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Research Paper :

Theoritical relationship between softness parameters and the stability of thiocyanate bridge in bimetallic tetrathio cyanate complexes

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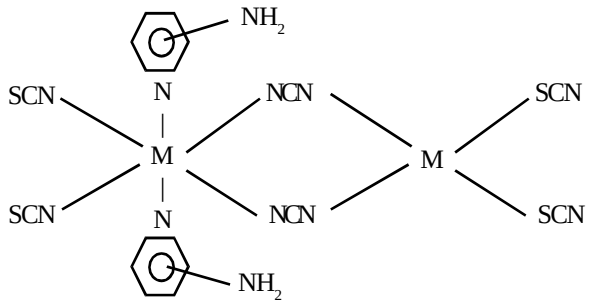
ABSTRACT

The softness parameters of M and M' in respect of the O/m/p-amino pyridine of MM'$(NCS)_4$ type of complexes, have been evaluated.



MNDO calculations were made to get precise values of softness of M and M'. Therefore stability of thiocyanate bridge in M and M' $(NCS)_4$ (M=Co, M' = Hg, Cd, Zn) is given below :

Co/Hg > Co/Cd > Co/Zn

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Complexes of metal thocyanates and selenocyanates have the subject of interest, and different workers have studies their different aspects. Burmeister (1966) described the effects of a large number of ligands on the change of M-SCN bonding to M-NCS and also reviewed linkage isomerism (1968) which included thiocyate ions. Bailey *et al.* (1971) discussed the infrared spectra of bimetallic tetrathio cyanates and selenocynates and described the effect of change of metal on the infrared active bands associated with the thiocyanate and selenocyanate ions. The Lewis-acid character of bimetallic tetra thiocyanate and selenocyanate of $CoHg(XCN)_4$ (X=S,Sc) type have been described in a review article by Singh. The corresponding selenocyanates have also been studied but comparatively less is reported in the literature.

Both bimetallic tetra thiocyanates and selenocyanates of general formula MM' $(XCN)_4$, M=Mn(II), Fe(II), Co(II), Ni(II), M'= Zn(II), Cd(II), Hg(II), Pd(II), X=S, Se can be used as Lewis acids because the co-ordination numbers of M and M' in MM' $(XCN)_4$ are four rather than their maximum of six.

Singh *et al.* extended the work to other bimetallic tetrathiocyanates and also studied the corresponding tetra selenocyanated (1979). They observed that the nature of these tetra thoicyanates and selenocyanates depends mainly upon the nature of M and M' in MM' $(NCS)_4$ (X=S, Se) and also upon the base strength of the lignads.

MATERIALS AND METHODS

The quantum mechanical equation which has been used for quantitative evaluation of softness values of metal and base ions is given below:-

$$E_n^{\#} = IP_n - b_2 (IP_n - EA_n) - (X_s(C_s^n)^2 / R_s) (1-1/\check{C}) + q_s - 2b^2 X_s (C_s^n)^2 \quad .....(I)$$

$$E_m^{\#} = IP_m - a^2 (IP_m - EA_m) - (X_r(C_r^m)^2 / R_r) (1-1/\check{C}) + q_r - 2b^2 X_s(C_s^m)^2 \quad .....(II)$$

The ionisation potential (IP), charge (q), radius (R), electron affinity (EA), desolvation energy (DE) are the essential requirements for the solution of the above equation. These values are available for ions, but in neutral molecules these values are not available.

The original equation is modified, for evaluation of softness values in neutal Lewis acids and bases. With the help of modified equation the softness of a large number of neutral Lewis acids and neutral Lewis bases were calculated. The values so calculated are termed as