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Spectroscopic, Physical, Thermal and Magnetic Studies of Tricine (L) Complexes

Eman A Hassan, Nagwa Nawar, Ebrahim Abdel-Galil and Mohsen M Mostafa*

Department of Chemistry, Mansoura University, Mansoura, Dakahlia Governorate 35516, Egypt

***Corresponding author:** Mohsen M Mostafa, Department of Chemistry, Mansoura University, Mansoura, Dakahlia Governorate 35516, Egypt, Tel: 00-202-01067446662; E-mail: amohsenmostafa@yahoo.com

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Abstract

New metal complexes derived from the interaction of tricine with some metal salts (Cu^{2+} and Co^{2+}) were synthesized and characterized by spectral (IR, UV-vis.), magnetic, conductance and thermal analyses (TGA) measurements. The results suggest that L coordinate in bidentate manners via the COO and NH groups. Spectral and magnetic studies suggest an octahedral geometry around the investigated metal ions. Material studio program has been used for calculating HUMO, LUMO and DFT parameters on the atoms to confirm the geometry of complexes.

***Keywords:** Metal complexes; Spectral and magnetic studies; Metal ions; Solvents; IR spectra; Electronic spectra*

Introduction

Tricine (L) exhibits several donor groups [1] and hence it acts as a good chelating agent. Hence, the main goal of our work is to prove that tricine has the flexibility to bind with several metal ions in unidentate, bidentate and/or tridentate manners [2-12]. In continuation of our earlier work [13] and others [14,15] we extend this work to throw the light on the importance of L in different fields with biological studies.

Experimental

Tricine, chemicals and solvents used in the present investigation were of AR quality and used as reported earlier [13]. Also, all instrumentation and (IR, UV-visible), magnetic and physical studies were carried out as reported earlier [13].

Synthesis of complexes in EtOH

A hot EtOH solution of the metal chlorides [$CuCl_2.2H_2O$ (1.0 mmol, 0.851 g) and $CoCl_2.6H_2O$ (0.59 g) was added to hot solution of tricine (1.0 mmol, 0.896 g) dissolved in EtOH (25 ml) and few drops of redistilled H_2O. The pH of the reaction

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mixture was adjusted with sodium acetate in case of Cu^{2+} while in case of Co^{2+} complexes NaOH was used till the pH of the reaction mixture reaches 7.5. The reaction mixture was refluxed on hot plate for 3 h. The complexes formed were filtered off, washed several times with EtOH and diethyl ether and finally dried in vacuum desiccator over anhydrous $CaCl_2$. The Cu^{2+} complex is readily soluble in redistilled H_2O, DMSO and is partially soluble in EtOH, DMF but the Co^{2+} complex is partially soluble in H_2O, EtOH, DMSO and DMF.

$[Co(tric)_2Cl_2].2H_2O$

Yield: 90%; brown powder; m. p. > 300 °C. IR (KBr; cm^{-1}): 3415, 3227 [OH (H_2O)], OH (EtOH), 2966 (NH), 2880 (OH, acid), 1602 (CO), 521 (M-O). Calcd.: for $C_{12}H_{30}CoN_2O_{12}Cl_2$ (%): C.27.5; H, 5.76; Co, 11.24, Cl, 13.52. Found: C, 26.8; H, 5.46; Co, 11.49, Cl, 13.00. Λ_m (DMSO): 8 Ω^{-1} cm^2 mol^{-1}. μ_{eff}: 5.79 BM. UV (cm^{-1}): 25252 (LMCT), 18726 ($^4A_{2g}$ F → $^4T_{1g}$ P; v_3), 16666 ($^4A_{2g}$ → $^4T_{1g}$; v_2). The values of v_1 ($^4A_{2g}$ → $^4T_{2g}$; v_1), B and β were calculated and found to be 8928 cm^{-1}, 400 cm^{-1} and 0.41, respectively. The β value indicates that the bond between the L and Co^{2+} ion is covalent in nature.

$[Cu(tric)_2]Cl_2.3H_2O$

Yield: 95%; torques powder; m. p. 195 °C. IR (KBr; cm^{-1}): 3322, 3235 [OH (H_2O), OH (EtOH), 2895 (OH, acid), 2968 (NH), 1620 (CO), 557 (M-O). Calcd.: for $C_{12}H_{32}CuN_2O_{13}Cl_2$ (%): C, 26.35; H, 5.9; Cu, 11.62, Cl,12.96. Found: C, 26.14; H, 5.42; Cu, 11.5, Cl, 13.3. Λ_m (DMSO): 65 Ω^{-1} cm^2 mol^{-1}. μ_{eff}: 3.13 BM. UV (cm^{-1}): 31847 cm^{-1} (*LMCT*), 12626 cm^{-1} (^2E_g → $^2T_{2g}$).

Results and Discussion

All the tricine complexes reported earlier in literature [1-15] shows that tricine coordinates to the metal ions in a mononuclear, binuclear and tridentate manner. The results of spectral and magnetic measurements suggest that the ligand coordinates in a bi- and/or tridentate manner and the isolated complexes have an octahedral structure around the metal ions [13].

IR spectra, electronic spectra, magnetic moments and conductance studies

The IR spectrum of tricine (FIG. 1.) was compared with the of the spectra of Co^{2+}, $[Co(tric)_2Cl_2].2H_2O$ and Cu^{2+} $[Cu(tric)_2]Cl_2.3H_2O$ (FIG. 2 and 3.) complexes. The results indicate that L coordinates to the Co^{2+} and Cu^{2+} ions in a bidentate manner through the carboxylate oxygen and amido groups without displacement of a hydrogen atom from the former group [16-18].

