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## **Supporting Information**



Positive ion mass spectrum of ions from a low power input (0.5W) plasma of acrylic acid.

Scheme from Ref. 10:



Scheme 1

Selected Ion flow Tube Studies to Investigate the Formation of Acrylic and Propionic Acid Protonated Clusters in Low Power, Low Pressure RF Plasmas (C A Mayhew & R D Short)

## Gaussian Calculations:

Gaussian 3, *Revision C.02*, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria,
M.A. Robb, J.R. Cheeseman, J.A.M. Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M.
Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N.
Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J.
Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.
E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R.
Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W.
Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V.
G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A.
D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S.
Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I.
Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A.
Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, M. W. Chen, W. Wong, C.

Figure (below) provides an image of a structure of the protonated dimer of acrylic acid, produced using Gaussian (B3LYP +G(d,p)). The calculations have shown that there are a number of hydrogen bonded complexes with similar energies for formation. All structures show that the two acrylic acids are bound through a hydrogen bond via the sharing of a proton.



Structure of the hydrogen bonded protonated acrylic acid dimer determined using Gaussian. For this structure the enthalpy of formation is  $\Delta H = -133 \text{ kJ mol}^{-1}$ . (Other comparable hydrogen bonded structures have been calculated with similar energies with the range of  $\Delta H$  being 124-137 kJ mol<sup>-1</sup>.)

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