Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Supramolecular $Fe^{II}_4L_4$ cage for fast ammonia sensing

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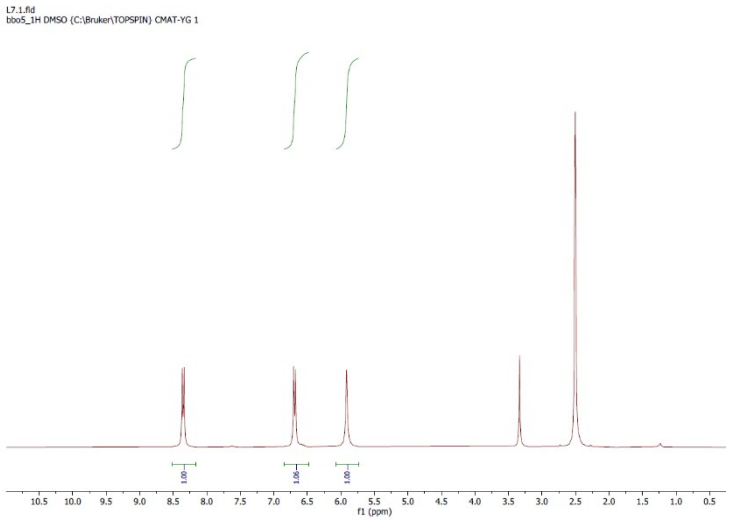
Contents

General information

All chemicals were purchased from commercial companies and used as supplied without further purification. NMR spectra were recorded on a Bruker AVANCE 300MHz spectrometer. Proton chemical shifts (δ) are reported relative to the solvent residual peak (2.50 ppm for dimethyl sulfoxide). High resolution electrospray ionization mass spectra (HRMS) were measured on a Q-Exactive ThermoFisher spectrometer. Elemental analyses (C, H, and N) were measured by MEDAC Ltd, UK. Thermogravimetric analyses (TGAs) were performed in $N_{2(g)}$ (100 mL min^{-1}) at a heating rate of 10 ^{o}C min^{-1} from 25 ^{o}C to 850 ^{o}C using a Mettler Toledo TGA/SDTA 851e analyzer. Fourier transformed infrared (FT-IR) spectroscopy were recorded by a Equinox 55 (Bruker) equipped with an ATR modulus and an MCT detector. Diffuse reflectance spectra (DRS) were performed with a PerkinElmer Lambda 9 UV/vis/NIR spectrophotometer equipped with a 60 mm integrating sphere and converted into absorption spectra by using the Kubelka−Munk function, using $BaSO_4$ as a reference. Raman Spectrum were obtained on a Horiba LabRAM HR Evolution with λ = 514 nm laser source equipped with temperature controller. The microstructure was studied by field emission scanning electron microscopy (SEM) using a Mira3-TESCAN microscope from Oxford Instruments Inc. Powder X-ray diffraction (PXRD) patterns were collected on a D8-Advance diffractometer (Bruker, Germany) with Cu Kα radiation (λ = 1.5148 Å). XPS analyses were carried on SSI-X-probe (SSX 100/206) photoelectron spectrometer from Surface Science Instruments (USA) using Al Kα as the X-ray source. All binding energies were calculated according to the C 1s peak fixed at 284.4 eV. Magnetic susceptibility for microcrystalline MOC-1 was measured on a Quantum design MPMS-5s SQUID magnetometer under an applied field of 1 T. Magnetic data were corrected for the sample holder and diamagnetic contributions. ^{57}Fe Mössbauer spectra were measured in transmission geometry with a constant acceleration mode conventional spectrometer equipped with a 50 mCi $^{57}Co(Rh)$ source and a Reuter Stokes proportional counter. The powdered samples were sealed in aluminum foil and spectra were recorded at 298 K. The spectra were fitted using Recoil 1.05 Mössbauer Analysis software and isomer shift values are given with respect to α-Fe at room temperature. NH_3 concentration detection was performed with a commercial ammonia gas detector (smart sensor, AR8500). The resolution is 0.1 ppm and the measuring range is 0~100 ppm. Relative humidity was monitored with a hygrometer from TFA Dostmann.

Synthesis of triazine-based subcomponent ligand 2,4,6-tris-(4-aminophenyl)triazine (TATP)

0.295 g (2.5 mmol) 4-aminobenzonitrile was placed in a round bottom flask at 0 ºC. Then, trifluoromethanesulfonic acid (1 mL, 11.1 mmol) was added dropwise for 25 min at 0 ºC. The mixture was stirred for 24 h under $Ar_{(g)}$ at room temperature. After that, distilled water (10 mL) was poured into the mixture and NaOH (2M) was added dropwise until the pH of the solution reached 7. The resultant light-yellow product was filtered and washed with distilled water several times, and then dried in a vacuum oven overnight. Yield: 0.239 g, 81%. ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ: 8.3-8.4 (s, 6H), 6.73-6.64 (d, 6H), 5.91 (s, 6H). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ: 169.7, 153.3, 130.5, 123.2, 113.4. HRMS (ESI, *m/z*): $[M+H]^+$ calcd for $C_{18}H_{18}N_4$: 355.16. Found: 355.16. The spectra are shown below.



^{1}H NMR spectrum for TATP.

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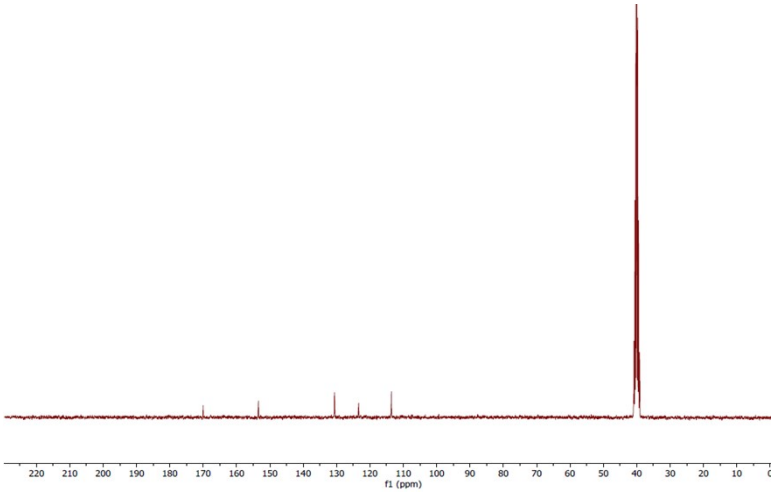
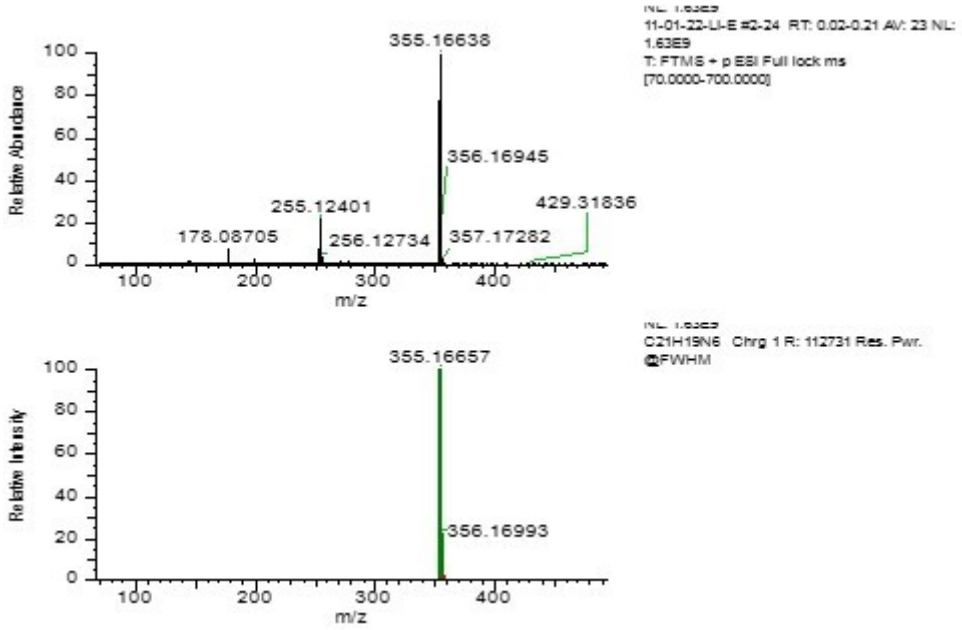
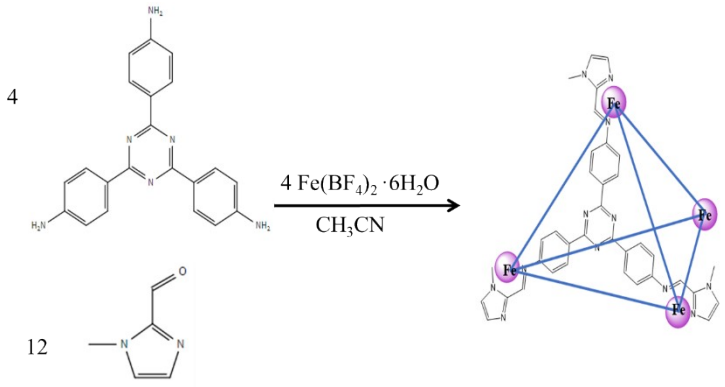


