Journal of Chemical, Biological and Physical Sciences

An International Peer Review E-3 Journal of Sciences

*Available online at*www.jcbsc.org

Section A: Chemical Sciences

CODEN (USA): JCBPAT Research Article

Thermodynamic Behaviors of Hypersensitive Transition Observed In Some Praseodymium Doped Systems with Various Amide Group Containing Ligands

Suresh Purohit

Department of Chemistry, ECB Polytechnic College, Bikaner, (Raj.) India

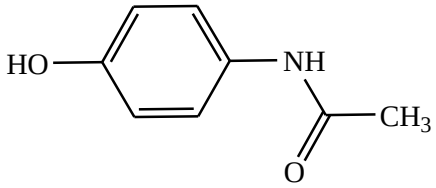
Received: 19March 2017**; Revised:** 02April 2017; **Accepted:** 10 April 2017

Abstract: In the present research paper we have studied the thermodynamic behaviors of hypersensitive transition observed in some praseodymium doped system with alcoholic saturated solutions of amide group containing ligands. For this purpose we have choose three ligands i.e., Paracetamol, Indomethacin and Lidocaine. These ligands are drugs in nature and contain amide group. It has been observed that amide group containing ligands play very important role in biological chemistry, since proteins made up of amino acids which contain amide group in their structure. Study is based on doped crystal phenomenon. In this research paper we have choose thermodynamic efficiency (TET) and work function (A) of hypersensitive transition. Both of these parameters are very important to explain the stability of a complex. Uses of computational chemistry have been explored in order to develop better and easier methods of calculations.

Keywords: amide group containing ligands, thermodynamic efficiency (TET), work function (A), hypersensitive transition etc.

INTRODUCTION

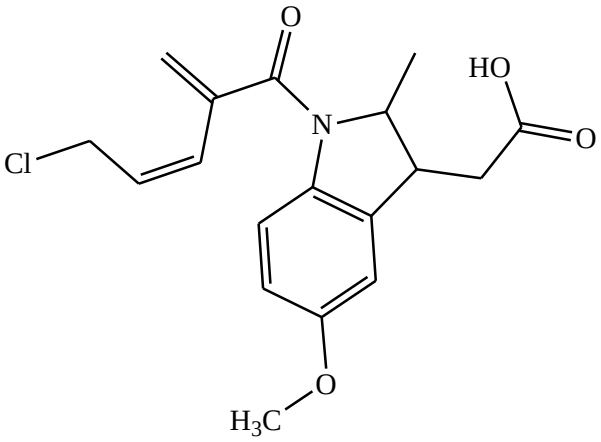
Paracetamol is a widely used analgesic anti-pyretic drug[1-3] Paracetamol is also known as Acetaminophen. It is a pain reliever and a fever reducer. The exact mechanism of is not known. It is used to treat many conditions such as headache, muscle aches, arthritis, backache, toothaches, colds, and fevers. It relieves pain in mild arthritis but has no effect on the underlying inflammation and swelling of the joint. Paracetamol may also be used for other purposes not listed in this medication guide.



N-(4-hydroxyphenyl)acetamide (Paracetamol)

Fig. 1: Chemical Structure of Paracetamol

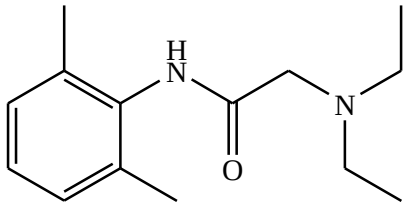
Indomethacin is a non-steroidal anti-inflammatory drug[4-6]. It is used to relieve pain, swelling, and joint stiffness caused by arthritis, gout, bursitis, and tendonitis. It is also used to relieve pain from various other conditions. This medication is known as a non-steroidal anti-inflammatory drug (NSAID). It works by blocking your body's production of certain natural substances that cause inflammation. This effect helps to decrease swelling and pain.



2-(1-(4-chlorobenzoyl)-5-methoxy-2-methylindolin-3-yl)acetic acid

Fig. 2: Chemical Structure of Indomethacin

Lidocaine is a local anesthetic[7-10]. Lidocaine topical jelly or ointment is used on different parts of the body to cause numbness or loss of feeling for patients having certain medical procedures. It is also used to relieve pain and itching caused by conditions such as sunburn or other minor burns, insect bites or stings, poison ivy, poison oak, poison sumac, minor cuts, or scratches



2-(diethylamino)-*N*-(2,6-dimethylphenyl)acetamide

Fig. 3: Chemical Structure of Lidocaine

In these drugs amide group is present as a main functional group. Amide plays a very important role in the living organism. All types of proteins are made up from amino acids and thus amide group acts as fundamental building block in living organism[11-13].

