98th Indian Science Congress

January 3-7, 2011, Chennai

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Vibrational Spectroscopy: An Excellent Tool for Characterisation of Biomolecules

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Abstract : Vibrational spectroscopy is one of the most powerful methods for the characterisation of biomolecules. Spectroscopic investigations of nucleic acid bases may help to throw light on the role of them in biological systems. With the development of experimental technology in past decade, the spectroscopic studies on the vibrational properties of biological macromolecules, such as nucleic acid bases and their derivatives have been developed quickly. The structural and vibrational properties of uracil and its 5-substituted derivatives (5XU; X=F,Cl, Br, I, CH_3, NH_2 ,NO_2) are presented with special emphasis on anticarcinogenic drug 5-fluorouracil as representative.

1 Introduction

Spectroscopy originating from the solar spectrum observed for the first time by Sir Issac Newton's in 1866 has been developed today into a number of branches apparently independent of one another. Among the various branches of spectroscopy, the vibrational spectroscopy which employs Infrared and Raman experimental techniques is of special importance for getting an insight into the molecular properties. The vibrational spectroscopy is undergoing rapid developments and above all IR and Raman techniques have become highly multidisciplinary. The introduction of laser during 1960's stimulated and revolutionized vibrational spectroscopy and perhaps Raman spectroscopy has most benefited from lasers, which could easily be visualized by the fact that by using powerful tunable lasers and principles of nonlinear optical mixing, it is now possible to record vibrational spectra of many compounds, which could previously not be observed by other conventional sources of light. In fact, its versatility, ease of sampling via coupling to fiber optics, macrooptical arrangements and microscopes, non-destructive, non-invasive and very often highly selective, and the ability to sample through glass which permit to be used to study the species in all physical forms including solution, have converted Raman spectroscopy, a very powerful analytical technique. Physicists, chemists, molecular-

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biologists, medical doctors and engineers all contribute to the multifaceted developments in methodologies and applications of vibrational spectroscopy. New strategies are evolving to push the molecular size limits to even higher values, the systems being investigated are getting bigger and bigger and even the nucleic acids and metal complexes are being investigated to understand the mechanism of specific recognitions occurring in living systems.

Now-a-days the investigation of the behavior as well as the metabolism of biomolecules on a molecular level has become centre to scientific field such as medical, pharmaceutical, microbiological diagnostics. Understanding of cellular processes is necessary for the development of new biotechnologies, medical diagnostics, newly designed drugs, as well as in food and environmental technology. So far standard techniques such as optical microscopy, fluorescence spectroscopy and immunoarrays have dominated the field of bioanalysis because of its high sensitivity. However, all these methods suffer from the lack of specificity and reveal only little or no molecular information. Vibrational spectroscopy provides information on a molecular level without labelling the biomolecule, [1]

The number of groups active in the field underline the potential of vibrational spectroscopy and specially Raman spectroscopy as a powerful tool in biological, medical, pharmaceutical and environmental applications. Puppels and colleagues have reviewed a variety of biomedical applications, where the status of the field and the technical requirements for the clinical implementation were critically discussed [2, 3].

IR and Raman Spectroscopy

When light is incident on matter (e.g on a biological cell, tissue, microorganism or mineral) it can interact with the atoms or molecules in different manners. Photons can be absorbed directly or can be scatterd. Absorption of light is most likely if the wavelength of the radiation is in the infrared (IR), visible (VIS) or in the ultraviolet UV spectral region. The IR absorption results in an excitation of vibrational modes of the molecule, while the VIS or UV absorption results in the excitation of an electronic transition which is often followed by a radioactive emission called fluorescence [B Schrader, *Infrared and Raman Spectroscopy: Methods and Applications,* VCH, Weinheim, 1995]. In Fig 1 the mechanism of fluorescence (A) and IR absorption (B) are shown.

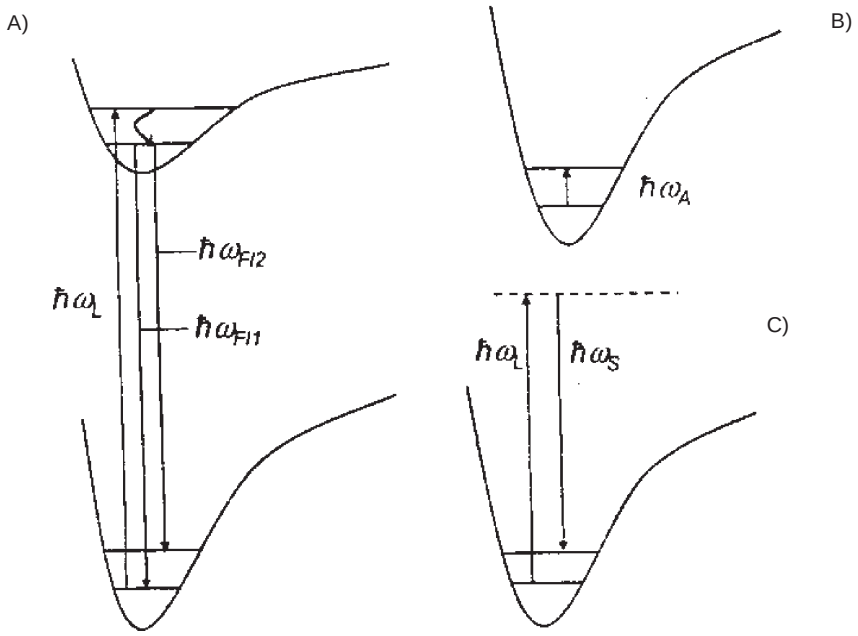


Fig 1. Simple model illustrating
(A) Fluorescence, (B) IR Absorption and (C) Raman scattering

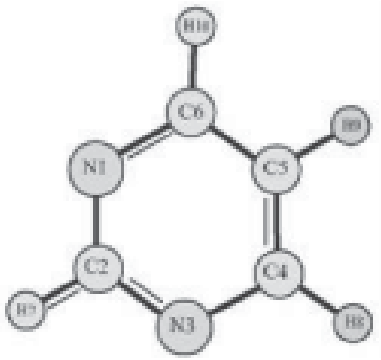
When light is scattered from a molecule most photons are scattered elastically. The scattered photons have the same energy (wavelength) as the incident photons. However, a small fraction of light (approximately 1 out of 10^8 photons) is scattered at optical frequencies different from the frequency of the incident photons. The process leading to inelastic scattering is called Raman effect. An energy transfer occurs as a result of the coupling between the incident radiations and the quantized states of the scattering system (schematically depicted in Fig 1 c). Depending on the coupling the incident photons either loose (Stokes) or gain (anti-Stokes) energy on the vibrational-rotational level or on the electronic level [J Popp, W Kiefer, Encyclopedia of Analytical Chemistry, ed. R A Mayer, Vol. 21, John Wiley & Sons, N Y, 2000, pp 13104-13143]. The scattered light with lower energy as compared to the incident laser light is called Stokes Raman scattering and the radiation with higher energy is referred to as anti-Stokes Raman scattering

Nucleic Acids Base Derivatives

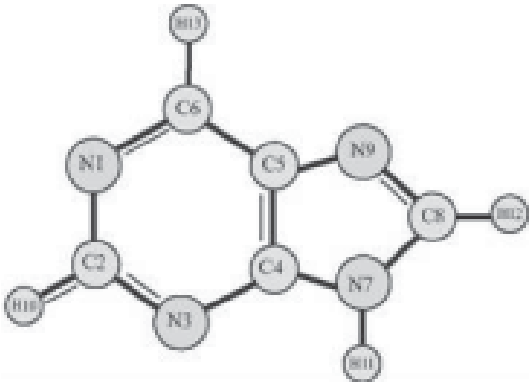
Cell is the first step in the creation of life. The fundamental structural units of a cell are the nucleic acids, the proteins and the phosphates. The most significant constituents of the nucleic acids, which impose upon them their biological activity, are the purine and

pyrimidine bases- Adenine, Guanine, Thymine, Cytosine and Uracil, which are conjugated heterocyclic molecules. These molecules and their derivatives are of considerable importance, because some of them are the basic constituents of DNA and RNA and play an important role in constitution and properties of nucleic acids. Recent spectroscopic studies of these compounds and their derivatives have been motivated because the vibrational spectra of free base molecules is very useful for the understanding of specific biological processes and in the analysis of relatively complex systems. Along the macromolecular double- helix chain, the vibrational modes of each base interact with those of other bases through hydrogen bonds or stacking effects and these interaction affect the ring vibrations.

The largest and most fascinating molecules, found in living organism today are the nucleic acid molecules. All the evidences indicate that the nucleic acids are the molecules



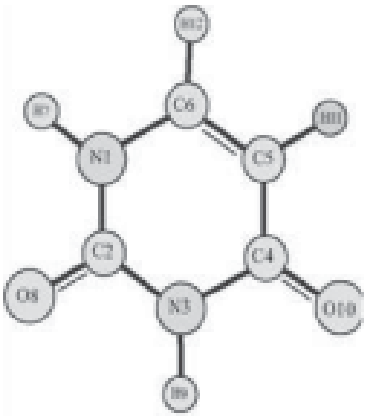
Pyrimidine (First isolated by Gabriel and Colman, 1899)
(a)



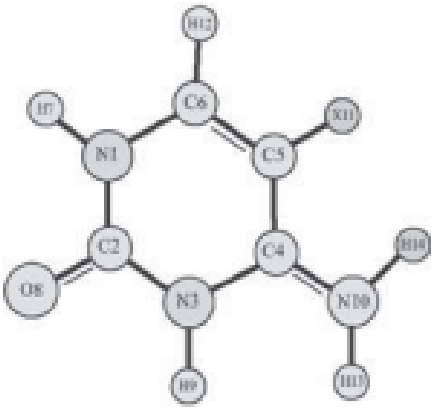
Purine
(b)

Fig 2. Structures of (a) Pyrimidine and (b) Purine

that exert primary control over the basic life processes in all organisms. The nucleic acids consist of two types of nitrogen bases: pyrimidines and purines. Though pyrimidine does not exist in nature but pyrimidines are considered to be important because they are the integral part of genetic material, viz. DNA and RNA as nucleotides and Nucleosides. The important pyrimidine bases found in the nucleic acid comprise cytosine, uracil and thymine. Of these, uracil and its derivatives are most useful and have been found to exhibit interesting biological and chemotherapeutic properties.



(a)
Uracil



(b)
Cytosine

(c)
Thymine

Fig 3: Structures of (a) Uracil , (b) Cytosine, and (c) Thymine

2. Theoretical Methods of Predicting Vibrational Spectra

In general the motivation for predicting vibrational spectra is to make vibrational spectroscopy a more practical tool. Computational methods can be used to assign the bands of the spectra.

Quantum chemical methods using the Density Functional (DFT) [6] theory provide a very good overall description of medium-size molecules. Among the DFT methods, those obtained by B3LYP, were selected as more appropriate. Moreover, for the wavenumber calculations [1] they appear more accurate than HF and MP2 [7] methods, and at lower computational cost. The Becke's three-parameter exchange functional (B3) [8] in combination with the correlation functional of Lee, Yang and Parr (LYP) [9], i.e. B3LYP, appears as the best and more used. The results obtained with several basis set differing in size and contraction are shown in the different Tables, starting with the 6-31G**. The 6-311++G(3df,pd) basis set represents the most accurate for geometrical parameters, but it is prohibited in computational memory required for wavenumber calculations. The 6-311+G(2d,p) basis is optimum for this purpose. The B3LYP results were determined with the GAUSSIAN 03 [10] program package.

Section I: The main interest of this section is to give an accurate molecular structure and vibrational wavenumbers of uracil molecule.

The importance of uracil (in short U) and its derivatives is indicated actually by the considerable number of publications appeared in the bibliography. Uracil is a pyrimidine base and it belongs to a group of the most important pyrimidines that play a fundamental role in the structure and function of enzymes and drugs.

Geometry Structure and Vibrational Wavenumbers of Uracil Molecule

Many studies have been reported on this molecule and its structure has been clearly established, Fig. 4. Although theoretically, geometrical optimizations at the MP2/6-311G* [11] level have been reported, the most accurate results today are shown in Table 1. The labeling of the atoms appears in Fig. 4. Experimental data have been reported by x-ray [12] and by ED [13]. Crystalline uracil is constituted by four molecules of C_s point symmetry per unit cell. The four molecules are arranged into two hydrogen-bonded dimers. All the experimental and theoretical studies on uracil have shown that the dioxo-dilactam tautomer U1, (Fig. 4), is the predominant form either in the gas phase or in solution or even in the solid state.

Table 1. Equilibrium geometries of uracil, bond lengths in **Å** and bond angles in degrees. The calculated values are with different DFT methods and basis set.

Parameters	B3LYP					MPW1	B97-1[a]			CCSD[a]	RX[b]	RX[c]	ED[d]
	6-31G**	6-311++G (2d,p)	6-311++G (3df,pd)	aug-cc-pVDZ	aug-cc-pVTZ	6-31G**	6-31G**	6-311+G (2d,pd)	aug-cc-pVDZ	6-31G**			
Bond lengths													
N1-C2	1.3947	1.3906	1.3893	1.3937	1.3895	1.3873	1.396	1.392	1.395	1.386	1.371	1.374	1.399[e]
C2-N3	1.3843	1.3805	1.3792	1.3842	1.3794	1.3775	1.386	1.382	1.385	1.385	1.377	1.381	1.399[e]
N3-C4	1.4129	1.4093	1.4076	1.4123	1.4080	1.4046	1.414	1.410	1.413	1.405	1.371	1.380	1.399[e]
C4-C5	1.4601	1.4554	1.4548	1.4599	1.4546	1.4556	1.464	1.459	1.463	1.466	1.430	1.444	1.462
C=C	1.3499	1.3443	1.3435	1.3528	1.3435	1.3463	1.353	1.348	1.356	1.347	1.340	1.343	1.343
N1-C6	1.3755	1.3722	1.3705	1.3763	1.3709	1.3688	1.376	1.373	1.377	1.382	1.359	1.370	1.399[e]
C2=O	1.2169	1.2120	1.2103	1.2189	1.2117	1.2124	1.217	1.212	1.219	1.218	1.215	1.219	1.212[f]
C4=O	1.2195	1.2146	1.2129	1.2110	1.2143	1.2148	1.220	1.215	1.221	1.219	1.245	1.233	1.212[d]
Bond angles													
N-C2-N	112.81	113.13	113.07	113.17	113.06	112.87	112.8	113.1	113.1	113.0	114.0	115.4	114.6
C2-N-C4	128.31	127.88	127.96	127.94	127.97	128.40	128.4	128.0	128.0	128.4	126.7	126.4	1260
N3-C4-C5	113.39	113.68	113.64	113.70	113.61	113.38	113.3	113.6	113.6	113.5	115.5	114.1	115.5
C4-C=C	119.93	119.83	119.80	119.78	119.85	119.78	119.9	119.7	119.7	119.7	118.9	120.7	119.7
N3-C2=O	124.47	124.18	124.23	124.17	124.23	124.41							
C4-N3-H	116.16	116.38	116.31	116.37	116.32	116.13							
N3-C4=O	120.37	120.22	120.25	120.14	120.23	120.39	120.4	120.3	120.2	120.6	119.2	120.5	120.2
C4-C5-H	118.14	118.24	118.26	118.31	118.23	118.24	118.2	118.3	118.4	118.2			

[a]From ref. [14]. The B97-1 DFT method appear described in ref. [15]. [b]Ref. [12a]. [b]Ref. [13]. [e]r(C-N) mean value [f]r(C=O) mean value

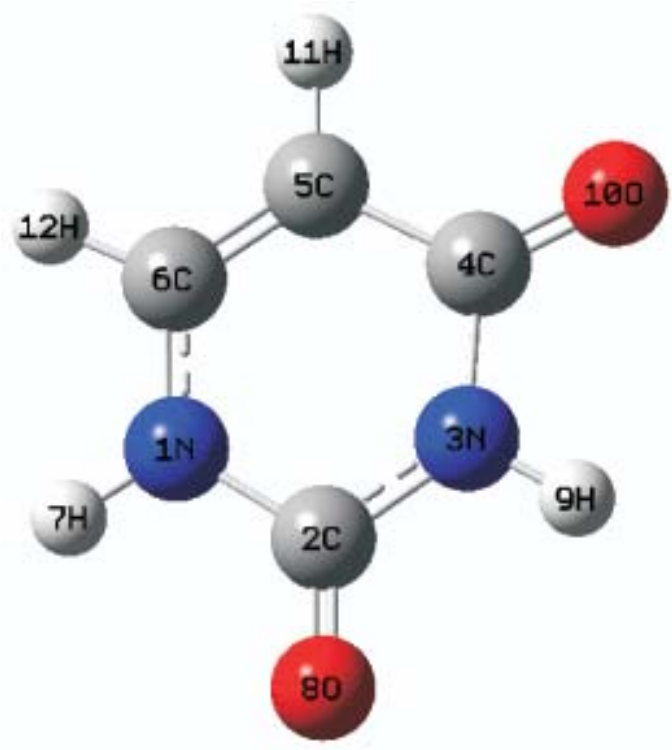


Fig. 4. Labeling of the atoms in uracil molecule.

Table 2 shows a comparision of the experimental and calculated harmonic wavennumbers and in Fig. 5 the ring modes characterized at B3LYP/6-31G** level in uracil molecule are plotted .

Section II

A survey of large number of synthetic pyrimidines having interesting biological properties reveals that in such compounds, the position of importance are C-5 and C-6 positions.

Uracil and its derivatives, constituents of the genetic material, play a fundamental role in basic biological processes. The transformation of uracil into 5-X Uracil (X= F,Cl, Br,I) significantly changes its chemical and spectroscopic properties, as well its *in vivo* activity. The biological activity of 5-XU (X= F, Cl,Br,I) is not fully understood and requires continuous studies.

5-Fluorouracil (5-FU) is a drug that is used in the treatment of Cancer. It belongs to the family of drugs called Antimetabolite. It is a pyrimidine analogue.

Table 2a. Comparison of the experimental wavenumbers (ν, cm^{-1}) and calculated harmonic values (ω, cm^{-1}) with the 6-31G** basis set, together with their relative (A, %) infrared intensities, relative Raman scattering activities (S, %), force constants (f, mDyne/Å), and characterization obtained in the normal ring modes of uracil molecule with some of the methods used.

No.	Characterization[a]	HF	MP2[c]	B3P86	B3PW91	B3LYP				B3LYP[e]		Infrared[b]		
		ω	ω	ω	ω	ω	ω[d]	A	f	ω	S	Ar matrix[f]	gas[g]	gas[h]
1	puckering N3	167	139	151	151	150	147	0	0.12	154	0			
2	puckering N1	179	161	171	171	170	165	0	0.10	171	0	185 w	185 w	
3	δ(OCNCO)	426	383	385	385	385	387	4	1.07	384	1	391 m	377 m	374 vw
4	γ(C=C-H12)	429	379	397	396	396	395	4	0.26	405	1	411 m	411 m	395 w
5	δ(ring)	561	518	519	518	519	523	4	1.26	519	2	516.5 m	527 m	512 w
6	δ(ring) + δ(C=O)	593	541	543	542	541	543	1	1.09	539	4	536.4 m		
7	δ_{as}(ring) + δ(C=O)	609	560	560	559	558	547	1	0.20	556	2	559 w	588 w	
8	γ(N1-H)	588	566	571	570	563	560	8	1.24	580	0	551.2 m	556 m	545 w
9	γ(N3-H)	730	698	693	692	687	677	14	0.31	699	1	662.1 s	633 m	659.5 w
10	γ(C4=O) + γ(C5-H)	803	782	732	731	729	728	2	0.63	727	0	718 w		717.4 vw
11	γ(C2=O)	862	722	760	759	752	765	10	2.73	763	0		769 s	756.5 w
12	ν(ring)	829	738	781	779	772	769	0	2.92	769	23	759.2 sh?		
13	γ(C5-H) + γ(C4=O)	905	799	814	814	813	819	10	0.97	821	0	804 s	810 s	802 w
14	ν(C-C) + δ(N-H)	1053	990	975	970	965	962	1	1.43	962	3	958.3 w	946 vw	952 w
15	γ(C6-H)	1110	930	971	973	970	972	0	0.72	970	2	963 w	974 w	972 sh

16	δ(NCC)	1076	999	994	993	990	994	1	3.43	988	1	982 w	999 w?	990 sh
17	ν(ring) + δ(C5-H)	1175	1113	1098	1097	1091	1086	1	1.42	1085	6	1073 w	1089 s?	1082 m
18	ν(C-N)+δ(C6H,N1H)	1306	1236	1210	1209	1198	1191	14	2.03	1195	0	1184 vs		1172 s
19	δ(C5-H) + δ(N-H)	1347	1273	1240	1237	1231	1227	1	1.22	1224	15	1217.4 w	1228 m	
20	δ(N3-H) + δ(C-H)	1530	1413	1388	1387	1382	1382	3	2.28	1378	13	1359.3 vw	1360 m	1356 sh
21	ν(C-N) + δ(N3-H)	1554	1436	1417	1415	1407	1406	20	2.95	1401	2	1388.7 vs	1380 s	1387 s
22	δ(C6-H) + δ(N-H)	1557	1449	1428	1426	1422	1423	3	2.08	1411	1	1399.6 vs	1396 ms	1400 s
23	δ(N1-H) + ν(N1-C)	1647	1536	1520	1518	1506	1498	18	3.41	1497	10	1472 ms	1480 s	1461 s
24	ν(C=C)	1847	1712	1704	1701	1690	1670	12	8.51	1672	24	1644 m	1632 vs	1641 s
25	ν(C4=O)	1995	1826	1830	1826	1808	1757	100	14.68	1760	55	1741 vs	1688 vs	
26	ν(C2=O)	2012	1868	1868	1864	1845	1791	92	15.17	1791	24	1757.5 vs	1734 vs	1756 vs
27	ν(C6-H)	3394	3263	3234	3231	3221	3200	1	6.59	3212	90		3076 w	
28	ν(C5-H)	3429	3304	3281	3278	3264	3242	0	6.78	3251	100	3084[i]	3101 w	3124 m
29	ν(N3-H)	3863	3612	3643	3642	3620	3592	11	8.19	3588	68	3434.5 s	3427 w	3436 s
30	ν(N1-H)	3902	3656	3682	3681	3658	3636	17	8.40	3632	89	3484.3 s	3450 w	3484 s

[a]Abbreviations: ν, stretching; δ, in-plane bending; γ, out-of-plane bending. [b] Notation: sh, shoulder; vs, very strong; s, strong; m, medium; w, weak; vw, very weak. [c]With the 6-31G* basis set. [d]With the 6-311+G(2d,p) basis set. [e]With the aug-cc-pVDZ basis set. [f]Refs. [17-19]. [g]Refs. [18-19]. [h]Ref. [20]. [i]Raman, ref. [18].

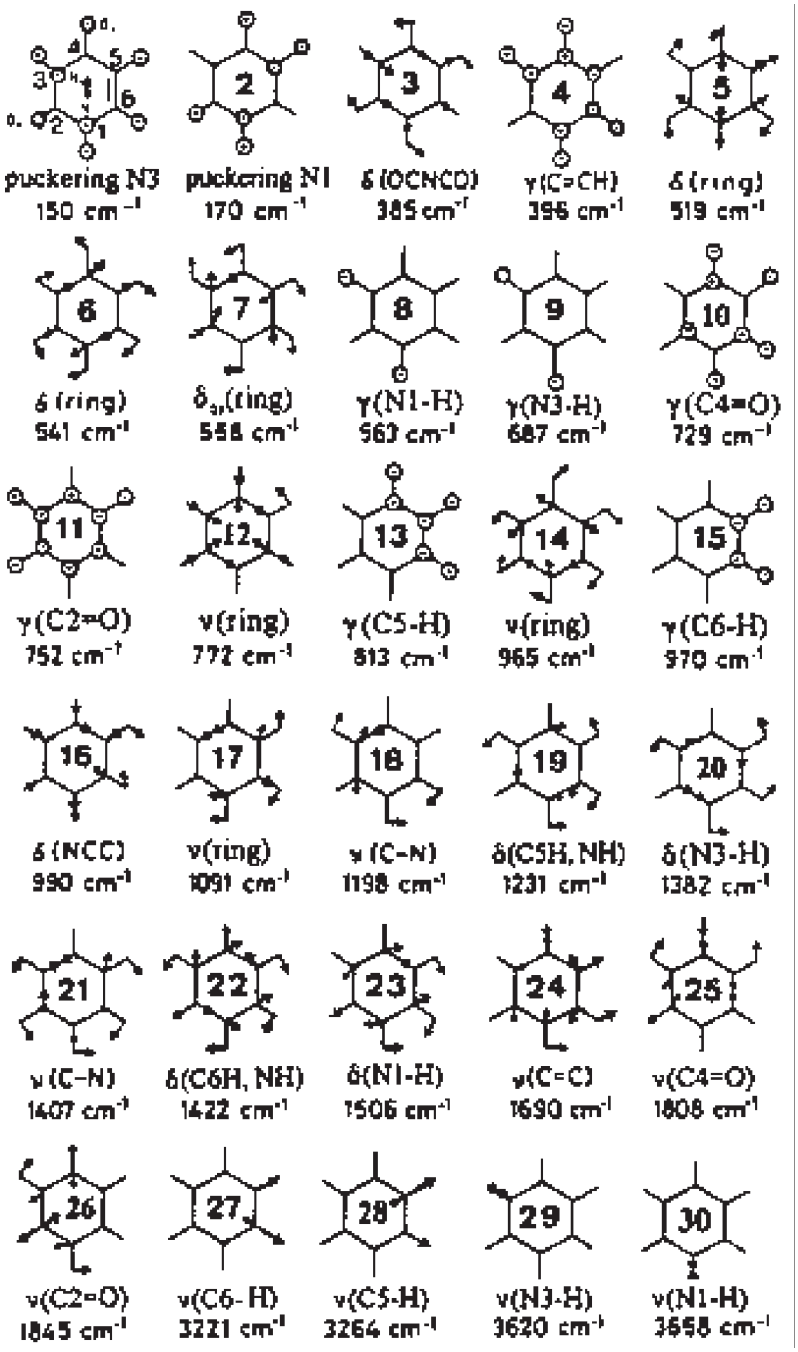


Fig 5. Characterisation of the normal modes in uracil molecule at B3LYP /6-311+ G level**

5-Chlorouracil (5-ClU) has also antitumor activity and forms complexes with some metal (II) ions . It has been suggested that peroxidases secreted by human phagocytes facilitate the formation of 5-ClU and 5-bromouracils (5-BrU) in the human inflammatory tissue.

The essential biological importance of 5-bromouracil is that it is one of the well known uncommon nucleotide bases and has the ability to coordinate with metals or to bind to tissues via metals, which interface with the growth of cancer cells. [M A Palafox. J Talaya, A Guerreo-Martinez, G Tardajos, Hitesh Kumar, J K Vats and V K Rastogi, Spectroscopy Letts,43(2010)51)].

5-Iodouracil is an important antimetabolite like other halogenated uracils, being in the case of 4-aminobutyrate aminotransferase the most effective inhibitor[Presant CA, Wolf W, Waluch V, Wiseman C, Kennedy P, Blaney D, Brechner RR, *Lancet* 343(1994)1184; Nakajima T *World J Surgery* 19(1995)570]. Some of the 5- iodouracil derivatives also posses antitumor activity [Singh UP, Singh BN, Ghosh AK, Singh RK, Sodhi A, *J Inorg Biochem* 44(1991)277], and have been used in the treatment of hepatitis B infections [Adair DW, Smiles KA, King D Eur Path Appl EP 565412 A1,(1993) 51]. Some 5-IU based nucleoside analogues were found to be selective inhibitors of herpes simplex viruses.

Other 5-substituted uracils also play an important role in biochemistry and pharmacology, such as 5-methyluracil or thymine (5-MeU), 5-aminouracil (5-AU), and 5-nitrouracil (5-NU), and therefore they have been included in the present work . 5-MeU (thymine) is a natural constituent of DNA and its structure is of particular importance in understanding the mechanism of the biological functions of DNA.

Since it is well known that the vibrational spectra constitute an important characteristic of a molecule and the common application of theoretical data and experimental results allows to draw detailed conclusions concerning the relation between the structure of molecule and the exhibition of its specific properties in real conditions, therefore in this section we present the results on 5-substituted uracils.

As a representative we first analyse the vibrational spectra of anticarcinogenic drug 5-Fluorouracil.

3. Experimental

The mid infrared spectrum of 5-FU from 400-4000 cm^{-1} was recorded with Perkin Elmer FTIR model 1760X, using KBr technique with 1 mg sample per 300 mg KBr. For the spectrum acquisition, 4 scans were collected at 1 cm^{-1} resolution, Fig. 9b.

The FT-Raman spectrum of 5-FU was recorded in powder form in the region 50-4000 cm^{-1} on a Bruker IFS 66 optical bench with an FRA 106 Raman module attachment at room temperature. The sample was mounted in the sample illuminator using an optical mount and no sample pretreatment was undertake. The NIR output (1064 nm) of an Nd:YAG laser was used to excite the spectrum. The laser power was set at 250 mW and the spectrum was recorded over 500 scans at a fixed temperature at a resolution of 4.0 cm^{-1} The FT-Raman spectra of 5-FU is shown in Fig 6.

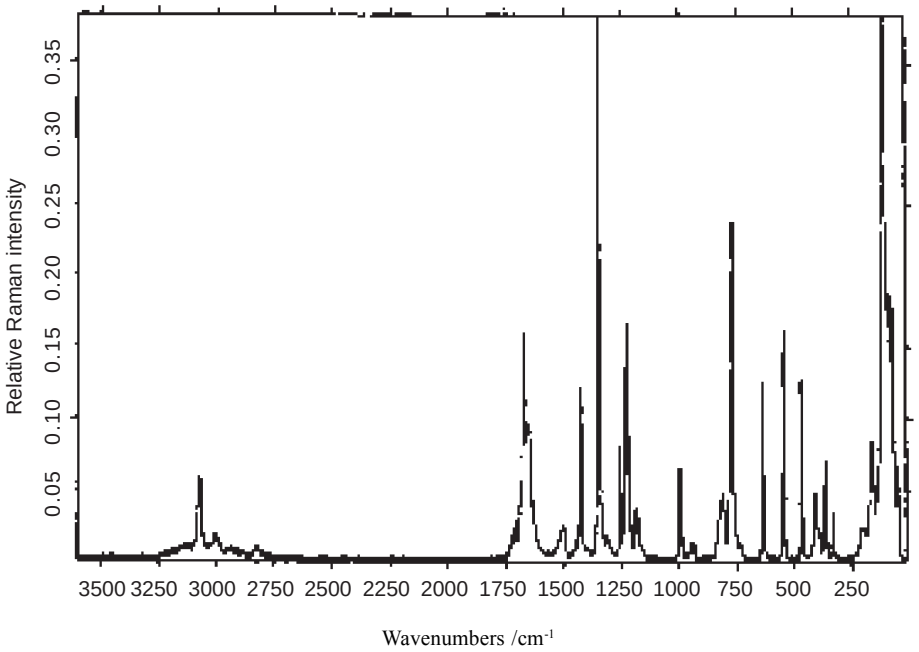


Fig 6. FT-Raman spectrum of 5-FU

5-FU is a planar, six membered N-heterocyclic molecule, which exhibits 30 normal vibrations, 21 of which are in-plane (a" species) and 9 are out-of-plane (a" species). The optimized dimer form of 5-fluorouracil, with the labelling of the atoms is shown in Fig 7.

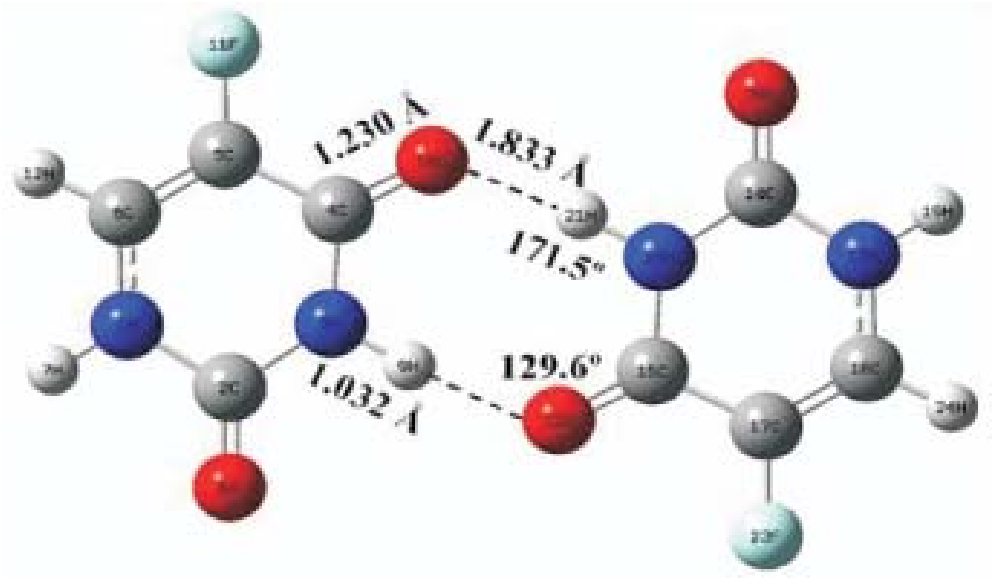


Fig. 7. Optimized dimer form of 5-fluorouracil, with the labelling of the atoms and several parameters of interest.

Fig 8 shows the vibrational displacement vector diagram of 5-FU, whereas experimental IR spectra is shown in Fig 9.The computed wavenumbers together with IR data in KBr pellets and Raman values in the solid state are collected in Table 3,whereas simulated scaled IR spectrum at the B3LYP level : in the isolated state (monomer form), in the dimmer form and in the isolated state of Tautomer T2 is shown in Fig 10. Fig 11 shows the comparision of the experimental Raman spectra of 5-FU with simulated scaled IR spectrum at the B3LYP level in the isolated state (monomer form), and in the dimmer form.

Table 3. Comparison of the calculated harmonic vibrational wavenumbers (ω, cm^{-1}) in the dimer form of 5-fluorouracil at the B3LYP/6-31G** level, Relative infrared intensities (A, %), relative Raman scattering activities (S, %), scaled wavenumbers and experimental IR data (cm^{-1}) in the solid state of 5-FU in KBr pellets.

calculated			scaled[a]	Experimental IR		Experimental Raman			No.[c]	Characterization
ω	A	S		ref. [32]	ν[b]	SERS, ref. [13].	ν[b]	ref. [3]		
3659	9	37	3491	3141 vs	3135	3146 sh		3142.9	30	ν(N1-H)
3300, 3258	**100**, 0	0, 100	**3152**, 3112	3069 vs	3067	3073 w	3069	3066.5	29	ν(N3-H)
3243	0	28	3098	3001 vs	3020	3001 vw		3002.0, 3028.1	27	ν(C6-H)
						2932,2892,2824 vw		2934.2, 2450.2, 2820.9		combinations modes
1851, **1849**	0, **39**	3, 0	1783, **1781**	1722 s	1720	1725 vw, 1707 vw	1706		26	ν(C2=O) + ν(C4=O) + δ(N-H)
								1724.5, 1704.9	25	ν(C4=O) + ν(C2=O) + δ(N3-H)
1773, 1766	**63**, 0	0, 22	**1710**, 1703	1671 vs	1670	1672 m	1671	1670.4	24	ν(C5=C6) + ν(ring)
1731, **1730**	0, **3**	9, 0	1670, **1669**	1662 vs	1650	1659 w	1655	1658.3	23	δ(N1-H) + ν(ring)
1520, 1519	**4**, 0	0, 3	**1471**, 1470	1502 m	-	1506 vw	1504	1503.6	22	ν(ring) + δ(N1-H)
1480, 1479	**2**, 0	0, 9	**1433**, 1432	1430 s	1435	1447 vw, 1425 w	1425	1448.2, 1424.1	20	δ(N3-H) + δ(N1-H) + δ(ring)
1429	4	1	1385	1349 m	1345	1350 vs	1349	1348.5		combinations modes
				1312 w		1313 vw		1311.3, 1119.3	21	δ(C6-H) + ν(ring) + δ(N1-H)
1355, **1354**	0, **2**	11, 0	1315,**1314**		1260	1258 w	1257	1256.8	28	ν(C-F) + ν(ring)
1287, 1286	**18**, 0	0, 3	**1250**, 1249	1225 m	1222	1225 m	1226	1224.0	18	δ(C6-H) + δ(N3-H) + δ(ring)
1219, **1218**	0, **2**	2, 0	1186, **1185**	1181 m		1187 vw	1185	1186.8	19	δ(CCH) + δ(N1-H) + δ(ring)
1169	3	1	1139	1158 sh	970	987 vw	996	996.3, 985.5	14	δ(N3-H) + δ(C6-H) + δ(ring)
979, 975	**3**, 0	0, 2	**959**, 956	949 w		950 vw		949.5	9	γ(N3-H)
937, 908	**9**, 0	0, 0	**920**, 892			937 vw		936.0	15	γ(C6-H)
892, 890	**1**, 0	0, 1	**877**, 875	880 m	875	887 vw		894.8	17	δ(ring)
823, 820	**3**, 0	0, 1	**812**, 809	813 s		810 vw	811	809.1	12	δ(ring)
762, **755**	0, **1**	6, 0	754, **748**	771 w		779 sh, 769 m	768	767.9	11	γ(C2=O) + γ(C4=O) + γ(ring)
748, 747	**1**, 0	0, 0	**741**, 740	751 m	740	738 vw		734.7		

									10	γ(C-N3-H) + γ(ring)
728	1	0	722	730 w					7	δ(ring)
639, 631	**1**, 0	0, 2	**638**, 631	643 m, 635 vw	615	639 w, 634 vw	637	638.3, 633.5	8	γ(N1-H)
559, 558	**7**, 0	0, 0	**563**, 562						5	6b[d], δ(ring)
541, 539	**2**, 0	0, 1	**546**, 544	551 s, 517 w	546	546 w	546	545.2	16	δ(C-F) + δ(C=O) + δ(ring)
464, 462	**1**, 0	0, 1	**473**, 471	469 s	450	466 sh, 471 w	470	470.0, 464	3	δ(OCNCO) + δ(ring)
408, 398	**3**, 0	0, 0	**420**, 411	419	419	414 vw	413	414	4	γ(C=C-H) + γ(ring)
388, **383**	0, **1**	1, 0	401, **396**			399 sh, 366 vw	367	365		
									13	γ(NC=CF) + γ(ring)
346	1	0	361			372 vw		371	6	δ(OCCF) + δ(ring)
324, **321**	0, **0.2**	0, 0	341, **338**			333 vw	332	331	1	γ(C=O) + γ(N3-H) + γ(ring)
177, 165	0	0, 0	202, 190			207 vw	210	207	2	γ(C=O)+ γ(C-F)+ γ(N1-H)+ γ(ring)
117, 116	**0.2**, 0	0, 0	**145**, 144			167 vw	166	167		
111,80	0	0, 1	139, 110			110 ms	110	109		lattice modes
77,**65**	0, **0.2**	0, 0	107, **96**			92, 83, 68		91, 81, 76, 56		lattice modes

[a] With the scaling equation: $\nu_{scaled} = 34.6 + 0.9447 \cdot \omega_{calculated}$, ref. [10,40]. [b] Present work. [c] According to the notation of the uracil ring modes, ref. [40].
[d]The direction of the displacement vectors is analogous to mode 6b of benzene ring [24]

Table 4. Optimized geometrical parameters, bond lengths in , angles in degrees, calculated by B3LYP/6-31G** in 5-XU derivatives.

