

Proforma for information to be provided by the Teaching/ Academic/ Research Staff

1. **Name** : Ram Anjore Yadav

2. **Designation** : Professor



3. **Academic Qualifications:**

S. No.	Degree	Institution	Year	Division (% marks)
1	High School	U.P. Board, Allahabad	1972	79.0
2	Intermediate	U.P. Board, Allahabad	1974	76.6
3	B.Sc.	Banaras Hindu University	1976	76.3
4	M.Sc.	Banaras Hindu University	1978	67.9
5	Ph. D.	Banaras Hindu University	1984	-

4. **Area of Specialization: (brief write up, 200 words)**

Our current research focuses on two main areas of research

1) **Spectroscopy:** We are involved in the study of the vibrational characteristics of the following three types of molecules : (i) nucleic acid bases and their derivatives,(ii) molecules of medicinal importance and molecules of organic conductors and superconductors' classes. We study vibrational spectra experimentally using IR and Raman spectroscopy. To help analyze the IR and Raman spectra and have some more information regarding different molecular characteristics we perform ab initio and DFT computations employing the Gaussian soft-wares 03 and 09 versions. Five students have done Ph. D. in this area.

2) **Non-linear Optical Properties of Photorefractive Materials:** Photorefractive materials are very important class of materials in the sense that these offer a medium for the non-linear interaction of two or more light waves. Such interactions lead to many important applications of these materials. We have recently started working in this area and are presently involved in the study of some resonators and other related area in these materials. Two students have done Ph. D. in this area. Two students have done Ph. D. in this area.

3) **Electromagnetics and Fibre Optics:** Electromagnetics is a very important and active research area in engineering and physics. Fibre optics exploits this area for analyzing theoretically different components used in fibre optic communications. Using Maxwell's equations we have studied spherical dielectric resonators with metallic shields which protects energy from going out side the resonators. Two students have done Ph. D. in this area also.

5. **Contact Information:**

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Home: D-86 Ashokpuram Colony, Dafi (B. H. U.), Varanasi-221011
Tel: +91542-2368593

6. Projects Undertaken as PI / Co- PI:

1. UGC, New Delhi supported project on “ Vibrational study of some tri-fluoro- anilines , benzonitriles and benzoic acids” (2005-2008: ~ Rs. 5 lacs)
2. UGC, New Delhi supported project on “ Spectra and Vibrational Study of some Vitamins”(2011-2013 ~ Rs. 6 lacs)

7. Awards/ Recognitions/ Memberships if any:

- National Merit Scholarship holder from High School to M. Sc. (1972-1978)
- Gold Medal Recipient for standing first at the B. Sc. III Examination 1976 of Banaras Hindu University
- Life-Member, Laser and Spectroscopy Society of India
- Life-Member, Indian Association of Physics Teachers
- Life-Member, Indian Physics Association

8. List of 10 major Publications: (in order of importance)

1. Raman and infrared spectra and normal coordinate analysis for 1,2-di-iodo tetrafluorobenzene
R. A. Yadav, I. S. Singh and O. Sala
J. Raman Spectrosc. (G.B.) **14**,353-357 (1983).
2. Some comments on electronic and vibrational spectra and thermodynamic functions of dihalogen toluenes
R. A. Yadav
Spectrochim. Acta (G.B.) **42A**, 689-691 (1986)
3. Vibrational spectrum, force field calculations, thermodynamic functions and barrier to internal rotation for benzoyl fluoride
R. A. Yadav, R. Shanker, S. Ram and I. S. Singh
Spectrochim. Acta.(G.B.) **43A**, 901-910 (1987)
4. Raman scattering in magnetic materials
R. A. Yadav
Proc. Ind. Acad. Sci. (Chem. Sci.) **102**, 629-634 (1990)
5. Force fields for C \equiv N substituted benzenes : II. Planar and non-planar modes of the three isomeric di-cyanobenzenes
D. N. Singh, J. S. Singh and **R. A. Yadav**
J. Raman Spectrosc.(G.B.) **28**, 355-362 (1997)
6. Force field calculations and re-assignments of Raman and IR frequencies of pyrazine- N,N'-dioxide
R. A. Yadav , V Mukherjee, M Kumar and Rashmi Singh

