

Supplementary Information

Reduced electric field and gas temperature effects on chemical product dynamics in air surface dielectric barrier discharges: from macro-physical parameters to micro-chemical mechanisms

Kun Liu,^{*a} Jie Zuo,^a Congfu Ran,^a Minghao Yang,^a Wenqiang Geng,^a Shiting Liu^a and Kostya (Ken) Ostrikov^b

^aThe State Key Laboratory of Power Transmission Equipment & System Security and New Technology, Chongqing University, Chongqing 400044, People's Republic of China. E-mail: liukun@cqu.edu.cn

^bSchool of Chemistry and Physics, Centre for Materials Science, Queensland University of Technology, Brisbane, QLD, 4000, Australia.

Fig. S1 shows the maximum discharge current and voltage waveforms in our experiment.

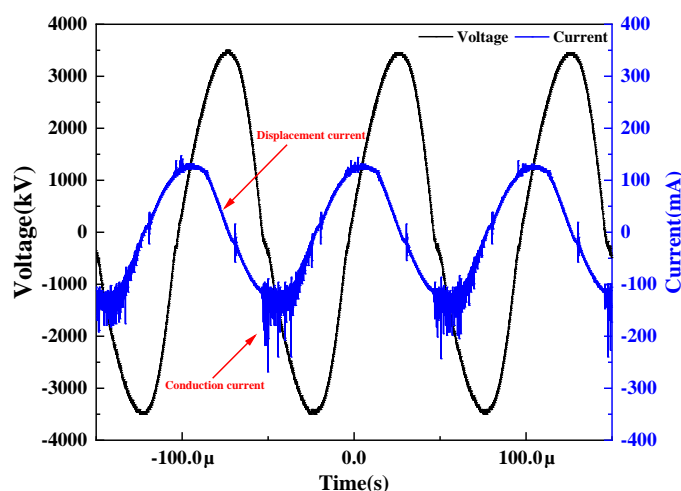


Fig. S1. Typical current-voltage waveforms of the SDBD at 10 kHz & 7 kV.

The gas temperature was obtained from the emission spectrum of molecular emission spectral data at 337.1 nm using Specair 2.2 and MATLAB. The method is as follows: firstly, the actual slit function obtained by the low-pressure mercury lamp was imported into the Specair 2.2 software. Secondly, the standard library was calculated by setting specific relevant software parameters, such as discharge gas composition, resolution, line shape, pressure and wave number to obtain the

standard library. Thirdly, the measured $N_2(C^3\Pi_u \rightarrow B^3\Pi_g, 0-0, 337.1\text{nm})$ spectral data was imported into Specair and normalized for comparison with the standard spectra to acquire the spectral lines closest to the actual measurement. And the corresponding temperature was to be considered as the gas temperature under that condition, as displayed in Fig. S2.

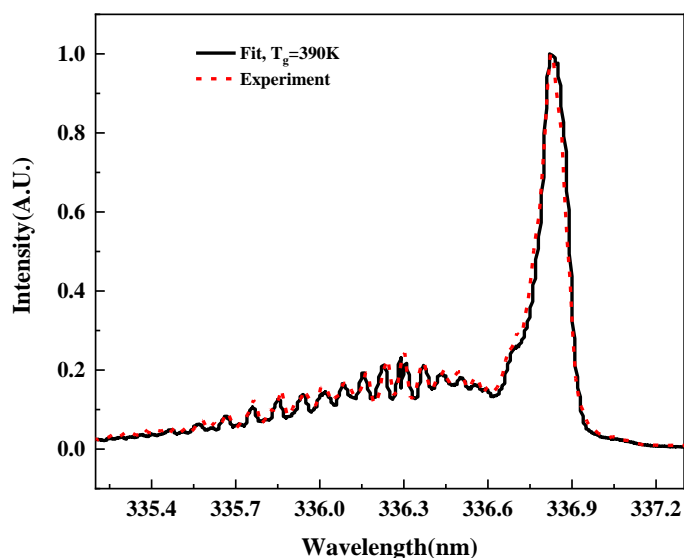


Fig. S2. The result of the gas temperature fitting at 6 kHz & 5.5 kV.

Fig. S3 shows the linearity of the measurement. As shown in Fig. S3(a) and (b), the linearity of FTIR was measured using air to dilute the NO standard gas. Fig. S3(a) displays the variation of NO absorption peaks measured at 450 ppm, 850 ppm, 1000 ppm, 1100 ppm, and 1450 ppm. To demonstrate the results more clearly, Fig. S3(b) was fitted with the absorbance at 1900 cm^{-1} . It can be observed that the linearity of the FTIR measurement is at a good level with $R^2 = 0.99722$. Due to the inability to acquire O_3 standard gas, the linearity of the UV absorption spectra was evaluated as follows: we employed an ozone generator to produce a fixed concentration of O_3 and passed it into the absorption chamber with 2 L/min. Then the air with 8 L/min, 3 L/min, 1.3 L/min, 0.5 L/min and 0 L/min was blown in, respectively, and the absorption spectra at the corresponding dilution contents (20%, 40%, 60%, 80%, 100%) could be obtained, as presented in Fig. S3(c). To better visualize the linearity of the measurement, Fig. S3(d) exhibits the absorbance

fit at 254 nm. It can be pointed out that the linearity of the UV absorption spectra is also at a good level with $R^2 = 0.99432$. Therefore, the calibration check above ensures the reliability of the experimental results.

