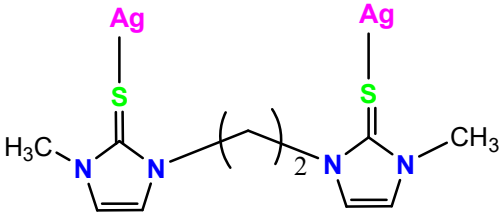
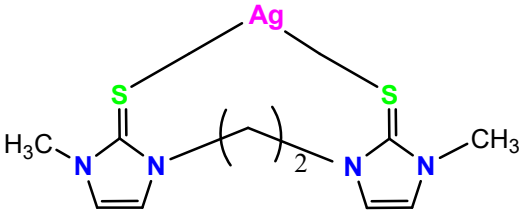
Electronic Supplementary Material (ESI) for CrystEngComm.

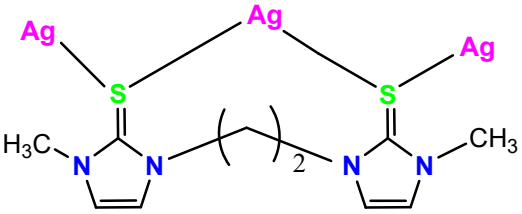
Supplementary



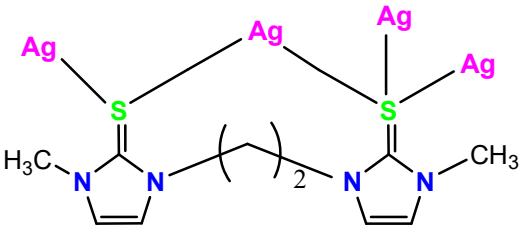
Bis-monodentate (**1**)



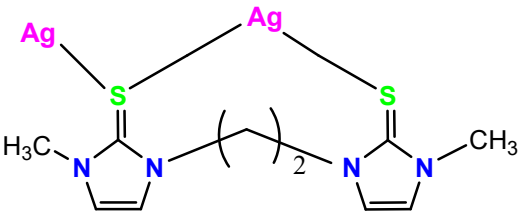
Chelating(**2**)



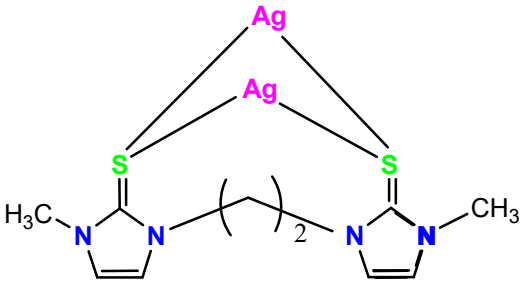
Chelating combining Bis μ_2-bridging (**3**)



Chelating combining μ_2 and μ_3-bridging (**4**)



Chelating combining monodentate and μ_2-bridging (**5**)

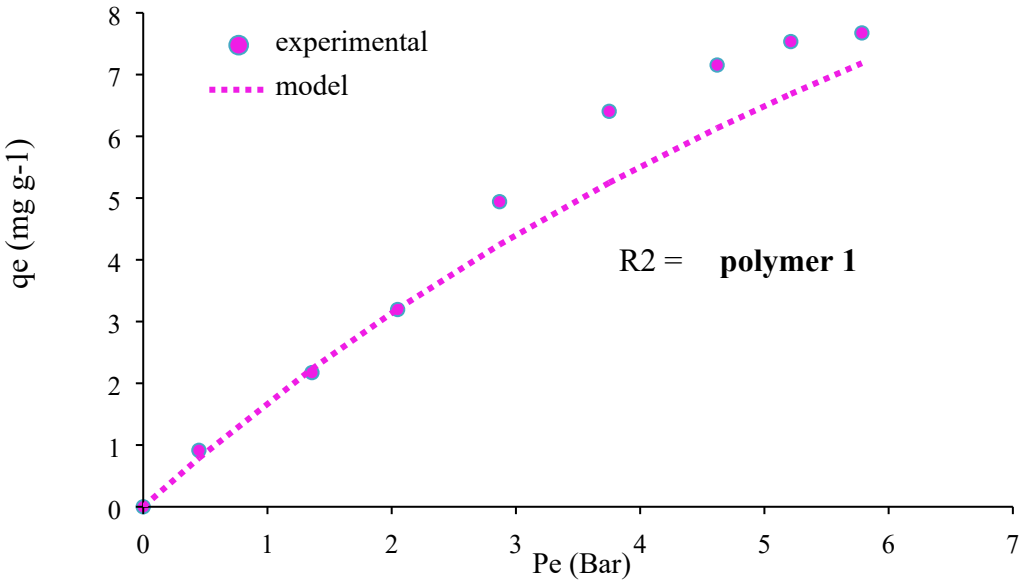


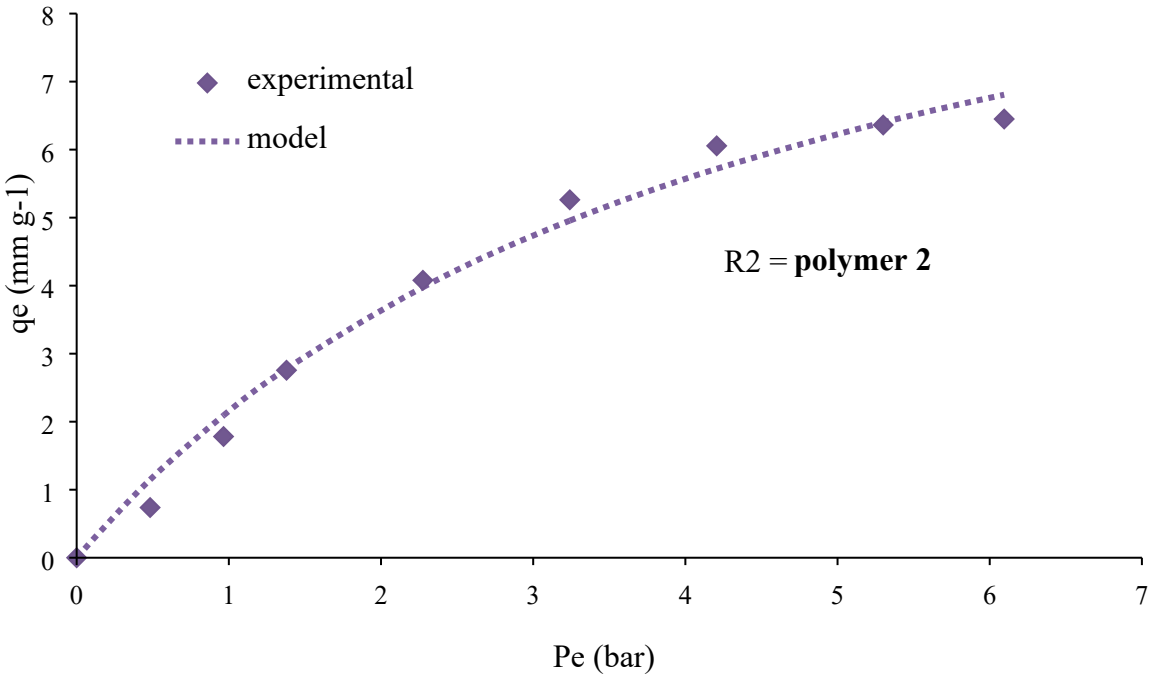
Bis-μ_2 chelating (**6**)

