

## REFERENCES

- [1] Ledesma, AE, Contreras, C, Svoboda, J, Vektariane, A & Brandan, SA 2010, 'Theoretical structures and experimental vibrational spectra of isomeric benzofused thieno [3,2-b] furan compounds', *Journal of Molecular Structure*, vol. 967, no.1-3, pp. 159-165.
- [2] Basoglu, A, Avci, D, Atalay, Y, Celik, F & Sahinbas, T 2011, 'Theoretical studies on molecular structure and vibrational spectra of 8-hydroxyquinolinium picrate', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 79, no. 5, pp. 1425-1429.
- [3] Kurt, M, Chinna Babu, P, Sundaraganesan, N, Cinar, M & Karabacak, M 2011, 'Molecular structure, vibrational, UV and NBO analysis of 4-chloro-7-nitrobenzofurazan by DFT calculations', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 79, no. 5, pp. 1162-1170.
- [4] Arivazhagan, M & Jeyavijayan, S 2011, 'Vibrational spectroscopic, first-order hyperpolarizability and HOMO, LUMO studies of 1,2-dichloro-4-nitrobenzene based on Hartree-Fock and DFT calculations', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 79, no. 2, pp. 376-383.
- [5] Ramalingam, S, Jayaprakash, A, Mohan, S & Karabacak, M 2011, 'Vibrational investigation on FT-IR and FT-Raman spectra, IR intensity, Raman activity, peak resemblance, ideal estimation, standard deviation of computed frequencies analyses and electronic structure on 3-methyl-1,2-butadiene using HF and DFT (LSDA/B3LYP/B3PW91) calculations', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 82, no. 1, pp. 79-90.
- [6] Yildirim, G, Senol, SD, Dogruer, M, Ozturk, O, Senol, A, Tasci, AT & Terzioglu, C 2012, 'Theoretical investigations of  $\alpha,\alpha,\alpha$ -trifluoro-3, -p and o-nitrotoluene by means of density functional theory', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 85, no. 1, pp. 271-282.

- [7] Xiao-Hong Li, Rui-Zhou Zhang & Xian-Zhou Zhang 2009, 'Natural bond orbital analysis of some *para*-substituted *N*-nitrosoacetanilide biological molecules', *Structural Chemistry*, vol. 20, no. 6, pp. 1049-1054.
- [8] Mehmet Karabacak, Leena Sinha, Onkar Prasad, Zeliha Cinar & Mehmet Cinar 2012, 'The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMO-LUMO analysis of monomeric and dimeric structures of 4-chloro-3,5-dinitrobenzoic acid', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 93, pp. 33-46.
- [9] Muthu, S & Isac Paulraj, E 2012, 'Molecular structure, vibrational spectra, first order hyper polarizability, NBO and HOMO-LUMO analysis of 4-amino-3(4-chlorophenyl) butanoic acid', *Solid State Sciences*, vol.14, no. 4, pp. 476-487.
- [10] Paulo, JA Ribeiro-Claro, Michael GB Drew & Vitor Felix 2002, 'C–H...O bonded dimers in 2-methoxy-benzaldehyde studied by X-ray crystallography, vibrational spectroscopy, and ab initio calculations', *Chemical Physics Letters*, vol. 356, no. 3-4, pp.318-324.
- [11] Jayashree Yenagi, Anita Shettar & Tonannavar, J 2012, 'On the anomalous vibration spectra and O–H...N bond dictated structure of 3-fluoroisonicotinic acid', *Vibrational Spectroscopy*, vol. 63, pp. 342-349.
- [12] Mehmet Karabacak, Mehmet Cinar, Sahin Ermec & Mustafa Kurt 2009, 'Experimental vibrational spectra (Raman, infrared) and DFT calculations on monomeric and dimeric structures of 2- and 6-bromonicotinic acid', *Journal of Raman Spectroscopy*, vol. 41, no. 1, pp. 2386-.2393.
- [13] Sebastian, S, Sundaraganesan, N & Manoharan, S 2009, 'Molecular structure, spectroscopic studies and first-order molecular hyperpolarizabilities of ferulic acid by density functional study', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 74, no. 2, pp. 312-323.
- [14] Epstein, LM, Shubina, ES, Ashkinadze, LD & Kazitsyna, LA 1982, 'Nitro group vibrations in spectra of nitroaromatic compounds with donor substituents', *Spectrochimica Acta*, vol. 38A, no. 3, pp. 317-322.