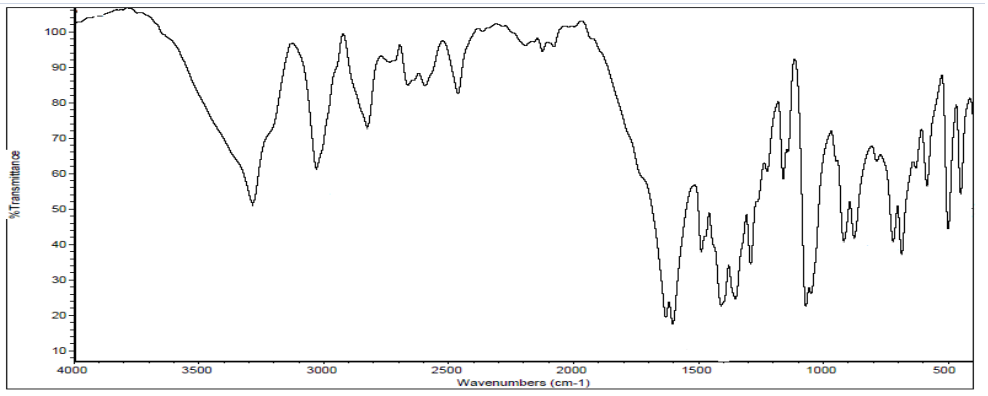


FIG. 1. **IR spectrum of tricine in KBr**.

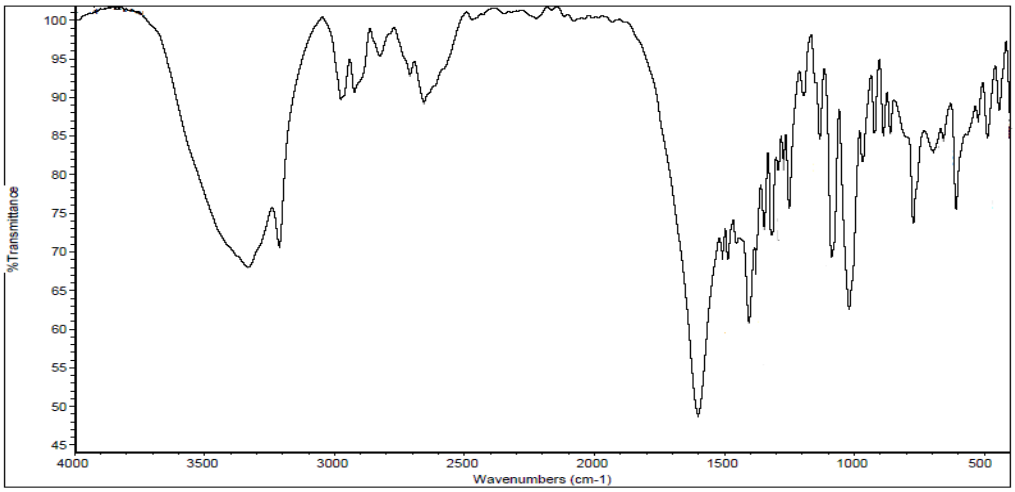


FIG. 2. **IR spectrum of $[Co(tric)_2Cl_2].2H_2O$ in KBr.**

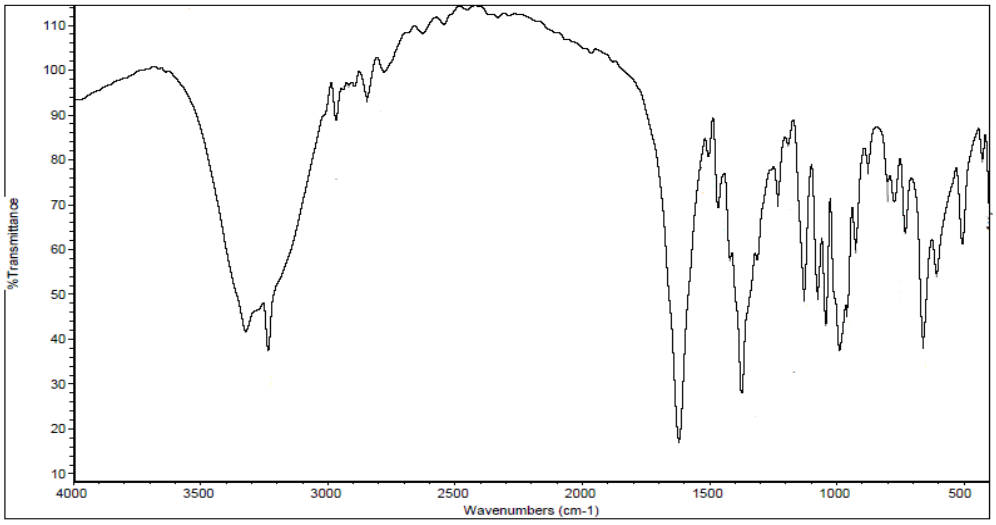


FIG. 3. **IR spectrum of $[Cu(tric)_2]Cl_2.3H_2O$ in KBr**.

The electronic spectra of all complexes were carried out in Nujol mull. The results of electronic spectra as well as the values of magnetic moments indicate that the complexes have octahedral geometry around the metal ions [19-21]. The values of conductance (8-12 ohm^{-1} cm^2 mol^{-1}) confirm that the two complexes are non-electrolyte in nature [22].