X =	H	H[a]	F	Cl	Br	I[b]	I[c]	CH_3[d]	NH_2	NH_2[e]	NO_2	NO_2[f]
C5-X	1.0808	1.002	1.3385	1.7347	1.8847	2.1132	2.11	1.5006	1.3926	1.3892	1.4574	1.437
C4-C5	1.4602	1.462	1.4651	1.4710	1.4699	1.4650	1.44	1.4679	1.4734	1.4685	1.4740	1.442
C5=C6	1.3498	1.343	1.3462	1.3519	1.3513	1.3504	1.32	1.3522	1.3550	1.3485	1.3601	1.359
N3-C4	1.4130	1.415	1.4066	1.4095	1.4087	1.4171	1.38	1.4076	1.3923	1.3892	1.4196	1.396
C2=O	1.2168	1.212	1.2163	1.2156	1.2157	1.2303	1.20	1.2177	1.2196	1.2135	1.2123	1.212
C4=O	1.2194	1.211	1.2164	1.2149	1.2156	1.2332	1.24	1.2217	1.2255	1.2175	1.2106	1.221
C4-C5-X	118.11	118.1	117.02	118.01	117.97	116.62	116.4	117.81	114.97	115.46	122.28	122.5
C4-C5=C6	119.94	119.7	121.62	120.43	120.37	120.60	122.0	118.19	118.54	118.38	120.65	120.9
N3-C4-C5	113.38	115.5	112.09	112.50	112.60	112.67	113.0	114.52	114.82	114.90	111.37	112.6
N1-C2-N3	112.79	114.6	112.82	112.62	112.63	112.44	114.9	112.49	112.48	112.69	112.43	114.2

[a]ED data, ref. [13]. [b]With the 3-21G** basis set. [c]X-ray data, ref. [37]. [d]In the form II. [e]At B3LYP/6-311++G(3df,pd) level. [f]X-ray with form I, ref. [44].

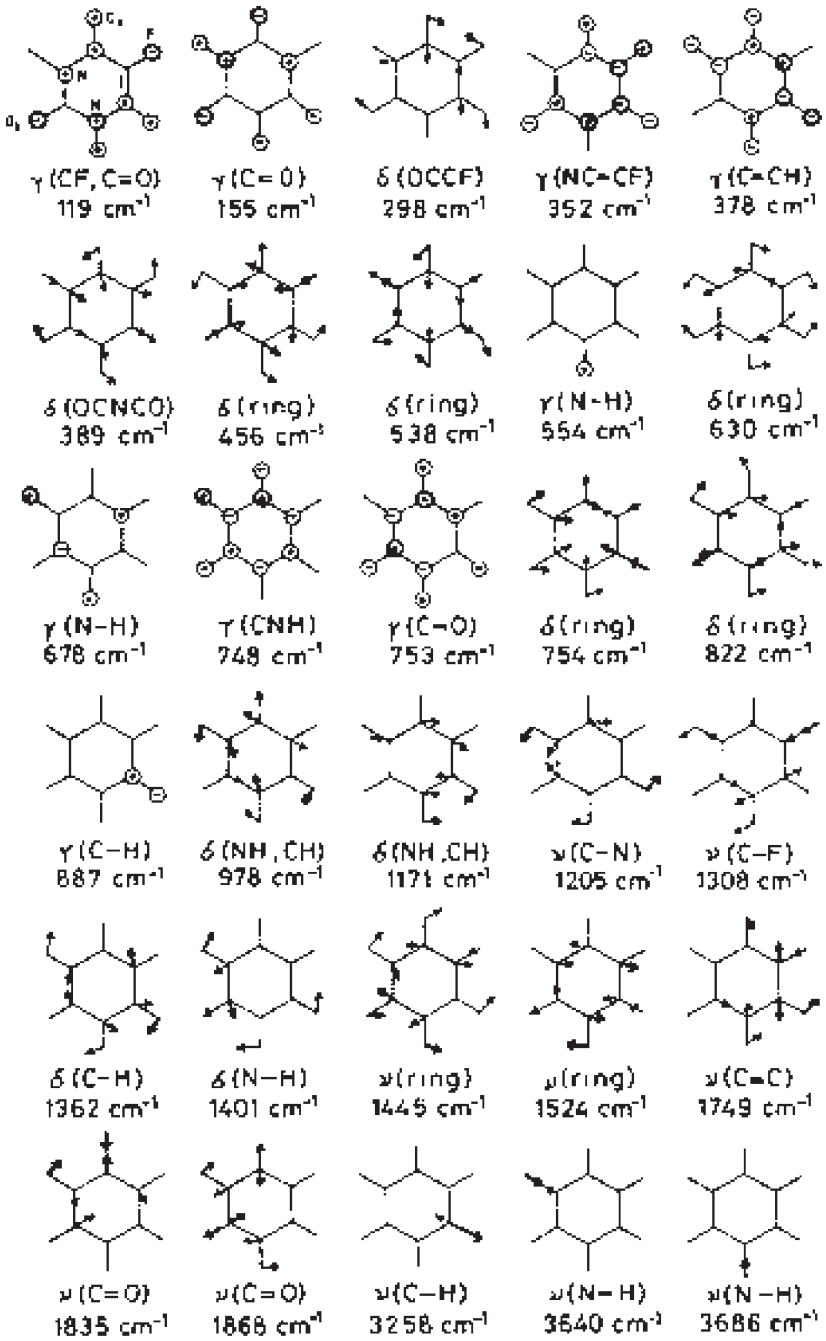


Fig 8. Characterisation of normal modes in 5-FU molecule at B3LYP /6-311+G level.**

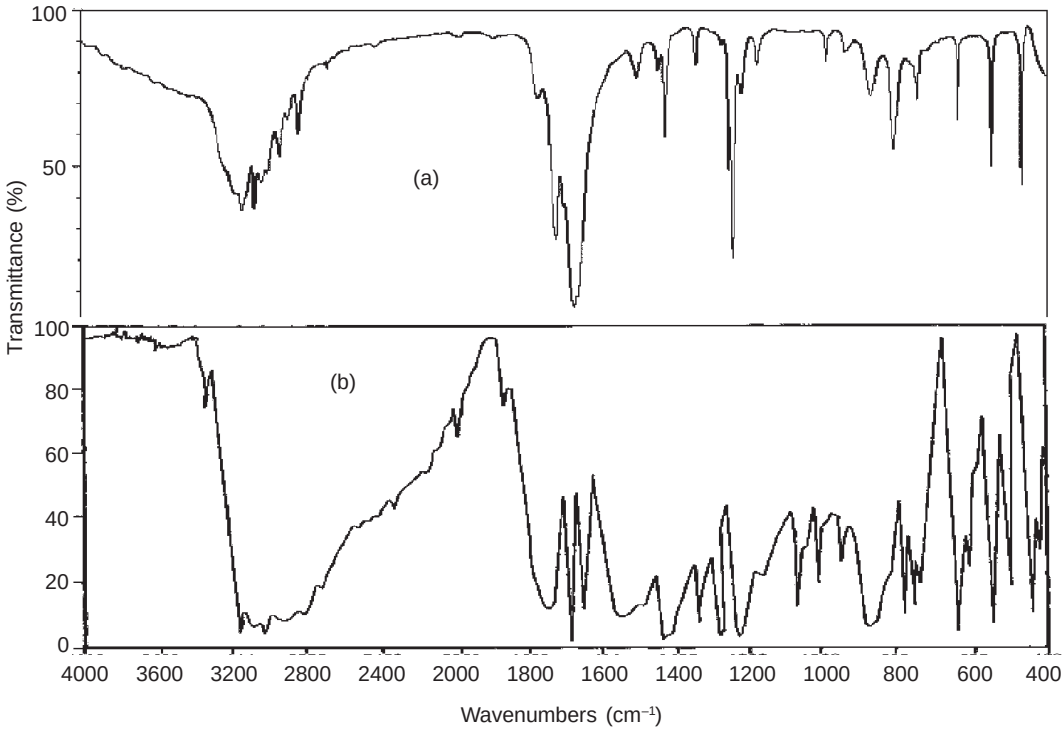


Fig. 9. Experimental IR spectra of 5-flurouracil: (a) from ref. [31]. (b) Our spectrum at higher concentration of the sample.

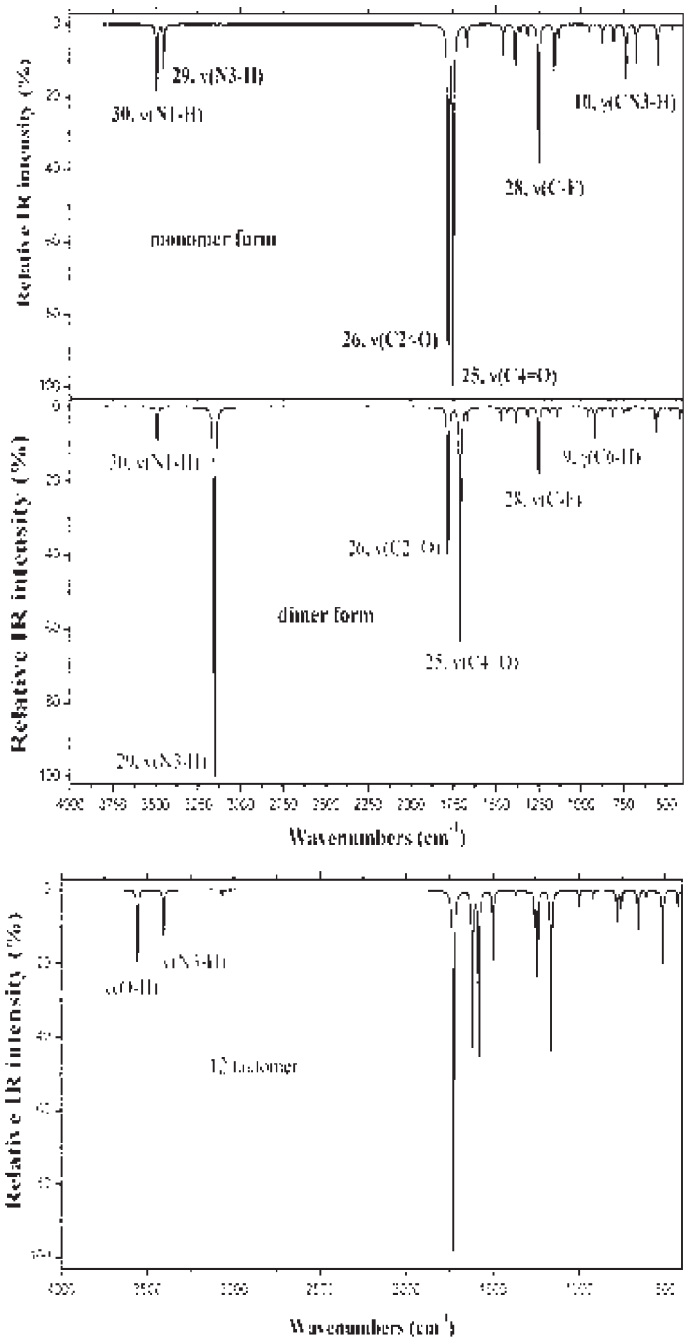


Fig. 10. Simulated scaled IR spectrum at the B3LYP level: in the isolated state (monomer form), in the dimer form, and in the isolated state of tautomer T2.

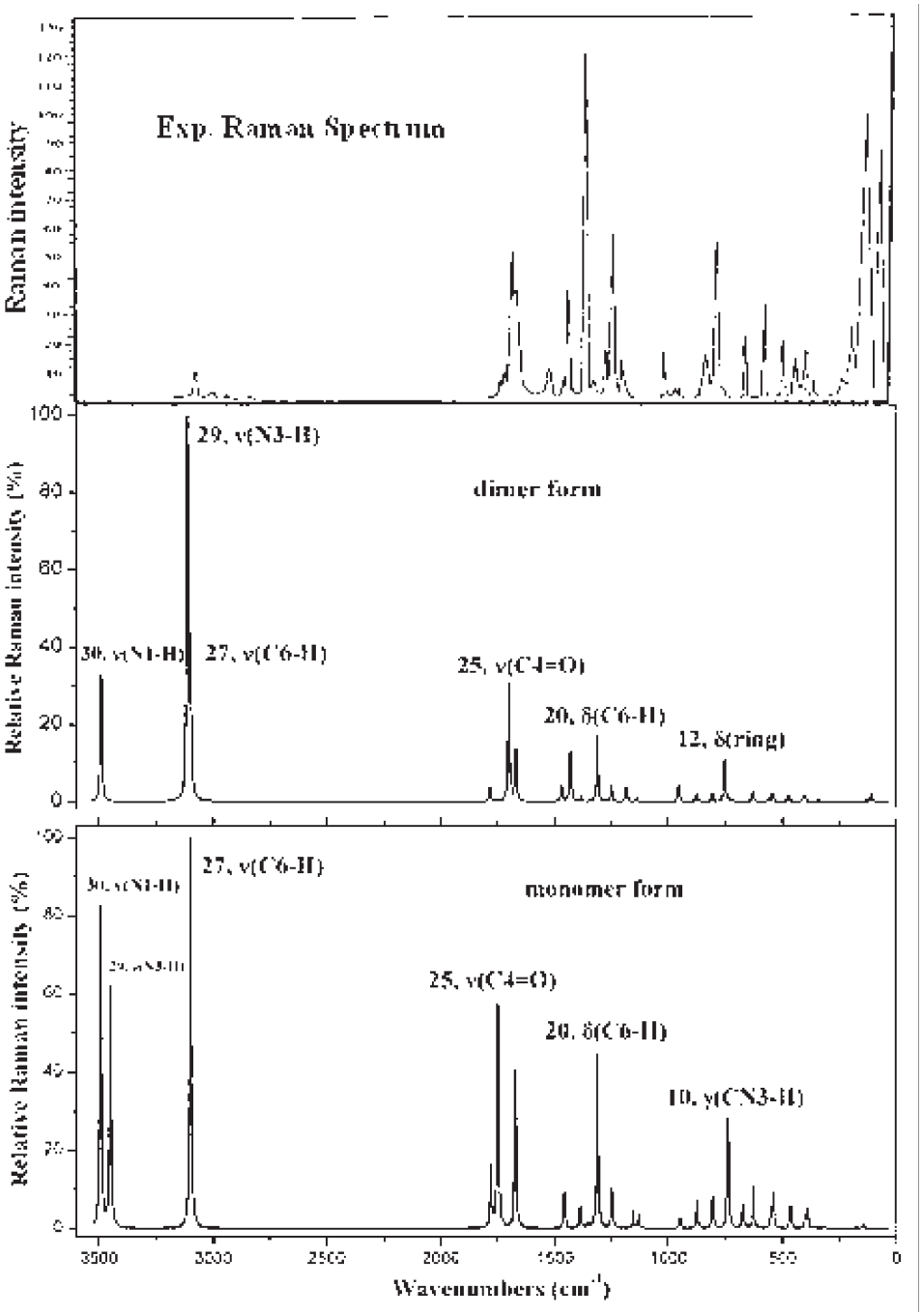


Fig. 11. Comparison of the experimental Raman spectra of 5-FU with the simulated scaled IR spectrum at the B3LYP level: in the isolated state (monomer form), and in the dimer form

4 Tautomerism

Studies of tautomerism phenomena have been valuable in many areas of chemistry as demonstrated by several reviews of experimental and theoretical studies in chemistry and biochemistry. The Fig 12 shows the tautomerism in 5-FU. The energies were calculated at MP2/6-31G** level. Tautomer T3 is least stable of the tautomers plotted in the figure.

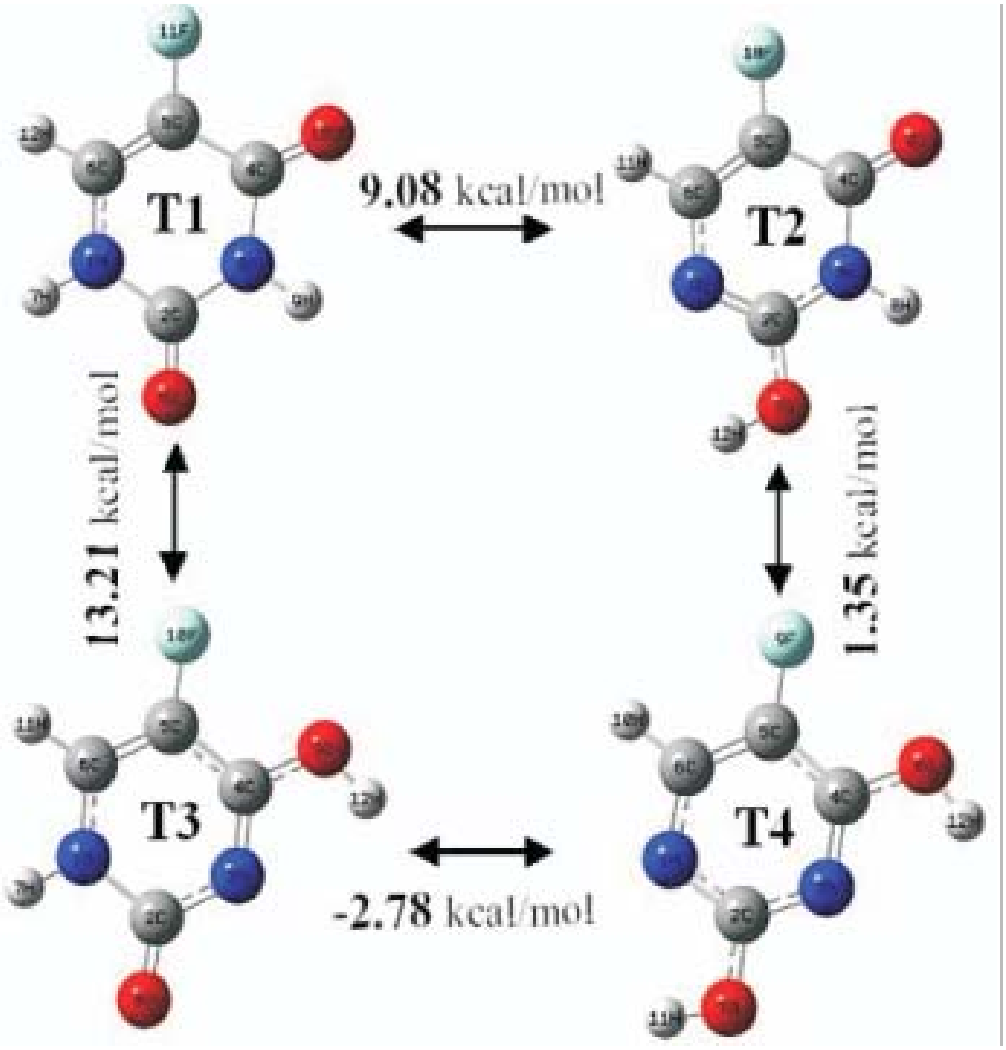


Fig. 12. Tautomerism in 5-fluorouracil. The energies were calculated at MP2/6-31G level. Tautomer T3 is the least stable of the four tautomers plotted.**

Section III

Due to the importance of the 5-XU, our interest in this section is to carry out a comparative analysis of their geometry and vibrational wavenumbers in relation to uracil molecule and to establish relationships between their parameters.

Geometry Structure of 5-XU

In 5-substituted uracil derivatives, experimental data have been reported only for 5-FU [39], 5-IU [40] and 5-NU [41] by x-ray. Therefore, due to lack of this experimental data for other uracil derivatives, DFT calculations appear as the only geometrical data. The selected calculated geometrical parameters of interest in the compounds under study are listed in Table 4. For comparison purposes, only the results at the B3LYP/6-31G** level are shown.

The optimized ring structure of the molecules under study is planar, in agreement with uracil and with the few experimental data available on these molecules. With the 5-substitution on the uracil ring, several key effects and certainly inter-related, can be underlined that produce the marked differences in the biological and pharmacological activities of these nucleobases:

(i) The first effect refers to the structural change mainly caused by the longer C-X bond than the C-H one of the uracil molecule.

(ii) The second effect, and the most important, is the drastic change of their functional ones expressed in terms of intermolecular interactions. This effect is specially pronounced with the 5-halo derivatives. The higher electronegativity of the halogen atom compared to hydrogen produce a perturbation in the electronic environment of the heterocyclic ring, and the new possibility of intermolecular H-bonds through this halogen atom. The halogen substitution also increases the polarizability of the nucleobases.

(iii) Other small effects also appear with the substitution, such as, a small increase of the C4-C5 bond and a shortening of the N3-C4 and C4=O bonds, while the C2=O, C2-N1 and C2-N3 bonds remain almost unchanged. This fact produces a slightly opening of the *ipso* angle C4-C5+C6, ~1-1.5º, and a slightly closening of the N3-C3-C5, while the N1-C2-N3 remains almost unchanged.

Table 5. Calculated by B3LYP/6-31G**, scaled with the scaling equation, and experimental IR wavenumbers in cm^{-1} in the molecules under study.

X =	H			F[a]			Cl				Br			
	calc.[b]	scal.	exp.[c]	calc.	scal.	exp.	calc.	calc.[d]	scal.	exp.[e]	calc.	calc.[d]	scal.	exp.[f]
ν(N1-H)	3658	3490	3484	3662	3494	3468	3655	3635	3487	3472.1[k]	3653	3632.7	3486	3471[m]
ν(N3-H)	3620	3454	3436	3617	3452	3416	3617	3590	3451	3425.7[k]	3616	3589.5	3451	3425[m]
ν(C6-H)	3221	3077	3076	3243	3098	3067	3238	3214	3094	3060	3237	3213.7	3093	3058
ν(C2=O)	1845	1778	1756	1846	1778	1754	1847	1793	1779	1768.4[k]	1847	1793.3	1779	1761
ν(C4=O)	1808	1743	1741	1813	1747	1742	1813	1763	1747	1735.5[k]	1808	1759.1	1743	1729
ν(C=C)	1690	1631	1641	1732	1671	1685	1685	1667	1626	1635	1679	1662.0	1621	1635
ν(C5-X)	3264	3118	3124	1285	1249	1224	661	662	659	639[l]	626	629.2	626	626

X =	I			CH_3			NH_2				NO_2		
	calc.[g]	scal.	exp.[h]	calc.[i]	scal.	exp.[c]	calc.	calc.[d]	scal.	exp.	calc.	scal.	exp.[j]
ν(N1-H)	3707	3478	3470	3659	3491	3484	3666	3643	3498	3402	3639	3472	3456
ν(N3-H)	3668	3433	3426	36193213	3453	3437	3622	3595	3456		3612	3447	3419
ν(C6-H)	3311	3086	3048[n]	1843	3070	3076	3227	3202	3083	3090.8[o]	3249	3104	3047[o]
ν(C2=O)	1794	1758	1765	1792	1776	1772	1839	1781	1772	1745	1859	1791	1773
ν(C4=O)	1742	1727	1723	1714	1728	1725	1781	1735	1717	1675	1833	1766	1752
ν(C=C)	1653	1622	1630[n]	1236	1654	1668	1724	1701	1663	1660.1[o]	1679	1621	1640
ν(C5-X)	243	260	235[n]		1202	1178	1294	1275	1257	1276	1224	1191	1194

[a]Ref. [4]. [b]Ref. [3]. [c]IR in the gas phase [20]. [d]With the 6-311+G(2d,p) basis set. [e]In the KBr matrix [46]. [f]IR in Ar matrix [42]. [g]With the 3-21G** basis set. [h]In Ar matrix [30]. [i]Ref. [4]. [j]IR in Ar matrix [43]. [l]Raman in the solid state [46]. [m]IR, ref. [45]. [n]In the solid state [47]. [o]In Raman.

Vibrational Wavenumbers of 5-XU

Table 5 collects selected calculated and experimental stretching vibrations. Gas phase experimental wavenumbers were included whenever they were available. To reduce the error of the calculated values, scaled values [2,3] are also included in Table 5.

The absence of a n(OH) band in the 3500-3700 cm^{-1} range and the appearance of n(C=O) modes as strong bands indicate that in the solid state these compounds exist in the Keto form. It appears that most of the uracil fundamentals absorb in relatively narrow wavenumber ranges. The strong coupling of the group modes in the uracil spectrum remains highly constant for their derivatives or its variation is directly related to the electron donating or withdrawing effects of substituents.

By comparing the results of Table 5, the following is also noticed:

(i) The carbonyl stretching motion in 5-XU couples significantly with the N1-H and N3-H bending motions, while in U it appears as an almost pure mode.

(ii) The calculated and experimental ν(C2=O) wavenumbers are only little affected by the different substituents. In general less than 10 cm^{-1}. The NO_2 group of 5-NU produces the highest interactions with the surrounding atoms, i.e. the largest differences from uracil. The ν(C4=O) wavenumbers are slightly more affected by the substituents than ν(C2=O). In 5-AU an intramolecular bond is formed between the H-atom of the NH_2 group and the O4 oxygen given rises to longer N-H and C4=O bonds, i.e. lower wavenumbers than U.

(iii) As far as the C=O fundamentals are concerned, the out-of-plane modes are almost insensitive to substitution with the exception of the wavenumber decrease (40-50 cm^{-1}) of γ(C4=O) in 5-substituted uracils. The fact that these out-of-plane C=O modes remain approximately (<1%) constant might be taken as evidence for almost pure C=O group modes (C2=O) or similar coupling (C4=O + C5-H) as in uracil molecule.

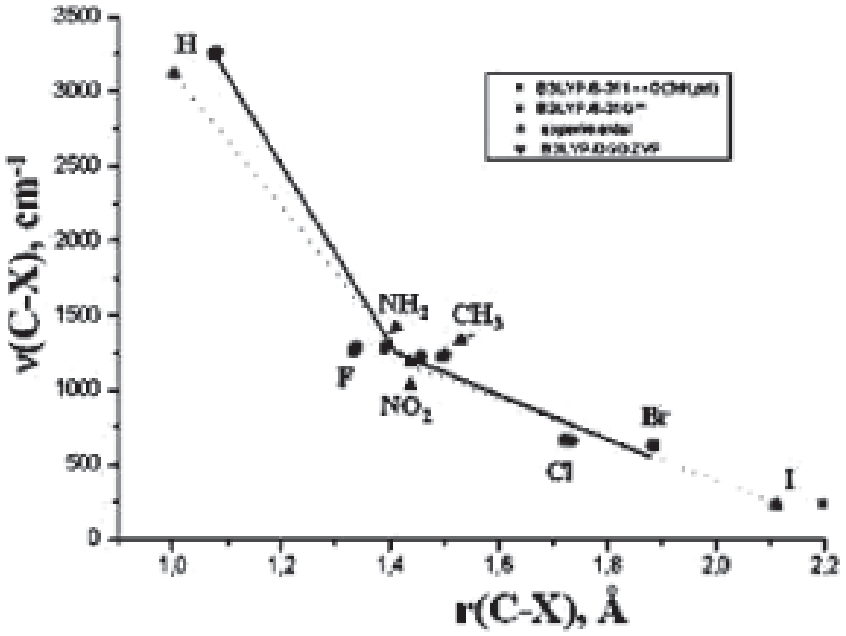
(iv) In these compounds and in U, it is noted that the N-H stretching modes are essentially pure group modes and substitution only induces shifts of about 1% or less. The calculated ν(N1-H) and ν(N3-H) stretching wavenumbers also appear little affected by the substituent, although their experimental values have larger differences, due to intermolecular interactions through the H-bonds, especially in 5-AU and 5-NU. The N-H in-plane bends are highly coupled to other groups or ring modes and the influence of substitution is not straightforward.

(v) The ν(C-X) stretching wavenumbers and the r(C-X) bond lengths appear correlated, Fig. 13a, with small deviations for the -F and $–CH_3$ groups. The only experimental point available for uracil was also included in the figure. However, no relationship is observed between ν(C-X) (or the C-X bond) and the MK charge on X.

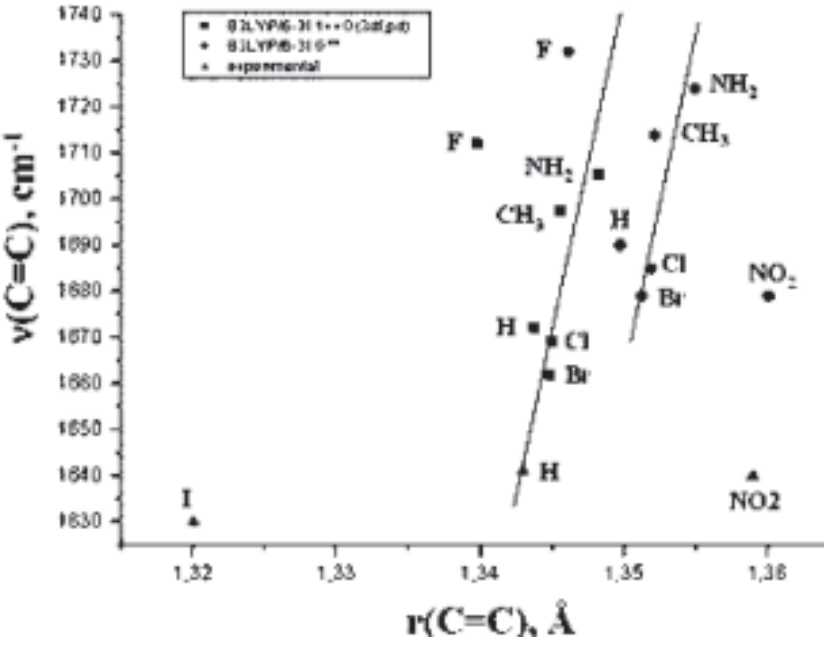
(vi) Since the C5=C6 bond is adjacent to the X-substituents, a significant effect of the various halogen substituents on the ν(C=C) frequency is expected. Although relationship was not obtained between ν(C=C) and r(C=C), the calculations show an increase in ν(C=C) with the slight increase in ν(C-X), Fig. 13b, experimentally and theoretically. It is also observed a large increase of the ν(C=C) frequency with the X-atom electronegativity, or with the increment in negative charge, Fig. 13c. These relations are linear, except for the Cl and Br halogens.

(vii) The atomic charge on the X and oxygen atom O8 appear approximately correlated, Fig. 13d. An increase in the positive charge on the X atom leads to a reduction in the negative charge on O8 atom.

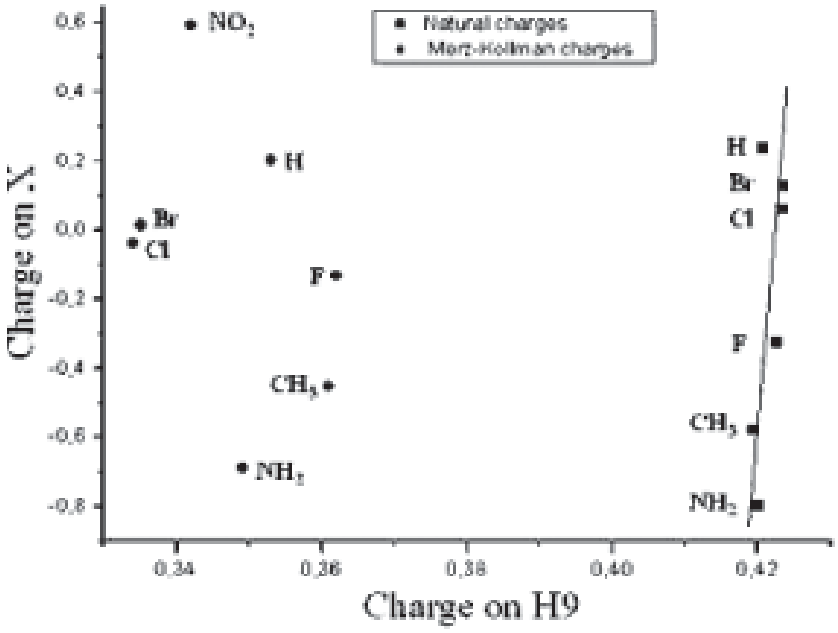
(viii) The experimental ν(C6-H) wavenumbers increase with the increment of negative charge on the X-atom, Fig. 13c. This relationship is almost linear, except for the U molecule. Correlation is not observed with the calculated wavenumbers.



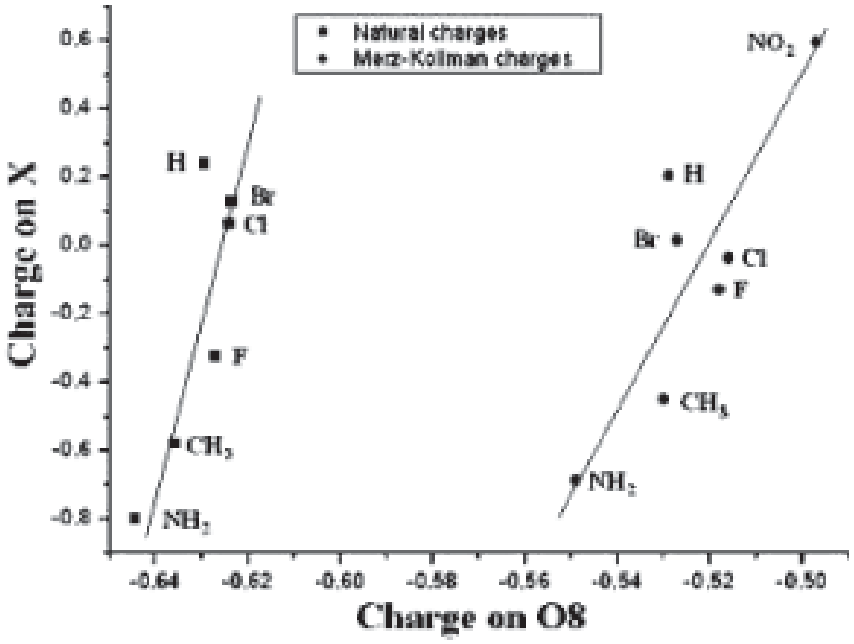
(a)


experimental
ν(C=C), cm⁻¹
r(C=C), Å
F
NH2
CH3
H
Cl
Br
NO2
I
NO2

(b)


Natural charges
Mert-Kollman charges
Charge on X
Charge on H9
NO2
H
Br
Cl
F
CH3
NH2

(c)



(d)

Fig. 13. Different relations established in the molecules under study: (a) Between the C-X stretching and the C-X bond length. (b) Between the C=C stretching and the C=C bond length. (c) Between the Merz-Kollman atomic charge on the X atom and on the H9 atom. (d) Between the Merz-Kollman atomic charge on the X atom and on the O8 atom.

A detailed description of the different modes in 5-XU is as follows:

N-H modes: The calculations predicted the two stretching N-H bands to occur within the range 3500-3450 cm^{-1} and the N-H oscillators to be uncoupled. The n(N1-H) band is estimated to occur by ca. 40 cm^{-1} wavenumbers higher than the n(N3-H) band. According to the harmonic wavenumber calculations, as the halogen mass is increased, the two bands shift slightly toward lower wavenumbers and the n(N-H) band separation is likely to decrease in Ar matrix [41]: 43, 40, 39, and 37 cm^{-1}, for 5-FU, 5-ClU, 5-BrU and 5-IU, respectively. The calculations predict no monotonous wavenumber shift of the n(N-H) bands to proceed with the increase in the halogen mass. The bands of U are located similarly to those of 5-FU molecule. The intensity of the N1-H stretching band is calculated to be higher by ca. 1.5 than that of the N3-H band. The scaled DFT wavenumbers overestimate the positions of the experimental bands by ca. 40 cm^{-1}. Nevertheless, the

presence of only two bands between 3400 and 3500 cm^{-1}, allows the assignment of the two n(N-H) bands beyond any doubt.

The IR intensities of the δ(N1-H) and δ(N3-H) modes tend to increase from 5-FU to 5-IU. The Raman activity of the δ(N1-H) mode of 5-XU molecules is ca. ten times greater than that of the δ(N3-H) mode, and the Raman activity of the δ(N3-H) mode decreases as the substituent mass is increased.

For U and halouracils, the γ(N3-H) out-of-plane mode is predicted to occur at ca. 675 cm^{-1}. The mode is nearly pure with PED ca. 85%. Its IR intensity is medium and it is supposed to increase slightly on passing from 5-FU to 5-IU and the Raman activity is predicted to remain unaffected by halogen substitution. The γ(N1-H) out-of-plane mode is practically pure with PED of 90% and is predicted to occur at ca. 570 cm^{-1}. In 5-FU this mode is calculated to occur ca. 15 cm^{-1} below those wavenumbers. Only a slight increase is observed on passing from 5-FU to 5-IU. The calculated IR intensity of the mode is medium and slightly decreases from 5-FU to 5-IU and the calculated Raman activity is constant.

C=O modes. For U and 5-XU one can distinguish three groups of C=O stretching bands: the first located at ca. 1765 cm^{-1}, the second in the region of 1745-1720 cm^{-1}, and the third between 1710 and 1705 cm^{-1}. The positions of the first and third group of C=O stretching vibration bands are almost insensitive to the change in the mass of the substituent, whereas the middle band shifts from ca. 1740 to 1720 cm^{-1}, on passing from the 5-FU to 5-IU molecule. For U molecule, the middle group of bands is positioned at the wavenumber similar to that for 5-BrU, i.e., at 1729 cm^{-1}, Table 6. Within each group of bands, the experimental bands in Ar matrix are split probably because of the formation of diverse Ar clusters surrounding the molecules in matrices. The most probable effect responsible for the increase in the number of groups of ν(C=O) experimental bands is a Fermi resonance.

The ν(C2=O) band position is predicted to remain almost unaffected by changes in the molecular structure under C-5 substitution. As the halogen mass is increased, the corresponding ν(C4=O) harmonic mode drifts slightly toward lower wavenumbers, from ca. 1742 cm^{-1} for 5-FU, to ca. 1723 cm^{-1} for 5-IU in Ar matrix. The two band intensities are practically equal for U and 5-FU. For heavier halogens, the ν(C2=O) band intensity increases, whereas the ν(C4=O) band intensity decreases proportionally so that, for the 5-FU molecule, the former is twice as intense as the latter.