- [15] Sangeetha, V, Govindarajan, M, Kanagathara, N, Marchewka, MK, Gunasekaran, S & Anbalagan, G 2014, 'Vibrational, DFT, thermal and dielectric studies on 3-nitrophenol-1,3,5-triazine-2,4,6-triamine (2/1)', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 118, pp. 1025-1037.
- [16] Agnieszka J. Abkowicz-Bienko, Zdzislaw Latajka, Dariusz C. Bienko & Danuta Michalska 1999, 'Theoretical infrared spectrum and revised assignment for *para*-nitrophenol. Density functional theory studies', *Chemical Physics*, vol. 250, no. 2, pp. 123-129.
- [17] Attila Kovacs, Vladislav Izvekov, Gabor Keresztury & Gabor Pongor 1998, 'Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study', *Chemical Physics*, vol. 238, no. 2, pp. 231-243.
- [18] Jianbo Zeng, Ji Qi, Fuquan Bai, Jorn Chi Chung Yu & Wei-Chuan Shih 2014, 'Analysis of ethyl and methyl centralite vibrational spectra for mapping organic gunshot residues', *Analyst*, vol. 139, no. 17, pp. 4270-4278.
- [19] Badawi, HM & Forner, W 2012, 'Analysis of the infrared and Raman spectra of the symmetrically substituted 1,3-diphenylurea and 1,3-diphenylacetone (dibenzyl ketone)', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 95, pp. 435-441.
- [20] Meganathan, C, Sebastian, S, Sivanesan, I, Keun Woo Lee, Byoung Ryong Jeong, Halil Oturak, Sudha, S & Sundaraganesan N 2012, 'Structural, vibrational (FT-IR and FT-Raman) and UV-vis spectral analysis of 1-phenyl-3-(1,2,3-thiadiazol-5-yl)urea by DFT method', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 95, pp. 331-340.
- [21] Leena Sinha, Onkar Prasad, Vijay Narayan & Shri Ram Shukla 2011, 'Raman, FT-IR spectroscopic analysis and first-order hyperpolarisability of 3-benzoyl-5-chlorouracil by first principles', *Molecular Simulation*, vol. 37, no. 2, pp.153-163.
- [22] Ravikumar, C & Hubert Joe, I 2010, 'Electronic absorption and vibrational spectra and nonlinear optical properties of 4-methoxy-2-nitroaniline', *Physical Chemistry Chemical Physics*, vol. 12, no. 32, pp.9452-9460.

- [23] Brown, GM 1962, 'The biosynthesis of folic acid II. Inhibition by sulfonamides', The Journal of Biological Chemistry, vol. 237, no. 2, pp. 536-540.
- [24] Peter A. Ajibade, Gabriel A. Kolawole, Paul O'Brien, Madeleine Helliwell & James Raftery 2006, 'Cobalt(II) complexes of the antibiotic sulfadiazine, the X-ray single crystal structure of  $[\text{Co}(\text{C}_{10}\text{H}_9\text{N}_4\text{O}_2\text{S})_2(\text{CH}_3\text{OH})_2]$ ', Inorganica Chimica Acta, vol. 359, no. 10, pp. 3111-3116.
- [25] Ogruc-Ildiz, G, Akyuz, S & Ozel, AE 2009, 'Experimental, *ab initio* and density functional theory studies of sulfadiazine', Journal of Molecular Structure, vol. 924-926, pp. 514-522.
- [26] Refat, MS, Sabry A El-Korashy, Ibrahim M El-Deen & Shaima M El-Sayed 2010, 'Experimental and spectroscopic studies of charge transfer reaction between sulfasalazine antibiotic drug with different types of acceptors', Drug Testing and Analysis, vol. 3, no. 2, pp.116-131.
- [27] Balachandran, V, Lakshmi, A & Janaki, A 2012, 'Conformational stability, vibrational spectral studies, HOMO-LUMO and NBO analyses of 2-hydroxy-4-methyl-3-nitropyridine and 2-hydroxy-4-methyl-5-nitropyridine based on density functional theory', Journal of Molecular Structure, vol. 1013, pp. 75-85.
- [28] Xianchang Li, Wei Li, Zhong'an Li, Xiaodong Zhou, Zhen Li, Jingui Qin & Jiming Hu 2011, 'Vibrational spectral investigation of four second order nonlinear optical azobenzene-containing materials: A combination of experimental and density functional theoretical (DFT) study', Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, vol. 79, no. 5, pp. 1976-1984.
- [29] Chaitanya, K 2012, 'Molecular structure, vibrational spectroscopic (FT-IR, FT-Raman), UV-vis spectra, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis, thermodynamic properties of benzophenone 2,4-dicarboxylic acid by *ab initio* HF and density functional method', Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, vol. 86, pp. 159-173.

- [30] Lin-Vien, D, Colthup, NB, Fateley, WG & Grasselli, JG 1991, *The Handbook of Infrared and Raman Characteristic Frequencies of Organic Molecules*, Academic Press, New York.
- [31] Aruldas, G 2008, *Molecular Structure and Spectroscopy*, Prentice-Hall of India Private Limited, New Delhi.
- [32] Griffiths, PR, De Haseth, JA 1986, *Fourier Transform Infrared Spectrometry*, Wiley, New York.
- [33] Bell, RJ 1972, *Introductory Fourier Transform Spectroscopy*, Academic Press, New York.
- [34] Skoog, DA James Holler, F & Stanley R Crouch 2007, *Principles of Instrumental Analysis*, Thomson Brooks/Cole, Haryana.
- [35] Smith, E & Dent, G 2005, *Modern Raman Spectroscopy – A Practical Approach*, John Wiley & Sons, Chichester, West Sussex, England.
- [36] Colin N. Banwell & Elaine M. McCash 2007, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Limited, New Delhi.
- [37] Nair, KPR 2006, *Atoms, Molecules and Lasers*, Narosa Publishing House, New Delhi.
- [38] Michael B. Smith & March, J 2007, *March's Advanced Organic Chemistry Reactions, Mechanisms and Structure*, John Wiley & Sons, New Jersey.
- [39] Peter Sykes 1986, *A Guidebook to Mechanism in Organic Chemistry*, Longman Scientific & Technical, New York.
- [40] Francis, R & Annick, R 2007, *Chemical Analysis Modern Instrumentation Methods and Techniques*, John Wiley & Sons, New York.
- [41] Tony Owen 1996, *Fundamentals of UV-visible Spectroscopy A Primer*, Hewlett-Packard Company, Germany.
- [42] Clark, BJ, Frost, T & Russell, MA 1993, *UV Spectroscopy: Techniques, Instrumentation and Data Handling*, Chapman & Hall, London.

