Catalytic ozonation of sulfamethoxazole using low-cost natural silicate ore supported Fe_2O_3: influencing factors, reaction mechanisms and degradation pathways

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Table S1 The main instruments used in the experiment

Instrument name	Instrument model	Manufacturer
Ozone generator	DHX-I	Harbin Jiujiu Electrochemical Engineering Co., Ltd
High performance liquid chromatography	LC-1200	Agilent, USA
Total organic carbon	TOC-V_{CPN}	Shimadzu, Japan
Inductively-Coupled Plasma Emission Spectrometer	OPTIMA 5300DV	Perkin Elmer, USA
Ion chromatograph	ICS-3000	Dionex, USA
Specific surface area and porosity analyzer	ASAP 2020M	Micromeritics, USA
X-ray powder diffractometer	D/max-RA	Rigaku, Japan
Fourier-Transform Infrared Spectrometer	Spectrum 2000	Perkin Elmer, USA
X-ray photoelectron spectrometer	AXIS ULTRA DLD	Kratos, UK
Scanning Electron Microscope	SU8000	Hitachi, Japan
Fluorescence spectrophotometer	FP6500	Hitachi, Japan
Liquid tandem mass spectrometry triple quadrupole	QTRAP ® 5500	AB SCIEX，USA

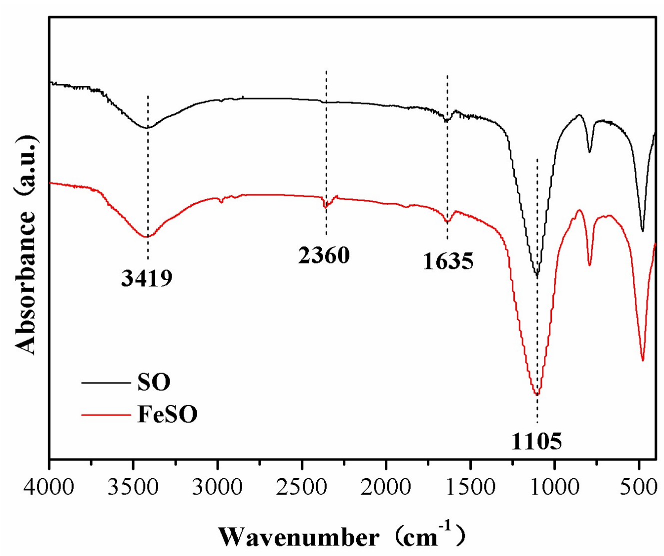


Fig. S1. FTIR spectra of SO and FeSO.

Table S2 LC-MS Liquid elution model

Gradient order	Time（min）	Flow rate（μl min^{-1}）	Acetonitrile（%）	Ultrapure water（%）
0	0.00	200	10	90
1	10.00	200	10	90
2	40.00	200	90	10
3	50.00	200	90	10
4	50.10	200	10	90
5	60.00	200	10	90

Table S3 Summary of N_2 adsorption − desorption results of catalysts.

Sample	BET (m^2 g^{-1})	Pore volume (cm^3 g^{-1})	Average pore size (nm)
SO	75.56	0.24	12.95
FeSO	53.45	0.16	11.78

Table S4 Dissolution of metal ions in FeSO catalytic ozonation of SMX

number of use	**dissolution of metal ions**（mg L^{-1}）
1	0.068
2	0.057
3	0.056
4	0.045
5	0.041