Thermal studies

The thermal analyses play a consequential role in studying the properties of the metal complex. To make sure about the proposed formula and the structure of the complex under investigation, the thermal analyses (TGA and DTG) curves was performed under a temperature range from 20 up to 1000 °C. The mass loses were estimated and computed up on the results

of the TGA of the calculated mass losses using the results of the microanalyses. The four steps of the decomposition of $[Co(tric)_2Cl_2].2H_2O$ complex is shown in FIG. 4. The temperature of the first step from 25-135 °C corresponds to the loss of two H_2O molecules and CH_2 (Found: 8.632%, Calcd.: 9.55%). The temperature of the second and third steps from 135-800 °C is referred to the loss of the fragments ($C_9H_{22}N_2O_6$ +2HCl) (Found: 62.199%, Calcd.: 62.036%). Finally, the residue appraises in the temperature range from 800-1000 °C corresponds to $CoNO_4C$, in which the calculated loss 28.412% which is in matching the found loss 29.1%.

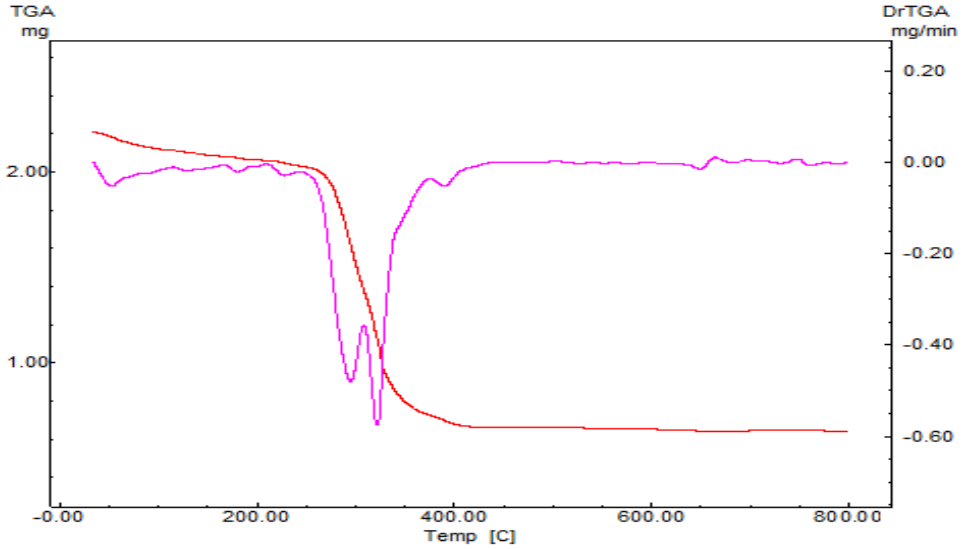


FIG. 4. **TGA curves of $Co(tric)_2Cl_2].2H_2O$.**

Modeling

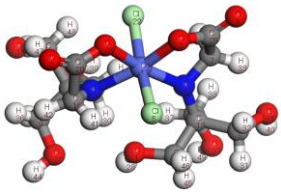
The molecular modeling drawing demonstrate the bond lengths, bond angles TABLES 1 and 2, chemical reactivity, energy components (Kcal/mol), kinetic energy (Kcal/mol) and binding energy (Kcal/mol) of tricine and its metal complexes are shown in TABLES 3 and 4 [23-30]. The DFT theory explains the results [31]. The data of bond angles and lengths illustrate the following comments:

1. The $[Co(tric)_2Cl_2].2½H_2O$ complex (FIG. 5. SCHEME 1) where the cobalt atom arranges in octahedral geometry. The ligand of two tricine acts as a bi-dentate manner coordinating ***via*** N(18), O(26), O(2) and N(11), additionally two chloride ions Cl(5) and Cl(22) complete the octahedral structure. There is a huge change in N(18)-C(26), N(11)-C(13), O(26)-C(20) and O(2)-C(25). The bond angles of tricine are adjusted upon coordination. The bond angles of tricine are lessened or expanded on complex arrangement as a result of bonding such as C(12)-N(18)-C(16), C(10)_C(13)-N(11), C(26)-C(20)-O(3) and C(6)-C(13)-N(11).

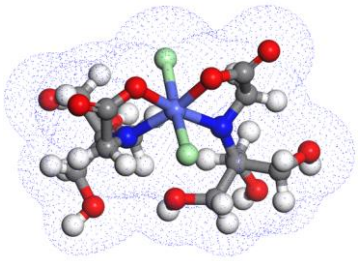
2. The $[Cu(tric)_2].Cl_2.3H_2O$ (FIG. 6. SCHEME 2) has an octahedral structure. The two ligand of tricine act as a tridentate chelating *via* O(6), O(8), N(14), N(19),O(4) and O(10). The bonds of all active groups joining in coordination are longer than that of now exist ligand such as NH. There is a huge variety in N(19)-C(4), N(14)-C(21),O(8)-C(17), O(6)-C(11), O(3)-C(16) and O(10)-C(13) bond lengths. The bond angles are diminished or expanded on complex arrangement as an outcome of bonding such as C(21)-N(14)-C(13), C(4)-C(11)-O(6).

