INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Magnetic Field Induced Transitions and Exchange Interactions in Columbites

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SHORT ABSTRACT

The studies on strongly correlated aspects of the Columbite family of compounds have become more intense in recent years because of their novel magnetic and electronic properties which provide impetus to the scientific community in searching for practical systems in the field of 'Quantum Magnets' that can be used to test the predictions of theoretically solvable models. Columbites are generally complex transition metal oxides with the chemical formula AB_2O_6, where both A and B site atoms are transition metal cations with divalent and pentavalent oxidation states, respectively. These systems are unique in the sense that they exhibit quantum critical behavior, magneto-electric coupling, tri-critical behavior, field-induced metamagnetic transitions, etc. The exotic physical properties of Columbites have been utilized in various industrial applications and they have huge commercial demand. In this thesis, we tried to establish the complete H-T phase diagram and understand the magnetic ground spin configuration of magnetic ions in the Columbite family of compounds. Nonetheless, we also focused on the determination of exchange constants between the magnetic cations by using different experimental results and theoretical models which is the strongest point of the current thesis. Also, the research work related to the dielectric response of columbites, mainly the analysis pertaining to the temperature and frequency dependence of ac-conductivity by using different theoretical models is unique. Magnetic measurements on $MnNb_2O_6$ reveal the robust anti-ferromagnetic ordering below T_N = 4.33 K which is further confirmed by heat capacity measurements (T_N = 4.36 K). The high-temperature paramagnetic susceptibility is fitted with modified Curie-Weiss law ($\chi = \chi_0 + C/(T-\Theta)$) which yields Θ = -17 K and C = 4.38 emu K $mol^{-1}Oe^{-1}$. Using these magnitudes, we further estimated the magnitude of effective magnetic moment μ which is ~ 5.920 μ_B per Mn^{2+} ion in $MnNb_2O_6$ system, and the corresponding g-factor 2.001 for Mn^{2+}. Moreover, this compound shows magnetic field-induced spin-flop transition at H_{sf} = 18 kOe. We provide a clear and vivid picture of the *H-T* phase diagram of the $MnNb_2O_6$ system which shows the triple point at T_{TP} (H, T) = (18 kOe, 4.06 K). Next, we employed the molecular field theory (MFT) and estimated the intrachain and interchain exchange constants whose magnitudes turn out to be J_0/k_B = -1.08 K and $J_\perp/k_B$ = -0.61 K, respectively. Furthermore, we presented the ac-conductivity ($\sigma(\omega,T)$) analysis exhibiting the thermally driven, Arrhenius-like behavior which is predominant at temperatures above 300 K. However the Double power law-based explanation of

the dispersive behavior of electrical conductivity $\sigma(\omega,T)$ studies provide evidence for the correlated-barrier hopping (CBH) conduction mechanism of charge carriers for temperatures between 173 K and 473 K. Moreover, the dynamical response of complex electric modulus spectra ($M^*(\omega,T)$) and the corresponding analysis using the Kohlrausch-Williams-Watts method shows the non-Debye type relaxation process is prevalent in the $MnNb_2O_6$ system with decay function exponent β lying between 0.794 and 0.840. Besides we presented the magnetic properties of tantalite Columbite $MnTa_2O_6$ which provide evidence of the AFM ordering with Néel temperature T_N = 5.97 K consistent with the T_N = 6.00 K determined from the peak in the C_p vs. T data. Further we estimated the critical exponents α = 0.10(0.13) for $T > T_N$ ($T < T_N$) from experimental data of C_p vs. T near T_N through the mathematical fits to the equation: $C_p = A|T\text{-}T_N|^{-\alpha}$. Magnetic studies reveals μ_{eff} = 5.96 μ_B per Mn^{2+} ion and yields the effective spin S = 5/2 with g = 2.015. Finally, we mapped the H-T phase diagram using the M-H isotherms and M-T data measured at different H yielding the tricritical point T_{TP} (H, T) = (17.0 kOe, 5.69 K) for $MnTa_2O_6$. Using the magnitudes of Θ and T_N and molecular field theory, the antiferromagnetic exchange constants J_0/k_B = -1.5 ± 0.2 K and $J_\perp/k_B$ = -0.85 ± 0.05 K are determined for the $MnTa_2O_6$ system. Further, we explored the magnetic ground state properties of $CoNb_2O_6$ which shows that the ground state of Co^{2+} has the effective spin S = 1/2 and not S = 3/2 expected from Hund's rules, the S = 1/2 ground state resulting from the combined effects of non-cubic crystalline field and spin-orbit coupling. On the other hand, by means of the experimentally obtained g value with S =1/2 and the experimental critical fields for spin flips we calculated the interchain antiferromagnetic exchange constants J_1/k_B (= -0.42 K) and J_2/k_B (= -0.67K) along with intrachain ferromagnetic exchange constant J_o/k_B = 6.2 K. Next, we further explored the rich magnetic properties of the $NiNb_2O_6$ system.