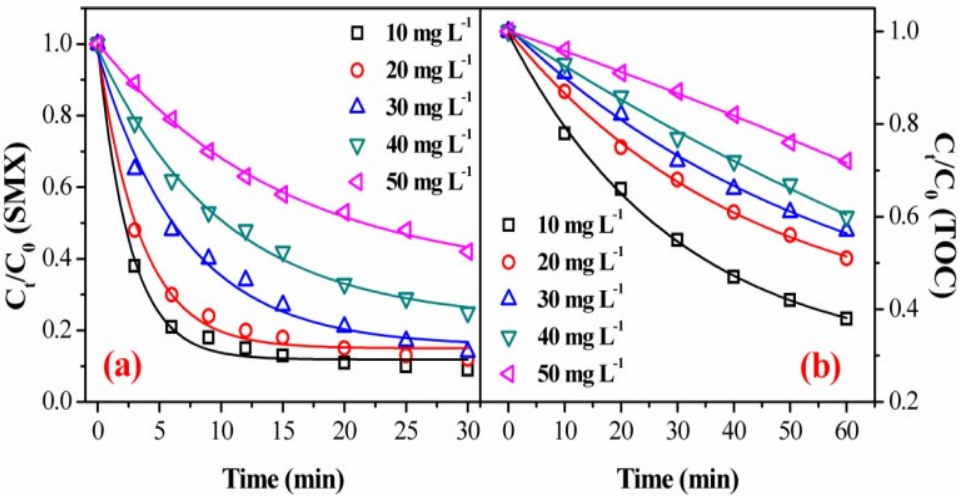
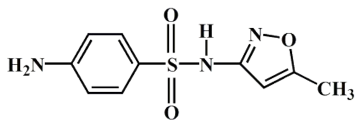
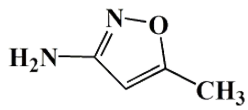
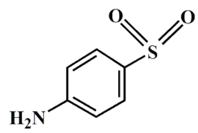
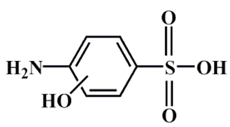
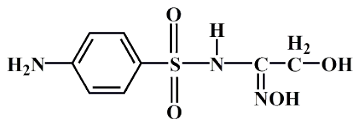
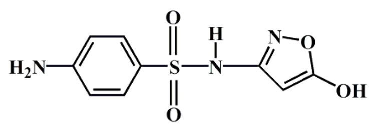
