Spectral study of some charge transfer complexes derived from some of drugs and acceptors in different solvents

A. A. K Al-Taiee   I. K. J. Al-dhmashee   S. D. Quddori

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Abstract

New charge-transfer (CT) complexes(10) were prepared from 3- methoxy 4- hydroxyl benzyldehyde(vanillin)، dimethyl aminebenzaladehyde with some aromatic amines (sulfa drugs) derivatives compounds as donor molecules with two acceptors molecules dinitrobenzene, and 2,4,6 trinitrophenol. The CT complexes were identified by FT-IR, melting points and UV-Vis spectra. The type of bonding between the donor and acceptor depends on the interaction between components were studies by UV-Vis spectra. The electronic absorption spectra of these compounds have been estimated under different polar solvents, some physical parameters of CT complexes have been calculated at the λ_{max} of each of them.Using Benesi-Hildebrands equation at25ºC, the equilibrium constant has been calculated.

Key Words: Schiff bases - Charge transfer complexes- polar solvent.

دراسة طيفية لبعض معقدات انتقال الشحنة المشتقة من بعض الأدوية والمستقبلات في مذيبات مختلفة

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الخلاصة

يتضمن البحث دراسة طيفية لبعض معقدات انتقال الشحنة المحضرة من تفاعل مشتقات مركبات (3- ميثوكسي -4 هيدروكسي بنزلديهايد و ثنائي مثيل امين بنزالديهايد مع بعض الامينات الاروماتية (ادوية سلفا) الجديدة (10 مركبات) والمشخصة طيفيا كجزيئات مانحة للالكترونات مع جزيئات مستقبلة للإلكترون هي ثنائي نيترو بنزين و 6,4,2 – ثلاثي نيترو فينول , وتم تشخيص هذه المعقدات المحضرة طيفيا باستخدام تقنية الأشعة تحت الحمراء وأطياف الأشعة فوق البنفسجية .ودرس هذا التداخل المعتمد على نوعية الجزيئتين المكونة للمعقد . بالإضافة إلى ذالك تم حساب بعض المعاملات الفيزيائية لهذه المركبات والمعقدات عند أقصى طول موجي λmax للمعقد ومطاوعة هذه المعقدات لمعادلة بنسي هلدبراند وفي مذيبات مختلفة القطبيةومنها تم حساب ثابت الاتزان في درجة حرارة 25 م°.

الكلمات الدالة: قواعد شيف – معقدات انتقال الشحنة – مذيب قطبي

Introduction

The study of the charge transfer complexes between several Schiff bases as electron donor and different electron acceptors such as [1] dinitrobenzene (DNB) ، (2, 4, 6-trinitro phenol (TNP). The equilibrium constants, the extinction coefficients of the CT complexes and the ionization potential of the acceptors were calculated. The Schiff bases were identified by using the IR and UV-visible and Mass Spectra [2-3], charge transfer complexes (CTC) with some acceptors exhibited wide applications [4]. Accordingly, much interest has been paid to molecular CTC. The formation of molecular complexes of (CT) type played an important role in many biological processes [5]. In another study, new molecular complexes of the CT type derived from the reaction Schiff bases derivative as a donor molecules with neutral molecules and acidic molecules as acceptors were synthesized [6].

Experimental

1-preparation of Schiff bases

Ten new Schiff bases were prepared by condensation of 3-methoxy-4-hydroxybenzaldehyde (vanillin) and Di-methyl amine benzaldehyde with five aromaticamine (Sulphadiazine, Sulphamirazine, Sulphadimine, Isoniazide, Sulphanilamide) in absolute

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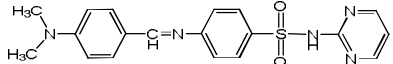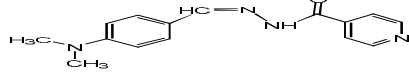
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ethanol [1,7,8,9,10] . The Schiff bases have been prepared as follows; equimolar quantities of the vanillin (1.53 gm, 1 mole) and the corresponding amine (1mole)were refluxed for (1hr) in (10-15 ml) absolute ethanol . Upon cooling a crystalline product was separated the solid was recrystallized from ethanol or normal hexane Table (1), the molecular structure of these Schiff characterized and identified by their melting point, element analysis, infrared (Shimadzu spectrophotometer Fourier transform (FTIR) as KBr disc) and spectra (recorded by uv-vis double –beam Schimadzu (UV-visible) spectrophotometer UV-1650 pc) using quartz cell (1cm) path length 2- Precipitation of CT complexes.

