

Supplementary Information

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

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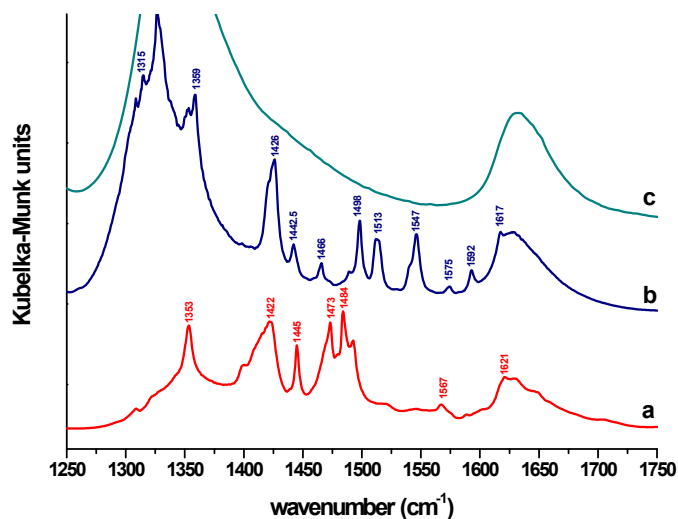


Figure S1: FTIR spectra recorded for 3HF incorporated in silicalite-1 (a), for 3HF adsorbed in CuZSM-5 (one year after mixing 3HF and zeolite powders) (b) and for CuZSM-5 zeolite (c).

Table S1: Cartesian coordinates (in angstroms) for [Cu(3HF),O₂Si(OH)₂]⁻

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

Table S2: Cartesian coordinates (in angstroms) for Cu(3HF)⁺

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

Table S3: Comparison of the Raman line positions (cm⁻¹) 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)₂].

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

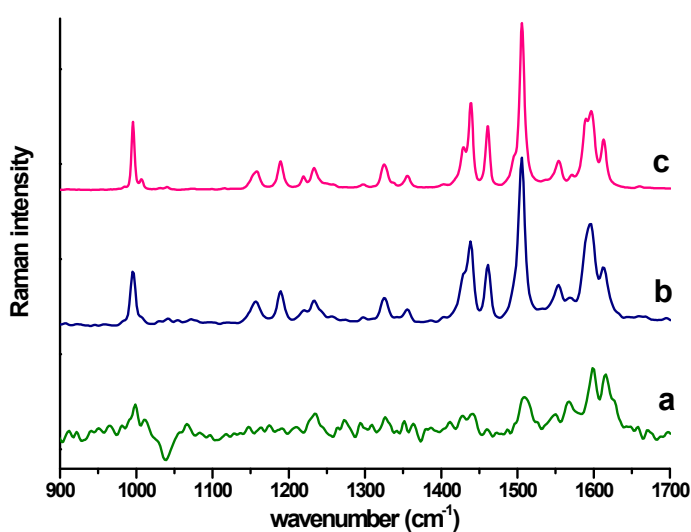


Figure S2: Experimental Raman spectrum obtained for 3HF-copper(II) solution after subtraction of methanol and free 3HF contributions (a). The spectrum is presented in comparison with the Raman spectrum of 3HF@CuZSM-5 (b) and with the spectrum of the collected yellow powder obtained after evaporation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