Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Toxic organic solvent adsorption by hydrophobic covalent polymer†

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Table S1. Crystallographic data of **CPCMERI-1.**

Crystal Data	
Formula	$C_{28}H_{20}N_2$
Formula Weight	384.46
Crystal System	monoclinic
Space group	'P 21/c'
a, b, c [Angstrom]	11.7907(4) 7.1668(2) 24.0105(7)
alpha, beta, gamma [deg]	90 98.472(2) 90
V [Ang**3]	2006.79(11)
Z	4
D(calc) [g/cm**3]	1.273
Mu(MoKa) [/mm]	0.074
F(000)	808
Crystal Size [mm]	0.22 x 0.20 x 0.18
Data Collection	
Temperature (K)	296(2)
Radiation [Angstrom]	MoKa 0.71073

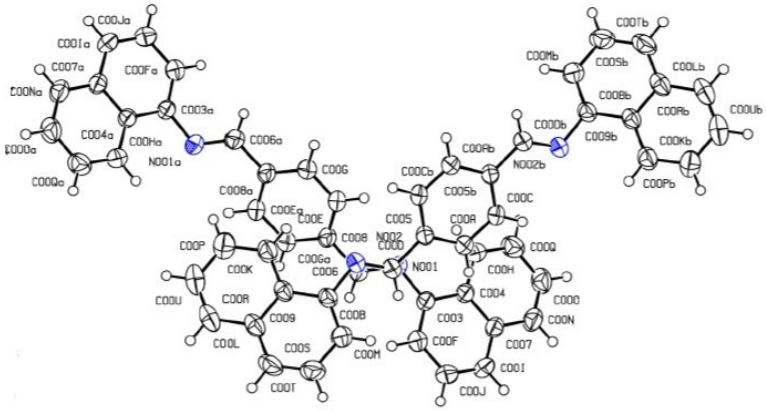

Fig. S1 ORTEP and atom numbering scheme of molecular analogue of CPCMERI-1.

Table S2. Coordinates for **CPCMERI-1** and Benzene energy optimized conformation.

N	0.2980262	4.7114446	9.4865247
C	0.6070581	3.6615416	8.6140320
C	1.5425791	3.9211193	7.5485015
C	-0.8950420	4.8771981	9.9240392
C	1.9012569	2.8503288	6.6612063
C	-1.2591839	5.9136803	10.8997330
C	-0.3084073	6.8069101	11.4327678
C	0.0977847	2.3761295	8.7803402
C	-0.6956435	7.7781649	12.3505871
C	2.1111240	5.2082945	7.3375726
C	1.3458003	1.5541380	6.8656297
C	0.4696185	1.3262384	7.9074126
C	2.8117007	3.1160619	5.5973651
C	3.3471304	4.3758103	5.4181406
C	2.9954077	5.4305991	6.2989892
N	-3.6017718	9.1018421	14.1607165
C	-3.9147260	10.1556852	15.0266947
C	-4.8780020	9.9085067	16.0703210
C	-2.4058757	8.9280056	13.7342150
C	-5.2409579	10.9830138	16.9513748
C	-2.0405511	7.8880435	12.7626269
C	-2.9909963	6.9936825	12.2308328
C	-3.3841813	11.4342493	14.8736321
C	-2.6037079	6.0221955	11.3133122
C	-5.4702423	8.6296084	16.2657485
C	-4.6610947	12.2708136	16.7627702
C	-3.7592174	12.4877165	15.7406580
C	-6.1785079	10.7289207	17.9943050
C	-6.7356458	9.4767190	18.1594794
C	-6.3802278	8.4185090	17.2842168
H	-1.7308185	4.2448366	9.5693807
H	0.7330789	6.7269769	11.1159540
H	-0.5723395	2.1670439	9.6175091
H	0.0484315	8.4680809	12.7588928
H	1.8354555	6.0176403	8.0156917
H	1.6316771	0.7426221	6.1907439
H	0.0575873	0.3267344	8.0710444
H	3.0806441	2.2989194	4.9216730
H	4.0449514	4.5640935	4.5976378
H	3.4274691	6.4244209	6.1530862
H	-1.5690324	9.5558245	14.0944047
H	-4.0324436	7.0733985	12.5478641
H	-2.6936467	11.6357085	14.0513432
H	-3.3478388	5.3320371	10.9054979
H	-5.1916906	7.8178297	15.5917592
H	-4.9489512	13.0850564	17.4335316
H	-3.3288509	13.4812846	15.5884609
H	-6.4502043	11.5487211	18.6656719
H	-7.4539043	9.2971771	18.9641611
H	-6.8302039	7.4309917	17.4183848