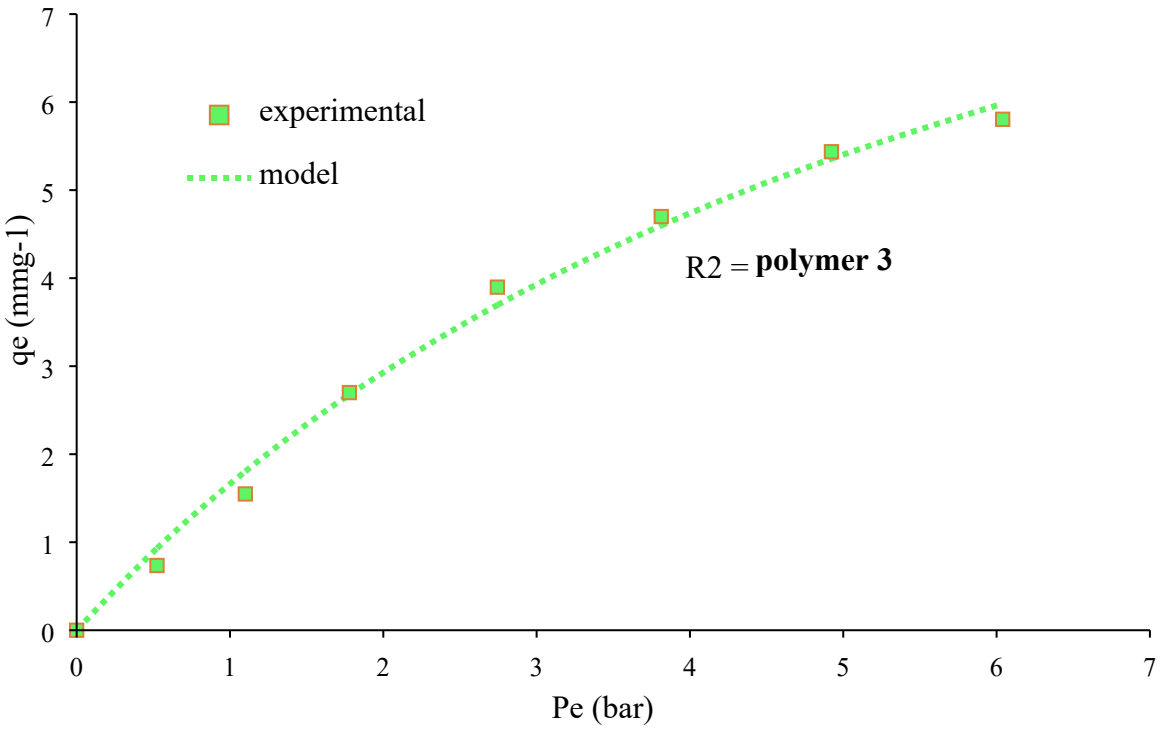
Chart S1: Types of 1, 2- bis (1-methylthioimidazolyl) ethane coordination fashion.

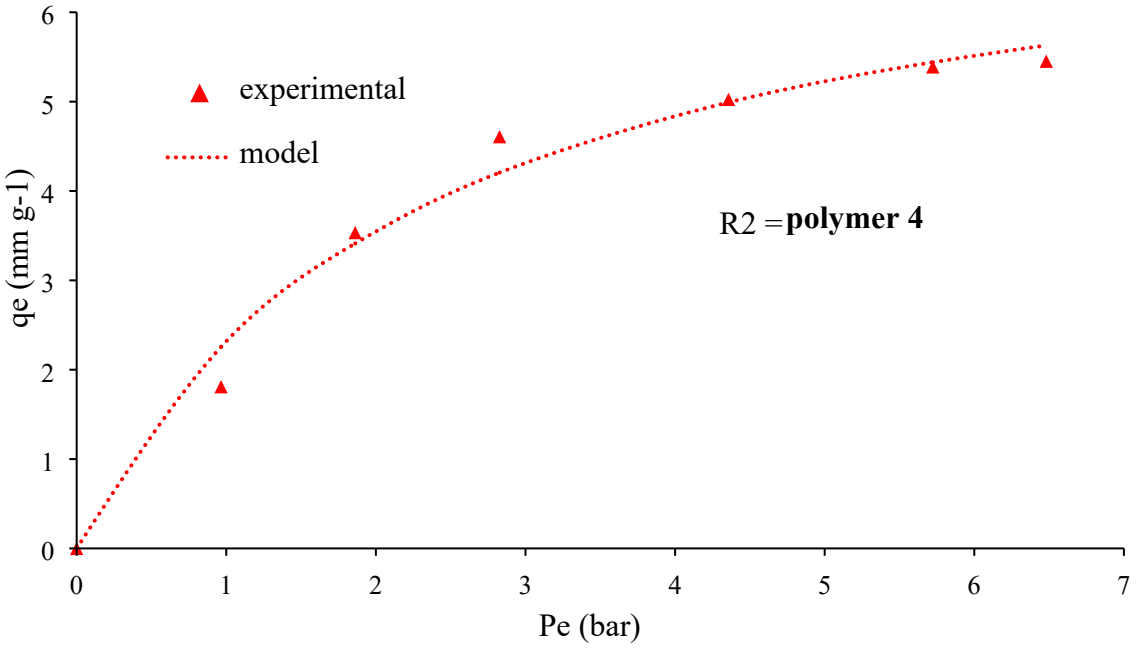
Table S1. Selected bond distances(Å) and bond angles (˚) for compounds **1- 5.**

