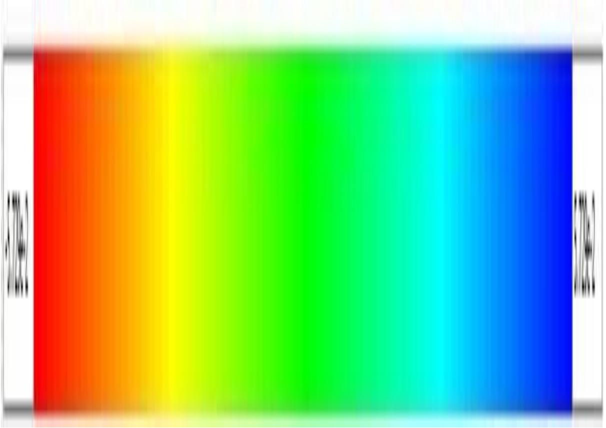


Fig.6: MEP (electron density indication) for succinic hydrazide ligand.

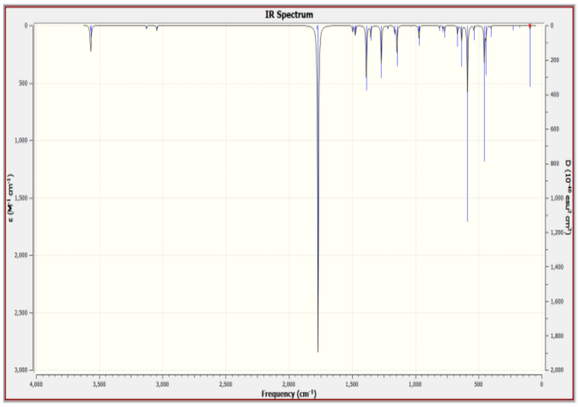


Fig.7: Theoretical IR for succinic hydrazide ligand.

The dipole moment and multiple pole moment (qudrupole), tracless quadrupole and hexasole moments for succinic hydrazide were given in **Tables(3-7)** with small values indicating little activity of succinic hydrazide. The different thermal energies were also calculated in **Table(8)** cited for succinic hydrazide ligand and it was found that the same of electronic + zero point energies, sum of electronic + thermal energies, sum of electronic + thermal enthalpies, sum of electronic + thermal free energies were the same indicating difference in vibrational motions.

Table(3): Dipole moment (field-independent basis, Debye) for succinic hydrazide ligand.

X= 0.0000	Y= 0.0000	Z= 0.4266	Tot= 0.4266

Table(4): Quadrupole moment of succinic hydrazide ligand.

Quadrupole moment (field-independent basis, Debye-Ang)		
XX= -44.8400	YY= -70.1343	ZZ= -38.1893
XY= -2.5536	XZ= 0.0000	YZ= 0.0000

Table(5): Tracless Quadrupole moment for succinic hydrazide ligand.

Traceless Quadrupole moment (field-independent basis, Debye-Ang):		
XX= 6.2145	YY= -19.0798	ZZ= 12.8652
XY= -2.5536	XZ= 0.0000	YZ= 0.0000

Table(6): Octapole moment for succinic hydrazide ligand.

Octapole moment (field-independent basis, Debye-Ang2):**				
XXX= .0000	YYY= 0.0000	ZZZ= -12.5893	XYY= 0.0000	XXY= 0.0000
XXZ= -2.0445	XZZ= 0.0000	YZZ= 0.0000	YYZ= -1.3711	XYZ= -4.5264

Table(7): Hexadecapole moment for succinic hydrazide ligand.

