

Hexaphenylbenzene and Hexabenzocoronene-Based Porous Polymers for the Adsorption of Volatile Organic Compounds

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Supplementary Information

Table of Contents

1. Synthesis Procedures	S3
2. FT-IR Characterization	S4
3. EDX Data	S4
4. Thermogravimetric Analysis	S5
5. PXRD Characterization	S5
6. Sorption Isotherms for CO ₂	S6
7. Sorption Isotherms for Vapours	S7
8. Vapour Adsorption Comparison Chart	S9
References	S10

1. Monomer Synthesis

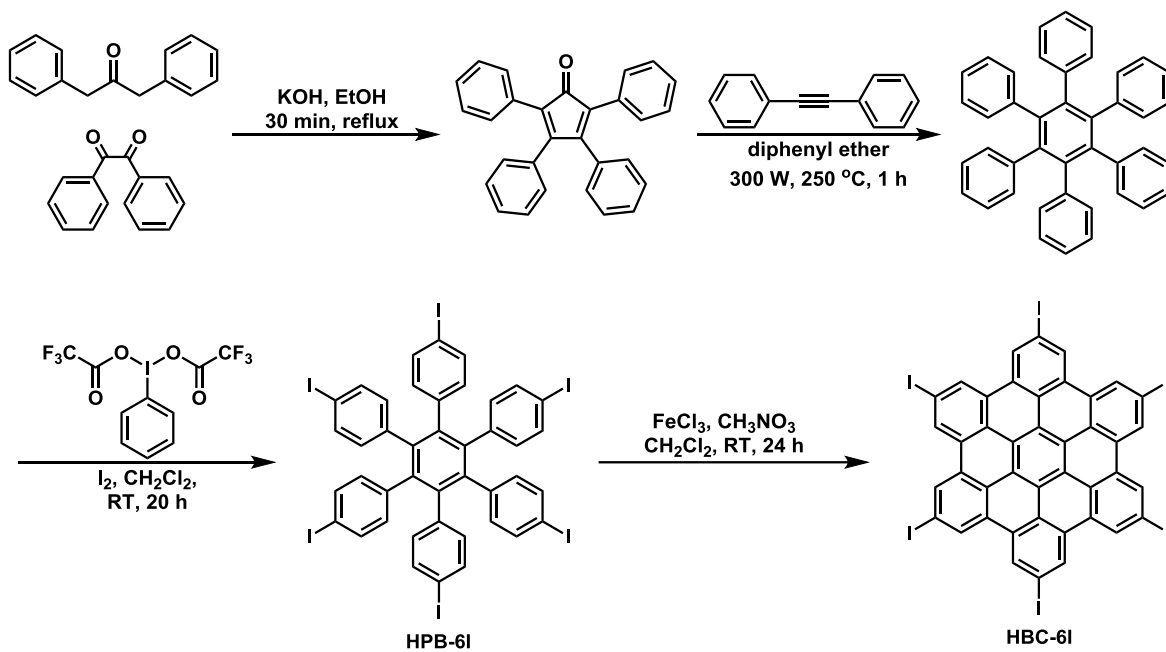


Fig S1: Synthesis of hexa(4-iodophenyl)benzene (**HPB-6I**) and hexakis(4-iodo)-perihexabenzocoronene (**HBC-6I**)¹⁻⁴