The δ(C=O) local modes, no. 7 in Table 2, absorb in Ar matrix [44] at 630, 605, 600 and 590 cm^{-1} for the 5-FU, 5-ClU, 5-BrU and 5-IU molecules, respectively. The analogous U mode is predicted to absorb at ca. 559 cm^{-1}. The theoretical IR intensity of the mode is

weak for all the spectra studied, and for 5-ClU it is practically inactive. This low intensity is the reason why the investigators [45, 46] have had difficulties in assigning the band in halouracil spectra.

Unlike for the δ(C=O) mode, the two γ(C=O) out-of-plane bending vibrations are mixed only slightly. The γ(C4=O) mode (no. 10) is predicted to occur at ca. 750 cm^{-1}, while the analogous in U is predicted to occur at ca. 720 cm^{-1} and has a significant contribution (PED ca 20%) in γ(C5-H) mode. The calculated IR intensity of this mode is medium and exhibits a tendency to increase as the halogen mass in increased. The band does not appear to be affected by halogen substituents. The assignment by Graindourze *et al.* for the 5-FU [45] and 5-BrU molecules is similar to that of Table 6, whereas that proposed by Nowak for 5-FU [44] and that by Stepanian *et al* for 5-BrU molecules [46] is different. The γ(C2=O) mode (no. 10) is predicted to occur at ca. 760 cm^{-1}. The theoretical IR intensity tends to decrease from U to 5-IU and it is predicted to be ca. two to three times lower than that of the γ(C4=O) mode. In contrast to the DFT results, the observed γ(C2=O) band intensity is ca. one half as large as that of the γ(C4=O) band.

C5-X modes. The ν(C5-F) local mode is predicted at 1250 cm^{-1}, which agrees with the Ar matrix band [41] at 1247.5 cm^{-1}. According to PED analysis, the ν(C5-Cl) local mode in 5-ClU is spread out between three normal modes that absorb at ca. 1070, 655 (the largest PED = 31%), and 370 cm^{-1}. A similar situation occurs for the ν(C5-Br) local mode, which is spread out between the normal modes at 1047, 623 and ca. 290 cm^{-1}. In the case of the 5-IU molecule, the ν(C5-I) mode contributes mainly to the vibration at 258 cm^{-1}.

The theoretical prediction of δ(C5-X) bending vibrations show a systematic decrease in the wavenumbers on passing from 5-FU to 5-IU molecule, an increases in its theoretical IR intensity, and decreases in its Raman activity. The γ(C5-X) vibrations are predicted to change significantly its position with the halogen atom mass from ca. 350 for 5-FU to ca. 250 cm^{-1} for 5-IU. For 5-ClU, 5-BrU and 5-IU the mode is practically IR inactive, whereas for 5-FU the mode has a rather low IR intensity.

C6-H modes. The calculations predict that, as the substituent mass at the position C-5 is increased, the ν(C6-H) shifts toward lower wavenumbers and its intensity decreases. The weak intensity of the ν(C6-H) band made it absent in the experimental spectra.

The δ(C6-H) mode wavenumber is predicted to occur at ca. 1315 cm^{-1}, while the analogous band in U (mode 22 in Table 2) is predicted to occur at ca. 1400 cm^{-1} and to be

coupled with the δ(N-H) mode. The theoretical IR intensity of this mode changes irregularly while the Raman activity is expected to decrease slightly as the halogen mass in increased. The Ar-matrix bands are located at ca. 1330 cm^{-1} in accordance to our calculations, and except for 5-FU, they exhibit quite low intensities. The low intensity of this mode may be a reason why other investigators have assigned it to other bands placed at 1182 cm^{-1} for 5-FU and at 1192 cm^{-1} [42] or 1189 cm^{-1} [43] for 5-BrU.

The γ(C6-H) out-of-plane vibrations are predicted to occur in the range of 875-905 cm^{-1} and to increase on passing from 5-FU to 5-IU, whereas for U (mode 15) it is predicted to occurs at ca. 970 cm^{-1}. The theoretical IR intensity of the mode is of medium intensity and decreases on passing from 5FU to 5-IU, while for U this mode is predicted to be almost inactive.

Ring vibrations. The C-N stretching mode (no. 18 of Table 2) is predicted to occur in the 1180-1150 cm^{-1} range. The IR intensity of the band is medium and it is little affected by substitution at the C5 atom. Mode 14 is defined as antisymmetric stretching of the opposite C4-C5 and N1-C2 bonds, and it is predicted to occur near 960 cm^{-1}, in accordance to the experimental results. The IR intensity of the band is medium and it is practically not affected by the substitution at the C5 atom. Mode 12 is predicted to occur at 760±10 cm^{-1}. The calculations indicate that its IR intensity should be very weak or almost null while the Raman intensity is expected to be strong.

Ring bending vibration mode (no. 16) is described as a δ(C5-X) mode, although its low wavenumber difficult the identification in the IR spectra. Mode 5 is the only local mode whose definition changes with halogen substitution; however, antisymmetric bending δ(N3-C4-C5) + δ(N1-C2-N3) is common for all those definitions. For the 5-ClU, 5-BrU and 5-IU molecules, mode 5 couples with the ν(C-X) vibration leading to a higher wavenumber. I.e. at 660, 625 and 610 cm^{-1} in the Ar matrix [41] spectra, for the 5-ClU, 5-BrU and 5-IU molecules, respectively, whereas for the 5-FU and U molecules, for which it is practically uncoupled with other local modes, it is located at lower wavenumber, at ca. 450 and 520 cm^{-1}, respectively. The mode is of medium IR intensity, except for 5-FU where it is much weaker.

3. Conclusions

Uracil and its derivatives, constituents of the genetic material, play a fundamental role in basic biological processes and vibrational spectroscopy is an excellent tool for characterization of these biomolecules.

This work shows the theoretical and experimental structure and vibrational spectra of uracil (U) and its 5-monosubstituted derivatives (5-XU; X = F, Cl, Br, I, CH_3, NH_2, NO_2). The effects in the geometry structure and vibrational wavenumbers by the different substituents in the 5-position of the uracil ring are analysed successfully and some correlations between the structure and spectra parameters are proposed.

It is expected that the present study may be very helpful in understanding the biological activity of 5-XU (X= F, Cl,Br,I) and in searching new novel antitumor/ anticancer drugs.

Acknowledgements

The author is thankful to Prof M A Palafox, Departamento de Química-Física I, Facultad de Ciencias Químicas, Universidad Complutense, Madrid-28040, Spain for reading the manuscript and making several suggestions. He is also thankful to Dr P K Tripathi, Indian Spectroscopy Society, KC 68/1, Old Kavinagar, Ghaziabad and Dr J K Vats, Physics Department, CCSU, Meerut for Proof Reading and making necessary corrections. The author is also thankful to Prof N K Taneja, Vice Chancellor, CCSU, Meerut for motivation and encouragement during the course of this work.

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98th Indian Science Congress

January 3-7, 2011, Chennai

II

ABSTRACT OF

PLATINUM JUBILEE LECTURE

PLATINUM JUBILEE LECTURE

Er^{3+}, Yb^{3+} Co-doped Gd_2O_3 Nano-crystalline Phosphor: A Multifunctional Material

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Rare earth dopants, such as Er^{3+}, Eu^{3+}, Ho^{3+}, Yb^{3+} etc. are known to produce excellent luminescence properties very useful for mankind. Recently we have developed Er^{3+}/Yb^{3+} co-doped Gd_2O_3 nano phosphor material which has interesting applications [1]. Laser radiation excitation with variable power shows optical switching and large heat generation from the sample which led this material as nano-volume optical heater [2, 3]. This kind of nano-volume heater can find application as the medicine for local hypothermal treatment of cells, for perforation of nanoholes in organics and metals etc.

The temperature dependent emission has shown this phosphor as temperature sensor [4]. Frequency upconverted emissions ($ë_{exc}$ = 976 nm) from two thermally coupled excited states $^2H_{11/2}$ and $^4S_{3/2}$ of Er^{3+} centered at 523 and 548 nm in the phosphor pumped by NIR source were recorded in the temperature range 300–900 K. The results imply that Er^{3+}:Yb^{3+} co-doped Gd_2O_3 phosphor can play an important role in high temperature measurements with a better sensitivity.

Further in continuation, this phosphor has been placed between the pole pieces of an electromagnet whose field can be varied up to 1 Tesla (1T). As the magnetic field is lowered from 1T to zero, the UC emission intensity shows a gradual increase. However, this increase does not follow the curve obtained when the magnetic field from was 0T to 1T. Thus in a complete cycle of magnetic field from 0T to 1T and from 1T to 0T one sees for the emission intensity a hysteresis much like as observed in M-H curve for ferromagnetic material. Thus an optically bistable emission is observed induced by the external magnetic field. This could find application in magneto-optic switches [5].

In a novel application we have used Gd_2O_3: Er^{3+}/Yb^{3+} phosphor as the detection of latent finger marks on the difficult surfaces like wood, glass plated and painted walls etc.

The intense green and red colour emitted by phosphor on excitation with probable 976 nm radiation has been used for the development of the finger marks in blue, green and red colour. The images can be monitored by simple camera with the aid of different filters [1].

Further, Pulsed laser ablation technique in liquid (distilled water) helped us to tailor the shape (spherical) and size (average diameter of ~12 nm) of this material. The colloidal transparent nano-particles of the phosphor material give intense emission in green and red region on excitation with 976 nm radiation and can be used efficiently for the tagging purposes for bio-imaging and in medical diagnostics [6].

The nanophosphor has been prepared through solution combustion method reagent grade Gd $(NO_3)_3$. $6H_2O$, Er $(NO_3)_3$. $6H_2O$ and Yb $(NO_3)_{3-}$. $6H_2O$ materials. The structure of the nanophosphor was verified by XRD and TEM methods

Optical studies have been carried out via absorption, upconversion (UC) studies (under 532 and 976 nm excitations) and lifetime measurements. Sample gives the intense UC band up to UV regions. All these potential results will be presented in this talk.

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98th Indian Science Congress

January 3-7, 2011, Chennai

III

ABSTRACT OF

YOUNG SCIENTIST AWARD PROGRAMME

YOUNG SCIENTIST AWARD

Microstructural Evolution and Tribiological Behavior in Al-Ga-Pd-Mn Quasicrystalline Thin Films

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Key words: *Thin Film, Quasicrystal, Electrical and Thermal Resistivities, X-Ray diffraction, Transmission electron microscopy.*

Thin film quasicrystal coatings have unique properties such as very high electrical and thermal resistivities and very low surface energy. A nano quasicrystalline thin film of icosahedral Al-Ga-Pd-Mn alloy has been produced by flash evaporation followed by annealing. The icosahedral phase of $Al_{65}Ga_5Pd_{17}Mn_{13}$ alloy has been used as a precursor material. The X-ray diffraction and transmission electron microscopy confirmed the formation of icosahedral phase in the thin film. The energy dispersive X-ray analysis investigations show the final stoichiometry maintained in the thin film. Icosahedral Al-Ga-Pd-Mn thin film provides a new opportunity to investigate the various characteristics including surface characteristics. The formation of icosahedral thin film in Al-Ga-Pd-Mn quaternary alloy by present technique has been studied for the first time. These films can be utilized as conversion coatings for Al substrates or incorporated into a full coating system containing an organic primer and a topcoat. Attempts will be made to discuss the micromechanisms for the formation of quasicrystalline thin film in Al-Ga-Pd-Mn alloys.

98th Indian Science Congress

January 3-7, 2011, Chennai

IV

ABSTRACTS OF
SYMPOSIUM/INVITED LECTURE

PROCEEDINGS

OF THE

NINETY EIGHTH SESSION OF THE

INDIAN SCIENCE CONGRESS

CHENNAI, 2011

PART II : ABSTRACTS OF SYMPOSIUM / INVITED LECTURE

SECTION OF
PHYSICAL SCIENCES

President **: Professor V K Rastogi**

1. Measurements by Light

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Light has fascinated and intrigued mankind since time immemorial. It has played a significant role in unraveling the mysteries of nature and advancement of knowledge.

Ever since we understood how light could be manipulated, its applications took roots. In turn the components to manipulate light required measurement of their properties so that better manipulation could be performed. Light therefore began to be used for measurement.

Most frequently used phenomenon for measurement is the interference phenomenon. It was used earlier to measure radii of curvature, film thickness and the wavelength of

light itself. The surface quality, performance quality and angle measurement on various optical components were routinely done in the workshop environment. Since wavelength of light was accepted as standard of length, measurement and calibration of length standards was done routinely.

Dramatic changes in the application of interference took place with the advent of lasers and availability of fast and area detectors. Other parameters which influence the length directly or indirectly began to be monitored by interferometry. The accuracy of measurement also increased tremendously. The measurement process became operator independent.

Holographic principles expanded the application of interferometry to real objects. Deformations due to load on real objects could be studied with interferometric precision. Whole objects like airplane wings could be evaluated in a single measurement. Vibration modes of real objects could be visualized and evaluated.

Application of interferometry did not remain limited to medium and large objects but was extended to the evaluation of performance of the MEMs devices.

Current accuracy of measurement is limited by the uncertainty principle but the optical physicists always find ways to overcome the limitations and the research continues in this direction.

The talk will take you on a journey through the wonderful world of interferometry – how it began and what it is accomplished so far and what are its ramifications to science and society.

2. Advances in Microwave Spectroscopy and Radioastronomy

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Microwave and millimeter waves are extensively used to study molecular structure and molecular interactions. These studies are not only important to elucidate the molecular structure and interactions but are also used as probes to investigate the interstellar media

and interstellar objects and in studying biological molecules. A new field of radio astronomy has already been originated and millimeter wave spectroscopy is used to study the interior properties of these astronomical objects. It is always advantageous to investigate the molecules in the laboratory and then use these microwave and millimeter spectra to seek the possibility of these molecules in the interstellar media.

3. Hypertelescope Imaging

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Single aperture interferometry by means of speckle imaging has made roads in several important fields in astrophysics. In recent years, the adaptive optics system at the telescope has produced spectacular results. However, the aperture of a telescope limits its resolving capacity. A diluted array of two or more telescopes is required to measure the brightness distribution across most stellar sources and many other objects of astrophysical importance. Such a technique, known as aperture synthesis, provides greater resolution of images than is possible with a single member of the array. Following the success of Interferometre a deux Telescope (I2T) and Grand Interferometre a deux Telescope (GI2T), the interferometry with phased arrays of multiple large sub-apertures has become a reality. These instruments are used to obtain results from the area of stellar angular diameters with implications for emergent fluxes, effective temperatures, luminosities and structure of the stellar atmosphere, dust and gas envelopes, binary star orbits with impact on cluster distances and stellar masses, relative sizes of emission-line stars and emission region, stellar rotation, limb-darkening, and astrometry. However, in order to obtain snapshot images of the astronomical sources, many-aperture optical array with arbitrarily diluted apertures is required to be built. The concept of 'hypertelescope' approach to imaging, which is viewed as a simple modification of the classical Fizeau interferometer by employing pupil densification, has a vast potential, since large array of relatively small apertures is easy to implement. In view of the present scenario, after a brief presentation on the interferometric techniques, the current trend and the path to future progress in optical interferometry using hypertelescope concept will be discussed.

4. Micro-optics and Nanophotonics Technologies for Defence Applications

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As the system volume and weight of a device decreases its utility increases manifold. Smaller instruments are less expensive and have increased manufacturing volume. For defence applications, reducing system volume and weight is critically important. For example, the camera in a helmet mounted display has to be as compact and light weight as possible. The additional burden of fitting a camera on the helmet of a soldier operating in battle-field has to be minimal. The same requirement holds true for a surveillance camera on an unmanned vehicle. Design using refractive and diffractive micro-optics can help in reducing the system volume and weight. This can be especially advantageous for IR optical systems where system volume and weight are considerably large. In an imaging system, using a refractive microlens array instead of a single lens reduces the optical system thickness (distance between the first optical element and detector array) and thereby the optical system volume and weight. Diffractive micro-optical elements may be used in conjunction with refractive elements to correct for aberrations in imaging systems and to achieve improved performance using reduced number of elements thereby reducing weight.

Structures with feature sizes of the order of nanometer have unique, controllable, and tunable optical properties.These properties arise from the fact that these structures are smaller the wavelength of light used to observe them. The optical properties of nanomaterials can be tailored for important defence applications most notable being compact, efficient and tunable light sources, detectors with enhanced capabilities, chemical and biological sensors. This paper discusses three areas in Nanophotonics that will have tremendous impact for defence applications namely Photonic Crystals, Metamaterials and Plasmonics.

Photonic crystals [1] are composed of periodic dielectric or metallo-dielectric nanostructures that affect the propagation of electromagnetic waves (EM) in the same way as the periodic potential in a semiconductor crystal affects the electron motion. The periodicity of the structure in one, two or three dimensions gives rise to dramatic changes

in the optical properties and possibily to the formation of a forbidden gap in electromagnetic spectrum referred to as 'Photonic Bandgap'. The photonic bandgap defines a set of frequencies for which light cannot propagate in the crystal. The tunability of the bandgap is achieved through control of dimensions and symmetry of the photonic structure providing exquisite frequency control of the propagation properties through the crystal. Photonic crystal promises to be a suitable material in which light could be created, transported and processed. In a two dimensional Photonic crystal typically created by drilling holes in a slab of high refractive index material like Silicon, many devices can be readily integrated like a waveguide (created by leaving a row of holes undone) or a microcavity (formed by leaving one or a few holes undone). When made of a luminescent material, these microcavities can turn into a lasing center and thus become light sources that can be integrated into photonic circuitry.

Metamaterials [2] are structured composite materials whose properties are determined primarily by the subwavelength sized structures. By designing the structures, one can tailor the optical / electromagnetic properties at specified frequencies for a given application. From a defence applications point of view, metamaterials holds immense promise for use in thermal radiation sensing. For thermal radiation sensing applications at LWIR frequencies (8-12 micron wavelengths), the metamaterial is designed to have exceptional impedance matching with vacuum for a wide range of angles and independent of polarization. Recent studies have shown that metamaterials having exceptional impedance matching along with very large absorption of upto 99.9% are possible.

In plasmonics [3], manipulation of light at nanoscale is based on the properties of surface plasmons arising from metal free-electron response. Surface plasmon are known to be very sensitive to any change occurring at the metal-dielectric interface. Plasmonics device hold immense promise for sensing, imaging and spectroscopy applications. Novel Plasmonic sensors will exploit nanoscale dispersion control and nanometric volumes, allowing improved sensitivity even at higher background levels. Hence, surface plasmon resonance (SPR) technique enjoys considerable advantages including higher versatility and accuracy over other optical techniques such as planar wave guiding, interferometry etc. Due to high sensitivity, the SPR technique has been exploited in the field of pesticide detection, gas or biomolecules sensing, detection of ultrathin films etc. Another application of plasmonics that is important to defence is to develop low-cost, rugged coatings that are highly absorptive at 1064 nm. As most laser range finders operate at 1064nm by using Nd-YAG or Nd-YVO_4 lasers, this would severely limit the range of the hostile laser range

finders. Crucial to this technology will be the design of plasmonic resonant particles or structures that will enable highly absorptive surfaces at the desired frequency.

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5. Discovery of Micropulses in the Bioluminescence of fireflies, oscillatory chemical reaction, Purkinje effect and a Model of Mode Locked Laser

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Bioluminescence is the process by which living organism like fireflies convert chemical energy into light. The enzyme luciferase catalyses the bioluminescence reaction, which uses luciferin, MgATP and molecular oxygen to yield an electronically excited oxyluciferin species. We recorded the in vivo emission and time resolved spectra of the firefly Luciola pracusta Kiesenwetter 1874 (Coleoptera: Lampyridae: Luciolinae). The time resolved spectrum reveals that a flash of 100 millisecond duration is, in fact, composed of a number of microsecond pulses (30, 000 pulses). The work also indicates the presence of oscillatory nature of chemical reaction (Bz), in the emission of fireflies, and we also show that the red sector in the bioluminescence spectrum of fireflies is not visible to the naked eye because of the Purkinji effect. A mode of the production of micropulses which is analogues to a mode locked laser is presented

6. Brownian Motion in Laser-cooled Atomic Clouds: Ob-servation of Super-ballistic Expansion

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The importance of fluctuations of the radiation force on the motion of atoms has been a subject of intense theoretical and experimental investigations since the seminal paper of Einstein on the quantum theory of radiation. While in the work of Einstein, the fluctuations are necessary to account for the Maxwellian distribution of atomic velocity in thermal equilibrium, in the more recent works on laser cooling and trapping of atoms the fluctuations give rise to diffusive spreading of velocities and that manifests as the temperature of laser-cooled atoms.

Very recently, we have demonstrated both experimentally and theoretically that in laser cooled atoms the fluctuations give rise to a new diffusion behavior of the type $x^2 \sim t^3$ for the mean square displacement. We term this behavior as the supper-ballistic behavior, which comes into play when a cold cloud of atoms is allowed to undergo one-dimensional expansion in the presence of two-dimensional near resonant laser beams. These experiments are conducted on cold cesium atoms generated in a magneto-optical trap, and they afford a direct visualization of the atomic random walk. We develop a model based on the theory of Brownian motion and show that the comparison of experimental results with theory provides a direct measure of the velocity diffusion coefficient. Another important issue related to these studies is that they provide a direct evidence for the radiation trapping force, the long-range repulsive force that arises from the multiple scattering of photons, which is of fundamental importance in astrophysics and plasma physics.

In this talk we discuss the ideas underlying these studies, the experimental configuration and results, the stochastic formulation of the problem and future directions.

7. Applications of a Technique on Photovoltaic Generation Using Thin Silicon Film in Studies on Solar Eclipse, Battery Charging and Earth Resources Studies

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Key words: *pn-junction, pnp transistor, Thin film, Visible region, Audio devices, Total solar eclipse, Solar battery charger, Earth resource detector*

In this work the photovoltaic generation in a thin film of p-n silicon junction has been discussed. The thin film was obtained by cutting p-n-p transistor at its top and adjacent electrodes (P and N) serving as a junction and source of photovoltaic effect on illumination. The photovoltaic effect has been measured for light intensities of different wavelengths in visible region. Light of different intensities and wavelengths were used to study the complete effect. The photo e.m.f. generated in such a thin films is much useful as it can derive many audio devices. Importance of this technique is that this device can be used in studies on solar eclipse as was done during total solar eclipse on July 11, 1991 by the author and his team. Further the technique is useful in studying earth resources and charging batteries through solar radiation.

8. Smith Chart and its Importance in Antenna Technology

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Key words: *Smith chart, Spectral simulation antenna parameters, Transmission Lines, Matching Circuits, Antenna Technology.*

The smith chart is a graphical aid or monogram designed for electrical and electronics engineers specializing in radio frequency to assist in solving problems with transmission

lines and matching circuits. It is an alternative to using tabular transformation. The Smith chart can be used to represent many parameters including impedances admittances, reflection coefficients, scattering parameters, noise figure circles, constant gain contours and regions for unconditional stability. The implementation of Smith chart plots with alternative graphics packages provides a great deal of insight into precession of both measured and theoretically computed data. The Smith chart is formed by complete circles of constant resistance, and partial circles of constant reactance. We use the fact that the reflection coefficient is one at the boundaries of the smith chart to find analytical expressions for the angular limits of the constant reactance circles. The equations are formulated in a way that they can be implemented conveniently with math CAD, in a computationally efficient fashion. Smith chart can look imposing, its nothing more than a special type of 2-D graph, much as polar and semilong log-log scales constitute special types of 2-D graphs. In this talk we shall present the basic idea of smith chart after that we shall discuss the utility of smith chart in antenna technology with the help of different graphs and figures.

9. Charge Transfer Interaction and First Order Hyperpo-larizability Studies For THz Application

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In the 21st century the Terahertz waves are expected to be utilized for the applications on ultrahigh-capacity telecommunication, medical diagnosis, device inspection, seeing-through analysis, environmental sensing, etc. Terahertz (THz) radiation is located in the spectral region 0.1-10 THz (3 cm^{-1}- 300 cm^{-1}) between the microwave and mid infra red region of the electromagnetic spectrum. The THz spectrum in the wavenumber range from 0.1 to 5 THz provides rich information on low wavenumber vibrational modes: crystalline lattice or inter-molecular vibrational modes, hydrogen bonding stretches, and some torsion vibrations in many chemical and biological compounds, including small biomolecules, pharmaceutical materials, and explosive. Normally the high second-order

nonlinear optical (NLO) process possibly to detect and generate the THz waves. The large value of second order polarizability, β which is a measure of the non-linear optical activity of the molecular system, is associated with the intramolecular charge transfer (ICT), resulting from the electron cloud movement through π conjugated framework from electron donor to electron acceptor groups. The electron cloud is capable of interacting with an external electric field and thereby altering the dipole moment and the second order non-linear optical activity. The simultaneous activation in the vibrational spectra shows the ICT of the system and thereby NLO activity. Density functional Theory and *ab initio* quantum-chemical computation can help to optimize the structure and predict the NLO properties for molecules designed. The physical properties of these conjugated molecules are governed by the high degree of electronic charge delocalization along the charge transfer axis and by the low band gaps. Vibrational spectral studies of the molecules can provide deeper knowledge about the relationships between molecular architecture, non linear response and hyperpolarizability and support the efforts towards discovery of new efficient materials for technological applications.

10. FTIR Studies on Nano Resin of Lactic Acid and Maleic Anhydrade

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Keywords: *Lactic acid, FTIR, Fluconazole, Nano Particles, Antifungal drugs.*

Controlled release drug delivery is a new way to treat the disease. Fluconazole is a trizole antifungal drug used in the treatment and prevention of superficial and systematic fungal infections. In a bulk powder form, it appears as a white crystalline powder, and it is very slightly soluble in water and soluble in alcohol. Like other imidazole and trizole – class antifungals fluconazole inhibits cytochrome P 450 enzyme 14α demethylase. Mammalian demethylase activity is much less sensitive to fluconazole than fungal demethylase. This inhibition prevents the conversion of lanosterol to ergosterol, an essential component of the fungal cytoplasmic membrane, and subsequent accumulation of 14á methyl sterols. To increase its retaining rate in the body flucanazole tablets were coated by a nano resin of lactic acid and maleic anhydride. Nano resin was prepared by the condensation reaction of lactic acid and maleic anhydride. Resin was characterized by

Fourier Transform Infrared spectra (FTIR). The peak at 1760 cm^{-1} is attributed to C=O stretching. The FTIR spectrum of nano resin was compared with FTIR spectra of lactic acid and maleic anhydride. The average size of particles was found 315 nm in this resin. The AFM picture shows that the new material have large polydispersity. Drug release rate of coated tablets was found faster than the uncoated tablet.

11. Abstract not Received

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13. Green Nanotechnology and its Application

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Nanotechnology is a new way to develop new novel materials by reducing their particle size down to 100 nm. Such nanosized materials can be manipulated to get new properties desired for specific applications. As such nanomaterials have excited science and enormous potentials. Many methods including chemical route, physical (evaporation, laser ablation, sputtering etc) and biological are used to synthesise these nanomaterials. Chemical route is very common and requires expensive chemicals, more time consuming

and often embedded with variation of particle size. Green nanotechnology has recently emerged where biological synthesis of nanoparticles, mostly metals, have been produced by chemical reduction of reducing agent present in the plant extracts. We in Amity Institute of Nanotechnology, initiated research in this area of Green nanotechnology. Plant extract mediated Ag nanoparticles have been synthesized, characterized and used for various purposes including antibacterial effects. Many instrumental techniques including AFM, UV vis spectrophotometer, Electrochemical analyzer, Dynamic Light Scattering system and TEM have been used in the present investigation. Results of the work in regard to nanoparticles formation and their applications will be highlighted in the presentation.

14. Negative Index Materials, Metamaterials and Photonic Band Gap Materials

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15. Studies on the Effect of Picolines on the Stereochemistry of Lanthanide (III) Nitrates Coordination Compounds of 4[N-Furfural) Amino] Antipyrine Semicarbazone

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In the present work the effect of α-, β- and γ picolines on the stereochemistry of the coordination compounds of lanthanides(III) nitrates derived from 4[N-(furfural) amino]-antipyrine semicarbazone (FFAAPS) has been studied. The general composition of the present coordination compounds is $Ln(NO_3)_3$(FFAAPS)pic (Ln = La, Pr, Nd, Sm, Gd, Tb, Dy or Ho; pic = α-, β-, or γ-picolines). All these coordination compounds were characterized by elimental analyses, molecular weight, molar conductance, magnetic susceptibility,

infrared and electronic spectra. The infrared studies suggest that the FFAAPS behaves as a neutral tridentate (N, N, O) while α-, β, or γ-picoline is coordinated to the central metal ion via heterocyclic N-atom. Nitrates are bicovalently bonded in these compounds. From electronic spectral data, nephelauxetic effect (β), covalence factor ($b^{1/2}$), Sinha parameter (δ %) and the covalence angular overlap parameter (η) have been calculated. Thermal stabilities of these complexes were studied by thermogravimetric analysis. In conclusion, the coordination number of lanthanides (III) in the present compound is found to be ten.

16. Developments in Atomic Structure Calculations

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Key words: *Atoms, Quantum objects, Wave functions, Partial differential equation, Dirac relativistic quantum mechanics.*

Atoms are quantum objects. Quantum objects are described by wave functions. Wave functions are obtained from wave equations. The wave equation describing the structures of an atom is a partial differential equation of eigenvalue type. The first partial differential equation for the wave function was invented by Schrödinger (1926). This equation does not include the relativity. For the first time, the effect of relativity was included by Klein-Gorden (1926) known as Klein-Gorden relativistic equation. But it does not give probability density overcome by Dirac (1928) known as Dirac relativistic quantum mechanics. These all quantum mechanical methods are for one electron systems. In nature, mostly atoms, molecules and ions are of multi-electron. One can set up the wave mechanical equations for multi-electron atoms but can not solve accurately. Approximations and numerical methods are developed for multi-electron systems. Now, the general availability of powerful electronic computers has resulted in a variety of developments in calculations of the electronic structure of atoms. The starting point is generally the Hartree-Fock (HF) approximation, which inadequately accounts for the motion of the electrons. A treatment of electron correlation has been the aim of most of the recent work in this field, and the methods which have been proposed are reviewed. The accuracy to which energies (or at least energy differences) can be evaluated, and the calculations of electron affinities and term ratios are considered. The evaluation of oscillator strength (transition probabilities)

and hyperfine structure are also covered. Available atomic structure programs based on the correlation methods (configuration interaction) are discussed. The role of correlation, relativity, quantum electrodynamics (QED), finite nuclear size (FNS) and parity non-conservation (PNC) in high precession theoretical investigation of properties of atoms and atomic ions are demonstrated. Tiwary and coworkers have extensively performed atomic structure calculations. At present, we do not have a comprehensive and practical atomic structure theory which accounts all these physical effects on an equal footing. Suggestions are made for future directions.

98th Indian Science Congress

January 3-7, 2011, Chennai

V

ABSTRACTS OF

ORAL /POSTER PRESENTATION

PROCEEDINGS

OF THE

NINETY EIGHTH SESSION OF THE

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PART II : ABSTRACTS

SECTION OF

PHYSICAL SCIENCES

President **: Professor V K Rastogi**

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PART II : ABSTRACTS

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PHYSICAL SCIENCES

President **: Professor V K Rastogi**

ORAL

1. R-Processes Nucleosynthesis in High Entropy Envir-onment in Explosion of Supernova Type II

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Key words: *Reflectivity, Near critical fluids, Nucleosynthesis, Entropy, Iron core, Supernova.*

It is generally acknowledged that type II supernova results from the collapse of iron core of a massive star which, at least in some cases, produces a neutron star. During collapse an outward bound shock wave forms in the matter falling onto the nearly stationary core which shows reflectivity of matter. The conditions behind the shock at 100 to 200 km are suitable for neutrino heating. The neutrino heating blows a hot bubble above the

proton eutron star and is the most important source of energy for supernova explosion. At this stage, we try to attain the R-process (rapid neutron capture process) path responsible for the production of heavy elements beyond iron, which are otherwise not possible to be formed by fusion reactions. The most interesting evolution occurs at temperature falls from 10^{10} K to 10^{9} K. At these high temperature conditions, the near critical fluids after fusion reactions are forbidden and transform into the respective atoms by R-process path which on beta decaying produce the ultimate elements of the periodic charts. Another astrophysical parameter needed for our analysis is neutron number density which we take to be greater than 10^{20} cm^{-3}. With these, at different entropy environments, we assign the neutron binding energy that represents the R-process path in the chart of nuclides. Along the path, the experimental data of observed elements matches our calculated one. We find that an entropy of H" 300 can lead to a successful R-proces.

2. Fluid Dynamics of Blood Flow in an Out-of-Plane Aorto-Left Coronary Sequential Bypass Graft

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Key words: *Coronary artery bypass grafting (CABG), Sequential bypass grafting (SBG), Multiple bypass grafting (MBG), Computational fluid dynamics (CFD), Wall shear stress (WSS), Wall shear stress gradient (WSSG), Side-to-side anastomosis, End-to-side anastomosis*

The sequential bypass grafting technique is a technique in which two or more coronary artery anastomoses are made with a single graft, usually the sapheneous vein. Despite the apparent advantages of using the sequential bypass grafting, this technique has been criticized on the basis that the entire revascularization depends on a single proximal anastomosis. Restenosis, a leading cause of bypass graft failure, can be correlated with

the geometric configuration and the hemodynamics of the bypass graft. The objective of this study was to use computational fluid dynamics (CFD) to investigate the hemodynamics in a three dimensional out-of-plane sequential bypass graft model, bypassing the partially occluded proximal portions of the obtuse marginal (OM) branches OM1 and OM2 arteries. Using a finite volume approach, quasi-steady flow simulations are performed at different instances of the cardiac cycle.

Plots of wall shear stress (WSS) and spatial WSS gradient (WSSG) distribution are shown in the aorto-left coronary bypass graft domain. The smooth flow patterns in the side-to-side anastomosis region indicate that a more uniform WSS and spatial WSSG distribution is observed in the side-to-side anastomosis configuration over the end-to-side anastomosis.

3. New Class of Dark Matter Objects and Their Detection

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Key words: *Dark Matter, Primordial black holes, Baryon load problem*

About one-fourth of the universe is thought to consisit of dark matter (DM). Yet there is no clear understanding about the nature of these particles. Common DM candidates includes WIMPs with masses from ~10 GeV-1TeV. These particles can gravitate to from a new class of objects in DM holos or around the galactic centre. We study in some detail many properties of these objects, their formation and possibilities of their detection, and implications on star formations. These could provide the possibility of forming primordial black-holes distinct from the usual Hawking black-holes and could also provide a scenario for short duration GRBs, avoiding the baryon load problem.

4. Effect of Nitrogen Doping on Ferromagnetism in (ZnO)n Clusters

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Keywords: *DFT, Doping in group II-VI and III-V semiconductors, ferromagnetism*

First principle calculations based on spin density functional theory have been performed for nitrogen doped $(ZnO)_n$ clusters (n = 1-8, 12, 16). The magnetic moment is observed in Zn_nO_n clusters when doped with N impurities at substitutional O site. The total energy calculation suggests that N is more stable at O site than that at the Zn site in ZnO clusters. A total magnetic moment of $1ì_B$ per N atom is introduced and the local magnetic moment is mainly localized on doped N atom. The N atom shows no tendency for clustering. The calculated results are in agreement with existing experimental and theoretical results.

5. A study of Sensitivity Properties of SC Filters Derived from LC Ladder Prototypes

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Key words: *Switched capacitor filter, LDI, Ladder and Passband filter, LC prototype filter.*

The sensitivity properties of a class of switched-capacitor LDI ladder filters are investigated. It is shown that , because of the frequency variation of the terminations in the equivalent circuit of such filters, the low passband sensitivity properties of the LC prototype filter is not retained. A modification to the input section of the filter is shown to result in low sensitivity.

6. Simulation studies for performance of diffraction free Airy and Bessel beams

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Keywords: *Diffraction, Propagation, Airy beam, Bessel beams, Gaussian beams, Light, Accelerating Airy beams, Linear axis*

Any ordinary optical beam of light spreads as it travels due to diffraction of light. Quite recently, non spreading freely accelerating Airy beams have been realized in optics community. In this paper, we have reported Airy beam as diffraction free beam, which consists of two important properties viz freely acceleration and nonspreading. We have carried out simulation study for both 1-D and 2-D Airy beam propagation, respectively. We have also made comparison among Airy beam, Bessel beam and Gaussian beam and our results infer that Airy beam propagates due to diffraction freely for a long distance in parabolic trajectory, while Bessel beam is less diffraction free and travels along linear axis.

7. EMIC Waves Study Around Earth's Environment by Particle Aspect Approach

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Key words: *Electromagnetic ion-cyclotron wave, Auroral acceleration region, Solar plasma, Earth's enviornment, Parallel electric field, Plasma density.*

Electromagnetic ion-cyclotron (EMIC) waves have been studied by single particle approach. The effect of EMIC instability in the presence of parallel electric field at different

plasma densities is evaluated. The dispersion relation, growth rate parallel and perpendicular resonance energies of the electromagnetic ion-cyclotron waves in a low (ratio of plasma pressure to magnetic pressure), homogeneous plasma have been obtained. The wave is assumed to propagate parallel to the static magnetic field. The whole plasma is considered to consist of resonant and non-resonant particles. It is assumed that resonant particles participate in energy exchange with the wave whereas, non-resonant particles participate in the oscillatory motion of the wave. The effect EMIC wave in the presence of parallel electric field at different plasma densities is to enhance the growth rate of EMIC waves. The results are interpreted for the space plasma parameters appropriate to the auroral acceleration region of the earth's magneto-plasma. The applicability of the present study is consistent with earth's environment according to the nature of EMIC waves.

8. Interdependence of Mechanical and Structural Properties in Sintered SnTe Films

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Key words: *Polycrystalline, XRD traces, Chalcogenides, Sintering technique, Lattice parameters, Crystallite size, Strain.*

In recent years, use of heavy metals especially lead, cadmium, and mercury in semiconducting industry, paints and coatings has been restricted throughout the world, on account of their detrimental effects on health. In order to replace such metals from various semiconductor and optoelectronic applications, it becomes quite necessary to search for their alternatives and look at possible compounds having similar properties with sufficient stability. To solve the purpose, tin based compounds have emerged as potential materials for their wide applications in industry and research . Tin chalcogenides SnS, SnSe and SnTe offer a group of promising materials for solar applications and optoelectronics in far

infra-red region of the spectrum as well as for thermo electric devices at medium high temperature.