Hexadecapole moment (field-independent basis, Debye-Ang3):**					
XXXX= 80.3580	YYYY= 959.7769	ZZZZ= 258.8460	XXXY= 28.4929	XXXZ= 0.0000	YYYX= 59.2144
YYYZ= 0.0000	ZZZX= 0.0000	ZZZY= 0.0000	XXYY= 140.6452	XXZZ= 59.5365	YYZZ=164.3859
XXYZ= 0.0000	YYXZ= 0.0000	ZZXY= 0.2166	N-N= 3.761504228607D+02 E-		
N=-1.725685959267D+03			KE= 4.145607858894D+02		

Table(8): Different energy for succinic hydrazide ligand.

Zero-point correction= (Hartree/Particle)	0.108797
Thermal correction to Energy=	0.115727
Thermal correction to Enthalpy=	0.116671
Thermal correction to Gibbs Free Energy=	0.078240
Sum of electronic and zero-point Energies=	-415.997864
Sum of electronic and thermal Energies=	-415.990934
Sum of electronic and thermal Enthalpies=	-415.989990
Sum of electronic and thermal Free Energies=	-416.028421

The translation E (thermal), CV (heat capacity at constant volume) and entropies (S) for the succinic hydrazide ligand were evaluated in **Table(9)**.

The partition function (Q values) for the succinic hydrazide ligand gave the vibration parameters for the different bonds with zero electronic entropy, slow translational and relational Q values. The Q values for vib (Bot) for all atoms from 1 to 9 were very great indicated that the vibration modes for succinic hydrazide ligand had heavy density function (DFT calculation), **Table(10)**.

Table (9): The translation energy ($E_{thermal}$), heat capacity at constant volume (CV) and entropies (S) for succinic hydrazide ligand.

	E(Thermal)[KCal/Mol]	**CV**[Cal/MolKelvin]	**S**[Cal/Mol-Kelvin]
Total	72.620	26.026	80.885
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.110
Rotational	0.889	2.981	26.497
Vibrational	70.842	20.065	14.278
Vibration1	0.602	1.954	3.587
Vibration 2	0.628	1.870	2.357
Vibration3	0.651	1.797	1.888
Vibration4	0.768	1.465	0.954
Vibration 5	0.788	1.414	0.872
Vibration 6	0.802	1.378	0.820
Vibration 7	0.813	1.350	0.781
Vibration8	0.894	1.165	0.568
Vibration 9	0.945	1.057	0.471

2. Quantum chemical calculations for copper complex.

The molecules structures with bond lengths for copper complex was given in **Fig(8)** and described by Mullikan charges, **Fig(9)**.

Mullikan charges are given in **Table(12)** for the 19 atoms of the complex. As shown in **Table (13)** in the checkout file of the discussed complex, the complex is very stable with electronic energy equal -2209.00106 HZ that is hard to dissolve in aqueous solvents. The dipole moment is about 5.4984 Debye which favorites high activity and dissolution in nonpolar solvents.

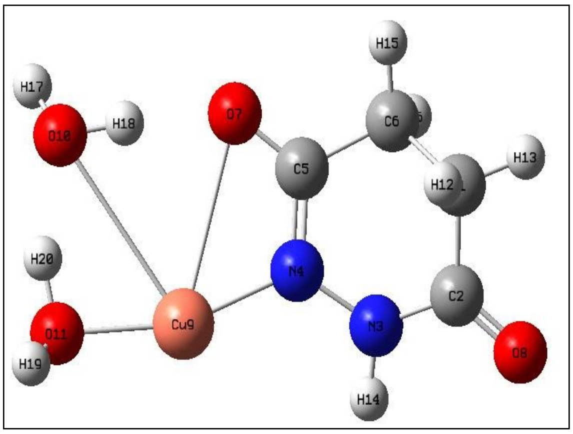


Fig.8: Optimizied structure for copper complex.