2-preparation of CT Complexes

The CT complexes form between two acceptors dinitrobenzene (DNB) ,tirnitrophenol (TNP) and Schiff base in (Absolute ethanol , methylene dichloride ($C_2H_4Cl_2$), chloroform (CHCl$_3$) ,carbon tetrachloride CCl$_4$ and (DMF) solvents for (1hr). The concentration of accepter ($1\times10^{-4}M$) were kept constant in every set of solution, while Schiff base concentrations were variable and were much greater ($\geq 1\times10^{-3}$) than the concentrations of the acceptors, This was done because bensi-Hildebrand's equation must be held for 1:1 molecular complex under this condition. The measurement of the electronic spectra of the CT complexes at λmax have been recorded

Table (1): physical properties of Schiff bases (donors).
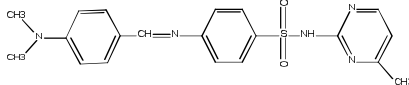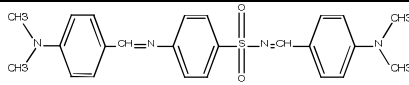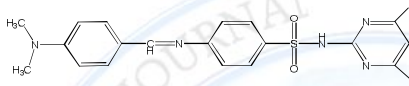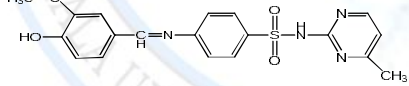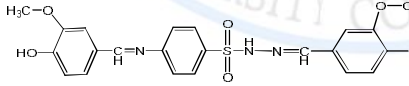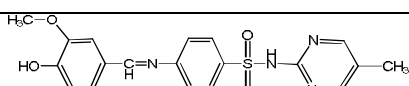
No. comp.	The name and the structure of Schiff base	M.p	W.MT g\mol	Color
A$_1$	4-(4-(dimethylamino)benzylideneamino)-N-(pyrimidin-2-yl)benzenesulfonamide	230-232	250.3	Yellowish Green
A$_2$	(Z)-N'-(4-(dimethylamino) benzylidene)isonicotinohydrazide	202-204	173.13	Yellow

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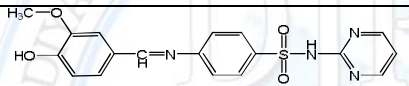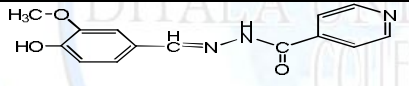|				
A$_3$	4-(4-(dimethylamino)benzylideneamino)-N-(4-methylpyrimidin-2-yl)benzenesulfonamide	220-222	264.31	Deep Yellow
A$_4$	N-(4-(dimethylamino)benzylidene)-4 (4(dimethylamino)benzylideneamino)benzenesulfona mide	219-221	172.21	Deep Yellow
A$_5$	4-(4-(dimethylamino)benzylideneamino)-N-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide	217-219	278.08	Reddish brown
C$_1$	4-(4-hydroxy-3-methoxybenzylideneamino)-N-(pyrimidin-2-yl)benzenesulfonamide	215-217	384.08	Pale Yellow
C$_2$	N'-(4-hydroxy-3-methoxybenzylidene)isonicotinohydrazide	227-229	271.09	Pale Yellow
C$_3$	4-(4-hydroxy-3-methoxybenzylideneamino)-N-(4-methylpyrimidin-2-yl)benzenesulfonamide	223-226	398.10	Pale Yellow
C$_4$	N'-(4-hydroxy-3-methoxybenzylidene)-4-(4hydroxymethoxybenzylideneamino)benzenesulfonohy ide	185-188	455.1	Deep Yellow
C$_5$	N-(4,5-dimethylpyrimidin-2-yl)-4-(4-hydroxy-3-methoxybenzylideneamino)benzenesulfonamide	184-185	412.12	yellowish orange