- Spectrochim. Acta (G.B.) **66A**, 964-971(2007)
- 7 . Infrared and ab initio studies of conducting molecules: 2,5-Diamino-3,6-dichloro-1,4-benzoquinone
R. L. Prasad, A. Kushwaha, Suchita, M. Kumar and **R. A. Yadav**
Spectrochim. Acta (G.B.) Part A, **69**(2), 304-311(2008)
 - 8 Normal modes and quality factors of shielded composite dielectric spherical resonators
R. A. Yadav, T. K. Yadav, M. K. Maurya, D. P. Yadav and N. P. Singh
Ind. J. Phy. , 83(10) (2009) 1421-1438.
 9. Study of modulation instability in a temporally incoherent photorefractive ring resonator below the threshold with incoherent light
M. K. Maurya, T. K. Yadav, Ruchi Singh, **R. A. Yadav** and D. P. Singh
Opt. Comm. ,283(11) (2010) 2416-2424
 - 10 Investigation of crystal structure, vibrational characteristics and molecular conductivity of 2,3-dichloro-5,6-dicyano-p-benzoquinone
P.Rani and **R.A.Yadav**
Spectrochimica Acta Part A 137, 2015, 1334-1347
- 9. Additional Information/ Achievements:**
- Reviewer, Spectrochimica Acta Part A
 - Reviewer Vibrational Spectroscopy
 - Reviewer , J. Optical Soc. Am
 - Reviewer, *Opt.Laser Tech*
 - Reviewer, J. Mol. Struct.
 - Reviewer, J. Mol. Struct.(Theochem)
- 10. Full List of Publications:** Total number of Papers published- **99**
with details as:
(i) Spectroscopy-75 , (ii) Electromagnetics-02 and (iii) Nonlinear optical effects in photorefractive materials-22

Research Publications of Prof. R. A. Yadav

Papers Published in Journals

(A) Spectroscopy

2. Vibrational spectra of three isomeric amino benzonitriles
S. Ram, **R. A. Yadav** and J. S. Yadav
The J. Sci. Res., BHU (India) **30(1)**, 207-226 (1980-81)
3. Raman and infrared spectra of terephthalaldehyde

- R. A. Yadav**, Ramakant, P. C. Mishra and I. S. Singh
Pramana (India) **18**, 311-315 (1982)
4. Raman and infrared spectra of 1,3-bis-(trifluoromethyl) benzene
R. A. Yadav, Shyampati, N. P. Singh and I. S. Singh
Ind. J. Pure Appl. Phys. **20**, 674-676 (1982)
 5. Raman and infrared spectra of 3-fluoro trifluoromethyl benzene
R. A. Yadav and I. S. Singh
Ind. J. Pure Appl. Phys. **20**, 677-680 (1982)
 6. Raman spectrum of phthalaldehyde
R. A. Yadav and I. S. Singh
The J. Sci. Res. BHU (India) **33(2)**, 1-4 (1982-83)
 7. Raman and infrared spectra and normal coordinate analysis for 1,2-di-iodo tetrafluorobenzene
R. A. Yadav, I. S. Singh and O. Sala
J. Raman Spectrosc. (G.B.) **14**, 353-357 (1983).
 8. Vibrational spectra of o- and m-ethyl phenols
R. A. Yadav and I. S. Singh
The J. Sci. Res., BHU (India) **33(2)**, 133-144 (1982-83)
 9. Vibrational studies of o-, m- and p-trifluoromethyl benzaldehydes
R. A. Yadav and I. S. Singh
Ind. J. Phys. **58B**, 556-569 (1984).
 10. Vibrational studies of trifluoromethyl benzene derivatives: p-trifluoromethyl aniline
R. A. Yadav and I. S. Singh
Spectrochim. Acta (G.B.) **41A**, 191-197 (1985)
 10. Vibrational spectra and normal coordinate analysis for substituted trifluoromethyl benzenes
R. A. Yadav and I. S. Singh
Proc. Ind. Acad. Sci. (Chem. Sci.) **95**, 471-487 (1985)
 11. Polarized Raman and infrared spectra and vibrational analysis for α Naphthylamine
R. Shanker, **R. A. Yadav**, I. S. Singh and O. N. Singh
Pramana (India) **24**, 749-755 (1985).
 12. Normal coordinate analysis for 2,4,6-trichlorophenol
R. A. Yadav, R. Shanker and I. S. Singh
Ind. J. Pure Appl. Phys. **23**, 522-524 (1985)
 13. Polarized Raman and infrared spectra of 2-chloro, 6-methyl aniline
R. Shanker, **R. A. Yadav**, I. S. Singh and O. N. Singh
Ind. J. Pure Appl. Phys. **23**, 343-345 (1985)
 14. Hydrogen bonding in o- and m-ethyl phenols
R. A. Yadav and I. S. Singh
Ind. J. Pure Appl. Phys. **23**, 627-627 (1985)