2. FT-IR Characterization

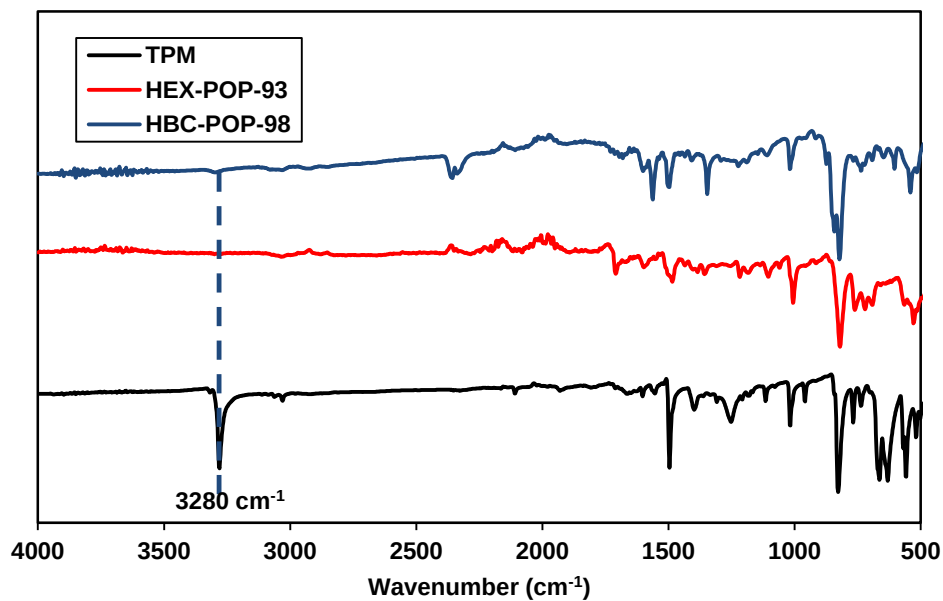


Fig S2: IR spectra of starting material: **TPM** and two POPs: HEX-POP-93 and HBC-POP-98

3. EDX Data

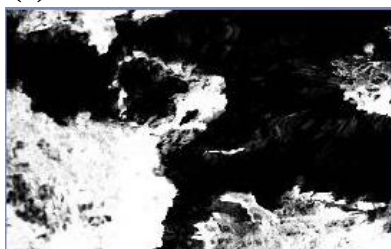
(a) HEX-POP-93



C map

I map

(b) HBC-POP-98



C map

I map

Fig S3: Carbon and iodine EDX maps of (a) HEX-POP-93 and (b) HBC-POP-98

Table S1: Elemental ratios in HEX-POP-93 and HBC-POP-98 for carbon, iodine, and palladium based on EDX analysis

Sample	Weight %		
	C%	I%	Pd%
HEX-POP-93	89.90	9.50	0.60
HBC-POP-98	90.34	9.00	0.65