^{13}C NMR spectrum for TATP.



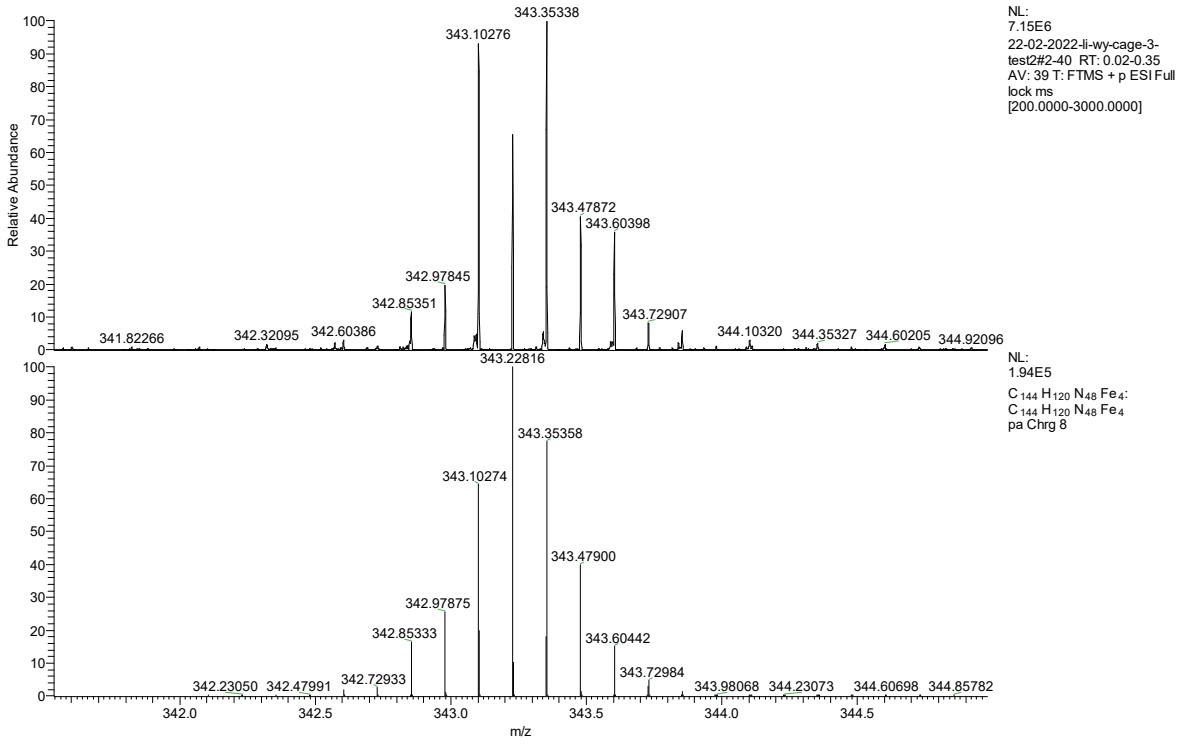
Mass spectrum for TATP.

Synthesis of MOC-1



Scheme. Formation of **MOC-1** in CH_3CN through subcomponent self-assembly approach.

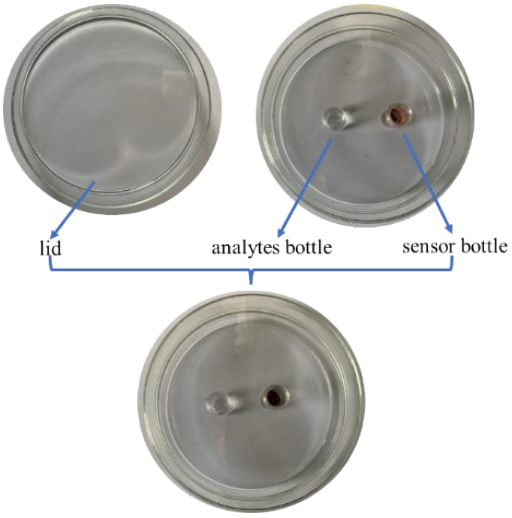
TATP (35.4 mg, 0.1 mmol), 1-methyl-2-imidazolecarboxaldehyde (33 mg, 0.3 mmol) and $Fe(BF_4)_2{\cdot}6H_2O$ (34 mg, 0.1 mmol) were added to a Schlenk flask with acetonitrile (30 mL). The reaction mixture was stirred at 65 °C overnight under argon atmosphere and then cooled to room temperature. The resulting solution was filtered and vapor-diffused with diethyl ether. After several days, single crystals of **MOC-1** were obtained. Yield: 18.9 mg, 22%. When a large amount of diethyl ether was directly added to the solution, a light brown microcrystalline precipitate appeared immediately. It was then filtered, washed with excess diethyl ether. Yield: 63.6 mg, 74%. ESI-MS: (*m*/*z*): $[Fe^{II}_4L_4]^{8+}$: 343.23. Elemental analysis of microcrystalline **MOC-1**: calcd. for $Fe^{II}_4L_4(BF_4)_8{\cdot}9H_2O$, $C_{144}H_{120}N_{48}Fe_4B_8F_{32}{\cdot}9H_2O$: C 48.01%, H 3.86%, N 18.66%; found: C 47.91%, H 3.73%, N 18.16%.



HRMS of **MOC-1** showing the $[Fe^{II}_4L_4]^{8+}$ peaks and the corresponding simulated isotopic patterns.

Sensing experiment device and cyclability test for the sensor

A home-made setup was assembled to detect different analytes (as shown below). About 8 mg of **MOC-1** and 0.5 mL different analytes solution were added into two small glass bottles, and then put in a glass cell culture dish. These were covered by a lid, sealed with parafilm, and incubated under ambient conditions. The discoloration photos were taken at a specific time by iPhone XR (iOS 15.4.1) with the setting of 'photo mode' 'tap to focus' and 'without flash'. The sensing experiments were carried out at room temperature (25 °C) and ambient relative humidity (RH) was about 25%. To control the RH in the sealed dish, another container with various amounts of water was put inside and the RH was monitor by hygrometer. In the cyclability study, after adsorbing $NH_{3(g)}$ molecules, **MOC-1** was termed as **MOC-1**@NH_3. **MOC-1** was exposed to ammonia vapor for 1 min at room temperature. Subsequently, **MOC-1**@NH_3 was placed into a vacuum oven at 70 °C overnight to regenerate **MOC-1** and this adsorption and desorption process was repeated five times. All sensing experiments used **MOC-1** as a microcrystalline powder and were all performed in triplicate.