- [43] Robert Withnall, Chowdhry, BZ, Stephen Bell & Trevor J. Dines 2007, 'Computational chemistry using modern electronic structure methods', *Journal of Chemical Education*, vol. 84, no.8, pp. 1364-1370.
- [44] David Young, 2001 *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, John Wiley & Sons, Inc., New York.
- [45] Ira N. Levine, 1991 *Quantum Chemistry*, Prentice Hall International, New Jersey.
- [46] Jan H. Jensen, 2010 *Molecular Modeling Basics*, CRC Press, Taylor and Francis Group, Florida.
- [47] Becke, AD 1998, 'Density-functional exchange-energy approximation with correct asymptotic behavior', *Physical Review A*, vol. 38, no. 6, pp. 3098-3100.
- [48] Lee, C, Yang, W & Parr, RG 1988, 'Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density', *Physical Review B*, vol. 37, no. 2, pp. 785-789.
- [49] Warren J. Hehre, 2003 *A Guide to Molecular Mechanics and Quantum Chemical Calculations*, Wavefunction, Inc., Irvine, CA.
- [50] Lewars EG 2011 *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*, Springer, New York.
- [51] Andrew R. Leach 2001 *Molecular Modelling: Principles and Applications*, Pearson Education, Harlow, England.
- [52] Frisch, MJ, Trucks, GW, Schlegel, HB, Scuseria, GE, Robb, MA, Cheeseman, JR, Scalmani, G, Barone, V, Mennucci, B, Petersson, GA, Nakatsuji, H, Caricato, M, Li, X, Hratchian, HP, Izmaylov, AF, Bloino, J, Zheng, G, Sonnenberg, JL, Hada, M, Ehara, M, Toyota, K, Fukuda, R, Hasegawa, J, Ishida, M, Nakajima, T, Honda, Y, Kitao, O, Nakai, H, Vreven, T, Montgomery, JA, Jr., Peralta, JE, Ogliaro, F, Bearpark, M, Heyd, JJ, Brothers, E, Kudin, KN, Staroverov, VN, Keith, T, Kobayashi, R, Normand, J, Raghavachari, K, Rendell, A, Burant, JC, Iyengar, SS, Tomasi, J, Cossi, M, Rega, N, Millam, JM, Klene, M, Knox, JE, Cross, JB, Bakken, V, Adamo, C,

- Jaramillo, J, Gomperts, R, Stratmann, RE, Yazyev, O, Austin, AJ, Cammi, R, Pomelli, C, Ochterski, JW, Martin, RL, Morokuma, K, Zakrzewski, VG, Voth, GA, Salvador, P, Dannenberg, JJ, Dapprich, S, Daniels, AD, Farkas, O, Foresman, JB, Ortiz, JV, Cioslowski, J & Fox, DJ 2010, Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT.
- [53] Dennington, R, Keith, T & Millam, J 2008, GaussView Version 5, Semichem Inc.
- [54] Glendering ED, Reed AE, Carpenter JE & Weinhold F 1998, NBO Version 3.1. TCI, University of Wisconsin, Madison.
- [55] Sundius, T 1990, 'MOLVIB – A flexible program for force field calculations', Journal of Molecular Structure, vol. 218, pp. 321-326.
- [56] Sundius, T 1991, MOLVIB a program for harmonic force field calculations, QCPE, program No. 604.
- [57] Sundius, T 2002, 'Scaling of *ab initio* force fields by MOLVIB', Vibrational Spectroscopy, vol. 29, no. 1-2, pp. 89-95.
- [58] O'boyle, NM, Tenderholt, AL & Langner, KM 2008, 'cclib: A library for package-independent computational chemistry algorithms', Journal of Computational Chemistry, vol. 29, no. 5, pp. 839 – 845.
- [59] Noury, S, Krokidis, X, Fuster, F & Silvi, B 1997, TopMod Package, Paris.
- [60] Flukiger, P, Luthi, HP, Portmann, S & Weber, J 2000, MOLEKEL 4.0, Swiss Center for Scientific Computing, Manno, Switzerland.
- [61] Foresman, JB & Frisch, A 1995, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., Pittsburgh, PA.
- [62] Ferraro, JR & Nakamoto, K 1994, Introductory Raman Spectroscopy, Academic Press, Inc., San Diego, CA.
- [63] Wilson, EB 1939, 'A method of obtaining the expanded secular equation for the vibration frequencies of a molecule', Journal of Chemical Physics, vol. 7, no. 11, pp. 1047-1052.