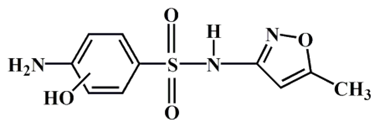
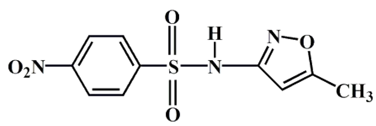
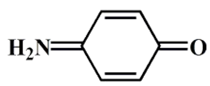
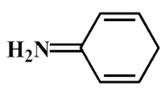
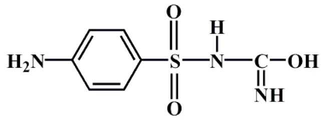
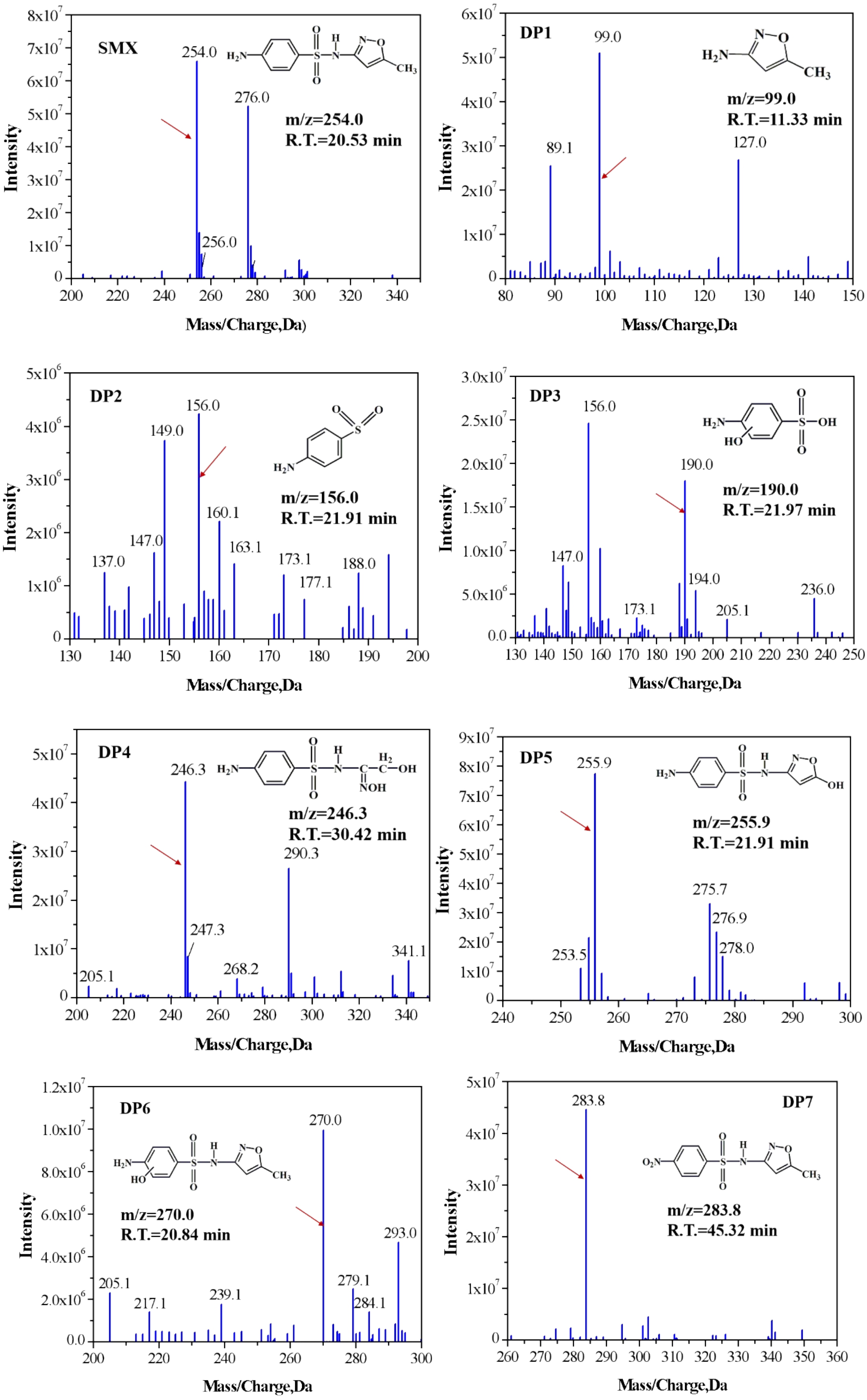


