## **Supplementary Information**

## Sorption of 3-hydroxyflavone in channel type zeolites: effect of confinement on copper(II) complexation

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**Figure S1**: FTIR spectra recorded for 3HF incorporated in in silicalite-1 (a), for 3HF adsorbed in CuZSM-5 (one year after mixing 3HF and zeolite powders) (b) and for CuZSM-5 zeolite (c).

## Table S1: Cartesian coordinates (in angstroms) for [Cu(3HF),O<sub>2</sub>Si(OH)<sub>2</sub>]<sup>-</sup>

С	4.675958	-1.967648	-0.053631
С	3.341988	-2.389442	-0.012389
С	3.064574	-3.770332	-0.030824
С	4.093417	-4.681003	-0.088695
С	5.427272	-4.235042	-0.129475
С	5.725551	-2.889333	-0.112377
Н	2.028552	-4.087672	0.001264
Н	3.881168	-5.744128	-0.103231
Н	6.234491	-4.958134	-0.175089
Н	6.747388	-2.528942	-0.143178
0	5.000401	-0.66738	-0.03817
С	2.322848	-1.383228	0.046117
С	2.71411	0.010119	0.056971
С	4.066252	0.319394	0.016145
0	1.089826	-1.651922	0.088743
С	4.66805	1.64759	0.025434
С	6.066974	1.787132	-0.017895
С	6.653999	3.042994	-0.007981
С	5.865498	4.189785	0.045197
С	4.481003	4.064004	0.088155
С	3.881427	2.811252	0.078691
Н	6.693206	0.904568	-0.059159
Н	7.735427	3.127132	-0.041828
Н	6.32763	5.171496	0.053047
Н	3.856503	4.95068	0.129774
Н	2.804762	2.713662	0.112235
0	1.745441	0.88027	0.107652
Cu	-0.013339	0.02574	0.160504
0	-1.141644	1.634219	0.201014
0	-1.779746	-0.806346	0.242508
Si	-2.451873	0.674377	0.259452
0	-3.348299	1.050866	1.626224
0	-3.512088	0.806985	-1.033768
Н	-4.213343	0.640252	1.681602
Η	-4.062988	1.592093	-1.041546

## Table S2: Cartesian coordinates (in angstroms) for Cu(3HF)<sup>+</sup>

С	-0.670418	2.484043	-0.001201
С	0.698174	2.200765	-0.000331
С	1.614125	3.267226	-0.000857
С	1.155087	4.566283	-0.002214
С	-0.222165	4.822416	-0.003063
С	-1.143419	3.788188	-0.002565
Η	2.673469	3.037558	-0.000175
Η	1.857011	5.391892	-0.002628
Η	-0.578098	5.846861	-0.004129
Η	-2.210865	3.974044	-0.003208
0	-1.610081	1.497001	-0.000748
С	1.109026	0.826591	0.001067
С	0.043384	-0.216588	0.001464
С	-1.330924	0.19556	0.000511
0	2.297642	0.465878	0.001941
С	-2.492147	-0.650418	0.000746
С	-3.773882	-0.050836	-0.000507
С	-4.909883	-0.831389	-0.000305
С	-4.802333	-2.223032	0.001155
С	-3.54801	-2.828637	0.002405
С	-2.399355	-2.060293	0.002211
Η	-3.862837	1.027612	-0.001644
Η	-5.886827	-0.361574	-0.001284
Η	-5.698767	-2.834063	0.001316
Η	-3.467969	-3.909717	0.003541
Η	-1.430077	-2.535883	0.003177
0	0.400777	-1.425376	0.002625
Cu	2.425104	-1.558717	0.003876

Table S3: Comparison of the Raman line positions (cm<sup>-1</sup>) for the spectra obtained after 3HF adsorption in CuZSM-5 and for 3HF-copper(II) solution after subtraction of methanol and free 3HF contributions. The subtracted spectrum is assigned to the 1:2 metal/ligand complex, [Cu(3HF)<sub>2</sub>].

3HF@CuZSM-5	<b>3HF/Cu solution</b>
1612	1615
1595	1598
1571 (weak)	1568
1554	1550
1506	1509
1461	1460
1439	1440
1428	1428
1324	1326
1233	1234



**Figure S2:** Experimental Raman spectrum obtained for 3HF-copper(II) solution after subtraction of methanol and free 3HF contributions (a). The spectrum is presented in comparison with the Raman spectrum of 3HF@CuZSM-5 (b) and with the spectrum of the collected yellow powder obtained after evaporation of 3HF-copper(II) solution (c).