- [64] Sundius, T 2002, MOLVIB, User's Guide, Helsinki. Available from: <<http://www.mv.helsinki.fi/home/sundius/MOLVIB/molv7man.pdf>>.[15 November 2018].
- [65] Schachtschneider, JH & Snyder, RG 1963, 'Vibrational analysis of the n-paraffins-II. Normal co-ordinate calculations', *Spectrochimica Acta*, vol. 19, no. 1, pp. 117-168.
- [66] Sellers, HL, Sims, LB, Lothar Schafer & Lewis, DE 1977, 'Vibrational analyses employing Cartesian coordinates', *Journal of Molecular Structure*, vol. 41, no. 1, pp. 149-151.
- [67] Mikosch, H & Bauer, G 1982, 'Normal coordinate treatment and force constant refinement in Cartesian coordinates', *Journal of Molecular Structure*, vol. 89, no. 3-4, pp. 355-364.
- [68] Gwinn, WD 1971, 'Normal coordinates: general theory, redundant coordinates and general analysis using electronic computers', *The Journal of Chemical Physics*, vol. 55, no. 2, pp. 477-481.
- [69] Wilson, EB, Decius, JC & Cross, PC 1955, *Molecular Vibrations*, Mc Graw-Hill, New York.
- [70] Sundius, T 1980, 'A New Damped Least-Squares Method for the Calculation of Molecular Force Fields', *Journal of Molecular Spectroscopy*, vol. 82, no. 1, pp. 138-151.
- [71] Pulay, P, Fogarasi, G, Pang, F & Boggs, JE 1979, 'Systematic *ab initio* gradient calculation of molecular geometries, force constants, and dipole moment derivatives', *Journal of the American Chemical Society*, vol. 101, no. 10, pp. 2550-2560.
- [72] Pulay, P, Fogarasi, G, Pongor, G, Boggs, JE & Vargha, A 1983, 'Combination of theoretical *ab initio* and experimental information to obtain reliable harmonic force constants. Scaled quantum mechanical (SQM) force fields for glyoxal, acrolein, butadiene, formaldehyde and ethylene', *Journal of American Chemical Society*, vol. 105, no. 24, pp. 7037-7047.
- [73] Keresztury G, Holly S, Besenyi G, Varga J, Wang A, Durig JR 1993, 'Vibrational spectra of monothiocarbamates-II.\* IR and Raman spectra,



- vibrational assignment, conformational analysis and ab initio calculations of S-methyl-N,N-dimethylthiocarbamate', *Spectrochimica Acta A*, vol. 49, no. 13-14, pp. 2007-2026.
- [74] Keresztury G, Chalmers JM & Griffith PR 2002, *Raman Spectroscopy: Theory in Handbook of Vibrational Spectroscopy*, John Wiley & Sons, Ltd., Chichester.
- [75] Reed, AE, Curtiss, LA & Weinhold, F 1988, 'Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint', *Chemical Reviews*, vol. 88, no. 6, pp. 899-926.
- [76] Fukui, K 1982, 'The role of frontier orbitals in chemical reactions (Nobel Lecture)', *Angewandte Chemie International Edition in English*, vol. 21, no. 11, pp. 801-876.
- [77] Francis A Carey 2000, *Organic Chemistry*, McGraw-Hill Companies, Inc., USA.
- [78] Thanthiriwatte, KS & Nalin de Silva, KM 2002, 'Non-linear optical properties of novel fluorenyl derivatives-*ab initio* quantum chemical calculations', *Journal of Molecular Structure (Theochem)*, vol. 617, no. 1-3, pp. 169-175.
- [79] Kleinman, DA 1962, 'Nonlinear dielectric polarization in optical media', *Physical Review*, vol. 126, no. 6, pp. 1977-1979.
- [80] Mulliken, RS 1955, 'Electronic population analysis on LCAO-MO molecular wave functions. I', *The Journal of Chemical Physics*, vol. 23, no. 10, pp. 1833-1840.
- [81] Kruszewski J & Krygowski TM 1972, 'Definition of aromaticity basing on the harmonic oscillator model', *Tetrahedron Letters*, vol. 13, no. 36, pp. 3839-3842.
- [82] Krygowski, TM 1993, 'Crystallographic studies of inter- and intramolecular interactions reflected in aromatic character of pi-electron systems', *Journal of Chemical Information and Computer Sciences*, vol. 33, no. 1, pp. 70-78.