Chemical reactivity

The assignment of energies of HOMO (π-donor) and LUMO (π-acceptor) are important parameters in quantum compound counts. The HOMO is the orbital that generally goes about as electron giver and the LUMO is the orbital that fundamentally goes about as electron acceptor. These molecular orbitals are also called frontier molecular orbitals (FMOs). The all negative value of E_{HOMO}, E_{LUMO} and their neighboring orbitals show that the prepared molecules are steady. The energy gap (E_{HOMO}-E_{LUMO}) is an important stability index serves to portray the chemical reactivity and kinetic stability of the molecule [31]. The gap (E_{HOMO}-E_{LUMO}) is connected to build up a hypothetical pattern for illustrating the structure in many molecular systems. The small gap in molecule means the molecule is more polarized and the molecule is known as soft molecule. The responsive of soft molecule is more than hard one as they easily offer electrons to an acceptor. The small energy gap in tricine shows that charge transfer easily happens in it. The ability of the molecule to give electron is weaker if the HOMO energy value is low. On opposite, the ability of the molecule is good if the HOMO energy value is high [31]. All the data are shown in TABLES 3 and 4.



Molecular modeling of [Co(tric)2Cl2].2H2O



Electron density of [Co(tric)$_2$Cl$_2$].2H$_2$O

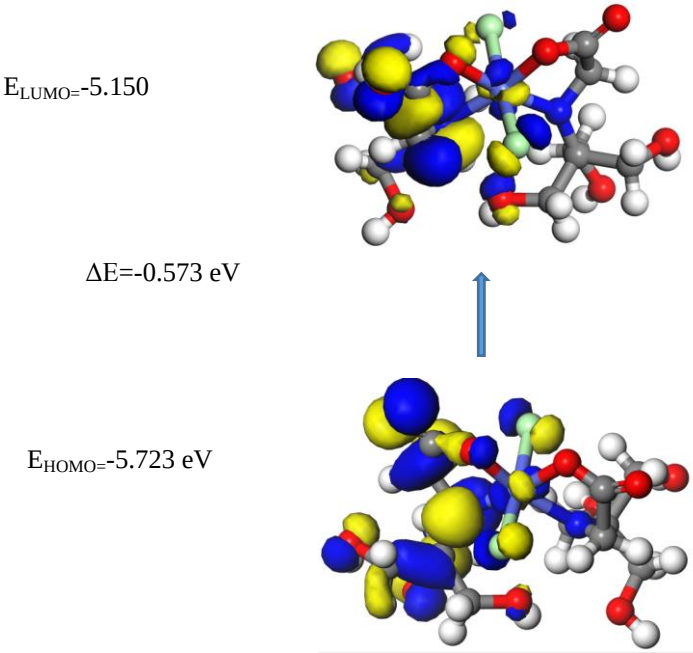


FIG. 5. (SCHEME 1**) Molecular modeling of [Co(tric)$_2$Cl$_2$].2H$_2$O.**

TABLE 1. **Bond lengths (Å) and bond angles of $[Co(tric)_2Cl_2].2H_2O$ using DFT-method from $DMOL^3$calculations.**

Bond	Length	Bond	Length
O(27)-H(49)	0.973	C(20)-C(16)	1.642
C(24)-H(48)	1.096	O(2)-C(25)	1.305
C(24)-H(47)	1.094	C(13)-C(10)	1.575
C(23)-H(46)	1.096	C(6)-O(15)	1.427
C(23)-H(45)	1.098	N(11)-Co(17)	2.004
O(21)-H(44)	0.973	O(26)-C(20)	1.281
O(19)-H(43)	0.983	N(11)-C(7)	1.442
C(16)-H(42)	1.091	C(10)-O(27)	1.439
C(16)-H(41)	1.116	Co(17)-Cl(5)	2.313
O(15)-H(40)	0.977	N(18)-C(12)	1.433
O(14)-H(39)	0.973	C(12)-C(24)	1.684
C(10)-H(38)	1.099	C(24)-O(19)	1.391
C(10)-H(37)	1.094	C(13)-C(6)	1.597
C(9)-H(36)	1.099	N(11)-C(13)	1.471
C(9)-H(35)	1.101	C(25)-C(7)	1.549
C(7)-H(34)	1.109	C(9)-O(21)	1.431
C(7)-H(33)	1.095	C(12)-C(9)	1.566
C(6)-H(32)	1.097	C(20)-O(3)	1.227
C(6)-H(31)	1.1	C(12)-C(4)	1.546
C(4)-H(30)	1.099	C(25)-O(8)	1.238
C(4)-H(29)	1.093	C(13)-C(23)	1.557
O(1)-H(28)	0.972	Co(17)-Cl(22)	2.304
N(18)-Co(17)	2.096	C(16)-N(18)	1.391
O(26)-Co(17)	1.975	C(4)-O(14)	1.444
O(2)-Co(17)	1.941	C(23)-O(1)	1.426

Bond	Angle	Bond	Angle
H(49)-O(27)-C(10)	107.405	C(10)-C(13)-N(11)	107.333
Co(17)-O(26)-C(20)	114.468	C(10)-C(13)-C(23)	110.705
O(2)-C(25)-C(7)	114.852	C(6)-C(13)-N(11)	112.178
O(2)-C(25)-O(8)	124.412	C(6)-C(13)-C(23)	103.403
C(7)-C(25)-O(8)	120.72	N(11)-C(13)-C(23)	114.405
H(48)-C(24)-H(47)	112.377	N(18)-C(12)-C(24)	106.009
H(48)-C(24)-C(12)	103.962	N(18)-C(12)-C(9)	115.038