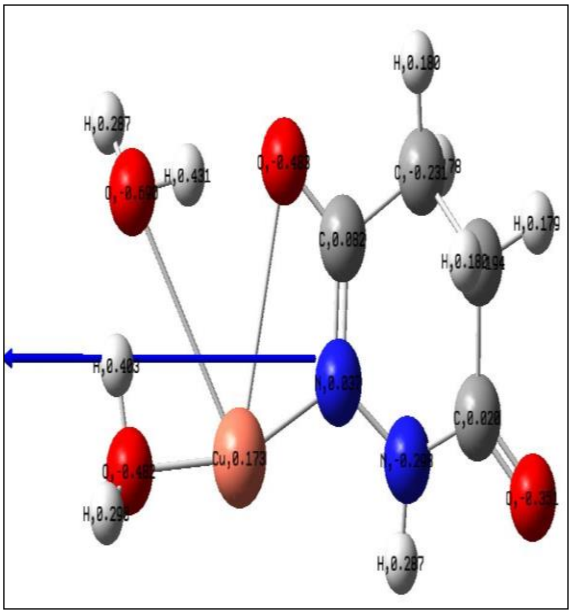


Fig.9: Mullikan charges for copper complex.

small activity of this ligand in liquid state media. The molecular electrostatic potential (MEP), **Fig (6)** was used to predict the electrophilic and nucleophilic sides [5]. The brown color was refered to electrophilic area for medium electron density [6]. The greenish blue and blue colors pointed to the nucleophilic region for attack and poor in electrons.

Table (10): The partition function values (Q) for the succinic hydrazide ligand.

	Q	**Log10(Q)**	**Ln(Q)**
Total Bot	0.102882D-35	-5.987662	-2.864653
Total V=0	0.113593D+15	14.055350	32.363640
Vib (Bot)	0.155897D-48	48.807162	-12.382644
Vib (Bot)	10.219879D+01	0.342184	0.787909
Vib (Bot)	2 0.113403D+01	0.054623	0.125775
Vib (Bot)	3 0.861243D+00	0.064875	0.149379
Vib (Bot)	4 0.442090D+00	.354489	-.816241
Vib (Bot)	5 0.410386D+00	-386808	0.890657
Vib (Bot)	6 0.390414D+00	0.408475	0.940549
Vib (Bot)	7 0.375383D+00	.425526	0.979810
Vib (Bot)	8 0.294559D+00	.530827	1.222275
Vib (Bot)	9 0.257071D+00	-589948	-.358404
Vib (V=0)	0.172127D+02	1.235849	2.845649
Vib (V=0)	1 0.275493D+01	0.440110	1.013391
Vib (V=0)	2 0.173936D+01	0.240390	0.553518
Vib (V=0)	3 0.149586D+01	0.174891	0.402702
Vib (V=0)	4 0.116742D+01	0.067226	0.154793
Vib (V=0)	5 0.114685D+01	0.059507	0.137020
Vib (V=0)	6 0.113437D+01	0.054754	0.126076
Vib (V=0)	7 0.112523D+01	0.051241	0.117987
Vib (V=0)	8 0.108031D+01	0.033550	0.077252
Vib (V=0)	9 0.106221D+01	0.026212	0.060356
Electronic	0.100000D+01	0.000000	0.000000
Ranslational	0.478694D+08	7.680058	17.683986
Rotational	0.137862D+06	5.139443	11.834005

The frontier energies of (E_{Homo}, E_{lumo}) which obtained by DFT were used to calculate some quantum chemistry parameters like band gap (E_{gap}), Global hardness (MG), global softness (SG), global electrophilicity index (W), electro negativity (X) and chemical

Table (11): Estimation of quantum parameters like Global hardness (η_G), global softness (S_G), global electrophilicity index ω, electronegativity (χ) and chemical potential (μ) from energy band gap (E_{HOMO}- E_{LUMO}) for succinic hydrazide ligand.