15. Some comments on electronic and vibrational spectra and thermodynamic functions of dihalogen toluenes
R. A. Yadav
Spectrochim. Acta (G.B.) **42A**, 689-691 (1986)
16. ab initio calculations of fundamental frequencies for isomeric di-fluorobenzenes
O. P. Singh, J. S. Yadav and **R. A. Yadav**
Proc. Ind. Acad. Sci.(Chem. Sci.) **99**, 159-166 (1987)
17. Vibrational spectrum of 1,2,4,5-tetrabromobenzene
R. A. Yadav and R. Shanker
J. Raman Spectrosc.(G.B.) **18**, 555-559 (1987)
18. Vibrational spectrum, force field calculations, thermodynamic functions and barrier to internal rotation for benzoyl fluoride
R. A. Yadav, R. Shanker, S. Ram and I. S. Singh
Spectrochim. Acta.(G.B.) **43A**, 901-910 (1987)
19. Vibrational studies of biomolecules . I. 2-thio-uracil
R. A. Yadav, P. N. S. Yadav and J. S. Yadav
Proc. Ind. Acad. Sci. (Chem. Sci.) **100**, 69-78 (1988)
20. Vibrational studies of biomolecules . II. 2-thio-cytosine
R. A. Yadav, P. N. S. Yadav and J. S. Yadav
Spectrochim. Acta.(G.B.) **44A**, 1201-1206 (1988)
21. Raman scattering in magnetic materials
R. A. Yadav
Proc. Ind. Acad. Sci. (Chem. Sci.) **102**, 629-634 (1990)
22. Infrared spectrum of N-t-BOC-Alanyl-Proline
K. Singh, **R. A. Yadav** and I. S. Singh
Ind. J. Phys. **65B**, 277-282 (1991)
23. Force fields of carbonic-di-halides
K. Singh, **R. A. Yadav** and D. K. Rai
Ind. J. Phys. **65B**, 283-285 (1991)
24. Vibrational studies of bio-molecules. III. 6-thio-guanine
K. Singh, **R. A. Yadav** and J. S. Yadav
Spectrochim. Acta (G.B.) **47A**, 819-820 (1991)
25. Vibrational spectra, thermodynamic functions and barrier to internal rotation for isomeric tri-fluoromethyl benzoylchlorides
Shanker, **R. A. Yadav**, I. S. Singh and O. N. Singh
J. Raman Spectrosc.(G.B.) **23**, 141-146 (1992)
26. Force fields for benzoylchloride : I-Vibrational assignments of non-planar modes revisited
R. A. Yadav

- Spectrochim. Acta (G.B.) **49A**, 891-895 (1993)
27. Surface enhanced Raman scattering of 2-cyanopyridine adsorbed on silver colloidal particle-comment,
R. A. Yadav
Pramana (India) **40**, C415 (1993)
 28. Vibrational studies, barrier height and thermodynamic functions for biomolecules: 5-trifluoromethyl uracil
R. Shanker, **R. A. Yadav** and I. S. Singh
Spectrochim. Acta (G.B.) **50A**, 1251-1258 (1994)
 29. Direction-cosines for barrier height determination: A general formalism
R. Shanker and **R. A. Yadav**
Asian J. Phys. (India) **5**, 225-229 (1996)
 30. IR and Raman spectra, force fields, barrier heights against internal rotations and Thermodynamic functions for isomeric trifluoromethyl anilines
D. N. Singh, R. Shanker, **R. A. Yadav** and I. S. Singh
J. Raman Spectrosc.(G.B.), **27**, 177-184 (1996).
 31. Laser Raman and IR spectra and force fields for 2,6-difluorobenzonitrile
V. K. Rastogi, C. B. Arora, S . K. Singhal , D. N. Singh and **R. A. Yadav**
Spectrochim. Acta (G.B.) **53A**, 2505 (1997)
 32. Force fields for $C \equiv N$ substituted benzenes : I. Force fields for benzonitrile
D. N. Singh and **R. A. Yadav**
Asian J. Phys. (India) **6**, 369-377 (1997)
 33. Force fields for $C \equiv N$ substituted benzenes : II. Planar and non-planar modes of the three isomeric di-cyanobenzenes
D. N. Singh, J. S. Singh and **R. A. Yadav**
J. Raman Spectrosc.(G.B.) **28**, 355-362 (1997)
 34. Force fields for CHO substituted benzenes : I. Planar and non-planar modes of benzaldehyde
D. N. Singh and **R. A. Yadav**
Asian Chem. Lett.(India) **2**, 65-73 (1998).
 35. Force fields for planar and non-planar modes of fluorobenzene revisited
J. S. Singh D. N. Singh and **R. A. Yadav**
Ind. J. Pure Appl. Phys. **37**, 97-103 (1999)
 36. Force field for planar modes of fluorobenzene revisited
J. S. Singh D. N. Singh and **R. A. Yadav**
Asian J. Phys.(India) **9**, 45-50 (2000)
 37. FT-Raman spectrum and ab-initio and density functional computations of the vibrational spectrum, molecular geometry, atomic charges and some molecular properties of anti-carcinogenic drug: 5-fluorouracil