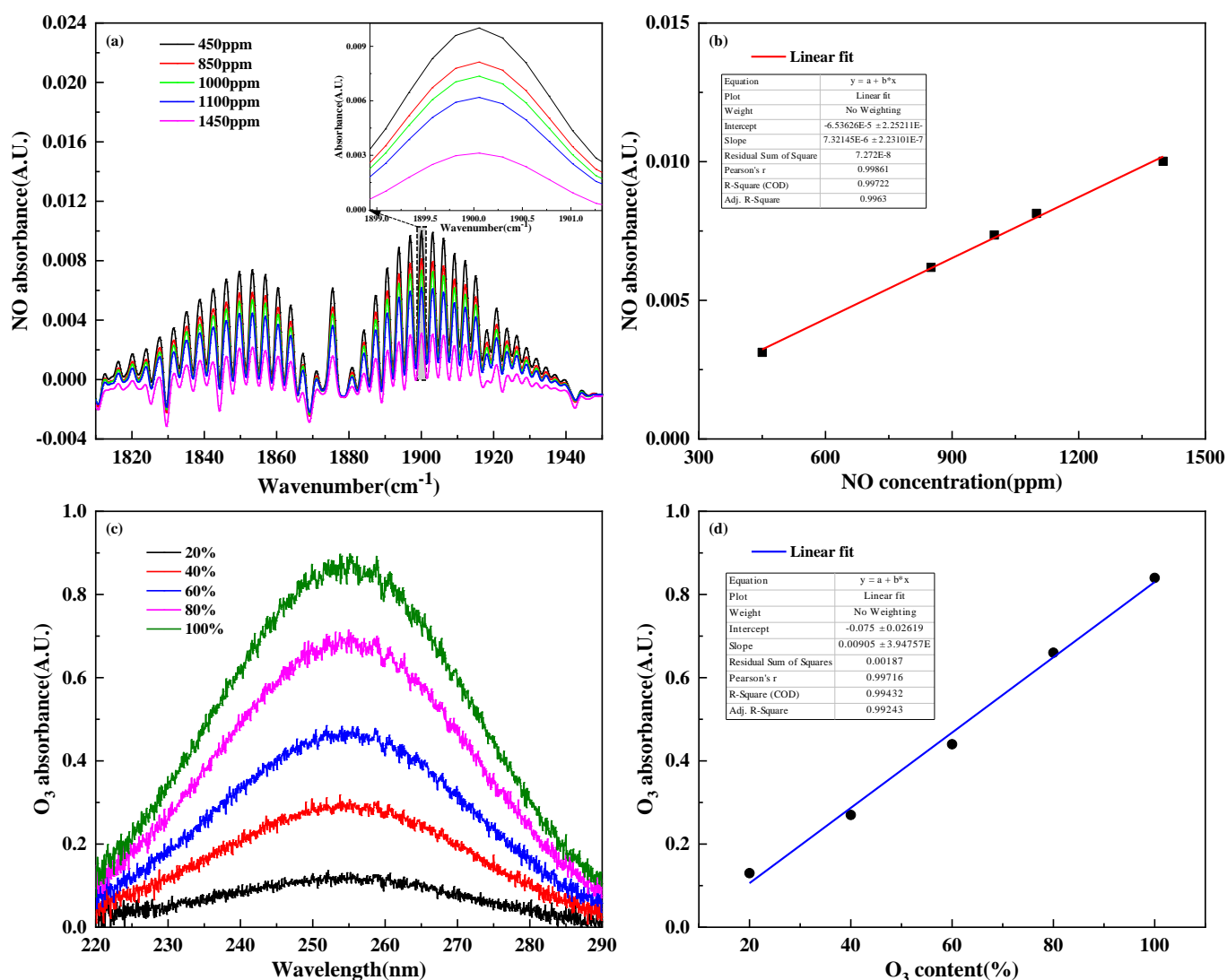
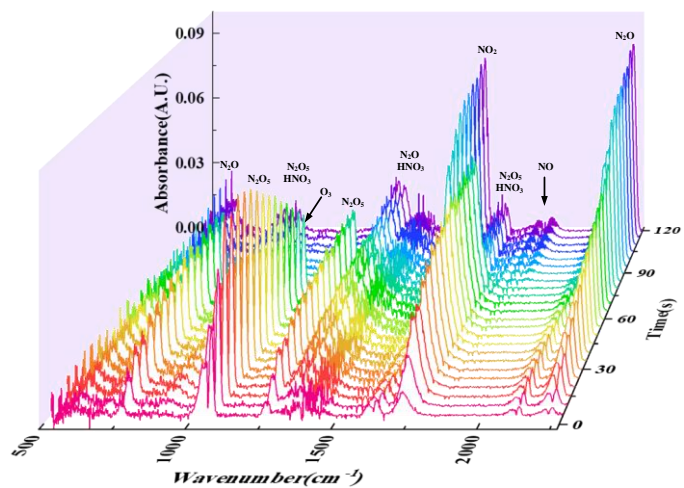