σ(e)	**ω(e)**	**S_G (e^1)**	**η_G (eV)**	**μ(e)**	**χ (V)**	**E_{LUMO} - E_{HOMO} (e)**	**E_{LUMO} (e)**	**E_{HOMO} (e)**
8.6184	0.1089	0.0580	0.1160	0.1476	0.1476	0.2320	.0316	0.2636

potential (M) as shown in **Table(11)** [3,4].

$$E_{gab} = E_{HOMO} - E_{LUMO} \quad (1)$$

$$\eta\text{-} = 0.5\ (E_{LUMO} - E_{HOMO}) \quad (2)$$

$$\sigma = 1/\eta\text{-} \quad (3)$$

$$\mu = -\chi = 0.5\ (E_{LUMO} + E_{HOMO}) \quad (4)$$

$$\chi = 0.5\ (E_{LUMO} + E_{HOMO}) \quad (5)$$

$$\omega = \mu 2/2 \quad (6)$$

All the calculated values for succinic hydrazide ligand were given and proved the

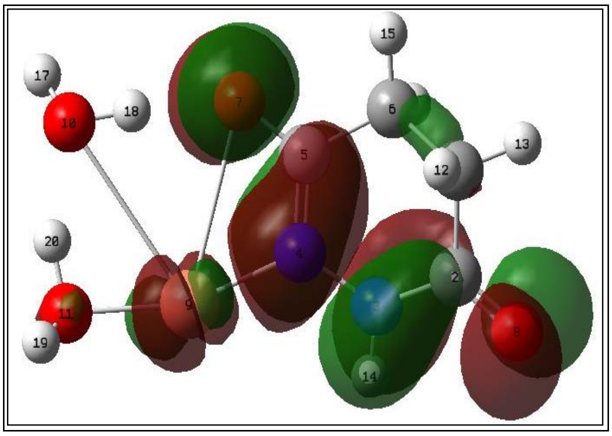


Fig.10: HOMO orbital for copper complex

Table(12): Mullikan charges for copper complex.

C	-0.194225
C	0.020073
N	-0.297885
N	0.037375
C	0.082374
C	-0.231057
O	-0.483095
O	-0.350503
Cu	0.172559
O	-0.690093
O	-0.482286
H	0.180147
H	0.179402
H	0.287476
H	0.180077
H	0.178288
H	0.286810
H	0.431335
H	0.289775

Table(13): Summary Gaussian checkout data for copper complex.

Copper complex (Opt step 99of 99)		
File type	Checkout	
Calculation Type	FOPT	
Calculation Method	RB3LYP	
Basis Set	6-311+G(D,P)	
Charge	0	
Spin	Singlet	
Solvation	None	
Electronic Energy	-2209.001006	HZ
RMS Gradient Norm	0.000029	HZ/Bohr
Dipole Moment	5.498470	Debye

The shapes of molecular orbitals for copper complex [Homo, Lumo and MEP] were shown in **Figs(10-12)**. Three zones were observed in **Fig.13**, the brown color belongs to electrophilic area and the other two areas greenish blue and blue belongs to the nucleophilic region. It was observed that the nucleophilic region was greater than the electrophilic region.

The IR evaluated theoretically was given in

Fig.14 giving vibrational which analyzed by using Gaussian 09 program.

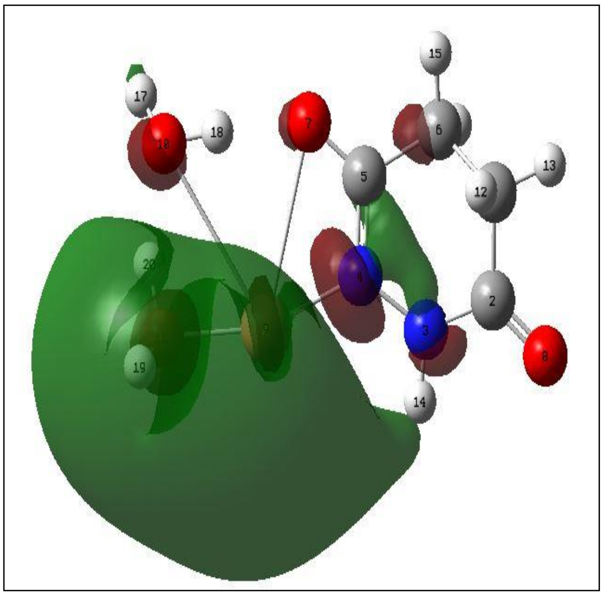


Fig.11: LUMO orbital for copper complex.

