Supporting Information for:

Impact of Metal and Anion Substitutions on the Hydrogen Storage Properties of M-BTT Metal-Organic Frameworks

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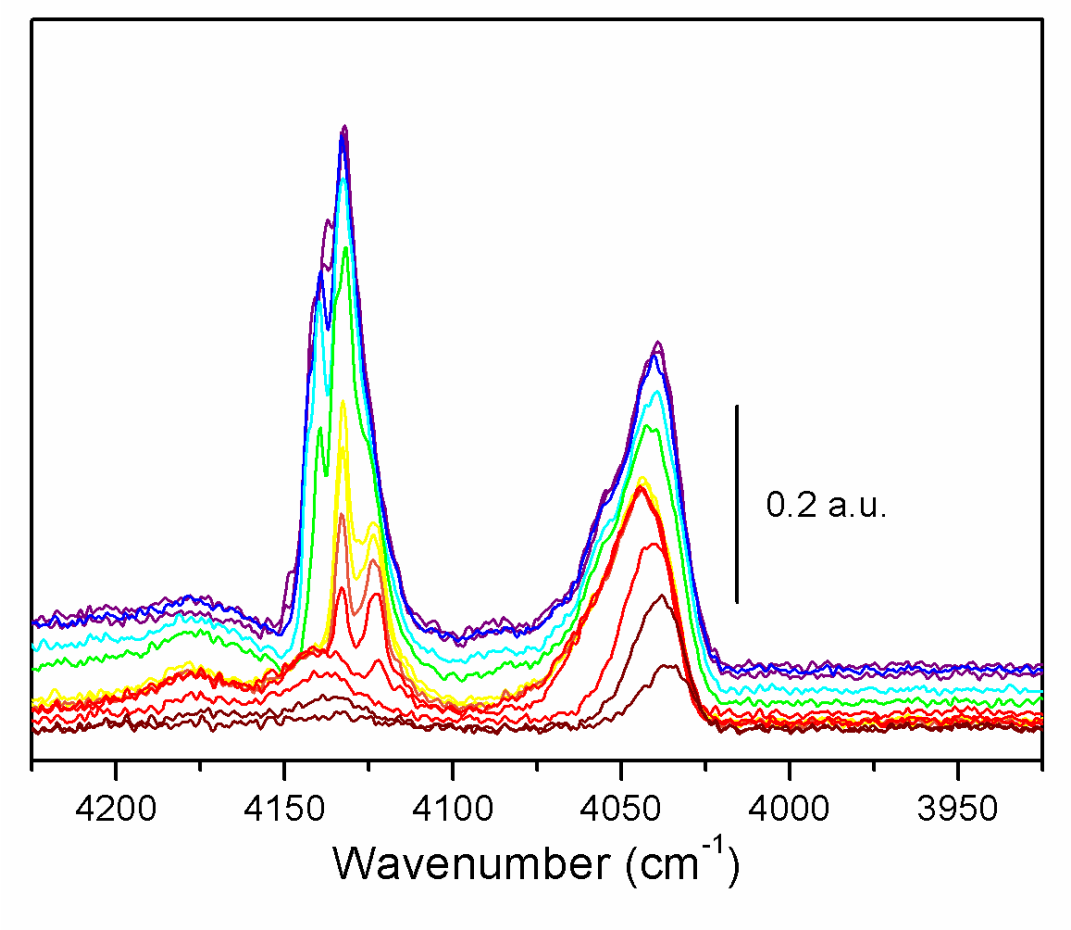

Figure S1. Infrared spectra for H_2 desorption recorded at 14 K for Mn-BTT, in which the pressure (and the total H_2 remaining in the system) was gradually reduced.