Fig. S2 Effect of initial concentration on (a) degradation and (b) mineralization of SMX in FeSO/O_3 (Experiment conditions: initial pH= 7.0, ozone dosage =0.4 mg min^{-1}, FeSO =1.0 g L^{-1} and T=20 ± 1℃).

Table S5 Decomposed products of SMX by catalytic ozonization degradation

Item	$[M + H]^+$(m/z)	Molecular formula	Structural formula
SMX	254	$C_{10}H_{12}N_3O_3S$	
DP1	99	$C_4H_7N_2O$	
DP2	156	$C_6H_6NO_2S$	
DP3	190	$C_6H_8NO_4S$	
DP4	246	$C_8H_{12}N_3O_4S$	
DP5	256	$C_9H_{10}N_3O_4S$	
DP6	270	$C_{10}H_{11}O_4N_3S$	
DP7	284	$C_{10}H_{10}N_3O_5S$	
DP8	108	C_6H_6NO	
DP9	92	C_6H_6N	
DP10	216	$C_7H_{10}N_3O_3S$	



SMX
254.0
276.0
256.0
m/z=254.0
R.T.=20.53 min
Intensity
Mass/Charge,Da)
DP1
99.0
89.1
127.0
m/z=99.0
R.T.=11.33 min
Intensity
Mass/Charge,Da
DP2
156.0
149.0
160.1
147.0
137.0
163.1
173.1
177.1
188.0
m/z=156.0
R.T.=21.91 min
Intensity
Mass/Charge,Da
DP3
156.0
190.0
147.0
194.0
173.1
205.1
236.0
m/z=190.0
R.T.=21.97 min
Intensity
Mass/Charge,Da
DP4
246.3
290.3
247.3
268.2
205.1
341.1
m/z=246.3
R.T.=30.42 min
Intensity
Mass/Charge,Da
DP5
255.9
275.7
276.9
278.0
253.5
m/z=255.9
R.T.=21.91 min
Intensity
Mass/Charge,Da
DP6
270.0
293.0
205.1
217.1
239.1
279.1
284.1
m/z=270.0
R.T.=20.84 min
Intensity
Mass/Charge,Da
DP7
283.8
m/z=283.8
R.T.=45.32 min
Intensity
Mass/Charge,Da

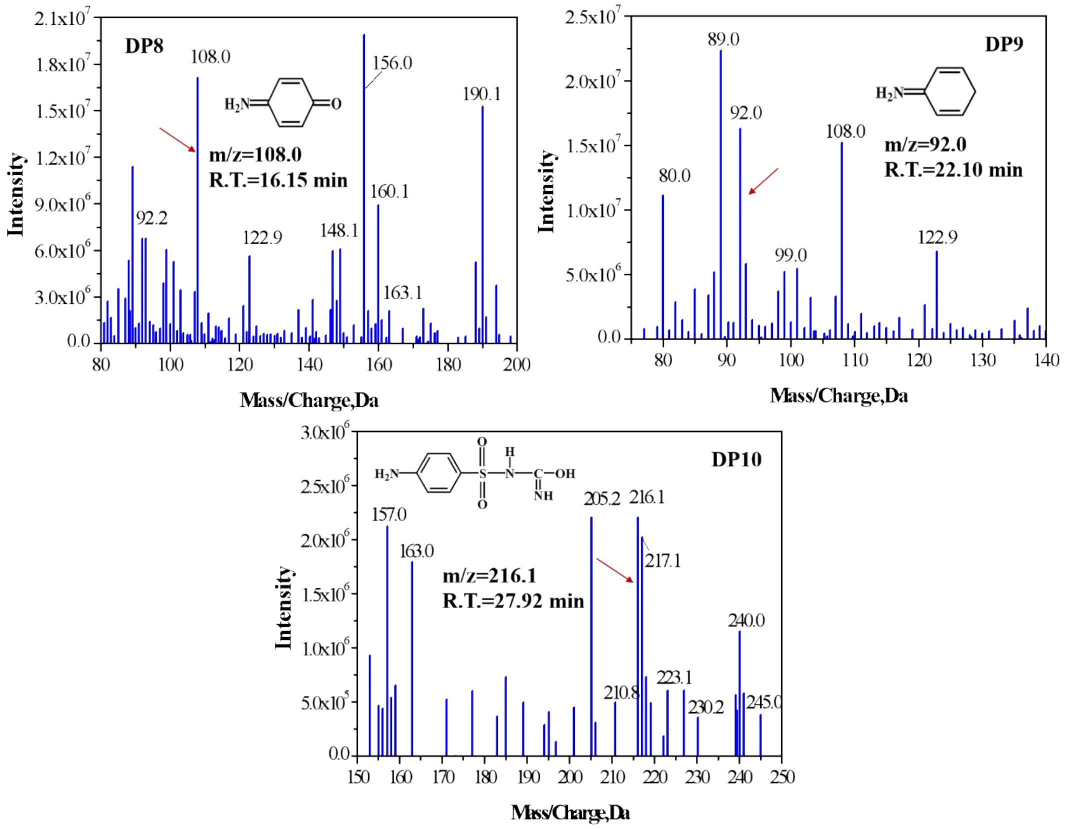


Fig. S3 LC-MS spectra of main intermediates of TCH