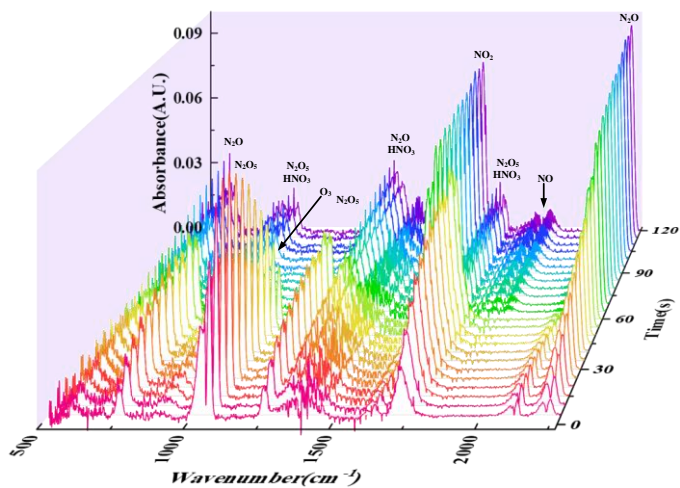
Fig. S3. Verification of the linearity in the relationship of the absorbance versus the concentration of molecules. (a) FTIR calibration spectra of NO; (b) Linear fit for FTIR measurement; (c) UV absorption calibration spectra of O₃; (d) Linear fit for UV absorption measurement.

Fig. S4 shows the *in-situ* FTIR results for all discharge conditions in our experiment. It is evident that O₃ existed at the early stages of the discharge. However, as time passed, O₃ disappeared at a certain moment. This moment was considered to be a sign for the accomplishment of the products change, with the signature product being NO. To be specific, the

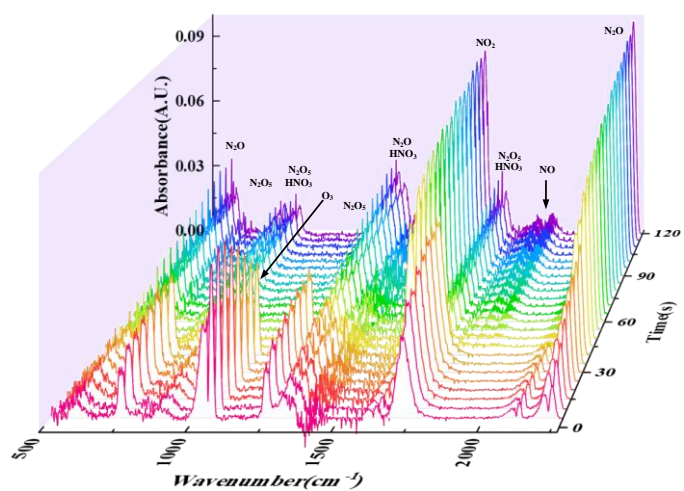
products change faster as the voltage or frequency increases. The following vibration bands were used for reactive species diagnosis: N_2O at 2235 cm^{-1} ; NO at 1900 cm^{-1} ; NO_2 at 1630 cm^{-1} ; N_2O_5 at 1720 cm^{-1} ; and O_3 at 1055 cm^{-1} .