4. Thermogravimetric Analysis

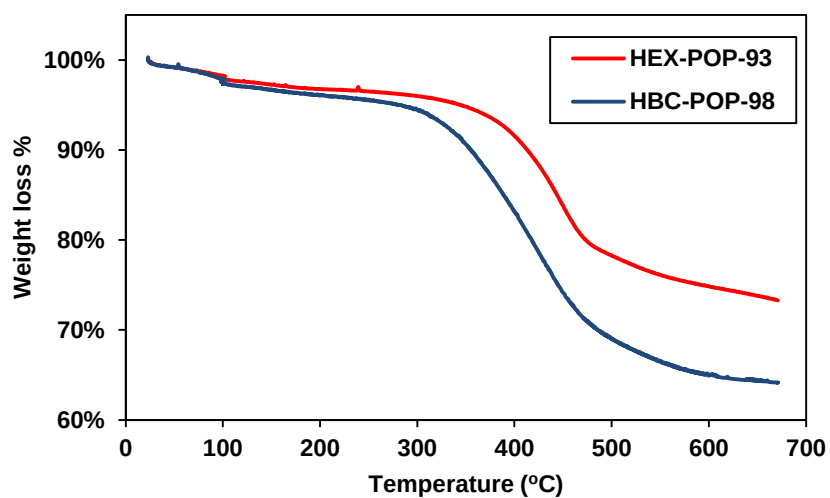


FIG S4: TGA curves of HEX-POP-93 and HBC-POP-98

5. Powder X-Ray Diffraction Characterization

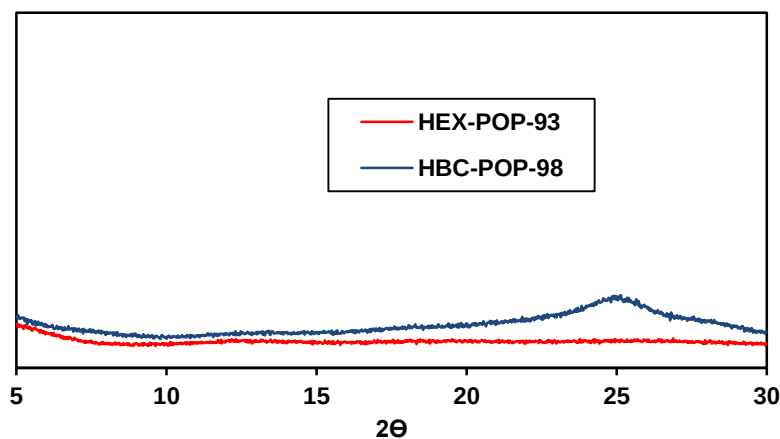
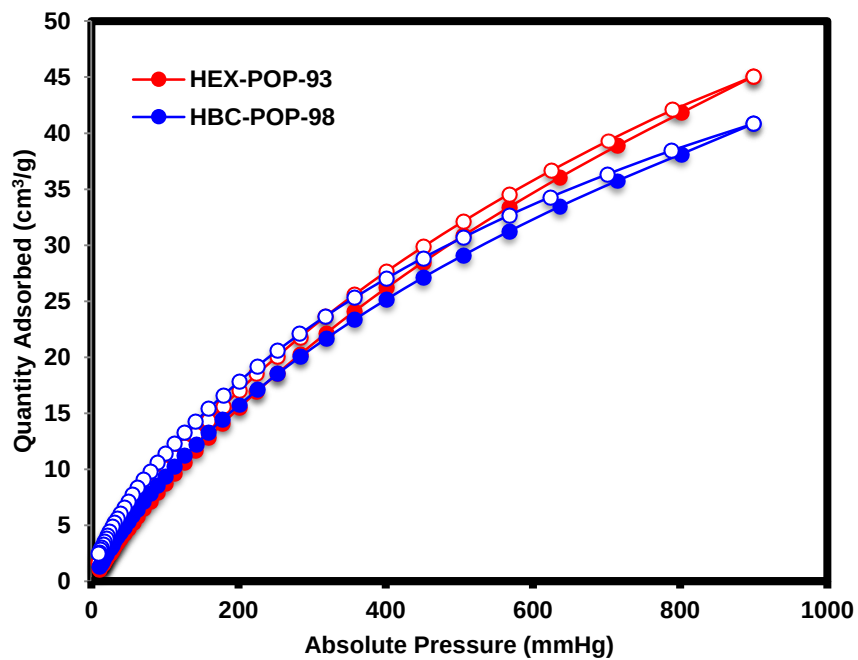


Fig S5: PXRD patterns of HEX-POP-93 and HBC-POP-98

6. Sorption Isotherms for CO₂

(a)



(b)

