COLLOQUIUM SPECTROSCOPICUM INTERNATIONALE XXXI

September 5-10, 1999 Ankara - Turkey

BOOK OF ABSTRACTS

Turkish Chemical Society

Middle East Technical University

The Scientific and Technical Research Council of Turkey

International Union of Pure and Applied Chemistry

BOOK OF ABSTRACTS

COLLOQUIUM SPECTROSCOPICUM INTERNATIONALE XXXI

September 5–10 • Ankara, Turkey

Hosted by:
The Turkish Chemical Society
Middle East Technical University

VIBRATIONAL INVESTIGATION AND THERMAL DECOMPOSITION KINETICS OF N,N-DIETHYL-N'-BENZOYLTHIOUREA AND ITS Pt(II), Pd(II) and Cd(II) COMPLEXES

Talat OZPOZAN[a], Sabri ÇAVUŞ[a], Nilgün ÖZPOZAN[a], Hakan ARSLAN[b], Melek MERDİVAN[c], Atilla AYDINLI[d]
[a]Erciyes University, Department of Chemistry, Kayseri, Turkey
[b]Mersin University, Department of Chemistry, Mersin, Turkey
[c]Balikesir University, Department of Chemistry, Balikesir, Turkey
[d]Bilkent University, Department of Physics, Ankara, Turkey

FTIR and RAMAN spectra of the ligand N,N-Diethyl-N'-Benzoylthiourea (DEBTU) and its Pt(II), Pd(II) and Cd(II) complexes in the form of ML_2 type (M: Pt, Pd, Cd, L: DEBTU) are obtained and their theoretical vibrational spectra are calculated. Unknown bands in the experimental vibrational spectra are assigned through simulation method. Thermal behaviours and thermal decomposition kinetics of the ligand and of its metal chelates are investigated.

The geometry (bond length, bond angle)[1] and force constants are used as input data for the calculation of frequencies; atomic radii, electronegativities are used as input data for the calculation of IR and Raman activities. Normal coordinate analysis are performed through point group symmetry of the compounds. The compounds are assumed to be isolated molecules for simplicity in calculations. The program package SPSIM (SPectrum SIMulation)[2] based on Wilson's GF matrix method[3] are used and valance force field type of force constants are employed for the calculations of frequencies.

The experimental and the calculated vibrational spectra are compared. The shifted frequencies in the calculated spectra are fitted by iteration technique to obtain new force fields for the compounds. By the aid of experimental spectra all the unknown bands in the calculated spectra are assigned and the validity of the results are discussed in comparison to the related literature.

Horowitz-Metzger[4] and Coats-Redfern[5] kinetic methods are used in the DTA/TG/DTG studies of complexes to calculate kinetic parameters (activation energy E^*, entropy ΔS^*, reaction order n, pre-exponential factor A) of the pyrolysis reactions. It was observed that the decompositions occurred in two stages and the % mass losses found experimentally and theoretically were in good agreement.

The reaction order for ligand is found to be unity for complexes at each stages are near to unity again. The first decomposition temperatures and the activation energies of the pyrolysis reactions are correlated to the radii of the metal ions of the complexes

1. M. Schuster, Dissertation, Frankfurter Universitat, Frankfurt, 1986
2. P. Fisher, D. Bougeard, B. Schrader, SPSIM Spektren Simulation, Universitat Essen, FRG, 1989
3. Wilson, Decius, Cross-Molecular Vibrations, Davor Publ. Newyork, 1980
4. H.H. Horowitz and G. Metzger, Anal. Chem., 35 (1963), 1464
5. A.W. Coats and J.P. Redfern, Nature, 201 (1964), 68