



Chemical modelling of the uptake process of carbonyl sulphide (COS) by the enzyme carbonic anhydrase

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Carbonic anhydrase (CA) is an ubiquitous zinc enzyme found in all living organisms. It is of vital importance in the CO₂ exchange process accelerating the reversible hydration of CO₂ by a factor of 10⁷ as compared to the uncatalyzed reaction. Furthermore, CA plays a very significant role in the global regulation of carbonyl sulphide (COS) in the atmosphere since it is the key enzyme for the biological uptake and consumption of this important trace gas. We have extended our investigations of the CA cycle with the model system [(H₃N)₃ZnOH]⁺ and CO₂ by studying the hydration of COS. CA is reported to convert COS into CO₂ and H₂S. We investigated the hydration mechanism of COS by using density functional theory to elucidate the details of the catalytic cycle. We demonstrate that nature selected a surprisingly elegant and efficient group of reactants, the [L₃ZnOH]⁺/CO₂/H₂O system, that helps to overcome any deactivation of the ubiquitous enzyme CA in nature.