C	4.8033982	5.3052192	10.5443090
C	6.0383923	5.4236962	11.1940237
C	6.1106016	5.3026757	12.5876693
C	3.6393366	5.0653777	11.2862565
C	3.7130515	4.9451072	12.6802371
C	4.9477678	5.0633268	13.3308635
H	4.7460066	5.3995249	9.4561268
H	6.9464130	5.6108857	10.6136297
H	7.0749477	5.3950669	13.0954986
H	2.6753710	4.9739338	10.7764473
H	2.8055724	4.7583514	13.2617096
H	5.0040151	4.9690412	14.4191424
C	-9.2794809	9.0813057	10.8349972
C	-8.0685644	9.1602397	10.1355240
C	-6.8538482	9.1094294	10.8310058
C	-9.2751892	8.9505946	12.2296238
C	-8.0600312	8.8998631	12.9241281
C	-6.8478614	8.9799182	12.2260806
H	-10.2282848	9.1213315	10.2922546
H	-8.0717244	9.2617324	9.0464354
H	-5.9088068	9.1711220	10.2836342
H	-10.2207680	8.8883801	12.7759100
H	-8.0560082	8.7975673	14.0130998
H	-5.8993755	8.9407298	12.7705364

Table S3. Coordinates for **CPCMERI-1** and Toluene energy optimized conformation.

N	0.3303109	3.5001931	10.3405696
C	0.9178736	2.3995455	9.7077961
C	1.3746887	2.5683212	8.3508797
C	-0.6630561	3.3566827	11.1371878
C	2.0054482	1.4629879	7.6854805
C	-1.2637457	4.4740290	11.8787152
C	-0.7893966	5.7948406	11.7496332
C	1.1302092	1.1846859	10.3550828
C	-1.3905134	6.8288557	12.4603581
C	1.2082793	3.7921890	7.6442330
C	2.1882232	0.2353866	8.3853074
C	1.7654626	0.1074640	9.6931300
C	2.4359204	1.6286868	6.3369383
C	2.2586889	2.8279841	5.6766265
C	1.6424032	3.9207098	6.3385031
N	-4.0919548	7.5475245	14.8390967
C	-4.5945327	8.6215383	15.5808205
C	-6.0231485	8.7146399	15.7503726
C	-3.0897920	7.6929258	14.0538111
C	-6.5635488	9.7904289	16.5330294
C	-2.4781748	6.5749995	13.3222226
C	-2.9495824	5.2536272	13.4549854

C	-3.7693950	9.5535905	16.2057851
C	-2.3518902	4.2205018	12.7403788
C	-6.9165415	7.7800008	15.1570446
C	-5.6790956	10.7259116	17.1434295
C	-4.3134313	10.6008202	16.9866490
C	-7.9775935	9.8892651	16.6804594
C	-8.8199811	8.9684751	16.0898201
C	-8.2827813	7.9021433	15.3238709
H	-1.1374695	2.3698809	11.2974262
H	0.0516756	5.9931089	11.0824471
H	0.8317030	1.0718675	11.3999397
H	-1.0184274	7.8517739	12.3522551
H	0.7330871	4.6291266	8.1585652
H	2.6768906	-0.5985459	7.8739097
H	1.9227158	-0.8305659	10.2325443
H	2.9129897	0.7837863	5.8317741
H	2.5952588	2.9401291	4.6423161
H	1.5116632	4.8692546	5.8105006
H	-2.6354629	8.6858050	13.8737616
H	-3.7897153	5.0563556	14.1237739
H	-2.6846970	9.4556577	16.1191193
H	-2.7260027	3.1980735	12.8461560
H	-6.4994096	6.9601521	14.5696780
H	-6.0985017	11.5372954	17.7447249
H	-3.6369609	11.3103961	17.4708909
H	-8.3860914	10.7120691	17.2743152
H	-9.9028376	9.0563097	16.2133467
H	-8.9559264	7.1722921	14.8657508
C	5.2942730	6.4679783	8.5288918
C	6.3599185	7.2105338	9.0488113
C	6.5410183	7.2726176	10.4362125
C	4.4196400	5.7927580	9.3891518
C	4.5903412	5.8427862	10.7834849
C	5.6643549	6.5968645	11.2913229
H	5.1396355	6.4153812	7.4471970
H	7.0429724	7.7401788	8.3788537
H	7.3683455	7.8530196	10.8550464
H	3.5881360	5.2175807	8.9705080
H	5.8142832	6.6558153	12.3741218
C	-8.8787011	12.9078971	11.6752339
C	-8.1306321	12.8852233	10.4912313
C	-7.3405455	11.7741049	10.1793323
C	-8.8267188	11.8100332	12.5406530
C	-8.0342465	10.6997422	12.2242598
C	-7.2803808	10.6615550	11.0388294
H	-9.4946257	13.7771766	11.9221109
H	-8.1606062	13.7390813	9.8080261
H	-6.7579292	11.7691974	9.2525283
H	-9.4027015	11.8165385	13.4704312
H	-7.9993890	9.8485700	12.9109253
C	3.6642152	5.0930074	11.7120553
C	-6.4427445	9.4557749	10.6827088