Compound	bond distances	(Å)	bond angles	(˚)
1	Ag(1)-S(1)	2.504	S(2)-Ag(1)-S(2)	110.44
	Ag(1)-S(2)	2.520	S(1)-Ag(1)-S(2)	104.27
	Ag(1)-S(2)	2.620	S(1)-Ag(1)-O(1)	76.33
	Ag(1)-O(2)	2.683	S(2)-Ag(1)-O(2)	77.57
	Ag(1)-O(1)	2.603	O(2)-Ag(1)-O(1)	48.37
	Ag(2)-S(2)	2.500	O(5)-Ag(1)-S(2)	117.90
	Ag(2)-S(1)	2.460	S(1)-Ag(2)-O(4)	91.20
	Ag(2)-O(4)	2.476	S(1)-Ag(2)-S(2)	147.37
	Ag(2)-O(5)	2.666	O(4)-Ag(2)-O(5)	50.04
2	Ag(2)-S(1)	2.464	S(1)-Ag(2)-S(2)	162.92
	Ag(2)-S(2)	2.432	S(1)-Ag(2)-O(5)	81.53
	Ag(2)-O(2)	2.647	S(2)-Ag(2)-S(5)	115.27
	Ag(1)-O(1)	2.440	S(1)-Ag(1)-S(1)	97.90
	Ag(1)-O(6)	2.485	S(1)-Ag(1)-S(2)	99.84
	Ag(1)-S(1)	2.702	O(1)-Ag(1)-O(6)	123.86
	Ag(1)-S(2)	2.485	O(1)-Ag(1)-S(1)	89.79
	Ag(1)-S(1)	2.665	S(2)-Ag(1)-O(6)	79.18
3	Ag(1)-S(1)	2.516	S(2)-Ag(1)- S(1)	123.79
	Ag(1)-S(1)	2.575	S(2)-Ag(1)-S(1)	109.64
	Ag(1)-S(2)	2.560	S(1)-Ag(1)-S(1)	126.19
4	Ag(1)-S(1)	2.608	S(1)-Ag(1)-S(1)	92.45
	Ag(1)-S(1)	2.703	S(1)-Ag(1)-S(2)	105.64
	Ag(1)-S(2)	2.564	S(1)-Ag(1)-S(4)	93.86
	Ag(1)-S(4)	2. 600	S(2)-Ag(1)-S(4)	108.41
	Ag(2)-S(2)	2. 651	S(2)-Ag(2)-S(3)	94.75
	Ag(2)-S(3)	2.465	S(2)-Ag(2)-S(4)	126.83
	Ag(2)-S(4)	2.497	S(3)-Ag(2)-S(4)	138.28
5	Ag(1)-S(1)	2.853	S(1)-Ag(1)-S(2)	95.29
	Ag(1)-S(2)	2.586	S(2)-Ag(1)-S(3)	105.27
	Ag(1)-S(3)	2.638	S(3)-Ag(1)-S(4)	84.14
	Ag(1)-S(4)	2.784	S(1)-Ag(1)-S(4)	84.50
	Ag(1)-S(4)	2.895	S(4)-Ag(1)-S(3)	116.30
	Ag(2)-S(3)	2.644	S(3)-Ag(2)-S(4)	88.77
	Ag(2)-S(4)	2.551	O(3)-Ag(2)-S(6)	123.27
	Ag(2)-S(5)	2.638	S(6)-Ag(2)-S(4)	122.77
	Ag(2)-S(6)	2.569	S(5)-Ag(2)-S(6)	87.51
	Ag(3)-S(1)	2.555	S(2)-Ag(3)-S(6)	84.41
	Ag(3)-S(2)	2.014	S(2)-Ag(3)-S(1)	92.15
	Ag(3)-S(5)	2.689	S(1)-Ag(3)-S(5)	106.80
	Ag(3)-S(6)	2.671	S(2)-Ag(3)-S(6)	114.84
	Ag(3)-S(6)	2.849	S(5)-Ag(3)-S(5)	118.88