This paper describes investigations on Pr(III) systems with alcoholic saturated solutions of amide group containing ligands. The study is based upon doped crystal phenomenon.

MATERIAL AND METHODS

In the present research Paracetamol, Indomethacin, Lidocaine, ethyl alcohol, distilled water etc. chemicals have been used. All solvents and chemicals used have AR grade. Their purity has checked by thin layer chromatography (TLC). The Pr(III) salt dissolved in suitable amount of ethanol and saturated amide ligands has been taken, i.e., Paracetamol, Indomethacin, and Lidocaine . Then both solutions have mixed together to form solutions of various ligands. Absorption spectra of doped systems have been recorded at pH-7. For this purpose double beam UV-Visible spectrophotometer has been used. In double beam spectrophotometer, the light ray is divided in to two parts or beams. One beam is passed through the reference material and other beam is passed through the sample. The reference beam intensity is taken as zero absorbance.

In this research paper we have choose two thermodynamic properties i.e., thermodynamic efficiency (TET) and work function (A) of hypersensitive transition. Those transitions are known as hypersensitive which are very sensitive to the ligand and solvent molecules. For such types of bands oscillator strength is found to be ~10-5. Oscillator strength of hypersensitive transitions exhibits greater variation than that of non-hypersensitive transitions[14,15]. Thermodynamic parameters support the covalency in metal-ligand interaction for hypersensitive transitions. Thermodynamic properties are of two types:

1. Thermodynamic Efficiency of Transition (TET)
2. Work Function (A)

Thermodynamic Efficiency of Transition (TET): Thermodynamic Efficiency of Transition (TET) may be calculated by the help of following formula:

$$\mathbf{TET = A / E} \qquad \mathbf{\ldots (1)}$$

Where, A = Work Function (cm^{-1}); E = Energy Absorbed for Transition (cm^{-1})

Work Function (A): Work function may be calculated by the help of following formula -

$$A = E - TS \ldots (2)$$

Where, T = Temprature (Kelvin); S = Absolute Energy (cm^{-1})

Since the value of S = K lnPobs , thus equation (2) may also be written as –

$$A = E - K\,T\,lnPobs \quad \ldots (3)$$

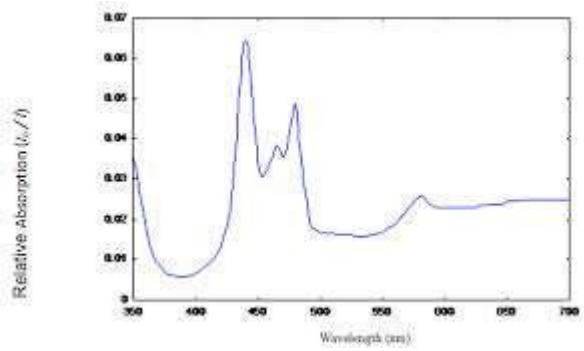
Where K = Boltzmann Constant = 0.6945 cm^{-1};Pobs = Oscillator Strength of Transition

The intensity of transitions can be explained by the oscillator Strength. In lanthanides two types of transitions such as f-f and f-d have been observed. In which f-f transitions give rise to sharp, narrow bands of comparatively weak intensities due to Laporte forbidden, whereas allowed f-d transitions are relatively broad and intense. The observed spectral transitions of the lanthanide ions are f-f transitions. Since the 4f-sub-shell of Pr(III) ions is well shielded by the filled 5s and 5p sub-shells, the energy levels of the 4f-electrons are only little influenced by the environment of Pr(III) ion. The intensity of f-f transition is weak, because these transitions are Laporte forbidden. Relaxation of this selection rule is very less effective than that of d-d transitions. This is because of the weak crystal field interaction.

The intensity of the absorption band in Pr(III) spectra has been studied Judd and Ofelt[16-23]. Most of the sharp lines like 4f↔4f transitions originating within the 4f-configuration of the lanthanide (III) ions are little affected by the environment of the lanthanide ions. Such transitions have been called hypersensitive transitions by Jorgensen and Judd (24). The oscillator strengths and shapes of the hypersensitive transitions can be used to probe complex formation, coordination geometry, ligand structure and chelate solvent interactions [13].

RESULTS AND DISCUSSION

The absorption bands of Pr(III) doped systems appears in the Visible region i.e., 400nm to 900nm. The four bands have appeared in the visible region. These bands appears due to the transitions from ground levels 3H4 to the excited J-levels, i.e., $^3P2$, $^3P1$, $^3P0$ and $^1D_2$.



By the help of oscillator strength, the observed and calculated values of thermodynamic parameters of various transitions including hypersensitive transition have been calculated at 7 pH. These values for hypersensitive transition have been given in the table-1:

Table -1:hypersensitive transitionvalues of metals.

