Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Adsorption Behavior and Structure Transformation of Mesoporous Metal-Organic Frameworks Towards Arsenates and Organic Pollutants in Aqueous Solution

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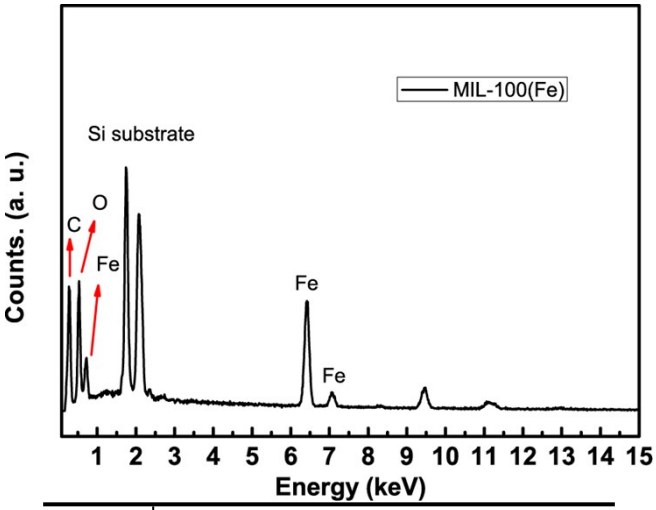
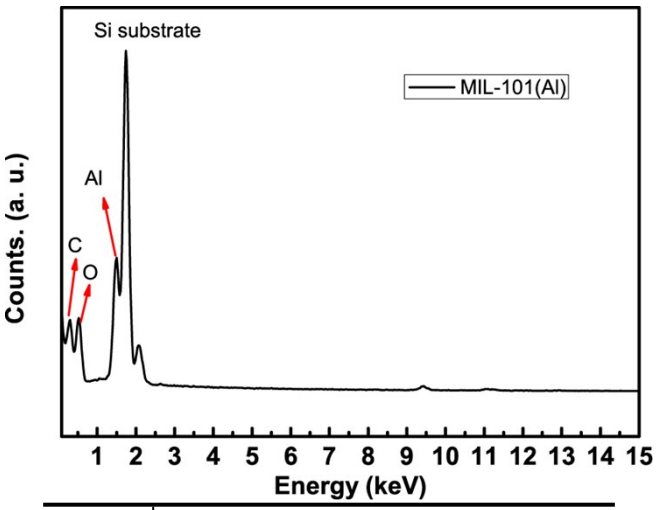
Supporting Information:



Element	weight %	Atom number %
C K	45.74	63.07
O K	28.21	29.20
Fe K	26.05	7.73
Total	100.00	

(a)



Element	weight %	Atom number %
C K	47.94	56.00
O K	47.42	41.59
Al K	4.65	2.42
Total	100.00	

(b)

Figure S1. EDS analysis and reports: (a) MIL-100(Fe), (b) MIL-100(Al). (the other peaks not

indexed came from Pt which was used in preparation of the samples for characterization)

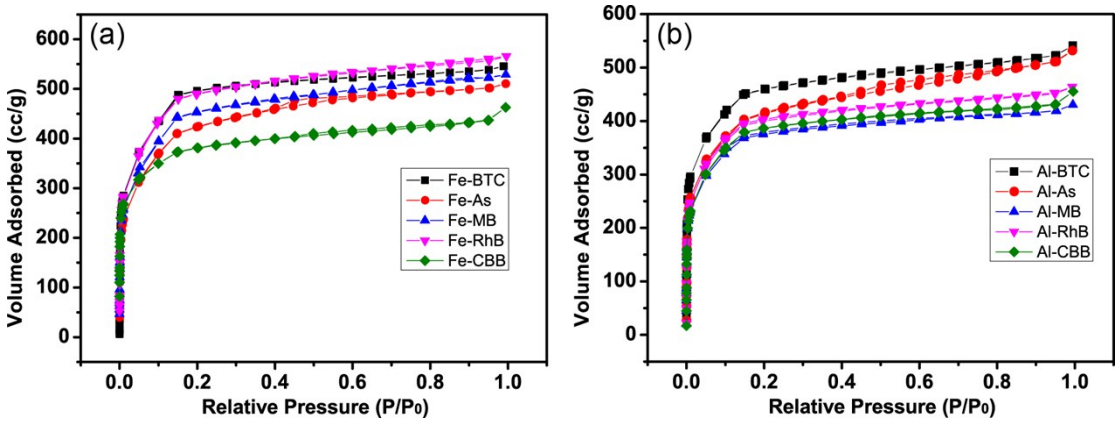


Figure S2. (a) Nitrogen adsorption-desorption isotherms of MIL-100(Fe) after adsorption in 100 ppm pollutants, (b) Nitrogen adsorption-desorption isotherms of MIL-100(Al) after adsorption in 100 ppm pollutants.

