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THE INVESTIGATION OF GEOMETRICAL PROPERTIES OF 2,5 PYRIDINEDICARBOXYLIC ACID, SYNTHESIS AND VIBRATIONAL PROPERTIES OF ITS SOME METAL HALOGEN COMPOUNDS

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Özet: In this work, the theoretical and experimental vibrational spectra of 2,5 pyridinedicarboxylic acid were studied. FT-IR spectra of the molecule in the liquid phase were recorded in the region 4000-400 cm^{-1}. The structural and spectroscopic data were calculated by using density functional method (B3LYP, HF, BLYP) with the 6-31G(d) basis set in the ground state. The vibrational frequencies were calculated and scaled values were compared with experimental FT-IR spectra. The observed and calculated frequencies are found to be in good agreement. In addition to these five new complexes of 2,5 pyridinedicarboxylic acid molecule Ni(2,5 PDA)Cl_2, Hg(2,5 PDA)Cl_2, Cu(2,5 PDA)Cl_2, Fe(2,5 PDA)Cl_2, Mn(2,5 PDA)Cl_2 [where; 2,5PDA: 2,5 pyridinedicarboxylic acid] were synthesized for the first time. The FT-IR spectra of the new complexes were recorded, and their C, H, and N analysis results were reported. The possible structures for complexes were proposed according to elemental analysis and FT-IR spectra.

Anahtar Kelimeler: *2,5 Pyridinedicarboxylic acid, DFT, vibrationalsSpectra*

2,5 PİRİDİNDİKARBOKSİLİK ASİT MOLEKÜLÜNÜN GEOMETRİK VE TİTREŞİMSEL ÖZELLİKLERİNİN ARAŞTIRILMASI VE BAZI METAL HALOJEN KOMPLEKSLERİNİN SENTEZLENMESİ

Abstract: Bu çalışmada 2,5 Piridindikarboksilik asit için deneysel ve teorik çalışma yapıldı. Molekülün FT-IR spektrumu sıvı fazda 4000-400 cm-^{1} aralığında kaydedildi. Yapısal ve spektroskopik hesaplar B3LYP, HF, BLYP metotlarında 6-31G(d) baz seti kullanarak yapıldı. Titreşim frekansları hesaplatıldı ve çarpım faktörü ile çarpılıp deneysel FT-IR spektrumu ile karşılaştırıldı. Gözlenen ve hesaplanan değerlerin uyumlu olduğu görüldü. Ayrıca 2,5 Piridindikarboksilik Asit için 5 yeni [formülü; Ni(2,5 PDA)Cl_2, Hg(2,5 PDA)Cl_2, Cu(2,5 PDA)Cl_2, Fe(2,5 PDA)Cl_2, Mn(2,5 PDA)Cl_2 ile verilen] kompleks sentezi ilk kez yapıldı. Komplekslerin FT-IR spektrumu kaydedildi. FT-IR spektrumu ve elemental analize göre yeni kompleksler için yapısı öngörüldü.

Anahtar Kelimeler: *2,5 Piridindikarboksilik asit, DFT, titreşim Spektrumu*

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1. INTRODUCTION

2,5 pyridinedicarboxylic acid (2,5PDA) with divergent function groups, which could give more possible to form bridging hydrogen bonds, in interesting and has potential for self assembly [1]. Recent studies concerning to use of 2,5PDA as a ligand towards transition metal salts [2-6] and lanthanide-transition metal salts [2,3] have shown that a great variety of polymeric structures can be obtained as a result of the different conformation and coordination modes of the 2,5PDA.More recently, the X-ray crystal structures and photo physical properties of four lanthanide complexes [7].

In this work, we have performed the experimental and theoretical vibrational analysis of 2,5 PDA for the first time. The molecular geometry, vibrational frequencies, have been calculated by using DFT, B3LYP method with 6-31G (d) basis set in the ground state. They are in good agreement with experimental results. Also the analysis of the experimental values indicates that there are some structure-spectra correlations. It was found that the frequency shift values depend on the metal in order Hg<Cu.