H	3.4251743	5.6887516	12.6078109
H	2.7210498	4.8201254	11.2145067
H	4.1337093	4.1578068	12.0661670
H	-6.9357010	8.8458275	9.9050477
H	-5.4598491	9.7518889	10.2819093
H	-6.2777192	8.8064025	11.5557077

Table S4. Coordinates for **CPCMERI-1** and Nitrobenzene energy optimized conformation.

N	0.3034387	5.4898726	8.7718346
C	1.2981694	4.8650462	8.0116605
C	1.4748346	5.2960194	6.6469683
C	0.4702970	5.7045428	10.0255937
C	2.4679058	4.6507263	5.8342344
C	-0.5788332	6.2706410	10.8843033
C	-1.8347198	6.6572395	10.3750600
C	2.0687981	3.8117565	8.4999869
C	-2.8010965	7.1899802	11.2222604
C	0.7027139	6.3490926	6.0817411
C	3.2391703	3.5861997	6.3834003
C	3.0342831	3.1752313	7.6852734
C	2.6512770	5.0946993	4.4922710
C	1.8887829	6.1217864	3.9731499
C	0.9026177	6.7517290	4.7751340
N	-3.4299303	8.1187717	14.7153515
C	-4.4235796	8.7460415	15.4746887
C	-4.6243153	8.2954033	16.8295614
C	-3.5923853	7.9141643	13.4593470
C	-5.6157142	8.9445633	17.6412359
C	-2.5429708	7.3485948	12.6007592
C	-1.2872227	6.9619184	13.1099983
C	-5.1695073	9.8207896	14.9951320
C	-0.3205271	6.4300548	12.2627234
C	-3.8779490	7.2191909	17.3857014
C	-6.3610482	10.0321154	17.1013396
C	-6.1331353	10.4610860	15.8091957
C	-5.8233782	8.4811697	18.9730305
C	-5.0858851	7.4316361	19.4833612
C	-4.1013258	6.7977256	18.6825500
H	1.4267642	5.4816686	10.5311427
H	-2.0343603	6.5337214	9.3087370
H	1.9051710	3.4535501	9.5190476
H	-3.7700407	7.5008935	10.8219486
H	-0.0549294	6.8300243	6.7026962
H	3.9871655	3.0944999	5.7553205
H	3.6165216	2.3465907	8.0975924
H	3.4110561	4.6037074	3.8772315
H	2.0405006	6.4508377	2.9414770
H	0.2972975	7.5590717	4.3538220

H	-4.5453721	8.1447899	12.9508234
H	-1.0879410	7.0851890	14.1764322
H	-4.9852464	10.1931999	13.9847389
H	0.6484876	6.1197393	12.6627232
H	-3.1211239	6.7354225	16.7658579
H	-7.1075337	10.5267563	17.7288854
H	-6.6956469	11.3069406	15.4044580
H	-6.5815930	8.9754045	19.5874011
H	-5.2563297	7.0876714	20.5072191
H	-3.5161496	5.9721314	19.0968973
C	7.1053527	3.9254089	13.5565305
C	6.9500223	2.7448786	14.2950425
C	5.6923797	2.1370359	14.4048714
C	6.0057491	4.5067085	12.9235578
C	4.7597342	3.8832368	13.0466525
C	4.5819539	2.7044977	13.7783527
H	8.0874612	4.3964374	13.4729774
H	7.8152819	2.2953868	14.7887258
H	5.5750935	1.2164196	14.9811779
H	6.1018253	5.4246462	12.3442206
H	3.5938798	2.2505475	13.8498002
C	-10.2041293	11.3371474	9.9228746
C	-8.9264644	11.8486604	9.6600379
C	-7.7932146	11.1738946	10.1161835
C	-10.3568344	10.1457632	10.6443152
C	-9.2346348	9.4574759	11.1075068
C	-7.9688799	9.9864579	10.8342612
H	-11.0872895	11.8707389	9.5626793
H	-8.8113034	12.7776988	9.0969978
H	-6.7894365	11.5519576	9.9239620
H	-11.3545953	9.7500336	10.8474467
H	-9.3282910	8.5291702	11.6705560
N	3.5958381	4.4885712	12.3847464
O	2.5118904	3.9287731	12.4954697
O	3.7636558	5.5228686	11.7522464
N	-6.7813870	9.2695564	11.3196521
O	-6.9484702	8.2254373	11.9358595
O	-5.6796431	9.7532170	11.0892210