Table S1. BET surface areas, pore size distribution and pore volume analysis.

Samples	S_{BET} m^2/g	V_{micro} cc/g	Pore Size/nm	Samples	S_{BET} m^2/g	V_{micro} cc/g	Pore Size/nm
Fe	1369.6	0.710	1.107	**Al**	1370	0.665	0.969
Fe-As	1131	0.589	0.581	**Al-As**	1200	0.567	0.960
Fe-MB	1223	0.636	0.628	**Al-MB**	1084	0.547	0.960
Fe-RhB	1345	0.712	0.628	**Al-RhB**	1149	0.584	0.951
Fe-CBB	1223	0.553	0.452	**Al-CBB**	1082	0.565	0.951

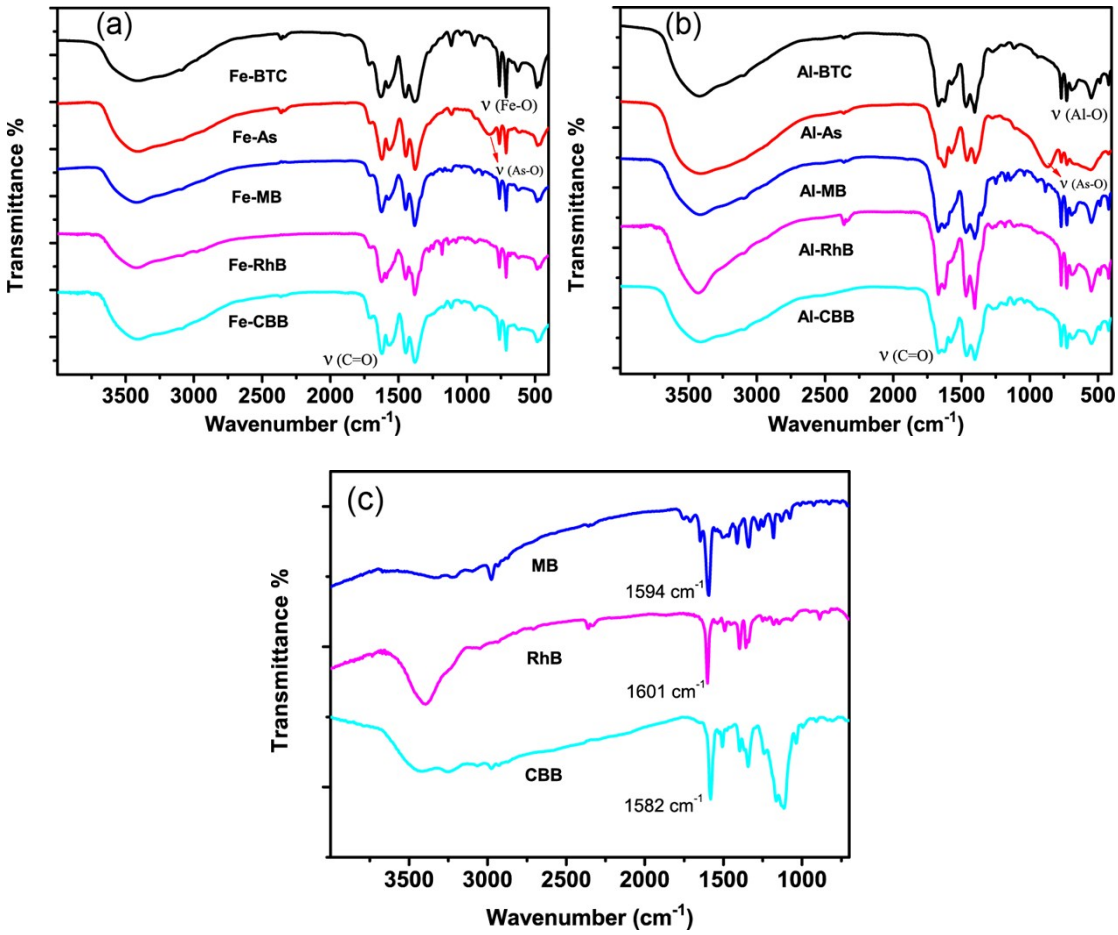


Figure S3. (a) FT-IR spectra of MIL-100(Fe) and the corresponding adsorbed samples, (b) FT-IR spectra of MIL-100(Al) and the corresponding adsorbed samples, (c) FT-IR spectra of MB, RhB and CBB.