2. CALCULATIONS

2,5 pyridinedicarboxylic acid in the ground state is computed by performing DFT/B3LYP methods 6-31G(d) basis set. The wave numbers in the ranges from 4000-1700cm^{-1} and lower than 1700 cm^{-1} are scaled with 0.958 and 0.983, respectively [8]. All calculations are performed by using GaussView molecular visualization program [9] and GAUSSIAN 03 program package on the personal computer [10]. In addition to these we prepared and reported the FT-IR spectra of some metal (II) halide complexes 2,5 PDA for detecting any possible relationship between the ligand vibrational values and the metal, and presented their IR data.

3. EXPERIMENTAL

All the chemicals (Aldrich, Sigma) were reagent grade and were used without further purification. Metal iodide (1mmol) was dissolved in absolute hot ethanol (10ml). The appropriate quantity of 2,5 PDA was added to the solution. The mixture was stirred magnetically at room temperature for 24 hr. The precipitated complexes were filtered, washed with the ether and dried (Figures 1-3).

The prepared samples were analyzed for C, H and N with a GmbH varioMICRO CHNS analyzer with the results in Table 1. The infrared spectra of discs (KBr) of fresh samples were recorded on Mattson 1000 FT-IR (4000-400 cm^{-1}) spectrometer

Table 1. Elemental analysis results related to complexes.

Complexes	(Analyses Results) Found /Calculated		
	C %	H %	N %
Ni(2,5 PDA)Cl$_2$	38,94/36,42	4,00/2,15	5,66/6,06
Hg(2,5 PDA)Cl$_2$	40,34/38,25	3,00/2,23	7.43/6,90
Cu(2,5 PDA)Cl$_2$	42,38/41,84	2,44/2,49	6,90/6,97
Fe(2,5 PDA)Cl$_2$	24,51/28,58	2,60/2,38	3,87/3,98
Mn(2,5PDA)Cl$_2$	54,56/49,29	4,47/2,51	7,06/7,04

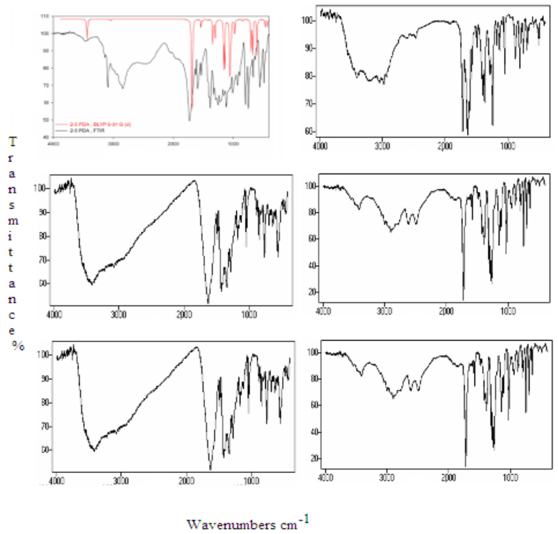

Figure 1. The spectrum of free 2,5 PDA, Ni(2,5PDA)Cl$_2$, Hg(2,5 PDA)Cl$_2$, Cu(2,5PDA)Cl$_2$,Fe(2,5 PDA)Cl$_2$ and Mn(2,5PDA)Cl$_2$, respectively.

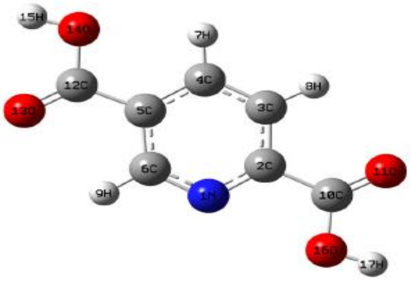

Figure 2. The theoretical geometric structures of 2,5 PDA molecule.