- V. K. Rastogi, C. B. Arora, **R. A. Yadav**, C. Singh and M. A. Palafox
J. Raman Spectrosc.(G.B.) **31**, 595-604(2000)
38. Laser Raman and IR spectra and force fields for 2,4-dichlorobenzonitrile
V. K. Rastogi, V. Jain, M. A. Palafox, D. N. Singh and **R. A. Yadav**
Spectrochim. Acta (G.B.) **57A**, 209-216 (2001)
39. Vibrational studies of trifluoromethyl benzene derivatives I: 2-amino-5-chloro and
2- amino-5-bromo benzotrifluorides
N. P. Singh and **R. A. Yadav**
Ind. J. Phys. **75B**(4), 347-355 (2001)
40. Vibrational spectra and force fields for 2, 3-; 2, 4-; 2, 5- and 3, 4-dihydroxy-
benzaldehydes
D.N. Singh, I. D. Singh and **R. A. Yadav**
Ind. J. Phys. (India) **76B**, 35-46 (2002)
41. Infrared and Raman spectral studies and evaluation of force fields for the three isomeric
methoxy benzaldehydes
D. N. Singh, I. D. Singh and **R. A. Yadav**
Ind. J. Phys. **76B**,307-318 (2002).
42. Vibrational studies of trifluoromethyl benzene derivatives II: 5-amino-2-fluoro and
5- amino-2-chloro benzotrifluorides
R. K. Yadav, N. P. Singh and **R. A. Yadav**
Ind. J. Phys. **77B**, 419-425(2003).
43. Vibrational spectra and force field calculations for 2-amino-5-chloro- and 2-amino-
5- bromo- benzotrifluorides
R. A. Yadav, R. K. Yadav and N. P. Singh
Spectrochim. Acta (G.B.) **64A**, 454-463(2006)
44. Force field calculations and re-assignments of Raman and IR frequencies of
pyrazine- N,N'-dioxide
R. A. Yadav , V Mukherjee, M Kumar and Rashmi Singh
Spectrochim. Acta (G.B.) **66A**, 964-971(2007)
45. Infrared and ab initio studies of conducting molecules: 2,5-Diamino-3,6-dichloro-
1,4-benzoquinone
R. L. Prasad, A. Kushwaha, Suchita, M. Kumar and **R. A. Yadav**
Spectrochim. Acta (G.B.) Part A, **69**(2), 304-311(2008)
46. Quantum chemical determination of molecular geometries and interpretation of
FTIR and Raman spectra for 2,3,4-and 2,3,6-tri-fluoro-benzonitriles
V. Mukherjee, Karunakar Singh, N. P. Singh and **R. A. Yadav**
Vib. Spectrosc., **47**(1), 26-37(2008)
47. *ab initio* determination of molecular geometries and vibrational frequencies of
CX₃ COOH (X = H, F, Cl, Br)
R. A. Yadav, M. Kumar, R. Singh, P. Singh, S. Jaiswal, G. Srivastav, R. L. Prasad

- Spectrochim. Acta (G.B.) Part A, **71**(4), 1565-1570(2008)
48. Quantum chemical determination of molecular geometries and interpretation of FTIR and Raman spectra for 2,4,5- and 3,4,5-tri-fluoro-benzonitriles
V. Mukherjee, Karunakar Singh, N. P. Singh and **R. A. Yadav**
Spectrochim. Acta (G.B.) Part A, **71**(4), 1571-1580(2008)
 49. FTIR and Raman spectra and SQM force field calculation for vibrational analysis of 2,3,4- and 2,3,6-tri-fluoro-anilines
V. Mukherjee, Karunakar Singh, N. P. Singh and **R. A. Yadav**
Spectrochim. Acta (G.B.) Part A, **73**(1), 44-53(2009)
 50. FTIR and Raman spectra, DFT and normal coordinate computations of 2,4,5- and 2,4,6-tri-fluoroanilines
V. Mukherjee, N. P. Singh and **R. A. Yadav**
Spectrochim. Acta (G.B.) Part A, **73**(2), 249-256(2009)
 51. Structural and vibrational studies of molecular conductors using quantum mechanical methods: 1,3-Dithiole-2-thione, 1,3-dithiole-2-one, 1,3-dioxole-2-one and 1,3-dioxole-2-thione
S. Jaiswal, A. Kushwaha, R. Prasad, R. L. Prasad and **R. A. Yadav**
Spectrochim. Acta (G.B.) Part A, **74**(1),16-25(2009)
 52. Energetics and structural insights of molecular conductors using density functional theory methods : 1,3-dithiole-2-thione, 1,3-dithiole-2-one, 1,3-dioxole-2-one and 1,3-dioxole-2-thione
R. L. Prasad, A. Kushwaha, Rajendra Prasad, S. Jaiswal and **R. A. Yadav**
J. Theo. Comp. Chem., **8**(6), 1485-1495 (2009)
 53. Experimental and calculation aspects of vibrational spectra and optimized geometry of 2,3,4-tri-fluoro-benzoic acid dimer
V. Mukherjee, N. P. Singh and **R. A. Yadav**
Spectrochim. Acta (G.B.) Part A, **74** (5),1107-1114(2009)
 54. FTIR and Raman spectra, DFT and SQMFF calculations for geometrical interpretation and vibrational analysis of some trifluorobenzoic acid dimers
V. Mukherjee, N.P. Singh and **R. A. Yadav**
Vib. Spectrosc., **52**(2), 163-172 (2010)
 55. DFT study of molecular geometries and vibrational characteristics of uracil and its thio-derivatives and their radical cations
R. Singh, S. Jaiswal, M. Kumar, P. Singh, G. Srivastav and **R. A. Yadav**
Spectrochim. Acta(G.B.) Part A, **75**(1), 267-276 (2010)
 56. *ab initio* studies of molecular structures, conformers and vibrational spectra of heterocyclic organics: I. Nicotinamide and its N-oxide
M. Kumar, S. Jaiswal, R. Singh, G. Srivastav, P. Singh, T. N. Yadav and **R. A. Yadav**
Spectrochimica Acta(G.B.) Part A, **75**(1),281-292(2010)