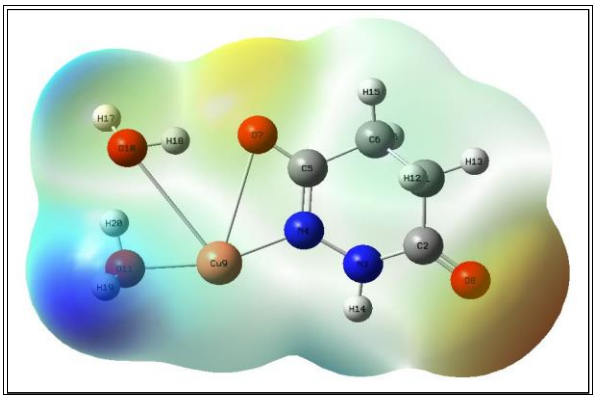


Fig.12: MEP for copper complex.

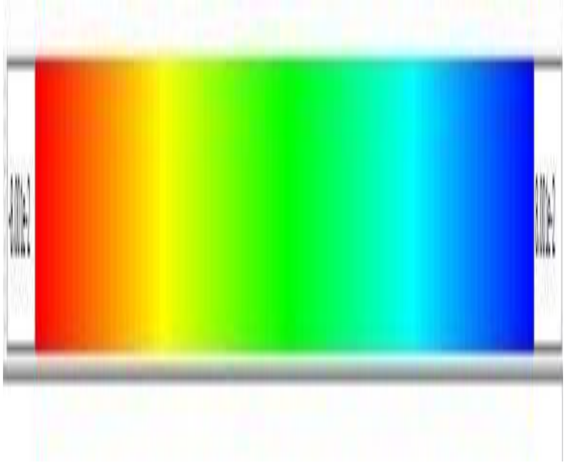


Fig.13: MEP (electron density indication) for copper complex.

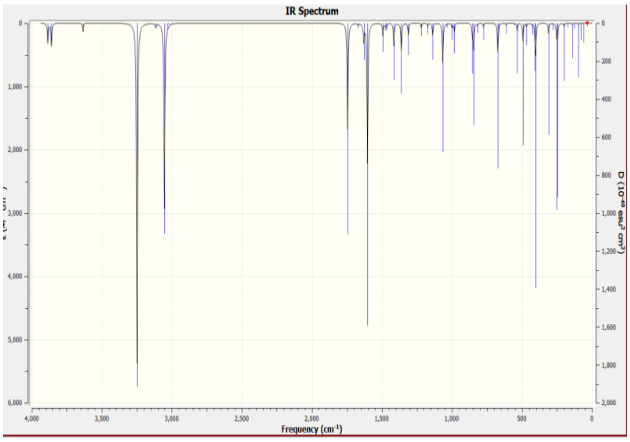


Fig.14: Theoretical IR for copper complex.

Dipole and multipole moment's data were extracted for the discussed complex from the Gaussian 09 calculations, **Tables(14-18)**. It was observed high dipole moment, total 5.4980 Debye. Other multi pole moments like quadrupole more tracless quadrupole moment, octopole moment and Hexadecapole moment were given with very high values for the complex than that of the ligand indicating very high activity of the complex in solvation studies.

Table(14): Dipole moment (field-independent basis, Debye) for copper complex.

X= 5.4903	Y= 0.0029	Z= 0.2917	Tot= 5.4980

Table (15): Quadrupole moment for copper complex.