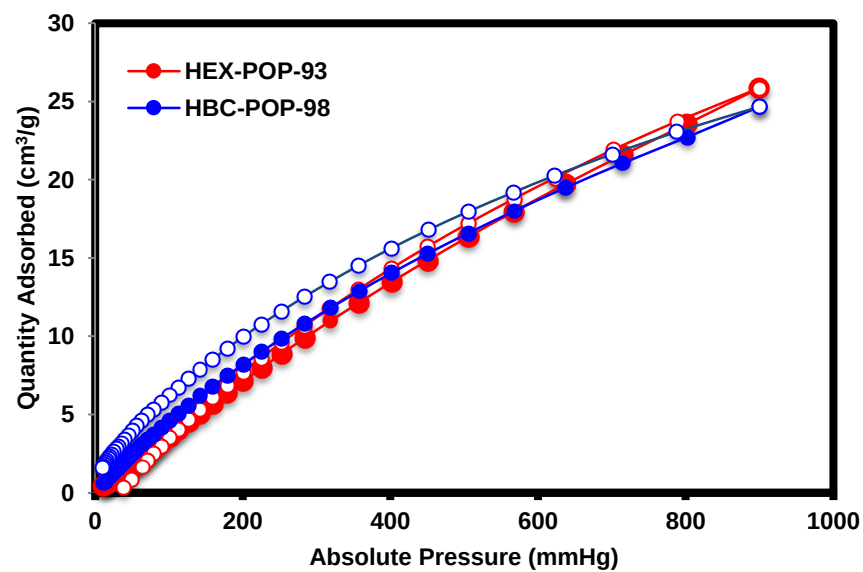


Fig S6: Adsorption (close circles) and desorption (open circles) isotherms of CO₂ for HEX-POP-93 (red) and HBC-POP-98 (blue) at (a) 273 K and (b) 298 K

7. Sorption Isotherms for Vapours

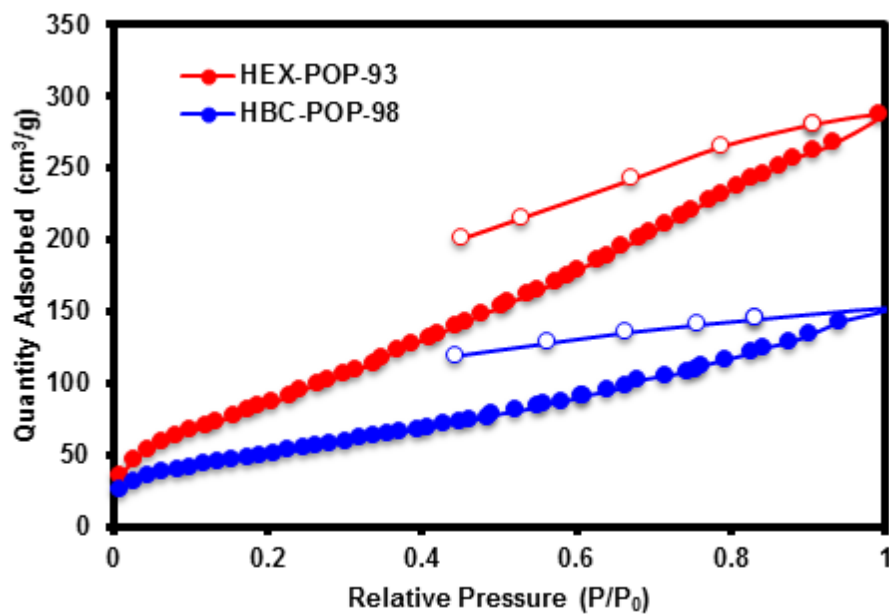


Fig S7: Adsorption and desorption isotherms of benzene vapour for HEX-POP-93 and HBC-POP-98 at 298 K

