Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Abiotic reduction of *p*-chloronitrobenzene by sulfate green rust: Influence factors, products and mechanism

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Text S1

GC-MS analytical method of *p*-chlorophenylhydroxylamine The temperature program was as follows: the initial temperature was 40 °C (held for 1 min), after which it was increased to 120 °C at a rate of 5 °C min^{-1}, and then to 120 °C at a rate of 10 °C min^{-1}, and finally to 280 °C at a rate of 30 °C min^{-1} (held for 2 min). The injection temperature was 250 °C, and the interface temperature was 280 °C. The injection port was operated in the splitless mode. The flow rate of the carrier gas (helium, 99.999%) was 1.0 mL min^{-1}. The mass spectrometer was operated in electron impact (EI) and selective ion monitoring (SIM) modes with a source temperature of 230 °C, and a solvent delay of 4.5 min.

GC-MS analytical method of *p*-nitrosochlorobenzene The temperature program was as follows: the initial temperature was 50 °C (held for 2 min), after which it was increased to 150 °C at a rate of 10 °C min^{-1}(held for 1 min), and finally to 270 °C at a rate of 20 °C min^{-1} (held for 5 min). The injection temperature was 250 °C, and the interface temperature was 280 °C. The injection port was operated in the splitless mode. The flow rate of the carrier gas (helium, 99.999%) was 1.0 mL min^{-1}. The mass spectrometer was operated in electron impact (EI) and selective ion monitoring (SIM) modes with a source temperature of 230 °C, and a solvent delay of 4.5 min.

