Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Heterogeneous reaction of toluene/NO_2/O_3 on α-Fe_2O_3 nanoparticles: The impacts of O_3, light illumination and relative humidity on the N-containing organic compounds (NOC) formation

Xiang He[1,2,3,*], Zhi-Cheng Ma[1,2,3], Xi Xi[1,2,3], Aiyilaiti Kudesi[1,2,3], Juan-Mei Wang[1,2,3]

[1] College of Ecology and Environment, Xinjiang University, Urumqi 830017, PR China

[2] Key Laboratory of Oasis Ecology, Ministry of Education, Xinjiang University, Urumqi 830017, PR China

[3] Xinjiang Jinghe Observation and Research Station of Temperate Desert Ecosystem, Ministry of Education, Xinjiang University, Urumqi 830017, PR China

[*]Correspondence and requests for materials should be addressed to X. He (xianghe@xju.edu.cn)

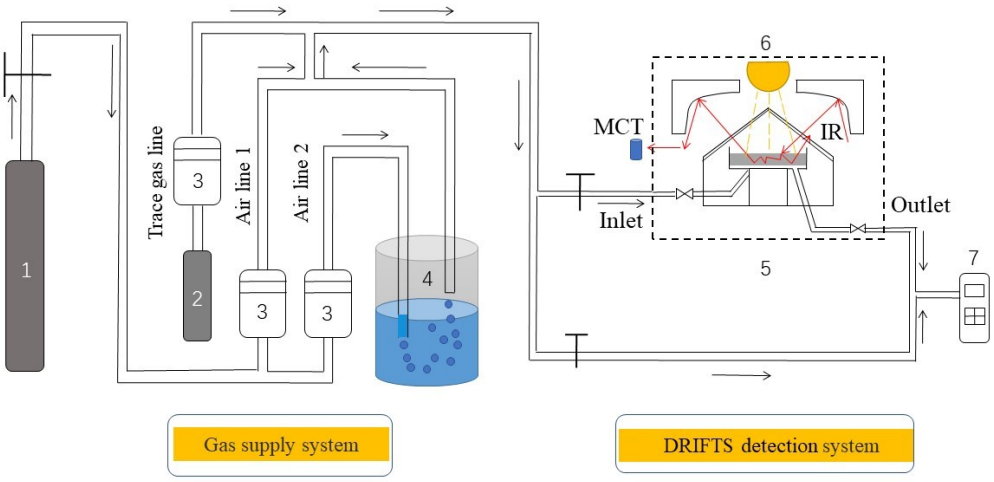

Fig. S1. The schematic diagram of the DRIFT reaction system. Note: 1. High-pure air cylinder; 2. Trace gas generator; 3. Mass flow meter; 4. Water vapor generator; 5. Reaction chamber; 6. Xenon lamp generator; 7. Hygrometer.

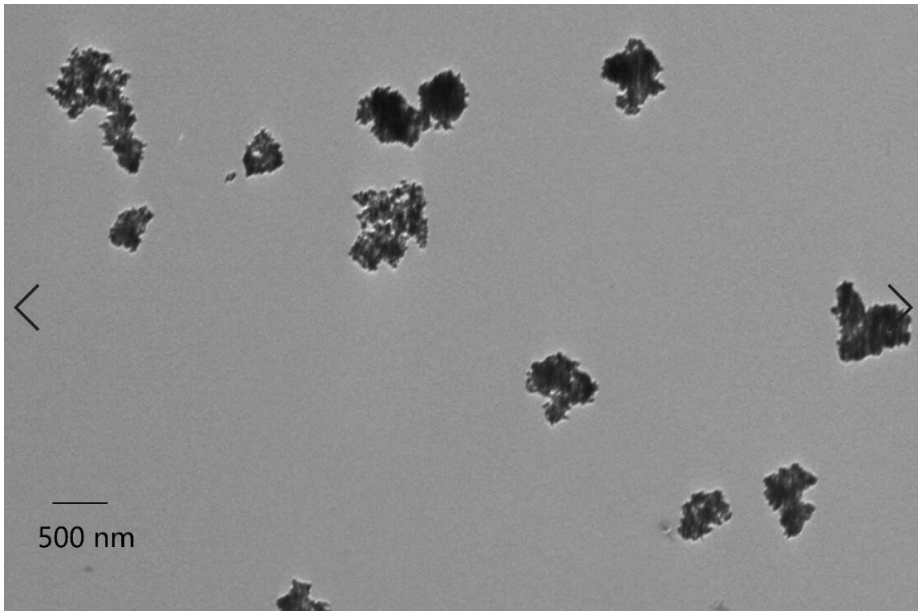

Fig. S2. TEM images of the α-Fe_2O_3 nanoparticles.