- [83] Becke, AD & Edgecombe, KE 1990, 'A simple measure of electron localization in atomic and molecular systems', *The Journal of Chemical Physics*, vol. 92, no. 9, pp. 5397-5403.
- [84] Matito, E & Sola, M, 2009, 'The role of electronic delocalization in transition metal complexes from the electron localization function and the quantum theory of atoms in molecules viewpoints', *Coordination Chemistry Reviews*, vol. 253, no. 5-6, pp. 647-665.
- [85] Birjmohun, RS, Hutten, BA, Kastelein, JJP & Stroes, ES 2005, 'Efficacy and safety of high-density lipoprotein cholesterol-increasing compounds: a meta-analysis of randomized controlled trials', *Journal of the American College of Cardiology*, vol. 45, no. 2, pp. 185-197.
- [86] Rodney, G, Uhlendorf, P & Maxwell, RE 1976, 'The hypolipidaemic effect of gemfibrozil (CI-719) in laboratory animals', *Proceedings of the Royal Society of Medicine*, vol. 69, no. 2, pp. 6-10.
- [87] Garg, A & Grundy, SM 1989, 'Gemfibrozil alone and in combination with lovastatin for treatment of hypertriglyceridemia in NIDDM', *Diabetes*, vol. 38, no.3, pp. 364-372.
- [88] Goldberg, R, La Belle, P, Zupkis, R & Ronca, P 1990, 'Comparison of the effects of lovastatin and gemfibrozil on lipids and glucose control in non-insulin-dependent diabetes mellitus', *The American Journal of Cardiology*, vol. 66, no. 8, pp. B16-B21.
- [89] Shen, DC, Fuh, MMT, Shieh, S-M, Ida Chen YD & Reaven, GM 1991, 'Effect of gemfibrozil treatment in sulfonylurea-treated patients with noninsulin-dependent diabetes mellitus', *Journal of Clinical Endocrinology and Metabolism*, vol. 73, no. 3, pp. 503-510.
- [90] Steiner, G 1991, 'Altering triglyceride concentrations changes insulin-glucose relationships in hypertriglyceridemic patients', *Diabetes Care*, vol. 14, no. 11, pp. 1077-1081.
- [91] Vinik, AI & Colwell, JA 1993, 'Effects of gemfibrozil on triglyceride levels in patients with NIDDM', *Diabetes Care*, vol. 16, no. 1, pp. 37-44.

- [92] Kahri, J, Vuorinen-Markkola, H, Tilly-Kiesi, M, Lahdenpera, S & Taskinen, M-R 1993, 'Effect of gemfibrozil on high density lipoprotein subspecies in non-insulin dependent diabetes mellitus. Relations to lipolytic enzymes and to the cholesteryl ester transfer protein activity', *Atherosclerosis*, vol. 102, no. 1, pp. 79-89.
- [93] Lahdenperä, S, Tilly-Kiesi, M, Vuorinen-Markkola, Kuusi, T & Taskinen, M-R 1993, 'Effects of gemfibrozil on low-density lipoprotein particle size, density distribution, and composition in patients with type II diabetes', *Diabetes Care*, vol. 16, no. 4, pp. 584-592.
- [94] Spencer, CM & Barradell, LB 1996, 'Gemfibrozil: A reappraisal of its pharmacological properties and place in the management of dyslipidaemia', *Drugs*, vol. 51, no. 6, pp. 982-1018.
- [95] Bruni, B, Coran, S, Di Vaira M & Giannellini, V 2005, '5-(2,5-Dimethylphenoxy)-2,2-dimethylpentanoic acid (gemfibrozil)', *Acta Crystallographica Section E*, vol. E61, no. 7, pp. o1989-o1991.
- [96] Benitta, TA, Balendiran, GK & James, C 2008, 'Vibrational spectral studies of gemfibrozil', *Proceedings of the second international conference on perspectives in vibrational spectroscopy*, pp. 218-222.
- [97] Frisch, MJ, Trucks, GW, Schlegel, HB, Scuseria, GE, Robb, MA, Cheeseman, JR, Montgomery, JA, Vreven, T, Kudin, TKN, Burant, JC, Millam, JM, Iyengar, SS, Tomasi, J, Barone, V, Mennucci, B, Cossi, M, Scalmani, G, Rega, N, Petersson, GA, Nakatsuji, H, Hada, M, Ehara, M, Toyota, K, Fukuda, R, Hasegawa, J, Ishida, M, Nakajima, T, Honda, Y, Kitao, O, Nakai, H, Klene, M, Li, X, Knox, JE, Hratchian, HP, Cross, JB, Bakken, V, Adamo, C, Jaramillo, J, Gomperts, R, Stratmann, RE, Yazyev, O, Austin, AJ, Cammi, R, Pomelli, C, Ochterski, JW, Ayala, PY, Morokuma, K, Voth, GA, Salvador, P, Dannenberg, JJ, Zakrzewski, VG, Dapprich, S, Daniels, AD, Strain, MC, Farkas, O, Malick, DK, Rabuck, AD, Raghavachari, K, Foresman, JB, Ortiz, JV, Cui, Q, Baboul, AG, Clifford, S, Cioslowski, J, Stefanov, BB, Liu, G, Liashenko, A, Piskorz, P, Komaromi, I, Martin, RL, Fox, DJ, Keith, T, Al-Laham, MA, Peng, CY, Nanayakkara, A, Challacombe, M, Gill, PMW, Johnson, Chen, BW, Wong, MW, Gonzalez, C, & Pople, JA 2004, *Gaussian 03*, Revision D.01, Gaussian, Inc., Wallingford CT.