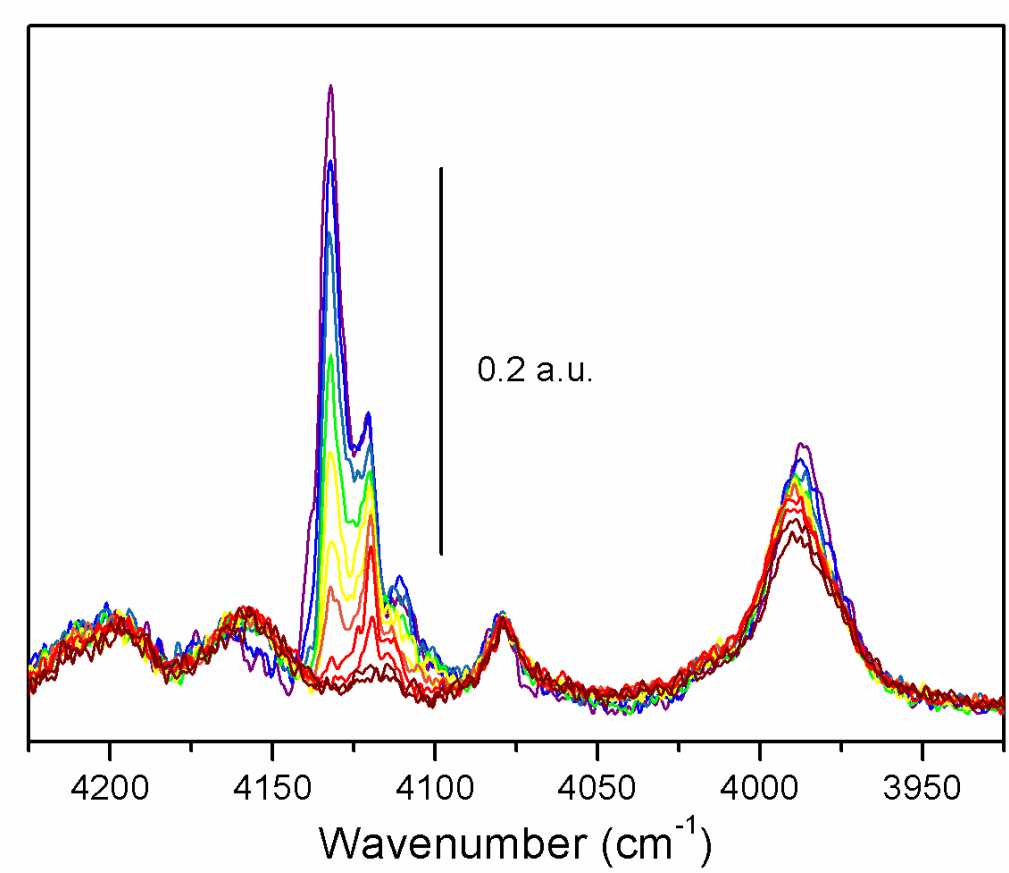

Figure S2. Infrared spectra for H_2 desorption recorded at 14 K for Fe-BTT, in which the pressure (and the total H_2 remaining in the system) was gradually reduced.