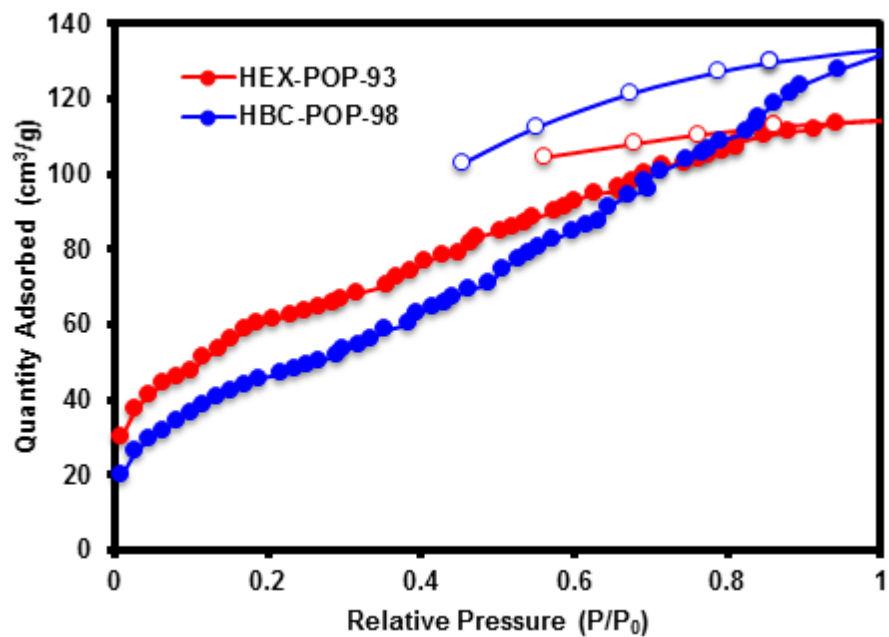


Fig S8: Adsorption and desorption isotherms of toluene vapour for HEX-POP-93 and HBC-POP-98 at 298 K

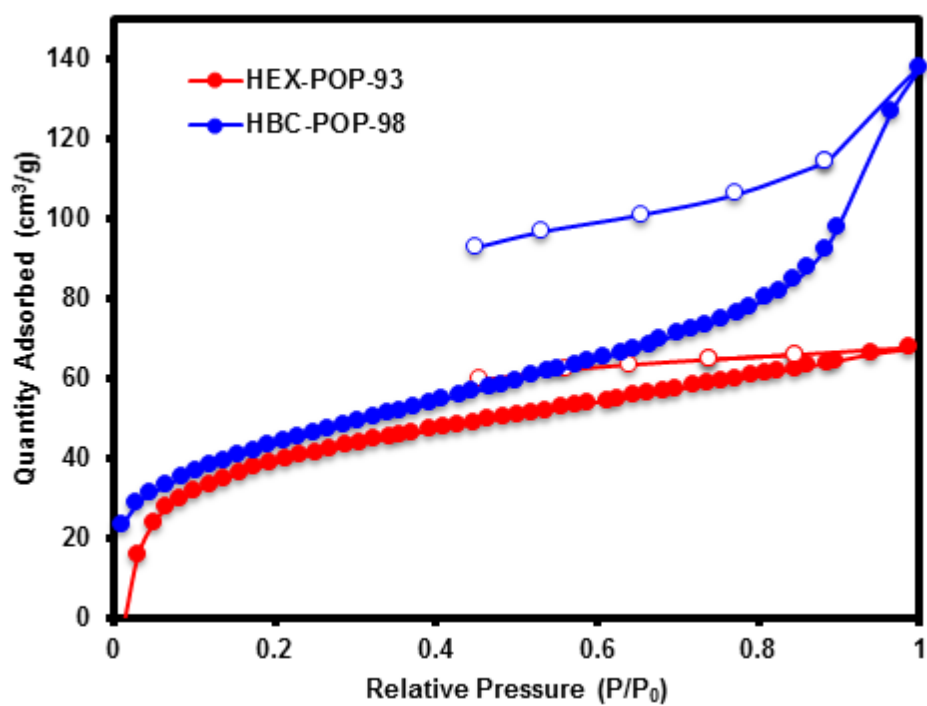


Fig S9: Adsorption and desorption isotherms of cyclohexane vapour for HEX-POP-93 and HBC-POP-98 at 298 K