Experimental set up for the colorimetric sensor **MOC-1**.

Data analysis methods

After obtaining the discoloration photographs, Color Name App in iPhone XR was employed to convert the photos into digital information, which included RGB (red, green, and blue) and HSB1 (hue, saturation, and brightness). These data were analyzed by standard chemometric methods using hierarchical clustering analysis (HCA) and principal component analysis (PCA). HCA, a multivariate statistical analysis method whose main purpose is to divide the analytes into discrete groups based on the characteristics of their respective responses. It involves measuring the distance or similarity between objects and their clustering. PCA is another powerful and effective statistical tool using orthogonal transformation to convert a set of possibly related observations into a set of principal components and the values of these principal components are linearly uncorrelated. In this paper, HCA and PCA was performed on the average values of RGB and HSB1 in triplicate. Euclidean distance[1], representing the total color response, was calculated by the following equation:

$$\text{Euclidean distance} = \sqrt{(R - R_0)^2 + (G - G_0)^2 + (B - B_0)^2 + (H - H_0)^2 + (S - S_0)^2 + (B1 - B1_0)^2}$$

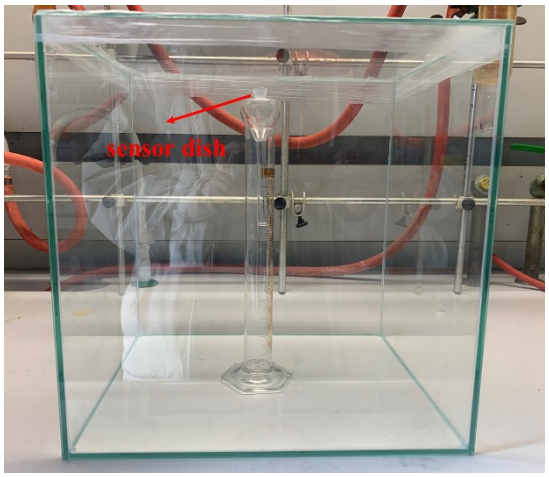
Where values of *R, G, B, H, S, B1* are color of sensor in different conditions and R_0, G_0, B_0, H_0, S_0, $B1_0$ are the control sensor.

Calculation of NH_3 gas concentration in sensitivity experiment

The concentration in ppm was calculated according to the following Eq.[2]

$$C(ppm) = \left(\frac{10\ CRTd_v V_{injected}}{PM_w V_{chamber}}\right)$$

where $C\ (ppm)$ is concentration of $NH_{3(g)}$ in *ppm*, C (wt%) is NH_3 aqueous solution concentration, R is the gas constant, T is the temperature in absolute scale, d_v is the liquid mass density (g/cm^3), $V_{injected}$ is the injected volume in μL, P (atm) is the pressure inside the chamber, M_w is the molecular weight, (g/mol), $V_{chamber}$ is the volume of chamber. In this work, C is 28%; P is 1 atm; M_w is 17 g/mol; T is 298 K. We used a home-made chamber and the $V_{chamber}$ is 26 L (32x27x32 cm), as shown below. The sensor dish is mounted on top of the chamber. After injecting the NH_3 aqueous solution to the chamber by injection syringe, a heating source was used to evaporate the solution to gaseous NH_3.



The schematic diagram of the home-made 26 L seal chamber for sensitivity experiment.

Single-crystal X-ray diffraction analyses

X-ray diffraction analyses for **MOC-1** was carried on MAR345 image plate using Mo-Kα radiation (λ = 0.71073Å), generated by an Incoatec IμS generator equipped with Montel Mirrors. Prior to data collection the crystals were flash frozen at 100 K. Data integration and reduction were performed with CrysAlis^{PRO} (CrysAlis^{PRO} Software System, Vol. Rigaku Corporation: Oxford, UK, 2015.) and the implemented absorption correction was applied. The structures were solved by SHELXT and refined by full-matrix least squares on F^2 using SHELXL2018/3. All non-hydrogen atoms were refined anisotropically and hydrogen atoms were added in calculated positions and refined in riding mode. The crystals of **MOC-1** were quite small and unstable. As diethyl ether was used as anti-solvent, crystals readily redissolved into the mother liquid when exposed to air. To be able to manipulate the crystals prior to data collection, a solvent transfer to THF was performed, assuring the necessary time to isolate and harvest the crystals. Although more data was collected in the low temperature measurements, the final resolution limit was set at 1.21 Å, beyond which the crystal diffracted poorly. The crystal also shows a single large cavity representing 26% of the unit cell volume, the electron density inside this cavity was taken into account by the SQUEEZE procedure in PLATON. All ring systems and their substituents were refined to be planar and the aromatic benzene rings were constraint to be perfect hexagons. The BF_4^- anions were idealized and refined as rigigd groups allowed to rotate and move around the central boron atom. Isotropic and rigid bond restraints were used on all non-metal atoms. The extensive use of restraints make that only global features should be discussed. Final crystallographic data and refinement values for **MOC-1** are listed in Tables S1. CCDC 2157667 contains the supplementary crystallographic data for this paper.

SHELXT:

Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3-8.

Crysalis^{PRO}:

Rigaku (2015). *CrysAlisPro Software System*, Version 1.171.38.41. Rigaku Oxford Diffraction

PLATON SQUEEZE:

Spek, A. L. (2015). *Acta Cryst.* C**71**, 9-18.

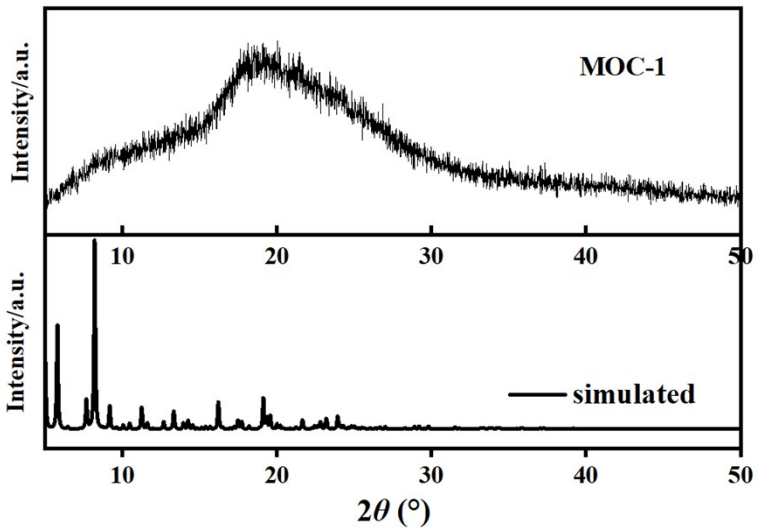


Fig. S1 Powder XRD and simulated PXRD for **MOC-1**.

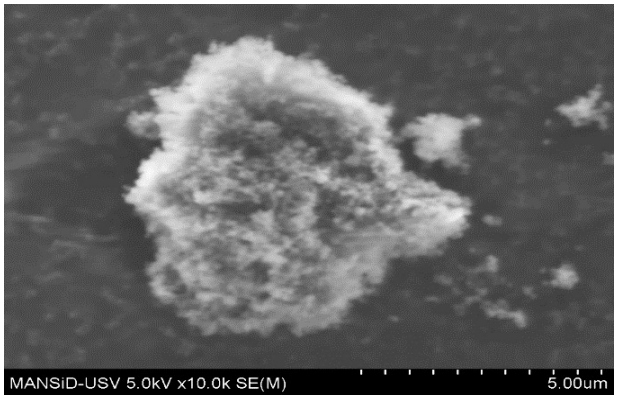


Fig. S2 SEM image for **MOC-1**.