experimental
model
qe (mg g-1)
Pe (Bar)
R2 = polymer 1
0
1
2
3
4
5
6
7
8


experimental
model
qe (mm g-1)
Pe (bar)
R2 = polymer 2
0
1
2
3
4
5
6
7
8


experimental
model
R2 = polymer 3
qe (mmg-1)
Pe (bar)
0
1
2
3
4
5
6
7


experimental
model
R2 = polymer 4
qe (mm g-1)
Pe (bar)
0
1
2
3
4
5
6
7

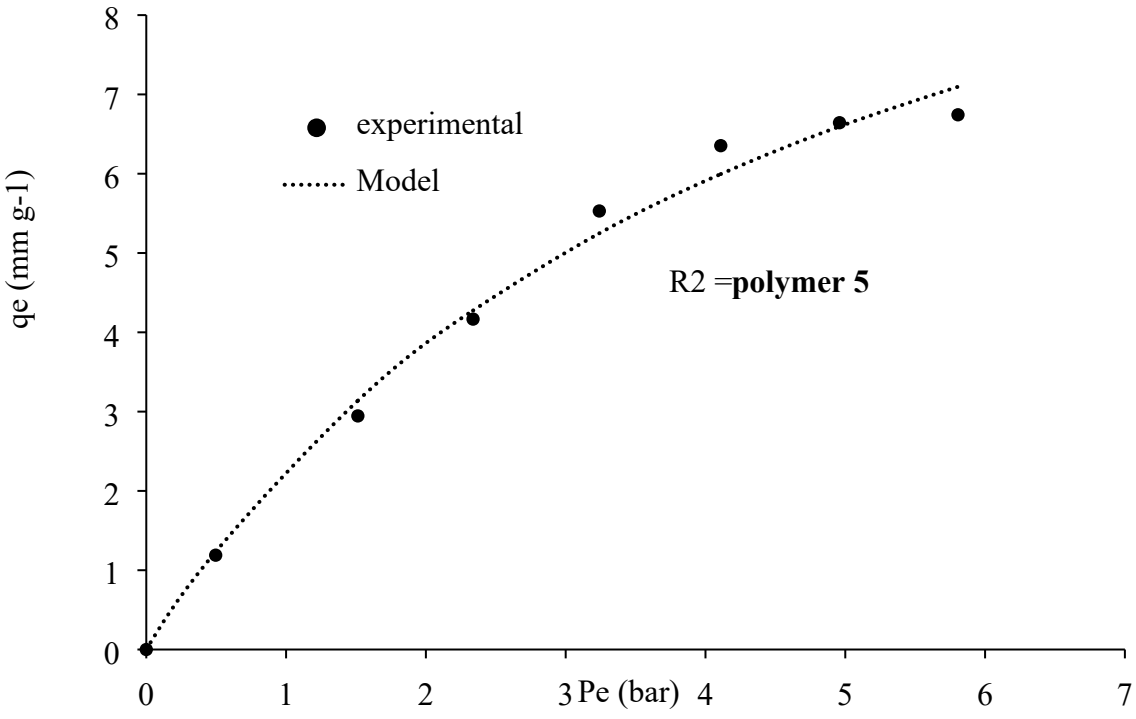
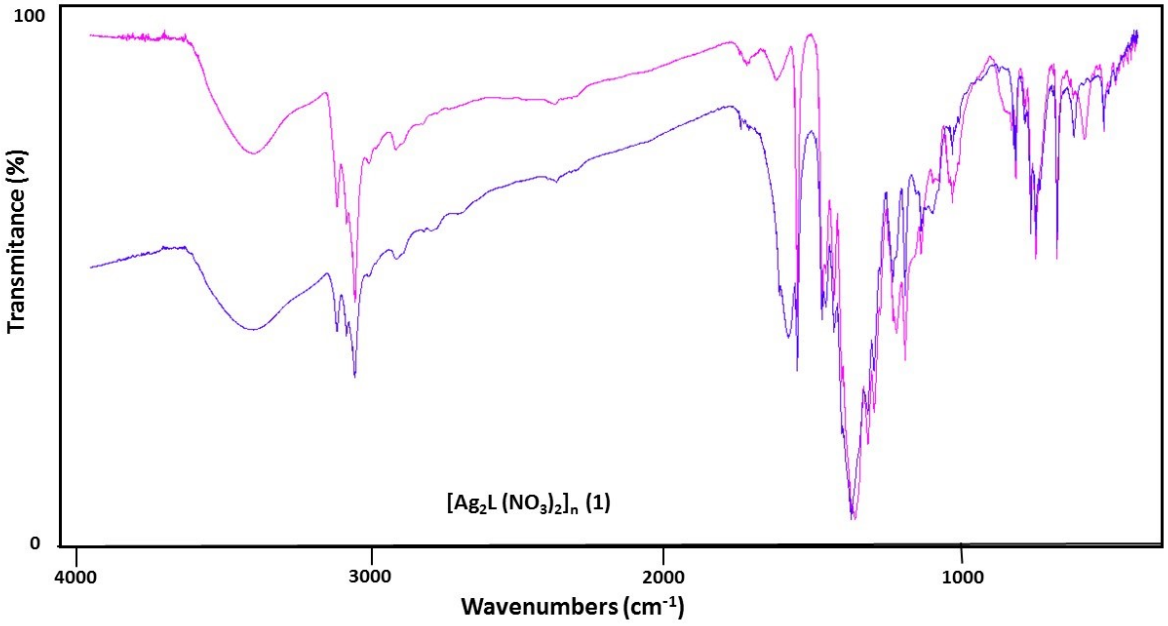
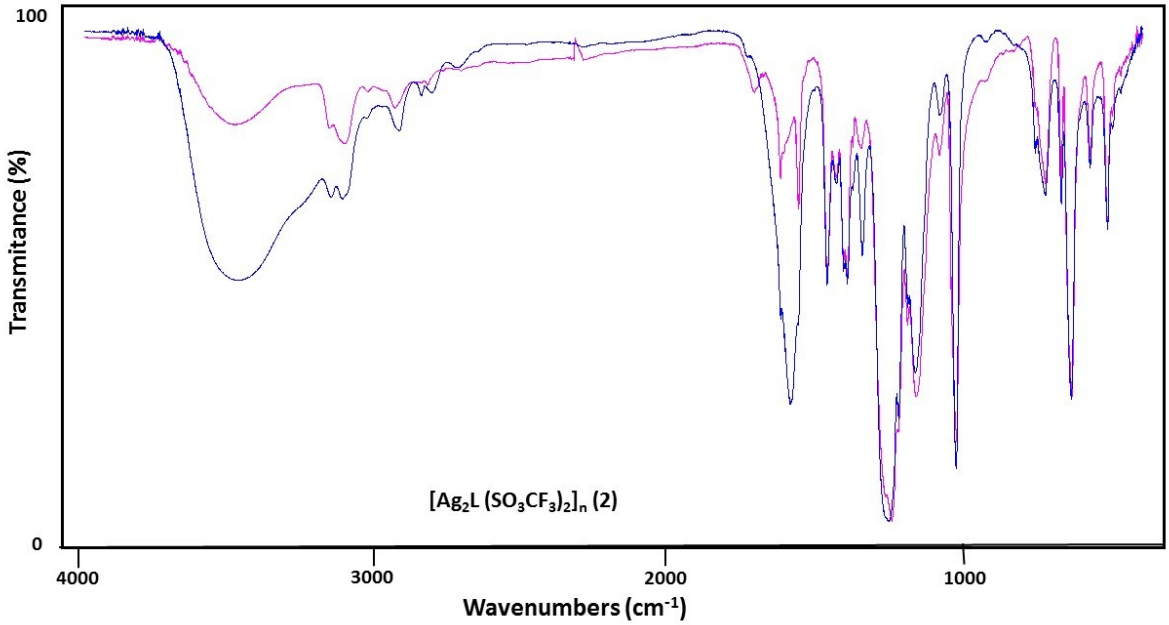
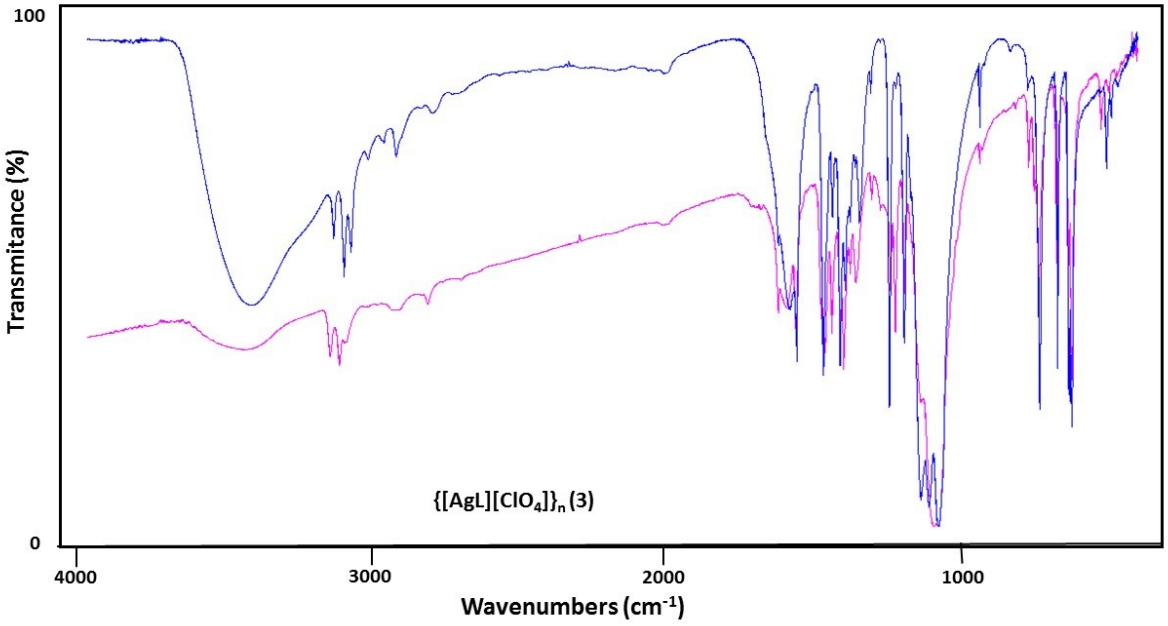
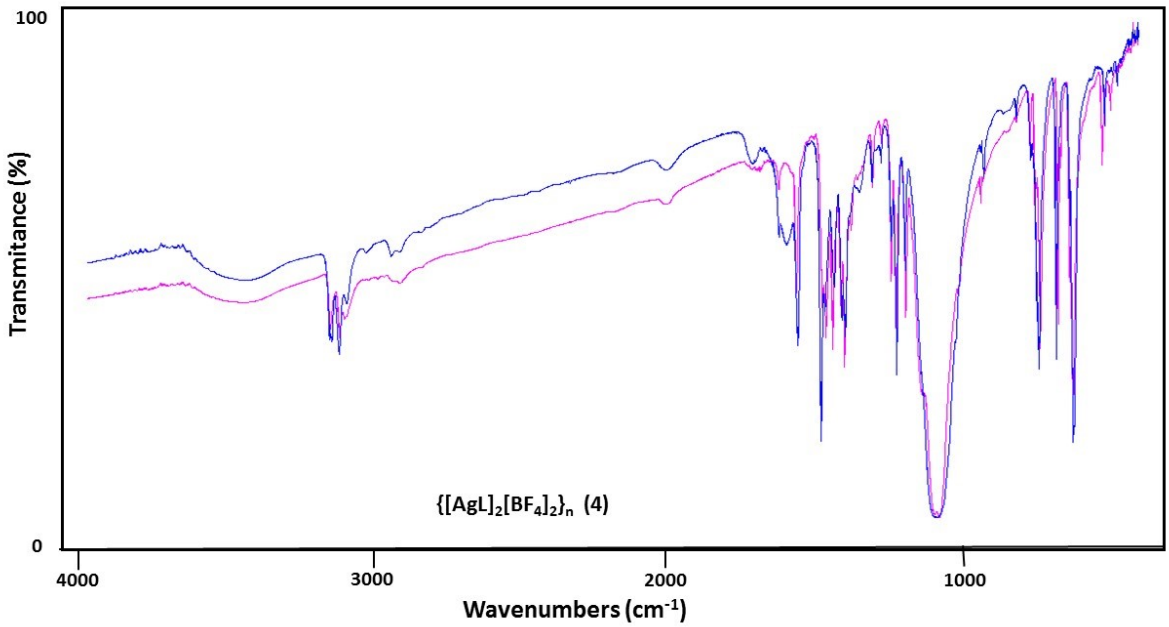