The technological interest in polycrystalline based devices is caused mainly due to their low production cost which makes them suitable for large scale applications. SnTe belongs to a class of self doping compounds i.e. metal chalcogenides. It is known to be a p-type semiconductor with strong self compensation of p-type conduction. Different workers have prepared SnTe films by vacuum based expensive techniques, however in the present investigation the sintering technique is employed to prepare SnTe films which is simple and commercially viable.We report here the results of physical properties of SnTe films particularly structural and mechanical. The XRD studies, interplanner spacing, lattice parameter, crystallite size and strain have been determined for the sintered films of different thicknesses and an attempt to establish an explicit co-relation between various quantities has been made. The XRD traces showed that strain was tensile in nature. The crystallite size increases with thickness while strain decreases.

9. Dielectric Properties of TM (= Cr^{3+}, Mn^{2+}, Fe^{3+}) Doped BiNbO4 Ceramic Powders

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This paper reports the dielectric properties of $Bi_{0.95}Tm_{0.05}NbO_4$ ceramic powders sintered at 800 $^{\circ}$C using solid state reaction method. For those materials, SEM images and EDAX elemental profiles have been obtained to understand their particle sizes and compositions. The XRD profiles of the samples were taken to understand their structure and nature. The dielectric properties of the samples prepared were measured by using PSM 1700 (LCR meter) from range 1 Hz – 1 MHz. It is interesting to mention dielectric constant (ε') and dielectric loss (tan δ) of all the samples were decreased where as ac conductivity (σ_{ac}) increases with increasing frequency. The Cole-Cole plots of all the

three samples show the bulk resistance (R_b) decreases with increase of the crystallite size, resulting the increase in dc conductivity (σ_{dc}). The present work has provided a provision to identify those three ceramic powders as technically important low temperature (800°C) sintered microwave dielectric materials for microwave applications.

10. Scattering of Positrons by Alkali Atom

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Key words: *Elastic scattering of positrons, Differential cross section, Distorted wave method, Polarization potential*

Large number of channels including continuum are open in positron-atom scattering at intermediate energies. In practice it is difficult to include effects of all channels including continuum in calculation. Although all the dynamics of the system can not be incorporated in a single distorted wave method. A suitable distorted wave method that accounts for the effect of higher excited states and continuum is required to predict cross-sections.

In the present investigation, using a method form of Born approximation differential cross section for elastic scattering of positrons by alkali atoms, potassium have been calculated in intermediate energy range. Attempts have been made to modify and to improve the Born approximation by taking into account the effect of nuclear interaction terms in the form of distorted wave (screened Coulomb Waves). To analyze the impact of polarization effect differential cross sections have been reported. The agreement between present set of results with corresponding theoretical predictions of S P Khare and Vijayshri is fair [Khare SP, Vijayshri, Physics with Positron, Procd Natinal Advances Research Workshop, London, (1987), p 417.]

11. Cubic $CuFe_2O_4$ Nanoparticles: Effect of Particle Size and Doping on the Structural and Magnetic Properties

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Key words: *Cubic $CuFe_2O_4$, Nanoparticles Mossbauer spectra, Doping*

Ferrite nanoparticles have attracted tremendous attention of researchers due to their wide application in industry and technology [J Appl Phys, 76 (1994) 7506; J Magn Magn Mater, 111 (1992) 29; J Magn Magn, 281 (2004) 353]. Studies on spinel ferrites have indicated that most of the properties are a function of the distribution of various cations on the octahedral (B) and tetrahedral (A) sites of spinel lattice [Phys Rev Lett, 68 (1992) 3112]. The unusual properties of ferrite nanoparticles can probably be explained on the basis of the dependence of cation distribution of these ferrites on their particle size. The particle size and cationic distribution depends on the method of preparation. Size dependent study of nanocrystalline ferrites have been reported by several workers [J Colloid Int Science, 146 (1991) 38; Phys Rev B, 54 (1996) 9288; J Appl Phys, 91 (2000) 2211]. In this work, we have studied size effects on the structural and magnetic properties of $CuFe_2O_4$.

Cubic $CuFe_2O_4$ is reported to exist at high temperatures. In this paper we describe the preparation of cubic $CuFe_2O_4$ nanoparticles at little above room temperature via chemical route. The experimental conditions have been controlled to produce nanoparticles with average particle sizes 18 nm to 3.2 nm. The cubic spinel structures of copper ferrites have been confirmed by XRD and FT-IR. Mossobauer studies of our samples show transformation from ferromagnetic to super-paramagnetic behaviour with the reduction in size and that in all the samples, iron is present as Fe^{+3} in both tetrahedral as well as octahedral sites and Cu^{2+}_{oct} content matches well with that required for cubic structure. Effect of doping nonmagnetic Zn^{2+} and magnetic Ni^{2+} in $CuFe_2O_4$ nanoparticles are discussed.

I. ASTROPHYSICS

12. Possible Upper Limits on Lorentz Factors in High Energy Astrophysical Process

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Key words: *Gamma–ray bursts, Lorentz factor, Relativistic effects*

Gamma-ray bursts (GRBs) are the most luminous physical phenomena in the universe. The relativistic effect on the blast wave associated with the GRB introduces the gamma factor. Here we put an upper limit on the gamma factor via constraints on maximal power allowed by GR and hence set upper limits on other observable quantitites such as decleration distance. Also upper limits are set on high frequency radiation due to constraints set by CMB.

13. Coronal Mass Ejections and Cosmic Ray Modulation

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The modulation of galactic cosmic rays due to solar activity has been known since almost five decades. Many mechanisms have been proposed to express the decreasing GCR flux in inner heliosphere. Theory of galactic cosmic ray modulation is based on four components (Parker, 1965). This theory combines four modulation mechanisms: the convection effect, adiabatic, gradient and curvature drifts and diffusion. The convection effect is due to the outward solar wind flux, which can reduce the cosmic ray intensity at any point in the heliosphere. The expanding solar wind comes the adiabatic energy change of cosmic ray particles, which is more important in the inner part of the heliosphere. Gradient and curvature drifts in the large scale heliospheric magnetic field, as well as

drift related to the heliospheric current sheet(HCS), have a major effect on the GCR modulation during the period of minimum solar activity(Potgieter,1997). Merged Interaction Regions(MIRs) and Global MIRs(GMIGs) were proposed by Burlaga et al(1993) as diffusing propagating barriers in the outer heliosphere in order to explain the modulation of galactic cosmic rays. GMIRs are thought to be due to various flows the sun including coronal mass ejections(CMEs) Recently several researchers have proposed that the agent which is transporting the solar activity information in the form of magnetic perturbations and causing effect in cosmic rays are coronal mass ejections(Lara et al,2005;Shrivastava and Singh, 2005).

CMEs are Magnetized structures, which produce large fluctuations in the heliospheric magnetic field.CMEs traveling in different speeds tend to merged into what are known as complex ejecta, which are seen often in interplanetary medium during the period of high solar activity. In this presentation I will discuss in detail the Coronal Mass Ejections and Cosmic Ray modulation.

14. On Main Sequence Stars

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Key words: *Main sequence stars, Mean matter density, Temperature, Pressure, Standard model, Perfect gas law, Mass, Radius.*

In the Hertzsprung-Russel diagram, where the ordinate represents brightness expressed as absolute magnitude and the abscissa as spectral types, at least 90 percent of the stars occupy a diagonal band extending from top left to bottom right. This is known as main sequence.

We consider twenty stars. Their mass and radius are known. Mean matter density is calculated mathematically. dP/dr is calculated using Arthur Eddington's 'Standard Model'. The expression for the temperature at the centre of the star is determined from the perfect gas law and this central temperature is calculated mathematically. Central pressure is estimated using Subrahmanyan Chandrasekhar's formula.

15. Flare Related Coronal Mass Ejections and Their Relation with Forbush Decreases of Higher Magnitude

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Key words: *Forbush decreases, Coronal mass ejections and interplanetary shocks, Sun, Solar plasma materials.*

CMEs are large-scale magnetized plasma structures originating from closed magnetic field regions on the sun and are the most energetic solar events in which vast amount of solar plasma materials are expelled from the solar corona into interplanetary space .They are responsible to generate disturbances in solar wind plasma parameters, interplanetary shocks and Forbush decreases in cosmic ray intensity. We have studied Forbush decreases magnitude e”10!, observed at Oulu super neutron monitor, during the period of 2000-2006 with coronal mass ejections CMEs), interplanetary shocks and disturbances in solar wind plasma parameters (velocity, density, interplanetary magnetic field). We have found that all Forbush decreases are associated with X ray solar flare related halo coronal mass ejections (CMEs). We have found positive co-relation with co-relation co-efficient 0.68 between magnitude of Forbush decreases (Fds) and speed of associated CMEs. All the Forbush decreases (Fds) are related to interplanetary shocks and the related shocks are forward shocks. Further, we have obtained negative correlation between magnitude of Forbush decreases and magnitude in jump in solar wind plasma velocity and density with correlation coefficient -0.34 between magnitude of Forbush decreases and magnitude of jump in solar wind plasma velocity, -0.36 between magnitude of Forbush decreases and magnitude of jump in solar wind plasma density. We have concluded that Forbush decreases in cosmic ray intensity are caused by coronal mass ejections associated with X ray solar flares and interplanetary shocks that they generate.

16. On Study of Acceleration of CMEs

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Key words: *Sun, Coronal Mass Ejections, Acceleration, Speed*

We present a statistical study on the acceleration of CMEs. This study is based on 8553 CME events observed by SOHO/LASCO during January 1996 to December 2009, which observes the inner corona from 1.1 to 30 RS. In our study we distribute CMEs in three groups: Narrow, Normal and Halo CMEs. Our study shows that narrow CMEs are completely biased towards to deceleration and normal and halo CMEs are almost equally distributed towards acceleration and deceleration. Our study shows that correlation between acceleration and speed of CMEs is high for halo CMEs.

2. ELECTRONICS AND COMMUNICATION

17. Scattering of High Frequency Pulsed Wave by Moving wedge

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Key words: *Wedge-shaped object, Dirac delta function, Dispersion phenomena, Relativistic velocity.*

A high frequency pulsed wave scattering by wedge-shaped object moving with relativistic velocity in free space is described in this paper. The incident pulse is a plane signal described by a Dirac delta function. In order to reduce the mathematical difficulties,

inherent to both the configuration and the motion of the scatterer, we apply the frame hopping method to analyze the interaction of the pulse incident field with a perfectly conducting wedge. The analytical solution to this scattering problem is found and the physical interpretation is given. In this analysis, we neglect any dispersion phenomena connected with the surrounding medium. It is shown that the field distribution in the frame of reference where the incident field is defined, is not simply a moving image of that in the frame where the wedge is at rest.

18. Analysis of a Cylindrical Dielectric Resonator Antenna with a Parasitic Conducting Strip

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Keywords: *Dielectric resonator, Q-factor, Dielectric resonator, Antenna, radiation patterns.*

Dielectric resonators (DR), by virtue of their high Q-factor and very low conduction loss have been found worthy of applications such as microwave and millimeter wave filters and antennas. An interesting feature of DR is that certain low Q-modes can be excited, which can radiate energy rather than confining it over a considerable frequency band. This paper discusses the experimental analysis on a cylindrical dielectric resonator antenna with parasitic conducting strip, loaded coplanar with the 50 Ù microstripline feed. The antenna offers an impedance bandwidth as high as 17.33% at a center frequency of 2.77 GHz, as a result of the enhanced coupling produced by the coplanar strip. The return loss, impedance, polarization and radiation characteristics of the antenna are studied. The radiation patterns are broad and the low cross polarization levels confirm that the antenna is linearly polarized over the entire impedance bandwidth.

19. Antenna Miniaturization Using a Reactive Impedance Substrate

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Keywords: *Wireless, Radio Frequency, Patch Antenna, Antenna miniaturization, Substrate, Impedance, Surfaces and Planar antennas.*

The growing number of wireless applications has presented RF (Radio Frequency) engineers with a continuing demand for low cost, power efficient and small size system designs. This paper presents theory, design and fabrication of a class of reactive impedance surface (RIS) substrates. The objectives in such a design process are to minimize the adverse effects of the antenna interaction with the substrate such as the mutual coupling between the antenna and its image, and accentuate positive interactions such as an appropriate spectral trend of stored electric and magnetic energy which can result in enhanced bandwidth and/ or antenna miniaturization.

The simulations compare very well with measured results obtained from a prototype $\lambda/10$ miniaturized patch antenna fabricated on an RIS substrate. This antenna shows measured relative bandwidth, gain and radiation efficiency of BW = 6.7%, G = 4.5 dBi, and ε_r = 90% respectively, which constitutes the highest bandwidth, gain, and efficiency for such a small size thin planar antenna.

20. The Enhancing Bandwidth and Size Reduction of Broadband Patch Antenna

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Key words: *Broadband antenna, Microstrip patch antenna, Slotted patch antenna, L-probe fed, Thin Substrate, Simulated impedance.*

With the ever-increasing need for mobile communication and the emergence of many

systems, it is important to design broadband antennas to cover a wide frequency range. The design of an efficient wide band small size antenna, for recent wireless applications, is a major challenge. Microstrip patch antennas have found extensive application in wireless communication system owing to their advantages such as low profile, conformability, low cost fabrication and ease of integration with feed network. The enhancing bandwidth and size reduction mechanism that improves the performance of a conventional microstrip patch antenna on a relatively thin substrate (about 0.01 λ_0), is presented in this research. The design adopts contemporary techniques; L-probe feeding, inverted patch structure with air-filled dielectric, and slotted patch. The composite effect of integrating these techniques and by introducing the novel slotted patch, offer a low profile, broadband, high gain, and compact antenna element. The simulated impedance bandwidth of the proposed antenna is about 23%. The proposed patch has a compact dimension of 0.543 λ_0 × 9.276 λ_0 (where λ_0 is the guided wavelength of the centre operating frequency). The design is suitable for array application with respect to a given frequency of 1.839-2.293 GHz.

21. Study of Electromagnetic Diffraction by Dielectric Slab

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Key words: *Electromagnetic Diffraction, Dielectric Slab, magnetic properties, surface-integral equations.*

There is a significant interest in scattering from thin layers of materials with combined dielectric and magnetic properties. In these cases, the computational problem reduces to solving a systems of surface-integral equations. In this paper we describe an integral equation approach to a fundamental scattering problem of transverse dielectric (TE) illumination of an infinite slot in a conducting screen situated between two dielectic slabs having different electromagnetic properties. The numerical results are given for the magnetic current for selected cases.

22. Patch Antenna with Substrates Having Different Di-Electric Constants for UWB Applications

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Key words: *Patch, antenna, Di-electric substrate, Ultrawide Band (UWB), coplanar waveguide (CPW), High frequency Simulator Software (HFSS).*

The interest in ultraband technologies led us to design a cedar patch antenna fed by coplanar waveguide for ultrawide band applications. Using two dielectric substrate cedar patch antenna were designed. The numerical simulation and analysis for this class of antenna are performed using HFSS. The simulated radiation pattern at two operating frequencies in the band width 5 and 9 GHz exhibited omnidirectional pattern with a return loss less than -10 dB throughout the entire bands. The antenna also exhibits reasonable gain values over the same frequency band.

23. Analysis of MIMO Channel Capacity in Tunnels

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Key words: *Wireless communication, MIMO (multiple-input multiple output) Tunnels, Propagation channel.*

Wireless communication in tunnels have been extensively studied but there is now growing interest in implementing multiple input multiple-output system in order to improve the communication performancar. This paper reports with the problem of multiple input

multiple output (MIMO) wireless channels in rectangular shaped tunnels. First, a reference scenario corresponding to the use of plane dense transmitting and receiving arrays is studied. The interest of such a canonicals array configuration is that it is able to characterize intrinsic MIMO performance in tunnel, regardless of the number of array elements. Simple analytical formulae to calculate the channel capacity are proposed. However, in practical applications, the number of array elements is quite limited. Therefore, the capacity which can be practically achieved, either the optimized linear arrays or with uniform linear arrays, is discussed in the second part of this communication and compared to the results of the reference scenario.

24. Reconfigurable Broadband Microstrip Antenna

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Key words: *Microstrip antenna, Coplanar wave guide, Broad impedance bandwidth, Substrate layers.*

We present a two layer microstrip antenna with a novel feeding technique that uses a coplanar wave guide and a slot loop combination in this paper. The proposed antenna offers broad impedance bandwidth as well as reconfigurability for multiband operation by incorporating switches in the feed. Furthermore broad impedance bandwidths were obtained by using two substrate layers consisting of a high $å_r$ substrate that contains the feed network and a low $å_r$ substrate that contains two patches, one patch on either side of the substrate. The two substrates are not separated by a ground plane. Impedance bandwidths of about 23% were obtained for two selectable frequency bands using two switches. The two frequency bands obtained for the parameters chosen in this paper are 8.73-10.95 GHz and 7.68-9.73 GHz. The difference in F/B ratio is due to the fact that when the two switches

are off, the excitation of the patches is mainly due to the loop portion of the feed which is near resonance, whereas when the two switches are on the excitation will be due to the small capacitive slot at the end of the CPW feed resulting in very small back radiation.

25. Radiation Characteristics of Circular Microstrip Antenna Array in Weakly Ionised Dusty Plasma Medium

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Key words: *Antenna array, Communication, Plasma, Characteristics, Directivity, Radiation Conductance, Radiated Power.*

Vast development in the field of communication needs investigation on microstrip antenna. A number of workers have successfully worked in this direction. To improve the characteristics of microstrip antenna, for higher gain, beam scanning or sterring capability, it is necessary to combine discrete radiation to form arrays, which provide a fixed beam of specified shapes . In this investigation we have attempted to study the radiation characteristics of circular microstrip antenna arrays using the concept of linear array. It is concluded that there is a significant change in working capability of circular microstrip antenna arrays in weakly ionized dusty plasma medium in comparison to free space and the radiation pattern for circular antenna array in weakly ionized dusty plasma medium enhances the directivity of the pattern.

26. Performance Comparison of Astable Multivibrator Circuit Using Various Circuit Designing SPICE Softwares

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Key words: *Astable mutivibrator, Transient analysis, Simulation. Electronic circuit design, Computer programs.*

This paper addresses performance of astable multivibrator using different spice softwares. Traditionally, electronic circuit design was verified by building prototypes, subjecting the circuit to various stimuli and then measuring its response using appropriate laboratory equipments. Prototype building is somewhat time consuming, but produces practical experience from which we judge the manufacturability of the design. Computer programs that simulate the performance of an electronic circuit provide a simple cost effective means of confirming the intended operation prior to circuit construction and of verifying new ideas that could lead to improve the circuit performance. Such computer programs are revolutionized the electronic industry which provides the products in the service of human being. In this paper we have performed the transient analysis of the same circuit in different spice software's to study the reliability of these softwares. It is essential to use these softwares for the efficient progress in the learning the electronics. The accuracy of the circuit performance and reliability is reported by using three test tools. The results are explored with browsing output data facility.

27. Role of Antennea and Propagation for MIMO Wireless Communication

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Key words: *MIMO systems, Antennae and Multiple Channels, multipath signal, Communication systems.*

Multiple-input multiple-output (MIMO) antenna systems represent one of the most important advances in communication systems. They take advantage of the use of a number of transmitting antennae and receiving antenna to exploit the spatial properties of the radio channel. The dramatic increase in the channel capacity achievable by MIMO systems makes this technology most promising for future wireless wideband Internet services. The aim of this paper, based on estimated multipath signal parameters in MIMO communication systems, we propose a novel approach to determine the position of mobile station using only one Base station. This approach intends to minimize the error occurring from the estimation of multiple paths.

28. Study of Electromagnetic Field Effects for Transmission Lines Transposition

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Key words: *AC system, Transmission lines, MATLAB programming, Magnetic field, Electric field.*

In the AC system, double-cicuit transmission lines consists of 6 conductors running in parallel. Transposition in case of long distance distribution of the 6 conductors results in electric and magnetic field distribution that may cause some serious harm surrounding

the transmission line. Therefore, in this investigation we study the electric and magnetic fields distribution resulting from six types long distance distributing transposition employing MATLAB programming to simulate electric field and magnetic field distribution for 500 kV, double -circuit, four bundled power transmission lines. From the simulation results it is apparent that the six types of transmission lines transposition in case of long distance distribution will not affect changing electric field and magnetic field which surround the transmission line.

29. Bandwidth Enhancement of Rectangular Compact Dielectric Resonator Antenna (DRA) for Broadband Applications

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Key Words: *DRA, Microstrip Patch Antenna and Bandwidth, Microwave spectrum, bandwidth.*

The present day technology demands continuing growth in electronic systems operating in the RF and microwave spectrum. These systems are designed to provide high efficiency, wide bandwidth and reduced equipment size. Recent advances in wireless communications has resulted in development of antenna that can be embedded into wireless products. Since the last two decades two classes of antenna i.e., the microstrip patch antenna and the dielectric resonator antenna have been under investigation for modern wireless applications. However, compared with the microstrip antenna, DRA has much wider impedance bandwidth. This is because the microstrip antenna radiates only through two narrow radiation slots, whereas the DRA radiates through the whole antenna surface except the ground part. Therefore, in this presentation the main focus has been done on the compact rectangular DRA for bandwidth enhancement for the application of wireless communication systems. The obtained results have been simulated using Ansoft HFSS.

30. Correction Factor for Admittance in Coaxially Excited Cylindrical Antennas

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Key words: *Antenna admittance, Antenna theory, Cylindrical antennas, TEM approximation, Coaxial source geometry.*

A longstanding problem in cylindrical antenna theory has been the accurate calculation of the admittance of a cylindrical antenna driven from a coaxial line. In the early days of cylindrical antenna theory the problem of dealing with the coaxial source region was circumvented by employing the so called "deltafunction" gap model and using experimentally derived correction factors. While reasonably accurate results have been obtained for a range of problems using the so called "TEM approximation" for the coaxial aperture electric field, these results nonetheless contain an error of small but unknown extent. In this work by examining the infinite coaxially excited antenna problem this approximation error has been quantified and a simple approximation factor has been deduced. This correction factor is applicable to a range of antenna problems having a coaxial source geometry.

31. Enhancing The Bandwidth of Dual-Band Monopole Antenna With Stagger-Tuned Arms

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Key words: *Monopole antenna, Dual-band radiation patterns, Finite Integration Technique, WLAN transceivers, Printed monopole.*

Dual band monopoles have recently been reported which cover frequencies employed

by WLAN systems in the US [Yeh S H and Wong K L, Microwave Optical Technology Letts, 34(2002)24]. Two branch monopoles have been employed in printed form but do not have sufficient bandwidth for the high band.

In the present work we describe a dual-band miniaturized printed monopole for integration in modern wireless systems. The printed monopole is augmented with two arms, resonant at slightly different frequencies, providing a broadened response for the upper band. The achieved bandwidth for the high band is 36%. These antennas are proposed for the emerging dual-mode multi-band WLAN transceivers, which operate over a wide range of bands as dictated by national authorities. Measured and simulated data including return loss, antenna gain and radiation patterns are presented. The numerical method employed was the finite integration technique.

32. Use of Computational Method for the Radiation Pattern of Tapered Dielectric Radiator

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Key words: *Tapered dielectric radiator, Local mode theory, Radiation pattern, Polarization current.*

The tapered dielectric radiators have been known for over past half century, but have not been applied very extensively as microwave antennas. Although experimental studies on tapered rod antennas have been undertaken, theoretical studies have involved strong simplifications and have provided general guidelines [Antenna Handbook, NY, 1988, p 173]. Rigorous approaches like full theories [Continuous transitions in open waveguides, Chicago, IL: Golem Press, 1971] formulated for the wedge waveguide are very complicated.

An efficient computational method to obtain the radiation pattern of tapered dielectric radiator is presented. The approach uses a local mode theory to determine polarization current distribution in the dielectric region and invokes the equivalence principle to calculate the far-field radiation pattern from this current distribution. This method provides a convenient design capability for wedge type dielectric radiators. The numerical results

confirm that dielectric wedge antennas fed by a uniform dielectric waveguide of the same permittivity radiate a main beam of modestly high directivity gain.

33. Study of Rectangular Dielectric Resonator Antenna with a Finite Ground Plane

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Key words: *Dielectric resonator antenna (DRA), input impedance, method of moments (MoM), ground plane.*

A probe-fed rectangular dielectric resonator antenna (RDRA) placed on a finite ground plane is numerically investigated using method of moments (MoM). The whole structure of the antenna is exactly modeled in our simulation. The feed probe, coaxial cable and ground plane are modeled as surface electric currents, while the dielectric resonator (DR) and the internal dielectric of coaxial cable is modeled as volume polarization currents. The effect of ground plane size, air gap between dielectric resonator and ground plane, probe length, and position on the radiation performance of the antenna including resonating frequency, input impedance, radiation pattern, and bandwidth are investigated. Moreover, it is shown that the MoM results are more accurate than other simulator results using software package such as High frequency structure Simulator (HFSS).

34. Study of Use of Dielectric Phase Shifted for Mechanically Storable Antennas

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Key words: *Wireless broadband communications, Element antenna, Security, Numerical simulations.*

The need for wireless broadband communications has increased rapidly in recent

years demanding quality of service, security, handover, and increased throughout for the wireless communication systems. Wireless communication is widely recognized as one of the fastest growing industries in today's market place. A mechanically steerable antenna was designed using an adjustable phase shifter which employs a dielectric slab placed close to a coplanar TL. Numerical simulations using Ansoft HFSS were conducted at 6 GHz, and a 4-element antenna was tested. A similar design can be used for a digital phase shifter with a matched impedance at the designed frequency.

35. Study of Compact Differential Antenna with Stacked Patches

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Key words: *Differential antenna, Dual frequency antenna, Stacked patches, wireless communications.*

With the development of wireless communications, compact and multi-band antennas for mobiles terminals are demanded. A compact differential dual-frequency antenna with stacked configuration has been presented. Compared with the conventional stacked dual-distributed on two layers and connected through via holes, thus the dimension of the antenna is reduced effectively. In order to improve the bandwidth at the first resonant frequency (f_1), a reflecting board is introduced and connected with the ground plane through three holes. As a result, a new resonant frequency close to f_1 can be excited and the band width at f_1 is enhanced. Both differential antennas with and without the reflecting board are fabricated and measured. The realized antennas have a compact size of 15 mm × 15 mm, which equals to 0.23 λ_1 × 0.23 λ_1 (λ_1, the guided wavelength at f_1). Good agreement between the simulated and measured resulted found in literature is obtained.

36. Effects of Wind on Intensity and Power Spectrum of Tropospheric Scintillation

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Key words: *Tropospheric Scintillation, Satellite Communication, Wind Speed, Fluctuations in amplitude.*

Attenuation of microwave signals is a common problem faced by telecommunication service providers all over the world. On the other hand, level of service quality and budget must be controlled to meet the customers' requirement. Tropical disturbances are perturbation of the wind flow. For the systems operating at high frequencies and low elevation angles tropospheric scintillation contribute a significant impairment. Scintillations are rapid fluctuations in amplitude and phase of the received signal arising from random fluctuation in the atmospheric refractive index due to turbulent irregularities in temperature humidity and pressure.

In the present work an analysis of the effects of wind on the intensity and power spectrum of tropospheric scintillation on the basis of propagation data available in the literature has been presented. The results show a strong correlation between the corner frequency and transverse wind speed, a weaker correlation with overall wind speed and a negligible correlation between scintillation intensity and transverse wind speed. Also a reduced correlation of the corner frequency with wind speed has been observed.

37. TE Scattering by Perfectly Conducting Arbitrarily Connected Strips

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Key words: *Conducting strips, Electromagnetic scattering, Integral- differential operators, Polygonal cross-section.*

The analysis of objects with edges by means of integral-differential operators, requires

the appropriate selection of the functional space where the solution has to be searched for. Mexiner derived conditions for the electromagnetic field which in turn imply a proper edge behavior of the currents induced on the scatter. Therefore, such conditions characterize the functional space to which the solution has to belong. In this paper the scattering by an arbitrary collection of perfectly conducting connected strips is analyzed for TE incidence. The studied configurations include both closed and open polygonal cross-section cylinders, as well as more complicated structures in which more than two strips are connected at a point. The proposed method is very efficient as few expansion functions are needed in a Galerkin scheme.This is achieved by means of expansion functions factorizing the correct edge singularity of the electromagnetic field and ensuring the continuity of the current at connecting points.

38. Study of Limitation on the Amplitude of the antenna Impulse Response

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Key words: *Antenna impulse response, Maximum amplitude, Effective aperture, Antenna directivity.*

Simple expressions for the maximum feasible peak value for the antenna impulse response have been derived from the properties of the antenna transfer function. Limits are derived on the maximum amplitude of the antenna impulse response and its derivatives, for the general case and for the special cases of constant directivity and constant effective aperture. It is shown that in general the maximum feasible amplitude is directly proportional to the square root of maximum antenna directivity, but proportional to the logarithm of the bandwidth ratio. Comparisons with published impulse response data show that measured and stimulated data are compatible with the computed limits.

39. Broadband Fractal Microstrip Antenna

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Key words: *Fractal, Wide bandwidth, Coupling substrate, Microstrip antennas, Resonance frequencies*

As wireless communication applications require more and more bandwidth, the demand for wideband antennas increases as well. One of the most applicable frequency band is X-band (8-12 GHz). Fractal passive Microstrip antennas are simple and novel structures that attract much attention recently. In this paper, a new microstrip modified and fractalized antenna using multiplayer structure for achieving wideband behavior in X-band is designed, optimized and simulated. Using fractal deflection in patch, multi higher order modes are inspired for coupling a much wider bandwidth. Roggers TMM3 ($\varepsilon_r = 3.38$) is used in this antenna as substrate. Working range for this antenna is from 7.7 GHz to 16.7 GHz (BW = 9 GHz). This antenna has simple structure, small size and 4 resonance frequencies.

40. Drop Size Distribution Model for Rain Attenuation

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Key words: *Dead-time problem, Drop diameters, Gamma distribution, Rain attenuation, Rain drop size distribution.*

A model is proposed for rain drop size distribution which is less sensitive to errors in the extremely small and large drop diameters. The rain rate estimated using measured drop size distribution shows that the contributions of lower drop diameters are small as

compared to the central drop diameters. This is expected since the sensitivity of the Joss distrometer are small as compared to the central drop diameters. The lower drop diameters are therefore removed from the drop size data and the gamma models is redesigned for its moments.

This paper finds the contributions of drop size diameters from the calculation of rain rate using measured data. Truncated gamma models are designed with removal of lower bins. This shows that Brawn's recommendation to ignore the small drop diameters due to the dead time problem is valid for the calculation of slant path rain attenuation of microwave limits. The 3rd, 4th & 6th moments are proposed to model gamma DSD in which consecutive bins are removed starting from the smallest drop size distribution. It is concluded that the sensitivity of the Joss distrometer affects the rain rate estimation at low rain rates.

41. Study of Transport Dielectric Resonator Antennas for Optical Purposes

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Key words: *Dielectric resonator, antennas, Optical components, Solar energy, Input impedance, Reflection coefficient.*

The dual function transparent hemispherical DRA made up of borosilicate crown glass has been investigated for the first time. It simultaneously functions as a radiating element and an optical foucing lens. It can also serves as a protective cover for its underlaid solar cell. Since the DRA is transparent, the light can pass through it and illuminate on the underlaid solar cell. Because of the focusing effect of the DRA, the voltage and current outputs of the solar cell can be increased. The weight of the DRA can be a concern in its

practical applications, but it can be possibly reduced by the advancement of future material technologies.

The proposed transparent DRAs can provide a higer gain (~ 4 dBi) than for the State-of- the Art transparent microstrip antennas (~-5dBi to 0 dBi). Also the proposed configuration can potentially be used for applications that need a self-sustaining power.

42. Enviornmental Effects on Voltage Comparator Circuit-A Simulation Study Performed Using MULTISIM

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Keywords: *MULTISIM, Simulation, Temperature analysis, EMI vibrations, Mechanical and Electronic design.*

Electronic products reliability is very important to both user and manufacturer. Desigining products to survive harsh environments is expensive in time and money. An optimum design is one that meets its requirements at minimum cost. Different factors such as humidity, radiatons, EMI, vibrations, shock, water leakage, fungal growth, chemical attack, damage due to abuse and many others would also play as disaster. In the industrial processes temperature is a main factor. Many of these factors put constraints on the mechanical and electronic design.

This paper presents simulations of typically chosen representative circuit of analogue electronics using MULTISIM 10.1. The circuit performance is tested by simulating under specified temperature range. The results are plotted as a function of temperature to show performance degradation of circuit operation. This study would then help the pool for bridging the gap between the customers need and manufacturer which would cut down the product waste cost, time and efforts manufacturering new product.

III. SPACE AND ATMOSPHERIC PHYSICS AND PLASMA

43. Numerical Analysis of Lattice Parameters of Acoustically Perturbed Brillouin Active Magnetised Semiconductor Plasma

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Key words: *Lattice parameters, Plasma, Modulation of light, Susceptibility, Semiconductor, Wavenumber, Hydrodyna-mical model.*

The numerical study of modulation of light by acousto-optic interaction is used in a number of applications including light modulation, beam deflections, spectrum analyzer and processing of informations. In the present numerical analytical investigation, the lattice displacement or vibration, acousto-optical susceptibility, and acousto-optical gain constant, which are arising due to the induced nonlinear current density and acousto-optical process are deduced in a acoustically perturbed Brillouin active magnetized semiconductor plasma using the hydrodynamical model of plasma and coupled mode scheme.

The influence of scattering angle, wavenumber and magnetic field has been explored. The numerical analysis has been applied to centrosymmetric crystal. Numerical estimates are made for type INSb crystal duly irradiated by adoubled frequency 10.6μm CO2 laser. It is found that lattice displacement/vibration , susceptibility and acousto-optical gain constant increase linearly with incident wavenumber and applied dc magnetic field, while decrease with scattering angle, the maximum values are obtained of the order of 55.19 $\times 10^{-15}$ m, 161.487 $\times 10^{-19}$ mks and 8.616×10^{-22} mks, respectively. Results are found to be well in agreement with literature values.

44. Alfven Surface Waves in a Partially Ionized Resistive Medium

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Key words: *Viscosity, Resistivity, Ion-neutral collisions, Alfven surface waves, Boundary Conditions, Neutral gas*

In this investigation we study the joint effects of viscosity, resistivity and ion-neutral collisions on Alfven surface waves propagating along a partially ionized plasma - vacuum interface. Partially ionized resistive medium consists of viscous incompressible ionized gas and neutral gas componenets. Applying boundary conditions at plasma-vacuum interface, we obtain the dispersion relation for Alfven surface waves and solve it numerically. For different values of resistivity and neutral gas friction parameters, the variations of real and imaginary parts of wave number k with viscosity parameter are shown graphically. It is found that two mode structure of Alfven surface waves results due to the effects of resistivity, viscosity and ion-neutral collisions taken simultaneously. These results might be useful for studying the behavior of Alfven surface waves in laboratory and space plasmas.

45. A Historical Analysis of Dusty Plasma in the Presence of Mass and Charge Variation (Theoretical Model)

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Key words: *Dusty Plasma, Dust Acoustic Waves (DAW), Debye length, Electrostatic field, Charge and mass fluctuation.*

The recent experimental observation from satellites and space studies suggest that dust is a abiquitous component of the cosmic environment, interstellar media, comentory tails, planetary rings, circumsteller shells, dark interiors of molecular clouds, nova ejecta, the out flow of red giant stars, star envelops, addretion disks, ionosphere and plasma processing are the example of dusty plasma. In laboratory plasmas, dust appears as trapped impurities and can lead to series contamination problems during the plasma aided manufacture of semiconductors. Most of the grain in the astrophysical environment are made of silicate or graphite. The interaction of the dust grain with plasma is due to charge on the dust grain which may be due to photoelectric emission stimulated by the ultraviolet radiation, collisional charging by ions and electron etc. In the present investigation we studied the history of theoretical model for the dusty plasma in the presence of massand charge variation. We have noted that a collapsing dust cloud with its size of the order of critical Jeans size, should exhibit a pulsational mode of star formation. However, the considerations of all possible drag effect and also magnetic field are required to explain recent experimental observations.

46. Study of Electron Inertia Effect on KAW in Earths Magnetoplasma

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Keywords: *Inertial kinetic Alfven waves, Cusp region, Wave particle interaction, Kinetic theory, Earth's environment.*

The effect of electron inertia on kinetic Alfven wave has been studied. The expressions for the dispersion relation, damping rate and damping length of the inertial kinetic Alfven wave (IKAW) are derived using the kinetic approach in cusp region. The Vlasov-kinetic theory has been adopted to evaluate the dispersion relation, damping rate and damping length with respect to the perpendicular wave number $k_{\perp}\rho_i$.The polar cusp is an ideal laboratory for studies of nonlinear plasma processes important for understanding the basic plasma physics, as well as the magnetospheric and astrophysical application of these processes.

47. Study of Beam Effect on EMIC Waves With Hot plasma Around Earth,s Magnetosphere

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Key words: *EMIC wave, Auroral acceleration region, Particle aspect analysis, Space plasma (waves and instabilities), Loss-cone distribution function.*

The effect of ion beam velocity on the growth rate of the EMIC wave with general loss-cone distribution function in hot anisotropic plasma is discussed by the trajectories of the charged particle. It is found that the effect of the ion beam is to reduce the energy of transversely heated ions, whereas the thermal anisotropy acts as a source of free energy

for the EMIC wave and enhances the growth rate. The effect of steepness of the loss-cone is to enhance the growth rate of the EMIC wave in hot plasma. These results are determined for auroral acceleration region.

48. An Analytical Study of Optical Emission from Venus Atmosphere during Night Time

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Key words: *Nightglow, Optical emissions, Transitions, Quantum State, Dissociative Recombination.*

Optical emissions at different wavelength from Venus atmosphere during night time have been observed by various space scientists. The emission features are assigned to excited atoms and molecules of oxygen and Nitric oxide. A variety of physical and chemical process responsible for producing these excited atoms and molecules have been investigated. In this paper we present an account of the possible mechanisms leading to optical emissions from Venus night atmosphere.