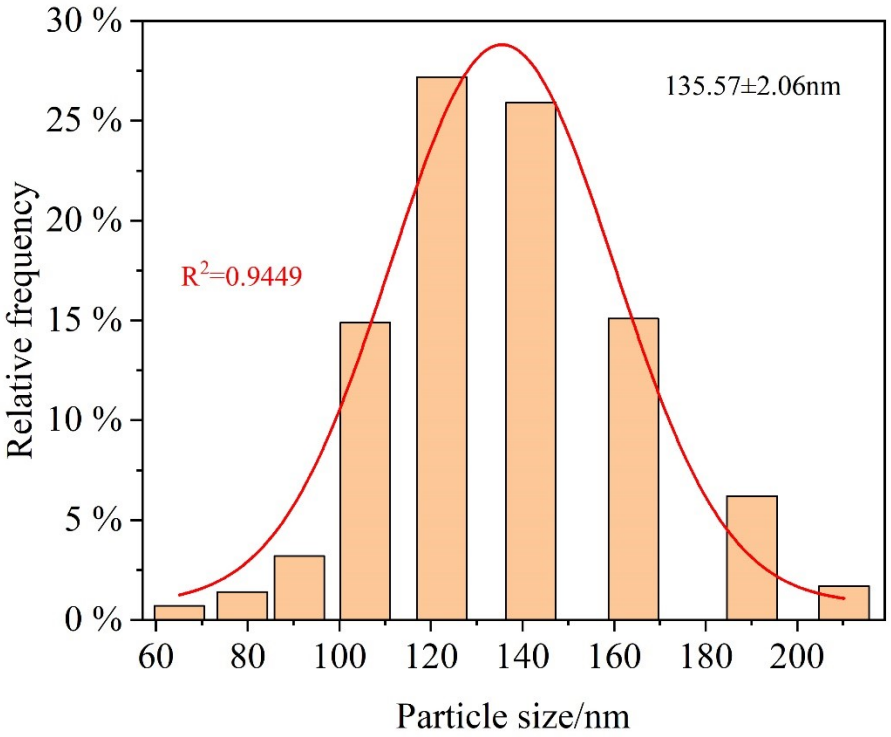

Fig. S3. Particle size distributions of the α-Fe_2O_3 nanoparticles.

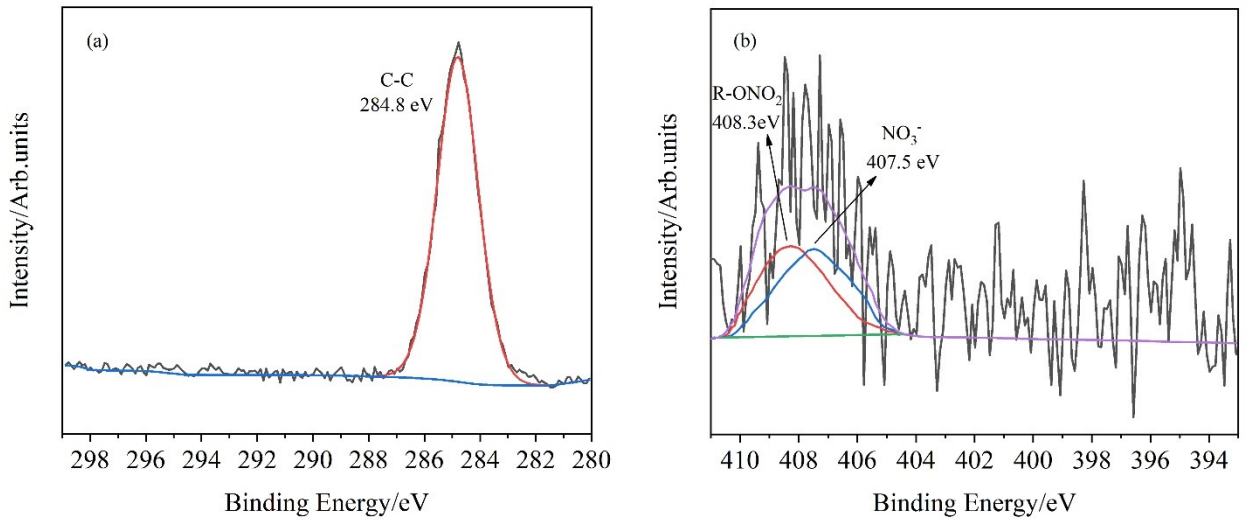

Fig. S4. Products after the heterogeneous reaction of toluene/NO_2 with α-Fe_2O_3 nanoparticles observed by (a) C 1s and (b) N 1s regions by XPS.