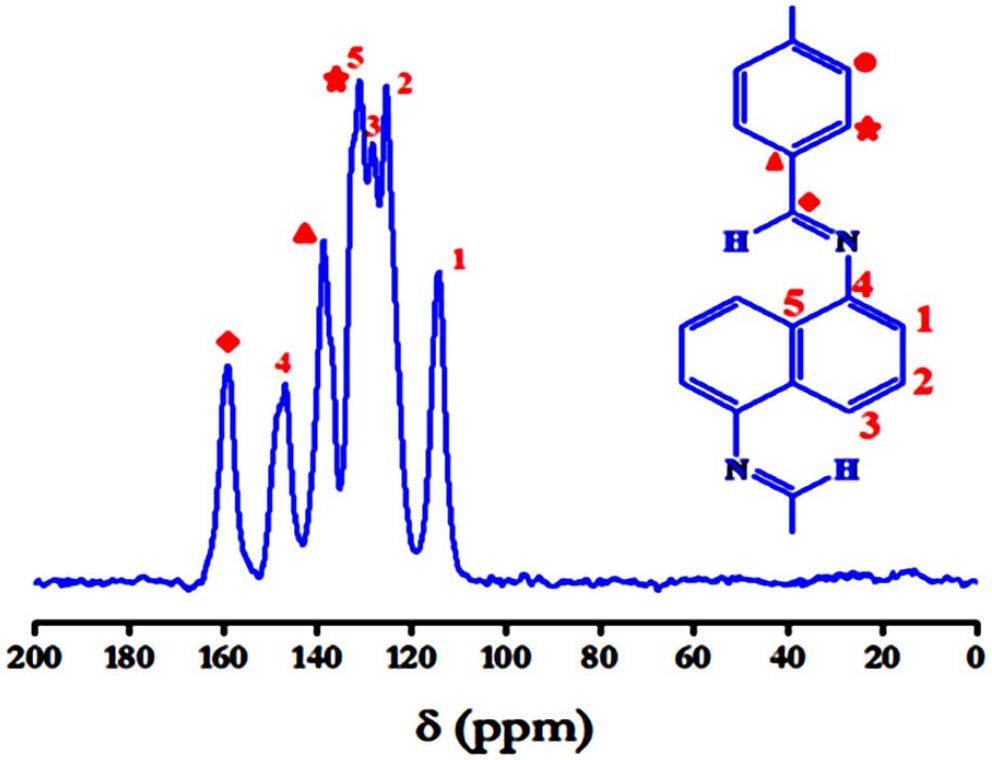

Fig. S2 Solid state 13C cross polarisation NMR spectra of CPCMERI-1 with peak assignment.

Table S5. Assignment of Solid state 13C cross polarisation NMR peaks of **CPCMERI-1**.

Sl No.	Peak Position δ in ppm)	Assignment Mark	Assigned Carbon
1	158.8	◆	Imine Carbon
2	100-150	1-5	Different carbons of naphthalene moiety
3	138.6	▲	Carbon of Terephthalaldehyde moiety
4	128.2	●	Carbon of Terephthalaldehyde moiety
5	130.8	★	Carbon of Terephthalaldehyde moiety