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Results and Discussion

1-IR Spectra

Table **(2)** represent the important bands were recorder for Schiff bases in the IR spectra, which indicate the formation of these compounds

Table (2): The major bands in IR spectrum for Schiff bases in (cm⁻¹).

No. comp.	C-H Alph	C=N	C═C	OH	SO$_2$	N-H Sulpha	Other
A$_1$	2937	1652	1492	-----	1325 1155	3257	C=NPyridine 1579
A$_2$	2923	1604	1434	-----	……..	3288	C=N Pyridine 1575 C=O 1662
A$_3$	2921	1633	1427	………..	1367 1180	3251	C=N Pyridine1525
A$_4$	2918	1652	1433	------	1371 1178	3274	C=N Pyridine 1606
A$_5$	2921	1650	1434	------	1369 1151	3253	C=N Pyridine 1598
C$_1$	2931	1654	1440	3421	1325 1155	3257	C=N Pyridine 1579 C-O 1261
C$_2$	3016	1631	1433	3487	1396 1188	3384	C=N Pyridine 1600 C-O 1280 C=O 1741
C$_3$	2846	1654	1450	3417	1365 1191	3230	C=N Pyridine 1577 C-O 1290
C$_4$	2846	1637	1413	3415	1365 1190	3230	C=N Pyridine 1575 C-O 1292
C$_5$	2964	1633	1431	3465	1380 1149	3253	C=N Pyridine 1596 C-O 1203

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Each of the compounds (1-10) under study was structurally characterized by melting points, and infrared. The absorption spectra of solutions in ethanol solvent were prepared for spectral registration in Schimadzu Rocco- 1650 UV-Vis at 25°C, in a quartz cell. From Table (2), the ultraviolet spectra of the compounds are characterized by three peaks between 307 – 237 nm, assigned to σ,π transition (of various origin) and charge transfer transition respectively. However, these three spectral bands exhibit different behaviors according to the nature of the substituents on the molecular structure of the compounds (1-10). Thus, we have observed two main effects according to the electron - donor and electron – acceptor roles of the substitute

Table (2) represent the important bands in the IR spectra of Schiff bases (1-10)$\nu_{C=C}$, $\nu_{C=N}$ and $\nu_{NH,}$ The IR spectra of compounds showed well defined bands; the stretching vibration modes of N-H group correspond to ν (amide) and ν (C=N), respectively, others appearance and disappearance of some bands in the IR spectra of these compounds respectively this indicating the formation of the synthesized compounds. The study has involved precipitation of that molecular charge transfer (CT) complexes by condensation molar quantities (1: 1).

Each one of our compounds (1-10) as charge donor and dinitrobenzene, trinitrophenol, as charge accepter. The solid complexes obtained are investigated by spectral and electrical methods, these tools (complexes were identified by their, IR and melting points, Tables (4-13), proved to be very helpful in investigating the type of interactions ,the nature of the bonding in these compounds and the nature of the acceptor neutral molecules (molecular compounds through electron transfer) .The acidic molecule will be formed through proton and electron transfer .The IR spectra of the CT complexes compared to those of the free components exhibit a new group with different intense bands, the varioustypes of interactions are discussed in the following:-

i - The ν_{C-H} bands of the donors part of the CT complexes are shifted to higher wave numbers where as those of the acceptors are shifted to lower values. This shift is observed with CT complexes involving π interaction in which a π- electron is transferred from the HOMO on the donor to the LUMO of the acceptor. This behavior reveals that, the electron transfer to the