49. Study of Frequency of Plasmons and Polaritons on the Cylindrical Surface of Carbon Nano Tube

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A Lot of interest has been shown in the study of carbon nano tube. The properties of the plasmons and polaritons on surface of carbon nano tube can be studied by deriving

the dispersion relation. However, no attempts have been made towards the derivation of the dispersion relation in the non-local limit for the coupled surface polariton waves in the case of cylindrical polar semiconductors for K ≠ 0. In the present investigation, the dispersion relation for surface Plasmon-polariton modes for K ≠ 0 is derived for long cylindrical interface in the non-local limit. This dispersion relation has then been reduced to the local limiting case in order to compare the dispersion relation for K= 0. The effect of spatial dispersion on surface Plasmon-polariton mode is discussed. The surface frequency of Plasmon varies with propagation constant K on the surface of carbon nano tube when it was placed in epoxy resin. However, this property of Plasmon was not seen when it was placed in other medium. This study is important in the field of microelectronics, laser integrated optics and nano technology.

IV. THEORETICAL PHYSICS

50. Cluster Expansion Monte Carlo Study of Phase Stability of Vanadium Nitrides

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Key words: *Cluster expansion, Monte Carlo simulation, Electronic structure, Phase stability, vanadium nitrides Density Functional Theory (DFT)s.*

Phase stability of stable and metastable vanadium nitrides is studied using density functional theory (DFT) based total energy calculations combined with cluster expansion-Monte Carlo simulation and super cell methods (Ravi et al, Phys Rev, B1(2010)104111). We have computed the formation enthalpy of the various stable and metastable vanadium nitride phases considering the available structural models and found that the formation

enthalpies of the different phases decrease in the same order as they appear in the experimental aging sequence. DFT calculations are known to show stoichiometric V_2N to be polymorphic in ε-Fe_2N and ζ- Fe_2N structures within a few MeV and VN to be more stable in WC (Bh) phase than in the experimentally observed NaCl (B1) structure. As these nitrides are known to be generally nonostoichiometric due to presence of nitrogen vacancies, we used cluster expansion and supercell method for examining the effect of nitrogen vacancies on the phase stability. It is found that the nitrogen vacancies stabilize ε-Fe_2N phase of V_2N_{1-x} and NaCl phase of VN_{1-x} compared to ζ- Fe_2N and WC(Bh) phases, respectively, rendering the computed phase stability scenario to be in agreement with experiments. Analysis of supercell calculated electronic density of states (DOS) of VN_{1-x} with varying x, shows that the nitrogen vacancies increases the DOS at Fermi level in WC(Bh) phase, whereas they decrease the DOS in NaCl phase. And this serves as the mechanism of enhancement of the stability of the NaCl phase. Monte Carlo simulations were used for computing the finite temperature formation enthalpies of these phases as a function of nitrogen- vacancy concentration and found close agreement for NaCl (B1) phase of VN_{1-x} for which measured values are available.

51. Mathematical Beauty of Physical Equations in Quantum Physics

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Key words: *Differential equations, Tensors, Dirac equations, Klein-Gorden equations, Spin, Relativistic equation.*

All elegant, beautiful and powerful equations in physics are differential (partial or total) equations of order zero or one or two as all physical quantities are tensors of rank zero (scalar) or one (vector) or two (tensor). Zero order differential equations are algebraic equations. First order differential equation is Dirac equation in relativistic quantum physics. First order differential equations describes of spin-1/2 as Dirac equation describes electron of spin-1/2. Second order differential equation describes particles of spin 0 or 1 as Klein-Gorden equation describes pion of spin-0 as well as photon of spin-1(Maxwell equations for electromagnetic wave are of second order, Newton equations for motion of particle are also of second order). Thus, it is clear from above that order of relativistic equation is connected with spin of particles (spin is natural outcome of relativity). It is well known

that there is an intimate relation between spin and quantum statistics. Hence, order of relativistic equations and spin are well interlinked. Because of this close relation, in quantum field theory (also known as second quantization, a true relativistic theory), Klein-Gorden equation can be quantized only by using -Bose-Einstein statistics and Dirac equation only by Fermi-Dirac statistics whereas non-relativistic Schrodinger equation can be quantized employing both statistics.

We will demonstrate all above facts with illuminating, illustrating and interesting examples available in the existing scientific literature in the poster session.

V. OPTICS/LASER/SPECTROSCOPY/ MOLECULAR PHYSICS

54. Optical Study of Polyaniline Electrolyte

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Key words: *PANI electrolyte, Refractive index, NaCl, UV, Oxidation, Concentration, Refractive index, Undoped PANI.*

Dark green coloured chlorinated water-soluble conducting Polyaniline was synthesized by oxidation of aniline with ammonium persulfate in hydrochloric acid at 0°C. The solubility was found to be 29.228ge/dm^3 and the concentration was found to be 0.1 moles/ dm3. PANI electrolyte of different molar concentration were prepared by addition of water (0.01, 0.02, 0.03 0.04, 0.05, 0.06 moles/dm^3). NaCl was used as a dopant and was added in all above PANI electrolytes of different molar concentration. It is found that the refractive index for NaCl doped PANI electrolyte is greater than undoped PANI electrolyte. Refractive index increases with molar concentration, whereas in NaCl doped PANI electrolyte, refractive index decreases with increasing molar concentration. UV study revealed that as polymer concentration in PANI electrolyte increases, polaron becomes more sensitive to π-π^* type transition. The broadening of the peak is observed in case of doped PANI electrolyte and maximum for 0.1 and 0.06 moles/dm^3 concentration because of the decoiling of the polymer.

55. CI and MCHF Optical Oscillator Strengths for the $3p^6 3d\,^2D^e \rightarrow 3p^5 3d^2 P^o$, $^2D^o$, $^2F^o$ Transitions in Ti^{3+}

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Key words: *Relativistic velocity, Dirac delta function, Frame hoping method, Conducting wedge, Hartree-fock*

Configuration interaction (CI) and multiconfiguration Hartree-fock (MCHF) optical oscillator strength (OOS), of bond length (f_L) and velocity (f_V) forms, have been calculated for the $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d\ ^2D^e \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5\ 3d^2\ ^2P^o$, $2D^o$, $2F^o$ transition in Ti^{3+} ion of the potassium isoelectronic sequence exactly in the same way as we did in our earlier work (Tiwary *et al*, Pramana- *J. Phys.* **46**, 381 (1996)2010). Comparison has been made with available relevant experimental data and our earlier theoretical results obtained by employing the configuration interaction (CI) method (Tiwary *et al*, *J. Phys. B*: At. Mol. Phys. **16**, 2457 (1983)). Our present investigation clearly demonstrates that the MCHF method is more accurate then the CI method.

56. Absorption, Fluorescence and FT-IR Spectra of Fifteen Medicinal Plant Leaves and a Co-relation Between Characteristic Features

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Key words: *Fluorescence and FT-IR spectra, Intensity, Chlorophyll extract, Empirical relation, Key bands, Absorption band.*

In the present work we report the absorption, fluorescence and FT-IR spectra in fifteen plant leaves of medicinal importance. The plant leaves of medicinal importance selected for the work are *Vinca major Linn, Paederia foelida Linn, Clitoria ternatea Linn, Clerodendron Colebrookianum, Monochoria vaginalis presel, Mesua ferrea L, Occimum*

canumsims.syn, Hibiscusrosa sinensis L, Trminalla arjuna (Roxb), Spilathes acmella, cinnamonum tamala nees, Centalla asiatica Linn, Curcuma Longa L, Terminalia chebula Retz and *Zingiber officinalis Rox.* The bands originating from different groups (N-H, O-H, C-H, C=O, C=C and C=N) may be termed as key bands and one can follow their absorption characteristics and differentiate individual plant leaves or tissues. These observations also make it evident that the manifestation of bands in the infrared regions result from the chlorophyll molecules masking or suppressing the appearance of all other bands due to other molecular origin, which if at all appear, it does with extremely low intensities. In the present work we have also correlated the fluorescence intensity from the chlorophyll extract of the medicinal plant leaves with the absorption band width by a simple empirical relation.

57. Effect of Argon on the LIBS Spectra of Nitro Compounds

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Key words: *Laser Induced Breakdown Spectroscopy (LIBS), Plasma, Nitro compounds, Cu matrix,4-nitroaniline, Ambient atmosphere.*

Detection of nitro compounds and their residues is very important for homeland security. An emerging optical technique named as Laser Induced Breakdown Spectroscopy (LIBS) is found most suitable for this purpose. It is a spectroscopic analysis technique that utilizes the light emitted from laser-generated micro plasma to determine the composition of sample, based on elemental and molecular emission intensities. The unique feature of LIBS which play significant role for the present object is its intrinsic capability for minimally destructive, *in situ*, real-time detection and multi-elemental analysis of chemical species. LIBS spectra of nitro compounds such as 4-nitroaniline and 4-nitrotoluene in Cu matrix have been acquired in air as well as argon atmosphere. Our result reveals that the flow of argon gas across sample surface reduced the effect of ambient atmosphere

and hence improved the quality of LIBS spectra. So, the effect of argon play significant role for analyzing the LIBS data with greater precision and accuracy.

58. Surface Enhanced Raman Shift in Novel Materials

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Key words: *Raman spectroscopy, Surface Enhanced Raman Spectroscopy, Nano materials, Laser semiconductors*

Raman spectroscopy born in India 80 years ago is now widely used as powerful tool for the applications in various areas such as pharmaceuticals, polymers, thin films, semiconductors, mineralogy, petrochemical, carbon and another nanomateirals for chemical identification, characterization of molecular structures and stress measurements etc. The name "Surface Enhanced Raman Spectroscopy" implies that it provides the same information that normal Raman spectroscopy does, but with a greatly enhanced signals. The discovery of SERS has opened up a promising way to overcome the low sensitivity problem plaguing traditional Raman spectroscopy. SERS not only improves the surface sensitivity which makes Raman spectroscopy more applicable, but also generates a stimulus for the study of the interfacial processes involving enhanced optical scattering from adsorbates on metal surfaces (*Chem Phys Lett*, 26(1974)163; *Rev Mod Phys*, 57(1985)783). Focusing of the exciting laser on the surface gives probing spots of the order of 1 ìm depending on the specifications of the set up. In this presentation we will show that surface enhanced Raman spectroscopy can be used to study the properties of nano structured materials.

59. Density Functional Theoretical Modeling and HOMO- LUMO Energy of *p*-hydroxy Benzoic Acid Dimer

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Key words: *Dimer; NIR FT-Raman; FT-IR; HOMO-LUMO, p-Hydroxy benzoic acid, Hydrogen bonding, Red shift, B3LYP level.*

p-hydroxy benzoic acid is subjected to the vibrational spectral investigation using NIR FT- Raman, and IR spectroscopic techniques. The geometry and vibrational spectra of *p*-hydroxy benzoic acid dimmer have been computed using B3LYP level 6-31 G(d) basis set. Vibrational spectral investigation confirms the formation of strong O-H…O hydrogen bonding between the carbonyl oxygen lone electron pairs. The red shift of the O-H stretching wavenumbers suggests the existence of strong intermolecular O-H…O hydrogen bonding. The lowering in the HOMO and LUMO energy gap explains the charge transfer interactions taking place within the molecule.

60. Charge Transfer Interaction and Vibrational Spectral Investigation of a Nonlinear Optical Material L- Glutamine Picrate: A DFT Study

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Key words: *Charge transfer interaction, NIR, FT-Raman, FT-IR, NLO, L-Glutamine Picrate, Hydrogen bonding, Density Functional Theory*

Charge transfer interaction, vibrational spectra and DFT computation of L-Glutamine

Picrate has been analyzed. The equilibrium energy, bonding features and harmonic vibrational wavenumbers have been investigated with the help of density functional theory method. The natural bond orbital analysis confirms the occurrence of strong intermolecular hydrogen bonding in the molecule. The vibrational modes found in molecular crystalline materials should be described as phonon modes with strong coupling to the intra molecular vibrations.

61. DFT and Vibrational Spectral Analysis of Non Linear Optical Crystal 1-(4-N, N-Dimethyl Amino Pyridinium) Acetic Acid Bromide Monohydrate

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Key words: *Density functional theory, Fourier transform, FT-Raman, FT-IR, NLO molecules, O-H…O interactions, Vibrational Spectra*

FT-Raman and FT-IR spectra of the crystallized nonlinear optical (NLO) molecules, 1-(4-N, N-Dimethylaminopyridinium) acetic acid bromide mono hydrate (DMAPAB) have been recorded and analyzed. The equilibrium geometry, vibrational wavenumbers and the first order hyperpolarizability of DMAPAB have been calculated with the help of Density Functional Theoretical (DFT) computations. The assignment of the vibrational spectra have been carried out with the help of Scaled Quantum Mechanical (SQM) force field theory. Optimized geometry gives the charge transfer interaction of the pyridine ring and the amino group in the electron donor side of the NLO chromophore. Electron-phonon coupling and O-H…O interactions in making the molecule NLO active have been analyzed on the basis of the vibrational spectral features.

62. Squeezing and Photon Statistics in CARS and CAHRS

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Key words: *Higher-order squeezing of radiation, Sub-poissonian photon statistics, Photon-number operator, CARS, CAHRS.*

The effect of squeezing and sub-poissonian nature of an optical field in coherent anti-Stokes Raman scattering (CARS) and coherent anti-Stokes hyper Raman scattering (CAHRS) are investigated under short time approximation. The coupled Heisenberg equations of motion involving real and imaginary parts of the quadrature operators are established and solved under short-time scale. The dependence of squeezing on the number of photons is also investigated. It is also shown that higher-order squeezing allows a much larger fractional noise reduction than lower order squeezing. The present work shows that squeezing is greater in CAHRS than the corresponding squeezing in CARS. It is also shown that squeezing is greater in stimulated process than corresponding squeezing in spontaneous interactions. The conditions for obtaining maximum and minimum squeezing are obtained. The photon statistics of the pump mode in the processes has also been investigated and found to be sub-poissonian in nature.

63. Spatial Hole Burning in Lasing Without Inversion

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Key words: *Spatial hole burning, Lasing without inversion, Stimulated decay, Laser noise.*

The semi classical theory of laser noise considers the spontaneous emission fluctuations as the major noise sources, and they have influences on gain in a number of ways. The phenomenon like spatial hole burning, heating are mainly responsible for gain suppression in laser cavity. The phenomenon of spatial hole burning appears naturally in semi classical theory of laser. This appears in the graph of normalized population difference versus axial coordinate along laser axis. Though the hole is burned by the field of intensity for a non moving atom the effect is inherently present as noise in laser oscillators and amplifiers. The basic principle of spectral hole burning was indeed applied by Arnald in the case of complicated structures like quantum wells. It was shown that the constant voltage driven laser diodes generates amplitude squeezed light. The phenomenon of spatial hole burning has also been used to explain few characteristics of quantum wells. In the last decade lasing without inversion (LWI) , has attracted tremendous attention. LWI gives the production of light with greatly reduced noise which could be useful in x ray laser and new type semiconductor laser. In the present work we show that phenomenon of spatial hole burning in semiclassical theory remains unaffected in lasing without inversion. This fact has not been discussed in earlier works.

64. Synthesis, Structural and Dielectric SpectroscopyStudy of $(1 - x)Ba(Fe_{0.5}Nb_{0.5})O_{3-x}BaTiO_3$, where x = 0, 0.10 Ceramics

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Key Words: *X-ray diffraction (XRD), Monoclinic crystal systems, Barium iron niobate, Electroceramics, Tangent loss, Dielectric constant, Polarisation.*

Barium iron niobate; $BaFe_{0.5}Nb_{0.5}O_3$ (BFN) is one of the interesting material from the technology point of view. In recent years, many workers have studied BFN, including Yokosuka [*Jpn J Appl Phys*, 34 (1995) 5338]; Tezuka et al [*J Solid State Chem.*, 154 (2000) 591]; Raeski et al , *J Appl Phys*, 93 (2003) 4130; Saha & Sinha ,J Phys: Condens Matter, 14 (2002) 249; Phys Rev, B65 (2002) 134103] and they have reported that the BFN-based electroceramics exhibit a relaxor behavior by showing very attractive dielectric properties over a wide range of temperatures. In the present investigation we report the synthesis, structural and spectroscopy study of polycrystalline samples of $(1-x)Ba(Fe_{0.5}Nb_{0.5})O_{3-x}BaTiO_3$, (where x = 0, 0.10) which were synthesized by the traditional solid state reaction method. Preliminary studies of X-ray diffraction (XRD) patterns at room temperature suggest that compound formed is a single phase with the monoclinic crystal systems. Detailed studies of dielectric and electrical properties of the material in a wide range of frequency (100 Hz to 5 MHz) and temperatures (30-270ÚC) showed that these properties are strongly temperature and frequency dependent. The abnormal behavior of dielectric constant (ε′) shows that 0.90 BFN + 0.10 BT ceramic experiences a ferroelectric to paraelectric transition around 260ºC. It is observed that dielectric constant (ε′) and tangent loss (tan δ) rapidly increases by making solid solution of BFN with 10% of BT. The higher value of å' at the low frequency region has been explained using Maxwell Wagner polarization effect.

65. Enhancement of Forster Resonance Energy Transfer (FRET) in Single Optical Microcavities

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Key words: *Whispering gallery modes (WGMs), Forster resonance energy transfer (FRET), Microcavity, Emission spectra.*

The dye-embedded single dielectric optical microcavities exhibit whispering gallery modes (WGMs) in their spontaneous emission spectra. Theoretical simulations for the experimentally observed WGMs have been carried out by using Lorenz-Mie theory. Forster resonance energy transfer (FRET) in a dye pair has been studied in single microcavities by using picoseconds time-resolved fluorescence microscopy. It is found that the efficiency of excitation energy transfer is enhanced by a factor of two in smaller microcavities as compared to that of the bulk. This enhancement has been explained mainly due to increase in the overlap integral and decrease of inter-molecular distance in the microcavity.

66. Extended Red Emmision (ERE) in a Meteorite of Type H4/5 Chondrite

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Key words: *Dergaon meteorite, Spectrum, Green diode-pumped Solid-state laser,Wavelength.*

In the present work we report the emission system in the visible sector of the spectrum from a meteorite that fell at Mahadevpur near Namsai town, India [Meteoritics & Planetary Science p 1570-Meteoritical Bulletin No. 94.] (27°.40' N, 95°.47' E), at 9:10 am Indian

Standard Time, February 21, 2007, and make a competitive study with the emission exhibited by the

Dergaon meteorite. This Mahadevpur meteorite belongs to the type of ordinary chondrite (H4/5). Laser induced fluorescence spectrum of Mahadevpur (near Namsai) meteorite of type H4/5 ordinary chondrite was excited with the help of a 25-mW green diode-pumped solid-state laser (532 nm), and a diffuse spectrum was photographed on a graph spectrograph in the wavelength of 5400-6500 Å. The band system is attributed to silicate (olivine), a major component of the meteorite. A comparison of the emission system that of Dergaon meteorite of type H5 ordinary chondrite was made.

67. FT-IR and Raman Spectroscopic Studies of Anti-cancer Active Molecule N-{(Meta-Ferrocenyl) Benzoyl}-Glycine-L-Alanine Ethylester

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Key words: *DFT, PED, Bioorganometallic, FT-Raman spectrum, FT-IR spectrum, Peptide mimetic models, Harmonic vibrational wavenumbers*

Bio organometallic chemistry has recently developed as a rapidly growing area, the main focus being the peptide mimetic models, macromolecular assemblies for molecular recognition and anti-cancer drugs [*Organometallic*, 22 (2003) 2166; *Organomet Poly Mat*, 15 (2005) 3; *J Am Chem Soc,* 110 (1988) 2615.]. In the present work FT-Raman and FT-IR spectra of anti-cancer active compound N-{(Meta-Ferrocenyl) Benzoyl}-Glycine-L-Alanine Ethylester (MFBGA) have been recorded and analyzed. The geometrical parameters and harmonic vibrational wavenumbers of MFBGA were predicted with the help of density functional theory

The FT-Raman spectrum, of MFBGA was recorded on Bruker RFS 100/S FT-Raman spectrometer and FT-IR was taken with a Perkin Elmer RXI spectrometer with the sample

in KBr. Gaussian 03 software package [Vibrational Spectra of Benzene Derivatives, Academic Press, New York, 1969.] was used for theoretical calculation. The quantum chemical calculations were performed applying DFT method, with Becke-3-Lee-Yang-Parr (B 3LYP) supplemented with the standard 6-31G (d,p) basis set. The optimized geometry corresponding to the minimum on the potential energy surface has been obtained by solving self-consistent field equation iteratively. PED is calculated using the software VEDA [*J Mole Struct*, 787 (2006) 172.]. Vibrational assignment of the molecule is done by using potential energy distribution analysis. Vibrational spectral studies of MFBGA are analyzed. The predicted vibrational wavenumbers well fit with the experimental spectra.

68. Vibrational Spectra of 4-Methoxy-2-Nitroaniline: DFT Study

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Key words: *Nitroaniline, Microscopic, Nonlinear susceptibilities, Polarizability, FT-IR spectrum, NIR-FT Raman spectrum.*

Nitroaniline based compounds are found to exhibit large microscopic second order nonlinear susceptibilities [Molecular Nonlinear Optics: Materials, Physics and Devices, academic Press, New York, 1994]. The π-conjugated organic structures show enhanced third order optical nonlinearities because of their high polarizability due to the presence of delocalized electrons along the side chain. The present work deals with the vibrational spectral analysis alongwith density functional theory (DFT) computations to investigate the structure, conjugation, inter and intra molecular interactions of the molecule 4-methoxy-2-nitroaniline (MONA).

The FT-IR spectrum of NA was recorded in the region 4000 -400 cm^{-1}, with samples in the KBr pellet, using Nicolet Magna 560 FTIR spectrometer. The resolution of the spectrum is 4 cm^{-1}. The NIR-FT Raman spectrum of NA crystal was obtained in the range 3500-50 cm^{-1} using Bruker RFS 100/S FT Raman spectrometer with a 1064 nm Nd:YAG laser source of 100 mW power.

The equilibrium geometry and the harmonic vibrational wavenumebrs of compound MONA have been calculated using Gaussian' 98 program package [Gaussian 98, Gaussian Inc, Pittsburgh PA, 1998.]. DFT quantum computations at B3 LYP/6-31 G* level has been used to compute the geometry and vibrational spectrum of MONA. The predicted vibrational spectra are in fair agreement with experiment.

69. Vibrational Investigation of Organic Compound L-Prolinium Picrate

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Key words: *DFT; FT-Raman; FT-IR, Hydrogen bonding, L-prolinium, ð donor-accepter, Molecular architecture.*

Vibrational spectral studies of the molecule can provide deeper knowledge abiut the relationships between molecular architecture and bioactivity. L-prolinium is one of the members of the amino acid family and the donor residue. L-prolinium picrate is a ð donor-accepter in which L-proline acts as donor and picric acid as accepter.

FT-Raman and IR spectroscopic techniques have been used to study structure-property relationship of the nonlinear optical material L-prolinium picrate (LPP).

Single crystals of LPP were synthesized from L-proline and picric acid taken in 1:1 ratio in triple distilled water. Homogeneous mixing was made possible by using a magnetic stirrer. The solution was filtered using macro filter paper and kept under room temperature for slow evaporation. The FT-IR spectrum of LPP in the region 400-4000 cm^{-1} was recorded using a Perkin-Elmer FT-IR spectrometer with the sample in KBr matrix. The FT-Raman spectrum was recorded on a Bruker RFS 100/S NIR-FT instrument using powdered form of the sample in the range 400-3500 cm^{-1}. The structural analysis of a picrate derivatives have been reported earlier [*Acta Cryst, C 62 (2006) 567; J Chem Crystallogr, 31 (2001) 345*.]

In the present study, Gaussian 03 package was used to optimize the structure and calculate the vibrational wavenumebrs of LPP at the B3LYP/cc-PVDZ level. The vibrational spectral studies show strong O-H…O and N-H…O intramolecular interactions exist between L-prolinium and picrate ions. Mulliken population analysis also supports transfer of charges and thereby bioactivity.

70. Quantum Chemical Modeling and Spectroscopic Analysis of 2, 4, 5-Trichlorobenzene sulfonyl chloride (TCBSC)

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Key words: *TCBSC, FTIR, FT-Raman, Vibrational analysis, Bioactivity, Pigments, Fluorescence.*

The wide bioactivity of 2, 4, 5-trichlorobenzene sulfonyl chloride (TCBSC) has led to perform vibrational spectral studies to understand its structural and bonding features. TCBSC is a novel pharmaceutical compound used in dyes, pesticides, pigments, as fluorescence brighteners and intermediate for agricultural chemicals in the manufacture of insecticides. Its derivatives are also used as a sweetner for sour crude oil and gasoline, hardener for silicon-carbide for electronic circuits. FTIR (4000-400 cm^{-1}) and FT-Raman (3500-50 cm^{-1}) spectral measurements have been made for the solid sample of TCBSC. The electronic structure calculations have been performed using Gaussian 09W program package. The optimized structures, energies, depolarization ratios, infrared intensities, Raman activities, Mulliken's charges, reduced mass and thermodynamic functions have been calculated at *ab initio* (HF)level, adopting the standard 6-311++G(d, p),6-311+G(d, p) basis sets. This geometry was then re-optimized again at B3LYP level using the above mention basis sets, for better description of polar bonds of the title compound. Further, to check whether the set of vibrational frequencies contribute maximum to the potential

energy associated with the normal coordinates of the molecule, the potential energy distribution is calculated using MOLVIB program package. The calculated potential energy distribution of the fundamental vibrations is satisfactory thereby confirming the frequency assignment of the molecule.

71. IR and Raman Studies of 7-Bromo-5-Chloro-8-Quinolinol Aided by DFT Analysis

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Key words: *7-Bromo-5-Chloro-8-Quinolinol, HOMO, LUMO, DFT.*

Quinoline family compounds are widely used as a parent compound to make drugs, fungicides, biocides and alkaloids dyes, rubber chemicals and flavouring agents. Also it is used as catalyst corrosion inhibitor, preservative and as solvent for resins and terpines. Spectroscopic techniques are inevitable powerful tool of investigation in any field of research. Fourier transform infrared spectroscopy (FTIR) is a technique that is widely used to identify organic and some inorganic materials. Infrared spectrometry (IR) provides a useful way for the identification of drugs. The FT- Raman and FTIR spectra of 7-Bromo-5-Chloro-8-Quinolinol (7BCQ) have been recorded in the regions 3500-100 cm^{-1} and 4000-400 cm^{-1}, respectively.

The geometry, intermolecular bond length, bond angle, harmonic vibrational frequencies and intensities, Highest Occupied Molecular Orbitals (HOMO), Lowest Unoccupied Molecular Orbital (LUMO) energy gaps and thermodynamical properties like zero point vibrational energies, rotational constants, entropies and dipole moment of 7BCQ have been computed using density functional theory (DFT) at the B3LYP/6-31+G and B3LYP/6-31++G levels.

72. DFT Simulations and Vibrational Analysis of FT-IR and FT-Raman Spectra of 4-Chloro-2,6-Dimethoxy Pyrimidine

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Key words: *Pyrimidine, Nucleotides, Nucleic acids, Living organisms, Uracil, FT -IR and FT - Raman spectra , Cytosine.*

Pyrimidine and its derivatives, components of individual nucleotides and of nucleic acids, are the most important biopolymers. Pyrimidine belongs to the family of nucleic acids. Nucleic acids are of great interest, since they control the manufacturing of proteins and the functions of the cells in living organisms. They also occur in many biologically active substances, including antibiotics . In the present work Quantum mechanical calculations of energies, geometries and vibrational wavenumbers of 4-Chloro -2, 6-Dimethoxy Pyrimidine (CDMP) were carried out using Density Functional Theory (DFT / B3LYP) method using 6 -31 + G and 6 -311 ++ G basis sets. The optimized geometrical parameters obtained by B3LYP method show good agreement with experimental data. The difference between the observed and scaled wavenumber values of most of the fundamentals is very small. A detailed interpretation of the infrared spectra of CDMP was also reported. Thermodynamic properties like entropy, heat capacity and zero point energy have been calculated for the molecule.

73. Molecular Structure and Vibrational Spectra of 1-Chloronaphthalene(CN) by *ab initio* and Density Functional Methods

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Key words: *CN, FT-IR, FT-Raman, Density Functional Method, Vibrational spectra, Naphthalene*

Naphthalene and its derivatives are known for their biological and pharmaceutical importance. Naphthalene is mainly used as a precursor to other chemicals. The single largest use of naphthalene is the industrial production of phthalic anhydride. The most familiar use of naphthalene is as a household fumigant. Refined naphthalene finds use in ball flakes and pellets, largely for use as an insect repellent. It is also used in the production of plastics, making dye stuffs, synthetic resins, coatings, tanning agents and celluloid. Naphthalene is found in both middle and heavy oil fractions at crude oil and is obtained by fractional crystallization. The structure of naphthalene is benzene-like having two six membered ring fused together. In the present work,the structure of 1-chloronaphthalene (CN) was analyzed by recording Fourier transform infrared (FTIR) (4000-400 cm^{-1}) and FT-Raman (3500-50 cm^{-1}) spectra at room temperature. The fundamental vibrational frequencies, intensity of vibrational modes and the ground state geometries of the title compound have been evaluated using density functional theory (DFT) and *ab initio* methods with the standard basis sets B3LYP/6-311++G (d,p) and HF/6-311++G (d,p) which yield a good agreement between observed and calculated frequencies.

74. Scaled Quantum Chemical Studies of the Structure and Vibrational Spectra of 2,4,6-Trimethyl Benzaldehyde (TMBA)

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Key words: *2, 4, 6-Trimethylbenzaldehyde,ab initio and DFT Methods, FT-IR and FT-Raman spectra.*

TMBA an aromatic aldehyde with three methyl groups is a clear liquid and it is used in the synthesis of other organic compounds including pharmaceuticals, agrochemicals, dyes and plastic additives. It is an important intermediate for the processing of perfumes and flavouring compounds. In the present work, FTIR and FT-Raman spectra of 2, 4, 6-trimethylbenzaldehyde have been recorded in the regions 4000-400 cm^{-1} and 3500-100 cm^{-1} , respectively. The optimized geometry, frequency and intensity of the vibrational bands of TMBA have been obtained by DFT method with complete relaxation in the potential energy surface using 6-31+G (d,p) and 6-31++G (d,p) basis sets. A complete vibrational assignment aided by the theoretical harmonic frequency analysis has been proposed. The observed and the calculated frequencies are found to be in good agreement. Simulation of infrared and Raman spectra utilizing the results of these calculations led to excellent overall agreement with the observed spectral patterns.

75. Experimental Vibrational Spectra (FT-IR and FT-Raman) and DFT Calculations of 1,3-Dibromo-5-Chlorobenzene

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Key words: *DFT, ab initio, B3LYP, Scaled Quantum Mechanical Method, Benzene, 1,3-Dibromo-5-Chlorobenzene.*

Spectroscopy is one of the powerful tools available for the study of atomic and

molecular structure and used in the analysis of a wide range of compounds. Spectroscopy has been becoming increasingly important and useful in the quantitative and qualitative analysis for materials. Benzene is an important solvent and precursor in the production of drugs, plastics, synthetic rubber and dyes. In the present work, Fourier transform infrared and Raman spectra of 1,3-dibromo-5-chlorobenzene have been recorded in the region 4000-400 cm $^{-1}$ and 3500-50 cm^{-1}, respectively. The optimum molecular geometry , normal mode wavenumbers , infrared intensities and Raman scattering activities have been investigated with the help of B3LYP density functional theory (DFT) and *ab initio* HF methods . The computed values of frequency are scaled using a suitable scale factor to yield good coherence with the observed values. The fundamental frequencies are used to calculate the thermodynamic functions namely, the enthalpy, entropy, heat capacity and free energy. Reliable vibrational assignments were made on the basis of total energy distribution (TED) calculated with scaled quantum mechanical (SQM) method.

76. Vibrational Spectroscopic Investigations of 4-bromo-2, 6-Dichloroaniline Based on ab initio HF and Density Functional Theory Calculations

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Key words: *Fourier transform, Infrared spectrum, Raman spectrum, ab initio HF, Density Functional Theory, Molecular geometries, Vibrational analysis, 4-Bromo-2, 6- Dichloroaniline.*

The spectroscopic techniques are very sensitive tool for the study of atomic and molecular structure of compounds. One of the most important aromatic amines is aniline. Aniline and its derivatives have been widely used as starting materials in a vast amount of chemicals, pharmaceuticals, dyes, electro-optical and many other industrial processes. The conducting polymer of aniline namely poly aniline is used in microelectronic devices as diodes and transistors. Particularly, aniline and its derivatives are used in the production

of dyes, pesticides and antioxidants. Consideration of these factors led us to undertake the detailed spectral investigation of 4-bromo-2, 6-dichloroaniline.

The Fourier transform infrared and Fourier transform Raman spectra of 4-bromo-2, 6-dichloroaniline have been recorded in the region 4000-400 cm^{-1} and 3500-50 cm^{-1} ,respectively. The optimized molecular structure, vibrational frequencies, corresponding vibrational assignments of 4-bromo-2, 6-dichloroaniline have been investigated by using *ab initio* Hartree-Fock (HF) and Density Functional Theory methods at B3LYP level using 6-31+G (d,p) basis set. Results obtained at this level of theory were used for detailed interpretation of the IR and Raman spectra. The good agreement between the observed and calculated frequencies is observed.

77. Spectroscopic Investigation of Arsenic(As) in Ground Water of Titabor in Jorhat District (Assam, India)

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Key words: *UV1 spectrophotometer, As in Ground Water, Minerals and ores, Toxic element.*

Arsenic (As) is an ubiquitous bio accumulative toxic element. It is widely distributed throughout the earth and crust. Arsenic is induced into water through the dissolution of minerals and ores, and in ground water, in some areas, it elevates as a result of erosion from local rocks. Combustion of fossil fuels is an another source of arsenic in the environment. Inorganic arsenic can occur (Environ Sci Tech, 85(2001)262) in the environment in several forms but in natural way, in ground water, it is mostly found as trivalent Arsenic [As (III)] or pentavalent Arsenic [As (V)]. Arsenic and its compounds are naturally present in low concentration at places with high geothermal activities . Long term exposure to elevation level of Arsenic may cause serious health hazards. Worldwide, the main reason for chronic human intoxication with Arsenic is the intake of contaminated ground water.

In Assam, the maximum arsenic was observed in Jorhat, Lakhimpur, Nalbari and Nagaon district. In the present work, an investigation has been made on Arsenic in gound water of Titabor, Jorhat district, Assam using UV-1 spectrophotometer . Location wise coutour is plotted to investigate the arsenic free region.

78. FT-IR and FT-Raman Spectra, ab initio and Density Functional Computations of the Vibrational Spectra, Molecular Geometry, and Some Molecular Properties of the 4-Amino-3,5-Dichlorobenzonitrile

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The experimental FT- IR (in different matrices) and FT-Raman spectra (in solid state) of 4-Amino-3, 5- Dichlorobenzonitrile molecule were recorded. The results were compared with theoretical values. Geometry, vibrational wavenumbers and thermodynamic parameters were calculated using DFT Qunatum Chemical Methods and several basis sets. With the help of specific scaling procedures, the experimentally observed FTIR and FT-Raman vibrational wavenumbers were analysed and assigned to different normal modes of the molecule. The error obtained was, in general, very low. The distorsions produced in the phenyl ring by the substituents are explained by the superposition principle.

The contributions of the different modes to each wavenumber were determined using potential energy distributions (PEDs). The geometry of the -Ca”N group is insignificantly affected by a new substitutent on the ring. Hence, the vibrational wavenumbers of the cyano group remains almost unchanged from the benzonitrile molecule. The Ca”N stretching mode is highly localized on the bond with a PED of 86%, and is assigned at 2230 cm ^{1} in Raman spectra. In-plane and out-of-plane bending modes of Ca”N group, by contrast, appear with weak IR intensity and with null Raman activity, and strongly coupled with CCC modes.

79. 2-Amino-5-bromobenzonitrile: ab Initio Calculations, FTIR and FT-Raman Spectra

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Key words: *FT-IR and FT-Raman spectra, 2-amino-5-Bromobenzonitrile, Thermodynamic parameters*

From the spectroscopic point of view, the vibrational spectra of benzonitrile (in short BN), mono substituted and disubstituted benzonitriles have been studied extensively [M A Palafox, V K Rastogi and J K Vats, J Raman Spectrosc, 37(2006)85]. In the present investigation geometry, vibrational wavenumbers and several thermodynamic parameters were calculated using *ab intio* quantum chemical methods for 2-amino-5-bromobenzonitrile molecule for the first time. The results were compared with experimental values. With the help of specific scaling procedures, the observed vibrational wavenumbers were analyzed and assigned to different normal modes of the molecules. The error obtained was in general very low. Using PED's were determined the contribution of the different modes to each wavenumber. The molecular geometry, the atomic charges, the total energy, the rotational constants, zero point energy, the room temperature entropy (translational, rotational, and vibrational) and dipole moment were determined. Other general conclusions were also deduced. As in benzonitrile and its derivatives the Ca ≡ N stretching mode appears at 2232 cm^{-1} with the strongest Raman intensity. In-plane and out-of-plane bending modes of Ca ≡ N group, by contrast, appear with weak IR intensity and with null Raman activity.

80. On the Nature of Quenching of Emission Spectra of N_2 of *m*-Nitrobenzaldihyde in Discharge

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Key words: *Fluorescence, Quenching, Molecular interactions, Excited-state reactions, Aromatic structure, Polymer.*

Fluorescence quenching is a process, which decreases the fluorescence intensity of a sample by a variety of molecular interactions such as excited-state reactions, molecular rearrangement, energy transfer, ground state complex formation and collisional quenching [*Indian J Pure & Appl Phys*, 34 (1996) 244; *Rad Measurement*, 26 (1996)117; *Procd DAE-BRNS Nat Laser Symp*, (2003) 578]. The quenching is concentration dependent. The quenching for the vapor of nitro compounds is fast and related to the vapor pressure. The quenching mechanism was attributed to the strong electron withdrawn property of the nitro group. It has been established that aromatic structure and numbers of nitro groups have almost no effect on the quenching properties. During recent years the authors have carried out extensive studies on laser induced fluorescence of various polymer containing nitrogen with respect to their quenching behavior. The silent feature observed is the first positive band of molecular nitrogen in the region 6068.5-6545 Å while the entire region belonging to the first positive is quenched or suppressed [Changmai R and Baruah GD, *Indian J Phys*, 82 (2008) 679, *Changmai et al*, 79 (2005) 1063]. In the present work we report the first positive band system due to molecular nitrogen in the region 5692.9-6545 Å which is severely quenched where a sample of *m*-nitrobenzaldyhyde is excited in uncondensed transformer discharge.