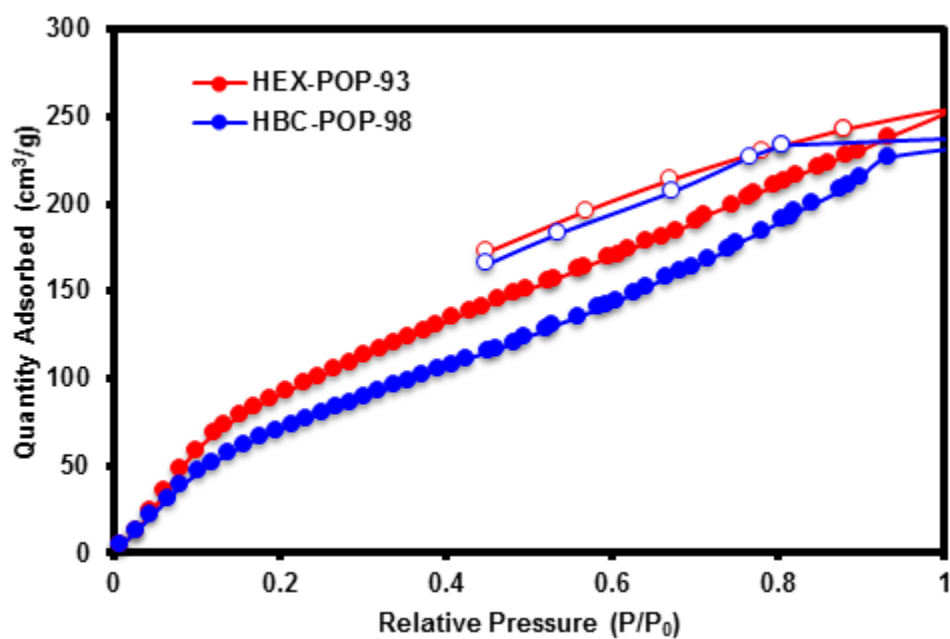


Fig S10: Adsorption and desorption isotherms of methanol vapour for HEX-POP-93 and HBC-POP-98 at 298 K

8. Vapour Adsorption Comparison Chart

Table S2: Adsorption capacities for POPs in this work and other materials.

Material	BET surface area	Adsorption wt%					Reference
		Benzene	Toluene	Cyclohexane	Methanol	Water	
HEX-POP-93	687	99.9	47.1	25.4	36.2	1.0	^a
HBC-POP-98	548	53.0	54.6	51.7	34.0	0.5	^a
MIL-101	3900	130.4 ^b	-	-	-	-	5
MIL-101	3980	129.1 ^c	109.6 ^c	-	-	-	6
PAF-1	5600	130.6 ^c	135.7 ^c	-	-	-	7
PAF-2	891	13.8 ^c	-	0.7 ^c	-	-	8
PAF-5	1503	128.6 ^c	111.4 ^c	-	94.9 ^c	-	9
PAF-11	704	87.4 ^c	78.0 ^c	-	65.4 ^c	3.5 ^c	10
SMPI-0	574.4	134.7	-	42.5	60	14.9	11
SMPI-10	112.0	104.7	-	42.8	83.4	30.4	11
CE-1	960	58.5	-	-	-	22.0	12
CE-2	588	35.1	-	-	-	6.9	12
PBI-1	62	54.4	-	-	-	32.9	13
MPI-1	1454	119.8	-	50.1	-	16.7	14
MPI-2	814	76.6	-	44.8	-	9.9	14
NPI-1	721	90.5	-	58.1	-	14.1	15
PI-ADPM	868	99.2	-	59.7	-	28.45	16
PSN-3	865	80.5	-	63.7	-	6.4	17
PSN-DA	1045	86.1	-	77.9	-	-	18
PCN-AD	843	98.0	-	57.4	-	-	19
PAN-1	925	72.6	-	52.7	-	8.4	20
PAN-2	1245	69.2	-	38.3	-	10.4	20
PBI-Ad-1	1023	98.0	-	53.6	-	-	21
PBI-Ad-2	926	76.5	-	46.3	-	-	21

^a in this work, ^b calculate from given mmol g⁻¹ values, ^c calculated from given mg g⁻¹ values

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