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acceptor would originate from the donor, such CT interaction leads to obvious shifts in the NO_2 bands of the acceptors to lower wave numbers.

ii- The C=N bands of the donor parts of the CT complex showed different behavior depending on the n, π-electron densities beside to the proton transfer from the acceptor to the homogenous atom linkage, beside to the $v_{C=C}$, conjugated - C=N-N=C-, v_{SO2} and v_{C-O-C} bands in the CT complex shift to the lower wave number. A comparison between the IR spectra of the free components and those of the CT complexes revealed the presence of the interaction between the two molecules and formation of CT complexes .The appearance of $v_{OH \ bands}$ due to OH group indicating to the intermolecular hydrogen bonding involving the OH group (represented by the presence of broad band).

Table (3): The major bands in IR spectrum for CT In (cm^{-1}).

NO	No. of comp.	$vC-HAr\,cm^{-1}$	$v\ C=N\,cm^{-1}$	$v\ C=C\ cm^{-1}$	$vOH\,cm^{-1}$	$v\ N-H\,cm^{-1}$	$v\ N=O\ cm^{-1}$
1	$1A_1$	3034	1633	1492	......	3228	1328
2	$2A_2$	3033	1591	1529	....	3190	1326
3	$3A_3$	3041	1633	1492	......	3232	1328
4	$4A_4$	3080	1610	1451	.....	3334	1326
5	$5A_5$	3247	1598	1429	......	3397	1336
6	$6C_1$	3074	1581	1494	3423	3259	1325
7	$7C_2$	3033	1566	1469	3465	319	1321
8	$8C_3$	3078	1568	1473	3357	3263	1342
9	$9C_4$	3253	1622	1458	3442	3274	1321
10	$10C_5$	3037	1579	1492	3423	3259	1325
11	$11A_1$	3074	1598	1436	......	3240	1363
12	$12A_2$	3099	1583	1492	......	3256	1323
13	$13A_3$	3043	1589	1427	.....	3193	1367
14	$14A_4$	3037	1851	1494	......	3234	1325
15	$15A_5$	3101	1579	1440	......	3257	1325
16	$16C_1$	3035	1581	1494	3423	3256	1367
17	$17C_2$	3045	1591	1476	3407	3176	1365
18	$18C_3$	3076	1631	1492	3485	3244	1344
19	$19C_4$	3063	1596	1492	3483	3232	1328
20	$20C_5$	3076	1596	1494	3485	3242	1433

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2-Charge transfer complex (CT)

The solution of all complexes in ethanol (CH_3CH_2OH), ethylene di Chloride ($C_2H_4Cl_2$), $CHCl_3$, CCl_4 and DMF are obeyed Benesi-Hildbrand equation (1) (Fig-1) show a typical example of the application of this equation . The solution of our Schiff bases with TNP and DNB absorb light in the visible region Tables (4-13). The Schiff base may act as an n-electron donor and the molecules as electron acceptors. Equation (1) was used to calculate the extinction coefficients and equilibrium constants for our CT complexes.

$$\frac{[A_0]L}{Abs} = \frac{1}{\varepsilon_{CT}} + \frac{1}{K.\varepsilon_{CT}} \cdot \frac{1}{[D_o]} \ldots\ldots(1)$$

[Ao] and [Do] are the concentrations of the electron acceptor and Schiff bases (electron donor) respectively, L is the path length, O.D$_{CT}$ the optical density of CT complex at λmax. ε_{CT} the molar extinction coefficient and K the equilibrium constant. Equation (2) was used to calculate the equilibrium constant[11].