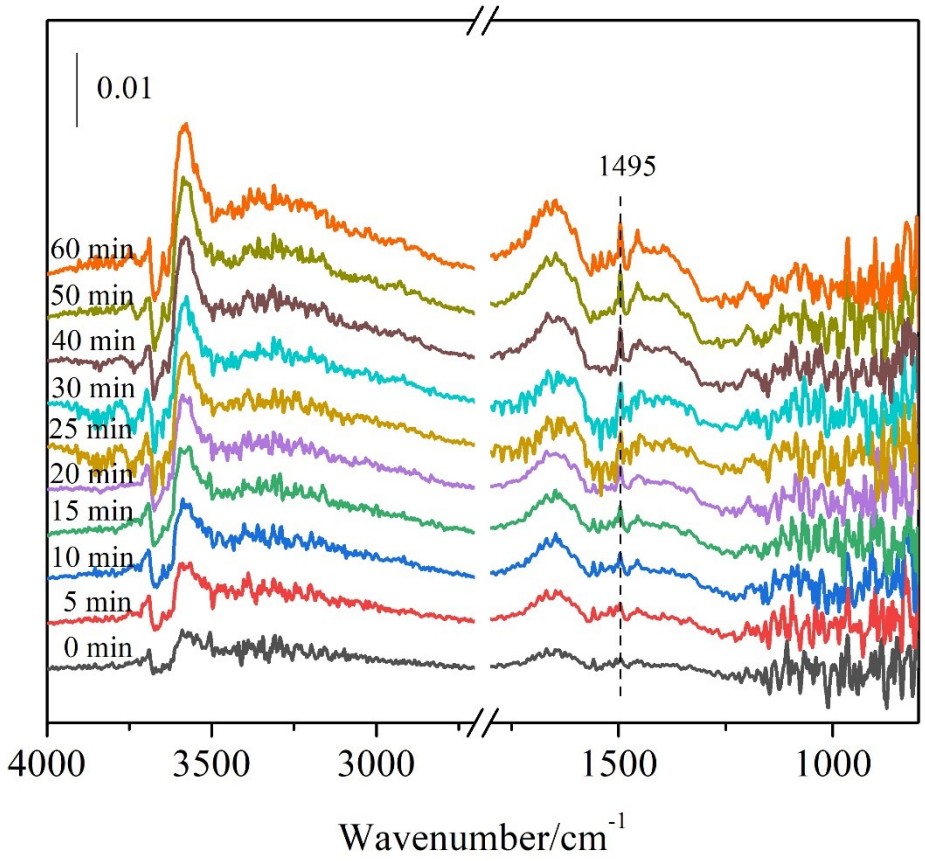

Fig. S5. In situ DRIFTS spectra of heterogeneous reaction of toluene with α-Fe_2O_3 nanoparticle as a function of time under dark condition. Conditions: [toluene] ~7.4×10^{14} molecules · cm^{-3}. The Y-axis stands for absorbance.