Table S2. Arsenates adsorption performances of MIL-100(Fe) and MIL-100(Al) under different pH values in 10 ppm arsenate solution (T = 25 °C; adsorbent doses = 0.4 g L^{-1}).

Samples	As(V) concentrations of solutions (ppm)		
	pH 4	pH 7	pH 11
Before adsorption	10	10	10
MIL-100(Fe)	6.30	2.46	0.57
MIL-100(Al)	2.95	1.04	0.11

Table S3. The selectivity experiments of MIL-100(Fe, Al) in 10 ppm arsenate solution with 50 ppm disturbing ions (T = 25 °C; adsorbent doses = 0.4 g L^{-1}).

Samples	Concentrations of As(V) and disturbing ions (ppm)							
	As(V)	Cl^-	As(V)	SO_4^{2-}	As(V)	NO_3^-	As(V)	HCO_3^-
Before adsorption	10	50	10	50	10	50	10	50
MIL-100(Fe)	3.77		2.51		3.75		0.191	
MIL-100(Al)	1.33		1.55		1.53		0.122	

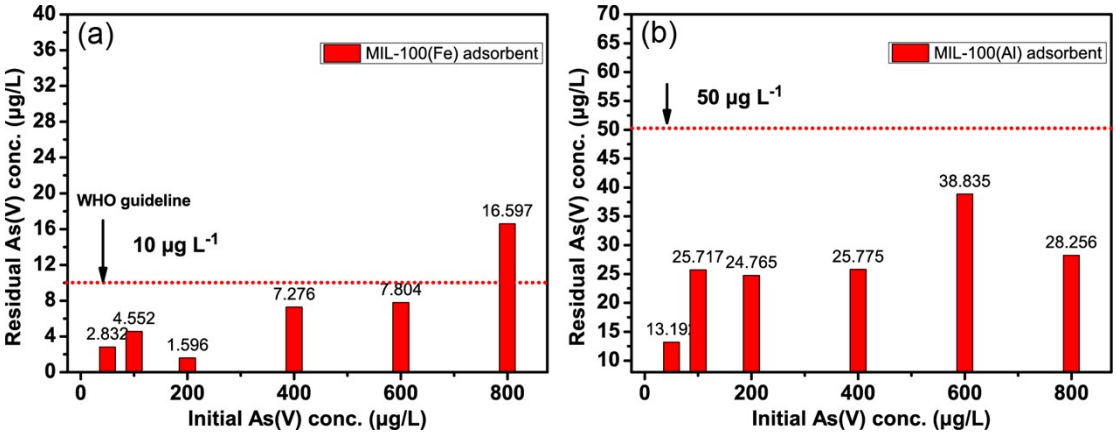


Figure S4. (a) The residual arsenate concentrations exploiting MIL-100(Fe) as the adsorbent for low-level arsenate removal. (b) The residual arsenate concentrations exploiting MIL-100(Al) as

the adsorbent for low-level arsenate removal (T = 25 °C; adsorbent doses = 0.5 g L^{-1}).