The plot of

$$\frac{[A_0]L}{Abs} VS. \frac{1}{[D_o]}$$

Gave a straight line of slop ……… $\dfrac{1}{K.\varepsilon_{CT}}$

And intercept ……………….. … $\dfrac{1}{\varepsilon_{CT}}$

Form the value of intercept calculated and the ε_{CT} value of slope and intercept was used to calculated equilibrium constant as follow

$$K_{CT} \frac{Intercept}{Slop} = \frac{1}{\varepsilon_{CT}} \bigg/ \frac{1}{K.\varepsilon_{CT}} \qquad \ldots\ldots\ldots.. (2)$$

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Tables (4-13) represent the values of ε_{CT} and K_{CT}. The ionization potential (IP) of Schiff bases , Its value can be determined form the electronic absorption spectra , and the dissociation energies of the excited state (W) of their CT complexes were calculated using following equation[11] (3)

$$hv_{CT} = Ip - E_A - W$$
....(3)

E_A is the electron affinity of the acceptor derived in terms of simple valance- bond description. Similar linear relationships have been described for complexes of many other acceptors .In general:

$hv_{CT} = a\, Ip + b$ ……………………(4)

This equation (4) is very important to estimate the value of the acceptor factor (a,b). the electron transfer originates from the same position of each Schiff bases and not affected by the other group of molecules to the acceptors , forming CT complex of the same geometry for all Schiff bases and obey Benesi–Hildebrand'sequation for 1:1 complexes (the ratio of these complexes) and the only unoccupied orbital available in acceptors ,is the π^* and the molecules Schiff bases are very rich in n-electrons ,therefore ,the value of the physical parameters with the same Schiff bases similarly the type of CT complexes with accepters are $(\pi \rightarrow \pi^*)$.

Table (4): The some physical parameters of Schiff bases and their CT complexes with the acceptor in C_2H_5OH

Com NO.	λ_{max} (nm)	K_{Ct} (mol^{-1} . dm^3)	hv_{cT}(eV)	Ip(eV)	W(eV)	ε_{max} m^2.mol^{-1}
1	429	166	2.89	7.98	3.78	1000
2	406	142	3.06	8.15	3.78	1000
3	435	200	2.85	7.94	3.78	5000
4	451	250	2.75	7.84	3.78	1000
5	405	250	3.06	8.15	3.78	1000
6	433	285	2.87	7.14	2.96	5000
7	409	150	3.03	8.12	3.78	3333
8	450	200	2.76	7.85	3.78	1666
9	457	300	2.71	7.80	3.78	3333
10	405	250	3.06	8.15	3.78	2000

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Table (5): The some physical parameters of Schiff bases and their CT complexes with the acceptor TNP DNB in C_2H_5OH

Com NO.	λ_{max} (nm)	K_{cT} ($mol^{-1} . dm^3$)	$h\nu_{cT}$(eV)	Ip(eV)	W(eV)	ε_{max} $m^2.mol^{-1}$
1	406	571	3.91	9.01	4.63	2500
2	404	333	3.06	8.15	3.78	3333
3	410	444	3.04	8.14	3.78	2500
4	413	500	3.00	8.09	3.78	2500
5	400	624	3.07	8.17	3.78	2000
6	408	666	2.76	7.85	3.78	1666
7	405	400	3.06	8.15	3.78	5000
8	414	666	2.75	7.85	3.78	2500
9	430	500	3.22	8.31	3.78	5000
10	390	666	3.01	8.10	3.78	5000

Table (6): The some physical parameters of Schiff bases and their CT complexes with the acceptor TNP in CCl_4

Com NO.	λ_{max} (nm)	K_{cT} ($mol^{-1} . dm^3$)	$h\nu_{cT}$(eV)	Ip(eV)	W(eV)	ε_{max} $m^2.mol^{-1}$
1	376	1333	3.30	8.39	3.78	3333
2	357	888	3.48	8.57	3.78	1250
3	377	1500	3.29	8.38	3.78	3333
4	400	1000	3.10	8.19	3.78	3333
5	357	1200	3.48	8.57	3.78	1666
6	380	2500	3.27	8.36	3.78	2000
7	358	1000	3.47	8.56	3.78	1666
8	385	1650	3.22	8.31	3.78	3333
9	402	1333	3.09	8.15	3.75	2500
10	358	1666	3.47	8.56	3.78	2000