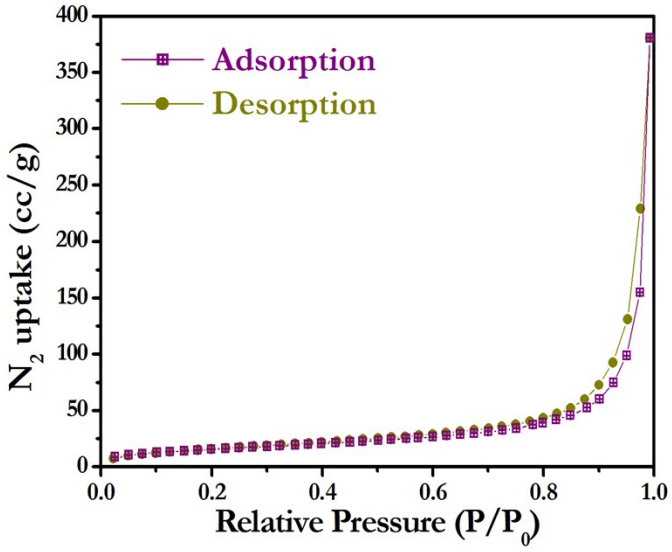

Fig. S3 N_2 adsorption/desorption isotherm of CPCMERI-1 after adsorption of benzene.

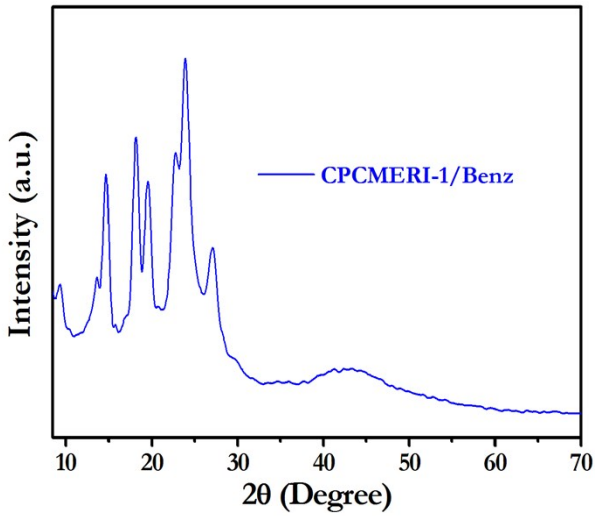

Fig. S4 Wide angle PXRD pattern of CPCMERI-1 after adsorption of benzene.

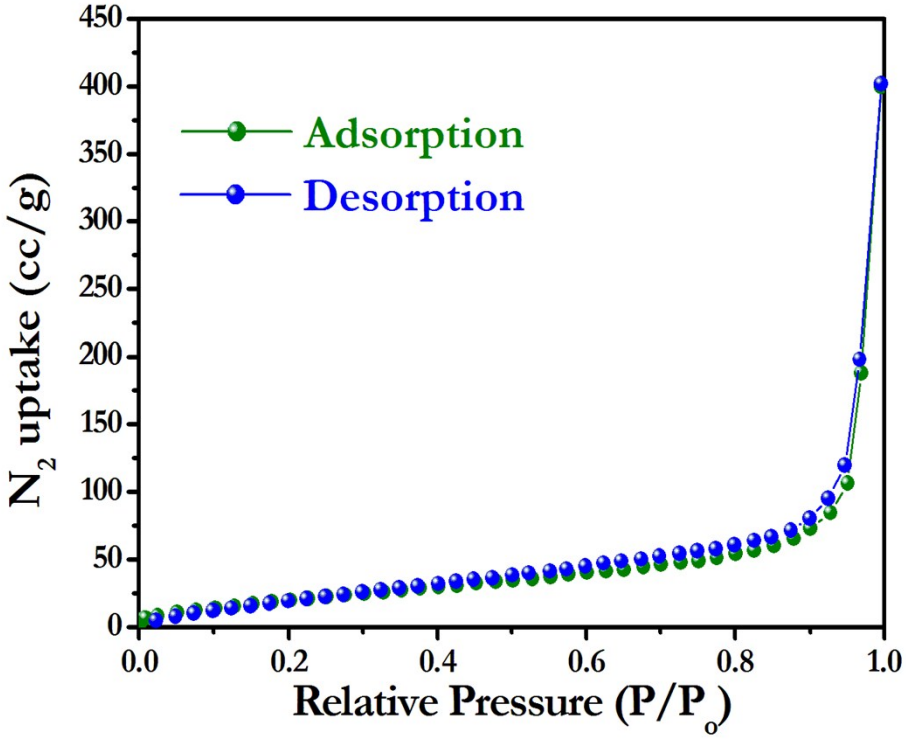

Fig. S5 N_2 adsorption/desorption isotherm of CPCMERI-1 synthesized via acid catalyzed pathway.