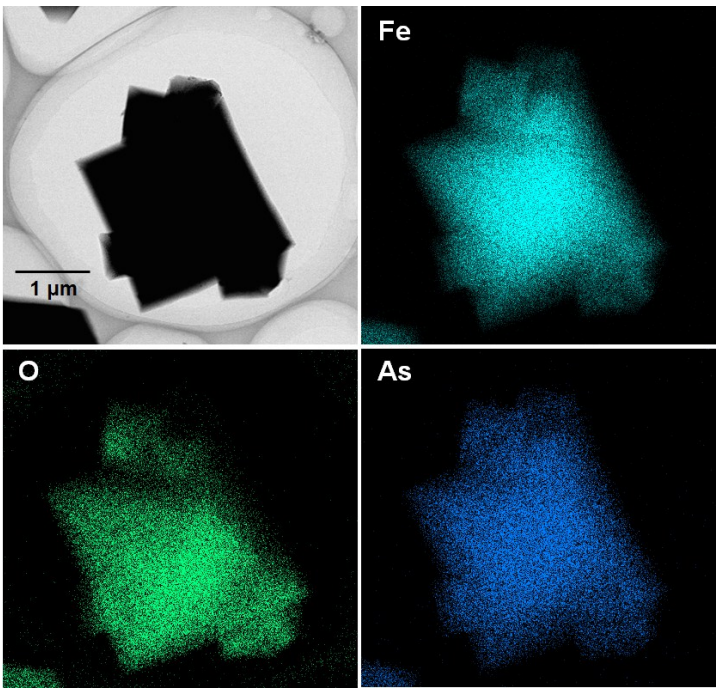


Figure S5. STEM images and elements dispersion of the arsenate adsorbed MIL-100(Fe).

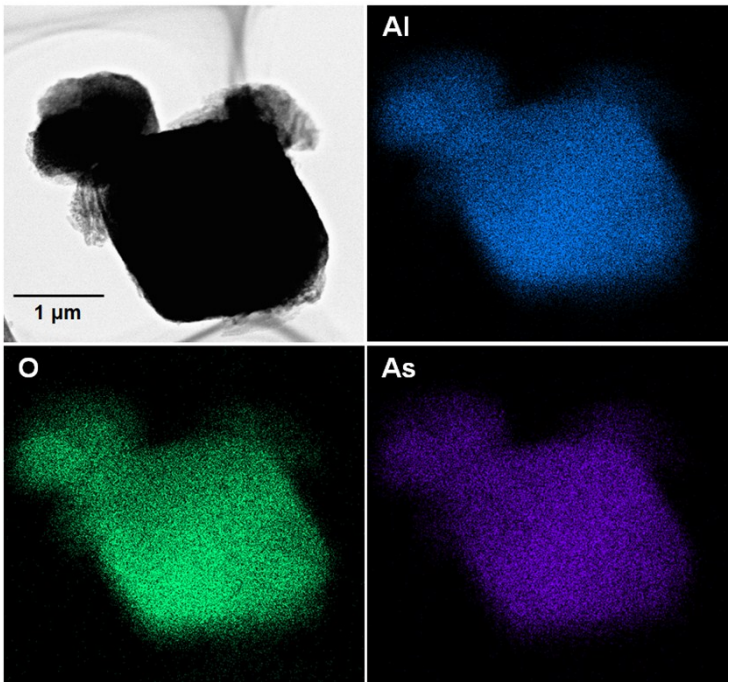


Figure S6. STEM images and elements dispersion of the arsenate adsorbed MIL-100(Al).

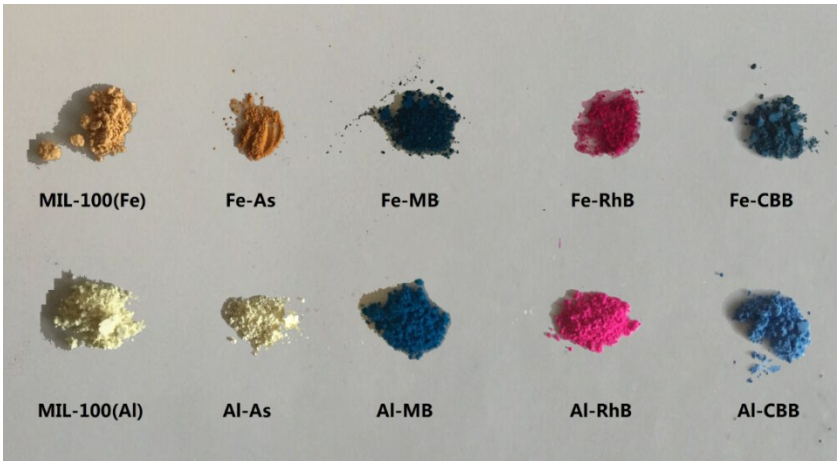


Figure S7. Digital photo images of the adsorbed MIL-100(Fe) and MIL-100(Al).