Quadrupole moment (field-independent basis, Debye-Ang		
XX=76.7517	YY=70.8148	ZZ=70.4369
XY=13.1145	XZ= 1.6672	YZ=3.6749

Table (16): Tracleless Quadrupole moment for copper complex.

Traceless Quadrupole moment (field-independent basis, Debye-Ang		
XX= 4.0839	YY= 1.8530	ZZ=2.2309
XY= 13.1145	XZ= 1.6672	YZ=3.6749

Table (17): Octapole moment for copper complex.

Octapole moment (field-independent basis, Debye-Ang2**			
XXX=204.4318	YYY=33.8928	ZZZ= 2.0693	XYY=41.6009
XXY=42.5162	XXZ= 6.7461	XZZ= 23.6586	YZZ= 11.5699
YYZ= -4.8672	XYZ=20.8181		

Table (18): Hexadecapole moment for copper complex.

Hexadecapole moment (field-independent basis, Debye-Ang3**			
XXXX=-590.2542	YYYY=- 02.2852	ZZZZ= -112.1944	XXXY= 196.4366
XXXZ=-33.3289	YYYX= 20.0748	YYYZ= -11.2606	ZZZX= -6.2154
ZZZY=-5.5366	XXYY=-97.0848	XXZZ= -399.0757	YYZZ= -134.6382
XXYZ=-66.5962	YYXZ= 1.3744	ZZXY= 17.7624	N-N= 9.300614153774D+02
E-N=-7.121284227781D+03		KE= 2.205649586790D+03	

The different thermal analysis data for the Cu-succinic hydrazide complex were given in **Table(19)** and showed that the sum of electronic zero point energies, sum of electronic + thermal energies sum of electronic + thermal enthalpies and sum of electrostatic + thermal free energies have all equal values indicating the only difference in vibrational modes for the complex studied.

Table(19): Different energies for copper complex.

Zero-point correction=	0.148290 (Hartree/Particle)
Thermal correction to Energy=	0.161602
Thermal correction to Enthalpy=	0.162546
Thermal correction to Gibbs Free Energy=	0.107504
Sum of electronic and zero-point Energies=	-2208.852716
Sum of electronic and thermal Energies=	-2208.839404
Sum of electronic and thermal Enthalpies=	-2208.838460
Sum of electronic and thermal Free Energies=	-2208.893502

The translation E (thermal), CV (heat capacity at constant volume) and entropies (S) for the complex discussed had small values only the vibrational values. E(thermal), CV and S for the different atoms were evaluated having great values indicating the activity of copper complex, **Table (20)**.

The molecular partition function (Q) values for copper complex were extracted from the output file in thermal analysis data, it was observed from the data formed in **Table (21)** that the electronic translation and rotational Q values are small values in comparing to the individual vibrational Q values for the different atoms and bonds in the vibrational modes [7-9].

Table (20): The translation energy ($E_{thermal}$), heat capacity at constant volume (CV) and entropies(S) for copper complex.

	E(Thermal) [KCal/Mol]	**CV**[Cal/Mol-Kelvin]	**S**[Cal/Mol-Kelvin]
Total	101.407	47.041	115.846
Electronic	0.000	0.000	0.000
Translatinal	0.889	2.981	41.958
Rotational	0.889	2.981	31.347
Vibrational	99.629	41.079	42.541
Vibration1	0.594	1.982	5.477
Vibration2	0.597	1.973	4.445
Vibration3	0.600	1.962	3.878
Vibration4	0.603	1.951	3.502
Vibration5	0.611	1.927	3.006
Vibration 6	0.615	1.913	2.804
Vibration7	0.627	1.875	2.398
Vibration 8	0.637	1.841	2.141
Vibration9	0.660	1.771	1.765
Vibration10	0.664	1.758	1.713
Vibration11	0.680	1.711	1.536
Vibration12	0.699	1.654	1.360
Vibration 13	0.768	1.465	0.954
Vibration14	0.774	1.450	0.929
Vibration15	0.789	1.411	0.868
Vibration16	0.825	1.322	0.745
Vibration17	0.832	1.304	0.722
Vibration18	0.849	1.265	0.675
Vibration19	0.889	1.174	0.577
Vibration 20	0.911	1.127	0.532
Vibration21	0.971	1.006	0.429

Table (21): The molecular partition function values (Q) for copper complex.