81. Spectroscopic Characterization of Terephthalamide synthesized from PET waste and its complex with Lanthanum Nitrate

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Keywords: *Terephthalamide, Pet Waste, Spectroscopic analysis, FTIR, UV, NMR Lanthanum Nitrate, Polymers*

Poly Ethylene terephthalate (PET) has excellent mechanical properties in comparison with other commodity polymers especially when it is used as a film or fiber. Terephthalamide, the depolymerised end product of PET waste has been synthesized from the degradation of PET waste through ammonolysis by using NH_3. It was further used for the synthesis of terephthalamide–Lanthanum complex with the help of Lanthanum-Nitrate to make better antifungal agent. Both the compound and the complex were characterized by different spectroscopic techniques like FTIR, UV, NMR and other analytical techniques.

82. Performance of DFT Functionals for the Calculation of EPR Hyperfine Coupling Constants for Some 3d Transition Metal Complexes

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Key words: *Density Functional Theory (DFT), Transition Metal Complexes, Hyperfine coupling constants*

We have investigated the performance of several DFT functionals for the calculation of EPR spectral parameter hyperfine coupling constants for some 3d transition metal

complexes, namely [Cu $(CO)_3$], [$Ni(CO)_3H$] and [Mn $(CO)_5$]. For these calculations, BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, BHP86 functionals have been used and the results obtained have been compared with experimental values. The hyperfine coupling constant values obtained from different density functionals have been found in the order of BLYP > BP86 > BPW91 > B3LYP > B3PW91 >BHLYP> BHPW91 > BHP86 > EXP for [Cu $(CO)_3$], BHPW91 > BHP86 > BHLYP > B3PW91 > BLYP > BP86 > BPW91 > B3LYP > EXP for [Mn $(CO)_5$]; and BHPW91 > BHP86 > BHLYP > B3PW91 > B3LYP > BLYP > BPW91 > BP86 > EXP for [$Ni(CO)_3H$] complex. We have inferred that although the results obtained by some of the DFT functionals are in close agreement with the experimental values but the performances of the different functionals for different transition metal complexes are not same. The performance of the functional BHP86 has been found better for [Cu $(CO)_3$], BP86 for [$Ni(CO)_3H$] and B3LYP for [Mn $(CO)_5$] metal **c**omplex.

83. Density Functional Calculations of EPR Hyperfine Coupling Constants of Some First Row Transition Metal Complexes

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Key words: *Density Functional Theory (DFT),Transition Metal Complexes, Hyperfine coupling constants*

We have calculated the EPR spectral parameter hyperfine coupling constants of some first row transition metal complexes, namely $[Fe(CO)_5]^+$, $[Mn(CN)_5NO]^{2-}$ and $[Co(CO)_4]$ using Density Functional Theory. For these calculations, BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, BHP86 functionals have been used. The hyperfine coupling constants

values obtained from different density functionals have been found in the order BHPW91 > BHP86 > BHLYP > B3PW91 > BLYP > BP86 > BPW91> B3LYP > EXP for [Fe $(CO)_5]^+$, BHPW91 > BHP86 > BHLYP > BLYP > BP86 > BPW91 > B3PW91 > B3LYP >EXP for [Mn $(CN)_5NO]^{2-}$ and BHPW91 > BHP86 > BHLYP > BLYP > BP86 > BPW91 > B3PW91 > B3LYP > EXP for $[Co(CO)_4]$ complex.We have inferred that DFT functional B3LYP is best functional for the estimation of hyperfine coupling constant for [Fe $(CO)_5]^+$, [Mn $(CN)_5NO]^{2-}$ and $[Co(CO)_4]$ metal complexes .

84. Density Functional Calculations of EPR Parameter Hyperfine Coupling Constants of $[Ni(CO)_3H]$ and [Co $(CO)_4$] Transition Metal Complex

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Key words: *Density Functional Theory (DFT), Transition Metal Complexes, Hyperfine coupling constants.*

We have calculated the EPR spectral parameter hyperfine coupling constants of **[**$Ni(CO)_3H$] and [Co $(CO)_4$] transition metal complex using Density Functional Theory. For this calculation, BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, functionals have been used and the results obtained are compared with experimental values. The results obtained from the density functional methods have been found in close agreement with the result obtained from the experiments. We have also found that the performance of the different functionals for both complexes is not same. The performance of the functional BP86 has been found better for **[**$Ni(CO)_3H$] ,whereas B3LYP functional is better for [Co $(CO)_4$]complex .

85. Density Functional Calculations of EPR Parameter Hyperfine Coupling Constants for [Cu $(CO)_3$], [Mn $(CN)_5NO]^{2-}$,and $[Mn(CN)_4]^{2-}$ Transition Metal Complexes

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Key words: *EPR, Density Functional Theory, BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, BHP86, Transition Metal Complexes, Hyperfine coupling constants*

We have calculated the EPR spectral parameter hyperfine coupling constants of [Cu $(CO)_3$], [Mn $(CN)_5NO]^{2-}$ $[Mn(CN)_4]^{2-}$ transition metal complex using Density Functional Theory. For these calculations, BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, BHP86 functionals have been used and the results obtained have been compared with experimental values. The results obtained from the density functional methods have been found in close agreement with the result obtained from the experiments. We have also found that the performances of the different functionals for different transition metal complexes are not same. The performance of the functional BHP86 have been found better for [Cu $(CO)_3$], B3LYP for [Mn $(CN)_5NO]^{2-}$ and BHPW91 for $[Mn(CN)_4]^{2-}$ transition metal complexes . We have also observed that performance of BLYP functional is very poor for [Cu $(CO)_3$], BHPW91for [Mn $(CN)_5NO]^{2-}$ and BLYP for $[Mn(CN)_4]^{2-}$ transition metal complexes .

86. Spectroscopic Study of Some Copper (II) Complexes

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Key words: *Square pyramidal, Tetragonally distorted octahedral.*

1-Phenylazo- 2-Naphthol (PANH) has three potential donor sites and thus it acts as a very good chelating agent. This ligand has been used for complexation with Cu(II) ions to synthesise the complexes of general formula: $Cu(PAN)_2Ln$, where L = secondary ligands like pyridine, picoline, H_2O and n = 0, 1 and 2. These complexes have been characterized by their elemental analysis, conductivity, measurement and magnetic moment at room temperature infrared spectra and electronic spectra. The ligand PANH is found to be coordinated through deprotonated phenolic oxygens and azonitrogen forming an six membered chelate with two conjugate ð-bonds in chelate ring. The magnetic moment values reveal the mononuclear nature of the complexes while their electronic spectra reveal the geometry of the complexes. $Cu(PAN)_2$ complex is found square planer while $Cu(PAN)_2$ L and $Cu(PAN)_2$ L_2 are found square pyramidal and tetragonally distorted octahedral.

87. FT-IR, FT-Raman Spectra and Density Functional Computation of 2,6-Dichlorobenzonitrile Molecule

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The usefulness of vibrational spectroscopy has expended rapidly over a last decade the development of FT-IR and FT-Raman instrumentation. The benzonitrile and its derivatives have many important applications [VK Rastogi et al, International J Quantum Chem, 94 (2003) 189]. From the spectroscopic point of view many derivatives of benzonitriles have been studied [VK Rastogi et al, J Raman Spectroscopy, 37 (2006) 85

& references therein], however to the best of our knowledge the complete study of vibrational spectra of 2, 6-dichlorobenzonitrile is not available in literature. Hence, in the present investigation, we study the vibrational spectra of this molecule and identify the various normal modes of vibration with the help of DFT computations.

The FT-Raman spectrum of 2,6-dichlorobenzonitrile was reported at room temperaturein the powder form in the region 50-4000 cm^{-1} on a Bruker IFS66 optical bench with an FRA 106 Raman module attachment. The sample was undertaken. The NIR output (1064 nm) of an Nd:YAG laser was used to excite (the probe) the spectrum. The instrument was equipped with a liquid nitrogen-cooled Ge detector. The laser power was set 100 mW and the spectrum was recorded over 100 scans at a fixed temperature. The spectral resolution was 6 cm^{-1} after apodisation. The mid infrared spectrum of the compound from 40-4000 cm^{-1} was recorded with a Perkin Elmer FT-IR model 1760X instruments, using the KBr techniques with 1 mg sample per 300 mg KBr. For the spectrum acquisition four scans were collected at 4 cm^{-1} resolution.

Density functional technical (DFT) computations od DBN performed by using Gaussian 03 program package at the Backe-Lee-Yang-Parr hybrid exchange-correlation three-parameter functional (B3LYP) level with standard 6-31G(d, P) basis set to derive the complete geometry optimization. All the optimized geometry corresponding to minimum on the potential energy surface has been obtained by solving self-consistent field equation iteratively. The calculated harmonic vibrational wavenumbers have been analytically calculated by taking second order derivatives of energy using the similar level of theory. The calculated frequencies were scaled with scaling factor.

88. Chromium Detection in Residue of Industrial Waste Water

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Key words: *LIBS, Cr, Industrial waste, filter paper*

In continuation of our work on the detection/monitor in quantification of heavy and toxic metals present in Environment, the present paper is an attempt to find the heavy

metals in industrial waste water. Jajmau is the prominat centre of leather tanning industries along the bank of River Ganga. Laser induced breakdown spectroscopy has been utilized to detect and quantify the heavy metals like Cr present in industrial waste water. Samples were collected from the different sections of water treatment plant situated in Jajmau and brought to the laboratory in packed air tight container. Water samples were filtered using whatman (no.1001) filter paper. LIBS spectra of residue deposited on the above filter paper have been recorded by focusing the laser beam of 532 nm of Nd:YAG laser (continuum surelite III-10). Laser induced plasma was created at its surface and emission from plasma is collected and analyzed by spectrometer and CCD detector (LIBS2000+). The spectral lines of Cr along with other heavy elements are seen in the LIBS spectra of waste water residue. To quantify the concentration of the Cr present in residue calibration curve was drawn using of Cr (267.7nm). The concentration of Cr was found higher than then the limit set by Environmental Protection Agency. Therefore government should take proper action on dumping the waste material from the industries.

89. Study of black pigment gallstone using LIBS

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Key words: *LIBS, Gallstone, Calcium, Copper*

Laser-induced breakdown spectroscopy (LIBS) is a versatile technique for analysis of variety of materials (in any phase: solid, liquid and gas) including biomaterials. The present study uses the LIBS technique for the compositional analysis of human gallbladder stone samples. LIBS spectra of black pigment gallstone samples have been recorded in air and argon for the spectral range 200-900 nm. Several elements like calcium, copper, magnesium, silicon, sodium, potassium etc. and lighter elements like carbon, hydrogen, nitrogen and oxygen are detected in the gallstone samples. The LIBS spectra of gallstone obtained in argon atmosphere is compared with the spectra recorded in air. The appreciable

increment in intensity of LIBS spectra is observed when the spectra are recorded in argon atmosphere.

90. Dispersion Characteristic by Different Modes in an Optical Fiber Wave Guide

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Key words: *Dispersion, Linearly polarized, TE_{01} mode, HE_{11} mode, Cutoff frequency, Phase velocity, Bessel function, attenuation.*

In this investigation we find out the dispersion characteristic for the linearly polarized HE_{11}, and TE_{01} modes and compare the phase velocity of the HE_{11} and TE_{01} modes in THz frequency range i.e. 10^{12} Hz. The additional dispersion due to dielectric layer is found to be small for the HE_{11} mode and the phase velocity is primarily determined by the waveguide radius.

The mode profile is determined by the transverse component of the mode wave factor $K_{-\ell}$which is proportional to the cutoff frequency $\omega_c = K_{-\ell}C$. The mode profile can be used to determine the corresponding cutoff frequencies. The characteristic wave factor K_{-l} can be found directly from the approximation for the HE_{11} mode.

$E(r, \theta) = E_0 J_0 (K_{-\ell} r)$; $E_y(r,\theta) = 0$

Where J_0 is the Bessel function of zeroth order and E_0 is the electric field amplitude at the waveguide centre. The phase velocity of HE_{11} mode follows the standard dispersion relation with region of low attenuation.

91. Spectral and Antimicrobial Studies of Co(II), Ni(II) and Cu(II) Complexes with Nitrogen, Oxygen and Sulphur Containing Schiff Base

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Key words: *Schiff base/ Co(II), Ni(II) and Cu(II)/ Semicarbazone/ Antimicrobial/ Antifungal Screening*

Hexacoordinated complexes of the general formula $[M(PPQS)_2]$ and $[M(PPQT)_2]$ where M = Co(II), Ni(II) and Cu(II), PPQS = 1- phenyl pyrazolo [4, 5-c] quinolin-4 [5H] semicarbazone, PPQT = 1- phenyl pyrazolo [4, 5-c] quinoline-4 [5H] thiosemicarbazone have been prepared. The ligand and metal complexes have been characterized by elemental analyses, molar mass, magnetic susceptibility, infrared spectra, molar conductivity and electronic spectra. The infrared spectral data proposes the coordination of the ligand, PPQS/ PPQT through N atom of quinoline ring, azomethine N and oxygen or sulphur atoms of either semicarbazone or thiosemicarbazone moiety. The electronic, spectral and magnetic susceptibility values propose octahedral geometry for the complexes. The molar conductivity value were found in the range 4.7-9.3 ohm^{-1} cm^2 mol^{-1} indicating all the complexes are non-electrolytic in nature. The ligand as well as metal complexes were screened for their antimicrobial activity.

92. Synthesis and Spectral Characterization of Coordination Compounds of Co(II), Ni(II) and Cu(II) with Nitrogen and Sulphur Containing Schiff Base Ligands

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Key words: *DHDBT/ Schiff base/ Co(II), Ni(II), Cu(II)/ complexes/ Antimicrobial studies, Azomethine N, Thione S*

Metal complexes of Schiff base derived from 8, 8-dimethyl-2,3,4,5,7,8 hexahydro diazepino [2,1-b] benzothiozol-10(9H) thiosemicarbazone [DHDBT] are reported and characterized based on elemental analyses, molar mass, IR, electronic spectra, magnetic susceptibility and molar conductance measurements. The complexes are found to have general formula $[M(DHDBT)_2X_2]$; where M = Co(II), Ni(II) and Cu(II); DHDBT = 2,3,4,5,7,8 hexahydro diazepino [2, 1-b] benzothiozol-10(9H) thiosemicarbazone; X = Cl^-, Br^-, I^- and NO_3^-. Schiff base and their metal complexes were also evaluated for their antifungal screening against *Aspergillus niger* and *Candida albicance* by disc diffusion method. Schiff base and complexes have been found active as antifungal agent.

On the basis of above mentioned studies the compound DHDBT acts as neutral bidentate ligand and coordination proposes through azomethine N and thione S atom of thiosemicarbazone moiety. The remaining positions of metal ion are satisfied by negative ions such as Cl^-, Br^-, I^-, NO_3^-. Thus, the complexes are proposed to be octahedral in geometry on the basis of electronic spectra and magnetic measurements.

93. Molecular structure, Vibrational Spectra and Nonlinear Optical Properties of L-Valine Hydrobromide:DFT Study

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Key words: *FT IR and Raman spectra, Nonlinear Optical Material, L-Valine Hydrobromide, Harmonic, Vibrational wavenumbers*

FT IR and Raman spectra of the nonlinear optical material L-Valine Hydrobromide crystal have been recorded and analyzed. The equilibrium geometry, bonding features and the harmonic vibrational wavenumbers of LVB have been calculated with the help of density functional theory (DFT) calculation. The lowering of N-H stretching wavenumber indicates the formation of N-H….Br hydrogen bonding. The calculated First order hyperpolarizability value shows that LVB is the potential candidate for the NLO applications. The electronic effects and the hydrogen bonding were explained using natural bond orbital analysis.

94. Vibrational Investigation of Organic Compound L-Prolinium Picrate

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Key words: *DFT; FT-Raman; FT-IR; hydrogen bonding*

FT-Raman and IR spectroscopic techniques have been are used to study structure-property relationship of the nonlinear optical material L-prolinium picrate (LPP). In the

present study, Gaussian '03 package was used to optimize the structure and calculate the vibrational wavenumbers of LPP at the B3LYP/cc-PVDZ level. The predicted vibrational wavenumbers well fit the experimental spectra. The vibrational spectral studies show strong O-H· · ·O and N-H· · ·O intramolecular interactions exist between L-prolinium and picrate ions. Mulliken population analysis also supports charge transfer and thereby bioactivity.

95. FT-IR and RAMAN spectroscopic studies of anti-cancer active molecule N- {(meta-ferrocenyl)Benzoyl} – glycine – L-alanine ethyl ester

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Key word: *DFT, PED, Bioorganometallic*

In the present work FT- Raman and FT-IR spectra of anticancer active compound N-{(meta-ferrocenyl). Benzoyl}-glycine -L-alanine ethyle ester (MFBGA) has been recorded and analyzed. The geometrical parameters and harmonic vibrational wave numbers of MFBGA predicted with the help of density functional theory. Vibrational assignment of the molecule is done by using potential energy distribution analysis.

96. Charge transfer interaction and vibrational spectral investigation of a nonlinear optical material L-Glutamine Picrate: A DFT study

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Keywords: *Charge transfer interaction; NIR FT-Raman; FT-IR; NLO.*

Charge transfer interaction, vibrational spectra and DFT computation of L-Glutamine

Picrate has been analyzed. The equilibrium geometry, bonding features and harmonic vibrational wavenumbers have been investigated with the help of density functional theory method. The natural bond orbital analysis confirms the occurrence of strong intramolecular hydrogen bonding in the molecule. The vibrational modes found in molecular crystalline materials should be described as phonon modes with strong coupling to the intra molecular vibrations.

97. Spectroscopic Characterization of Complex of La^{+3} with 5-Nitrouracil

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Among the biomolecules, the N-heterocyclic molecules e.g. pyrimidine, cytosine, thymine, uracil and their derivatives are of considerable importance and play an important role in constitution and properties of nucleic acids. Recent studies of uracil derivatives and their metal complexes have been motivated because they function as antitumor agents against many types of tumors by inhibiting DNA and protein synthesis. It has been found that certain metal complexes of uracil derivatives show enhanced antitumor activity with respect to free ligand. The lanthanides have long been known as blood anticoagulant and therapeutical application of rare earth compounds are still in vogue. Lanthanide metal ions have also been used as biological probe. Since 5-nitrouracil possesses chelating ability ,therefore in the present investigation, we report the synthesis and characterization of the complex of La(III) with 5-nitrouracil. Stable complex of La^{+3} with 5-nitrouracil of the composition $[(C_4H_3N_3O_4)_3]Cl_3$ has been isolated in the solid state for the first time. The newly synthesized compound is characterized on the basis of chemical analysis, magnetic

measurement, and infrared and Raman spectral studies and it has been concluded that (i) the ligand 5-nitrouracil acts as bidentate, and (ii) the complex possesses octahedral environment around the central metal ion.

98. DFT Study on Tautomerism of 5-aminouracil

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Among the 5-substituted uracils, 5-aminouracil (5-AU) plays special attention [*V K Rastogi et al,* Chem Phys, 340(2007)17] It is a pyrimidine nucleobase analogue of thymine in which the methyl group is replaced by amino group, adding therefore new hydrogen bonding sites. The compatibility of 5-AU has been recognized in the central position of a DNA triplex, causing damage in the genome or mitotic cell division.

Due to the feasible relationship between the occurrence of the rare enol tautomeric forms of uracil and point mutations developing during RNA replications, numerous studies have been reported on the tautomerism of nucleic acid bases, using both theoretical and experimental approaches.Much of the interest in the present work is due to the fact that tautomers induce alterations in the normal base pairing, leading to the possibility of spontaneous mutations in the DNA or RNA helices.. In the present work ,the calculations have been carried out using Density Functional Theory (DFT), with the Becke's three-parameter exchange functional (B3) in combination with the correlation functional of Lee, Yang and Parr.The main findings of this study are: (i)The special characteristic of the amino group has been accurately reproduced by B3LYP. (ii) The ring of 5-AU shows a small non-planarity.(ca 1.5°) due to an intramolecular H-bond, which is formed between the oxygen O10 and the amino hydrogen. As a consequence of this H-bond, the NH_2 group is much more affected than the C=O moiety.and (iii) ten tautomeric forms of 5-AU were determined and optimized. Six of them are related to those of uracil, with a similar stability order.

99. DFT Simulations and Vibrational Analysis of FT-IR and FT-Raman Spectra of 2-Hydroxy-4-Methyl Pyridine

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Key words: *Vibrational spectra, 2-Hydroxy-4-Methyl Pyridine, DFT Calculations, FT-IR, FT-Raman.*

Pyridine and its related derivatives are found in the structure of many drugs. A vast literature pertaining to the medical aspects of these drugs is available. This work deals with the vibrational spectroscopy of 2-hydroxy-4-Methyl Pyridine (HMP) by means of quantum chemical calculations. The mid and far FT-IR and FT-Raman spectra were measured in the condensed state. Hartree-Fock (HF/6-31 G*) and density functional theory (DFT, B3LYP/6-31G*) ab initio methods have been performed to interpret the observed vibrational spectra. The vibrational spectra were interpreted with the aid of normal coordinate analysis based on scaled density functional force field. The results of the calculations were applied to simulated infrared and Raman spectra of the titled compound, which showed excellent agreement with the observed spectra.

100. FT- Raman and FTIR Spectra and ab initio and DFT Calculation of 5-Amino-2-Nitrobenzoic Acid

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Key words: *FTIR and FT- Raman spectra, 5-Amino-2-nitrobenzoic acid, Geometrical parameters, DFT, Minimum energy, Conformer.*

The FTIR and FT- Raman spectra of 5-amino-2-nitrobenzoic acid (ANB) have been

recorded. From the standard geometrical parameters the geometry of ANB was optimized at ab initio and DFT levels of theory with complete relaxation in the potential energy surface using 6-311++g(d,p) basis set. Several thermodynamic parameters were also calculated for the minimum energy conformer at ab initio and DFT level of theories. The harmonic vibrational frequencies were calculated and the scaled values have been compared with the experimental FTIR and FT-Raman spectra. Majority of the computed wave numbers were found to be in good agreement with the experimental observations. The experimental spectra also coincide satisfactorily with those of the theoretically constructed spectrograms. The hydrogen bonding interaction involving the carboxyl and the nitro groups has also been discussed.

101. Vibrational and Nuclear magnetic Resonance Spectra of N, N' Bis-(2-Propenamido) Benzene 1, 4 Dicarboxamide Synthesized From Terephthalic Dihydrazide)

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Key words: *PET waste, amide, UV Curing, FTIR, NMR*

The aromatic amide has been synthesized by using Terephthalic dihydrazide, depolymerized end product of PET waste with hydrazine monohydrate and acryloyl chloride. The synthesized aromatic amide was characterized with the help of FTIR and NMR spectroscopic techniques alongwith other analytical methods. In the N-H stretch region of FTIR spectrum, there is a single band at 3188 cm^{-1} instead of a pair of bands due do symmetric and asymmetric N-H stretch of NH_2 group. The absence of doublet in the N-H stretch region indicates that acrylic moiety has been attached to both ends of terephthalic dihydrazide. The data obtained give good support for the proposed structure confirming the reaction of aminolysed end product with acryloyl chloride at both ends. It has potential for many applications such as adhesives and UV cured coatings.

102. FT-IR and XRD Spectroscopy for the Characterization of Ancient Ceramic Clay Mineralogy

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Key words: *Ancient pottery sherds, XRD and FT-IR.*

Potteries are the representative tool for material culture that results the interaction between man and his territory. They also allow us to reconstruct the whole manufacturing process from the preparation of the paste to the firing of artifacts. Each of the pottery production reveals us the potter's technical skills, their artistic sense and their practical necessities. In this regard, scientific analysis applied to pottery give the possibility of evaluating the ceramic raw materials and of the clay type. X-ray diffraction and Fourier transform Infrared Spectroscopic analysis of grey pottery fragments from an intensively studied Alagankulam archaeological site, Ramanathpuram district, Tamilnadu, India belonging to first century BCE is detailed in this work. By knowing the crystalline phase and chemical composition of minerals present in the pottery sherds through the XRD and FT-IR respectively we tried to determine the minerals used by the potters, and the clay origin. We also examined the changes of phases produced by the heating which could furnish information on the manufacturing conditions. Hence, both of these methods enable us to reveal differences in the mineralogy of a components, and characteristic minerals as "fingerprint" which may allow distinguishing potteries of different provenance and origin.

103. Crystal and Molecular Structure of 2-ethoxy-4-Methyphenyl-4-Toluene Sulfonate

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Sulfones and Sulfonates have a wide variety of applications in many fields including pesticides, fungicides, medicines and several other areas. Only a few para toluene sulfonates have so far been studied by single crystal XRD. In this paper a freshly synthesized para toluene sulfonate bearing the name given in the title has been subjected to single crystal XRD studies.

The title compound crystalises in the triclinic system with space group P-1 with cell parameters a = 7.8095 Å, b = 9.2787 Å, c = 11.4058 Å, $\alpha = 104.678^{o}$,$\beta = 99.653^{o}$, $\gamma = 94.906^{o}$.

The structure was solved by direct methods using SHELXS-97 and refined by SHELXL-97 programs. ORTEP-32 was used for thermal ellipsoid plots. The R-factor converged to a value of 0.0384 for 1870 unique reflections.

The structural details with regard to bond lengths, bond angles, torsion angles and plane orientations are discussed. The intermolecular features are also studied and the hydrogen bonding patterns are tabulated.

104. Bose-Einstein Condensation, Atom Laser and Application of Semiclassical Theory of Laser to Atom Laser

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Key words: *Laser, Atom laser, Bose-Einstein Condensation (BEC), Bosonic atom, Semiclassical theory of laser, Dispersion curves.*

The invention of optical maser is an important breakthrough of 20th century science. To an ordinary person laser is a pin thin beam of brightly colored light but for an expert it is a coherent beam of photons locked in identical quantum states. Now a beam of atoms can also travel together in quantum lock up, like the photons in a light laser. The realization of Bose-Einstein condensation in trapped dilute atomic vapour enables us to think in terms of the resulting matter wave as an atom laser in close analogy with an optical maser. In a Bose-Einstein Condensate (BEC), a macroscopic fraction of the bosonic atom occupies the ground state of the system and so can be described by a single wave function. The Bose-Einstein Condensation (BEC) is itself analogous to the coherent build up of radiation in a cavity mode and therefore in some sense a laser. However, it is the extraction of atoms from the Bose-Einstein Condensate (BEC) without loss of coherence which is called the atom laser. At present there exists a considerable amount of literature dealing with the subject of atom laser and Bose-Einstein Condensation. But, our present objective is not to discuss the various aspects of atom laser.

There is a host of experiments where Bose-Einstein Condensate (BEC) and atom lasers generated from them can make dramatic improvements in the measurements of fundamental constants in physics and we can also expect new horizons to open up. Semiclassical theory of laser as developed by Lamb and Coworkers has described a large number of laser phenomena.. It may be noted that the theory was initially applied in stationary atoms and subsequently for moving atoms. In the present work we apply this theory for stationary atoms in BEC and atom laser and analyse the role of the semiclassical theory of laser as formulated by Lamb and his coworkers in explaining the behaviors of

atom laser. Bose-Einstein Condensation (BEC) is essentially stationary and therefore semiclassical theory of laser may be particularly relevant to atom laser. In this investigation we work out the dispersion curve for two level atom lasers and show that the dispersion curves exhibit interesting features like broadening near threshold. It occurs when the decay rate is sufficiently high.

105. Study on the molecular interactions of antibiotic with Biomolecules

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Key words: *Doxycycline hyclate, Fatty acid, Molecular interaction, Ultrasonic.*

Many pharmacologically active compounds are of amphiphilic nature. As a result, they tend to self associate and to interact with biological molecules. This review focuses on the self-aggregation properties of antibiotic doxycycline hyclate, as well as on their interaction with oleic acid molecules at physiological condition. These chemical interactions are likely to have localized and special effects, which may be more-or-less stable or they may be complexes due to relatively weak forces, such as polar or ionic forces, hydrogen-bonding or dispersion forces. Dilute solution viscometry (DSV) technique is employed to find the hydrodynamic molecular interactions between the non-Newtonian doxycycline hyclate and the essential fatty acid – the oleic acid in the presence of ethyl methyl ketone. The acoustical properties of blend solutions have shown that ultrasonic velocity and its derived parameters provide much information on molecular interactions. The results of these techniques identify the dominated thermodynamic solute-solute interactions of doxycycline hyclate and oleic acid and the excess thermoacoustic parameters identified the dipolar and dispersive forces in the blends with respect to the compositions and elevation of temperatures from 303K to 310K and 313K.

106. Computation of(3 /2)$^+$ Resonance in ^{15}C: Bound State in the Continuum

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In the present investigation, a novel theoretical technique is used to calculate the low-lying $(3/2)^+$ resonance state of ^{15}C using a two-body model (^{14}C+n). Supersymmetric Quantum Mechanics (SSQM) can be used to construct an isospectral potential with a bound state in the continuum (BIC). This isospectral potential develops a deep well followed by a high barrier which can effectively trap the system giving rise to a BIC and hence facilitates the calculation of resonance energy easily and more accurately than the original shallow potential. Application of this method for the calculation of resonance energy (E_R) of the $(3/2)^+$ state of ^{15}C yields 3.555 MeV which agrees extremely well with the experimental value. The width of this state is found to be 2.201 MeV which is also in reasonable agreement with the experimental value.

107. Fourier Transform Raman Spectrum of Antithyroid Drug 2-Thiouracil

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Extensive work has been done with the structural analogues of uracil and its derivatives

and many of them have been found to exhibit interesting biological and chemotherapeutic properties. The nucleic acid bases with sulfur atom instead of oxygen have been a subject of considerable interest since they were detected in natural t RNAs. Thiouracil derivatives attract much attention because of their pharmacological activities. For example, 6-*n*-propyl-2-thiouracil is a potent antithyroid drug, fluorinated-2-thiouracil derivatives reveal antitumours and antithyroid activity, 5-cyano-2-thiouracils and their derivatives are a new class of leishmanicides. A series of 1-amino-5-substituted 4-thio or 2, 4-dithio-uracils analogues were assayed for anti-conflict and anestethic activity in rats or mice. In addition to these well known medicinal properties of thiouracils (TU), others have recently appeared e.g. as marine corrosion inhibitors for steel, or as dental adhesives in the treatment with metal surface.

In the thiouracils, 2-thiouracil(2TU) offers special importance. 2-thiouracil has been identified in t-RNA and it plays an important role in anticancer and antiviral activity. The chemotherapeutic activity of-2TU is due to its ready incorporation into the nucleic acid, impeding the melanoma tumors growth. 2-TU also induces modifications in the thyroid gland, and thus it is known as an antithyroid drug.

Structural studies of 2-TU and some thioanalogues have been reported at the semiempirical level. Tautomerisation, hydrogen bonding, solvent effect etc in 2-TU have been a subject of many rigorous *ab initio* studies. However, its complete vibrational analysis is not yet available in literature. Therefore, in the present work, FT-Raman study of antithyroid Drug 2-Thiouracil was carried out. Ab initio and density functional computations of the vibrational spectrum, the molecular geometry, the atomic charges (Mulliken Charges), the total energy , the zero point energy, the rotational constants, the room temperature entropy and dipole moment were carried out. The observed Raman wavenumbers were analysed in light of the computed vibrational spectra. The agreement between the calculated and experimental structure of 2-TU was satisfactory. The substitution of S atom in place of O atom has little effect on the molecular structure.

108. FT-IR, FT-Raman Spectra and Density Functional Computation of 2, 6-Difluorobenzonitrile

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Benzonitrile is monosubstituted benzene and is an aprotic polar solvent with a dipole moment of 4.18D and for this reason it has been extensively used in chemistry as a solvent. It has many other important uses. From the spectroscopic point of view the vibrational spectra of benzonitrile and mono- and di-substituted benzonitriles have been extensively studied . To the best of our knowledge a complete study of vibrational spectra of 2,6-difluorobenzonitrile has not been made so far. Hence, the present investigation was undertaken, to study the vibrational spectra of 2,6- difluorobenzonitrile and to identify the frequencies of different modes of vibration in this molecule.

Quantum chemical calculations were carried out using density Functional theoretical methods (DFT), including the Becke's three parameters exchange functional (B3) with the correlation functional of Lee, Yang and Parr (LYP). Several basis sets were used, starting with 6-31 G** to 6-311 ++ G (3df, pd). The basis set 6-31 G** leads to results that represent a compromise between accuracy and computational cost [2]. In the present study it is found that the two fluorine atoms only increase the ν(C ≡ N) by 10 cm^{-1} . Further, the study indicates that the bond length of C≡N bond remains almost unchanged with the substitution of F atoms on the ring at different positions.

109. FT-IR, FT-Raman Spectra and Some Molecular Properties of 2, 4-Dichlorobenzonitrile

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Keywords: *Benzonitrile, 2,4- Dichlorobenzonitrile, FTIR and FT-Raman spectra, Scale factor, Raman intensity.*

From the spectroscopy point of view benzonitrile and its mono- and disubstituted derivatives have been studied extensively (V K Rastogi et al, Indian J Pure & Appl Phys,47(2009)844;V K Rastogi et al, Indian J Phys, 84(2010)151; V K Rastogi et al, Indian J Pure & Appl Phys, 48(2010)85.]. However, a vibrational analysis on 2,4-dichlorobenzonitrile molecule has not been completely and rigousley studied yet, although its vibrational spectra have been studied earlier. Therefore, in the present investigation FTIR and FT-Raman spectra were recorded and analyzed on the basis of *ab initio* and density functional computations with complete relaxation in the potential energy surface using 6-311G (d,p) basis set.

An accurate assignment of the vibrational bands was carried out with the help of B3LYP ab initio method and a reassignment of several fundamentals was performed. The specific scale factor procedure gives rise to a more noticeable improvement on the predicted frequencies than when scaling equations are used. The nitrile stretching frequency appears at 2230 cm^{-1} in IR and at 2240 cm^{-1} in Raman in agreement with its scaled value at 2270 cm^{-1}. This frequency is highly localized within in the CN group because the potential energy distribution (PED) for this wavenumber contains contributions from the C-CN (13%) and CN (88%) stretching force constants only. Further, as reported in other benzonitriles, this stretching mode appears with the strongest Raman intensity

110. 2, 4-Difluorobenzonitrile: *Ab intio* Calculation, FT-IR and FT-Raman Spectra

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Key words: *F-T Raman spectrum,FT-IR spectrum, Cynosubstituted organic compounds, 2, 4-Difluorobenzonitrile.*

The idea of combining theoretical and experimental results for predicting vibrational wavenumbers is not new, and a variety of different approaches have been suggested and reviewed recently [Palafox M A, Rastogi V K, Mittal L, Int J Quantum Chem, 94 (2003) 189.] .The nitriles are cynosubstituted organic compounds and benzonitrile derivatives have several important applications . From the spectroscopic point of view the vibrational spectra of benzonitrile and mono- and di- substituted benzonitriles have been extensively studied. However, to the best of our information, the vibrational analysis of 2, 4-DFBN has not been completely and rigorously studied yet. Therefore, in the present work FTIR and FT-Raman spectra were recorded and analyzed on the basis of *ab initio* and density functional computations with complete relaxation in the potential energy surface using 6-311G (d,p) basis set. Geometry, vibrational frequencies, atomic charges and several thermodynamic parameters were calculated using *ab initio* quantum chemical method. Specific scale factors were also deduced and employed in the predicted frequencies.

The mid-infrared spectra of 2, 4-DFBN in the region 200-400 cm^{-1} has been recorded on Perkin Elmer FTIR model 1760 X, using KBR techniques. For the FT-IR spectra, 4 scans were collected at 4 cm^{-1} resolution. FT- Raman spectrum in the region 50- 4000 cm^{-1} was recorded on a Brukker IFS 66 optical bench with an FRA 106 Raman module attachment at room temperature. The laser power was set at 100 mW and the spectrum was recorded over 100 scans at a fixed temperature.

In general the values obtained in bond lengths and angles are very similar and they are in accordance with the microwave data and NMR results reported in the case of

benzonitrile molecule. The difference between the observed and computed wave numbers values of most of the fundamentals is very small, and therefore the assignment seems to be correct. On the basis of theoretical computations the wavenumbers 2220 and 1218 cm^{-1} correspond to ν(C≡N) and ν(C-CN) modes, respectively. The small distorsions of the benzene ring are explained in terms of the change in hybridization affected by the substituents at the carbon site to which it is appended. On the basis of vibrational analysis at B3LYP / 6-31G (d,p) and HF/6-31 G (d,p) levels several thermodynamic parameters are also calculated.

111. Optical Camouflage

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Key words: *Artificial intelligence, Living or non-living object, Optical physics, Nanotechnology.*

Mankind always sensed the milestones of science as wonders.

Desigining of things and applications that the humans may not even dream of had become the ultimate aim of the scientists and researchers. Here, I present one of such creative and awesome technology that emerged as a landmark in the field of artificial intelligence.

In this unique paper, my aim is to explain how to turn any living or non-living object invisible. This is not a magic and is made possible by the revolution in the field of optical physics. The application of augmented reality and nanotechnology are the pillars behind this concept. A new concept called retro reflection, made possible through nano technology is also demonstrated. The entire set up and the process behind this including projector, digital computer and the cloak made of weeds is elucidated very clearly by including some real life and commercial applications. Finally, we discussed the concept of head mounted displays, which made tele-conferencing an ease and also made the same person's presence at multiple places at the same time.

In a single statement, my innovative paper deals with the concept of optical camouflage, which holds the key in making a desired object or a person, look invisible and can even project a person at different places at the same time by using the fundamentals of optical physics. To be clearer, our concept delivers similar experiences to that of harry potter's individual cloak.

112. Pattern Classification Using Wavelet Fourier Descriptor and Their Recognition Using Hybrid Correlator

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Key words: *Wavelet transform, Fourier descriptor, Shape retrieval, Fingerprint classification, Hybrid correlator, Wavelet modified MACH filter*

In this paper, we report retrieval and classification of fingerprint's shape based objects employing wavelet Fourier descriptor (WFD) technique. This technique has been applied to a database consisting of different class's shapes. Very similar objects can be classified correctly by virtue of wavelet moments and its multi-resolutions properties. We have applied wavelet transform to polar-form of binary shapes of object. The Fourier transform has been taken of wavelet moments to select less number of feature vectors. The Euclidean distance has been calculated as a similarity measure parameter for fingerprint classification. To study the effect of noise on the retrieval and classification of shapes of different objects, additive and multiplicative noise of various variances were applied to the database. For retrieved shape recognition, an optical experiment employing hybrid correlator architecture has been carried out. Wavelet modified maximum average correlation hight (MACH) filter have been used for hybrid correlator.

