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Review

The role of metal substitution in the promiscuity of natural and artificial carbonic anhydrases

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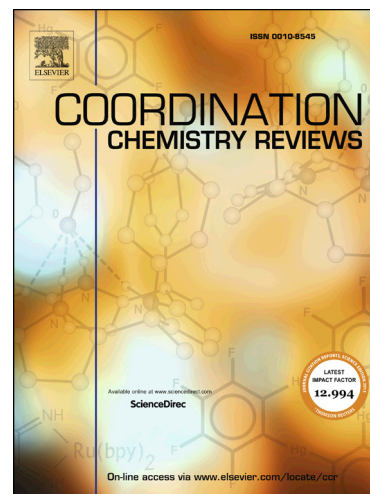
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The role of metal substitution in the promiscuity of natural and artificial carbonic anhydrases

Paolo Piazzetta^{a*}, Tiziana Marino^{a*}, Nino Russo^a and Dennis R. Salahub^b

^aDipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, I-87036 Rende, Italy

^bDepartment of Chemistry, CMS – Centre for Molecular Simulation, IQST – Institute for Quantum Science and Technology, Quantum Alberta, University of Calgary, 2500 University Drive N.W., Calgary, Alberta, Canada T2N 1N4 and Department of Chemistry, Henan University of Technology, Zhengzhou, 450001, China

Highlights:

- Insight is gained into the mechanisms of reactions catalyzed by the promiscuous carbonic anhydride enzyme family.
- Substituting Zn for Co slightly increases the efficiency while Cu decreases the activity of the enzyme.
- The Cd variant, which has two cysteine residues in its first coordination shell, chooses a different reaction mechanism from the native Zn enzyme, Cd preferring a bidentate mode of binding bicarbonate.
- Carbodiimide acts as a competitive inhibitor.
- Rh-CA is predicted to be an effective catalyst for the hydrogenation of CO₂, aided by two explicit water molecules that lower the activation barrier of the rate-limiting step, the release of the product.

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