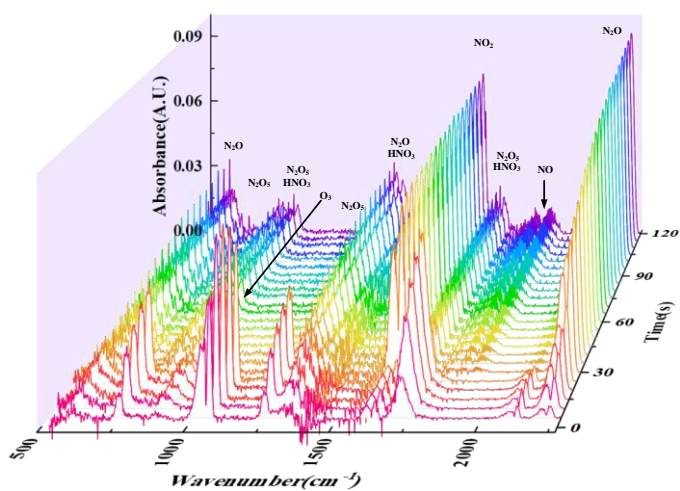
(a) 6kHz & 5.5kV



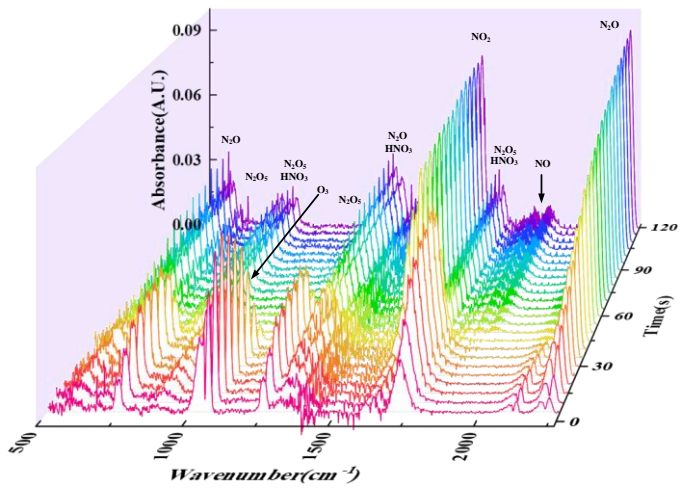
(b) 6kHz & 6kV



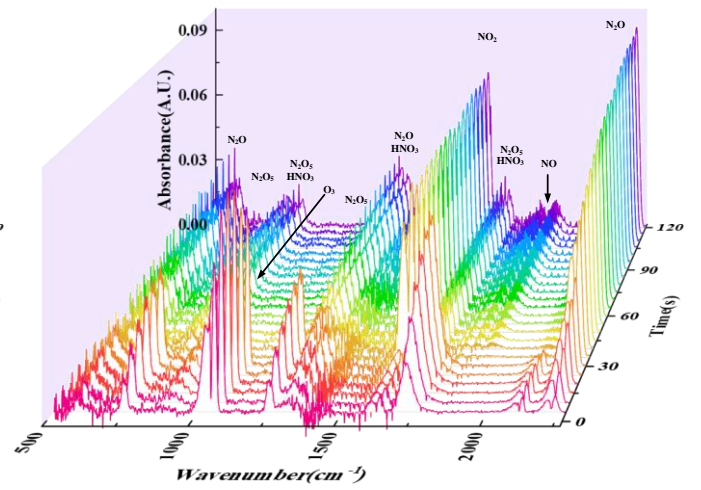
(c) 6kHz & 6.5kV



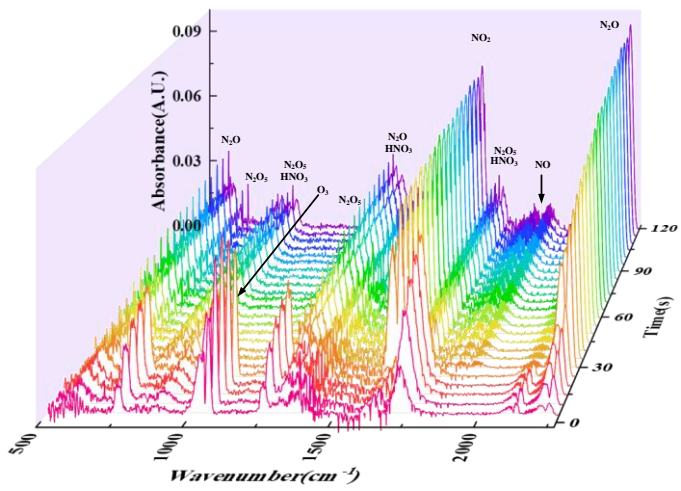
(d) 6kHz & 7kV



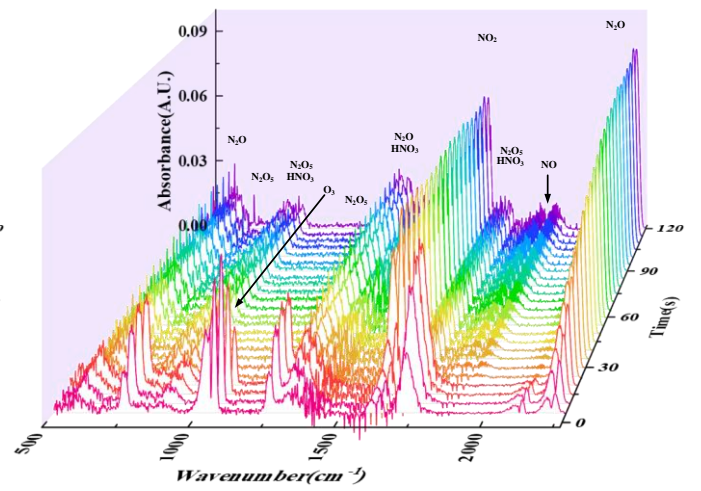
(e) 7kHz & 5.5kV