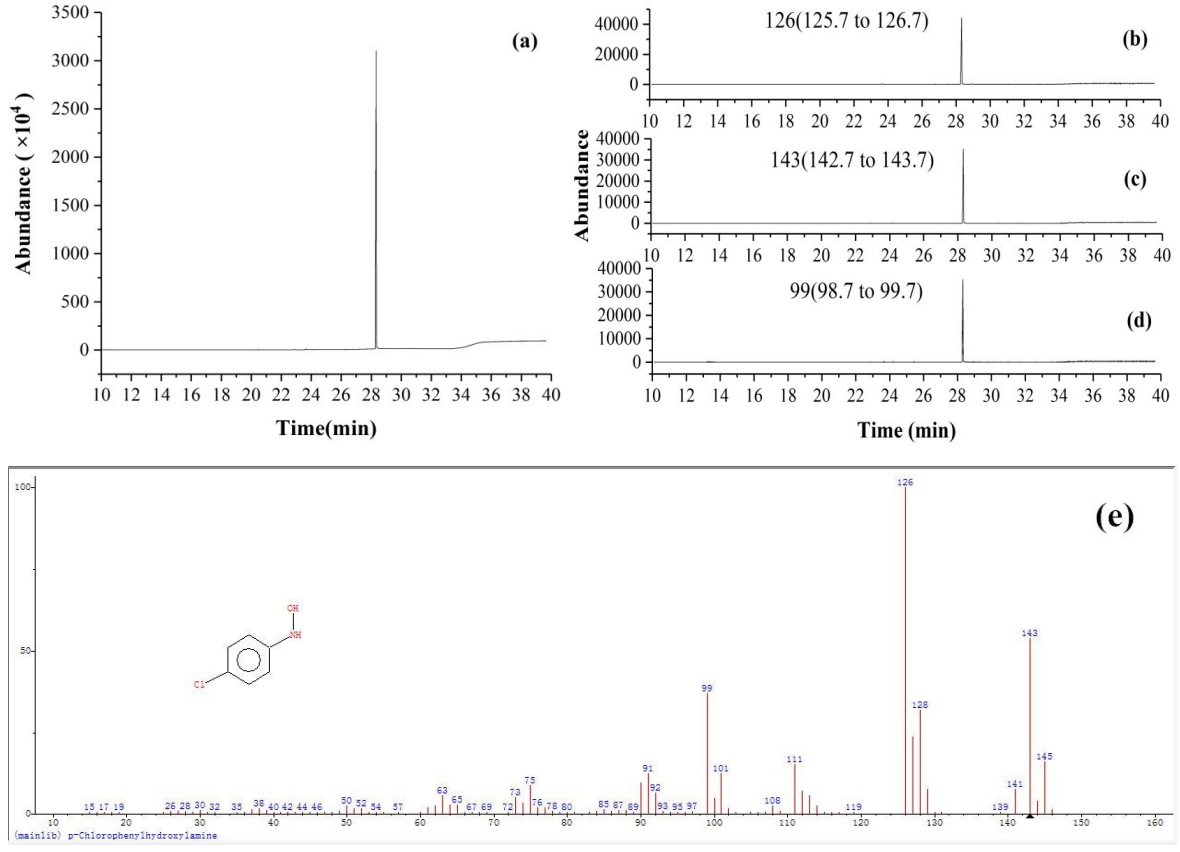

Fig. S1 GC-MS chromatogram of *p*-chlorophenylhydroxylamine (a) Total ion (b) m/z=126 (c) m/z=143 (d) m/z=99 (e) Mass spectrum and corresponding substance

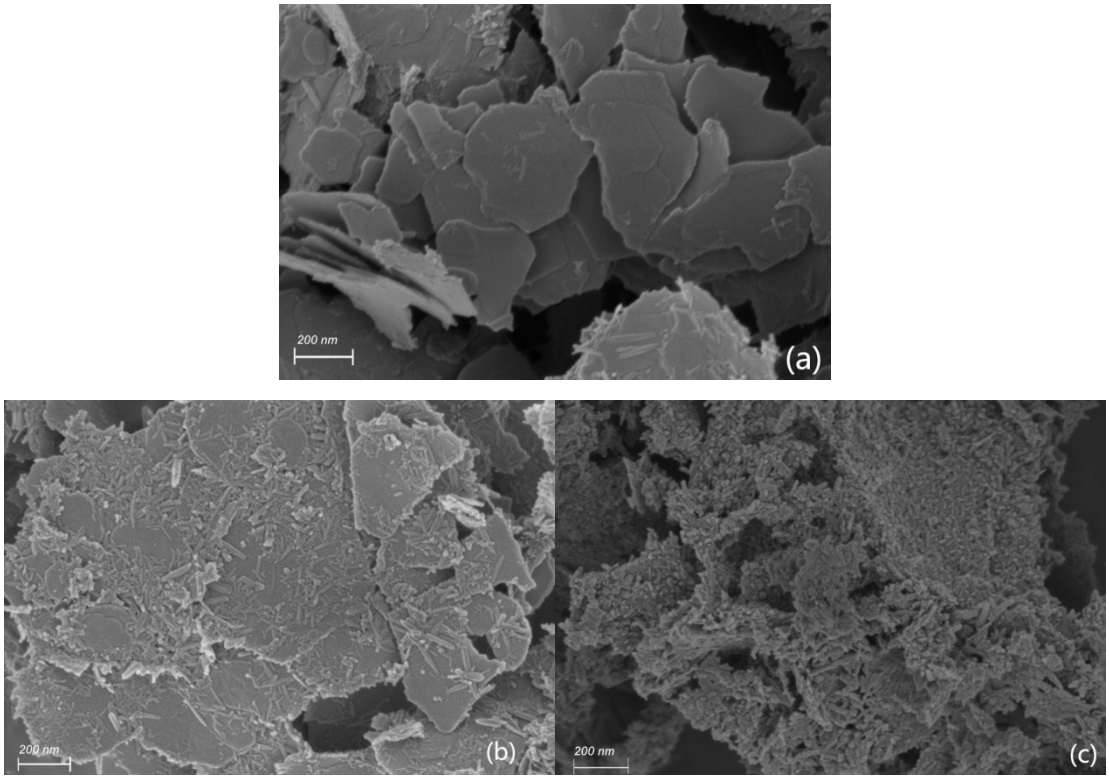

Fig.S2 SEM image of powders at (a) 0 min, (b) 15 min and (c) 40 min.