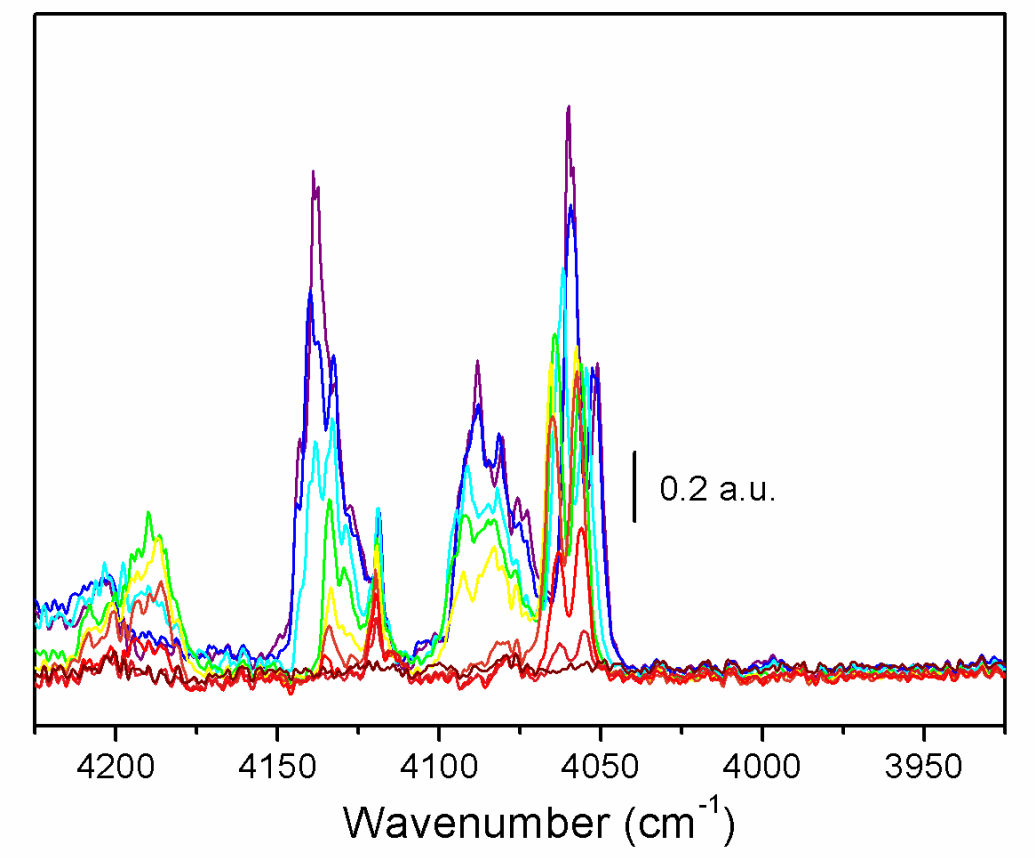

Figure S3. Infrared spectra for H_2 desorption recorded at 14 K for Cu-BTT, in which the pressure (and the total H_2 remaining in the system) was gradually reduced.