Pr(III) Doped System	Pr(III) + Paracetamol	Pr(III) + Indomethacin	Pr(III) + Lidocaine
$E_{obs.}$	22497.188	22466.861	22471.91
$E_{cal.}$	22528.884	22497.733	22491.766
$P_{obs.}$	1.0801721	1.4843655	0.8780754
$P_{cal.}$	0.5417739	0.8097885	0.4615273
$A_{obs.}$	25341.011	25244.887	25358.612
$A_{cal.}$	25515.542	25401.193	25511.607
$TET_{obs.}$	1.1264079	1.1236499	1.1284582
$TET_{cal.}$	1.1325702	1.1290557	1.1342643

CONCLUSION

Some doped systems of Pr(III) ion with three ligands such as Paracetamol, Indomethacin and Lidocaine in ethanolic medium have been taken. Solution spectra of each doped system have been recorded in UV-Visible and near IR range. By the help of some spectral data, thermodynamic efficiency (TET) and work function (A) have been determined.

It has been concluded from the table that the observed values of work function (Aobs) has less than that of calculated values (Acal) for all types of doped systems. Similarly the observed values of TET (TETobs) has also less than that of calculated values (TETcal) for all types of doped systems. The significance of thermodynamic parameters is well understood but their computation from spectroscopic data proposes a microscopic behavior of the f-f transition. The present study finds that the microscopic behavior with respect to TET for Pr(III) doped systems is almost the same.

REFERENCES

1. C. J. Nikles, M. Yelland, C. D. Marc, D. Wilkinson, Am. J. Therap., 2005, 12(1), 80.
2. N. F. Atta, A. Galal, S. M. Azab, Int. J. Electrochem. Sci., 2011, 6, 5082.
3. J. Parojcic, K. Karljikovic-Rajic, Z. Duric, M. Jovanovic, S. Ibric, Biopharm. Drug, 2003, 24, 309.
4. X. Q.Chen, Y. T. Jin Y Y, G. Tang G, New Pharmacology, People Health Publishing House, 2003, 186.
5. L. Mason, J. Edward, R. A. Moore, H. J. NcQuay, Cochrane Database System Review, 2004, 4, 43.
6. L. U. Bin, R. Wen, Y. Hong, H. E. Yingju, Int. J. of Pharmaceutics, 2007, 333, 43.
7. R. H. Dworkin, A. B. O' Connor, J. Audette et al., Mayo Clin Proc., 2011, 85 Suppl, 3:S3-S14.
8. A. Nicolaou, B. Nicholson, G. Hans, L. Brasseur, J of Pain Research, 2011, 4, 25.
9. R. Baron, V. Mayoral, G. Leijon et al., Curr. Med. Res. Opin., 2009, 25, 1663.
10. R. Baron, V. Mayoral, G. Leijon et al., Curr. Med. Res. Opin., 2009, 25, 1677.

11. S. Purohit, Int. J. of Chemical and Pharmaceutical Analysis,DOI : http://dx.doi.org/10.21276/ijcpa.
12. S. Purohit, N. Bhojak, Research and Reviews: Journal of Chemistry, 2013, 2(2).
13. H. S. Bhandari, D. D. Gudesaria, S. Purohit, N. Bhojak, Int. J. Chem. Sci., 2010, 8(1), 393.
14. P. C. Mehta, S. P. Tandon, S. P. Sinha, Mol. Phys., 1972, 23, 807.
15. D. E. Henrie, G. R. Chopin, J. Chem. Phys., 1968, 49, 477.
16. B. R. Judd, Phys. Rev., 1962, 127, 750.
17. G. S. Ofelt, J. Chem. Phys., 1962, 37, 511.
18. W. T. Carnail, P. R. Field, K. Rajnak, J. Chem. Phys., 1968, 49, 4412.
19. A. Heller, J. Mol. Spect., 1968, 28, 208.
20. S. S. L. Surana, R. C. Mathur, S. P. Tandon, Solid State Phys., 1975, 8, 2323.
21. S. V. J. Lakshman, S. J. Buddhudu, Quant. Spectrosc. Radiat Transfer, 1987, 24, 251.
22. A. H. Qusti, and J. Chrysochoos, J. Less Common Metals, 1985, 112, 287.
23. J. Chrysochoos, A. H. Qusti, J. Less Common Metals, 1986, 126, 161.
24. C. K. Jorgensen, B. R. Judd, Mol. Phys., 1964, 8, 281.

Corresponding author: Dr. Suresh Purohit;

Lecturer Department of Chemistry, ECB Polytechnic College, Bikaner (Raj.)India

On line publication Date: 810.04.2017