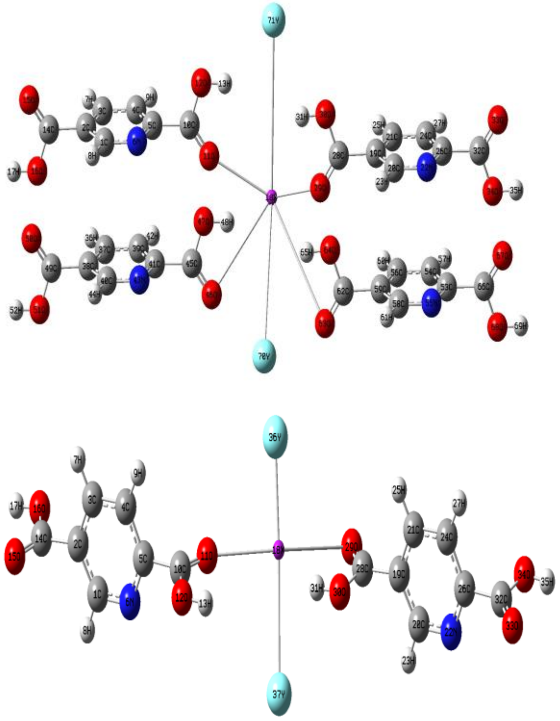

Figure 3. The proposed molecular structure of quadro and dual 2,5PDA complexes.

4. RESULTS AND DISCUSSION

The optimized structure of the 2,5 PDA compound is shown in Fig. 1 with numbering of the atoms. 2, 5 PDA has substitution in two para-position of the pyridine. If we assumed that the carboxyl groups (-COOH) had a single mass point all the molecules under consideration would belong to C_{2V} point group. It has 27 normal vibrations of which 19 are planar and eight are non-planar. In addition to these 27 ring vibrations there are nine vibrations due to the substitute carboxyl groups. The FT-IR spectra of free 2,5 PDA, $Ni(2,5PDA)_2Cl_2$, $Hg(2,5PDA)4Cl_2$, $Cu(2,5PDA)_4Cl_2$, $Fe(2,5PDA)_2Cl_2$ and $Mn(2,5PDA)4Cl_2$ complexes were given in Fig 1 respectively. The vibrational assignments were made of free 2,5 PDA by comparing with the assignments of pyridine [15, 16] and nicotinic acid [17]. The vibrational wave numbers of free ligand and synthesized complexes were listed in Table 2.

2,5 PDA has different coordination form and it is coordinated not only through the carboxylate group but through the nitrogen atom of the pyridine ring (Figure 2). This property leads to different constructions in the metal complexes. Similar structure variations were observed in the complexes studied here for different transition metal atoms.

The most important vibrational modes were ν(C=O) and pyridine ring vibrations to implying the coordination of the metal atom to ligand molecule. Because, it is known that if the coordination takes place through ring nitrogen, the ν(C=O) and pyridine ring vibrations shifts to the higher region in the complexes of pyridine and pyridine derivatives [11-13]. If the coordination takes place through carboxyl oxygen it is expected that the ν(C=O) vibrations strongly shifts to below region.

The ν(C=O) bands of pyridine derivatives containing carboxyl group were expected at higher than 1650cm^{-1} [15]. A strong band appeared at 1729 cm^{-1} in the infrared spectrum of free 2,5 PDA and it was assigned ν(C=O). This band was observed at 1718 cm^{-1} in the spectrum of $Ni(2,5PDA)_2Cl_2$ and 1717 cm^{-1} for $Hg(2,5PDA)_4Cl_2$, 1710 cm^{-1} for $Cu_2(2,5PDA)_4Cl_2$, 1702 cm^{-1} for $Fe_2(2,5PDA)_2Cl_2$ and 1722 cm^{-1} for $Mn(2,5PDA)_4Cl_2$ complexes. This significant shift was a result of coordination taken place through the two carboxyl oxygen to the Ni atom. On the other hand this band undergo slight negative shift in the spectrum of $Ni(2,5PDA)_4Cl_2$ complex and explained the influence of the hydrogen bindings, which led to formation of hydrogen-bonded frameworks and polymeric network structure of isonicotinic acid as in Ref. [14].