	Q	**Log10(Q)**	**Ln(Q)**
Total Bot	0.356223D-49	-9.448278	-13.858868
Total V=0	0.575736D+19	18.760223	43.197010
Vib (Bot)	0.185550D-63	-3.731539	-46.747292
Vib (Bot)	1 0.577437D+01	0.761505	1.753430
Vib (Bot)	2 0.342114D+01	0.534171	1.229973
Vib (Bot)	3 0.255660D+01	0.407663	0.938678
Vib (Bot)	4 0.210436D+01	0.323119	0.744009
Vib (Bot)	5 0.161924D+01	0.209312	0.481959
Vib (Bot)	6 0.145274D+01	0.162189	0.373454
Vib (Bot)	7 0.116064D+01	0.064696	0.148968
Vib (Bot)	8 0.100146D+01	0.000634	0.001460
Vib (Bot)	9 0.797981D+00	-0.098008	-0.225671
Vib (Bot)	10 0.771869D+00	-0.112456	-0.258940
Vib (Bot)	11 0.687762D+00	-0.162562	-0.374313
Vib (Bot)	12 0.608860D+00	-0.215483	-0.496167
Vib (Bot)	13 0.442218D+00	-0.354364	-0.815953
Vib (Bot)	14 0.432640D+00	-0.363873	-0.837849
Vib (Bot)	15 0.408651D+00	-0.388647	-0.894893
Vib (Bot)	160.361693D+00	-0.441660	-1.016960
Vib (Bot)	17 0.352986D+00	-0.452243	-1.041327
Vib (Bot)	18 0.335000D+00	-0.474955	-1.093623
Vib (Bot)	19 0.298050D+00	-0.525711	-1.210495
Vib (Bot)	20 0.280699D+00	-0.551759	-1.270472
Vib (Bot)	21 0.240928D+00	-0.618112	-1.423255
Vib (V=0)	0.299890D+05	4.476962	10.308587
Vib (V=0)	1 0.629598D+01	0.799063	1.839911
Vib (V=0)	2 0.395748D+01	0.597419	1.375608
Vib (V=0)	3 0.310503D+01	0.492066	1.133024
Vib (V=0)	4 0.266294D+01	0.425361	0.979431
Vib (V=0)	5 0.219468D+01	0.341372	0.786038
Vib (V=0)	6 0.203638D+01	0.308859	0.711174
Vib (V=0)	7 0.176375D+01	0.246438	0.567445
Vib (V=0)	8 0.161934D+01	0.209338	0.482020
Vib (V=0)	9 0.144169D+01	0.158871	0.365814
Vib (V=0)	10 0.141966D+01	0.152186	0.350420
Vib (V=0)	11 0.135030D+01	0.130431	0.300329
Vib (V=0)	12 0.128785D+01	0.109866	0.252975
Vib (V=0)	13 0.116750D+01	0.067257	0.154865
Vib (V=0)	14 0.116119D+01	0.064905	0.149449
Vib (V=0)	15 0.114575D+01	0.059091	0.136061
Vib (V=0)	16 0.111711D+01	0.048095	0.110743
Vib (V=0)	17 0.111204D+01	0.046122	0.106201
Vib (V=0)	18 0.110185D+01	0.042123	0.096992
Vib (V=0)	19 0.108209D+01	0.034265	0.078898
Vib (V=0)	20 0.107340D+01	0.030763	0.070835
Vib (V=0)	21 0.105502D+01	0.023260	0.053559
Electronic	0.100000D+01	0.000000	0.000000
Translatioal	0.121315D+09	8.083915	18.613903
Rotational	0.158251D+07	6.199345	14.274520