57. ab initio Determination of Geometries and Vibrational Characteristics of Building Blocks of Organic Superconductors: 4,5-ethylenedithio-1,3-dithiole-2-thione, and 4,5-ethylenedithio-1,3-dithiole-2-one
S. Jaiswal, Deepshikha Singh, R.L. Prasad and **R.A. Yadav**
Spectrochimica Acta(G.B.) Part A, **76**(3-4),297-310(2010)
58. Vibrational study on the molecular structure of 1,4-naphthoquinone and 2- methyl-1,4-naphthoquinone and their radical anions by using density functional theory.
Priyanka Singh, N.P. Singh and **R.A.Yadav**
J. Chem.. Pharmacy. Res. 2(2010) 199-224
59. Study of the optimized molecular structures and vibrational characteristics of neutral L-Ascorbic acid and its anion and cation using density functional theory
J. Chem.. Pharmacy. Res. 2(2010) 656-681
Priyanka Singh, N.P. Singh and **R.A.Yadav**
60. FTIR and Raman spectra and optimized geometry of 2,3,6-tri-fluorobenzoic acid dimer: A DFT and SQMFF study
V. Mukherjee, N.P. Singh, R.A. Yadav
Spectrochimica Acta Part A **77**(4), 787-794 (2010)
61. Quantum mechanical studies of conformers, molecular structures and vibrational characteristics of heterocyclic organics: Nicotinic acid and 2- fluoronicotinic acid
Priyanka Singh, N.P. Singh and **R.A.Yadav**
J. chem.. pharmacy. Res. (2011)
62. Comparative structural and vibrational studies of 6-amino purine (Guanine) and its radical species using density functional theory.
Rashmi Singh, M.Kumar,, P.Singh, and **R.A.Yadav**
J. Chem.. Pharmacy. Res. 3 (2011) 25-37
63. Experimental IR and Raman Spectra and quantum chemical studies of molecular structures, conformers and vibrational characteristics of L- ascorbic acid and its anion and cation.
R.A.Yadav, Poonam Rani, Priyanka Singh, M Kumar, R.Singh, N.P.Singh
Spectrochim Acta 84(2011)6-21.
64. Experimental IR and Raman Spectra and quantum chemical studies of molecular structures, conformers and vibrational characteristics of nicotinic acid and its N-oxide.
M.Kumar, **R.A.Yadav**
Spectrochim Acta 79(2011) 1316–1325
65. Optimized geometry and vibrational spectra and NBO analysis of solid state 2,4,6 - tri-fluorobenzoic acid hydrogen bonded dimer
V. Mukherjee, N.P. Singh, **R.A. Yadav**
Journal of Molecular Structure, Volume 988, Issues 1-3, 24-34 (2011)
66. Vibrational studies and electron-molecular vibrational coupling of tetrafluorotetracyanoquinodimethane

P. Rani , R.A. Yadav

Bulletin of Laser and Spectroscopy Society of India, ISSN:2229-3752; Special issue dedicated to late Prof. D. K. Rai, 19, 97-112(2011-2012)

- 67 *ab initio* determination of geometries and vibrational characteristics of building blocks of organic super-conductors: TTF and its derivatives
P. Rani, R.A. Yadav
Spectrochimica Acta Part A, 99, 2012, 303-315
- 68 DFT study of vibrational spectra of 2-(2-hydroxyphenyl) Benzothiazole
U. Pandey, R. P. Singh, M. Srivastava, R. A. Yadav
Bulletin of Laser and Spectroscopy Society of India, ISSN:2229-3752; Special issue dedicated to late Prof. A. N. Singh, 20, 57-70(2012-2013)
- 69 Vibrational studies of benzene, pyridine, pyridine-N-oxide and their cations
M. Kumar, Mayuri Srivastava, R.A. Yadav
Spectrochimica Acta Part A, 111, 2013, 242-251
- 70 Experimental and theoretical studies of vibrational spectrum and molecular structure and related properties of pyridoxine (vitamin B6)
Mayuri Srivastava, P. Rani, N.P. Singh, R.A. Yadav
Spectrochimica Acta Part A 120, 2014, 274-286
71. Experimental Raman and IR spectral and theoretical studies of vibrational spectrum and molecular structure of Pantothenic acid (vitamin B5)
Mayuri Srivastava, N.P.Singh, and R.A.Yadav
Spectrochimica Acta Part A 129, 2014, 131-142
72. Synthesis, characterization and quantum chemical investigation of molecular structure and vibrational spectra of 2,5-dichloro-3,6-bis-(methylamino)1,4-benzoquinone
B. P. S. Gautam, Mayuri Srivastava, R. L. Prasad and R.A. Yadav
Spectrochimica Acta Part A 129, 2014, 241-254
73. DFT Study of Conformational and Vibrational Characteristics of 2-(2-Hydroxyphenyl) Benzothiazole Molecule
Urmila Pandey, Mayuri Srivastava, R.P.Singh and R.A.Yadav
Spectrochimica Acta Part A 129, 2014, 61-73
74. Raman and IR studies and DFT calculations of the vibrational Spectra of 2, 4-Dithiouracil and its cation and anion
R. Singh and R. A. Yadav
Spectrochimica Acta Part A 130, 2014, 188-197
75. Investigation of crystal structure, vibrational characteristics and molecular conductivity of 2,3-dichloro-5,6-dicyno-p-benzoquinone
P.Rani and R.A.Yadav
Spectrochimica Acta Part A 137, 2015, 1334-1347

