Supplemental Information

Online Monitoring the Hydrolysis of Uranium Hexafluoride for Intermediates by Cryogenic Layering and FTIR

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Chart, line chart

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Figure S1. Infrared spectrum of the UF6 hydrolysis at (a) initial cryogenic layering and (d) final product state. Principal component analysis provides two principal components**,** PC1 (b) and PC2(c) that can better show the differences in stable intermediate formation.

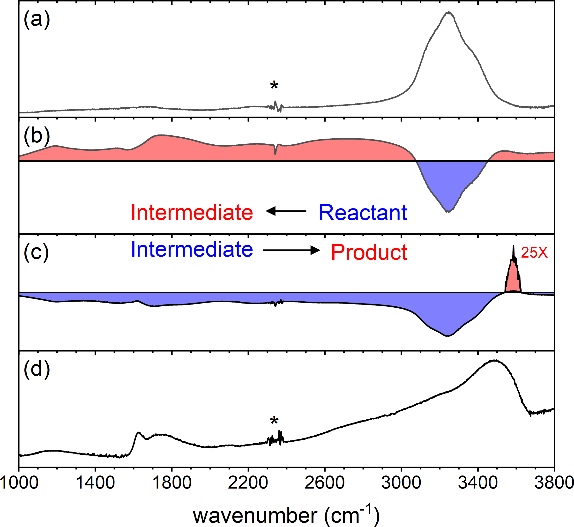


Figure S2. Infrared spectrum of the UF6 hydrolysis at (a) initial cryogenic layering and (d) final product state. Principal component analysis provides two principal components, PC1 (b) and PC2 (c) that can better show the differences in stable aqueous spectrum and proton transfer process.



Figure S3. Score plot of the data set showing a clear reaction pathway is captured by PC1 and PC2.

Table of PCA Eigen Values and Variances:

|  |  |  |  |
| --- | --- | --- | --- |
| Principal Component Number | Eigenvalue | Percentage of Variance (%) | Cumulative (%) |
| 1 | 0.27076 | 86.35469 | 86.35469 |
| 2 | 0.02269 | 7.23675 | 93.59145 |
| 3 | 0.0104 | 3.31771 | 96.90915 |
| 4 | 0.00415 | 1.32202 | 98.23117 |
| 5 | 0.00301 | 0.9603 | 99.19148 |
| 6 | 0.00117 | 0.37356 | 99.56504 |
| 7 | 5.07E-04 | 0.16158 | 99.72661 |
| 8 | 3.20E-04 | 0.10208 | 99.8287 |
| 9 | 1.50E-04 | 0.04769 | 99.87638 |
| 10 | 8.34E-05 | 0.0266 | 99.90298 |
| 11 | 6.25E-05 | 0.01994 | 99.92292 |
| 12 | 4.34E-05 | 0.01383 | 99.93675 |
| 13 | 3.62E-05 | 0.01156 | 99.9483 |
| 14 | 2.49E-05 | 0.00795 | 99.95625 |
| 15 | 2.14E-05 | 0.00681 | 99.96306 |
| 16 | 1.78E-05 | 0.00567 | 99.96874 |
| 17 | 1.22E-05 | 0.0039 | 99.97264 |
| 18 | 1.06E-05 | 0.00339 | 99.97603 |
| 19 | 7.63E-06 | 0.00243 | 99.97846 |
| 20 | 6.76E-06 | 0.00216 | 99.98062 |
| 21 | 5.98E-06 | 0.00191 | 99.98252 |
| 22 | 5.18E-06 | 0.00165 | 99.98417 |
| 23 | 4.92E-06 | 0.00157 | 99.98574 |
| 24 | 3.35E-06 | 0.00107 | 99.98681 |
| 25 | 3.18E-06 | 0.00102 | 99.98783 |
| 26 | 2.97E-06 | 9.48E-04 | 99.98877 |
| 27 | 2.83E-06 | 9.02E-04 | 99.98968 |
| 28 | 2.33E-06 | 7.44E-04 | 99.99042 |
| 29 | 2.18E-06 | 6.95E-04 | 99.99112 |
| 30 | 2.16E-06 | 6.90E-04 | 99.9918 |
| 31 | 1.81E-06 | 5.79E-04 | 99.99238 |
| 32 | 1.65E-06 | 5.27E-04 | 99.99291 |
| 33 | 1.60E-06 | 5.11E-04 | 99.99342 |
| 34 | 1.50E-06 | 4.78E-04 | 99.9939 |
| 35 | 1.36E-06 | 4.35E-04 | 99.99433 |
| 36 | 1.31E-06 | 4.16E-04 | 99.99475 |
| 37 | 1.15E-06 | 3.68E-04 | 99.99512 |
| 38 | 1.13E-06 | 3.60E-04 | 99.99548 |
| 39 | 1.03E-06 | 3.30E-04 | 99.99581 |
| 40 | 9.49E-07 | 3.03E-04 | 99.99611 |
| 41 | 8.96E-07 | 2.86E-04 | 99.9964 |
| 42 | 8.56E-07 | 2.73E-04 | 99.99667 |
| 43 | 8.11E-07 | 2.59E-04 | 99.99693 |
| 44 | 7.49E-07 | 2.39E-04 | 99.99717 |
| 45 | 6.91E-07 | 2.20E-04 | 99.99739 |
| 46 | 6.32E-07 | 2.02E-04 | 99.99759 |
| 47 | 5.97E-07 | 1.91E-04 | 99.99778 |
| 48 | 5.82E-07 | 1.86E-04 | 99.99797 |
| 49 | 5.33E-07 | 1.70E-04 | 99.99814 |
| 50 | 5.08E-07 | 1.62E-04 | 99.9983 |
| 51 | 4.87E-07 | 1.55E-04 | 99.99845 |
| 52 | 4.69E-07 | 1.50E-04 | 99.9986 |
| 53 | 4.40E-07 | 1.40E-04 | 99.99874 |
| 54 | 4.28E-07 | 1.37E-04 | 99.99888 |
| 55 | 3.87E-07 | 1.24E-04 | 99.999 |
| 56 | 3.69E-07 | 1.18E-04 | 99.99912 |
| 57 | 3.36E-07 | 1.07E-04 | 99.99923 |
| 58 | 3.11E-07 | 9.93E-05 | 99.99933 |
| 59 | 2.90E-07 | 9.25E-05 | 99.99942 |
| 60 | 2.65E-07 | 8.45E-05 | 99.9995 |
| 61 | 2.38E-07 | 7.60E-05 | 99.99958 |
| 62 | 2.29E-07 | 7.29E-05 | 99.99965 |
| 63 | 2.17E-07 | 6.91E-05 | 99.99972 |
| 64 | 2.03E-07 | 6.48E-05 | 99.99979 |
| 65 | 1.86E-07 | 5.93E-05 | 99.99985 |
| 66 | 1.76E-07 | 5.62E-05 | 99.9999 |
| 67 | 1.60E-07 | 5.10E-05 | 99.99995 |
| 68 | 1.44E-07 | 4.60E-05 | 100 |
| 69 | 8.14E-32 | 2.60E-29 | 100 |
| 70 | 1.11E-34 | 3.53E-32 | 100 |
| 71 | 1.84E-35 | 5.87E-33 | 100 |