We observed two ring vibrations related to nitrogen atom at 1627cm^{-1}, 1594 cm^{-1} of the spectrum of 2,5 PDA. These bands were assigned ν (C=N) + ν (CC) and ν (C-N) + ν (C C). It is known that the donor power of pyridine ring nitrogen is strong [18]. Similar bindings were also seen in different isonicotinic acid metal complexes [14]. As a result of elemental analysis and interpreting of frequency shifts, the proposed structures of $Ni(2,5PDA)_2Cl_2$ and $Fe(2,5PDA)_2Cl_2$ complexes are two ligand molecule with an octahedral environment and $Hg(2,5PDA)_4Cl_2$, $Cu(2,5PDA)_4Cl_2$ and $Mn(2,5PDA)_4Cl_2$ complexes are two ligand molecule with an octahedral environment as in Fig 3. The structural and spectroscopic data were calculated by using density functional method (B3LYP, HF, BLYP) with the 6-31G(d) basis set in the ground state. Theoretical computations and Table 4 show that B3LYP is the most compatible than HF, BLYP. Therefore molecular geometry, vibrational frequencies, have been calculated by using DFT, B3LYP method with 6-31G(d) basis set in the ground state. This data are in good agreement with experimental results. One can see these results Tables 2-3. We don’t use dihedral angels in table inadequacy of paper.

Table 2: The vibrational wave numbers (cm-^{1}) of free 2,5 PDA and complexes

$Ni(L)_2Cl_2$	**$Hg(L)_4Cl_2$**	**$Cu(L)_4Cl_2$**	**$Fe(L)_2Cl_2$**	**$Mn(L)Cl_2$**	**FREE L**	**Vibrational assignments**
3110 m	3095 s	3082 s	3073 m	3107 m	3095m	i.p OH strain
1718 s	1717 s	1710 s	1702 s	1722 vw	1729 s	C=O strain
1638 m	1629 s	1599 m	1626 s	1619 w	1627s	C=N + CC strain
1574 m	1596 m	1571 m	1621 s	1578 m	1594 m	C-N + CC strain
1543 m	1540 m	1485 s	1485 m	1530 m	1537 w	OH torsion + C-O strain
1369 m	1388 m	1397 m	1401 m	1385 m	1385 zw	i.p CH torsion
1288 m	1297 m	1293 m	1339 m	1289m	1293 m	i.p CH torsion
1267 m	1226 s	1260 m	1282 m	1267w	1252 m	i.p CH torsion
1240 vw	1220 m	1216 m	1233 m	1215 m	1217m	i.p CH torsion
1174 m	1218 m	1215 m	1174 m	1175 m	1216 m	C-O strain
1129 m	1162 s	1171 s	1153 s	1141 w	1160vw	COH torsion
1089 w	1118 m	1129 s	1121 m	1111 m	1116 m	Ring breathing
1025 m	1014 m	1013 vw	1038 m	1025 vw	1009 m	Ring corruption
943 w	945 m	942 m	949 m	943 m	930 m	o.o.p CH torsion
877 m	893 m	895 s	877 w	877 m	892 m	o.o.p CH torsion
798 m	801 m	816 m	804 w	798m	799 m	o.o.p CH torsion
750 s	749 s	753 w	757 m	745 s	748 m	o.o.p CH torsion
690 w	693 m		731 s	693m		C_P-C_{COOH} strain + COH tortion
625 s	673 s	686 vw	686 m	646 m	669 vw	o.o.p COOH corruption
622 m	635 m	594 m	664 m	605 w	633 m	OCO twist+ ring corruption
544 m	563	519 m	550 w	543 w	544 m	Ring torsion + COOH torsion
458 m	488 m	460 m	466 w	485 m	487 m	o.o.p Ring corruption
421 m	436 m	454 m	433 w	448 w	448 m	o.o.p Ring corruption
	4021 w	404 w				o.o.p OH torsion

L:2,5 PDA, m;middle, w;weak, vw;very weak, s;strong, i.p; in plane, o.o.p; out of plane