VI. SOLID STATE PHYSICS/CONDENSED MATTER PHYSICS/THIN FILMS

113. Synthesis and Study of CdS Nanoparticles

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Keywords: *CdS, nanoparticles, Chemical synthesis, Capping agent, FTIR, Brus Equation.*

The present paper deals with synthesis of CdS nanoparticles synthesized using a chemical solution method using urea as a capping agent. This method is simple, fast and can be developed at room temperature. The obtained particles were characterized using X-ray diffraction (X-RD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR) and Ultraviolet-visible absorption spectroscopy (UV-Vis spectrum). The X-RD analysis suggested that the CdS nanoparticles were of the cubic structure. The particle size was estimated by two different methods Scherrer formula and Brus equation; and an average particle size was 26.5 nm with a good agreement between both the techniques.

114. Synthesis and Characterization of ZnO Nanoparticles

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Keywords: *Nanoparticles, Zinc Oxide, Charring, Brus equation, Chemical solution method*

This work evaluates the structural and optical properties of ZnO nanoparticles

synthesized by simple chemical solution method. The diameter of particle ranges from 20 nm to 150 nm with an average diameter of 85 nm. Addition of oxalic acid and glycol acts as shape and size controlling agents. The prepared ZnO nanoparticles are studied by X-Ray Diffraction (X-RD), Scanning electron microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR) and UV-Vis Absorption. The direct band gap energy of the ZnO nanoparticles obtained from UV-Vis spectra is of the order of 3.43 eV. This band gap energy value was further used in the Brus equation for determination of particle size, which is in good agreement with the particle size determined from X-RD pattern.

115. Degradation Study of LDPE/STARCH Composites

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Keywords: *Biodegredation, LDPE, Starch, X-RD, SEM, Thin films Microbial organisms*

1, 5, 15 & 25 wt. % starch filled LDPE thin films (20 μm) have been prepared by solution evaporation technique. For biodegradation study, soil burial technique is used. Experimental samples are characterized by X-RD and SEM. Biodegradability has been studied after 90 & 180 days by SEMs. It is observed that biodegradability increases with starch content and it is due to microbial organisms.

116. Effect of Pressure and Temperature on Elastic Properties of Mono-atomic Solids: TI-DFT Approach

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Keywords: *ElasticProperties, Mono-atomic Solids, TI-DFT,Pressure, Temperature*

We have applied the Time Independent-Density Functional Theory (TI-DFT) to investigate the effect of pressure and temperature on the elastic properties of mono-atomic solids. For this we have derived the total crystal energy in momentum space from valance electron eigen values and using thermodynamical relations we have computed the variation of elastic parameters with pressure and temperature. The computed results are well in accordance with the available experimental values. The knowledge of elastic properties and their dependence on pressure and temperature is useful for further studies related with equation of state, phase transition, structural stability, etc.

117. Synthesis and Characterization of Functionalized Graphene Sheets

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Keywords: *Graphene, Graphite oxide,Preparation, characterization, Flat monolayer*

Graphene has attracted significant interest in recent years due to its potential applications in many different areas. Graphene is defined as a flat monolayer of carbon

atoms tightly packed into a two-dimensional (2D) honeycomb lattice. Because of their novel properties, such as exceptional thermal and mechanical properties, high electrical conductivity, graphene sheets have been extensively studied in synthesizing nanocomposites and fabricating various microelectrical devices, such as field-effect transistors, ultrasensitive sensors etc. Graphene sheets with mono or few layers were synthesized by variety of techniques including micromechanical cleavage of highly ordered pyrolytic graphite, exfoliation of graphite oxide, arc discharge of graphite, chemical vapor deposition and solvothermal method. In the present investigation, functionalized graphene sheets have been synthesized by thermal exfoliation of graphite oxide. Graphite oxide is a graphite derivative with covalently attached oxygen-containing groups to its layers. The graphite oxide has been prepared by chemical treatment of graphite powder with conc. sulfuric acid, nitric acid and potassium chlorate. The functionalized graphene sheets have been synthesized by thermal exfoliation of as prepared graphite oxide. The as-prepared functionalized graphene sheets have been characterized by X-ray diffraction, scanning electron microscopy, high resolution transmission electron microscopy and Fourier transform infrared spectroscopy.

118. An Evaluation of Magnetic Field Dependence on Conduction Electron Effective mass [m*(H)/m] for Pr Metal

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Key words: *Higher-order squeezing of radiation, Sub-poissonian photon statistics, Photon-number operator, Effective mass*

In this paper, we have evaluated effective mass [$m^*(H)/m$] in the presence of magnetic field for Pr Metal, using the theoretical formulation of Nakajima, which includes the boson propagator obtained from the magnetic excitation of the self energy. By modifying the coupling of the boson propagator and taking the effect of CEF (Crystalline Electric Field), we have computed Sommerfield constant ã as a function of H. Our theoretically evaluated results were compared with the experimental data and the agreement is found very good. We have also computed [$m^*(H)/m$] as a function of H. Our theoretically evaluated values decrease with H as per experimental finding.

119. Thermoluminescence, Temperature Dependence and Isothermal Decay of $BaSrSiO_4$ Phosphor Activated with Dy and Eu

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Key words: *Thermoluminescence, Isothermal decay, BaSrSiO4, phosphor, Activator*

The basic idea involved in luminescence studies of the phosphors is to obtain some deviation from the perfect crystal structure in order to modify the output patterns which may be exploited for desired purposes. This may be obtained by structural imperfections developed during synthesis (self activated phosphors) or due to presence of small quantities of foreign impurities (impurities activated phosphors).

In the present communication the thermoluminescence studies of Barium Strontium silicates activated with Dysprosium and Europium, in various combinations of host matrix and activator concentrations are being reported. The composition of the host matrix i.e. ratios of Ba and Sr phosphors is found to have an appreciable effect.

The temperature dependence and isothermal decay studies of the same group of phosphors are also being reported which underline the effect of activator concentration and the dose of excitation. The rate of decay of phosphorescence is found to be remarkaby modified with the addition of second activator-Europium in the phosphor matrix.

Moreover, phosphor [$BaSrSiO_4$: $Dy_{0.5}Eu_{0.001}$], in particular, has been found to behave somewhat different from other members of the group.

These studies allow the theoretical interpretation of the experimental findings as they indicate the formation of different "trapping centers" and the transfer rate to these centres from the "host lattice". Such information regarding phosphors is vital and can be exploited in their industrial implications.

120. Lattice Dynamical Properties of Semiconducting Compound CdTe

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Key words: *Lattice dynamics, Phonon, Dispersion relations, Density of states, Bonding and Structural properties, Solids.*

Lattice dynamical calculations are one of the important tools in understanding the thermodynamical, structural, bonding and numerous other solid state properties. Consequently, the lattice dynamical calculations of various compounds have been widely studied by experimental techniques. The experimental techniques give quite precise information about the vibrations of phonons.

Phonons, being one of the elementary excitations of solids, provide complete information about the inter-atomic forces in solids. The inter-atomic forces are of paramount importance as their study leads to an understanding of bonding and structural properties of the compounds. All the properties depend upon constituent atoms of the crystal and can be obtained with the help of theoretical models for lattice dynamical calculations.

The semiconducting compound CdTe having zinc-blende structure is a promising candidate material for numerous experimental and theoretical investigations. Since neutron scattering experiments provide a reliable data for phonon dispersion in CdTe crystals, a considerable efforts have been made for the theoretical studies of this compound. In the present wok, lattice dynamical properties of semiconducting compound CdTe have been studied using Three-body shell model (TBSM). This model incorporates the effect of the short range repulsive interactions including the second nearest neighbors, in addition to the long range coulombic interactions in the frame work of rigid shell model. Our three-body shell model involves in total eleven disposable parameters . These parameters are two-body interaction (A, A_1 and A_2), three body interaction (γ_1, γ_2, and γ_3), electronic polarizability (α_1 and α_2), distortion polarizability (d_1 and d_2) and effective charge parameter (Z'). Using above proposed model the phonon dispersion relations, phonon density of states and the Debye characteristic temperature have been calculated and plotted for the compound CdTe. We find good agreement between theoretical and experimental results.

121. Pinned Flux Line Lattice in a Type II Superconductor

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Key words: *Pinning centre, Flux line lattice, Inhomogeneities, Type II superconductors, Deformation, Low temperature region.*

The research on type II superconductors (high and low temperature region) is much significant from technological point of view. Pinning centers arise due to in- homogeneities in a superconductor. Large and randomly arranged pinning centers cause a strong deformation of a flux line lattice so that each pinning centre acts on the lattice with a maximum force. In the present work the temperature and field force dependences are determined by the type of inhomogeneties and their sizes.

122. Analysis of Crystal Structures of Some High-Temperature Superconductors

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Key words: *Superconducting ceramic materials, Twinning, Crystal structure.*

The present paper reports some structural characteristics of YBCO and MgB_2 type superconductor compounds. The YBCO has in common the presence of copper oxide

layers, with superconductivity taking place between these layers. The more layers of CuO_2, the higher are T_c 123 compounds containing Cu-O planes and chains. The planes have an important role in the superconductivity mechanism and the chains are filled or empty "tanks of electrons", depending on the oxygen content or dopant. The crystal structure of a new binary intermetallic superconductor with a remarkably high superconducting transition temperature T_c is presented. It is complex lattice with two layers of boron and magnesium.

123. Magnetization Reversal Induced by Spin Accumulation in Ferromagnetic Transition–Metal dots

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Key words: *Magnetization, Ferromagnetic, & Transition–metal.*

In this paper, we have presented orthodox theory to study current–induced magnetization reversal in ferromagnetic quantum dots. Current–induced spin accumulation causes a free energy charge comparable to the charging energy. The free energy charge depends on the direction of the equilibrium magnetization, and the characteristic features of transition–metal electronic states. Magnetization reversal occurs when the free energy charge is comparable to the anisotropy energy, which is experimentally feasible.

124. Humidity Sensing by Polyaniline-metal Oxide Composites

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Key words: *Polyaniline-metal oxide composite, Al2O3, humidity.*

Polyaniline-metal oxide composites with 4, 8, 10, and 30% Al_2O_3 were synthesized

by traditional chemical route. XRD spectra of PANI-10% Al_2O_3 composite shows diffraction peaks at 2è values of 30.925°, 41.875° and 47.825°. The change in the resistance with relative humidity for PANI-metal oxide composites was monitored using a laboratory set-up. The resistance of the composites was seen to decrease as the of relative humidity was increased. Composite with 4% Al_2O_3 is most sensitive to humidity as compared to other composites.

125. Giant Magneto Resistance of (001) Fe/(001) Cr Magnetic Super Lattices

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Key Words: *Giant Magneto Resistance, Super Lattices, Molecular Beam*

We have studied the magneto resistance of (001)Fe/(001) Cr super lattices prepared by molecular-beam epitaxy. A huge magneto resistance is found in super lattices with thin Cr layers: For example, with t_{Cr} = 9 Å, at T = 4.2 K, the resistivity is lowered by almost a factor of 2 in a magnetic field of 2T.We ascribe this giant magneto resistance to spin-dependent transmission of the conduction electrons between Fe layers through Cr layers.

126. Computer Simulation Study of High Pressure Behavior of RbCl and RbBr Crystals

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Key words: *Computer simulation, phase transition, Many- body interactions, and Elastic constants.*

The alkali halides are well known to undergo a structural phase transformation from B1 (NaCl) to B2 (CsCl) structures between 0 .5 Gpa to 30 Gpa. No insulator to metal transition in these solids has been reported so far. Several theoretical attempts have been made by various workers to interpret the equation of states, phase transition pressures using both ab intio and model theories. With the availabilities of more precise experimental data it has been found that these theories are quite inadequate to explain the equation of states of simple ionic solids. Model calculations are performed using Born – Mayer type potential. The breathing shell models have also been not successful in finding a good agreement with the experimental results, as the correction due to electron shell deformation at high pressure has not been considered in their potential functions. In the present work, we investigate the effects of these many-body interactions on structural phase transitions and elastic constants of Rubidium Halides. In the present work, we have studied the pressure-induced structural phase transition and elastic constants at high pressure for two Rubidium Halide crystals namely RbCl and RbBr. The study is made using a model potential that includes many body interactions due to electron shell overlap. The present model potential has only one parameter and other constants have been obtained from overlap integrals. The theoretically predicted phase transition pressures and other structural properties of these solids agree reasonably well with measured data. The computer simulated structural phase transition pressures for RbCl and RbBr are 0.90 Gpa and 0.78 Gpa respectively.

127. Gupta Free Energy of Mixing of AlGa and AlGe Molten Alloys

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A theoretical investigation of the free energy of mixing of AlGa and AlGe molten alloys has been made in the framework of statistical mechanical theory. Analytical expressions for free energy of mixing depends sensitively on ordering energy 'w', coordination number 'z' and concentration 'c', have been utilized to extract microscopic structural information from the bulk thermodynamical properties. The free energy of mixing data of these alloys suggest that AlGa is a segregating system while AlGe is a weak interacting system.

128. Piezoelectric and Pyroelectric properties of PSZT Samples

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In this work we describe the piezo and pyro electric properties of the newly synthesized PSZT samples. The longitudinal piezo electric strain coefficient (d_{33}) and the transverse piezo electric strain coefficient d_{31} are estimated by using piezometer. The hydrostatic piezo electric coefficient (d_h) is calculated using the relation $d_h = d_{33} + 2d_{31} \times d_{31}$. The piezoelectric properties ($d_{33,}$ d_{31} and d_h) have been studied for PSZT (8/53/47) composition and compared with PZT(53/47), PSZT(2/53/47), PSZT(4/53/47) compositions studied earlier. Other piezoelectric coefficient (g_{33}, g_h, & $g_h d_h$) have also been studied for PZT(53/47), PSZT(2/53/47), PSZT(4/53/47), PSZT(6/53/47) and PSZT(8/53/47) composition.

The variation of pyroelectric coefficient with temperature for PZT(53/47), PSZT(2/53/47), PSZT(4/53/47), PSZT(6/53/47) and PSZT(8/53/47) compositions have been measured using a measurement cell and pyroelectric coefficient has been found to be increasing with temperature.

129. Growth and Morphological Studies of CdZnTe Thin Films

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Key words: *Thin films, CdZnTe, Electrodeposition , admium zinc telluride (CdZnTe)*

The present work deals with the electrodeposition of cadmium zinc telluride (CdZnTe) thin films and their characterization using XRD, SEM, EDAX. The electrochemical bath was made up of aqueous solutions of $CdCl_2.2H_2O$, $ZnCl_2$ and Te reacted with nitric acid for CdZnTe. Conducting tin oxide (SnO_2) layers grown on plane glass slide by a CVD method were used as substrates for the electrochemical growth of films. X-ray diffraction (XRD) studies reveal that the films are single phase with the fcc structure and the (111) orientation. Scanning electron microscopy (SEM) shows that the surface of the films is uniformly covered with grains of one micron size. Energy dispersive analysis of X-rays (EDAX) shows that the composition of the films is close to the required stoichiometry.

130. CdO Surface Modified Barium Stannic Titanate Oxide ($BaSnTiO_3$) Thick Film Resistor as a Chlorine (Cl_2) Gas Sensor

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Key words: *BaSnTiO3, thick film resistor, Perovskite, Gas sensor, dipping*

High sensitivity semiconductor oxide gas sensors are strongly needed in the fields of

environmental monitoring, bad-smelling gas detection, medical applications, and so on. In the present work the perovskite $BaSnTiO_3$ (BST) was prepared and used in form of thick film resister to sense gases in controlled ambient environment and results of pure and surface modified thick film are presented.

The perovskite $BaSnTiO_3$(BST) was prepared mechanochemically from $Ba(OH)_2$. H_2O and $SnCl_2$ and$TiCl_2$. The XRD confirms the polycrystalline single-phase perovskite phase. The films of pure $BaSnTiO_3$(BST) were prepared by simple screen printing technique. The gas sensing performance of these films was tested to various gases by using static gas sensing system at various operating temperatures. Film is then surface modified to have Cd as doped. Sintered film is then checked for gas sensing performance, and results of said thick film are presented.

131. Study of Voltage Noise in High-T_c YBCO Thin Films at Different Frequency, Temperature and Bias Current

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The study of noise in high T_c materials may give important information about the physics of the transition. Noise characteristics depend on the operating temperatures, bias current and modulation frequency. This includes the onset of several stages of transition, the inter-grain critical currents, the effect of magnetic fields, the role of inhomogenieties and other kinds of disorder and the dynamics of the vortex motion in the material. There has been considerable work on the noise related to the dynamics of vortices in an applied magnetic field. The results of the measurements of voltage noise at different frequency, temperature and bias current are discussed. Voltage noise, S_v versus temperature and bias current are presented both in normal and superconducting states and the possible governing mechanism for the noise behavior of the samples are proposed and discussed. To understand

the effect of sample quality on voltage noise, measurements were performed on sample of different phases and orientations.

132. Fabrication and Characterization of Large Area ZnO Thin Films

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Zinc oxide has attracted considerable attention these days because of its wide band gap behavior which confirms a host of potential applications in gas sensors [Nanotechnology, 21 (2010) 085502/1-085502/5.], solar cells [Crystal Research & Technolgy, 45 (2010) 292-298; Material Science & Processing, 98 (2010) 595-599.], catalysis [J. Mater. Chem., 19 (2009) 4044-4060.], organic light emitting diodes [Japanese J Appl. Phys, 48 (2009).], microelectronic devices [Japanese J Appl. Phys, 48 (2009); PCT Int. Appl. (2009); Chemistry Lett., 38 (2009) 566-567; IEEE Transducers on Electron Devices, 54 (2007) 1301-1307; Japanese J Appl. Phys, 46 (2007) 2645-2649.] particularly like electronic devices with highly non-liner current-voltage relationships called varistors [J Soc. Information Display, 13 (2005) 547-554; Appl. Phys. Lett., 92 (2008) 023506/1-023506/3; Material Transaction, 50 (2009) 1060-1066; Appl. Physics Lett., 94 (2009) 252108/1-252108/3; J Am. Ceram. Soc., 91 (2008) 3742-3745.].

In the present work different chemical methods such as chemical bath deposition (CBD), spray pyrolysis, successive ionic layer absorption and deposition, electro deposition etc. have been used to obtain ZnO films. As compared to other deposition methods, CBD has its own simplicity, reproducibility, nonhazardous, cost effectiveness, etc. The CBD method is found to be well suited for large area thin films. A procedure that improves the efficiency of CBD method during the growth of the different ZnO films is adopted. By means of this procedure, the precipitation process occurs only upon glass substrate. The structural, electrical and morphological characterization of the films with different treatment temperatures has also been done.

133. ANb_2O_6 (A=Ba, Sr) : Optical Ceramics

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Key words: *X-ray diffraction, SEM,UV-visible spectrum, Photoluminescence.*

ANb2O6 (A= Ba, Sr) ceramics are prepared through the solid state ceramic route which includes calcinations at 1175 °C and sintering at 1225 °C for 4 hr. Structure is determined by XRD analysis and surface morphology by SEM. BaNb2O6 (BNO) has orthorhombic structure and SrNb2O6 (SNO) has monoclinic structure. Optical band gap determined from UV-visible spectrum analysis is 2.85 eV for SNO. Powdered samples of BNO and SNO are excited at 435 nm and 504 nm respectively. Obtained emission spectra are analyzed and the corresponding transitions are identified. The samples can find the field of optoelectronics.

134. Effect of ZnO Doping on $Nd_{0.23}Y_{0.77}TiTaO_6$ Microwave Ceramics

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Key words: *Microwave, X-ray Diffraction, SEM Analysis, Conductance*

The ZnO doped $Nd_{0.23}Y_{0.77}TiTaO_6$ compositions are prepared through the solid state ceramic route. The samples are sintered in the range 1300 °C-1400 °C. The structural analysis is done using XRD and the surface morphology is situated using SEM. The dielectric properties of the sample are measured in the ratio and microwave frequency regions. Doping of ZnO reduced the sintering temperature (about 160°C) and increased the dielectric constant (ε_r) and the temperature coefficient of resonant frequency (τ_f). Most of the samples have high ε_r and τ_f, hence suitable for microwave applications.

VII NUCLEAR PHYSICS

135. Inelastic Scattering of Electron From Argon

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Key words: *Differential cross section (DCS), Argon, Electron atom collision, Breit-Pauli relativistic model (BPRM), Atomic collisison*

The accurate determination and understanding of electron impact induced atomic collision processes is important for a number of reasons. From the practical perspectives, the modeling of many systems of environmental and technological interest relies on the incorporation of cross section data to describe collision processes at microscopic scale. These cross section predicts reaction rates for the range of possible collision outcomes comprising elastic scattering, excitation and ionization. Thus the provision of precise cross section data is vital to these applications.

In the area of electron atom collision the electron-noble gas system has been a prime focus of study over many years.

We have computed inelastic differential cross section (DCS) of Argon by electron impact using Breit-Pauli relativistic model (BPRM) in the low energy range i.e. at 12.5 eV. The results are found in excellent agreement with available experimental measurements. The other theoretical calculation shows similar behavior with lesser magnitude. However, some discrepancies suggested that more and more theoretical as well as experimental works are required. Recently, we have presented positron impact excitation cross section (ECS) results of Argon. The detailed results of our present study will be displayed during the presentation.

136. Scattering of Positrons by Cesium Atom

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Key words: *Positron, Cesium atom, Alignment angle, Relativistic distorted wave method, Incident energy.*

In recent reports the relativistic effect in electron alkali atom scattering process have received considerable interest, particularly on the inertial electron. This effect on the atomic structure becomes more important with an increase of atomic number, i.e heavy atoms like Rb, Cs etc .This relativistic effect should explicitly be included in the scattering process [*J Phys*, B14(1981)559].The study of scattering of electron from cesium atom has been of considerable interest from the theoretical point of view as it is widely used in atomic clocks and in thermodynamic conversion in plasmas. To the best of our knowledge up till now none experiment is performed on positron cesium atom excitation. Therefore, in the present work, the observable quantities like orientation parameters and alignment angle of cesium atom excited from ground to first excited state by position impact are calculated. The energy range is 20 eV to 100 eV, but here we are presenting the results only at 20 eV incident energy. We have used relativistic distorted wave method for these calculations. The observed results are compared with distorted wave method, and found interesting features with these results. However, experimental results are required for comparison of these parameters. The detailed results will be presented at the congress venue.

137. Estimation of Natural Radioactivity in Some Soil Samples

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Key words: *Uranium, Thorium, Potassium, Radon, Soil samples, HPGe detector, Canister Technique, Gamma-rays Spectrometry.*

Natural radioactivity in soils comes from ^{238}U and ^{232}Th series and natural ^{40}K. Radon is formed from the decay of radium which in turn is formed from uranium. In the present study the soil samples have been collected from various locations of North-Eastern Haryana, India. The places are in the vicinity of Shivalik range of Himalayas. For the estimation of U, Th and K a non-destructive technique by a high resolution gamma-rays spectrometry with HPGe detector has been used. Gamma spectroscopy is based on the identification and quantification of nuclide-specific emission lines, and uses emission probabilities and detector efficiencies to relate peak area to total activity or concentration. Alpha sensitive LR-115 type II plastic track detectors have been used for measuring the radon concentration in different soil samples using "Canister Technique". Based upon the data, the mass and the surface exhalation rates of radon emanated from the samples have also been calculated. A positive correlation (0.461) between equivalent activity and the redon surface exhalation rate has been observed.

138. Analysis of Complex Fragment Emission for the Study of the Fermi Energy Domain Nuclear Collisions

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Key words: *Fermi energy, CF emission & Domain Nuclear Collisions*

In this paper, complex fragment production in the Fermi energy domain heavy ion

collisions has been studied. The physics used for the description of the various remnants produced in the entrance channel is based on fireball model taking into account the kinematic and dynamic features of the collision partners, and the decay processes are simulated by a version of the statistical binary decay model. Applications have been shown to the target-like products for reactions of copper with 24.0, 31.1, 38.5 and 46.4 MeV/u12C. Absolute comparisons with experimental data give a very well overall agreement.

139. Analysis of Complex Fragment Emission for the Study of the Fermi Energy Domain Nuclear Collisions

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Key words: *Complex fragment, Energy domain, Fermi energy domain, Nuclear Collisions, Statistical model, Compound nuclei.*

Complex fragment (CF) emission in intermediate energy nuclear reactions has been a subject of both experimental and theoretical interest for many years (*Prog Part Nucl Phys*, 21(2006)401). The process of CF emission from excited compound nuclei has been systematically studied for reactions (X + Be, C, Al) from 8.0 MeV/u upto 100 MeV/u (*Phys Rev Letts*, 51(2005)2187; *Nucl Phys*, A476(2007)516; *Nucl Phys*, A483(2003)371).

In the present work, a refined statistical model calculation has been proposed to study the mechanisms of complex fragment produced in intermediate energy nuclear collisions. As example of first application , the mass distributions measured in the reaction 24.0-46.4 MeV/u 12C with 64Cu has been examined. The excellent agreement between theoretical estimations and experiments show the common origin of the entire complex. Fragments indicate the important role of compound nuclei in intermediate energy heavy ion reactions.

140. Study of Some Heavy Ion Induced Reactions at Energy 5 to 7 MeV/A

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Key words: *Heavy ion reactions, Incomplete and complete fusion, Excitation functions, Offline gamma ray spectroscopy*

The excitation function for ^{59}Co(C, p4n) ^{66}Ge and ^{59}Co(C, áp4n) ^{62}Zn have been measured using well established activation techniques followed by offline ã-ray spectroscopy. The measured excitation functions have been compared with the theoretical predictions as obtained from statistical model codes ALICE-91, CASCADE and PACE4. The effect of variation of different parameters including level density parameter involved in these codes has also been studied. Excellent agreement was found between theoretical and experimental values in the fusion evaporation reaction channel (C, p4n). However, significant enhancement of cross section observed in á-emission channel (C, áp4n) may be due to incomplete fusion process and/ direct reaction process. To the best of our knowledge, excitation functions for these channels in the considered energy range have been reported for the first time.

141. Nuclear Isomers 90g, mZr, 89g, mZr, 89g, mY and 85g, mSr Formed by Bombardment of 89Y with Protons of Energies from 4 to 20 MeV

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Keywords: *Excitation functions, Isomeric ratio, Preequilibrium reactions*

The study of the formation of nuclear isomeric pairs in nuclear reactions may be used as an aid in the investigation of the mechanism of nuclear reactions. It will provide important information on the angular momentum transfer and coupling in nuclear reactions and production of each nucleus. Qaim et al have shown [S M Qaim, S Sud´ar and A Fessler, *Radiochim. Acta* ,93, 503 (2005)] that the isomeric cross-section ratio is primarily governed by the spins of the two levels involved, rather than their separation and excitation energies. However, the onset of pre-equilibrium emission at relatively higher incident energies may distort this smooth behavior

Keeping above facts in mind, as part of systematic study of nuclear reactions induced by light and heavy ions, in the present work we determined the isomeric population ratio of the nuclei 90g, mZr, 89g, mZr, 89g, mY, and 85g, mSr formed in reactions 89Y(p,?)90g,mZr, 89Y(p,n)89g,mZr, 89Y(p,p)89g,mY, and 89Y(p,?n)85g,mSr, respectively, for energy ranges from threshold to 20 MeV.

142. Analysis of Cosmic Ray Mass Composition at Ultra High Energies

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Detection of UHE Cosmic Rays (Ep >1017eV) provides important information on characteristics of High Energy nuclear interaction and also helps to solve astrophysical problems of Cosmic Ray origin, beyond the Greisen-Zatsepin-Kuz'min cut off (> 1020

eV). Èerenkov Radiation (CR) associated with Ultra High Energy Cosmic Rays passing through earth's atmosphere are detected using a Èerenkov detector consisting of a 5 inch photo multiplier tube (PMT, type 9792KB make EMI) to be operated in coincidence with the mini-array of Physics Department, Gauhati University, India . It is well known that the characteristics of these optical pulses are correlated with the longitudinal shower development and hence the mass composition of the primary particle. The Èerenkov detector is calibrated using Èerenkov photons produced in a tank of distilled water through which secondary cosmic rays (mainly muons) of known average flux pass. In this paper, we report Èerenkov pulse spectrum using Multi Channel Analyser (MCA) for calibration and simulated spectrum triggered by mini-array events within the energy window 1017 – 1018 eV.

143. Rotational Excitation of CO_2 by Electron Impact

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Key words: *Rotational excitation, Regional wave approximation, Differential cross section.*

We have used regional wave approximation (RWA) to calculate elastic cross section of carbon dioxide (CO_2) by electron impact, at 40 eV. The main advantage of using this method to calculate cross section is that the incident electron can be represented by plane wave in the region greater than cut off parameter. No doubt a high degree of accuracy is achieved by using regional wave approximation method. On the other hand when the present result is compared with other available experimental results, it shows a better agreement. So this method gives better results for elastic cross section scattering. However, detailed results of present study will be discussed at the congress meet.

144. Ground State Excitation of Helium by Positron Impact

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In this paper, we focus our attention and deal with positron impact excitation of n = 2 state of Helium from its ground state with the point of view of angular correlation parameter (ã) at 50 eV. To calculate this parameter, distorted wave approximation theory with different choices of distorted potential has been used. The result for 1^1S-2^1S transition is compared with available theoretical and experimental data. We found that the obtained results are quite sensitive to the choice of distortion potential used. The detailed results shall be presented at the venue of congress.

145. Higher Dimensional Cosmological Model For L –Dark Energy

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Key words: *Cosmological constant, Higher dimensional space time, Dark Matter, Theory of Gravitation*

In this paper we have obtained a set of solutions for a kinematical Λ viz, $\Lambda \propto (\dot{R}/R)^2$ by assuming the barotropic equation of state in the context of Kaluza-Klein type theory of gravitation. Some results of cosmic density Ω and deceleration parameter q have been

obtained with consideration of two-fluid structure instead of usual uni-fluid cosmological model.

VIII. PHYSICS OF NANOMATERIALS

146. Contrast and Resolution of Nanowires in Electrostatic Force Microscopy

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Key words: *Lateral resolution, Metallic nanowires, Mutual polarization, Dielectric sample, Metallic objects.*

In the present work a detailed analysis of the contrast and lateral resolution between a dc-biased tip and metallic nanowires over a dielectric sample is presented. The theoretical technique used to analyze the interaction intrinsically includes the mutual polarization between the tip- sample, and the metallic objects. We have demonstrated that a good selection of the microscope setup parameters (dielectric constant of the reference sample and tip-sample distance) can increase the contrast by more than an order of magnitude. Depending on the tip-sample distance, the contrast of a single nanowire can be highly increased using dielectric samples instead of metallic ones. In particular, the contrast can be 12 times greater for dielectric samples when $D \approx R_{tip}$. On the other hand, the dielectric constant does not have any influence in the lateral resolution. The key parameters in this case are the tip-sample distance and the tip radius. Analysing the properties of the sample, we have found a constant difference of 1 – 2 nm in the lateral resolution between spherical particles and nanowires. Although the difference can be considered small, it reduces the lateral resolution by up to 20% when the tip-sample distance is small compared to tip radius.

147. Nanocomposites – Technology Emerging trends & Applications in plastics

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Key words: *Nanocomposite, Organically Modified Layered Silicates, Plastic, Nanoscale, Polymer-filler, Intercalation.*

In the last 2-3 years one of the most significant technological breakthroughs in the plastics industry is the development of polymer nanocomposites, i.e. plastic resins reinforced with nanosize additives. In short, a shift to nanoscale fillers (i.e., polymer nanocomposites) offers the potential to improve numerous material properties with negligible negative consequences. Of particular interest is a recently developed nanocomposite technology consisting of a polymer and layered silicate. This combination often exhibits remarkably improved mechanical and various other properties when compared to pure polymers or conventional composites (both micro- and macro composites). These improvements can include high moduli, increased strength and heat resistance, decreased gas permeability and flammability, and increased biodegradability of biodegradable polymers. On the other hand, these materials have also proven to be unique model systems for the study of the structure and dynamics of polymers in confined environments, the main reason for these improved properties is interfacial interaction between matrices and organically modified layered silicates (OMLSs), as opposed to conventional composites. Layered silicates (LSs) have layer thickness in the order of 1 nm and very high aspect ratios (e.g., 10–1,000). A small weight percentage of OMLSs that are properly dispersed throughout the matrix thus creates a much larger surface area for polymer-filler interfacial interactions than do conventional composites. Although the intercalation chemistry of polymers (when mixed with appropriately modified layered silicate and synthetic layered silicates has been understood for a long time, the study of

polymer/ layered silicate (PLS) nanocomposites has recently gained greater momentum. Though significant progress has been made in developing nanocomposites with different polymer matrices, a general understanding has yet to emerge. A major challenge to further development of nanocomposites is the lack of even simple structure-property models. Without such models, progress in nanocomposites has remained largely empirical. Similarly, predicting ultimate materials properties or maximum theoretical performance for different classes of nanocomposites is almost impossible at present. This paper is intended to highlight the major developments in this area during the last decade.

148. Study of Optical Properties of CdS Nanoparticle Thin Films Doped With Polyvinylalcohoal Solution Matrix

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Key words: *CdS Nanoparticles, Thin Films, PVA, X-RD, SEM, Photocurrent, Homo-Lumo transitions.*

0.1, 0.5, 1, 2, 5 wt % CdS doped polyvinyl alcohol thin films were prepared by solution evaporation techniques. The samples were characterized by X-RD, SEM and measuring time dependence and field dependent photocurrent. The particle size was 3 to 4 nm determined by X-RD and the % crystallinity decreases with increase in concentration of CdS with PVA. Time dependence photocurrent is explained on the basis of Homo-Lumo transitions, whereas field dependence on the basis of Onasagar theory of germination of recombination of ion pairs.

149. Structural and Optical Characterization of CdMgS Nanocrystalline Film by Chemical Deposition Method

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Key words : *Nanostructures, Chemical deposition, X-ray diffraction, Absorption spectroscopy.*

In this work we report the growth of CdMgS nanocrystalline films by chemical bath deposition method using sodium citrate as complexing agent. The obtained nanocrystalline film was characterized by x-ray diffraction technique (XRD), which indicates that the film is single phase in nature. The surface morphology and average crystalline size was determined by scanning electron microscopy (SEM). The average size of particles was found to be in the range of 115 nm. EDAX analysis confirmed the presence of Cd, Mg and S. The transmission spectra, recorded in the UV visible range reveals a relatively high transmission coefficient (80%) in the obtained films.

150. Structural Phase Transitions in AIN Nanoparticles

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Key words: *Nanoparticles, Equations of state, Density Functional Theory, Group III-nitride compounds, Optoelectronic devices.*

Group III-nitride compounds have attracted increasing attention in recent years due

to their significant applications, such as optoelectronic and field emission devices. As an important candidate of these compounds, AIN has various unique properties such as excellent thermal conductivity, high chemical resistance, high melting point, wide band gap and small electron affinity, which have gained considerable interests. In the present paper we have derived the analytical expressions for bulk modulus and equation of state from the *ab-initio* pseudopotential approach to the total nano-crystal energy within the framework of local density functional formalism and have used it to analyze the phase transition of AIN nanoparticles of 45 nm in size.

151. Optical Properties of Flourescent Dye Coupled with Gold Nanoparticles

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Key words: *AuNP's, ADS560EI, Absorption, Fluorescence, Optoelectronics, Raman scattering, Nanoparticles.*

Absorption and fluorescence spectroscopy are considered to be primary research tool in Physics, Chemistry and biological sciences. During the past 20 years there has been a remarkable growth in the use of fluorescence in all branches of science, since it reveals many important photophysical properties of the molecule.

There has been dramatic growth in the use of fluorescent dye nowadays. In this paper we have investigated the optical properties of fluorescent laser dye ADS560EI (3-Ethyl-2-[3-[3-ethyl-3H-benzothiazol-2-ylidene]-1-propenyl]-benzothiazolium iodide) coupled with green gold nanoparticles (AuNP's) of size 4-12 nm. ADS560EI lasr dye is widely used in industrial applications like security printing, Lithographic printing plates and many other printing applications.

The absorption and fluorescence spectra of chosen compound with/without gold nanoparticles in alcoholic solvents were obtained using UV-Visible spectrometer of Hitachi U-3200 and USB 4000 Spectrometer, respectively. From the observed results, it is found that optical absorption and fluorescence of ADS560EI in alcoholic solvents using gold nanoparticles possess excellent enhancement in optical absorption and fluorescence. Enhancement of quantum yield depends on the size and shape of gold nanoparticles coupling to adsorbed dye.

152. Car Painting With Nanotechnology

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Key words: *Nanotechnology, Nanolength, Nanopaint, Nanocoating, Waterproof, Ohm's law.*

Nanotechnology is frequently presented as one the brightest technology of the future which is growing worldwide. Nanotechnology is the creation of materials, devices and systems by control of matter on nanolength scale (10^{-9}m) and exploitation of novel phenomenon and properties of the same. It is a study of particle size of 1 to 100 nm.These structures are known as nanostructure. Anything smaller than nm in size is just a loose atom or small molecule floating in the space as a little speck of vapour. At the nanoscale fundamental properties of material changes. For example, a nanoscale wire does not necessarily obey Ohm's law.

Nanoscale gold particles can be orange, red or greenish instead of yellow depending on their nanosize. Using nanoparticle properties, we propose the idea for change of colour of paint. Nanopaint /nanocoating give better and tighter grip on the surface. This paint is waterproof, durable and tolerant to the detergents and chemicals. In this paper we proposed technology which changes colour of car paint very easily.

153. Use of Biomass Waste Blended Cement with Laboratory Synthesized nano-SiO_2

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Keywords: *nano-SiO, Fly ash, Rice husk ash, Strength, FTIR spectra , Solid waste*

Use of industrial solid waste for cement production is environmentally friendly. This paper presents a laboratory study on the properties of 25% (Rice husk ash and Fly ash) blended cement incorporated with laboratory synthesized 5% nano-SiO_2. The results were compared with those of nano-SiO_2 free blended cement. The study indicated the significant changes and the strength increases significantly in waste blended cement incorporated with nano SiO_2.

154. Computational Study of Tunneling Field Effect Transistor Based on Graphene Nanoribbon

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Key words: *Tunneling field-effect transistors (FETs), Graphene Nanoribbon (GNR), Bandstructure, Ambipolar, Subthreshold slope*

The recently discovered graphene nanoribbon (GNR) is ideal for tunneling FETs due

to its symmetric band structure, light effective mass and monolayer-thin body. In the present investigation, we have developed the physics of p-i-n GNR tunneling FETs using three dimensonal atomistic quantum transport simulations technique. The Important role of the edge bond relaxation in the device characteristics has also been identified. It is found that the asymmetric source-drain doping or a properly designed gate can effectively suppress the ambipolar *I–V* characteristics. A subthreshold slope and a significantly improved on–off ratio can be obtained by the p-i-n GNR tunneling FETs.