- [98] Sato, H, Dybal, J, Murakami, R, Noda, I & Ozaki, Y 2005, 'Infrared and Raman spectroscopy and quantum chemistry calculation studies of C–H···O hydrogen bondings and thermal behavior of biodegradable polyhydroxyalkanoate', *Journal of Molecular Structure*, vol. 744-747, pp. 35-46.
- [99] Varsanyi, G 1969, *Vibrational Spectra of Benzene Derivatives*, Academic Press, New York.
- [100] Roeges, NPG 1994, *A Guide to the Complete Interpretation of Infrared Spectra of Organic Structures*, Wiley, New York.
- [101] Brian Smith, C 1999, *Infrared Spectral Investigation– A Systematic Approach*, CRC press, USA.
- [102] Colthup, NB, Daly, LH & Wiberly, SE 1990, *Introduction to Infrared and Raman Spectroscopy*, Academic Press, New York.
- [103] Socrates G 2001, *Infrared and Raman Characteristic Group Frequencies: Tables and Charts*, John Wiley & Sons Ltd, Chichester.
- [104] Padmaja, L, Ravikumar, C, Sajan, D, Hubert Joe, I, Jayakumar, VS, Pettit, GR & Faurskov Nielsen, O 2009, 'Density functional study on the structural conformations and intramolecular charge transfer from the vibrational spectra of the anticancer drug combretastatin-A2', *Journal of Raman Spectroscopy*, vol. 40, no. 4, pp. 419-428.
- [105] Ravikumar, C, Hubert Joe, I & Jayakumar, VS 2008, 'Charge transfer interactions and nonlinear optical properties of push-pull chromophore benzaldehyde phenylhydrazone: A vibrational approach', *Chemical Physics Letters*, vol. 460, no. 4-6, pp. 552-558.
- [106] Svartz, N 1942, 'Salazopyrin, a new sulfanilamide preparation. A. Therapeutic results in rheumatic polyarthritis. B. Therapeutic results in ulcerative colitis. C. Toxic manifestations in treatment with sulfanilamide preparations', *Acta Medica Scandinavica*, vol. 110, no. 6, pp. 557–598.
- [107] Dick AP, Grayson MJ, Carpenter RG & Petrie A 1964, 'Controlled trial of sulphasalazine in the treatment of ulcerative colitis', *Gut*, vol. 5, no. 5, pp. 437-442.

- [108] McConkey B, Amos RS, Durham S, Forster PJG, Hubball S & Walsh L 1980, 'Sulphasalazine in rheumatoid arthritis', *British Medical Journal*, vol. 280, no. 6212, pp. 442-444.
- [109] Connell, WR 1996, 'Safety of drug therapy for inflammatory bowel disease in pregnant and nursing women', *Inflammatory Bowel Diseases*, vol. 2, no. 1, pp. 33-47.
- [110] Ashutosh Kar 2006, *Medicinal Chemistry*, New Age International (P) Ltd. Publishers, New Delhi.
- [111] Beryl West, Lendrum R, Hill MJ & Geoffrey Walker 1974, 'Effects of sulphasalazine (salazopyrin) on faecal flora in patients with inflammatory bowel disease', *Gut*, vol. 15, no. 12, pp. 960-965.
- [112] Berti-Mattera, LN, Kern, TS, Siegel, RE, Nemet, I & Mitchell, R 2008, 'Sulfasalazine blocks the development of tactile allodynia in diabetic rats', *Diabetes*, vol. 57, no. 10, pp. 2801-2808.
- [113] Gupta, AK, Ellis, CN, Siegel, MT & Voorhees, JJ 1989, 'Sulfasalazine: A potential psoriasis therapy?', *Journal of the American Academy of Dermatology*, vol. 20, no. 5, pp. 797-800.
- [114] Filip, LA, Caira, MR, Farcas, SI & Bojita, MT 2001, 'Triclinic polymorph of sulfasalazine', *Acta Crystallographica Section C*, vol. C57, no. 4, pp. 435-436.
- [115] Asha Chandran, Sheena Mary, Y, Hema Tresa Varghese, Yohannan Panicker, C, Pavel Pazdera, Rajendran G & Babu N 2011, 'FT-IR, FT-Raman spectroscopy and computational study of N-carbamimidoyl-4-{(E)-(2-hydroxyphenyl)methylidene]amino} benzenesulfonamide', *Journal of Molecular Structure*, vol. 992, no. 1-3, pp. 77-83.
- [116] Karabacak, M, Cinar, M, Coruh, A & Kurt, M 2009 'Theoretical investigation on the molecular structure, Infrared, Raman and NMR spectra of para-halogen benzenesulfonamides, 4-X-C<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>NH<sub>2</sub> (X=Cl, Br or F)', *Journal of Molecular Structure*, vol. 919, no. 1-3, pp. 26-33.
- [117] Topaçli C & Topaçli A 2003 '*Ab initio* calculations and vibrational structure of sulfanilamide', *Journal of Molecular Structure*, vol. 644, no. 1-3, pp. 145-150.

