

Supporting Information for

**Temperature and Size Dependence of Characteristic
Hydrogen-Bonded Network Structures with Ion Core
Switching in Protonated (Methanol)₆₋₁₀ -(Water)₁ Mixed
Clusters: A Revisit**

Marusu Katada[†], Po-Jen Hsu[§], Asuka Fujii^{*†}, and Jer-Lai Kuo^{*§}

[†]Department of Chemistry, Graduate School of Science, Tohoku University,
Sendai 980-8578, Japan.

[§]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617,
Taiwan.

* To whom correspondence should be addressed. E-mail:

asukafujii@m.tohoku.ac.jp (A.F.); jlkuo@pub.iams.sinica.edu.tw (J.-L.K.).

Contents

Figure S1 Comparison between the IR spectra of bare H⁺(MeOH)_n(H₂O)₁ (*n* = 7 - 10) measured by monitoring two different dissociation channels.

Complete Reference 75

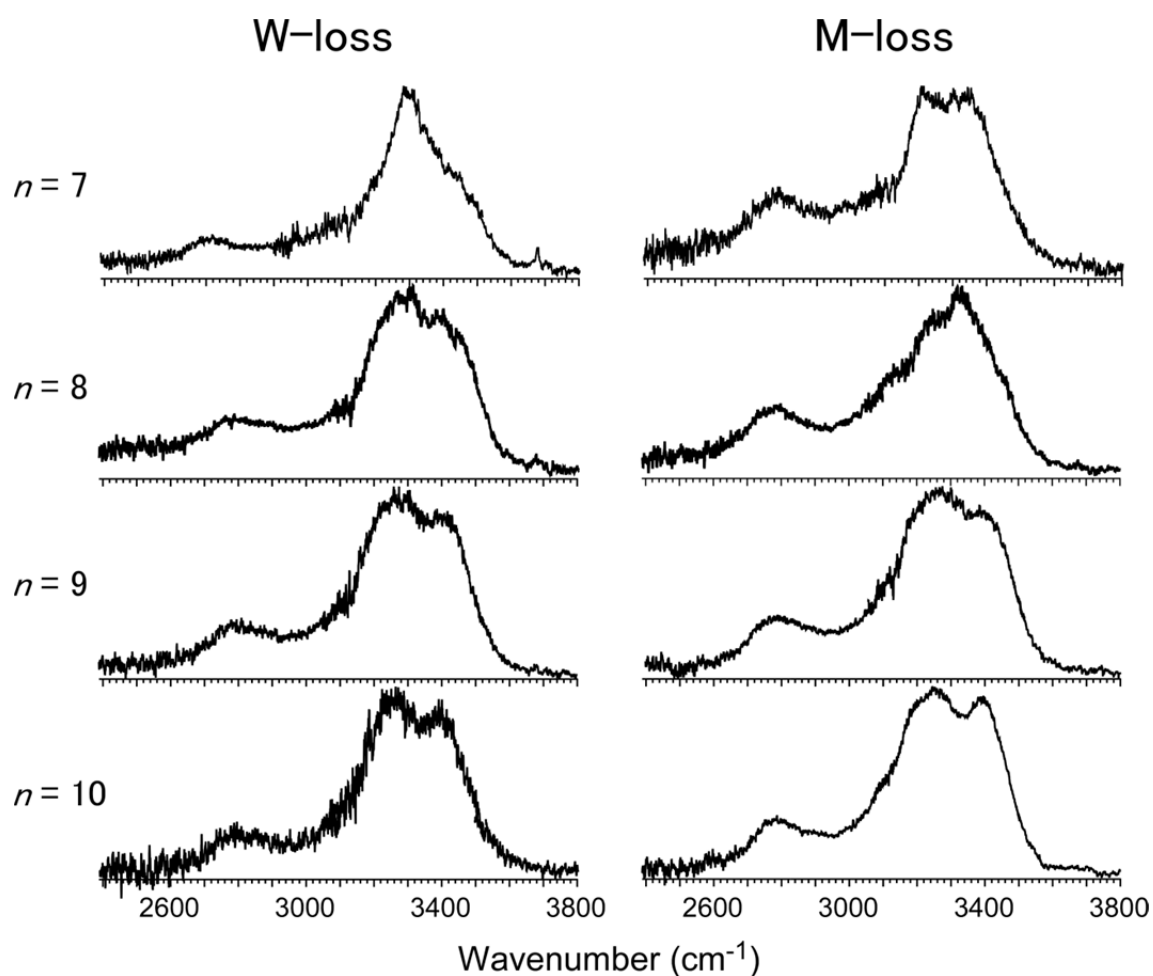


Figure S1 Comparison between the IR spectra of bare $\text{H}^+(\text{MeOH})_n(\text{H}_2\text{O})_1$ ($n = 7 - 10$) measured by monitoring the water (W) -loss dissociation channel (left column) and the methanol (M) -loss dissociation channel (right column). Note that differences between the spectra at the same size become negligible with increasing cluster size (n).

Complete Reference 75

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision E.01, Gaussian, Inc., Wallingford CT, 2009.