155. Nano Materials: Oxide Based Diluted Magnetic Semiconductors

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Key words: *DMS, Semiconductor materials, Alloys, Spintronics applications, Ferromagnetism, Stoichiometry, Dopant.*

Diluted magnetic semiconductors (DMSs) which are alloys with magnetic elements embedded in semiconductor materials, have been extensively studied in last decade for their unique semiconducting and magnetic properties. The observation of ferromagnetism in the Mn-doped III-V semiconductor at fairly high temperatures has made DMS a promising candidate for spintronics applications. Generally, oxide semiconductors have wide band gap, i.e transparent for visible light, and can be doped heavily with n-type carrier. This feature serves an important role as transparent conductor that is used for various applications. From the viewpoint of DMS, this feature can be promising for strong ferromagnetic exchange coupling between localized spins due to carrier induced ferromagnetism, such as Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and double exchange interaction when localized spin is introduced in the oxide semiconductor. This situation prompted us to make oxide based DMS. Unfortunately, however except for a couple of favourable cases of materials systems, the promise of the field appears to have been clouded by materials issues arising from questions about dopant uniformity, defect states, and secondary phases. This has been particularly the case with most oxide-based DMS systems, because oxygen non stoichiometry during materials synthesis sensitively affects the microstate, including dopant clustering and defect formation.

156. Visible Emission from as Prepared ZnO:Ca Nanocrystals

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Key words: *Photoluminescence, ZnO, Nanoparticles, Ca doping.*

Undoped and 5, 10, & 15 at% Ca doped ZnO crystals are prepared by a wet chemical route. The particle size calculated using x-ray diffraction data in Debye-Scherer formula is obtained nearly 15 nm, showing the nanocrystalline nature of the particle. Effect of excitation wavelength on the photoluminescence emission spectra of the nanocrystals is investigated. In doped samples the peak around 459 nm is found slightly blue-shifted with excitation changing from 350 to 325 nm and then to 300 nm. The increase in dopent concentration leads to comparable PL emission in the blue and green regions although with diminished overall intensity.

157. Degradation Study of LDPE/ Starch Composites

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Key words: *Biodegredation, LDPE, Starch, X-RD, SEM*

1, 5, 15 & 25 wt. % starch filled LDPE thin films (20 μm) have been prepared by solution evaporation technique. For biodegradation study, soil burial technique is used. Experimental samples are characterized by X-RD and SEM. Biodegradability has been studied after 90 & 180 days by SEMs. It is observed that biodegradability increases with starch content and it is due to microbial organisms.

158. Mahua (Madhuca Indica) Leaf Extract: A Novel Mediator for Synthesis of Silver Nanoparticles

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Silver nanoparticles have been prepared by green chemistry route involving the chemical reduction of Ag^+ ions into Ag from $AgNO_3$ solution through Mahua leaf extract. In the present investigation the particles size and their distribution have been studied. The formation of silver nanoparticles has been confirmed by the colour change, oxidation reaction and Atomic Force Microscope images. It is found that initially the size of particles was smaller, but they grow with time, and thereafter gain uniform size and distribution. AFM images after 5 min 2h and 24 h clearly show the above. Structure of Ag nanoparticles and capping around it has also been demonstrated through Atomic Force Microscope images. Average particle size was 30-40 nm inclusive of capping of organic compounds of the extract. However, the average size of the Ag nanoparticles was only 12 nm. This is a unique behavior contradictory to the non-conventional methods. The antibacterial effect of the particles has also been recorded. Modern techniques like Atomic Force Microscope, UV visible spectrophotometer, Dynamic Light Scattering and Electrochemical Analyzer have been used for analysis of the sample solutions. Implications are discussed.

159. Ginger (Zingiber Officinale) Root Extract: A Source of Silver Nanoparticles and Their Application

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Ginger root extract has been used for chemical reduction of Ag^+ ion producing Ag nanoparticles. It is observed that chemical reduction is slow as compared to pudina or

other leaf extracts reported by other authors. The observations of non-uniform particle size in the early stages of reaction, and subsequent appearance of uniform size distribution at the later stages have been accounted for the slow reduction process of ginger root extract. 3D Atomic Force Microscope (AFM) images of Ag nanoparticles reveal hill like structures around them. Attempt has been made to explain the mechanism of formation of such particles. It is believed that polyol (oxalic/ascorbic acid) and water soluble heterocyclic components of the root extract play a key role in chemical reduction and stabilization of Ag nanoparticles respectively. Tranmission Electron Microscope (TEM) images have been used as a complementary technique to see the shape and absolute size of Ag nanoparticles. In addition, the toxic effect of Ag nanoparticles to E. coli starin has been demonstrated.

160. Synthesis and Studies of Nanocrystalline $La_{0.8}Ba_{0.2}MnO_3$ Manganite

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Key words: *Nanocrystalline, X-Ray Diffraction, Sol Gel Method, The optical Energy Band Gap, The Scanning electron microscope.*

Nanocrystalline $La_{0.8}Ba_{0.2}MnO_3$ manganite was prepared by Sol-Gel method. The broadness of XRD peaks indicates the nanocrystalline nature of the crystal and it was found to be orthorhombic-rhombohedral monoclinic with space-group R3c with average crystallite size of 81.6 nm. The scanning electron microscope (SEM) reveals that the compound is agglomerated with fine primary particles. The high temperature resistivity data were explained by using variable range hopping(VRH) mechanism. $La_{0.8}Ba_{0.2}MnO_3$ compound exhibit the insulator- metal behavior and the insulation to metal transition temperature is in the range of 357-362 K. The optical energy band gap was found to be of

the order of 3.52 eV. The larger value of the optical energy band gap as compared to bulk further confirms the nanocrystalline nature of $La_{0.8}Ba_{0.2}MnO_3$. The nanoparticles are rod shaped and more or less homogeneously dispersed.

161. Synthesis and Characterisation of Nanoparticles of Yttrium Barium Stannous Oxide by a Single Step Modified Combustion Route

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Key words: *Nano-particles, Combustion Synthesis, Optical Properties, Superconductivity, X Ray Diffraction, Thermogravimetric analysis.*

Synthesis of advanced ceramics and speciality materials as nanocrystals is one of the major fields in materials processing technology. Advantages of nanocrystalline materials are superior phase homogeneity, sinterability and microstructure leading to unique mechanical, electrical, dielectric, magnetic, optical and catalytic properties. The coarse-grained powders synthesized using the conventional solid state route have the disadvantages of larger particle size, high temperature processing and relatively lower purity. The $YBa_2SnO_{5.5}$, a high temperature polycrystalline material, developed through conventional solid-state route, has been reported in early communication. The $YBa_2SnO_{5.5}$ finds applications as substrates for high temperature superconducting materials, for their applications in microwave integrated circuits and transmission lines.

In this paper we report for the first time, synthesis of nanoparticles of $YBa_2SnO_{5.5}$ powder using a modified single-step combustion process. The $YBa_2SnO_{5.5}$ powder obtained by self sustained combustion of a precursor complex of respective metal ions is characterized by X-ray diffraction, thermogravimetric analysis, differential thermal analysis and Transmission Electron Microscopy. The particle size of the as prepared $YBa_2SnO_{5.5}$ was in the range of ~ 15 nm. Also we are first to report the photo luminescent property of the $YBa_2SnO_{5.5}$. Photo luminescent spectra of the sample show intense emission peaks. The chemical stability of $YBa_2SnO_{5.5}$ with HTS YBCO is also examined.

162. Structural and Optical Characterization of $Ba_{0.5}Sr_{0.5}MoO_4$ Nano Powder Synthesized Through an Auto-igniting Combustion Techniques

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Key words : *Nano crystalline $Ba_{0.5}Sr_{0.5}MoO_4$, X-ray diffraction (XRD) , Fourier transform infrared spectra*.

Nano crystalline $Ba_{0.5}Sr_{0.5}MoO_4$ has been synthesized through a novel single step auto-igniting combustion process. X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy analysis confirmed the formation of single phase nanocrystalline compound with a crystallite size of 22 nm as calculated using Scherrer's formula. Optical properties of the sample were studied using UV-Vis and photoluminescence spectroscopy. Photoluminescence spectrum was obtained by exciting the sample at 450nm. Our studies reveal the good luminescence properties and possible electrical applications of $Ba_{0.5}Sr_{0.5}MoO_4$ as a semiconductor.

IX. ULTRASONIC PHYSICS

163. Molecular Interaction in Binary Mixture of Poly (ethylene glycol) 200 with Ethanolamine, *m*-Cresol and Aniline at 298.15 K

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Key words: *Viscosities, velocities, refractive indices, Poly (ethylene glycol) 200, Lubricants, Protein crystallography.*

Poly ethylene glycol (PEG) is commonly used as a polar stationary phase for gas

chromatography, as a heat transfer fluid in electronic testers and in protein crystallography. PEGs are frequently used in pharmaceutical and cosmetic fluids as solvents, carriers, humectants, lubricants, binders, bases and coupling agents (*Principles of Polymer Science and Technology in Cosmetics and Personal Care; Marcel Dekker, New York, 1999*) and also for extraction, separation and purification of biological materials (*Partition of Cel Particles and Macromolecules, 3rd edn, John Wiley & Sons, 1986* ; *Polymer Applications for Biotechnology, Printice Hall,New Jersey, 1992*). Poly(ethylene glycols) are polymeric materials whose chain are composed of oxyethylene units and terminated by hydroxyl group at both ends.The thermodynamic and transport properties of polymers are especially relevant in polymer procesing and industrial applications.

In the present investigation, densities, absolute velocities, ultrasonic velocities and refractive indices of binary mixtures of poly (ethylene glycol) 200 with ethanolamine, *m*-cresol and aniline have been measured at 298.15 K and atmospheric pressure over entire composition range. The experimentally evaluated data has been used to calculate deviation in viscosity, excess molar volume, deviation in ultrasonic velocity, deviation in refractive index, deviation in isentropic compressibility, excess intermolecular free length, excess acoustical impedance and excess Gibbs free energy of activation for viscous flow. The results have been fitted to Redlich-Kister polynomial equation. The variation of these parameters with respect to the change in concentration of poly (ethylene glycol) 200 have been explained in terms of specific intermolecular and intramolecular interactions present in the mixture.

164. Thermo-acoustic Studies on Binary Liquid Mixtures of N, N Dimethylacetamide with Methanol, 1-Propanol and Water at 293, 303 and 313 K

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Key words: *Density (ρ_m), viscosity (η_m), Ultrasonic velocity (u_m) and refractive index (R_m), Gibbs **free** energy, Excess molar volume*

Molecular interaction studies on binary liquid mixtures have been one of the most important field of research. Density, viscosity, ultrasonic velocity and refractive index are

some of the important physical properties, used as a tool for binary liquid mixtures (*J Chem Eng Data*, 606(2000)45, *Fluid Phase Equib*, 17(2001)181; *Tnd J Phys*, 23(2002)76B). In recent years a considerable emphasis has been given to investigate both experimentally and theoretically excess thermodynamic properties of binary liquid mixtures to explain the nature and extent of intermolecular interaction between components of liquid mixtutres.

In the present study, the density (ρ_m), viscosity (η_m), ultrasonic velocity (u_m) and refractive index (R_m) for binary liquid mixtures of N, N-dimethylacetamide with methanol, 1-propanol and water, respectively have been measured at three temperatures (T = 293.303 and 313 K) over the entire composition range.

Using these experimental data, various excess thermodynamic properties namely excess molar volume (V_m^E), excess Gibbs free energy of activation for various flow (ΔG^{*E}), excess acoustical impedance (Z^E) and molar refraction deviation (ΔR_m) have been calculated and fitted to Redlich-Kister polynomial equation. The observed values of excess / deviation parameter were explained on the basis of strength of intermolecular interaction occurring in the components of liquid mixture. Density for all three mixtures for entire concentration range at different temperatures has also been calculated theoretically using HBT model and standard deviation in density. The study indicated that the presence of strong interaction through hydrogen bonding between unlike molecules is characterized by non-linear behavior of excess values of V_m^E, ΔG^{*E}, Z^E, and ΔR_m and parameters. The study also indicated that the interaction is strongest in DMA+ water system.

165. Estimation of Theoretical Ultrasonic Velocity in the Liquid Systems (Glucose + α-amylase) at 298.15K

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Key words: *Ultrasonic velocity, Glucose,á-amylase, Impedense dependence, aqueous amylase*

Various theoretical models have been applied to evaluate the sound velocity values

at 298.15K for the binary system of glucose with aqueous amylase and compared with the experimental values. The validity of Nomoto (NR), Van Deal-Vangeal (IMR), Impedense dependence relation (IDR), collision factor theory (CFT) and Nutsch-Kuhnkies (NK) method is cheaked and a comparative study of the above models is made. The non-ideal behavior of the systems is explained in terms of molecular interactions of the constituents of the mixture.

X. THEORY OF RELATIVITY

166. Flaws in Special Relativity

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Key words: *Special relativity, speed of light, length contraction, pions.*

Special theory of relativity is full of flaws. Some of the flaws discovered by me last year, were presented at 97th proceedings of the Indian Science Congress Association. Now, I found one more flaw in the length contraction. If length contraction is supposed right, then the sun's rays should reach the earth in no time which is impossible because the velocity of light is finite. However, it is known that the sun's rays take about eight minutes to reach the earth. Thus the special theory of relativity is wrong from this point of view also.

167. Incomplete derivation of $\Delta L=\Delta mc^2$ (or speculation of $\Delta E = \Delta mc^2$), its critical analysis; and applications of Generalized form $\Delta E = Ac^2\Delta m$

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Einstein's Sep. 1905 paper in which $\Delta L= \Delta mc^2$ (light energy –mass equation) is derived, is not completely studied; and is only valid under *handpicked* or *super—special conditions* of involved parameters. The origin of $\Delta E = \Delta mc^2$ from $\Delta L = \Delta mc^2$ is completely speculative in nature. This derivation (under general conditions) contradicts the *law of conservation of matter/energy.* In simple words it implies that when light energy is emitted then its mass must increase. The decrease in mass can be equal to L/c^2 or less or more than L/c^2.Thus self contradictions also exist in Einstein's derivation. *The factor c^2 has been arbitrarily brought in picture by Einstein.* Einstein applied binomial theorem in the end of the derivation then equation is "L = "mc^2 is obtained. If the same derivation is applied in the beginning, then result is $m_b = m_a$ i.e. no equation is obtained which involves c^2 or L. Thus conversion factor is arbitrarily brought in the picture. These are the limitations of the derivation.

Further, universe is formed? How *big bang* took place? Why universe is expanding? These fundamental questions are not explained by $\Delta E = \Delta mc^2$. An attempt has been made to explain such unanswered questions with help of mathematical model based upon $\Delta E = Ac^2\Delta m$. The universe has started its life (before Big Bang) with zeroans, this perception is consistent with NASA's Wilkinson Microwave Anisotropy Probe (WMAP) data, interpreted by Erickcek.

168. General Relativistic MHD Source Terms in 3 + 1 Form for the Gravitational Field Equations

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Key words: *Numerical MHD, General relativity, Einstein's equation, Ideal MHD.*

In this paper, the complilation of the complete set of Maxwell-Einstein-Magneto hydrodynamic equation s is done. These equations determine the self consistent evolution of a relativistic, ideal MHD fluid in a dynamical space time. Our aim is to set down a formulation of the equations that is suitable for numerical integeration in full 3+1 dimensions. Subsets of these equations have appeared elsewhere but we reconcile several seemingly different and equivalent forms of equations. Lastly we drive the MHD source terms that appear in Einstein equations. Some special features regarding this paper will be discussed at the time of presentation in congress.

XI. MISCELLANEOUS

169. Study of Thermopower of Cu-Zn Alloy at Low Temperatures

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Key words: *Metal alloys, Electron diffusion, Fermi energy, Phonon-drag and Mean free path, Thermoelectric power, Anharmonicity*

The thermoelectric power may give many necessary and useful information on the

behavior of metal and metal alloy at low temperatures, where conduction is complicated. The existing theoretical interpretation and derivation of thermoelectric power of metal and metal alloys have been separated into electron diffusion and phonon-drag components, which have many anomalies. The phonon-drag thermopower which arises due to the net anisotropy of phonon momentum transfer to conduction electrons in a temperature gradient is strongly attenuated on alloying. Since the anharmonicity of lattice wave is strong enough above the temperature $T = \theta_D/6$, where θ_D is Debye temperature, whole anomalous zone of thermopower lies between 0K to 20K. In this temperature zone anharmonicity of lattice wave may not be claimed because phonon-phonon mean free path is proportional to 1/T in this temperature zone. Thus the phonon –drag idea is unable to explain it.

We have made measurement of thermoelectric power of Cu-Zn alloy between 1K to 5K. The electron diffusion thermopower in this system has been satisfactorily explained in terms of impurity without the aid of phonon-drag effect. Thus we see that electrons are the sole contributors to the thermopower of Cu-Zn alloy at very low temperatures, where it is assumed to be effective.

170. Dielectric Properties and Electric Conductivity Studies of Some Minerals

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Some minerals viz corundum (A_2O_3), topaz [$Al_2(SiO_4)(OH,F)_2$], apatite [$(Ca_5(PO4)_3(OH,F,Cl)$], tourmaline [$Na(Fe,Mn)_3Al_6(BO_3)\ Si_6O_{18}(OH)_4$], opal ($SiO_2.nH_2O$) and talc [$Mg_6Si_8O_{20}$) $(OH)_4$] are collected from Khammam District of Andhra Pradesh, India and chemically analyzed. Although there are some studies on dielectric properties of the above mentioned minerals, a detailed study of temperature and frequency variations of dielectric constant and loss has not been carried out. Therefore, in the present investigation measurement of dielectric constant and loss of these minerals have been

carried out in the frequency range 100Hz to 100kHz at temperature ranging from room temperature to 400 ^{0}C. The room temperature measurements were extended to 10 MHz in order to obtain static dielectric constant. From the data on ε and tan δ, ac conductivity, a has been evaluated. The dc conductivity measurements have also been carried out upto a temperature of 400 ^{0}C.

171. Student's Alternative Frames About the Conceptual Dimensions of Optics Across Different Levels

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Key words: *Preconceptions, 'Misconceptions', Alternative frames and optics., Physics Education, Preconcepts, School Science*

A lot of studies have been conducted to know "How pupils learn Physics". Many research papers on this subject focus on what may be called as 'Preconceptions' and 'Misconceptions'. Preconcepts are everyday experiences, common sense theories, arrays of explanations, beliefs, naïve, world view and interactive knowledge or present status of knowledge by means of which the students make their own sense of environment they observe and experience. These have also been referred as 'Alternative Framework' (Driver 1981). During the last few decades, there has been much of interest in research studies on exploration and Misconceptions/ alternative frames of Physics among students learning physics at different levels [Physics Education (2005) 179; Physics Education (U K) 42 (2007) 516; School Science, 46 (2008) 41; Physics Education, 25 (2008) 79.]. Such studies are especially significant from the point of view of planning the teaching strategy. A study conducted on several groups of students learning physics at different levels (+2, U G I, U G II, U G III, U G IV) reveals a high level of misconceptions about understanding the conceptual dimensions of optics. Students' responses were taken by administering a tool followed by four practical activities. Analysis of the responses and transcriptions of video recorded interviews of students indicate a significant gap between the learning outcomes as expected from the curriculum given to the students and their real learning at all levels.

It is also noted that there is no significant difference amongst students at different levels. They face noteworthy difficulty with regard to applications of concepts of optics in different practical activities they performed. This may be attributed partly due to the dominance of their preconcepts on learning. It is suggested that a carefully planned system of instruction taking into consideration students' pre-concepts may help to improve the situation.

172. Semiempirical Study of Heterocyclic Molecule on Au (111) Contacts

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Keywords: *Molecular electronics, Extended Huckel theory, Non equilibrium Green's function, Quantum transport, Heterocyclic molecules*

The prime purpose of molecular electronics is to develop electronic devices since functional molecules constitute promising building blocks for future generation of nanoelectronic devices. Understanding of the fundamental processes of electron conduction through individual molecules is a most important requirement for the design of molecules for electronic functionalities. Considerable computational effect [Chem. Phys. 112(2000)1510; Chem. Phys, 125(2006)174718] have been devoted in the recent years and many devices properties have been demonstrated [Physica B 296, 72 (2001), Phys. Rev. B 66, 035322 (2002) 035322; Comp. Mat. Sci. 27, 151 (2003)]. The semi-empirical method is computationally flexible to capture several quantitative descriptions of molecules of moderate size. In the present work, we describe theoretically the electron transport properties for the model of heterocylic molecules such as pyrrole, furan and thiophene attached to two semi-infinite gold <111> electrodes using Non Equilibrium Green's

Function (NEGF) formalism [*Phys. Rev. B. Condens. Matter,* 65, (2002) 165401] coupled with the Extended Huckel Theory (EHT).

The electron transport properties of these molecular systems are affected by heterocyclic molecules and the molecule -to -electrode coupling strength. In the weak molecule-to-electrode coupling limit the conductance shows sharp peaks, while it broadened in the strong molecular coupling limit. We observed that the coupling strength yields significant variations in the behavior of I-V characteristics.

173. Dielectric Relaxation Studies of Formamide with Alcohol Mixtures by TDR

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Key words: *TDR, Amides, Alcohols, Relaxation time, The Kirkwood correlation factor, Excess dielectric constant*

Using Time Domain Reflectometry (TDR), dielectric relaxation studies have been carried out on binary mixtures of formamide with alcohols (1-butanol, 1-pentanol, 1-hexanol, 1-heptanol and 1-octanol) for various concentrations over the frequency range from 10 MHz to 10 GHz at 303 K. The Kirkwood correlation factor and excess dielectric constant properties were determined and discussed to yield information on the molecular interactions of the systems. The variation of relaxation time with the chain length of alcohols and formamide is noticed. The Bruggeman plot shows a deviation from linearity. This deviation was attributed to some sort of molecular interaction which may take place between the alcohols and substituted amides. The excess static permittivity and excess inverse relaxation time values vary from negative to positive for all the systems indicating the solute-solvent interaction to exist between alcohols and formamide for all the dynamics of the mixture.

174. Perturbation Effects on the Stability of Triangular Equilibrium Points in the Generalized Photogravitational Restricted Three Body Problem

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Key Words: *Stability/equilibrium points/Generalized/Photogravitatio-nal/RTBP, Perturbation effects, Triangular equilibrium.*

We have examined the liner stability of the triangular points photogravitational restricted three body problem when primary is a source of radiation and smaller primary is an oblate spheroid. We consider the effect of perturbation in coriolis and centrifugal force with the help of parameters α and β. We have found the triangular equilibrium points and characteristic equation of the problem. The position of triangular equilibrium points are affected by oblateness and radiation pressure force. We conclude that motion is stable for, $0 \leq \mu \geq \mu_c$ and unstable for $\mu_c \leq \mu \leq 1/2$.

175. A Study of Burgers Equations: Introduction and Applicablity

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Bihar, India

Key words: *Burgers equations, Taylor approximation and Douglas method, Numerical solutions, Weak-time dependent wave.*

In the present paper an attempt is made to give an introduction of Burgers equation, its origin and applicability in various fields and one example of weak-time dependent wave is illustrated. Numerical solutions are obtained for two problems by using restrictive Taylor approximation and it is concluded that Douglas method also performs well.

176. Study of Cost Effective Thin Film Crystalline SiliconSolar Photovoltaic Cells

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Key words: *Solar radiations, Thin films, Crystalline silicon, Monocrystalline silicon, Electrons, Holes, Electric Field.*

Solar cells based on crystalline silicon have dominated the Photovoltaic market since its birth. In crystalline silicon cells the bottom layer is doped with boron atoms to create electron- "holes" and the top layer is doped with phosphorus atoms to create excess electrons. The resulting sandwich of these two layers generates an electric field and is called a p-n junction. When solar radiation strikes the surface of the Solar Photovoltaic cell, it stimulates electrons, which are then induced by the electric field to flow through the connected electrical load. This current flow is directly proportional to the intensity of solar radiation striking the cell.

In this work we study the advantage of cost effective thin film crystalline silicon solar photovoltaic cell and show that monocrystalline silicon transfer techniques have opened an exciting avenue towards a low cost Solar Photovoltaic Cells production.

177. Analysis of Electromagnetic Scattering by PEC Cylinder at the Dielectric Rough Surface Interface

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Key words: *Dielectric rough surface, Electromagnetic (EM) scattering, Method of moments, Gaussian correlation function, Moisture content*

This paper reports the Gaussian rough surface with Gaussian correlation function which has been used to represent the statistical rough surface. Electromagnetic scattering from partially perfect electrically conducting (PEC) cylinder at the rough surface interface between two dielectric media has been analyzed for the case of TM wave incidence by applying the method of moments (MoM) with point matching. The effects of surface roughness and moisture content of the soil on the bistatic scattering cross section of the partially buried PEC objects at the rough surface interface has been investigated using the Monte Carlo procedure.

178. Analysis of Negative Magnetic Particle with Double Resonant Frequency Points

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Key words: *Magnetic **cell**, Inductor Resonant frequency, Quasi-Static Lorents theory, Permeability regioins*

In this paper, investigation has been carried out on a new structure which has double negative permeability regioins. By using a numerical code based on Quasi-Static Lorents theory, the effective permeability has been extracted and two negative permeability regions have also been observed. At the first region, the imaginary part is very small. By adding metallic rods into this double, resonant frequency structure, we can form low loss DNM materials.

179. A Study of Electromagnetic Scattering by an Object Located on a Rough Surface Using Time-Domain Integral Equations

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Key words: *TDIE, MoM-**IDFT**, &Transient Scattering.*

In this paper, some results of a numerical investigation on electromagnetic scattering by a 2-D target located on a time-evolving rough surface have been presented. The time responses of the current distributions and far-zone field have also been computed using TDIE approach. Finally, the MoM-IDFT scheme is introduced to depict the accuracy of the presented technique for the transient scattering by a complex object integrated with the rough surface.

180. Solar Desalination System Integrated with Flat Plate Solar Collector and SPV Pump for Purification of Flood Water

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Key words: *Solar energy, Desalination, Efficiency, Vacuum pressure, Regression, Photovoltaic Water Pump, Distillation System.*

In this paper we studied a solar desalination system which is made for purification of flood water. This system is very low cost and can provide 8 liters of purified water per

day. The experimental setup consists of a flat plate solar collector, a Solar Cell, a condenser, a solar photovoltaic water pump and vacuum pump. Efficiency of this system is found to vary from 15% to 25% with respect to 350 W/m^2 to 950 W/m^2. This distillation system has maximum distillate yield of 8.5 liters/day. The yield at different pressures is studied and the cost analysis is done for the case if electrical power is used in place of solar photovoltaic system. The running cost for production of purified water is as less as Rs 0.25 per litre. The purified water profile is tested and found safe for drinking.

181. Analysis of Ancient Pottery Sherds Recently excavated from Gangaikonda Cholapuram in Tamilnadu, India

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Keywords: *Archaeological pottery fragments, infra-red spectroscopy, X-ray diffractometry*

Pottery and its origins have been crucial tropes in cultural histories since ancient times. Pots and the raw materials and tools of their manufacture contributed rich imagery and metaphors for the ineffable skills of humankind. It also symbolizes a sophisticated merging of separate domains of human knowledge and experience. Therefore, the performance of a pottery clay material in relation to site and environmental conditions is essential. In this connection, the value of scientific studies is even more important for archaeological materials, because of lack of information deriving form other kinds of evidences. The specimens studied in the present work consist of three pottery fragments from an archaeological dig on Gangaikondacholapuram, Jayangondam Taluk of Perambalur District, Tamilnadu, India, dating back to about 1012-1044 CE. The samples were studied using X-ray diffractometry and FT-IR spectrophotometry. Analyses were aimed in particular to determine the most striking aspect of the finds and the difference in clay type between the sherds. The other main points investigated and discussed are related to the chemical and mineralogical composition of pottery specimens.

182. Acoustical Investigation on an Anionic Surfactant in the Presence of Builder and Fillers

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Key words: *Surfactant, builder, fillers, enzyme-lipase, acoustical parameters.*

Surfactants and builders are the two most important ingredients in laundry, household and personal-care cleaning products. They play a key role in washing processes. The enzyme lipase is coupled with three fillers in the presence of aqueous surfactant builder solutions with various concentrations. The efficiency of the detergents in the removal of dye colour has been investigated by acoustical studies. The behaviour of aqueous surfactant solutions were analysed by studying the variation of ultrasonic velocities (u) and densities (ρ). These measurements were carried out at the temperature of 303K using thermostatically controlled water bath whose temperature was maintained with an accuracy of ±0.1K. Various acoustical parameters such as adiabatic compressibility(β), free length (L_f), acoustical impedance (Z) and surface properties like surface tension(γ), surface area(Y) and molar surface energy(E) were determined and the results were discussed in terms of molecular interaction.

183. Apparent Porosity and Thermal Analysis to Determine the Firing Temperature of the Ancient Bricks Recently Excavated at Kottapuram Fort in Kerala, South India.

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Key words: *TG-DTA, Porosity and Archaeological Pottery.*

Archaeological pottery throws ample light on nature, culture and the development

of the civilization of ancient people. Promising techniques were employed to determine the firing temperature and porosity of the archeological brick samples. TG-DTA is commonly employed in research to determine the characteristics of materials. The archaeological brick shreds collected from the recently excavated archaeological site Kottapuram Fort, Kerala, South India were subjected to the apparent porosity measurement using water absorption technique and Thermal analysis using TG-DTA. The determined porosity value for the sample KTP2 is 40.51% and for the KTP3 is 29.40%. The analysis of the data obtained in the thermograph was utilized for the estimation of the firing temperature and weight loss of brick concerned. The firing temperature of the samples was determined below 800^{o}C.

184. Explicit Formulae for Computation of Averages of Ordered Operators using Wigner Function I: Single Mode Quantized Electromagnetic Field Case

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Key words: *Wigner function, Weyl ordered and s-ordered operators, higher order squeezing*

We obtain an expression for Wigner function corresponding to an arbitrary single mode quantized electromagnetic field state if the density operator is known in photon number state representation. This expression is then used to obtain explicit formulae for computation of averages of Weyl ordered operators. These results are extended to the case of s-ordered operators. Useful expressions for higher order field correlation functions, squeezing are obtained in terms of matrix elements of density operator in photon number state representation.

185. Acoustical Studies on the Ternary Mixture of Toluene + Chloroform + Cyclohexane Liquid Mixtures at 303.15, 308.15 and 313.15 K

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Key words: *Ultrasonic velocity; Organic liquids; Acoustical properties; Molecular interactions*

Ultrasonic velocity, density and viscosity of the ternary mixture of Toluene + Chloroform + Cyclohexane) were measured at 303 K. From these experimental data, various acoustical properties such as adiabatic compressibility (β), intermolecular free length (L_f), free volume (V_f), internal pressure (π_i), acoustic impedance (Z), molar sound velocity (R) and molar compressibility (W) were calculated. The results are interpreted in terms of molecular interactions occurring in the solutions.

186. Developing Innovative Practices for Concept Development of Science

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In the age of information and technology every development is incomplete without science. As I have experienced in all my 25 years teaching that teaching level of science is not satisfactory. After reading very heavy books of science the teachers and students

are also affected to negative attitude. Even today teachers teach too much facts and principles of science because they are not well versed in scientific concepts.

I have done some innovative practices to develop the understanding scientific concept in children. I have written a book "JANO TAB MANO" for supplementary reading material in Physics. In this book, I have dealt 20 concepts of physics in very simple lucid, interesting poetic and figuretic form. In this book, inertia, Newton's law, the motion of the earth, frequency of sound, jet motion, echo of the sound, motion of light etc. have been simplified causal relation of the twenty concept.

In the middle school of Madhyapradesh 1010 copies of "JANO TAB MANO" have been sent by Madhyapradesh Rajyapal to Shiksha Kendra Bhopal at 42 distinct under library scheme. Students and teachers are taking advantage of this book. Evaluators advised to send this book to National Curriculum Framework 05 in the "National Teachers Science Conference 2006" was held in Masore. Some portion of this book is included in this project.

In the direction of research wing DIET, Chhindwara and sponsored by Madhyapradesh Rajya Shiksha Kendra Bhopal, I have done an action research and my subject was- "At the middle school level students are not able to write correct chemical equations, because they do not know the symbols of elements and valency so they can not form compound".

I have done this action research with 40 students of class eighth of my school. I have developed a new method to teach chemical equations based on step by step teaching and got good result.

Facts and principles of science should be taught in very interesting and applied manner, only then students can enjoy and learn science as a subject.

187. Promoting Scientific Temper Through Cause Effect Relationship Study in Science and Other Areas of Daily Life

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Science is regarded as a body of logical, verifiable and systematic knowledge acquired through a sequence of processes. Science is characterized by its processes and skills. Basic Scientific processes and Skills consist of Observation, Measurement, Inference, Classification, Prediction and Communication. Formulating Hypotheses, Identifying Variables, Designing Investigations, Experimentation, measurement, Organizing of Data in Tables and Graphs, Describing Relationships between Variables, Analyzing Investigations and the Data and Formulating Models are some of the higher skills.

Teaching of Science is a pedagogical approach used in classrooms whereby teaching and learning is approached in the same manner as the Science itself. Science magazine [Scientific Teaching, 304 (2004) 521-522] describes scientific teaching as active learning strategies to engage students in the process of science and teaching methods that have been systematically tested to show results.

Scientific Teaching lists three major elements of science teaching [Jo Handelsman et al, Scientific Teaching (2007)]: Active learning, Assessment and Diversity.

In this presentation, it is concluded that the process approach of science is valid for every area of investigation. There exists definite similarity or resemblance between parameters of different phenomena under the process approach which provides richness to the understanding of the phenomena. A few examples from the point of view of cause-effect relationship have been cited above to highlight its importance. A process orientation of learning of a scientific phenomenon not only prepares learners construct one's own knowledge, learn to learn themselves and appreciate its application in diversified fields.

188. Analysis of Electromagnetic Wave Scattering From Slotted Conducting Wedge

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Key words: *EM scattering, Slotted conducting wedge, Mode- matching, Kontorovich- Lebedev transform, Electromagnetic Wave.*

Electromagnetic wave scattering plays significant role in electromagnetic wave propagation. Electromagnetic wave scattering from conducting wedges with slots is a canonical problem in antennas and microwave engineering. A number of studies have been performed to better understand wedge scattering characteristics, it is still of theoretical interest to derive a rigorous solution for scattering from a slotted conducting wedge. As such, we need to solve a boundary value problem of scattering from a slotted conducting wedge using the boundary conditions.

In the present work, the electromagnetic wave scattering from a slotted conducting wedge has been presented. The Kontorovich- Lebedev transform and the mode- matching were applied to obtain a convergent series solution. Computations were performed to illustrate EM scattering from slotted conducting wedges. The mode- matching formulation provides a stable and convergent series solution. Computed results agree well with other existing ones. The formulation of Kontorovich- Lebedev transform and mode- matching is very efficient for numerical computation and is expected to be useful for the study of slotted conducting wedge scattering.

189. Space Settlement-How Realistic in Our Near Future

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Key words: *Space Colonization, Centripetal & Centrifugal force, Newton's third law of motion, Corolis effect, Asteroid Mining, Low-g-Recreation, Space Tourism and Space Solar Power.*

We know where humankind is now in its limited ability to venture into space, and we can envision technologies that include routine space flight and large human populations in space; the challenge is to figure out how to get from where we are now to what we can envision. Although the technical challenges of space infrastructure development will be significant, the factors most responsible for preventing us from surmounting those challenges are politics and economics. Various rationales have been proposed by other authors and are summarized, with assessment of the hurdles involved in each. In an effort, the co-authors developed a compelling rationale for building the first community in space and the infrastructure required to support it, which passes the tests of economic necessity and political appeal.

190. A Water Lifting-Cum-Electricity Producing Non-Stop Working Machines

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A model for water lifting-cum electricity producing non-stop working machine is proposed. In this model there are 3 belts arranged on the pullies. On these belts big plates and small buckets are fixed at equal distances.The model of the machine will be displayed during presentation.

191. Unsteady Effect on MHD Free Convection and Mass Transfer Flow of Kuvshinshki Fluid Through Porous Medium With Constant Suction and Constant Heat and Mass Flux

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Key words: *Kuvshinshiki fluid, Convection, Mass transfer, Porous medium, Skin friction.*

An analysis of unsteady two-dimensional free convection and mass transfer flow of a Kuvshinshiki fluid through a porous medium bounded by a vertical infinite surface with constant Suction velocity and constant heat flux in the presence of a uniform magnetic field is presented. The effects of G_r and λ_1 with the time on the velocity, temperature, concentration distribution and skin friction are discussed with help of tables and graphs.

192. Particle Detection by Evaporation from Super Fluid Helium

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Key words: *Helium atoms, Solar Neutrinos, Particle Detection, á particles, p-p neutrinos, Compton scattering*

In this investigation we have detected helium atoms that have been evaporated from a super fluid bath by rotons excited by α particles and by recoil electrons from Compton scattering. We have measured the overall efficiency of this process and found it to be in reasonable agreement with expectations based on other experimental data. These results

provide experimental evidence upon which to base an estimate of the energy threshold for observation of solar neutrinos in a detector of sufficient mass (~ 10 tons) to have useful counting rates for *p-p* neutrinos. Such a detector might use 10^3 to 10^4 wafers. Allowing for geometric effects and for the analysis of the signals from a large numbers of wafers, it appears reasonable to expect a full detector threshold of 10 ≤ keV.

193. Computer Aided Design of Adiabatic Friction in a Nozzle for Turbomachinery and High Speed Vehicles

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**Satyabama University, Chennai, India

Key words: *Nozzle design, Computer aided design, Adiabatic friction, Green technology*

The paper describes the novel work and design and implementation of green sustainable technologies for hypersonic nozzles in hypersonic transport aircraft under design and implementation by DRDO.

194. Optical Properties of Vacuum Evaporated $CdS_{1-x}Se_x$ Thin Films

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CCS University Campus,
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Key words: *CdS thin films, Vacuum evaporated technique, Optical properties*

The optical, structural and electrical properties of the films depend upon the method of deposition and deposition parameters. In the present work we have prepared $CdS_{1-x}Se_x$

thin films by vacuum deposition technique. To study the optical properties absorption and transmission spectra of these films were taken at room temperature with the help of Hitachi Spectrometer model U-3400. The thickness of these films were measured by a spectrophotometric method using transmission spectra and thickness comes out to be 0.42 micron. Further study indicated that the refractive index and real part of dielectric constant decreases, while the extinction coefficient and imaginary part of dielectric constants increases with increase in wavelength .

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