(B) Electromagnetics

1. Normal modes and quality factors of homogeneous isotropic spherical

dielectric resonators : I- shielded dielectric sphere.

I. D. Singh and **R. A. Yadav**

Pramana (India) **62**,1255-1271(2004)

2. Normal modes and quality factors of shielded composite dielectric spherical resonators

R. A. Yadav, T. K. Yadav, M. K. Maurya, D. P. Yadav and N. P. Singh

Ind. J. Phy. , **83(10)** (2009) 1421-1438.

(C) Non-linear Optical Effects in Photorefractive Materials

1. Dependence of gain and phase-shift on crystal parameters and pump intensity in unidirectional photorefractive ring resonators
M. K. Maurya, T. K. Yadav and **R. A. Yadav**
Pramana, J. of Phy., **72 (4)** (2009) 709-726
2. Oscillation dependence of two-wave mixing gain for unidirectional ring resonator in photorefractive materials
M. K. Maurya, T. K. Yadav and **R. A. Yadav**
Opt. Laser Tech., **42(3)** (2010) 465-476
3. Minimization of the fluctuation in the signal beam intensity of a nonlinear optical medium with a transmission grating
M. K. Maurya, T. K. Yadav and **R. A. Yadav**
Opt. Laser Tech. **42(5)** (2010)775-782
4. Study of modulation instability in a temporally incoherent photorefractive ring resonator below the threshold with incoherent light
M. K. Maurya, T. K. Yadav, Ruchi Singh, **R. A. Yadav** and D. P. Singh
Opt. Comm. ,**283(11)** (2010) 2416-2424
5. Feedback method of the noise suppression in wave-mixing amplifiers based on non-linear materials with photorefractive response in a reflection grating configuration
M.K. Maurya, **R.A. Yadav**
Opt. Comm, **283(12)** (2010) 2615-2621
6. Effect of photoconductivity and dielectric constant of the photorefractive materials on two-beam coupling gain and phase-shifts for a single unidirectional photorefractive ring resonator
M.K. Maurya , **R.A. Yadav**
Opt. Laser Tech., **42(6)** (2010) 883-893
7. Oscillation characteristics of a coupled unidirectional ring resonators with Photorefractive crystals
M.K. Maurya, T.K. Yadav, Dheerendra Yadav and **R.A. Yadav**
Opt. Laser Tech., **43(7)** (2011) 1041-1053
8. Effect of photoconductivity and oscillation frequency shift on the signal beam intensity in two beam coupling in photorefractive materials
T. K. Yadav, M. K. Maurya, and **R.A. Yadav**

Optik **122** (2011) 1607-1614.

9. Dependence of space charge field and gain coefficient on the applied electric field in photorefractive materials
Ruchi Singh, M. K. Maurya, T. K. Yadav, **R. A. Yadav** and D. P. Singh
Opt. Laser Tech., **43(1)** (2011) 95-101
11. Luminescence and second harmonic generation in $\text{Eu}^{3+}/\text{Eu}^{2+}$ embedded B_2O_3 :
 LiNbO_3 non-linear glass-ceramics.
T. K. Yadav, A.K.Singh, K.Kumar and **R.A. Yadav**
Optical material, **33** (2011) 1732–1736
12. Dynamic study of the gain in two beam coupling in photorefractive materials
T. K. Yadav, M. K. Maurya, and **R.A. Yadav**
Optik, **123** (2012) 1329–1335.
13. Pattern formation in a passive incoherent ring resonator system based on nonlinear material with the self-focusing non-instantaneous Kerr response
M.K. Maurya, R.A. Yadav
Optics & Laser Technology, **44** (2012) 505-513
14. Study of photoconductive and dielectric dependence of gain and phase-shift in the coupled unidirectional ring resonators based on non-degenerate wave-mixing in photorefractive materials
M.K. Maurya, R.A. Yadav
Optics & Laser Technology, **44** (2012) 1191-1202
15. Enhancement of the diffraction efficiency of the hologram recorded in photorefractive media under the action of external electric field.
T. K. Yadav, M. K. Maurya, and **R.A. Yadav**
Optik, **123** (2012) 1120–1127.
16. Frequency detuning dependence of oscillation condition for a semilinear photorefractive optical resonator in a photorefractive material with reflection gratings
M.K. Maurya, R.A. Yadav
Optik, **123** (2012) 1260-1270
17. Theoretical analysis of the effects of frequency detuning dependence of photorefractive two-beam coupling coefficient on gain and phase-shifts of the signal beam for a coupled unidirectional photorefractive ring resonator
M.K. Maurya, R.A. Yadav
Optik, **124** (2013) 313-323
18. Theoretical study of properties of BaTiO_3 material with grating spacing and light intensity
Ruchi Singh, D.P. Singh, R.A. Yadav
Optik, **124** (2013) 466-469
19. Photovoltaic dependence of photorefractive grating on the externally applied dc electric field
M.K. Maurya, R.A. Yadav
Optics & Laser Technology, **47** (2013) 10-21
20. Two wave mixing in nonlinear Kerr medium and its dependence on photoconductivity