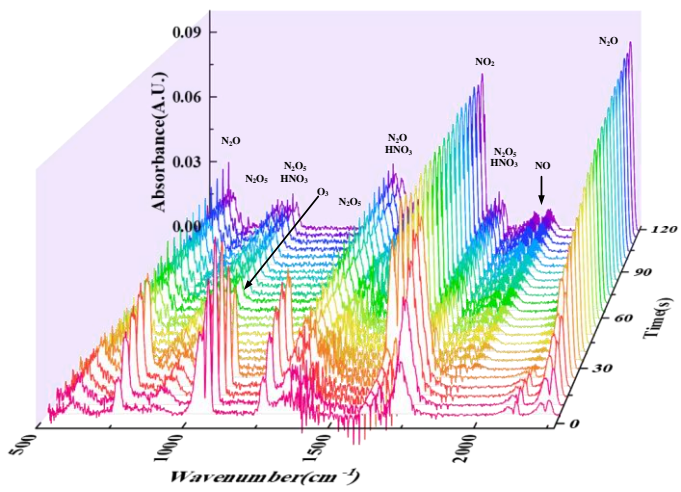
(f) 7kHz & 6kV



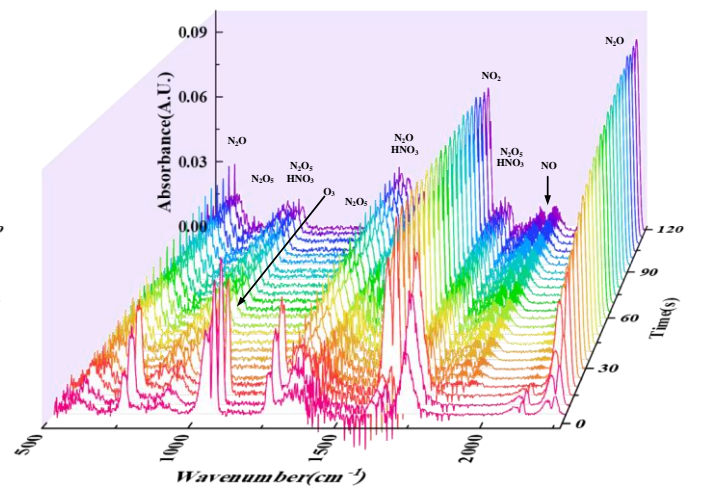
(g) 7kHz & 6.5kV



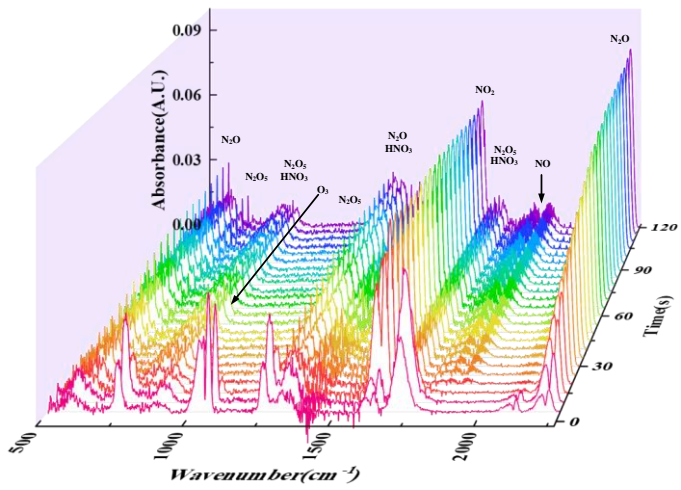
(h) 7kHz & 7kV



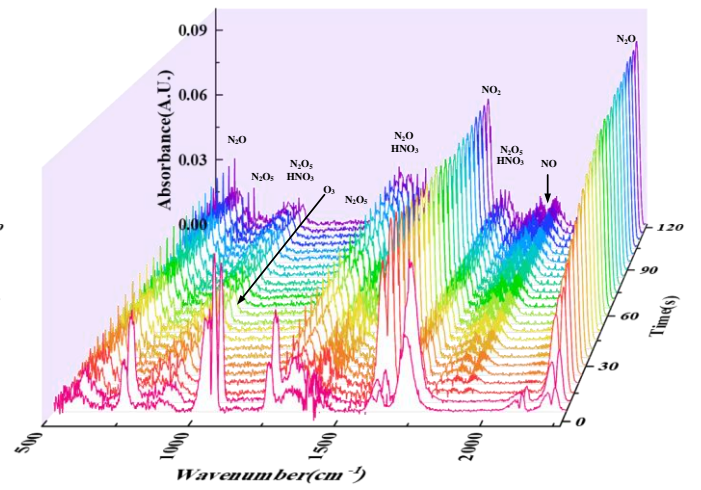
(i) 8kHz & 5.5kV



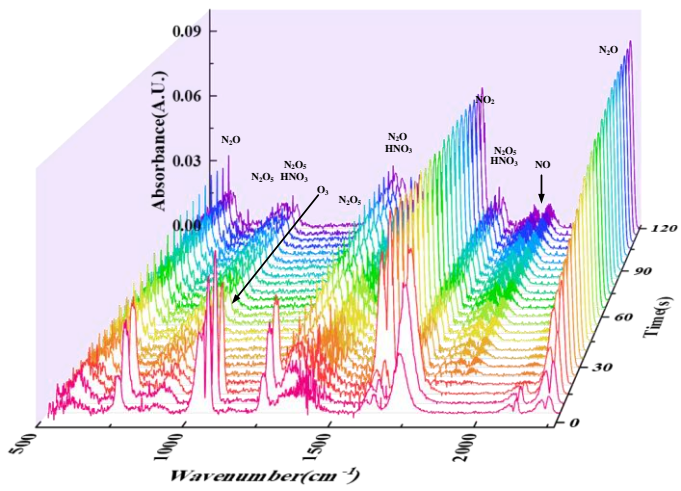
(j) 8kHz & 6kV