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Table (7): The some physical parameters of Schiff bases and their CT complexes with the acceptor DNB inCCl4

Com NO.	λ_{max} (nm)	K_{cT} ($mol^{-1} . dm^3$)	$h\nu_{cT}(eV)$	$I_p(eV)$	$W(eV)$	ε_{max} $m^2.mol^{-1}$
1	353	1333	3.25	8.34	3.78	3333
2	313	1000	3.97	9.06	3.78	2000
3	366	1750	3.39	8.48	3.78	1428
4	400	2500	3.10	8.19	3.78	2000
5	305	1250	4.07	9.16	3.78	2000
6	371	3333	3.35	8.44	3..78	3333
7	325	1500	3.82	8.91	3.78	3333
8	380	2222	3.27	8.36	3.78	5000
9	401	2666	3.09	8.18	3.78	1250
10	311	3000	3.99	9.08	3.78	3333

Table (8): The some physical parameters of Schiff bases and their CT complexes with the acceptor TNP in CHCl3

Com NO.	λ_{max} (nm)	K_{cT} ($mol^{-1} . dm^3$)	$h\nu_{cT}(eV)$	$I_p(eV)$	$W(eV$	ε_{max} $m^2.mol^{-1}$
1	399	777	3.11	8.20	3.78	1428
2	396	625	3.13	8.22	3.78	2000
3	405	875	3.06	8.15	3.78	1428
4	407	666	3.05	8.14	3.78	1666
5	378	888	3.28	8.37	3.78	1250
6	402	1333	3.09	8.18	3.78	2500
7	396	666	3.13	8.22	3.78	5000
8	406	1000	3.06	8.15	3.78	3333
9	408	714	3.04	8.13	3.78	2000
10	386	1000	3.22	8.31	3.78	1000

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Table (9): The some physical parameters of Schiff bases and their CT complexes with the acceptor DNB inCHCl₃

Com NO.	λ_{max} (nm)	K_{cT} (mol^{-1} . dm³)	$h\nu_{cT}$(eV)	Ip(eV)	W(eV)	ε_{max} m².mol^{-1}
1	380	1000	3.27	8.45	2.94	3333
2	371	777	3.35	8.50	2.94	1428
3	400	1333	3.10	8.25	2.94	1428
4	404	888	3.07	8.22	2.94	1250
5	346	1000	3.59	8.74	2.94	1666
6	400	1666	3.10	8.25	2.94	2000
7	383	875	3.24	8.39	2.94	2000
8	402	2500	3.09	8.24	2.94	3333
9	405	1000	3.06	8.21	2.94	1000
10	378	1333	3.28	8.43	2.94	2500

Table (10): The some physical parameters of Schiff bases and of their CT complexes with the acceptor TNP in (CH₂)₂Cl₂

Com NO.	λ_{max} (nm)	K_{cT} (mol^{-1} . dm3)	$h\nu_{cT}$(eV)	Ip(eV)	W(eV)	ε_{max} m².mol^{-1}
1	406	571	3.91	9.01	4.63	2500
2	404	333	3.06	8.15	3.78	3333
3	410	444	3.04	8.14	3.78	2500
4	413	500	3.00	8.09	3.78	2500
5	400	624	3.07	8.17	3.78	2000
6	408	666	2.76	7.85	3.78	1666
7	405	400	3.06	8.15	3.78	5000
8	414	666	2.75	7.85	3.78	2500
9	430	500	3.22	8.31	3.78	5000
10	390	666	3.01	8.10	3.78	5000