and dielectric properties of the medium.
T. K. Yadav, M. K. Maurya, and **R.A. Yadav**
Optik, **124** (2013) 876–882.

21. Effect of grating spacing on response time and sensitivity In photorefractive materials at large modulation depth
Ruchi Singh, D. P. Singh, and R. A. Yadav
Journal of Russian Laser Research, **34** (2) (2013) 185-191
22. Comparative study of signal to noise ratio and gain in photorefractive materials
Ruchi Singh, R.A. Yadav and D. P. Singh
Journal of Russian Laser Research, **34** (6) (2013) 509-514

18. Conferences/ Seminars/Symposia/Proceeding Abstracts

More than 40 abstracts (1/2 to 1 page) and extended abstracts (2 pages) included in the proceedings of different Indian and foreign conferences / seminars / symposia

1. . Thermodynamic properties of pentafluorobenzenes;
Proc. Conf. Thermal Systems, Dept. Mech. Engg., BHU 235-251(1986)
R.A. Yadav, O.N.Singh and R.Shanker
2. Thermodynamic function of benzoylfluoride
Proc. Conf. Thermal Systems, Dept. Mech. Engg., BHU 262-2661(1986)
R.A. Yadav, O.N.Singh and R.Shanker
3. Thermodynamic function of benzoylfluoride
Proc. Conf. Thermal Systems, Dept. Mech. Engg., BHU 262-2661(1986)
R.A. Yadav, O.N.Singh and R.Shanker
4. Normal modes of pentachlorobenzene
Proc. ICORS-X, Chem.Phys. Inst., Univ.Oregon(USA) 31 Aug- 5 Sept.,(1986)
R.A. Yadav and R.Shanker
5. Vibrational studies of biomolecules. II-2-thiocytosine
Proc. ICORS-XI, Chem.Phys. Inst., Univ.Oregon(USA) 31 Aug- 5 Sept.,(1986)
R.A. Yadav, P.N.S.Yadav and J.S.Yadav.
6. Doublet structure of carbonyl stretching in benzaldehyde and its derivatives;
Proc. ICORS-XI. Inst.,learning Univ.London(England) Sept 5-9.,(1988)
R.A. Yadav, P.N.S.Yadav and J.S.Yadav.
7. Aldehyde internal modes in benzaldehyde and its derivatives
Proc. ICORS-XII, Colllege of Sci. and Math, Univ. South Carolina(USA) 206-207(1990)
R.A.Yadav
8. The assignments of ν_1 and ν_{12} in substituted benzenes;

Proc. ICORS-XII, College of Sci. and Math, Univ. South Carolina(USA)
206-207(1990)

R.A.Yadav

9. Assignments of C=O bending modes in uracil derivatives;
Proc. ICORS-XIII, Univ. of Wurzburg, Germany. Aug. 31- Sept.4,(1992)
R.A.Yadav, R.Shanker
10. Force field for benzoylchloride – II vibrational assignments of planar modes revisited;
Proc. ICORS-XIII, The Honk Kong Univ. of Sci. and Tech., Hong Kong, 22-26 Aug., 1994, p-159(1994)
R.A.Yadav
11. IR spectrum of 4-amino, 2,6, -dihydroxy pyrimidine;
Proc. NCONS 97, 10-12 Feb., Chennai, p-159(1997)
R.A.Yadav, D.N.Singh, J.S.Singh, R.Shanker
12. IR spectrum of 4-amino, 2,4-dihydroxy -6-methyl pyrimidine;
Proc. NCONS 97, 10-12 Feb., Chennai, p-160(1997)
R.A.Yadav, D.N.Singh, J.S.Singh, R.Shanker
13. Force field for planar modes of fluorobenzene;
Proc. Nat. Conf. Mol. Spectr., Gorakhpur (1997)
R.A.Yadav, D.N.Singh and J.S.Singh
14. Laser Raman and IR spectra , force fields and the thermodynamic functions for 2,3- dihydroxy benzaldehyde;
Proc. NLS Dec. 14-16 (1998)
R.A.Yadav and D.N.Singh
15. Force field for non planar modes of fluorobenzene;
Proc. Nat. Conf. Mol. Spectr., Merrut, (1998)
R.A.Yadav, D.N.Singh and J.S.Singh
16. Normal modes of shielded spherical dielectric cell resonators;
Proc. Natl. Laser Symp. NLS-2003 , I.I.T Kharagpur,2003
D.P.Yadav, N.P.Singh and **R.A.Yadav**
17. Theoretical Study of IR and Raman Spectra of 5-Hydroxy Uracil
Rashmi Singh, M. Kumar,**R.A Yadav**, EUCMOS 2008, Molecular Structure p-33
18. Quantum Mechanical Studies, Molecular Structures and Vibrational Characteristics of the Amino Acid (L - Valine)
M. Kumar ,**R. A. Yadav**, AIP Conf. Proc. 1267(2010) 678-678, XXII INTERNATIONAL CONFERENCE ON RAMAN SPECTROSCOPY, Date: 8–10 August 2010 ,Location: Boston (MA)
19. R. Singh, M. Kumar, S. Jaiswal, P. Singh, G. Srivastav and **R. A. Yadav** “
DFT