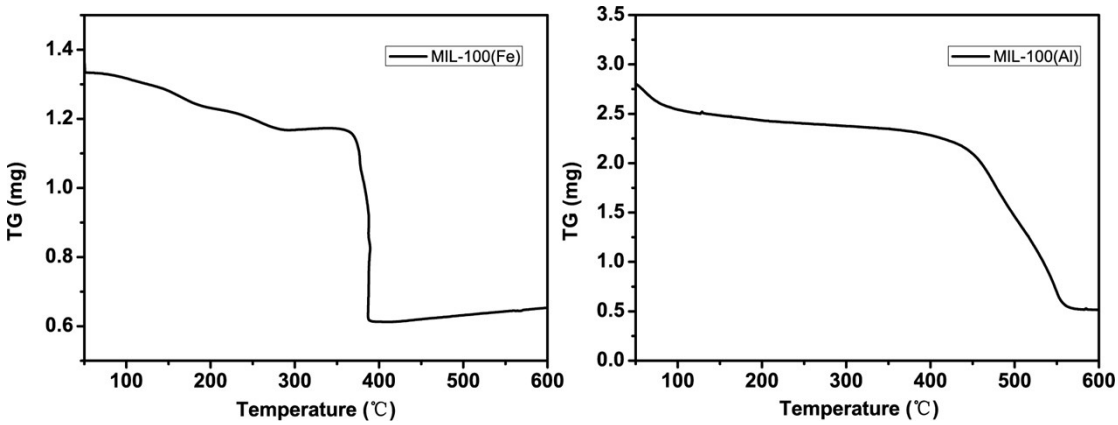


Figure S8. TG curve of iron and aluminum trimesate under air ambience (5 °C/min to 600 °C, hold at 50 °C for 30 min).

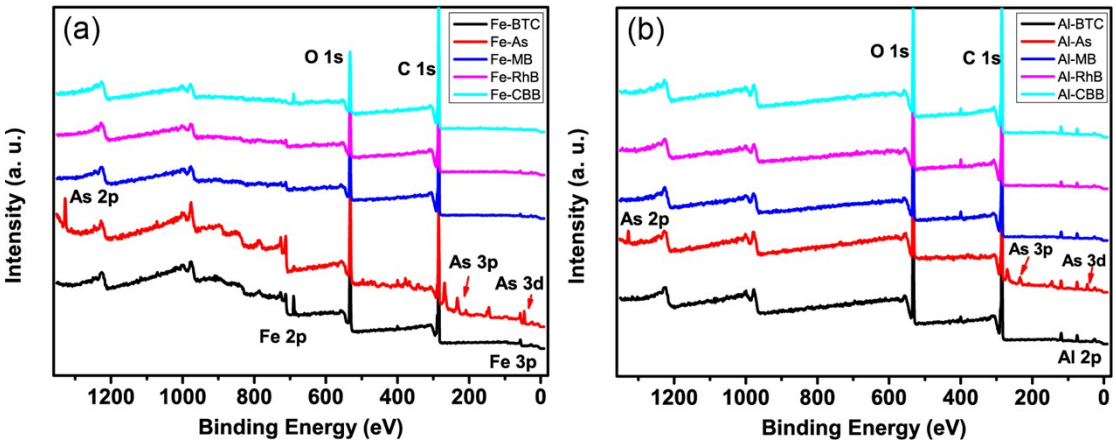


Figure S9. (a) XPS spectra of MIL-100(Fe) and adsorbed samples, (b) XPS spectra of MIL-100(Al) and adsorbed samples.

Table S4. Elements contents (atomic %) of XPS analysis.

Elements Contents (%)	C	N	O	Fe/Al	F	As	Na
Fe	68.18	0.93	25.09	1.94	3.87		
Fe-As	61.92	1.46	29.11	2.91	0.77	3.36	0.47
Fe-MB	79.62	--	19.09	0.75	0.54		
Fe-RhB	79.96	0.62	18.43	0.67	0.31		
Fe-CBB	80.86	0.5	16.99	0.28	1.54		
Al	68.45	1.89	24.98	4.68			
Al-As	71.47	--	22.86	4.39		1.28	--
Al-MB	71.2	2.33	22.46	4.01			
Al-RhB	74.22	2.19	20.62	2.97			
Al-CBB	70.65	1.76	23.52	4.07			