Spectral study of some charge transfer complexes derived from some

of drugs and acceptors in different solvents

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Table (11): The some physical parameters of Schiff bases and of their CT complexes

with the acceptor DNB in $(CH_2)_2Cl_2$

Com NO.	λ_{max} (nm)	K_{cT} ($mol^{-1} . dm^3$)	$h\nu_{cT}$(eV)	Ip(eV)	W(eV)	ε_{max} $m^2.mol^{-1}$
1	401	666	3.99	9.14	2.94	1666
2	396	500	3.13	8.28	2.94	2500
3	402	625	3.09	8.24	2.94	2000
4	405	571	3.06	8.21	2.94	2500
5	381	666	3.26	8.41	2.94	2500
6	404	714	3.07	8.22	2.94	2000
7	403	500	3.08	8.23	2.94	5000
8	405	875	3.06	8.21	2.94	1428
9	406	800	3.06	8.21	2.94	2500
10	385	777	3.22	8.37	2.94	1428

Table (12): The some physical parameters of Schiff bases and their CT complexes with

the acceptor TNP in DMF

Com NO.	λ_{max} (nm)	K_{cT} ($mol^{-1} . dm3$)	$h\nu_{Ct}$(eV)	Ip(eV)	W(eV)	ε_{max} $m^2.mol^{-1}$
1	438	100	2.83	7.92	3.78	5000
2	412	100	3.01	8.10	3.78	1000
3	452	112	2.75	7.84	3.78	10000
4	448	111	2.77	7.86	3.78	1000
5	419	125	2.96	8.05	3.78	1111
6	439	111	2.83	7.92	3.78	10000
7	428	100	2.90	7.99	3.78	1250
8	451	114	2.75	7.84	3.78	2000
9	457	140	2.71	7.80	3.78	1428
10	431	150	2.88	7.97	3.78	3333

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Table (13): The some physical parameters of Schiff bases and their CT complexes with the acceptor DNB inDMF

Com NO.	λ_{max} (nm)	K_{cT} (mol^{-1} . dm^3)	$h\nu_{cT}$(eV)	Ip(eV)	W(eV)	ε_{max} m^2.mol^{-1}
1	411	125	3.02	8.17	2.94	2000
2	407	100	3.05	8.20	2.94	3333
3	422	114	2.94	8.09	2.94	1250
4	430	200	2.89	8.04	2.94	1250
5	410	150	3.03	8.18	2.94	3333
6	418	200	2.97	8.12	2.94	1666
7	409	112	3.03	8.18	2.94	1111
8	421	142	2.95	8.10	2.94	1000
9	426	200	2.91	8.06	2.94	5000
10	412	166	3.01	8.16	2.94	1000

Table (14): the physical parameters of Schiff Bases and of their CT complexes with the acceptor TNP in different solvent

CH$_3$CH$_2$OH		CCl$_4$		CHCl$_3$		C$_2$H$_4$Cl$_2$		DMF	
$h\nu_{cT}$(eV)	K_{cT} (mol^{-1} dm^3)	$h\nu_{cT}$(eV)	K_{cT} (mol^{-1} . dm^3)	$h\nu_{cT}$(eV)	K_{Ct} (mol^{-1} . dm)	$h\nu_{cT}$(eV)	K_{cT} (mol^{-1} . dm)	$h\nu_{cT}$(eV)	K_{cT} (mol^{-1} . dm^3)
2.89	166	3.30	1333	3.11	777	3.91	571	2.83	100
3.06	142	3.48	888	3.13	625	3.06	333	3.01	100
2.85	200	3.29	1500	3.06	875	3.04	444	2.75	112
2.75	250	3.10	1000	3.05	666	3.00	500	2.77	111
3.06	250	3.48	1200	3.28	888	3.07	624	2.96	125
2.87	285	3.27	2500	3.09	1333	2.76	666	2.83	111
3.03	150	3.47	1000	3.13	666	3.06	400	2.90	100
2.76	200	3.22	1650	3.06	1000	2.75	666	2.75	114
2.71	300	3.09	1333	3.04	714	3.22	500	2.71	140
3.06	250	3.47	1666	3.22	1000	3.01	666	2.88	150