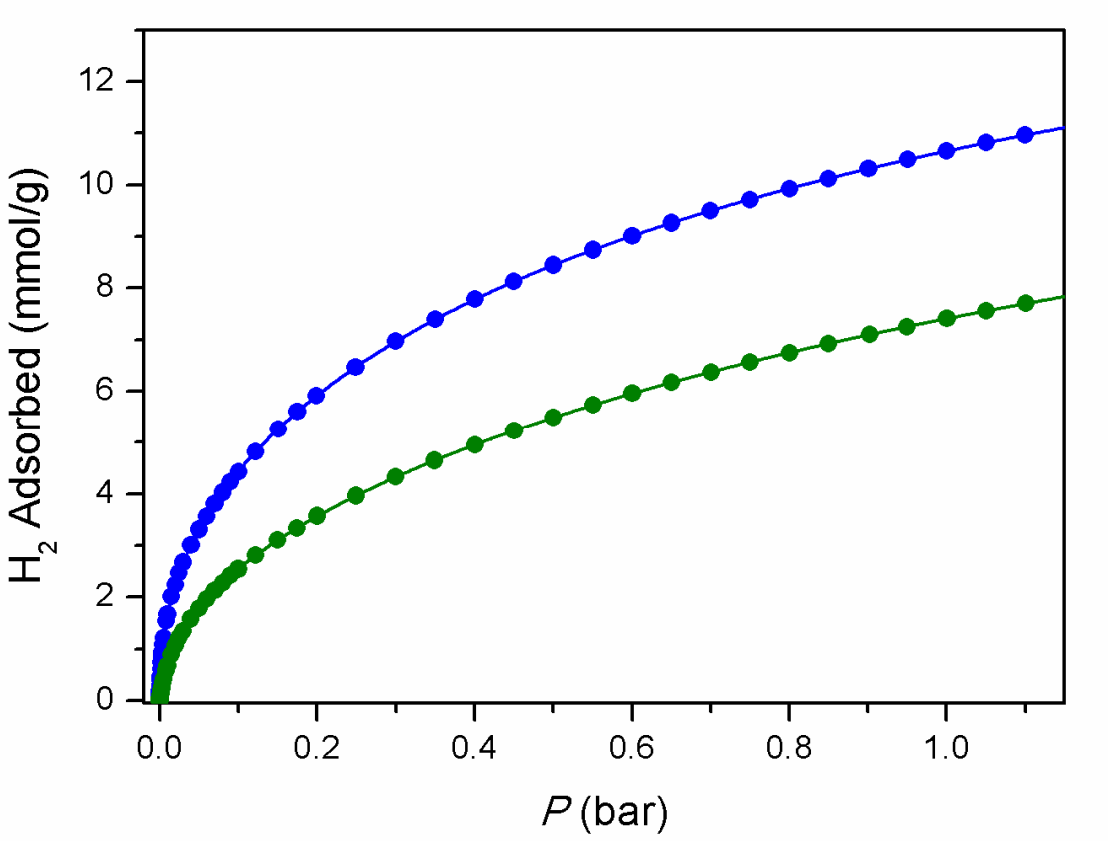

Figure S4. H_2 adsorption isotherms for Mn-BTT collected at 77 K (blue) and 87 K (green). The solid lines represent the dual-site Langmuir fit to the data, using the parameters tabulated in Table S1.