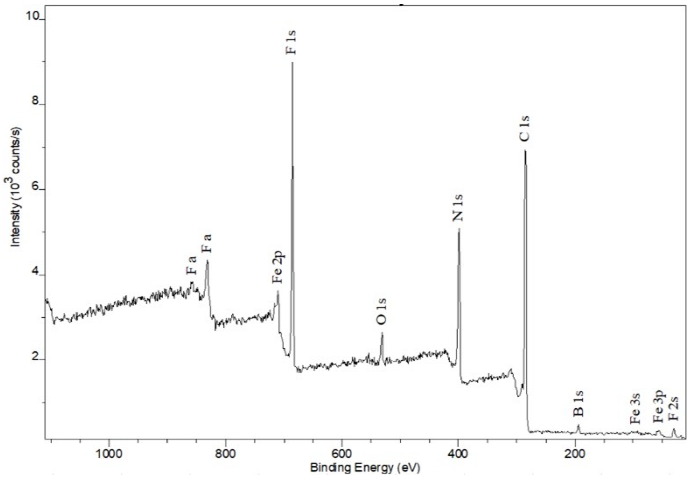


Fig. S3 Full XPS spectrum of **MOC-1**.

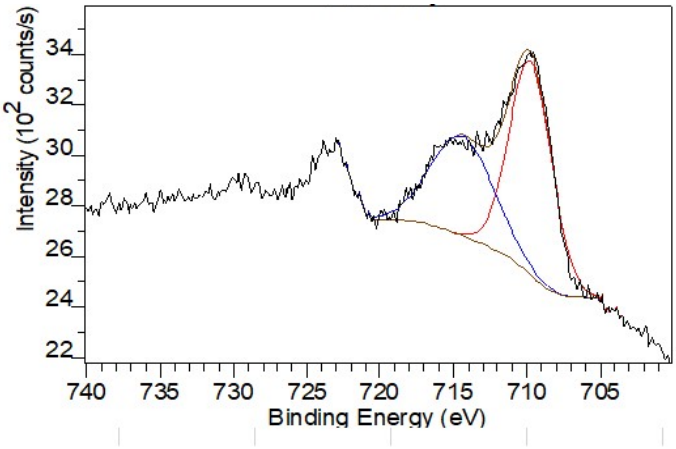


Fig. S4 High resolution Fe 2p XPS spectrum for **MOC-1**.

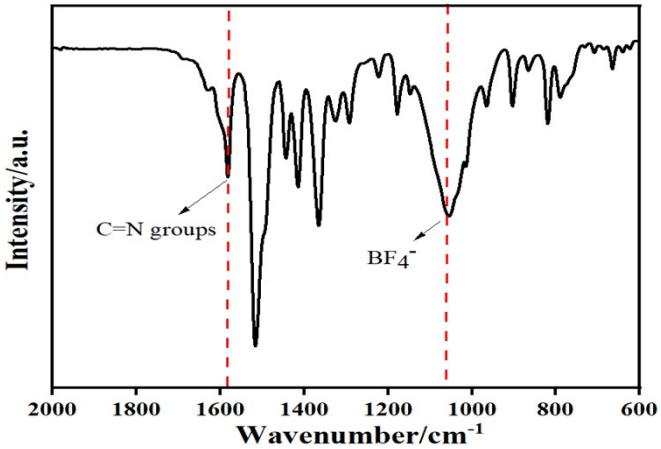


Fig. S5 FT-IR for **MOC-1**.

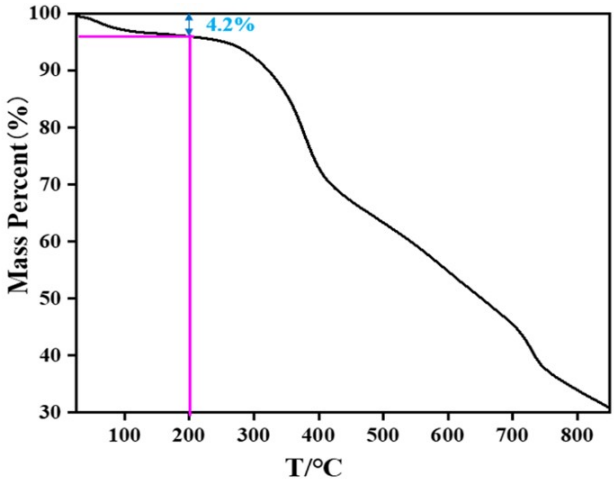


Fig. S6 TGA curve of **MOC-1** and the abscissa of the pink line is 200 ℃.

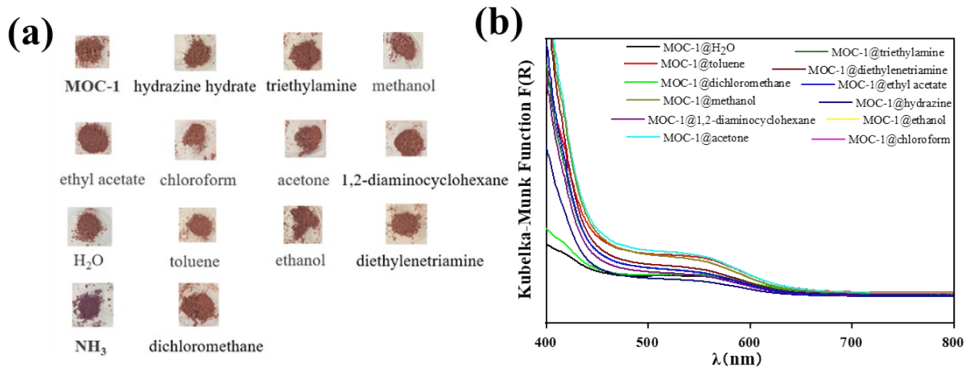


Fig. S7 Digital photographs of **MOC-1** after adsorption of 12 analytes (a) and corresponding diffuse reflectance spectra at r.t (b).

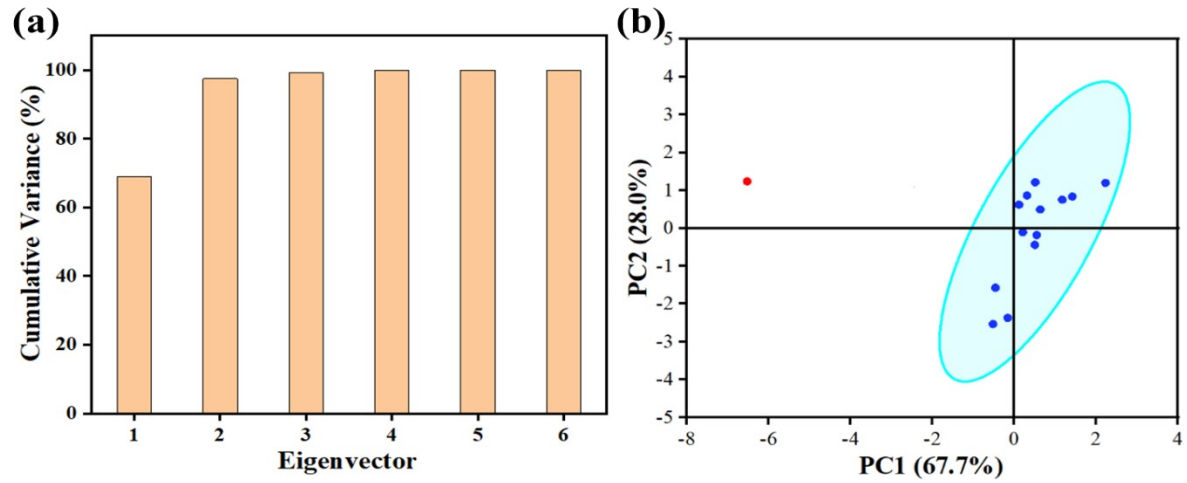


Fig. S8 PCA scree plot (a) and PCA score plot (b) of $NH_{3(g)}$ (red point) and 12 analytes (blue points) at r.t.