Figure S1: Volumetric adsorption isotherms of H2S measured at 278 K for polymer **1**-**5**.


100
0
Transmitance (%)
$[Ag_2L(NO_3)_2]_n$ (1)
4000
3000
2000
1000
Wavenumbers (cm^{-1})


100
0
Transmitance (%)
$[Ag_2L(SO_3CF_3)_2]_n$ (2)
4000
3000
2000
1000
Wavenumbers (cm^{-1})


100
Transmitance (%)
0
{[AgL][ClO4]}n (3)
4000
3000
2000
1000
Wavenumbers (cm-1)


100
Transmitance (%)
0
{[AgL]2[BF4]2}n (4)
4000
3000
2000
1000
Wavenumbers (cm-1)

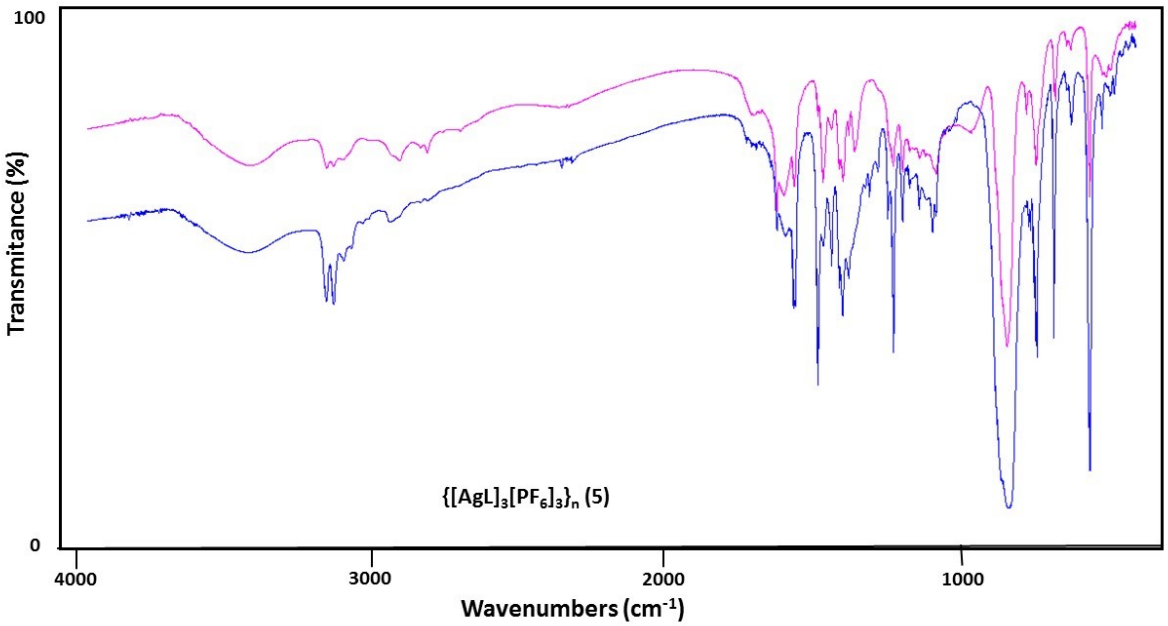


Figure S2. FT-IR spectra for coordination polymers **1**-**5** before (blue) and after (pink) exposure to H_2S gas.