Spectral study of some charge transfer complexes derived from some of drugs and acceptors in different solvents
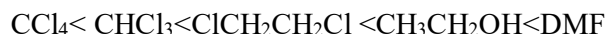
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Table (15): The physical parameters of Schiff Bases and of their CT complexes with the acceptor DNB in different solvent

CH₃CH₂OH		CCl₄		CHCl₃		(CH₂)₂Cl₂		DMF	
hv_{cT}(eV)	K_{ct} (mol⁻¹ . dm³)	hv_{cT}(eV)	K_{cT} (mol⁻¹ . dm³)	hv_{cT}(eV)	K_{cT} (mol⁻¹ . dm³)	hv_{cT}(eV)	K_{ct} (mol⁻¹ . dm³)	hv_{cT}(eV)	K_{cT} (mol⁻¹ . dm³)
3.91	571	3.25	1333	3.27	1000	666	3.99	3.02	125
3.06	333	3.97	1000	3.35	777	500	3.13	3.05	100
3.04	444	3.39	1750	3.10	1333	625	3.09	2.94	114
3.00	500	3.10	2500	3.07	888	571	3.06	2.89	200
3.07	624	4.07	1250	3.59	1000	666	3.26	3.03	150
2.76	666	3.35	3333	3.10	1666	714	3.07	2.97	200
3.06	400	3.82	1500	3.24	875	500	3.08	3.03	112
2.75	666	3.27	2222	3.09	2500	875	3.06	2.95	142
3.22	500	3.09	2666	3.06	1000	800	3.06	2.91	200
3.01	666	3.99	3000	3.28	1333	777	3.22	3.01	166

Conclusions

The compounds (1-10) under consideration, allowed to interact with acceptor molecules to form CT complexes under investigation takes place $\pi \rightarrow \pi^*$ type transitions .The solutions of all complexes obeyed to Benesi-Hildbrands equation. The ratio of Schiff bases derivative: acceptor in every cases is 1:1. the values of some physical parameters for all compounds and CT complexes (Ip , E_{CT} ,W, K_{CT} , ε_{CT}) were calculated , and found to be affected with both the nature of acceptors. The values of ionization potentials for the compounds (1-10) vary with the following order TNB>TNP, and for K_{CT} the following order DNB> TNP. The CT complex was spontaneously formation, but very weak in solution and have a slower rate of the hydrolysis was observed .It was also observed that the solvent significant effect on ultraviolet radiation spectra of charge transfers complexes where cause polar dislodge increase red as in following order:

$$CCl_4< CHCl_3<ClCH_2CH_2Cl <CH_3CH_2OH<DMF$$

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It was also calculate equilibrium constant of complexes consisting of Schiff bases that prepared from 3- methoxy -4-hydroxybenzaldehyde (vanillin) be greater than dimethyl amine benzaldehyde because of having a group (OH) driving electron
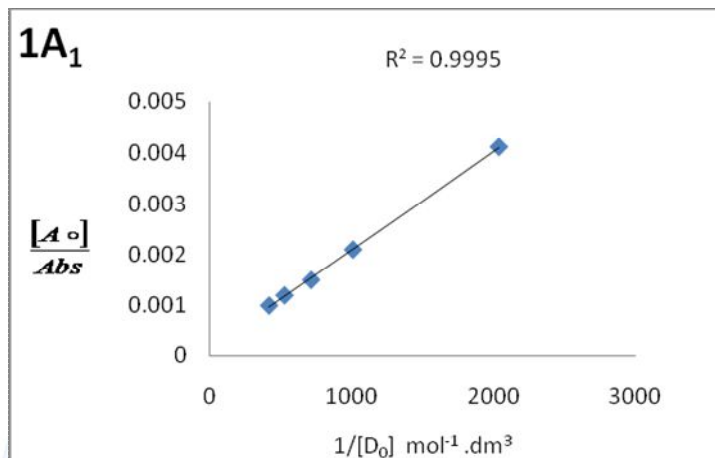
Figure (1): Application of Benesi-Hildbrands equation for the CT complex of Compound (1) with T.N.P in CH_3CH_2OH

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