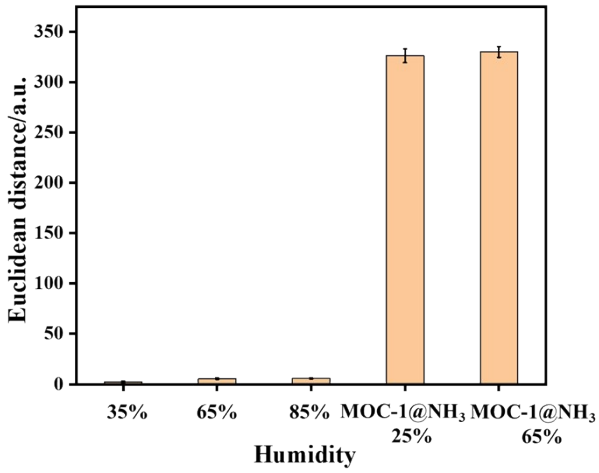


Fig. S9 Sensor performance under different relative humidity levels alone and **MOC-1**@NH_3 under 25% (normal condition) and 65% relative humidity.

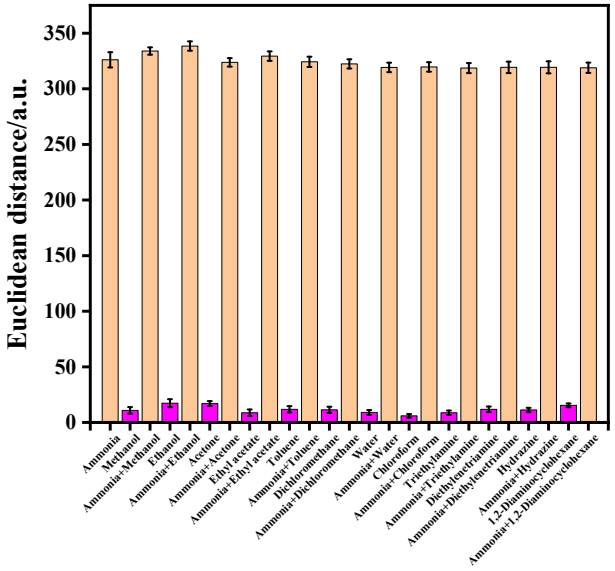


Fig. S10 Interference of various analytes vapours on the colorimetric response of $NH_{3(g)}$ at r.t.

	MOC-1@NH_3	Regenerated MOC-1
1st cycle		
2nd cycle		
3rd cycle		
4th cycle		
5th cycle		

Fig. S11 Digital photographs of **MOC-1**@NH_3 and the regenerated **MOC**-1 in the recyclability test.

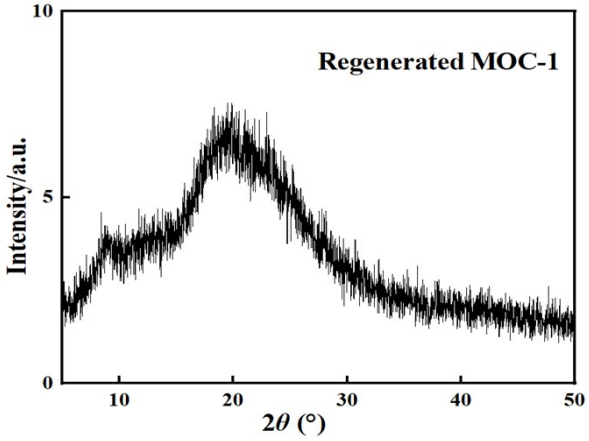


Fig. S12 Powder XRD for regenerated **MOC-1**.

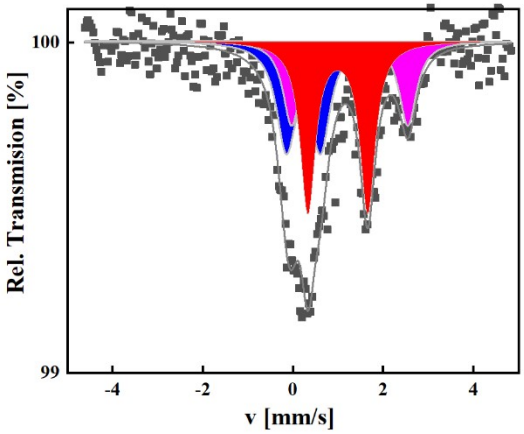


Fig. S13 ^{57}Fe Mössbauer spectrum for regenerated **MOC-1**.

^{57}Fe Mössbauer parameters for regenerated **MOC-1**.

Sample	Spin State Fe(II)	A/A_{tot} (%)	Mössbauer parameters		
			δ (mm s^{-1})	ΔE_Q (mm s^{-1})	$\Gamma/2$ (mm s^{-1})
Regenerated MOC-1	LS (blue)	33	0.23(6)	0.76(1)	0.26(1)
	HS-1 (red)	43	0.99(3)	1.33(5)	0.21(5)
	HS-2 (magenta)	24	1.26(6)	2.58(1)	0.23(1)

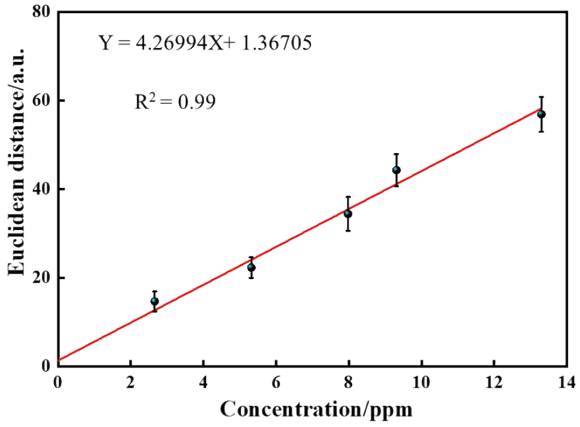


Fig. S14 Plots of the Euclidean distance of **MOC-1** after adsorbing different concentration $NH_{3(g)}$ for 1 h at r.t. The red line is the calibration curves. The noise was defined as the standard deviation among the control (exposure to air).

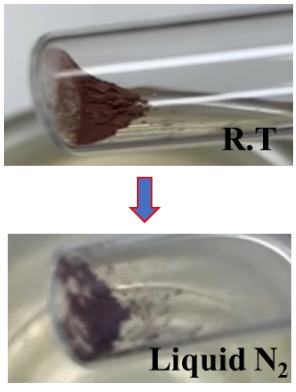


Fig. S15 Thermochromic property of **MOC-1**.

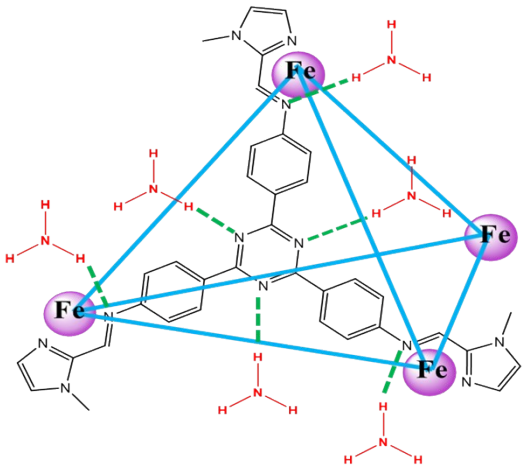


Fig. S16 Suggested discoloration mechanism for $NH_{3(g)}$. Green dots represent hydrogen bonding.