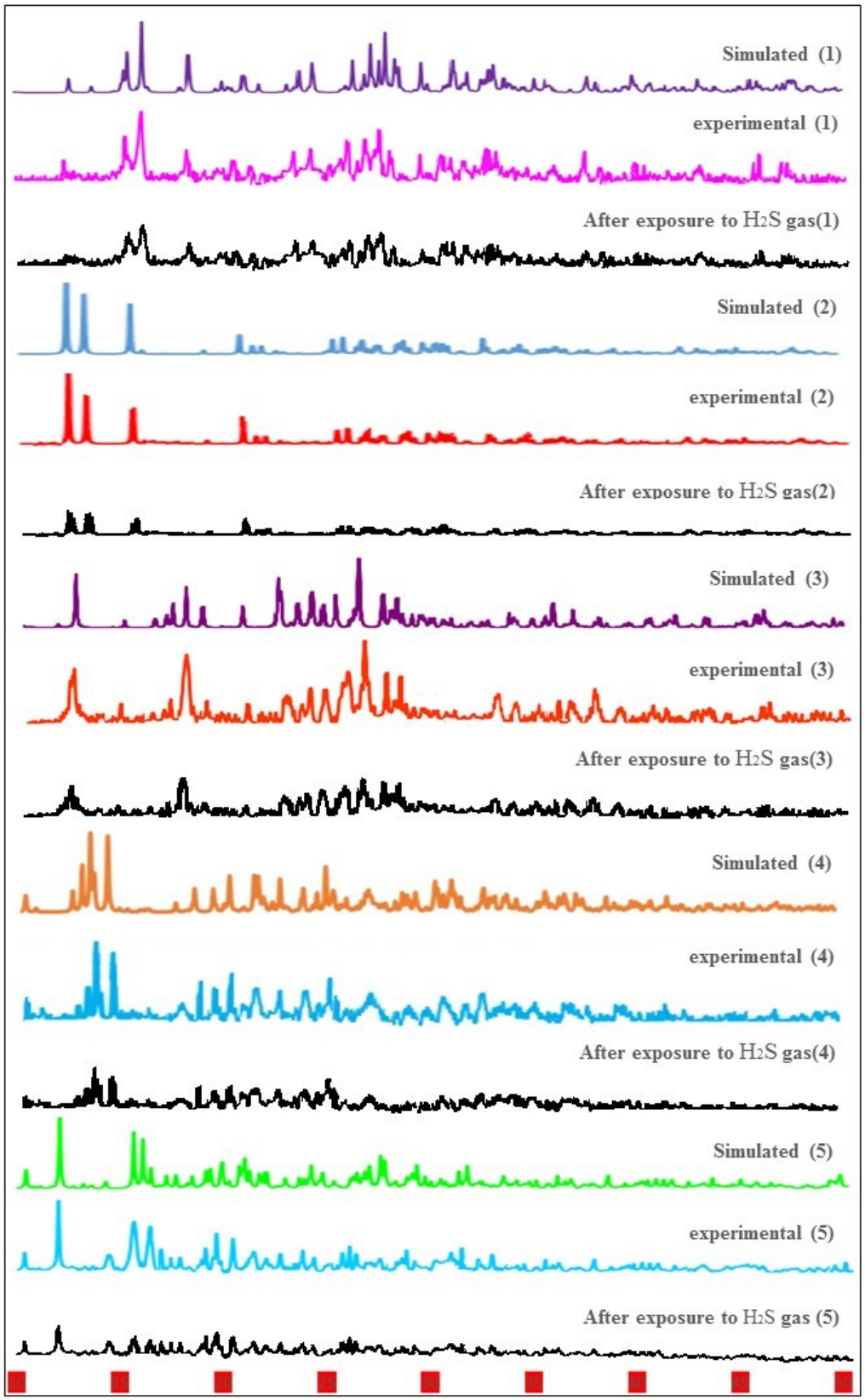
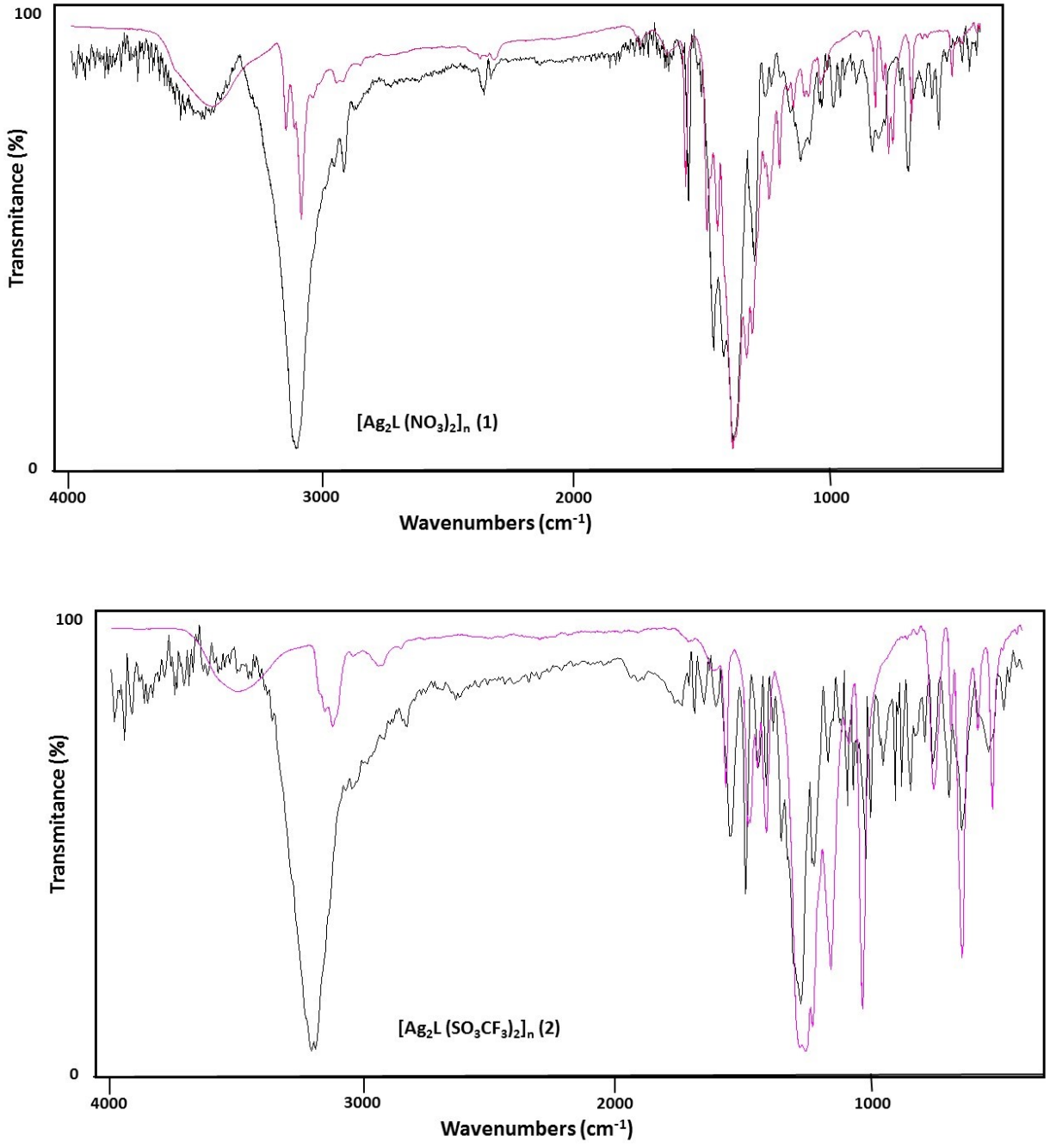
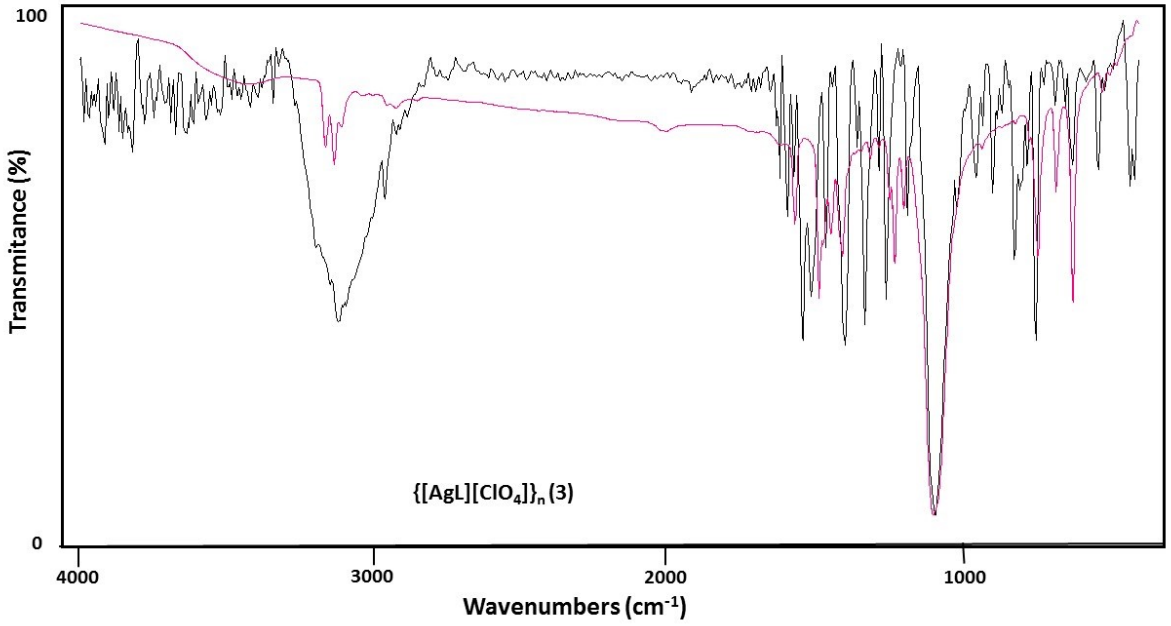
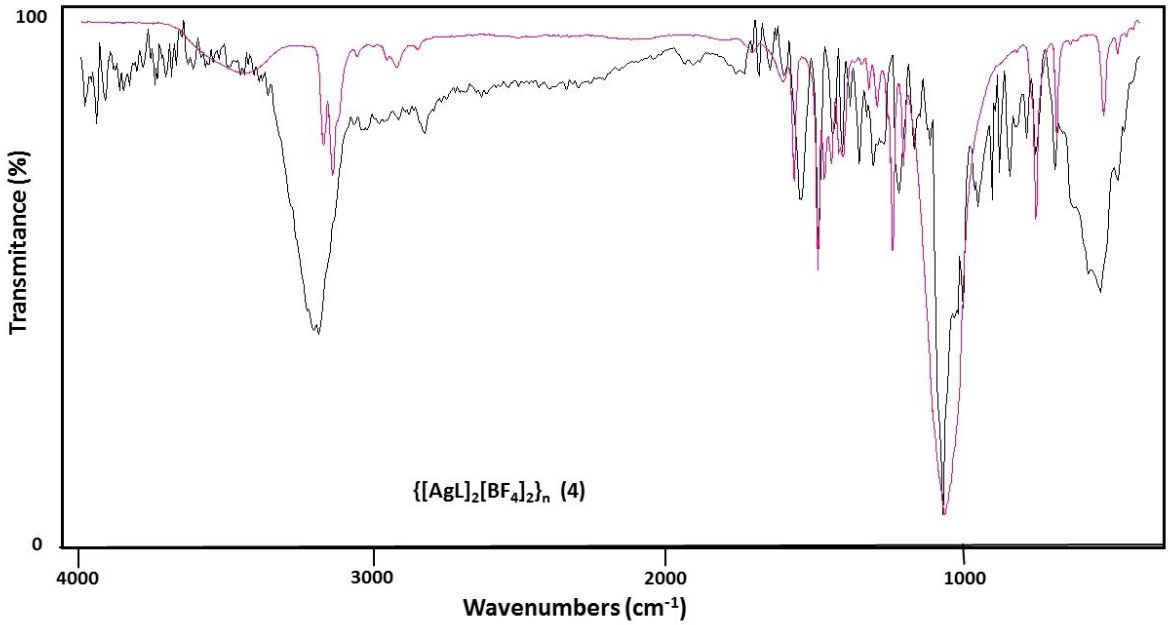