Table 3: The theoretical vibrational wave numbers (cm-^{1}) of free 2,5 PDA

HF			BLYP			B3LYP			FTIR		Assigments
Freq	IR-Intensty	Ram. Activity	Freq.	IR-Intensty	Raman Actvity	Freq.	IR-Intensty	Raman Actvity	Freq.	% Trans	
3468,53	99,55	162,32	3444,81	49,90	240,96	3450,03	81,37	191,34			ν(14O-15H)
3467,30	231,34	72,41	3436,39	45,49	221,44	3444,75	78,95	174,74	3095	68	ν(16O-17H)
2937,28	0,18	87,68	3078,49	1,47	111,35	3029,74	0,30	99,12			ν(3C-8H) +ν(4C-7H)
2920,17	1,29	51,13	3066,15	0,52	48,95	3016,04	0,48	50,40			ν(3C-8H) + ν(4C-7H)
2919,12	2,34	66,22	3040,68	4,67	75,76	2996,90	2,89	71,66			ν(6C-9H)
1730,17	124,47	59,95	1694,31	206,04	113,09	1706,62	223,11	92,79			ν(12C-13O)
1722,30	781,57	5,09	1683,57	261,18	72,98	1697,17	334,95	46,69	1729	49	ν(10C-11O)
1556,42	50,32	152,09	1538,83	24,71	248,64	1542,14	29,21	215,43	1627	76	ν(3C-4C) + ν(6C-N)
1519,13	21,44	1,52	1506,84	6,33	13,68	1509,55	8,44	6,43	1594	68	ν(2C-3C) + ν(4C-5C)
1427,45	35,72	3,90	1426,60	5,36	4,92	1423,07	15,51	4,86	1537	75	ν(5C-6C)
1335,63	240,13	1,21	1343,84	75,17	8,64	1339,25	131,63	8,31	1385	56	ν(3C-4C) + ν(6C-N)
1326,60	1,36	12,90	1323,18	12,76	26,97	1324,73	1,42	26,52			ν(C6-N) + δ(COH))
1287,74	167,67	2,07	1301,00	99,22	8,55	1295,06	139,73	5,84	1326	64	ν(5C-12C) + δ(14O-15H) + δ(4C-7H)
1229,01	0,85	3,11	1261,96	2,99	2,14	1245,62	0,91	1,18			ν(C-N) + ν(CC)
1169,46	140,33	12,13	1249,50	0,22	6,05	1233,26	0,51	3,48	1293	61	ν(6C-N) + δ(3C-8H) + δ(6C-9H)
1147,31	256,07	18,05	1158,56	144,86	47,67	1152,99	120,30	48,68	1252	58	ν(10C-2C) + δ(16O-17H) + δ(4C-7H)
1110,88	82,28	4,34	1141,75	139,17	51,33	1137,14	236,94	25,40	1217	60	ν(5C-12C) + δ(14O-15H)
1075,95	223,94	1,52	1098,02	4,91	13,88	1081,71	7,30	3,58	1160	64	□ (7H-4C-3C-8H)
1051,95	15,58	13,44	1057,82	298,38	1,00	1070,31	267,53	2,52	1116	57	ν(10C-16O) + δ(3C-8H)
1027,14	73,79	1,49	1039,59	117,98	3,27	1050,67	86,27	7,17	1009	65	ν(12C-14O) +□ (7H-4C-6C-9H)
973,33	0,15	1,17	978,94	69,97	0,09	972,46	43,38	0,14	930	69	Ring deformation + i.p.δ(CH)
964,17	20,58	0,64	951,14	0,00	1,20	947,38	0,00	1,12			o.o.p.δ(CH)
944,34	0,45	2,49	924,31	1,79	3,01	920,40	1,53	2,72			o.o.p. δ(CH)
852,26	6,13	0,37	843,46	9,77	1,70	838,05	8,58	1,18	892	75	o.o.p. δ(CH)
780,09	0,01	4,11	783,58	0,02	29,14	781,19	0,03	26,76			Pridine + □ COOH
773,59	0,01	26,54	768,57	0,01	1,59	767,45	0,00	2,02			o.o.p.[δ(pridine) + δ(COOH)]
722,36	156,90	0,43	704,40	112,91	0,27	705,32	119,78	0,34	799	58	o.o.p. w (COOH + CH)
677,00	178,80	0,04	685,94	15,84	3,14	679,19	26,80	1,79			o.o.p. w (COOH + CH)
671,08	50,82	0,63	674,36	109,44	0,25	675,02	134,16	0,14	748	56	□ COOH
614,69	0,07	4,73	618,92	0,70	11,38	614,14	0,21	9,01			□ COOH + pridine Wagging
591,99	2,52	4,62	606,14	112,94	0,39	598,61	2,21	1,81	669	74	□ COOH + pridine Wagging
562,37	180,78	0,35	603,76	1,77	0,99	593,24	131,09	0,47	633	84	Sym. δ(OH)
542,76	15,98	10,36	580,20	11,26	19,60	569,81	13,85	16,06			Asym.δ(OH)
493,62	1,72	0,88	499,82	0,80	1,08	496,90	1,00	0,99			δ(pridine-COOH)
461,25	44,83	0,02	469,86	24,86	0,06	466,87	29,71	0,05	544	68	δ(C-C=O)
420,37	18,96	0,01	430,80	23,85	0,02	427,90	25,54	0,01	487	71	δ(C-C-OH)
418,58	18,69	0,17	414,57	7,82	0,30	413,57	9,89	0,24	448	89	Wagging
394,81	3,83	0,19	383,97	3,87	0,31	384,95	3,93	0,28			Ring Torsion
271,00	0,01	3,78	279,11	0,01	3,81	275,88	0,01	3,57			COOH-pridine-□ COOH
229,17	1,11	0,54	234,11	0,94	0,86	230,20	1,03	0,74			z.z. δ(pridine-COOH)
225,15	0,28	1,22	224,06	0,22	0,39	222,64	0,23	0,62			wagging
135,63	3,09	0,02	139,06	2,41	0,02	136,63	2,67	0,02			Sym. δ(pridine-COOH)
73,82	0,04	0,01	70,64	0,00	0,01	71,26	0,02	0,07			□ agging
63,71	0,21	0,78	68,78	0,93	0,80	68,69	0,76	0,72			Torsion
40,13	5,30	0,09	46,85	3,04	0,00	47,75	3,62	0,01			COOH Torsion

