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A Semi-Empirical Study on Metal Ion/Murexide Complexation

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**Abstract:** Modeling of the metal ion/ligand complexation reactions between divalent metal cations ( $M^{2+}$ ) and hydrophilic tridentate ligand murexide ( $Mu^-$ ) in water, water+glycerol, and in glycerol was carried out. Kinetic studies showed that the rate of the reaction is very dependent on the metal ion, with  $Zn^{2+} > Ni^{2+}$ , but, reactions are slower in dispersed glycerol than in dispersed water. Theoretical calculations, which have shown a metal ion dependence, were consistent with the experimental observations. The entropy values calculated in all solvents were negative and were similar in value, indicating that these spontaneous reactions are enthalpy driven.

**Key Words:** Murexide, complexation, glycerol, metal ion.

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