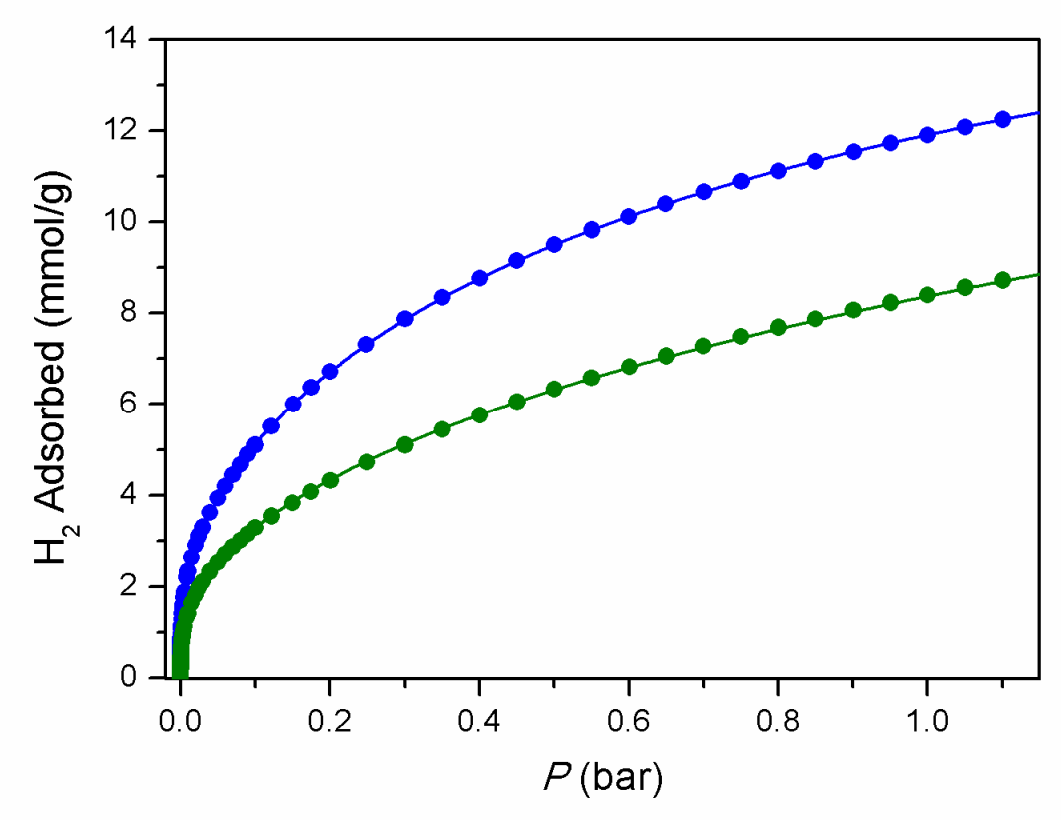

Figure S5. H_2 adsorption isotherms for Fe-BTT collected at 77 K (blue) and 87 K (green). The solid lines represent the dual-site Langmuir fit to the data, using the parameters tabulated in Table S2.

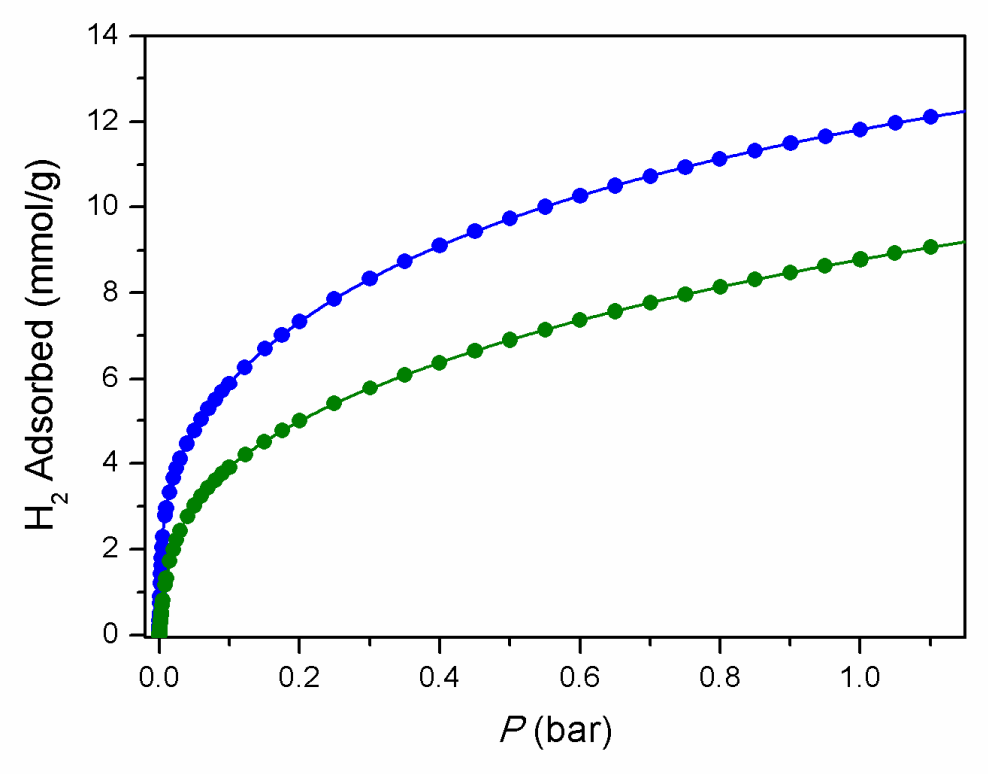

Figure S6. H_2 adsorption isotherms for Cu-BTT collected at 77 K (blue) and 87 K (green). The solid lines represent the dual-site Langmuir fit to the data, using the parameters tabulated in Table S3.