- [118] Refat, MS & Mohamed, SF 2011, 'Spectroscopic, thermal and antitumor investigations of sulfasalazine drug *in situ* complexation with alkaline earth metal ions', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 82, no. 1, pp. 108-117.
- [119] Soliman, AA 2006, 'Spectral and thermal study of the ternary complexes of nickel with sulfasalazine and some amino acids', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 65, no. 5, pp. 1180-1185.
- [120] Mohamed, GG, Soliman, AA & El-Mawgood, MA 2005, 'Structural and thermal characterization of cerium, thorium and uranyl complexes of sulfasalazine', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 62, no. 4-5, pp. 1095-1101.
- [121] Desiraju GR, Steiner T 1999, *The Weak Hydrogen Bond: In Structural Chemistry and Biology*, Oxford University Press, New York.
- [122] Peter J Larkin 2011, *IR and Raman Spectroscopy: Principles and Spectral Interpretation*, Elsevier, USA.
- [123] Robert M Silverstein & Francis X Webster 2003, *Spectrometric Identification of Organic Compounds*, John Wiley & Sons, Inc., New York.
- [124] Maren, TH 1976, 'Relations between structure and biological activity of sulfonamides', *Annual Review of Pharmacology and Toxicology*, vol. 16, no. 1, pp. 309-327.
- [125] Ferguson, AD, Kessler, AD & Scott, RB, 1954, 'Use of a quadruple sulfonamide mixture in acute bacterial infections of infancy and childhood', *The Journal of Pediatrics*, vol. 45, no. 6, pp. 655-661.
- [126] Golzar Hossain, GM 2006 'A new polymorph of sulfamerazine', *Acta Crystallographica Section E*, vol. E62, no. 6, pp. o2166-o2167.
- [127] Tommasino, J-B, Renaud, FNR, Luneau, D & Pilet, G 2011, 'Multi-biofunctional complexes combining antiseptic copper(II) with antibiotic sulfonamide ligands: Structural, redox and antibacterial study', *Polyhedron*, vol. 30, no. 10, pp. 1663-1670.

- [128] Esrafil, MD, Behzadi, H, Beheshtian, J & Hadipour, NL 2008, 'Theoretical  $^{14}\text{N}$  nuclear quadrupole resonance parameters for sulfa drugs: Sulfamerazine and sulfathiazole', *Journal of Molecular Graphics and Modelling*, vol. 27, no. 3, pp. 326-331.
- [129] Kurotani, M & Hirasawa, I 2008, 'Polymorph control of sulfamerazine by ultrasonic irradiation', *Journal of Crystal Growth*, vol. 310, no. 21, pp. 4576-4580.
- [130] Aitipamula, S, Chow, PS & Tan, RBH, 2011, 'Solvates and a monohydrate of  $\text{N}^4$ -acetylsulfamerazine: Structural, thermochemical and computational analysis', *Journal of Molecular Structure*, vol. 1005, no. 1-3, pp. 134-140.
- [131] Lu, J, Li, Y-P, Wang, J, Li, Z, Rohani, S & Ching, C-B, 2011, 'Pharmaceutical cocrystals: a comparison of sulfamerazine with sulfamethazine', *Journal of Crystal Growth*, vol. 335, no. 1, pp. 110-114.
- [132] Wheatley, PJ 1960, 'The crystal and molecular structure of pyrimidine', *Acta Crystallographica*, vol. 13, no. 2, pp. 80-85.
- [133] Savin, A, Silvi, B & Colonna, F 1996, 'Topological analysis of the electron localization function applied to delocalized bonds', *Canadian Journal of Chemistry*, vol. 74, no. 6, pp. 1088-1096.
- [134] Mohan, J 2001, *Organic Spectroscopy: Principles and Applications*, New Age International (P) Limited Publishers, New Delhi.
- [135] Higson, FK 1992, 'Microbial degradation of nitroaromatic compounds', *Advances in Applied Microbiology*, vol. 37, pp. 1-19.
- [136] Spain, JC 1995, *Biodegradation of Nitroaromatic Compounds*, Plenum Press, New York.
- [137] Spain, JC 1995, 'Biodegradation of nitroaromatic compounds', *Annual Review of Microbiology*, vol. 49, no. 1, pp. 523-555.
- [138] Munnecke, DM 1976, 'Enzymatic hydrolysis of organophosphate insecticides, a possible pesticide disposal method', *Applied and Environmental Microbiology*, vol. 32, no. 1, pp. 7-13.