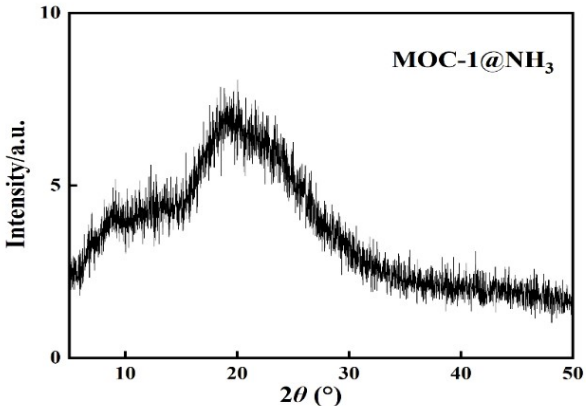
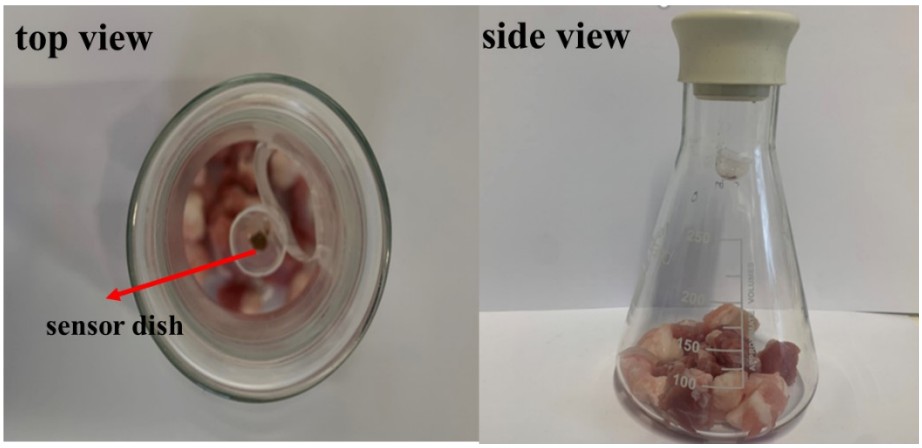


Fig. S17 Powder XRD for **MOC-1**@NH_3.

Application of MOC-1 sensor for monitoring pork spoilage

MOC-1 sensor (5 mg) in a small dish was glued on the top of a conical flask (250 mL) containing 45 g of fresh pork (bacon) bought in a local supermarket. The bottle was sealed by cap and parafilm and stored at 4 °C, as shown below. At specific time intervals (12 h, 36 h, 48 h, 60 h, 72 h, 84 h, 96 h), photographs of the sensor were taken and these data in Table S8 were analyzed by PCA. In addition, at each time interval, a commercial NH_3 gas sensor (AR8500) was used to detect the NH_3 gas concentration in the flask. Noted that in the process of cold chain transportation, the types, packaging, transportation conditions and weights of pork are different, so the experimental results of the spoilage of different pork may vary to some extent. More comprehensive experiments are needed in the future to study the range of MOC-1 in food safety assessment, but the sensor material and the corresponding analytical methods show great potential.



Experimental set up for monitoring pork spoilage.

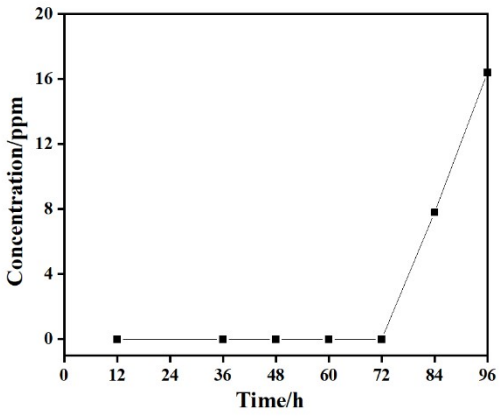


Fig. S18 Plots of $NH_{3(g)}$ concentration at different time internals.

Table S1. Crystal data and structure refinement details for **MOC-1**.

Table S2 HCA database for **MOC-1** and 13 analytes.

Formula	$C_{144}H_{120}Fe_4N_{48}(BF_4)_8 \cdot$[+solvent]
Formula weight	3440.75
Radiation (Å)	MoK_α (0.71073)
Crystal system	Monoclinic
Space group	Ia
T (K)	100
a (Å)	37.219(3)
b (Å)	60.858(2)
c (Å)	37.232(19)
α (°)	90
β (°)	109.597(7)
γ (°)	90
V ($Å^3$)	79448(9)
Z	16
ρ_{calc} ($g.cm^{-3}$)	1.151
θ range (deg)	2.1420 to 16.5170
F(000)	28032
Crystal size (mm)	0.15×0.15×0.10
Absorption coefficient (mm^{-1})	0.369
Data/restraints/parameters	43905/53460/7201
Goodness of fit on F^2	1.168
R_1^a, wR_2^b $(I>2\sigma(I))$	0.0943, 0.2096
R_1^a, wR_2^b *(all data)*	0.1635, 0.2499

MOC-1	**R**	**G**	**B**	**S**	**H**	**B1**
1	138	90	80	10	42	54
2	146	94	77	14	47	57
3	140	92	77	14	45	54
average	141.33	92	78	12.67	44.67	55
Water	**R**	**G**	**B**	**S**	**H**	**B1**
1	138	90	80	10	42	54

2	137	88	79	9	42	53
3	124	76	68	8	45	48
average	133.00	84.67	75.67	9.00	43.00	51.67
Chloroform	**R**	**G**	**B**	**S**	**H**	**B1**
1	144	88	78	9	45	56
2	147	91	79	10	46	57
3	145	89	80	8	44	56
average	145.33	89.33	79	9	45	56.33
Ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	108	71	88	342	32	42
2	110	71	88	344	35	43
3	106	68	86	332	35	41
average	108.00	70.00	87.33	339.33	34.00	42.00
Acetone	**R**	**G**	**B**	**S**	**H**	**B1**
1	137	84	76	7	44	53
2	149	94	84	9	43	58
3	135	81	75	5	44	52
average	140.33	86.33	78.33	7	43.67	54.33
Dichloromethane	**R**	**G**	**B**	**S**	**H**	**B1**
1	127	76	69	7	45	49
2	129	80	70	10	45	50
3	132	80	73	7	44	51
average	129.33	78,67	70.67	8	44.67	50
Hydrazine	**R**	**G**	**B**	**S**	**H**	**B1**
1	141	93	79	13	43	55
2	134	85	71	13	47	52
3	131	82	71	10	45	51
average	135.33	86.67	73.67	12	45	52.67
Methanol	**R**	**G**	**B**	**S**	**H**	**B1**
1	130	80	72	8	44	50
2	139	86	81	5	41	54
3	144	91	84	6	41	56
average	137.67	85.67	79	6.33	42	53.33
Ethanol	**R**	**G**	**B**	**S**	**H**	**B1**
1	128	75	68	6	46	50
2	130	77	69	7	46	50
3	124	72	65	7	47	48
average	127.33	74.67	67.33	6.67	46.33	49.33
Toluene	**R**	**G**	**B**	**S**	**H**	**B1**
1	150	98	80	15	46	58
2	146	94	77	14	47	57
3	149	96	79	14	46	58
average	148.33	96	78.67	14.33	46.33	57.67
Ethyl acetate	**R**	**G**	**B**	**S**	**H**	**B1**
1	134	81	74	6	44	52
2	136	82	76	5	44	53
3	140	87	79	7	43	54
average	136.67	83.33	76.33	6	43.67	53
Triethylamine	**R**	**G**	**B**	**S**	**H**	**B1**
1	136	86	78	8	42	53
2	144	94	83	10	42	56

3	140	90	81	9	42	54
average	140	90	80.67	9	42	54.33
Diethylenetriamine	**R**	**G**	**B**	**S**	**H**	**B1**
1	143	90	81	8	43	56
2	139	85	76	8	45	54
3	132	78	70	7	46	51
average	138	84.33	75.67	7.67	44.67	53.67
1,2-Diaminocyclo-hexane	**R**	**G**	**B**	**S**	**H**	**B1**
1	124	72	63	8	49	48
2	125	72	64	7	48	49
3	138	85	76	8	44	54
average	129	76.33	67.67	7.67	47	50.33

Table S3 PCA database for **MOC-1** and 13 analytes.