Table S1 Quantification Report of unreacted GR_{SO4} powders

Peak	Position BE (eV)	FWHM (eV)	Raw Area (cps eV)	RSF	Mass Conc (%)
Fe (2p)	710.9	4.242	144505.4	2.957	54.32
O(1s)	531.4	2.586	94278.9	0.780	36.10
C (1s)	284.8	2.039	8130.7	0.278	6.04
S (2p)	168.6	1.995	4895.9	0.668	3.09

Equation S1:

$$\text{Iron to Oxygen ratio} = \frac{\text{Raw Area}_{Fe(2p)}/\text{RSF}_{Fe(2p)}}{\text{Raw Area}_{O(1s)}/\text{RSF}_{O(1s)}} \quad \text{(S1)}$$

Table S2 Gupta and Sen multiplet peaks parameters used to fit Fe($2p_{3/2}$) spectra of GR_{SO4} with variable composition

Reaction time	Species	*Fe(2p)* (FHWM) (eV)	Area (%)
0 min	Fe(II)	709.0 (1.4)	7.5
		710.2 (1.4)	28.2
		711.4 (1.4)	17.5
	Fe(III)	710.9 (1.7)	15.3
		712.4 (1.7)	7.4
		713.0 (1.7)	15.8
		714.0 (1.7)	8.3
15 min	Fe(II)	709.5 (1.4)	14.0
		710.5 (1.4)	5.2
		711.4 (1.4)	7.2
	Fe(III)	710.3 (1.7)	11.5
		711.3 (1.7)	17.2
		712.4 (1.7)	22.5
		713.5 (1.7)	22.1
40 min	Fe(III)	710.4 (1.6)	17.5
		711.2 (1.6)	36.5
		712.3 (1.6)	25.6
		713.6 (1.6)	20.4

Table S3 Binding energy values, FHWM (full-width at half-maximum), peak areas and interpretation for O(1s) spectra of GR_{SO4} with variable composition

Reaction time	*O(1s)* (FHWM) (eV)	Area(%)	Species
0 min	529.9 (1.1)	15	Fe-O
	531.3 (1.2)	72	OH^-
	532.1 (1.3)	13	H_2O
15 min	530.5 (1.2)	21	Fe-O
	531.8 (1.3)	68	OH^-
	532.7 (1.2)	11	H_2O
40 min	530.0 (1.2)	31	Fe-O
	531.5 (1.3)	62	OH^-
	532.4 (1.2)	7	H_2O

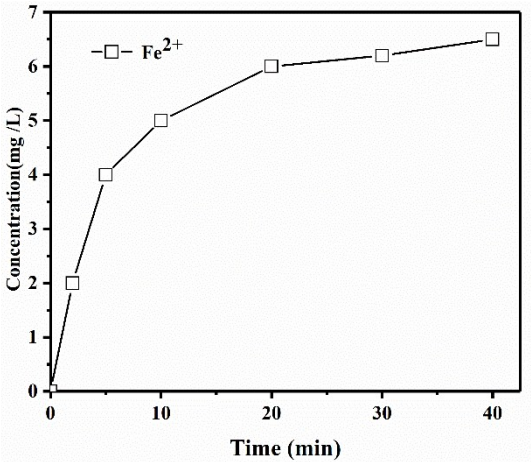

Fig. S3 Dissolved ferrous ions during the reaction. $[p\text{-CNB}]_0$ = 500 μg/L, $[GR_{SO4}]_0$=0.1 g/L, T = 20 ℃, pH = 6.5.

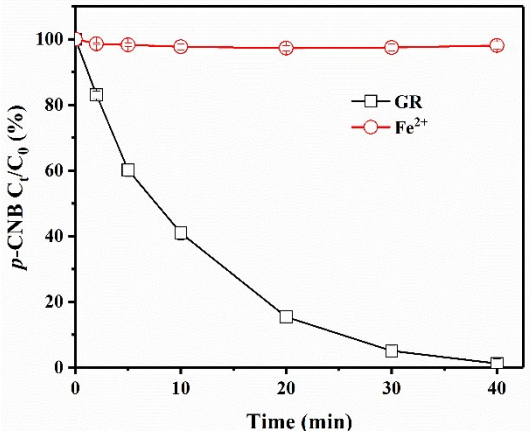

Fig. S4 Comparison of removals of *p*-CNB with Fe(II) and GR_{SO4}. $[p\text{-CNB}]_0 = 500$ μg/L, $[Fe(II)]_0 = 0.1$ g/L, $[GR_{SO4}]_0 = 0.1$ g/L, T = 20 ℃, pH = 6.5. Error bars represent one standard deviation (n = 3).