- [139] Stevens, TO, Crawford, RL & Crawford, DL 1991, 'Selection and isolation of bacteria capable of degrading dinoseb (2-*sec*-butyl-4,6-dinitrophenol)', *Biodegradation*, vol. 2, no. 1, pp. 1-13.
- [140] Abdel-Kader, MHK & Webster, GRB 1982, 'Analysis of fenitrothion and metabolites in stored wheat', *International Journal of Environmental Analytical Chemistry*, vol. 11, no. 2, pp. 153-165.
- [141] Li, C, Takahashi, S, Taneda, S, Furuta, C, Watanabe, G, Suzuki, AK & Taya, K 2006, 'Impairment of testicular function in adult male Japanese quail (*Coturnix japonica*) after a single administration of 3-methyl-4-nitrophenol in diesel exhaust particles', *Journal of Endocrinol.* vol. 189, no. 3, pp. 555-564.
- [142] Mi, Y, Zhang, C, Li, C, Taneda, S, Watanabe, G, Suzuki, AK & Taya, K 2009, 'Quercetin protects embryonic chicken spermatogonial cells from oxidative damage intoxicated with 3-methyl-4-nitrophenol in primary culture', *Toxicology Letters*, vol. 190, no. 1, pp. 61-65.
- [143] Bi, S, Wu, Y-Z, Zhou, Y-X, Tang, J-G & Guo, C 2009, '2-Methyl-4-nitrophenol', *Acta Crystallographica Section E*, vol. E65, no. 6, pp. o1378.
- [144] Dong, S-L & Cheng, X 2012, '3-Methyl-4-nitrophenol', *Acta Crystallographica Section E*, vol. E68, no. 2, pp. o518.
- [145] Mahadevan, D, Periandy, S, Karabacak, M, Ramalingam, S & Puviarasan, N 2012, 'Spectroscopic (FT-IR, FT-Raman and UV-vis) investigation and frontier molecular orbitals analysis on 3-methyl-2-nitrophenol using hybrid computational calculations', *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 86, pp. 139-151.
- [146] Kovacs, A, Izvekov, V, Keresztury, G & Pongor, G 1998, 'Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study', *Chemical Physics*, vol. 238, no. 2, pp. 231-243.
- [147] Tanaka, T, Nakajima, A, Watanabe, A, Ohno, T & Ozaki, Y 2004, 'Surface-enhanced Raman scattering of pyridine and p-nitrophenol studied by density functional theory calculations', *Vibrational Spectroscopy*, vol. 34, no. 1, pp. 157-167.



- [148] Syam Sundar, N 1985, 'The infrared absorption spectra of substituted phenols—4-nitro-3-methyl-, 2-amino-4-nitro- and 4-amino-3-methylphenol', *Spectrochimica Acta Part A: Molecular Spectroscopy*, vol. 41, no. 12, pp. 1449-1455.
- [149] <<http://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=IN&language=en&productNumber=422908&brand=ALDRICH&PageToGoToURL=http%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fproduct%2Faldrich%2F422908%3Flang%3Den>>. [1 September 2012]
- [150] <<http://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=IN&language=en&productNumber=M62654&brand=ALDRICH&PageToGoToURL=http%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fproduct%2Faldrich%2Fm62654%3Flang%3Den>>. [1 September 2012]
- [151] Davis, TL 1943, *The Chemistry of Powder and Explosives*, John Wiley & Sons, New York.
- [152] Ritter, H, Braun, S, Kaiser, M & Becher, C 2008, 'Stabilizer degradation in propellants: Identification of two isomeric forms of 2-nitro-N-nitroso-N-ethylaniline', *Propellants, Explosives, Pyrotechnics*, vol. 33, no. 3, pp. 203-208.
- [153] Lussier, L-S, Bergeron, E & Gagnon, H 2006, 'Study of the daughter products of akardite-II', *Propellants Explosives, Pyrotechnics*, vol. 31, no. 4, pp. 253-262.
- [154] Larranaga, MD, Lewis, RJ & Lewis, RA 2016, *Hawley's Condensed Chemical Dictionary*, John Wiley & Sons, Inc., New Jersey.
- [155] Harper, RJ, Almirall, JR & Furton, KG 2005, 'Discrimination of smokeless powders by headspace SPME-GC-MS and SPME-GC-ECD, and the potential implications upon training canine detection of explosives', *Proceedings of SPIE*, ed. Edward M. Carapezza, Bellingham, pp. 638-643.
- [156] Laza, D, Nys, B, Kinder, JD, Mesmaeker, AK & Moucheron, C 2007, 'Development of a quantitative LC-MS/MS method for the analysis of common propellant powder stabilizers in gunshot residue', *Journal of Forensic Sciences*, vol. 52, no. 4, pp. 842-850.

- [157] Betz, R, Gerber, T & Schalekamp, H 2011, '1,3-Diethyl-1,3-diphenylurea', *Acta Crystallographica Section E*, vol. E67, no. 4, pp. o827.
- [158] Dollish, FR, Fateley, WG & Bentley, FF 1974 *Characteristic Raman Frequencies of Organic Compounds*, John Wiley & Sons, New York.
- [159] Miertus, S, Scrocco, E & Tomasi, J 1981, 'Electrostatic interaction of a solute with a continuum. A direct utilization of *ab initio* molecular potentials for the prevision of solvent effects', *Chemical Physics*, vol. 55, no. 1, pp. 117-129.
- [160] Miertus, S & Tomasi, J 1982, 'Approximate evaluations of the electrostatic free energy and internal energy changes in solution processes', *Chemical Physics*, vol. 65, no. 2, pp. 239-245.
- [161] Cossi, M, Barone, V, Cammi, R & Tomasi, J 1996, '*Ab initio* study of solvated molecules: a new implementation of the polarizable continuum model', *Chemical Physics Letters*, vol. 255, no. 4-6, pp. 327-335.