Quantum chemical parameters for the complex density function theory (DFT) calculation were done from the properities of the optimized complex and evaluating E_{Homo} which equal -0.2105 ev and E_{lumo} equal -0.05061 ev, **Table(22)**

The first calculation is the energy gap (E_{gap}) [E_{Homo}-E_{lumo}] equal 0.16144 ev indicating better conduction of the complex than the succinic hydrazide ligand used. The other parameters for copper complex like global hardness (MG), global softness (SG), global electrophilicity index (W), electro negativity (X) and chemical potential (M) values were greater than that of the ligand values. All calculated values proved a little activity of the complex used.

Table (22): Estimation of quantum parameters like Global hardness (η_G), global softness (S_G), global electrophilicity index ω, electronegativity (χ) and chemical potential (μ) from energy band gap (E_{HOMO}- E_{LUMO}) for copper complex.

σ(e)	**ω(eV)**	**S_G (e^{-1})**	**η_G (eV**	**μ(e)**	**χ (e)**	**E_{LUMO} - E_{HOMO} (e)**	**E_{LUMO} (e)**	**E_{HOMO} (e)**
12.388	0.00862	0.0403	0.0807	0.1313	0.1313	0.1614	0.0506	0.2120

REFERENCES

1. D. CHU, D. TRYK, D. GERVASIO, E. B. YEAGER; (1989), "EXAMINATION OF THE IONOMER/ELECTRODE INTERFACE USING THE FERRIC/FERROUS REDOX COUPLE"; *J. ELECTRO ANAL.CHEM.INTERFACIAL ELECTROCHEM*; **272 (1-2),** 277-284.
2. E. A. Gomaa, r. T. Rashad; (2019), "thermal and thermodynamic parameters for glycine (gl) solvation in water theoretically*"; biomed. J. Sci. Tech.* Res.; **23 (2),** (17345 — 17348)a.
3. H. Sosdin, y. Bermiidez, o. Castellano, j. Hernandez; (2004), "effects of protonation on the dipole polarizability of monocyclic azines": a theoretical study. Chem. Phys. Lett. **396 (1-3)**, 117-121.
4. R. R. Da silva, t. C. Ramalho, j. M. Santos, j. D. Figueroa-villar; "on the limits of highest-occupied molecular orbital driven reactions": (2006), the frontier effective-for-reaction molecular orbital concept; *j. Phys. Chem. A;* **110 (3)**, 1031-1040.
5. M. Govindarajan, s. Periandy, k. Carthigayen; "ft-ir and ft-raman spectra, (2012), thermo dynamical behavior, homo and lumo, uv, nlo properties", computed frequency estimation analysis and electronic structure calculations on bromotoluene; spectrochim. Acta part a mol. Biomol. Spectrosc; **97**, 411-422.
6. H. Tanak, y. Koysal, s. Isik, h. Yaman, v. Ahsen; (2011), "experimental and computational approaches to the molecular structure of 3-(2-mercaptopyridine) phthalonitrile; bull. Korean chem. Soc ; **32 (2)**, 673-680.
7. N. S. Pagadala, k. Syed, j. Tuszynski; (2017) "software for molecular docking": a review. Biophys. Rev.;.**9 (2)**, 91-102.
8. G. M. Morris, d. S. Goodsell, r. S. Halliday, r. Huey, w. E. Hart, r. K. Belew, a. J. Olson; (1998), "automated docking using a lamarckian genetic algorithm and an empirical binding free energy function"; comput. Chem. **19 (14)**, 1639-1662.
9. G. Verkhivker, k. Appelt, s. T. Freer, j. E. Villafranca; (1995), "empirical free energy calculations of ligand-protein crystallographic complexes; protein eng. Des.sel. **8 (7)**, 11041