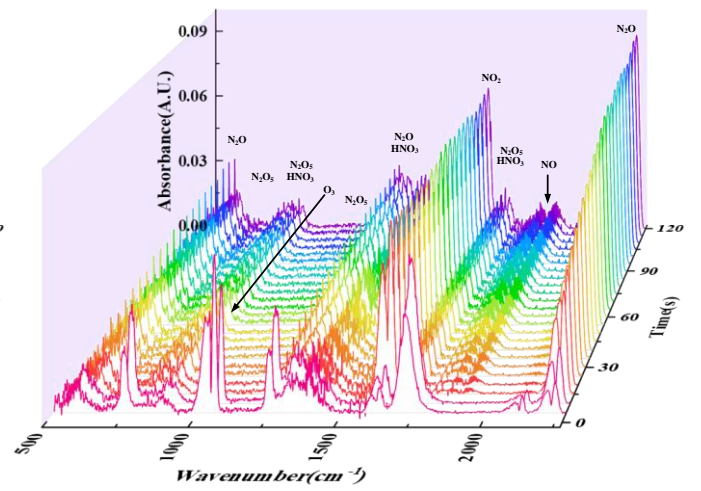
(k) 8kHz & 6.5kV



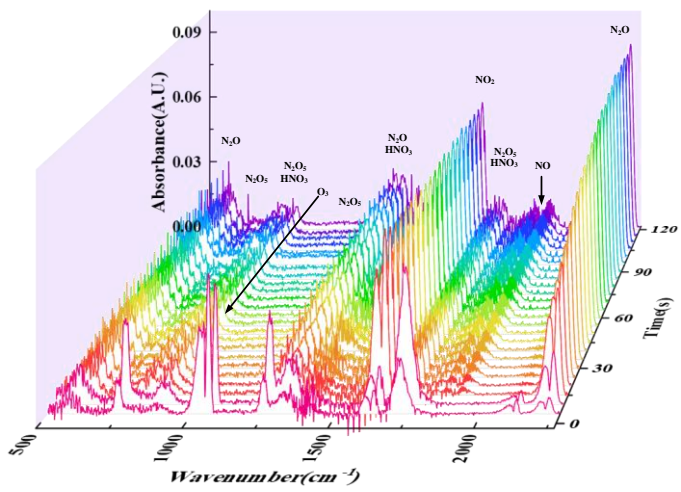
(l) 8kHz & 7kV



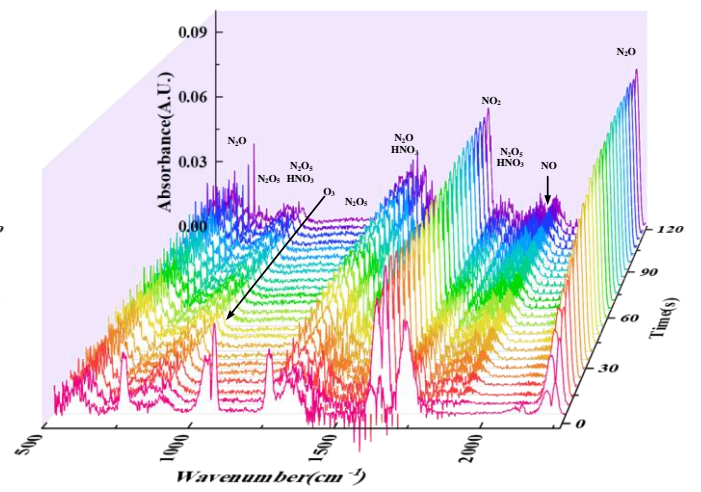
(m) 9kHz & 5.5kV



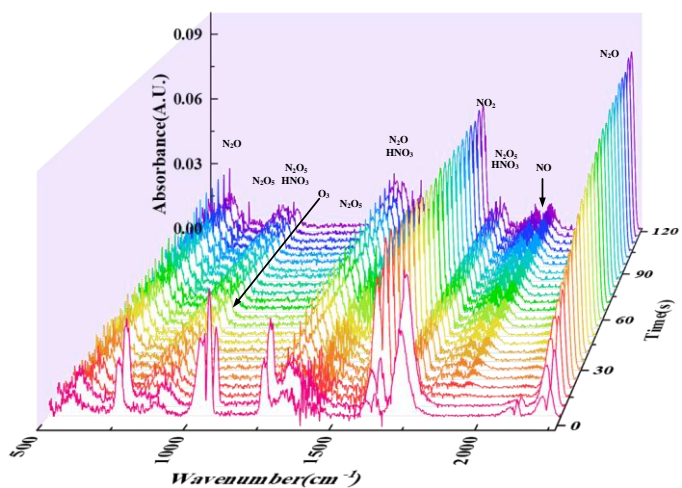
(n) 9kHz & 6kV



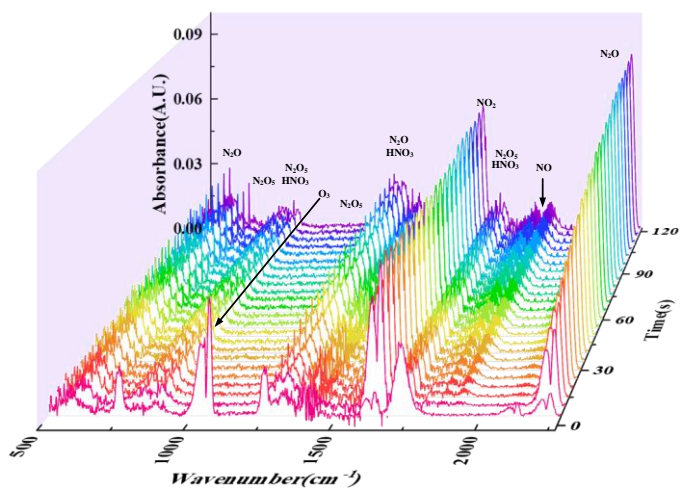
(o) 9kHz & 6.5kV