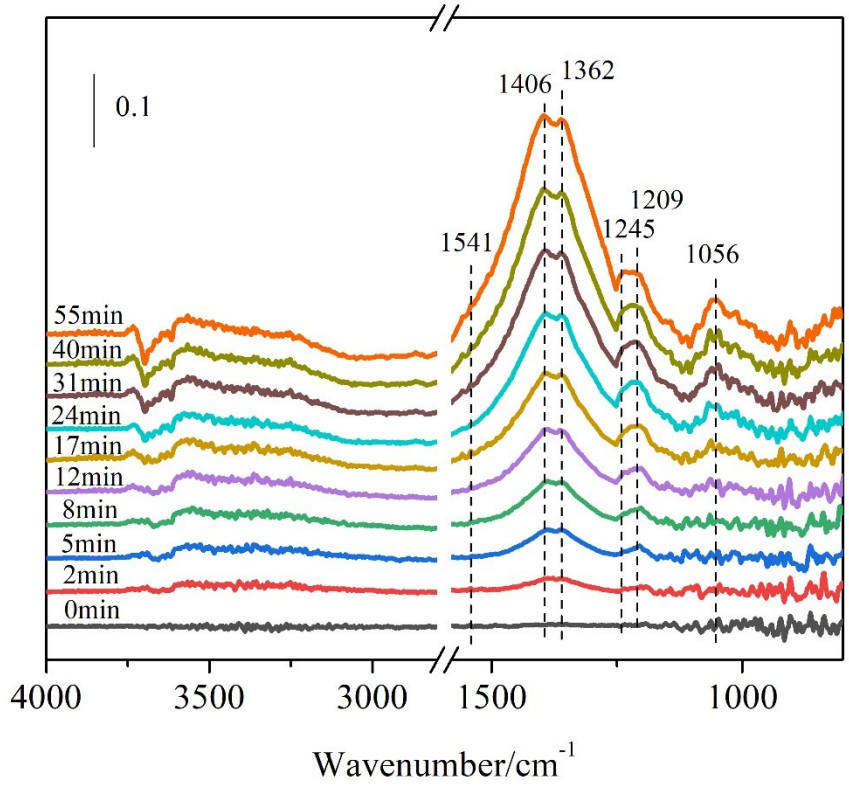

Fig. S6. In situ DRIFTS spectra of heterogeneous reaction of NO_2 with α-Fe_2O_3 nanoparticle as a function of time under dark condition. Conditions: [NO_2] ~7.4×10^{14} molecules · cm^{-3}. The Y-axis stands for absorbance.

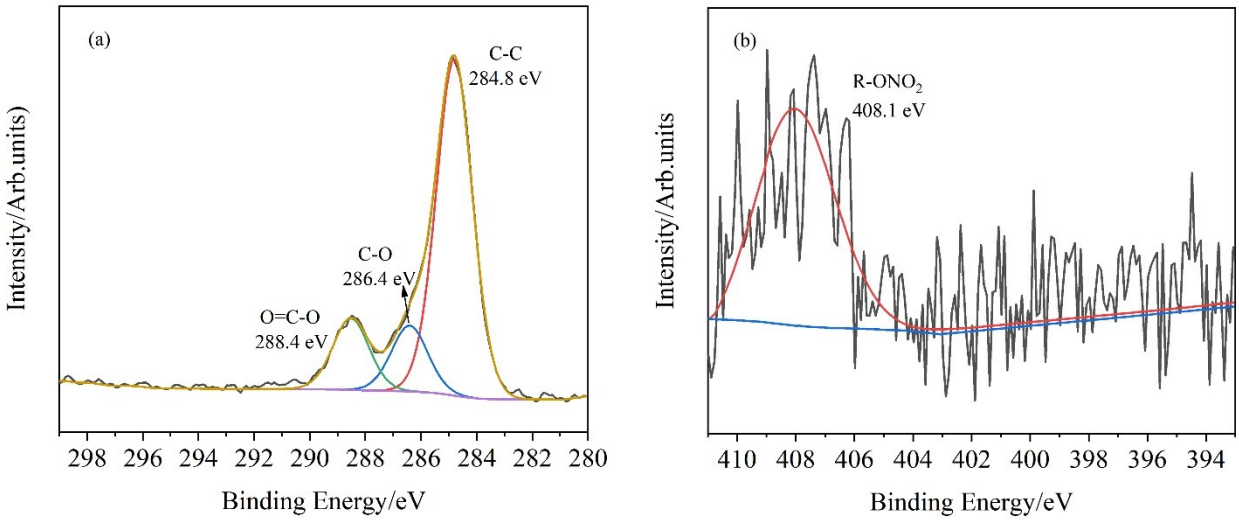

Fig. S7. Products after the heterogeneous reaction of toluene/NO_2/O_3 with α-Fe_2O_3 nanoparticles observed by (a) C 1s and (b) N 1s regions by XPS.