Analytes	**R**	**G**	**B**	**S**	**H**	**B1**
MOC-1	141.33	92	78	12.67	44.67	55
Hydrazine	135.33	86.67	73.67	12	45	52.67
Triethylamine	140	90	80.67	9	42	54.33
1,2-Diaminocyclohexane	129	76.33	67.67	7.67	47	50.33
Diethylenetriamine	138	84.33	75.67	7.67	44.67	53.67
Methanol	137.67	85.67	79	6.33	42	53.33
Ethanol	127.33	74.67	67.33	6.67	46.33	49.33
Chloroform	145.33	89.33	79	9	45	56.33
Acetone	140.33	86.33	78.33	7	43.67	54.33
Ethyl acetate	136.67	83.33	76.33	6	43.67	53
Dichloromethane	129.33	78,67	70.67	8	44.67	50
Toluene	148.33	96	78.67	14.33	46.33	57.67
Water	133.00	84.67	75.67	9.00	43.00	51.67
Ammonia	108.00	70.00	87.33	339.33	34.00	42.00

Table S4 Response time database for ammonia and humidity.

MOC-1@NH_3							
Time (s)	**Times**	**R**	**G**	**B**	**S**	**H**	**B1**
0	1	138	90	80	10	42	54
	2	146	94	77	14	47	57
	3	140	92	77	14	45	54
	1	157	109	108	1	31	61
	2	162	113	110	4	27	64

5	3	155	107	105	2	32	60
10	1	119	76	78	341	35	45
	2	118	71	73	342	36	43
	3	123	71	74	355	36	43
15	1	109	70	80	354	35	42
	2	113	74	83	344	34	44
	3	117	79	86	348	32	45
30	1	114	75	83	347	34	44
	2	112	72	81	353	35	43
	3	121	82	91	346	32	47
60	1	106	71	85	339	33	41
	2	105	67	82	346	36	41
	3	103	68	82	335	33	40
90	1	102	64	82	338	37	40
	2	105	65	84	341	38	41
	3	110	70	88	332	36	43
120	1	115	84	94	351	26	45
	2	108	78	87	340	27	42
	3	110	83	92	337	24	43
180	1	113	83	90	345	26	44
	2	110	80	88	337	27	43
	3	114	84	91	351	26	44
240	1	106	71	96	343	36	43
	2	102	67	93	329	36	41
	3	104	72	97	333	35	43
Humidity							
35%	1	138	90	77	12	44	55
	2	141	93	80	11	44	56
	3	139	91	78	12	45	55
65%	1	136	89	75	11	45	52
	2	140	92	81	13	43	50
	3	138	88	78	12	40	53
85%	1	137	89	77	11	44	53
	2	140	90	81	11	42	51
	3	138	88	79	12	41	53
MOC-1@NH_3 25%	1	106	71	96	343	36	43
	2	102	67	93	329	36	41
	3	104	72	97	333	35	43
MOC-1@NH_3 65%	1	105	70	96	344	36	43
	2	101	65	94	339	36	41
	3	104	73	98	333	34	42

Table S5 Different analyte vapours interference experiment database.

MOC-1@water	**R**	**G**	**B**	**S**	**H**	**B1**
1	147	90	81	11	46	58
2	149	94	80	10	43	56
3	152	93	79	9	46	58
average	149.33	92.33	80.00	10.00	45.00	57.33
MOC-1@water/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**

1	132	82	109	327	37	51
2	136	86	110	335	36	53
3	137	85	112	328	37	53
average	135.00	84.33	110.33	330.00	36.67	52.33
MOC-1@chloroform	**R**	**G**	**B**	**S**	**H**	**B1**
1	143	99	79	11	46	58
2	144	94	76	10	46	57
3	143	96	78	10	45	57
average	143.33	96.33	77.67	10.33	45.67	57.33
MOC-1@chloroform/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	135	86	110	330	36	52
2	133	85	109	335	36	52
3	139	89	115	326	35	54
average	135.67	86.67	111.33	330.33	35.67	52.67
MOC-1@acetone	**R**	**G**	**B**	**S**	**H**	**B1**
1	149	101	92	12	39	57
2	147	99	88	11	39	57
3	150	99	90	10	41	56
average	148.67	99.67	90.00	11.00	39.67	56.67
MOC-1@acetone/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	149	96	121	337	35	58
2	147	94	117	330	36	57
3	133	81	105	336	39	52
average	143.00	90.33	114.33	334.33	36.67	55.67
MOC-1@hydrazine	**R**	**G**	**B**	**S**	**H**	**B1**
1	151	93	79	12	42	55
2	154	89	81	10	44	58
3	151	92	71	9	43	56
average	152.00	91.33	77.00	10.33	43.00	56.33
MOC-1@hydrazine/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	130	81	105	336	37	49
2	129	82	106	325	36	50
3	130	81	105	330	37	55
average	129.67	81.33	105.33	330.33	36.67	51.33
MOC-1@ethanol	**R**	**G**	**B**	**S**	**H**	**B1**
1	150	102	92	10	38	58
2	148	98	87	11	40	56
3	152	99	89	9	40	55
average	150.00	99.67	89.33	10.00	39.33	56.33
MOC-1@ethanol/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	103	66	72	345	35	40
2	113	72	77	347	36	44
3	93	56	65	350	39	36
average	103.00	64.67	71.33	347.33	36.67	40.00
MOC-1@ethyl acetate	**R**	**G**	**B**	**S**	**H**	**B1**
1	142	93	87	10	40	54
2	144	93	86	10	41	55
3	145	98	89	9	38	56
average	143.67	94.67	87.33	9.67	39.67	55.00
MOC-1@ethyl acetate/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	102	69	79	341	32	40

2	110	79	88	342	28	43
3	113	77	89	335	31	44
average	108.33	75.00	85.33	339.33	30.33	42.33
MOC-1@diethylenetriamine	**R**	**G**	**B**	**S**	**H**	**B1**
1	149	96	81	10	44	55
2	149	95	86	9	45	54
3	153	98	84	11	46	55
average	150.33	96.33	83.67	10.00	45.00	54.67
MOC-1@diethylenetriamine/ ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	134	84	107	325	37	52
2	130	82	104	331	37	51
3	137	89	110	335	35	53
average	133.67	85.00	107.00	330.33	36.33	52.00
MOC-1@triethylamine	**R**	**G**	**B**	**S**	**H**	**B1**
1	147	96	80	12	42	53
2	143	98	83	10	44	55
3	148	101	81	13	45	54
average	146.00	98.33	81.33	11.67	43.67	54.00
MOC-1@triethylamine/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	140	94	120	328	34	56
2	132	84	110	325	36	51
3	138	90	113	334	34	54
average	136.67	89.33	114.33	329.00	34.67	53.67
MOC-1@1,2-diaminocyclohexane	**R**	**G**	**B**	**S**	**H**	**B1**
1	152	102	85	11	45	57
2	154	101	83	10	43	53
3	151	99	84	12	42	55
average	152.33	100.67	84.00	11.00	43.33	55.00
MOC-1@1,2-diaminocyclohexane/ ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	131	79	104	331	39	51
2	133	82	107	325	38	52
3	136	87	109	334	36	53
average	133.33	82.67	106.67	330.00	37.67	52.00
MOC-1@methanol	**R**	**G**	**B**	**S**	**H**	**B1**
1	150	98	85	11	43	58
2	147	94	82	11	43	56
3	149	98	84	12	43	58
average	148.67	96.67	83.67	11.33	43.00	57.33
MOC-1@methanol/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	115	72	81	347	37	45
2	109	67	76	340	38	42
3	112	73	82	346	34	43
average	112.00	70.67	79.67	344.33	36.33	43.33
MOC-1@toluene	**R**	**G**	**B**	**S**	**H**	**B1**
1	147	100	81	14	45	55
2	146	99	83	15	42	56
3	150	102	84	16	44	58

