

Visualisation and characterisation of voids in molecular crystals

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Supplementary Information

Table S1. Surface areas ($\text{m}^2 \text{g}^{-1}$) for MOFs plotted in Fig. 5.

MOF	0.002 au surface area	0.0003 au surface area	BET experiment	Langmuir experiment
MOF-74	1790	1514	950 ¹ , 783 ²	1072 ¹ , 1132 ²
MIL-53(Cr)	2915	1991	1026 ³	1500 ⁴
HKUST-1	2595	2606	1944 ¹ , 1507 ² , 1154 ⁵ , 692 ⁶ , 1680 ⁷ , 1850 ⁷ , 1296 ⁸ , 1502 ⁹	2257 ¹ , 2175 ² , 1958 ⁵ , 918 ⁶ , 2216 ⁹
IRMOF-18	3967	2895		1501 ¹⁰
IRMOF-13	3355	3008	1551 ²	2100 ²
IRMOF-11	3450	3083	1984 ¹	2337 ¹ , 1911 ¹⁰
IRMOF-1	3234	3403	3534 ¹ , 2296 ⁵ , 3100 ¹¹ , 3800 ¹¹ , 572 ¹² , 2800 ¹³	4171 ¹ , 3362 ¹⁰ , 3840 ⁵ , 3300 ¹¹ , 4400 ¹¹ , 2900 ¹⁴ , 3080 ¹⁵ , 1014 ¹²
IRMOF-20	3194	3469	4024 ¹ , 3409 ²	4593 ¹ , 4346 ²
IRMOF-6	3395	3514	2804 ¹ , 2476 ²	3305 ¹ , 3263 ² , 2630 ¹⁶
IRMOF-9	3666	3650	1904 ²	2613 ²
IRMOF-8	3563	3838		1466 ¹⁰ , 1818 ¹⁵
IRMOF-14	3734	4077	1453 ¹⁶	1936 ¹⁶
MOF-177	3865	4153	4746 ^{1,17}	5640 ^{1,17} , 4526 ¹⁰ , 4500 ¹⁸

Table S2. Pore volumes ($\text{cm}^3 \text{g}^{-1}$) for MOFs plotted in Fig. 5. PLATON values were obtained using the same crystal structures as modified in the present work, using a probe radius of 1.2 Å and a grid spacing of 0.2 Å.

MOF	0.002 au volume	0.0003 au volume	PLATON "solvent excluded volume"	PLATON "solvent accessible volume"	experiment
MOF-74	0.467	0.363	0.477	0.291	0.39 ²
MIL-53(Cr)	0.555	0.387	0.526	0.243	0.56 ⁴
HKUST-1	0.681	0.526	0.703	0.388	0.75 ² , 0.69 ⁸ , 0.76 ⁹
IRMOF-18	0.809	0.623	0.825	0.486	
IRMOF-11	1.041	0.837	1.071	0.650	0.73 ²
IRMOF-13	2.203	1.991	2.251	1.779	
IRMOF-9	1.232	1.047	1.270	0.871	1.13 ¹³ , 1.04 ¹⁴
IRMOF-6	1.232	1.047	1.270	0.871	1.53 ²
IRMOF-1	1.777	1.575	1.812	1.357	1.14 ² , 0.92 ¹⁶
IRMOF-20	1.817	1.602	1.865	1.384	0.90 ²
IRMOF-8	1.777	1.575	1.812	1.357	
MOF-177	0.467	0.363	0.477	0.291	0.69 ¹⁶
IRMOF-14	0.809	0.623	0.825	0.486	1.59 ¹⁸ , 1.69 ¹⁷

Table S3. Surface areas ($\text{m}^2 \text{g}^{-1}$) for COFs plotted in Fig. 7.

COF	0.002 au surface area	0.0003 au surface area	BET experiment	Langmuir experiment
COF-1	3776	2608	711, ¹⁹ 628, ⁸ 750 ²⁰	970 ²⁰
COF-5	2501	1989	1590, ¹⁹ 1670, ²⁰ 2027 ²¹	1990 ²⁰
COF-6	2093	1513	750 ²⁰	980 ^{20, 22}
COF-8	2673	1998	1350 ²⁰	1400 ^{20, 22}
COF-10	2616	2091	1760 ²⁰	2080 ^{20, 22}
COF-102	4786	4965	3472, ²³ 3620, ²⁰ 2926 ²¹	4452, ²³ 4650 ²⁰
COF-103	4889	5085	4210, ²³ 3530 ²⁰	5207, ²³ 4630 ²⁰
COF-105	4921	5423		
COF-108	4622	5131		
COF-18Å	2392	1895	1260 ²⁴	
TP-COF	2359	1942	868 ²⁵	
COF-202	4973	4653	2690 ²⁶	3214 ²⁶

Table S4. Pore volumes ($\text{cm}^3 \text{g}^{-1}$) for COFs plotted in Fig. 5. PLATON values were obtained using the same crystal structures as modified in the present work, using a probe radius of 1.2 Å and a grid spacing of 0.2 Å.

COF	0.002 au volume	0.0003 au volume	PLATON "solvent excluded volume"	PLATON "solvent accessible volume"	experiment
COF-1	0.412	0.231	0.391	0.084	0.32, ¹⁹ 0.36, ⁸ 0.30 ²⁰
COF-5	1.143	1.026	1.135	0.901	1.07 ²⁰
COF-6	0.385	0.289	0.376	0.198	0.32 ²⁰
COF-8	0.823	0.699	0.808	0.577	0.69 ²⁰
COF-10	1.487	1.364	1.484	1.236	1.44 ²⁰
COF-102	1.748	1.483	1.794	1.220	1.35, ²³ 1.55 ²⁰
COF-103	1.941	1.668	1.991	1.399	1.66, ²³ 1.54 ²⁰
COF-105	5.065	4.792	5.124	4.696	
COF-108	5.288	5.031	5.328	4.707	
COF-18Å	0.716	0.599	0.706	0.481	0.29 ²⁴
TP-COF	1.338	1.226	1.338	1.103	0.79 ²⁵
COF-202	1.264	1.002	1.282	0.734	1.09 ²⁶

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