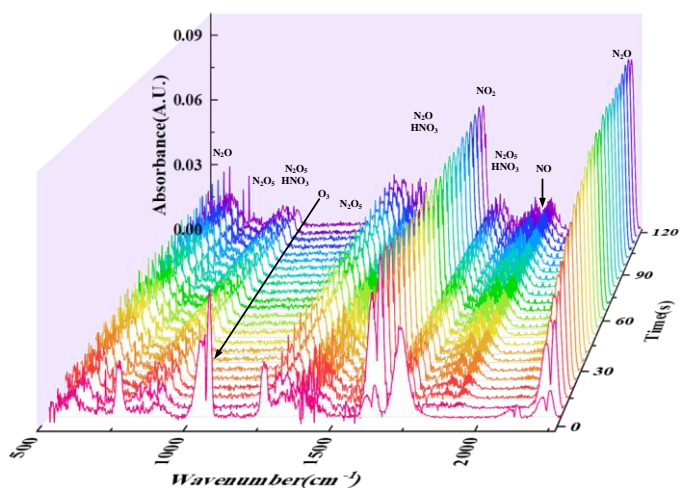
(p) 9kHz & 7kV



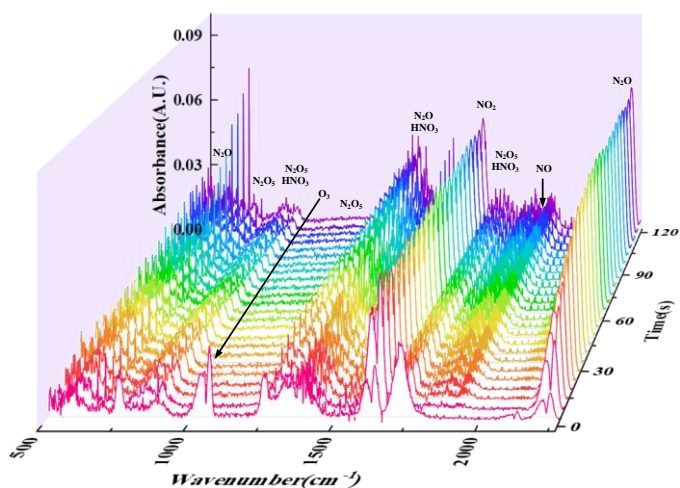
(q) 10kHz & 5.5kV



(r) 10kHz & 6kV



(s) 10kHz & 6.5kV

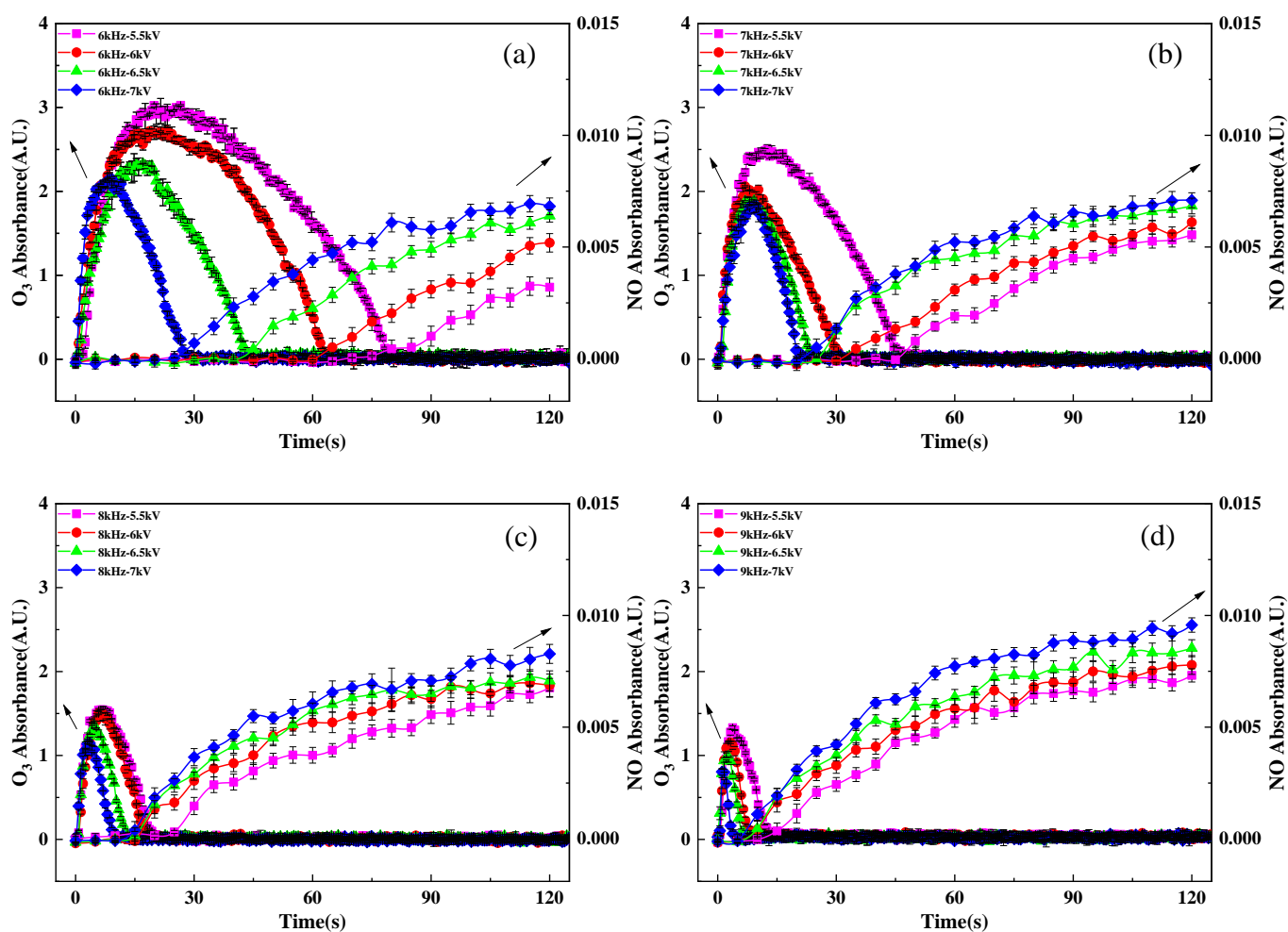


(t) 10kHz & 7kV

Fig. S4. The results of in-situ FTIR spectra at different applied voltages and frequencies.