ν; stretching, δ; in-plane bending, γ; out-of-plane (o.o.p.) bending, ρ; scissoring, ω; wagging, τ; torsion.

i.p; in plane, o.o.p; out of plane, asym:asymetric, sym: symmetric.

Table 4: Geometrical parametries of 2,5 PDA Bond Lenghts and Bond Angels

Bond	**HF**	**BLYP**	**B3LYP**	**Bond**	**HF**	**BLYP**	**B3LYP**
Lenghts (Å)	**6-31G(d)**	**6-31G(d)**	**6-31G(d)**	**Angels $^{(0)}$**	**6-31G(d)**	**6-31G(d)**	**6-31G(d)**
R(1,2)	1,321	1,356	1,341	A(2,1,6)	118,01	117,021	117,312
R(1,6)	1,314	1,344	1,332	A(1,2,3)	123,885	123,706	123,776
R(2,3)	1,384	1,41	1,399	A(1,2,10)	118,167	118,549	118,539
R(2,10)	1,504	1,511	1,503	A(3,2,10)	117,948	117,745	117,686
R(3,4)	1,383	1,4	1,391	A(2,3,4)	117,981	118,571	118,412
R(3,8)	1,071	1,091	1,084	A(2,3,8)	120,021	119,384	119,428
R(4,5)	1,385	1,41	1,399	A(4,3,8)	121,999	122,045	122,16
R(4,7)	1,073	1,091	1,085	A(3,4,5)	118,55	118,608	118,513
R(5,6)	1,392	1,415	1,404	A(3,4,7)	120,853	121,072	121,144
R(5,12)	1,487	1,496	1,488	A(5,4,7)	120,597	120,32	120344
R(6,9)	1,073	1,094	1,087	A(4,5,6)	118,497	118,213	118,412
R(10,11)	1,19	1,229	1,215	A(4,5,12)	122,919	123,339	123,341
R(10,16)	1,317	1,365	1,345	A(6,5,12)	118,586	118,449	118,447
R(12,13)	1,188	1,226	1,213	A(1,6,5)	123,08	123,882	123,576
R(12,14)	1,328	1,377	1,356	A(1,6,9)	117,111	116,887	117,105
R(14,15)	0,953	0,987	0,975	A(5,6,9)	119,809	119,231	119,32
R(16,17)	0,952	0,988	0,976	A(2,10,11)	122,675	123,46	123,154

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