Electronic Supplementary Information

Chiral recognition during adsorption on MOF [{Cu12I(trz)8}•4 Cl•8 H2O]n, obtained from achiral building blocks without external source of chirality

Yuliya F. Sharafutdinova, Ksenia S. Balandina, Irina N. Pavlova, Marat R. Agliullin, Vladimir Yu. Guskov



Figure 1S. Isotherms of limonene vapors adsorption at 90 °C



Figure 2S. Isotherms of limonene vapors adsorption at 100 $^\circ C$



Figure 3S. Isotherms of limonene vapors adsorption at 120 °C



Figure 4S. Isotherms of limonene vapors adsorption at 130 °C



Figure 5S. Isotherms of limonene vapors adsorption at 140 $^\circ C$



Figure 6S. Isotherms of limonene vapors adsorption at 110 °C



Figure 7S. Differential entropies of limonenes adsorption on CsCuCl3 crystals at 90 °C



Figure 8S. Differential entropies of limonenes adsorption on CsCuCl3 crystals at 100 °C



Figure 9S. Differential entropies of limonenes adsorption on CsCuCl3 crystals at 110 °C



Figure 10S. Differential entropies of limonenes adsorption on CsCuCl3 crystals at 120 °C



Figure 11S. Differential entropies of limonenes adsorption on CsCuCl3 crystals at 130 °C



Figure 12S. Nitrogen adsorption isotherm at 77 K



Figure 13S. FTIR spectrum

Table 1S. Approximation parameters for limonenes adsorption isotherms by DR equation. W_0 – icropore volume, E – characteristic energy

T, °C	W ₀		E		
	R-(+)-limonene	S-(-)-limonene	R-(+)-limonene	S-(-)-limonene	
90	0.104	0.097	13.5	13.3	
100	0.098	0.097	12.7	12.8	
110	0.071	0.082	13.0	12.5	
120	0.070	0.073	12.3	12.2	
130	0.060	0.060	12.3	12.2	
140	0.039	0.041	13.3	13.1	
150	0.035	0.035	13.1	13.1	
150	0.031	0.034	14.1	13.2	

P, Pa	р	P, Pa	р	P, Pa	р
36.3	0.3928	66.1	0.3547	97.6	0.3892
40.9	0.4144	70.9	0.3718	102.3	0.4506
45.7	0.4307	75.6	0.3934	107.1	0.1604
50.4	0.3679	80.3	0.3504	111.8	0.1711
55.2	0.3828	86.6	0.3513	116.6	0.3833
61.4	0.3880	91.4	0.3813		

Table 3S. P-values for pairs of points of limonenes adsorption isotherms at 100 °C ($\alpha = 0.05$).

Table 4S. P-values for pairs of points of limonenes adsorption isotherms at 110 °C ($\alpha = 0.05$).

P, Pa	р	P, Pa	р	P, Pa	р		
82.3	0.1092	121.0	0.0422	159.6	0.0137		
90.1	0.1282	131.2	0.0319	175.1	0.0173		
97.8	0.1653	136.4	0.0101	185.3	0.0145		
P, Pa	р	P, Pa	р	P, Pa	р		
34.2	0.2287	58.9	0.5974	87.6	0.9556		
38.3	0.2064	63.0	0.5264	91.7	0.9664		
42.4	0.8211	67.1	0.4755	95.8	0.8981		
46.5	0.9771	71.2	0.9057	100.0	0.8363		
50.6	0.6567	79.4	0.7906	104.1	0.7825		
54.8	0.6841	83.5	0.8735	110.9	0.9361		
105.5	0.0391	144.2	0.0113	193.0	0.0159		
113.2	0.0422	151.9	0.0124	200.8	0.0175		

Table 5S. P-values for pairs of points of limonenes adsorption isotherms at 120 °C ($\alpha = 0.05$).

P, Pa	р	P, Pa	р	P, Pa	р
77.0	0.0013	154.0	0.0314	267.5	0.0290
88.0	0.0027	165.0	0.0377	278.5	0.0372
99.0	0.0046	176.0	0.0463	289.5	0.0372
121.0	0.0163	245.5	0.0228	300.5	0.0447
132.0	0.0321	256.5	0.0275		

Table 6S. P-values for pairs of points of limonenes adsorption isotherms at 130 °C ($\alpha = 0.05$).

P, Pa	р	P, Pa	р	P, Pa	p
123.0	0.2147	245.9	0.0569	338.2	0.0141
138.3	0.2854	261.3	0.06865	353.5	0.0175
153.7	0.3835	276.7	0.08947	368.9	0.0200
169.1	0.4929	292.0	0.1103	384.3	0.0251
215.2	0.0367	307.4	0.1469	415.0	0.0418
230.6	0.0444	322.8	0.0122		