average	147.67	100.33	82.67	15.00	43.67	56.33
MOC-1@toluene/ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	135	86	110	330	36	52
2	133	85	109	339	36	52
3	139	89	115	336	35	54
average	135.67	86.67	111.33	335.00	35.67	52.67
MOC-1@dichloromethane	**R**	**G**	**B**	**S**	**H**	**B1**
1	146	98	87	11	40	57
2	148	95	82	12	42	55
3	151	99	84	13	44	59
average	148.33	97.33	84.33	12.00	42.00	57.00
MOC-1@dichloromethane/ ammonia	**R**	**G**	**B**	**S**	**H**	**B1**
1	132	83	107	330	37	51
2	129	81	106	338	37	50
3	133	85	109	332	36	52
average	131.33	83.00	107.33	333.33	36.67	51.00

Table S6 Recyclability database for five adsorption and desorption cycles.

	times	**R**	**G**	**B**	**S**	**H**	**B1**
MOC-1@NH_3 (1^{st} cycle)	1	116	81	97	325	30	45
	2	104	72	87	334	30	40
	3	110	76	92	327	30	43
Regenerated MOC-1	1	110	71	79	342	35	43
	2	112	75	81	354	33	43

(1st cycle)	3	116	78	85	345	32	45
MOC-1@NH_3 (2nd cycle)	1	195	125	106	12	45	76
	2	201	129	110	12	45	78
	3	194	120	105	10	45	76
Regenerated MOC-1 (2nd cycle)	1	124	109	88	27	34	52
	2	120	112	90	28	34	53
	3	132	109	88	26	34	52
MOC-1@NH_3 (3rd cycle)	1	105	74	90	327	29	41
	2	101	71	86	334	29	39
	3	117	82	99	326	29	45
Regenerated MOC-1 (3rd cycle)	1	117	92	71	24	42	48
	2	127	95	73	24	42	49
	3	125	94	73	24	41	49
MOC-1@NH_3 (4th cycle)	1	122	82	89	341	32	47
	2	137	96	103	355	29	53
	3	128	87	94	345	32	50
Regenerated MOC-1 (4th cycle)	1	124	109	88	27	34	52
	2	120	112	90	28	34	53
	3	132	109	88	26	34	52
MOC-1@NH_3 (5th cycle)	1	132	93	111	333	29	51
	2	123	88	104	326	28	48
	3	118	85	101	323	27	46
Regenerated MOC-1 (5th cycle)	1	116	101	92	23	25	48
	2	129	102	94	21	25	49
	3	119	99	92	24	25	48

	times	**R**	**G**	**B**	**S**	**H**	**B1**
control	1	138	90	80	10	42	54
	2	146	94	77	14	47	57
	3	140	92	77	14	45	54
2.66 ppm	1	150	88	81	7	40	53

	2	155	91	83	8	41	55
	3	156	87	79	8	41	52
5.32 ppm	1	156	102	87	17	46	62
	2	155	105	91	17	44	64
	3	153	103	88	17	45	62
7.98 ppm	1	163	108	93	13	41	62
	2	158	105	91	12	42	62
	3	165	114	95	12	38	67
9.31 ppm	1	166	116	97	17	43	65
	2	170	120	100	18	41	68
	3	168	119	98	18	44	64
13.3 ppm	1	168	127	117	11	31	66
	2	167	121	112	10	32	64
	3	165	123	115	12	34	63

Table S7 The Euclidean distance *vs*. $NH_{3(g)}$ concentration database

Table S8. Comparison of the sensing performances for **MOC-1** sensor developed in this work and some other previously reported.

PANI = polyaniline, FJU-56 = $[Co(H_{0.27}L)]\cdot 4H_2O\cdot 0.5DMF$ (L = Tris-(4-tetrazolyl-phenyl)amine),

sensors	Detection limit	Analytical method	operation temperature (℃)	Ref
$TiO_2/SnO_2/WO_3$	20 ppm	resistance	200	3
$PANI/rGO/SnO_2$	20 ppm	resistance	r.t.	4
MoO_3	10 ppm	resistance	500	5
PANI-RGO	100 ppm	resistance	r.t.	6
$Ni_3V_2O_8$	50 ppm	resistance	650	7
PANI-ZnO	10 ppm	resistance	r.t.	8
FJU-56	1.38 ppm	absorbance	r.t.	9
TMOF-6(Cl)	13 ppm	fluorescence	r.t.	10
$[Fe(trz\text{-}tet)_2(H_2O)_4]\cdot 2H_2O$	NA	image digitization	r.t.	11
$[Fe(H_2btm)_2(H_2O)_2]Cl_2$	0.58 ppm	image digitization	r.t.	12
MOC-1	2.8 ppm	image digitization	r.t.	This work

TMOF-6(Cl) = $[Pb_{1.5}Cl_2+][^{-}O_2C(C_6H_4)_2CO_2^{-}]\cdot 0.5H_2O$, trz-tetH = 5-(4H-1,2,4-triazol-yl)-2H-tetrazole, H_2btm = di(1H-tetrazol-5-yl)methane

Table S9 HCA data for pork spoilage experiment.

12 h	**R**	**G**	**B**	**S**	**H**	**B1**
1	158	105	97	7	38	61
2	165	112	104	7	36	64
3	152	99	90	8	40	59
average	158.33	105.33	97.00	7.33	38.00	61.33
36 h	**R**	**G**	**B**	**S**	**H**	**B1**
1	151	102	94	8	37	59
2	154	105	97	8	37	60
3	150	102	94	8	37	58
average	151.67	103.00	95.00	8.00	37.00	59.00
48 h	**R**	**G**	**B**	**S**	**H**	**B1**
1	153	103	96	7	37	60
2	164	115	106	9	35	64
3	147	97	90	7	38	57
average	154.67	105.00	97.33	7.67	36.67	60.33
60 h	**R**	**G**	**B**	**S**	**H**	**B1**
1	158	106	98	7	37	61
2	168	114	106	7	36	65
3	159	106	98	7	38	62
average	161.67	108.67	100.67	7.00	37.00	62.67
72 h	**R**	**G**	**B**	**S**	**H**	**B1**
1	157	114	96	7	36	63
2	152	112	94	8	39	62
3	164	110	102	8	38	64
average	157.67	112.00	97.33	7.67	37.67	63.00
84 h	**R**	**G**	**B**	**S**	**H**	**B1**
1	134	93	89	5	33	52
2	137	96	92	5	32	53
3	132	94	88	8	33	57
average	134.33	94.33	89.67	6.00	32.67	54.00
96 h	**R**	**G**	**B**	**S**	**H**	**B1**
1	110	83	75	13	31	43
2	114	86	78	13	31	44
3	111	83	76	11	31	43
average	111.67	84.00	76.33	12.33	31.00	43.33

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