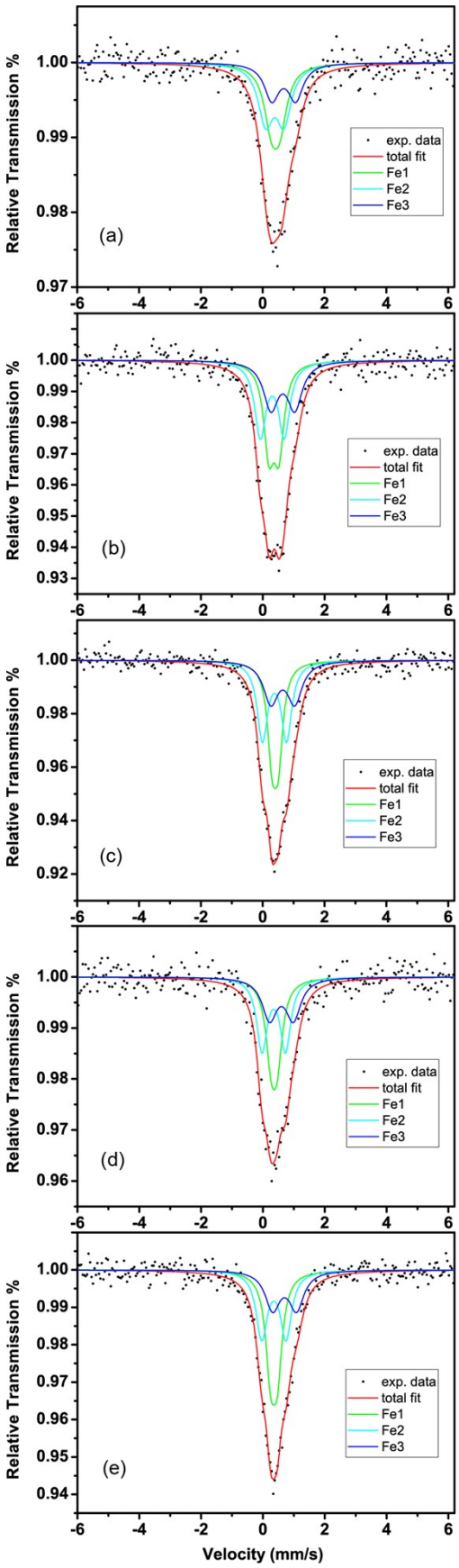


Figure S10. Mössbauer spectra of MIL-100(Fe) and adsorbed samples (a) before adsorption[1] (b) As(V)-adsorbed[1] (c) MB-adsorbed (d) RhB-adsorbed (e) CBB-adsorbed.

Table S5. Summary of Mössbauer parameters and assignment to iron species.

MIL-100(Fe)	δ(mm/s)[a]	*Qs* (mm/s)[b]	FWHM (mm/s)[c]	Area Ratio (%)
Fe1	0.41	0.27	0.56	36.0
Fe2	0.39	0.59	0.57	39.0
Fe3	0.68	0.77	0.58	25.0
Fe-As	**δ(mm/s)**	***Qs* (mm/s)**	**FWHM (mm/s)**	**Area Ratio (%)**
Fe1	0.36	0.32	0.40	36.2
Fe2	0.31	0.77	0.43	34.8
Fe3	0.65	0.77	0.58	29.0
Fe-MB	**δ(mm/s)**	***Qs* (mm/s)**	**FWHM (mm/s)**	**Area Ratio (%)**
Fe1	0.41	0.20	0.35	35.0
Fe2	0.38	0.78	0.40	37.0
Fe3	0.65	0.77	0.58	28.0
Fe-RhB	**δ(mm/s)**	***Qs* (mm/s)**	**FWHM (mm/s)**	**Area Ratio (%)**
Fe1	0.36	0.19	0.42	35.0
Fe2	0.35	0.76	0.41	36.0
Fe3	0.60	0.77	0.58	29.0
Fe-CBB	**δ(mm/s)**	***Qs* (mm/s)**	**FWHM (mm/s)**	**Area Ratio (%)**
Fe1	0.36	0.21	0.39	40.0
Fe2	0.35	0.78	0.43	34.0
Fe3	0.70	0.77	0.58	26.0

[a] Isomer shift or chemical shift (δ),

[b] Quadrupole splitting (*Qs*),

[c] Full width at half maximum (FWHM)

Reference:

[1] J. Cai, X. Wang, Y. Zhou, L. Jiang, C. Wang, Phys. Chem. Chem. Phys. 2016, 18, 10864-10867.