Simulated (1)
experimental (1)
After exposure to H2S gas(1)
Simulated (2)
experimental (2)
After exposure to H2S gas(2)
Simulated (3)
experimental (3)
After exposure to H2S gas(3)
Simulated (4)
experimental (4)
After exposure to H2S gas(4)
Simulated (5)
experimental (5)
After exposure to H2S gas (5)

Figure S3. PXRD patterns for polymers **1-5** the simulated and experimental before and after exposure to H_2S gas.




100
Transmitance (%)
0
{[AgL][ClO4]}n (3)
4000
3000
2000
1000
Wavenumbers (cm-1)


100
Transmitance (%)
0
{[AgL]2[BF4]2}n (4)
4000
3000
2000
1000
Wavenumbers (cm-1)

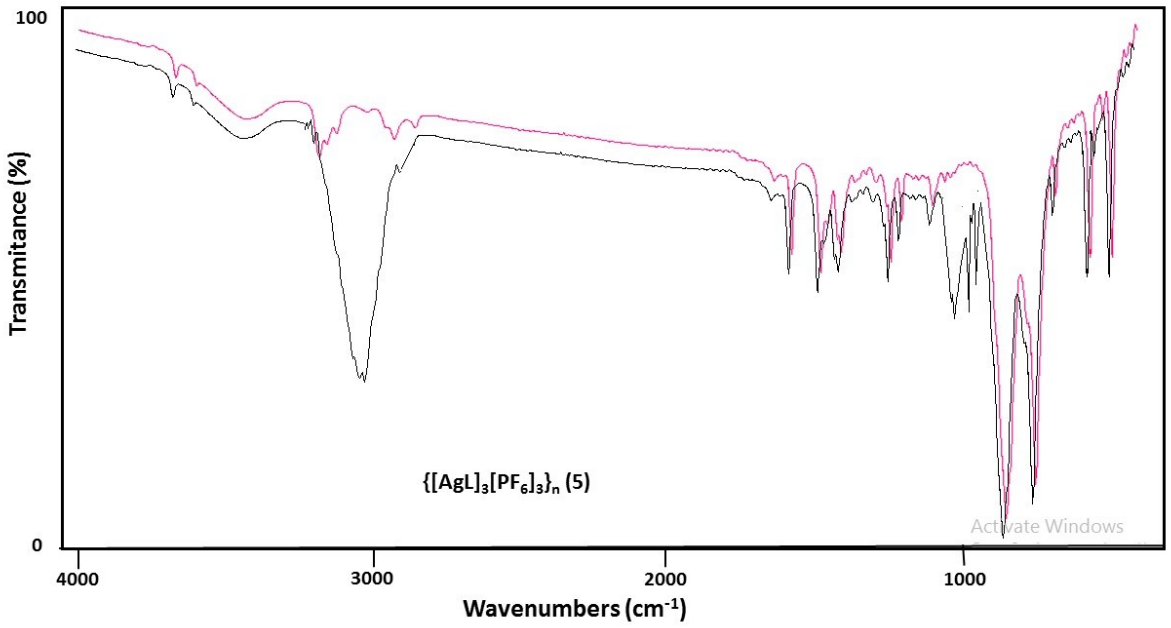


Figure S4. FT-IR spectra for coordination polymers **1**-**5** before (pink) and after (black) exposure to NH_3 gas.

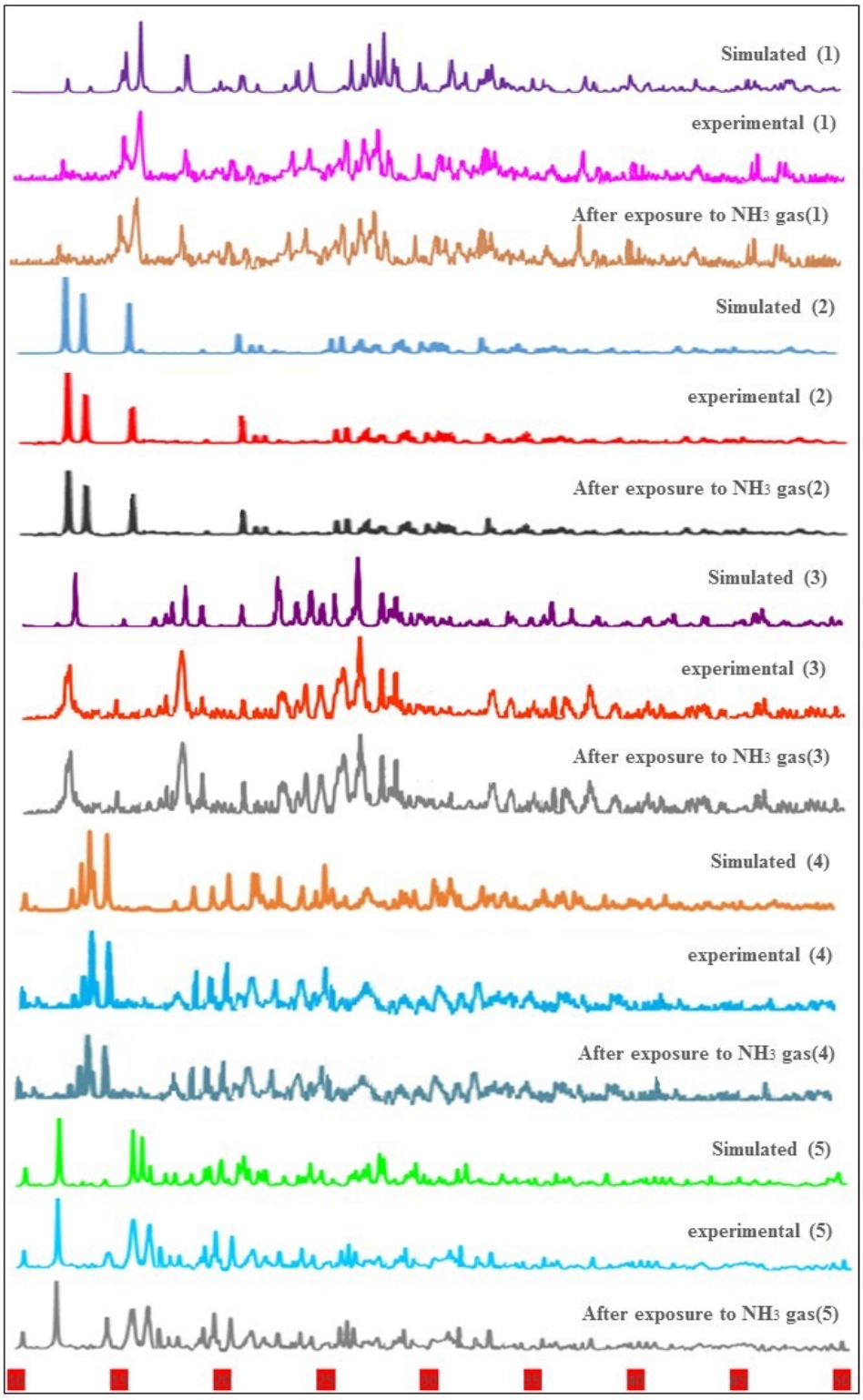
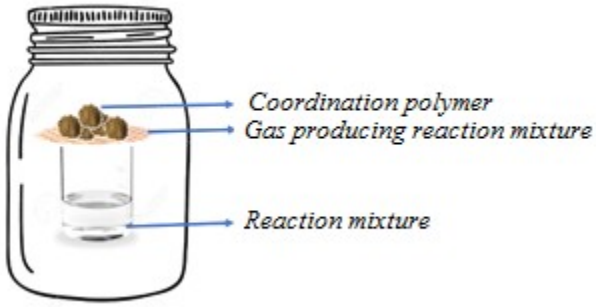


Figure S5. PXRD patterns for coordination polymers **1-5** the simulated and experimental before and after exposure to NH_3 gas.

SchemeS1. Experimental method for NH_3 adsorption

The NH_3 gas were selected to evaluate their adsorption capacities for the polymers **1** - **5**. Solid (powder) samples of these polymers were separately exposed to the gas producing reaction mixture in a breaker box (SchemeS6) for 4h at ambient conditions. The gas adsorption by the considered polymer were monitored by the infrared and X-ray powder diffraction techniques through the deposition of these polymers in the vicinity of gases.



SchemeS1. *NH_3 gas absorption system.*