H(48)-C(24)-O(19)	114.014	N(18)-C(12)-C(4)	112.236
H(47)-C(24)-C(12)	106.823	C(24)-C(12)-C(9)	104.343
H(47)-C(24)-O(19)	107.81	C(24)-C(12)-C(4)	107.85
C(12)-C(24)-O(19)	111.648	C(9)-C(12)-C(4)	110.693
H(46)-C(23)-H(45)	108.91	Co(17)-N(11)-C(7)	105.713
H(46)-C(23)-C(13)	107.941	Co(17)-N(11)-C(13)	137.971
H(46)-C(23)-O(1)	106.774	C(7)-N(11)-C(13)	116.09
H(45)-C(23)-C(13)	106.233	H(38)-C(10)-H(37)	108.87
H(45)-C(23)-O(1)	110.318	H(38)-C(10)-C(13)	108.941
C(13)-C(23)-O(1)	116.48	H(38)-C(10)-O(27)	109.943
H(44)-O(21)-C(9)	106.118	H(37)-C(10)-C(13)	109.487
C(16)-C(20)-O(26)	112.841	H(37)-C(10)-O(27)	110.726
C(16)-C(20)-O(3)	116.544	C(13)-C(10)-O(27)	108.847
O(26)-C(20)-O(3)	130.612	H(36)-C(9)-H(35)	107.241
H(43)-O(19)-C(24)	106.149	H(36)-C(9)-O(21)	111.301
Co(17)-N(18)-C(12)	137.244	H(36)-C(9)-C(12)	111.395
Co(17)-N(18)-C(16)	102.656	H(35)-C(9)-O(21)	110.969
C(12)-N(18)-C(16)	116.821	H(35)-C(9)-C(12)	105.469
N(18)-Co(17)-O(26)	80.109	O(21)-C(9)-C(12)	110.278
N(18)-Co(17)-O(2)	166.821	H(34)-C(7)-H(33)	107.953
N(18)-Co(17)-N(11)	110.215	H(34)-C(7)-N(11)	109.124
N(18)-Co(17)-Cl(5)	95.382	H(34)-C(7)-C(25)	103.551
N(18)-Co(17)-Cl(22)	90.897	H(33)-C(7)-N(11)	114.731
O(26)-Co(17)-O(2)	86.741	H(33)-C(7)-C(25)	112.312
O(26)-Co(17)-N(11)	169.61	N(11)-C(7)-C(25)	108.542
O(26)-Co(17)-Cl(5)	88.278	H(32)-C(6)-H(31)	108.079
O(26)-Co(17)-Cl(22)	88.107	H(32)-C(6)-O(15)	106.974
O(2)-Co(17)-N(11)	82.951	H(32)-C(6)-C(13)	108.727
O(2)-Co(17)-Cl(5)	85.039	H(31)-C(6)-O(15)	109.802
O(2)-Co(17)-Cl(22)	87.761	H(31)-C(6)-C(13)	105.967
N(11)-Co(17)-Cl(5)	89.532	O(15)-C(6)-C(13)	117.015
N(11)-Co(17)-Cl(22)	92.776	H(30)-C(4)-H(29)	110.16
Cl(5)-Co(17)-Cl(22)	172.115	H(30)-C(4)-C(12)	107.422

H(42)-C(16)-H(41)	113.087	H(30)-C(4)-O(14)	109.196
H(42)-C(16)-C(20)	110.527	H(29)-C(4)-C(12)	109.798
H(42)-C(16)-N(18)	118.296	H(29)-C(4)-O(14)	110.485
H(41)-C(16)-N(18)	109.176	Co(17)-O(2)-C(25)	113.811

