

Theoretical Study of Water Cluster Catalyzed Decomposition of Formic Acid

Satoshi Inaba^{*,†,‡}

*School of International Liberal Studies, Waseda University, 1-6-1 Nishiwaseda, Shinjuku-ku,
Tokyo 169-8050, Japan, and Department Terrestrial Magnetism, Carnegie Institution of
Washington, 5241 Broad Branch Road, NW, Washington, DC 20015-1305, USA*

E-mail: satoshi.inaba@waseda.jp

Phone: 81-3-5286-1730. Fax:

^{*}To whom correspondence should be addressed

[†]Waseda University

[‡]Carnegie Institution of Washington

Supporting Information Available

Table S1: The rate constants (1/s) for the decomposition of a cis-HCOOH and a trans-HCOOH catalyzed by n water molecules as a function of the temperature ($^{\circ}\text{C}$).

| cis-HCOOH | | | | | | |
|-------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Temperature | $n = 0$ | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ |
| 25 | 6.7×10^{-28} | 1.6×10^{-24} | 4.3×10^{-21} | 1.3×10^{-21} | 4.4×10^{-18} | 3.3×10^{-18} |
| 125 | 6.3×10^{-21} | 1.5×10^{-16} | 1.8×10^{-13} | 1.5×10^{-13} | 1.1×10^{-10} | 1.5×10^{-10} |
| 225 | 1.7×10^{-15} | 2.1×10^{-11} | 6.9×10^{-9} | 1.1×10^{-8} | 3.2×10^{-6} | 6.2×10^{-6} |
| 325 | 3.9×10^{-11} | 6.5×10^{-8} | 8.1×10^{-6} | 2.1×10^{-5} | 3.1×10^{-3} | 7.6×10^{-3} |
| 425 | 7.6×10^{-8} | 2.1×10^{-5} | 1.3×10^{-3} | 4.7×10^{-3} | 4.3×10^{-1} | 1.3 |
| 525 | 2.5×10^{-5} | 1.7×10^{-3} | 5.8×10^{-2} | 2.8×10^{-1} | 1.8×10^1 | 5.9×10^1 |

| trans-HCOOH | | | | | | |
|-------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Temperature | $n = 0$ | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ |
| 25 | 9.8×10^{-34} | 3.1×10^{-23} | 1.9×10^{-19} | 2.0×10^{-20} | 2.6×10^{-19} | 5.9×10^{-19} |
| 125 | 1.8×10^{-23} | 6.7×10^{-16} | 1.3×10^{-12} | 5.9×10^{-13} | 3.5×10^{-12} | 6.3×10^{-12} |
| 225 | 2.5×10^{-16} | 7.8×10^{-11} | 2.9×10^{-8} | 2.0×10^{-8} | 6.9×10^{-8} | 1.0×10^{-7} |
| 325 | 2.0×10^{-11} | 2.4×10^{-7} | 2.6×10^{-5} | 2.2×10^{-5} | 5.1×10^{-5} | 6.6×10^{-5} |
| 425 | 7.0×10^{-8} | 7.9×10^{-5} | 3.5×10^{-3} | 3.2×10^{-3} | 5.8×10^{-3} | 6.7×10^{-3} |
| 525 | 3.4×10^{-5} | 6.4×10^{-3} | 1.4×10^{-1} | 1.4×10^{-1} | 2.0×10^{-1} | 2.2×10^{-1} |

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