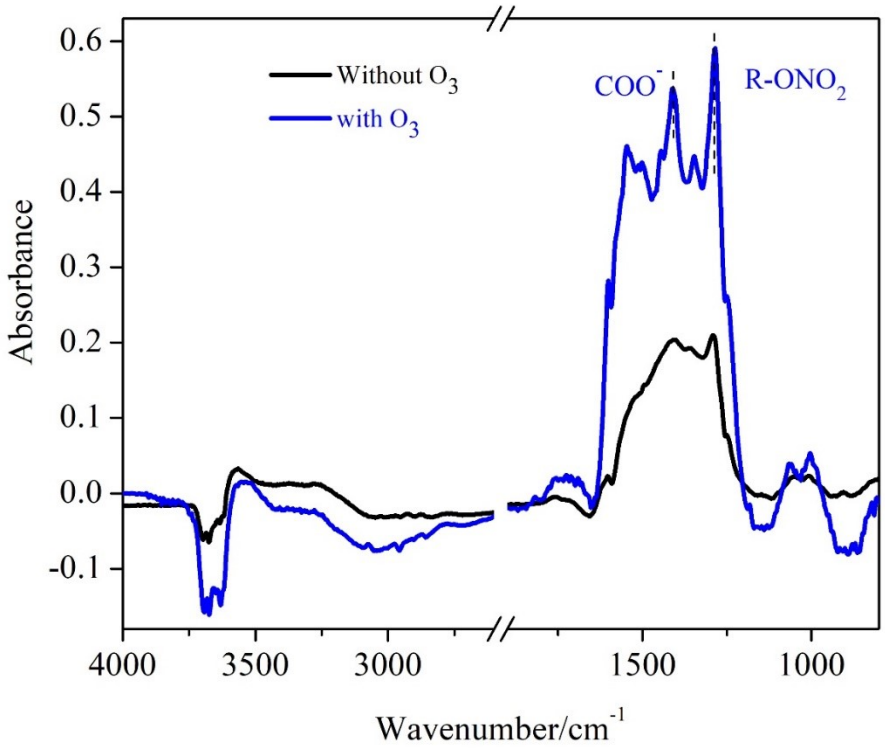

Fig. S8. Comparison of the final DRIFTS spectra for α-Fe_2O_3 after the reactions with toluene/NO_2 and toluene/NO_2/O_3. Conditions: [toluene] ~7.4×10^{14} molecules · cm^{-3}, [NO_2] ~7.4×10^{14} molecules · cm^{-3}, [O_3] ~7.4×10^{14} molecules · cm^{-3} and RH~0%.

.

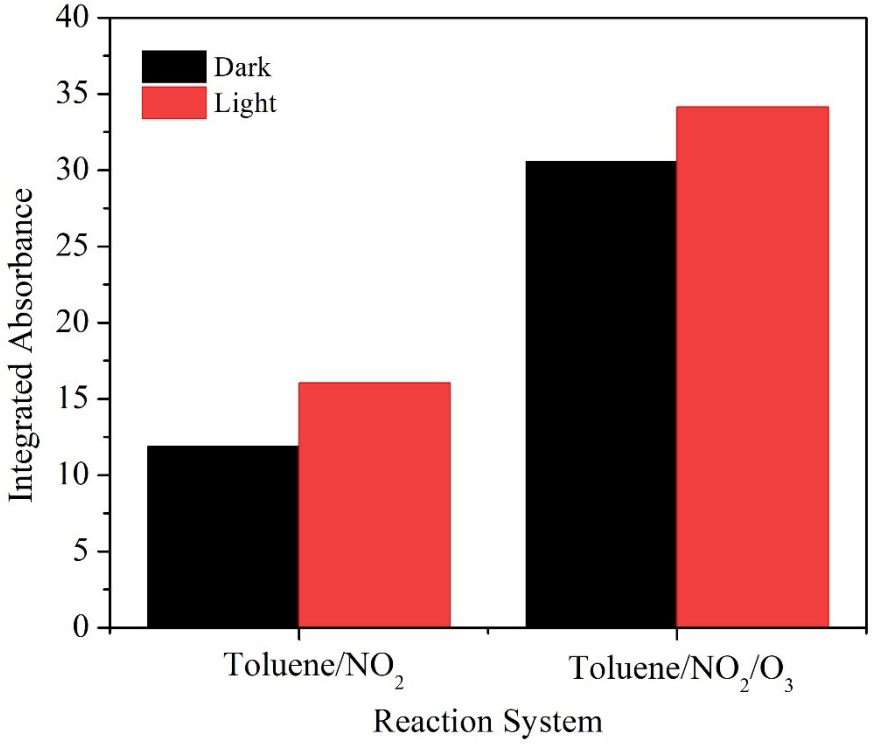

Fig. S9. The integrated absorbance of R-ONO species formed on the surface of α-Fe_2O_3 nanoparticles after reaction of toluene/NO_2 and toluene/NO_2/O_3 in the dark and light conditions.