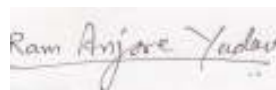
analysis of DTU and its radicals” 2nd one day conference on New Trends in Research - 2009, BHU Varanasi.

20. R. Singh, S. Jaiswal, M. Kumar, P. Singh, G. Srivastav and **R. A. Yadav** “Vibrational assignments with help of DFT calculations of Cytosine and Thiocytosine” National Symposium on Advances in Lasers and Spectroscopy - 2009, Dr. H. S. Gour University, Sagar.
21. R. Singh, M. Kumar and **R A Yadav** ” Vibrational spectra for uracile and its derivatives” 1st one day conference on new trends in research-2008, BHU, varanasi-221005.
22. R. Singh, M. Kumar and **R. A. Yadav**” Vibrational spectra of uracil and dithiouracil”2nd international conferences on perspective in vibrational spectroscopy (ICOPVS 2008) Mar Invanios college trivandrum.
23. R. Singh, S. Jaiswal, M. Kumar, P. Singh, G. Srivastav and R. A. Yadav “DFT study of Molecular geometries and vibrational characteristics of Uracil and its radical cation” MMSELTLA - 2009, University of Allahabad, Allahabad.
24. R. Singh, M. Kumar and **R. A. Yadav** ”Vibrational studies of 5-halo-uracil: 5- bromo- uracil” First Indo-US workshop on spectroscopy: Future trends in spectroscopy application to national security, organized by Dept of Phys. BHU (India) & Mississippi State University (USA) Jan. 9- 11 (2006) p-32. Vibrational studies of 5-halo-uraciles: 5- bromo- uracil
25. M. Kumar, Rashmi Singh and **R. A. Yadav**
First Indo-US workshop on spectroscopy:Future trends in spectroscopy application to national security, organized by Dept of Phys. BHU (India) & Mississippi State University(USA) Jan. 9- 11(2006) p-32
26. vibrational spectra for uracile and its derivatives
R. Singh, M. Kumar and **R A Yadav**
1st one day conference on new trends in research, BHU, Varanasi-221005, 24-28 Feb. 2008
27. Vibrational spectra of 2-thiouracil and dithiouracile
M. Kumar, R. Singh and **R. A. Yadav**
2nd international conferences on perspective in vibrational spectroscopy (ICOPVS 2008)
24-28 Feb, 2008, Mar Invanios college Trivandrum, Kerla, India
28. Vibrational spectra of uracile and dithiouracile
R. Singh, M. Kumar and **R. A. Yadav**
2nd international conferences on perspective in vibrational spectroscopy (ICOPVS 2008) 24-28 Feb, 2008, Mar Invanios college Trivandrum, Kerla, India
29. ab initio studies on structure and vibrational spectra of the Vitamin B₁₃ and its radical anion.
P. Singh, G. Srivastav, S. Jaiswal, R. Singh, M. Kumar and **R. A. Yadav**.

2nd one day conference on New Trends in Research - 2009, 17-01-2009,
Department of Physics, BHU Varanasi.

30. Theoretical vibrational spectroscopic study of Sulfanilamide.
G. Srivastav, P. Singh, R. Singh, M. Kumar, S. Jaiswal and **R. A. Yadav**.
National Symposium on Advances in Lasers and Spectroscopy - 2009,
27-28 Feb. 2009, Dr. H. S. Gour University, Sagar.
31. Molecular structure and vibrational spectra of Menadione : band
assignments based on density functional calculations.
P. Singh, G. Srivastav, R. Singh, M. Kumar, S. Jaiswal and **R. A. Yadav**.
National Symposium on Advances in Lasers and Spectroscopy - 2009,
27-28 Feb. 2009, Dr. H. S. Gour University, Sagar
32. Effect of applied electric field and grating spacing on performance of ring
Resonator International Conference on Material Science and Technology-2012
Ruchi Singh, D P Singh and **R A Yadav**
IOP Conf. Proc. (to be communicated).
33. Theoretical study of SNR in photorefractive materials
Ruchi Singh, D. P. Singh, and **R. A. Yadav**
AIP Conf. Proc. 1536, 709 (2013); doi: 10.1063/1.4810424

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Place: Banaras Hindu University



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