

## H08

FUNCTIONAL AND STRUCTURAL MODEL COMPLEXES OF  
ZINC METALLOENZYMES USING LIGANDS BASED ON  
*cis,cis*-1,3,5-TRIAMINOCYCLOHEXANE

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The zinc-containing metalloenzyme *Carbonic Anhydrase* has received much attention in recent years due to its very rapid reversible conversion of carbon dioxide and bicarbonate [1]. Small molecule models have been used to elucidate the roles of various amino acids in the enzyme's active site, and it has been proposed that models which mimic the secondary coordination sphere of the zinc (II) in the enzyme may act as functional models.

In an attempt to model the secondary coordination sphere of the zinc (II) ion in *Carbonic Anhydrase*, we have prepared a new ligand [2] that, when complexed to a metal, forms a stereochemically-rigid cavity, Figure 1. This cavity 'surrounds' exogenous ligands [2,3] which are bound to the metal ion, and as such, the cavity mimics amino acid residues that are in the zinc's secondary coordination sphere in the enzyme. We have synthesized a range of zinc (II) and cobalt (II) salts of the ligand. These include the zinc (II) and cobalt (II) hydroxide complexes which are structural models of the zinc and cobalt forms of the enzyme. Furthermore, we have shown that the cobalt (II) hydroxide complex is active in the reversible binding of CO<sub>2</sub>.

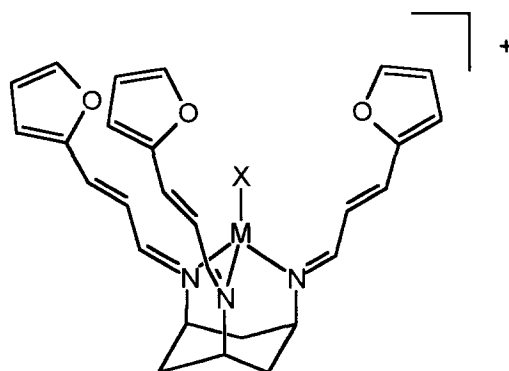


Figure 1.

#### References

1. E. Kimura, *Progress in Inorganic Chemistry*, Vol. 41, K. D. Karlin, Ed. Wiley & Sons, Inc., 1994, p443 and references therein.
2. L. Cronin, B. Greener, M. H. Moore and P. H. Walton, *J. Chem Soc., Dalton Trans.*, 1996, 3337.
3. B. Greener, M. H. Moore and P. H. Walton, *Chem. Commun.*, 1996, 27.