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Crystallographic Snapshot of an Arrested Intermediate in the Biomimetic Activation of CO_2

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The authors of this Communication now believe that a single crystal of a $[(n\text{-}C_4H_9)_4N]^+[CH_3CO_2]^-$ impurity in their bulk sample was misidentified as $[(n\text{-}C_4H_9)_4N]^+[O_2C\cdots OH]^-$ in their original report. This was interpreted as an arrested intermediate in the base-mediated activation of CO_2, indicating an egregiously long C—O(H) bond that is in fact the C—C bond of the $[CH_3CO_2]^-$ salt. However, the biomimetic nature of the hydrophobic pockets in $[(n\text{-}C_4H_9)_4N]^+[CH_3CO_2]^-$ still offers valuable insights into the substrate binding sites in human carbonic anhydrase II, since the geometry of the weak hydrogen bonding is identical to the interactions that tether CO_2 to the pockets of this metalloenzyme. Moreover, the computational component of the original study revealed a three-stage process for the base-mediated activation of CO_2, which is independent of the experimental structural study.