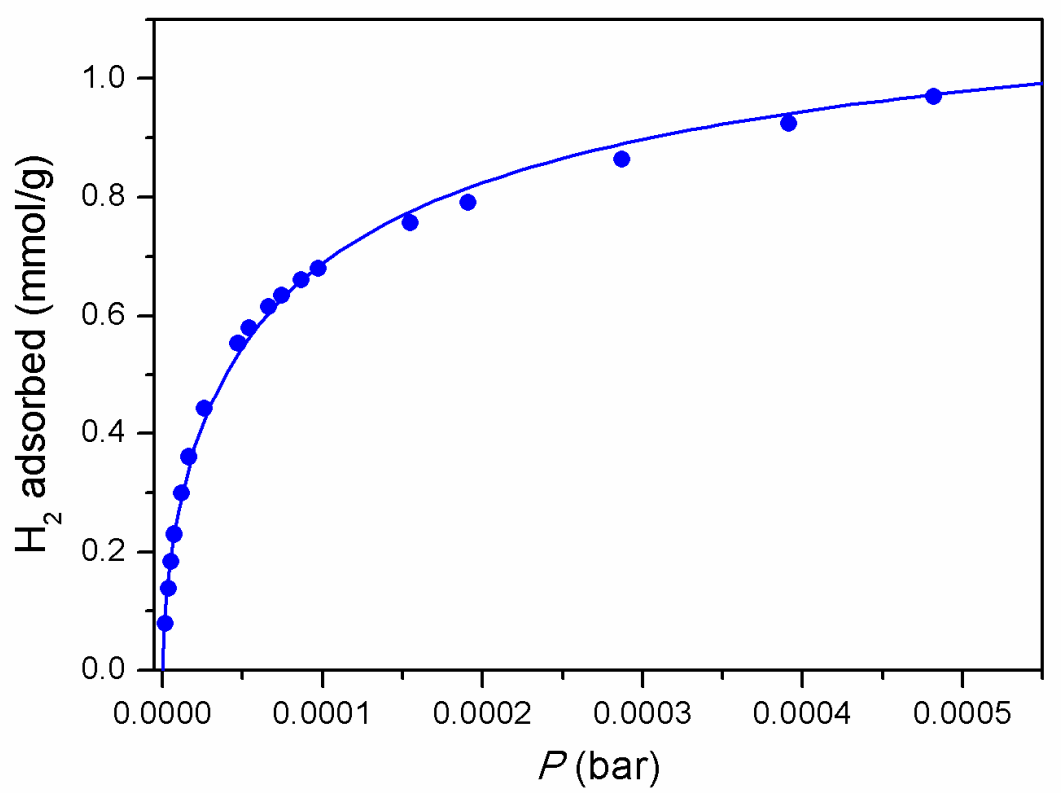

Figure S7. The lowest-pressure region of the H_2 adsorption isotherm for Fe-BTT collected at 77 K. The solid line represents the dual-site Langmuir fit to the data, using the parameters tabulated in Table S4.

Table S1. Dual-site Langmuir fit parameters for the H_2 isotherms for Mn-BTT in Figure S4.

Parameter	*T*	
	77 K	87 K
q_{sat1}	1.21214	1.34085
b_1	185.22316	32.77728
v_1	0.92104	0.93787
q_{sat2}	19.48467	16.67445
b_2	0.9409	0.57771
v_2	0.66854	0.77047

Table S2. Dual-site Langmuir fit parameters for the H_2 isotherms for Fe-BTT in Figure S5.

Parameter	*T*	
	77 K	87 K
q_{sat1}	7.9845	0.61692
b_1	1.59297	455.7024
v_1	0.97761	0.754
q_{sat2}	50.0	50.0
b_2	0.16279	0.18357
v_2	0.27638	0.51252

Table S3. Dual-site Langmuir fit parameters for the H_2 isotherms for Cu-BTT in Figure S6.

Parameter	*T*	
	77 K	87 K
q_{sat1}	2.75088	2.76398
b_1	456.97063	62.91413
v_1	1.03415	1.00654
q_{sat2}	18.30037	16.52023
b_2	0.98154	0.57883
v_2	0.66592	0.75204

Table S4. Dual-site Langmuir fit parameters for the lowest-pressure portion of the 77 K H_2 isotherm for Fe-BTT in Figure S7.

Parameter	*T*
	77 K
q_{sat1}	1.27932
b_1	417.16893
v_1	0.63856
q_{sat2}	0.00121
b_2	5.22471E-06
v_2	62.77542