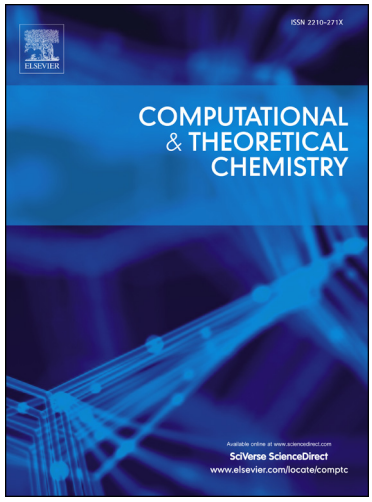

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Competing nitrile hydratase catalytic mechanisms: is cysteine-sulfenic acid acting as a nucleophile?

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ABSTRACT

The full catalytic mechanism for nitrile hydratase is explored, involving cysteine-sulfenic acid acting as a nucleophile, activating a water molecule to attack nitrile substrates. The iminol intermediate undergoes tautomerization to form the amide product. The computed enthalpies are closely related to experimental values, suggesting the current mechanism with two water molecules should be further investigated.

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