

D046 MAGNETIC PROPERTIES OF $[(CO)_3MoFe_3S_4(SR)_3]^{3-}$
(R=Bz,Et,Ph), A SYNTHETIC CUBANE-TYPE CLUSTER
SIMULATING THREE-IRON CENTERS IN PROTEINS.

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We have recently described the synthesis and certain physicochemical properties of the heterometal cubane-type cluster $[MoFe_3S_4]^0$ [1]. There is substantial interest in this type of complexes because of the presence of trinuclear magnetically coupled units in proteins [2].

The X-ray structure determination of $(Et_4N)_3$ revealed the familiar cubane-type structure but with long Mo-S and Mo-Fe bonds indicating that this anion can best be described as a weak complex of the $Mo(CO)_3$ unit and the $[Fe_3S_4(SR)_3]^{3-}$ cluster. EPR studies suggest that the total ground spin state has integer spin. Magnetic susceptibility studies exhibit Curie-type behavior at low temperatures and establish $S=2$ as the ground state.

The zero field Moessbauer spectra at 4.2 K for the anion with R=Bz consist of a superposition of two quadrupole doublets with intensity ratio 2:1 and isomer shifts of 0.44 and 0.34 mm/sec for the higher and lower intensity component respectively. These values are typical of a $Fe^{2+}-Fe^{3+}$ delocalized pair and an Fe^{3+} respectively. The magnetically perturbed Moessbauer spectra for applied fields up to 6T show two magnetically distinct subsites with intensity ratio 2:1. The first one has negative and the second has positive hyperfine coupling constants with average values of -117 and 136 kG respectively. The fine and hyperfine parameters are very similar to those obtained for D. gigas Ferredoxin II (2). The low temperature spectra of the other two complexes under study (R=Ph, R=Et) exhibit very similar patterns as in the case of R=Bz.

1. D.Coucouvanis, S.Al-Ahmad, A.Salifoglou, W.R.Dunham and R.H. Sands, Angew. Chem. Int. Ed. Engl. 27 (1988) 1353.
2. V.Papaefthymiou, J.-J.Girerd, I.Moura, J.J.G.Moura and E. Munck, J. Am. Chem. Soc. 109 (1987) 4703.