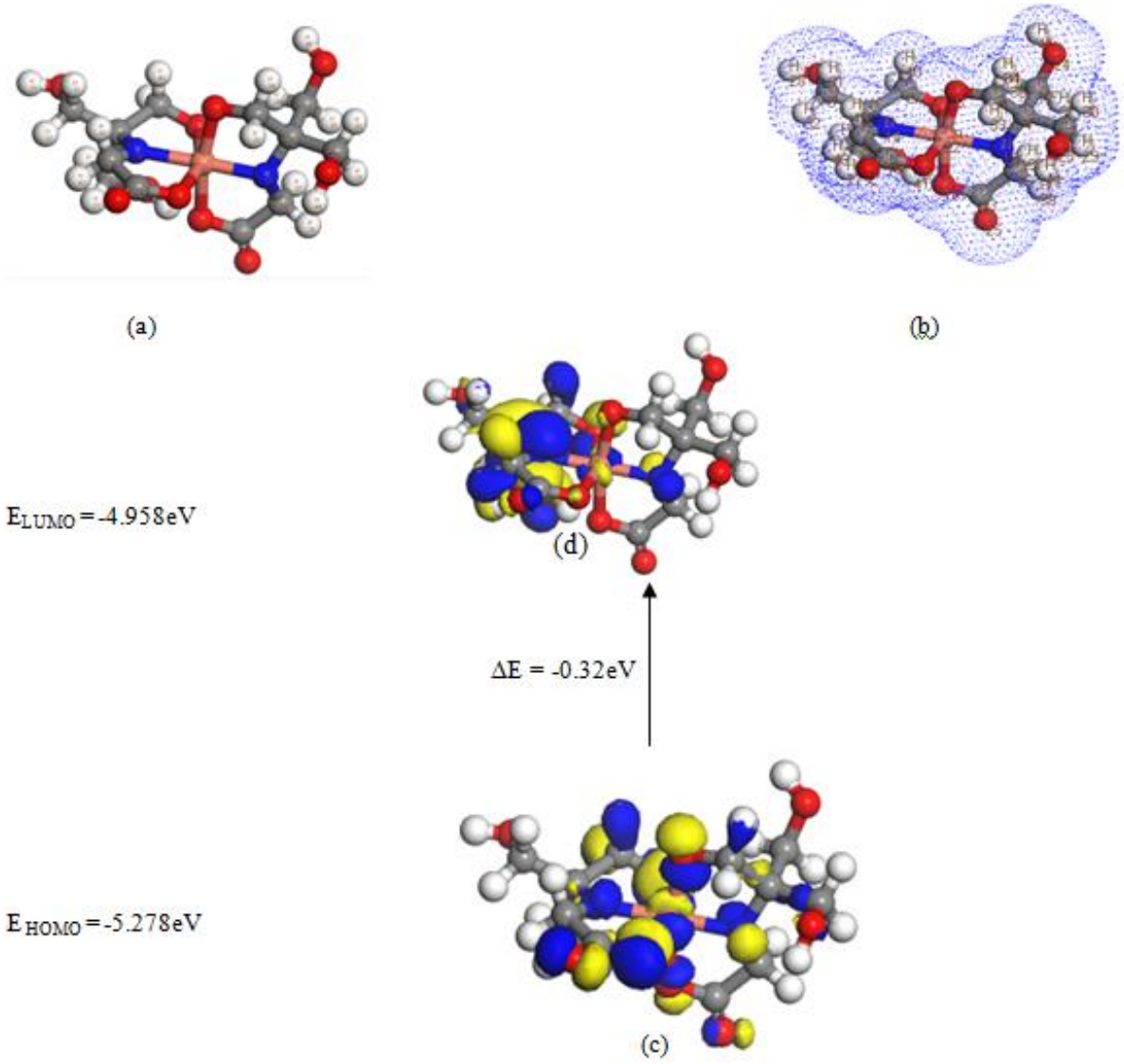


FIG. 6. (SCHEME 2**) Molecular modeling of (a) [Cu(tric)$_2$]Cl$_2$.3H$_2$O, (b) electron density,(c) HOMO and (d) LUMO.**

TABLE 2. **Bond lengths (Å) and bond angles of $[Cu(tric)_2]Cl_2.3H_2O$ using DFT-method from $DMOL^3$calculations.**

Bond	Length(Å)	Bond	Length(Å)
O(24)-H(45)	0.97	C(4)-C(7)	1.589
O(23)-H(44)	0.972	C(4)-C(11)	1.549
C(21)-H(43)	1.105	C(11)-O(6)	1.406
C(21)-H(42)	1.108	N(19)-C(4)	1.461
O(18)-H(41)	1	C(16)-O(2)	1.255
C(17)-H(40)	1.11	O(3)-Cu(22)	2.237
C(17)-H(39)	1.102	C(20)-C(9)	1.542
C(15)-H(38)	1.103	N(19)-Cu(22)	1.918
C(15)-H(37)	1.105	C(20)-C(17)	1.614
C(12)-H(36)	1.097	C(21)-N(14)	1.435
C(12)-H(35)	1.101	C(1)-O(18)	1.346
C(11)-H(34)	1.106	C(16)-C(21)	1.544
C(11)-H(33)	1.102	C(13)-O(25)	1.236
C(9)-H(32)	1.099	O(6)-Cu(22)	1.913
C(9)-H(31)	1.102	C(20)-C(1)	1.792
C(7)-H(30)	1.096	C(13)-C(15)	1.544
C(7)-H(29)	1.1	O(10)-Cu(22)	2.015
O(5)-H(28)	0.971	N(14)-C(20)	1.352
C(1)-H(27)	1.097	O(10)-C(13)	1.321
C(1)-H(26)	1.093	O(8)-Cu(22)	2.154
N(14)-Cu(22)	2	C(12)-O(24)	1.435
C(15)-N(19)	1.452	C(17)-O(8)	1.349
C(4)-C(12)	1.571	O(3)-C(16)	1.281
C(9)-O(5)	1.43	C(7)-O(23)	1.421

Angle	Degree (°)	Angle	Degree (°)	Angle	Degree (°)
H(45)-O(24)-C(12)	107.274	C(15)-N(19)-Cu(22)	110.1	H(34)-C(11)-H(33)	108.38
H(44)-O(23)-C(7)	107.774	C(4)-N(19)-Cu(22)	111.597	H(34)-C(11)-C(4)	111.689
N(14)-Cu(22)-O(3)	78.439	H(41)-O(18)-C(1)	111.206	H(34)-C(11)-O(6)	107.303
N(14)-Cu(22)-N(19)	175.925	H(40)-C(17)-H(39)	108.797	H(33)-C(11)-C(4)	108.087

