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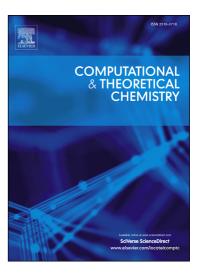
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Competing nitrile hydratase catalytic mechanisms: is cysteine-sulfenic acid acting as a nucleophile?

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ABSTRACT ARTICLE INFO 2009 Elsevier Ltd. All rights reserved. Article history: Received The full catalytic mechanism for nitrile hydratase is explored, involving cysteine-sulfenic acid Revised acting as a nucleophile, activating a water molecule to attack nitrile substrates. The iminol Accepted intermediate undergoes tautomerization to form the amide product. The computed enthalpies are Available online closely related to experimental values, suggesting the current mechanism with two water molecules should be further investigated. Keywords: Quantum mechanics/molecular mechanics Nitrile hydratase Sulfenic acid Amide-iminol tautomerism

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