The effects of discharge parameters including applied voltage and frequency on the characteristic products in both states were investigated. The applied voltages were set to 5.5, 6, 6.5, and 7 kV, respectively, and the absorbance of the products at the applied frequency of 6, 7, 8, 9, and 10 kHz were measured at each voltage condition, so that the products change at different voltages and frequencies were obtained. The residual gas of the last discharge in the chamber was evacuated with a vacuum pump, after which fresh air was blown in and the discharge device was

cooled to the initial temperature before the next experimental measurement. Fig. S5 shows the variation curves of the characteristic products for different discharge conditions, presented as fixed voltage and fixed frequency, respectively. It can be seen from Fig. S5 that the applied voltage and frequency have similar effects on the characteristic products. Specifically, the higher the voltage or frequency, the lower the maximum absorbance of O_3 and the higher that of NO ; moreover, the faster the disappearance of O_3 and the earlier the appearance of NO . This means the products were changed faster and faster.



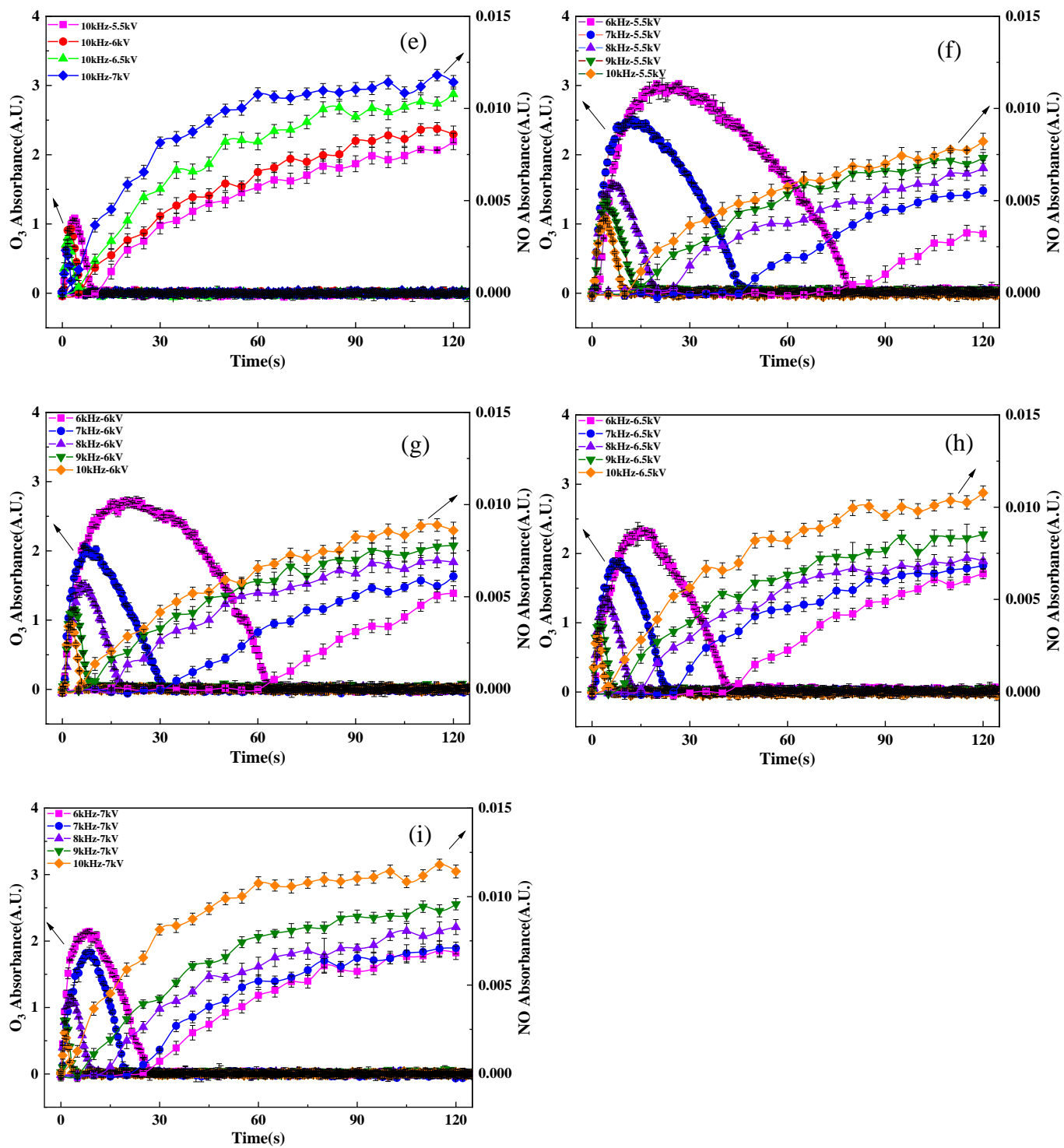


Fig. S5. The dynamic changes of characteristic product absorbance under different applied voltages and frequencies.