N(14)-Cu(22)-O(6)	93.485	H(40)-C(17)-C(20)	101.092	H(33)-C(11)-O(6)	111.947
N(14)-Cu(22)-O(10)	96.349	H(40)-C(17)-O(8)	113.132	C(4)-C(11)-O(6)	109.468
N(14)-Cu(22)-O(8)	80.029	H(39)-C(17)-C(20)	109.548	Cu(22)-O(10)-C(13)	111.882
O(3)-Cu(22)-N(19)	97.519	H(39)-C(17)-O(8)	111.415	H(32)-C(9)-H(31)	107.672
O(3)-Cu(22)-O(6)	92.302	C(20)-C(17)-O(8)	112.35	H(32)-C(9)-O(5)	111.276
O(3)-Cu(22)-O(10)	93.608	O(2)-C(16)-C(21)	118.132	H(32)-C(9)-C(20)	110.103
O(3)-Cu(22)-O(8)	158.415	O(2)-C(16)-O(3)	124.633	H(31)-C(9)-O(5)	111.469
N(19)-Cu(22)-O(6)	86.114	C(21)-C(16)-O(3)	117.235	H(31)-C(9)-C(20)	108.167
N(19)-Cu(22)-O(10)	84.361	H(38)-C(15)-H(37)	105.805	O(5)-C(9)-C(20)	108.113
N(19)-Cu(22)-O(8)	104.025	H(38)-C(15)-N(19)	109.831	Cu(22)-O(8)-C(17)	108.833
O(6)-Cu(22)-O(10)	169.371	H(38)-C(15)-C(13)	108.583	H(30)-C(7)-H(29)	108.813
O(6)-Cu(22)-O(8)	90.486	H(37)-C(15)-N(19)	114.864	H(30)-C(7)-C(4)	106.806
O(10)-Cu(22)-O(8)	87.262	H(37)-C(15)-C(13)	107.054	H(30)-C(7)-O(23)	106.545
H(43)-C(21)-H(42)	105.57	N(19)-C(15)-C(13)	110.439	H(29)-C(7)-C(4)	108.822
H(43)-C(21)-N(14)	111.465	Cu(22)-N(14)-C(21)	117.306	H(29)-C(7)-O(23)	111.922
H(43)-C(21)-C(16)	108.736	Cu(22)-N(14)-C(20)	118.651	C(4)-C(7)-O(23)	113.689
H(42)-C(21)-N(14)	110.122	C(21)-N(14)-C(20)	123.932	C(11)-O(6)-Cu(22)	107.119
H(42)-C(21)-C(16)	108.257	O(25)-C(13)-C(15)	122.404	H(28)-O(5)-C(9)	106.737
N(14)-C(21)-C(16)	112.413	O(25)-C(13)-O(10)	122.064	C(12)-C(4)-C(7)	107.444
C(9)-C(20)-C(17)	117.697	C(15)-C(13)-O(10)	115.263	C(12)-C(4)-C(11)	111.465
C(9)-C(20)-C(1)	104.649	H(36)-C(12)-H(35)	109.266	C(12)-C(4)-N(19)	113.885
C(9)-C(20)-N(14)	117.588	H(36)-C(12)-C(4)	107.815	C(7)-C(4)-C(11)	112.783
C(17)-C(20)-C(1)	100.397	H(36)-C(12)-O(24)	111.273	C(7)-C(4)-N(19)	109.955
C(17)-C(20)-N(14)	107.407	H(35)-C(12)-C(4)	108.883	C(11)-C(4)-N(19)	101.363
C(1)-C(20)-N(14)	107.126	H(35)-C(12)-O(24)	109.003	Cu(22)-O(3)-C(16)	113.028
C(15)-N(19)-C(4)	121.272	C(4)-C(12)-O(24)	110.558	H(27)-C(1)-H(26)	114.644

TABLE 3. **Calculated E_{HOMO}, E_{LUMO}, energy band gap (E_H-E_L), chemical potential (μ), electronegativity (ϰ), global hardness (Ƞ), global softness (S) and global electrophilicity index (ω) for tricine and its complexes.**

Compound	EH eV	EL eV	(EHEL) eV	ϰ eV	μ eV	Ƞ eV	S eV^{-1}	ω eV	σ eV
L^1; $C_6H_{13}NO_5$	-5.18	-0.678	-4.502	2.929	-2.929	2.251	1.1255	1.9056	0.4442
$[Co(L^1)_2Cl_2].2H_2O$	-5.723	-5.15	-0.573	5.437	-5.4365	0.287	0.14325	51.5803	3.49
$[Cu(L^1)_2]Cl_2.3H_2O$	-5.278	-4.958	-0.32	5.118	-5.118	0.16	0.08	81.856	6.25

TABLE 4. **Some of energetic properties of tricine and its complexes calculated by DMOL^3 using DFT-method**.

No.	Compound	HOMO (eV)	LUMO (eV)	Binding energy (Kcal/mol)	Total energy (Kcal/mol)
1	L1; C6H13NO5	-5.18	-0.678	-2483726	-4.189×10^5
2	[Co(L1)2Cl2].2H2O	-5.723	-5.15	-4863.411	-1.518×10^6
3	[Cu(L1)2]Cl2.3H2O	-5.278	-4.958	-4510.29	-9.751×10^5

Conclusion

The Cu^{2+} and Co^{2+} complexes coordinate in bidentate fashion. The geometry of the isolated complexes was determined by chemical, physical, spectral, conductance and magnetic measurements. The results of spectral and magnetic studies suggest octahedral geometry around the metal ions. The molecular modeling drawing demonstrate the bond lengths, bond angles, chemical reactivity, energy components (Kcal/mol), kinetic energy (Kcal/mol) and binding energy (Kcal/mol) of tricine and its metal complexes.