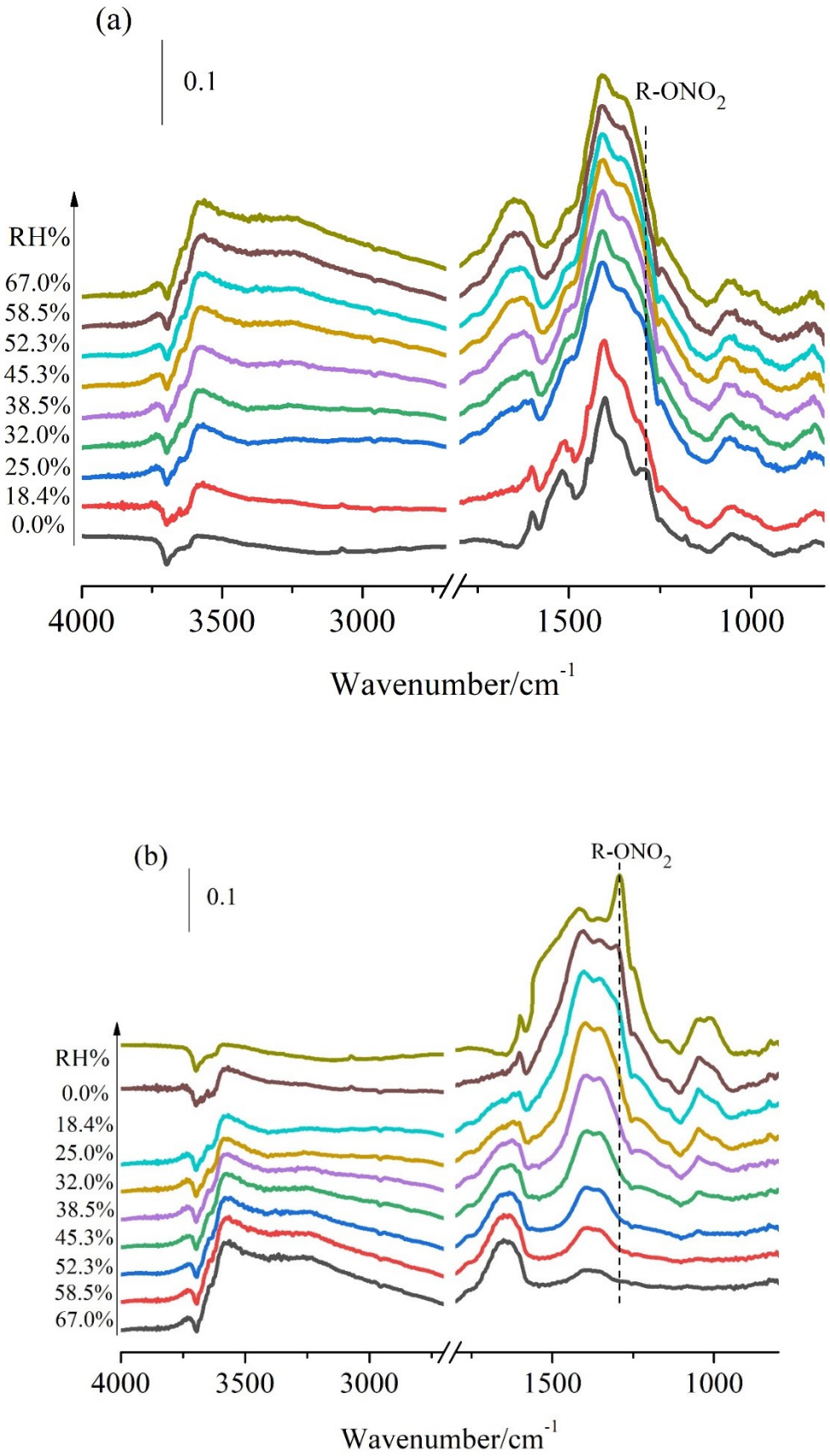

Fig. S10. DRIFTS spectra of the heterogenous reactions of toluene/NO_2/O_3 with α-Fe_2O_3 under simulated irradiation during the dehumidifying (a) and dehumidifying (b) processes. The Y-axis stands for absorbance.