REFERENCES

1. Crans DC, Ehde PM, Shin PK, et al. Structural and kinetic characterization of simple complexes as models for vanadate-protein interactions. J Am Chem Soc. 1991;113:3728-36.
2. Chakraborty D, Bhattacharya PK. Intramolecular interligand interactions in Cu (II) ternary complexes involving dipeptides and amino acids. J Inorg Biochem. 1990;39:1-8.

3. Manjula V, Chakraborty D, Bhattacharya P. Ternary complexes of Cu(II) involving histidine and another amino acid or dipeptide. Indian J Chem. 1990;29A:577-80.
4. Kapoor RC, Jailwal JK, Kishan JA. Complex Formation of N-[Tris (hydroxymethyl) methyl] glycine with Lead and Cadmium. J Inorg Nucl Chem. 1978;40:155-8.
5. Tripathi RM, Ghose R, Ghose AK. Heteroligand complexes of some transition-metals containing 2, 2'-bipyridyl and tricine as ligands in aqueous-solution. Indian J Chem. 1985;24A:565-7.
6. Vaidyan AV, Bhattacharya PK. Interligand interaction in ternary complexes of Zn (II) and Cd (II) with dipeptides and aminoacids. Can J Chem. 1994;72:1107-10.
7. de Castro B, Pereira J, Gameiro P, et al. Multinuclear NMR and potentiometric studies on the interaction of zinc and cadmium with cytidine and glycylglycine. The effect of the anion. J Inorg Biochem. 1992;45:53-64.
8. Pandeya KB, Patel RN. Ternary complexes of copper(II) with glycylglycine, glycylglyclglycine and some imidazoles. Indian J Chem. 1990;29A:602-4.
9. Kishan JAI, Kapoor R. Complex Formation of N-[Tris (hydroxy-methyl)methyl]glycine with Copper(II) and Zinc(II). Indian J Chem. 1984;23A:355-6.
10. Farkas E, Kiss T. Effects of side-chain donor groups on deprotonation of peptide amide in copper (II) complexes at high pH. Polyhedron. 1989;8:2463-7.
11. Hosny WM. Complexes of Vitamin B6. Ternary complexes of Cu(II) with pyridoxamine and amino acids, DNA units or peptides. Egypt J Chem. 1999;42:151-73.
12. Prenesti E, Daniele PG, Prencipe M, et al. Spectrum-structure correlation for visible absorption spectra of copper (II) complexes in aqueous solution. Polyhedron. 1999;18:3233-41.
13. Al-Radadi NS, Al-Ashqar SMA, Mostafa MM. Synthesis and characterization of some new binary and ternary CuII complexes. Synth React Inorg Met-Org and Nano Chem. 2011;41: 203-10.
14. Boraei AA, Ahmed IT. Synth React Inorg Met-Org and Nano Chem. 2002;32: 981-1000.
15. El-Roudi OM, Abd Alla EM, Ibrahim SA. Potentiometric studies on the binary complexes of N-[Tris (hydroxymethyl) methyl] glycine with Th^{4+}, Ce^{3+}, La^{3+}, and UO_2^{2+} and medium effects on a Th^{-} tricine binary complex. J Chem Eng Data. 1997;42:609-13.
16. Nakamoto K. Infrared and Raman spectra of inorganic and coordination compounds Part A. Theory and Applications in Inorganic Chemistry. 1997:88-97.
17. Ketcham KA, Garcia I, Swearingen JK, et al. Spectral studies and X-ray crystal structures of three nickel (II) complexes of 2-pyridineformamide 3-piperidylthiosemicarbazone. Polyhedron. 2002;21:859-65.
18. Bates RG, Roy RN, Robinson RA. Solute-solvent effects in the acidic dissociation of the ampholyte N-tris (hydroxymethyl) methylglycine (“tricine”) in 50 mass% methanol-water solvent. J Sol Chem. 1974;3:905-16.
19. Lever ABP. Inorganic electronic spectroscopy. Amsterdam, The Netherlands. 1968:420.
20. Tanabe Y, Sugano S. On the absorption spectra of complex ions I and II. J Phys Soc Jpn. 1954;9:753-66.
21. Earnshaw A. Introduction to Magnetochemistry. Acadmic Press. London. 1968.
22. Geary WJ. The use of conductivity measurements in organic solvents for the characterisation of coordination compounds. Coord Chem Revs. 1971;7:81-122.
23. Kivelson D, Neiman R. ESR studies on the bonding in copper complexes. J Chem Phys. 1961;35:149-55.

24. Singh B, Yadava BP, Aggarwal RC. Indian J Chem. 1984;23A:441-52.
25. Delley B. An all-electron numerical method for solving the local density functional for polyatomic molecules. J Chem Phys. 1990;92:508-17.
26. Delley B. A scattering theoretic approach to scalar relativistic corrections on bonding. Int J Quantum Chem. 1998;69:423-33.
27. Delley B. From molecules to solids with the DMol 3 approach. J Chem Phys. 2000;113:7756-64.
28. Wu X, Ray AK. Density-functional study of water adsorption on the PuO 2 (110) surface. Phys Rev. 2002;65:085403.
29. Kessi A, Delley B. Density functional crystal vs. cluster models as applied to zeolites. Int J Quant Chem. 1998;68:135-44.
30. Materials Studio v 5.0. Accelrys software Inc. 2009.
31. Linert W, Taha A. Co-ordination of solvent molecules to square-planar mixed-ligand nickel(II) complexes: A thermodynamic and quantum-mechanical study. J Chem Soc Dalton Trans. 1994:1091-5.