Supporting Information: Water Stability and Adsorption in Metal-Organic Frameworks

Nicholas C. Burtch, Himanshu Jasuja, and Krista S. Walton*

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, 311 Ferst Drive NW, Atlanta, Georgia 30332, United States

E-mail: krista.walton@chbe.gatech.edu

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*To whom correspondence should be addressed

Table S1: Criteria for MOF water stability classifications

Water Stability Ranking Criteria	
Thermodynamically Stable	Stable after long-term exposure to aqueous solutions: Week or greater in pure water, day(s) in acidic/basic or boiling conditions *Strong potential for a wide range of applications*
High Kinetic Stability	Stable after exposure to high humidity conditions: Decomposes after short exposure times in liquid water *Strong potential for industrial applications with high humidity conditions*
Low Kinetic Stability	Stable under low humidity conditions *Potential for applications with pre-dried gas conditions*
Unstable	Quickly breaks down after any moisture exposure *Potential for applications under moisture-free conditions*

Table S2: Summary of characterization results used in classifying thermodynamically stable MOFs.

MOF	Conf.	Ref.	Characterization summary
Bio-MOF-14	High	1	No loss of PXRD and only minor changes to SEM crystallite image after soaking in water for 2 months. CO_2 uptake nearly unaffected after soaking in water for 30 days
MIL-101(Cr)	High	2	Loss of PXRD and large loss of BET surface area after exposure to 50% steam at 300°C
		3	Normal adsorption/desorption behavior in vapor isotherm.
		4	No change in PXRD after immersion in water at 323 K for one day. Normal water adsorption/desorption behavior in vapor isotherm.
		5	No change in PXRD or BET surface area after soaking in boiling water for one week.
		6	No change in PXRD or BET surface area after soaking in boiling water for one week.
		7	Small decrease in water capacity after 40 water isobars cycles from 140°C to 40°C at a vapor pressure of 5.6 kPa. No subsequent change in BET surface area or pore volume.
		8	No change in PXRD or FTIR after soaking in water and acetonitrile for two days.
		9	Stated to be "stable" after months in air and various organic solvents at room temperature.
MIL-101-SO_3H(Cr)	High	3	Normal adsorption/desorption behavior in vapor isotherm.
		10	No change in PXRD or BET surface area after soaking in boiling water for more than a day.
MIL-96(Al)	High	11	No change in particle size or surface properties observed from SEM and AFM after immersion in pH 6 water for 100 days.
		12	No change in PXRD after 40 water isobar cycle tests between 40 and 140°C at 75% RH in helium.
$Ni_3(BTP)_2$	High	13	No change in PXRD or BET surface area after two week exposure to boiling aqeous solutions of pH 2-14.
PCN-222(Fe)	High	14	No change in the PXRD or BET surface area after soaking in water, boiling water, and 2 M, 4 M, and 8 M HCl for one day.
PCN-224(M)	High	15	No change in PXRD or BET surface area after soaking in pH 0-11 solutions for one day.

Table S3: Summary of characterization results used in classifying thermodynamically stable MOFs (continued).

MOF	Conf.	Ref.	Characterization summary
ZIF-8	High	2	No change in PXRD and a small decrease in BET surface area after exposure to 50 mol% steam at 200°C.
		4	Minor change to PXRD after one day in water at 323 K. No change in PXRD or BET surface area after water adsorption at 298 K.
		16	No change in PXRD after one week exposure to 80°C benzene, 65°C methanol, or boiling water. No change in PXRD after one day exposure to boiling 0.1M or 8M NaOH solutions.
		17	No change in PXRD after one week in water. Some additional PXRD peaks after three months of water exposure.
		18	No decrease in CO_2 or N_2 capacity or selectivity after as-synthesized material exposed to air at 68% RH at 26°C for three days.
Al-PMOF	Med.	19	No change in PXRD or dissolution of ligand evidenced from UV/Vis analysis after one week in neutral or pH 5 solution. Loss of crystallinity and ligand dissolution observed after 1 week in pH 8 solution
JUC-110	Med.	20	No change in PXRD after ten days in boiling water. Further stability implied from water isotherm behavior and GC water/alcohol seperation performance.
MIL-100(Cr)	Med.	17	No change in PXRD after one year in water.
		21	Reproducible adsorption/desorption behavior after 3x vapor isotherm cycles.
		22	Little change in water adsorption behavior after 2,000 adsorption/desorption cycles.
MONT1	Med.	23	PXRD and SEM unchanged after 15 days in boiling water.
$Pb_2(PTPTP)_2(H_2O)_2$	Med.	24	No change in unit cell parameters obtained from single crystal XRD after stirring in water, acid, and base solutions for 36 hours.
Pb_2(p-PDA) $(PTPTP)_2$	Med.	24	No change in unit cell parameters obtained from single crystal XRD after stirring in water, acid, and base solutions for 36 hours.

Table S4: Summary of characterization results used in classifying thermodynamically stable MOFs (continued).

MOF	Conf.	Ref.	Characterization summary
Pb_4(o-PDA)$_2$ (PTPTP)$_2$	Med.	24	No change in unit cell parameters obtained from single crystal XRD after stirring in water, acid, and base solutions for 36 hours.
LaBTB	Low	25	No change in PXRD after exposure to 60°C and 100°C aqueous HCl of pH 2, aqueous NaOH of pH 14, and water solutions for three days.
$H_3(Cu_4Cl)_3$-(BTTRI)$_8$	Low	26	No change in PXRD or TGA results after three days in boiling water or 1 day in pH 3 acid.
Zn(1,4-BDP)	Low	27	No change in PXRD after three days in boiling water.
Zn(1,3-BDP)	Low	27	No change in PXRD after three days in boiling water.
Cu_3(BTP)$_2$	Low	13	No change in PXRD after one day in boiling water or one day in pH 14 solution;
Zn_3(BTP)$_2$	Low	13	No change in PXRD after one week in 100°C aqueous pH 3 HCl solution; loss of PXRD after one hour in room temperature pH 14 NaOH solution or one day in boiling water.
Cu_2(TCMBT) (BPP)(OH)	Low	28	No change in PXRD after two months in boiling water.
NOTT-300	Low	29	No change in PXRD after exposing activated sample to air for one month or immersing in water methanol, ethanol, $CHCl_3$, CH_3CN, DMF, THF, benzene, or toluene for one week. Activated sample also yields no change in CO_2 uptake at 1bar after 3x exposure to 90-100°C water vapor for 1 hour followed by sample reactivation.
PCMOF-5	Low	30	Fresh sample boiled in water for 7 days with minor loss of PXRD and mass. Sample activation indicates a reversible loss of sample crystallinity.
SNU-80	Low	31	No change in PXRD after one week in liquid water. No change in PXRD or elemental analysis after adsorption/desorption at 298 K.

Table S5: Summary of characterization results used in classifying MOFs with high kinetic stability.

MOF	Conf.	Ref.	Characterization summary
CALF-25	High	32	No change in PXRD or BET surface area after adsorption to 95% RH at 313 K. No change in PXRD or decrease in CO_2 uptake after expsoure to 90% RH for one day at 353 K. Loss of PXRD peaks after 7 days in boiling water.
CAU-10	High	33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
DUT-51(Hf)	High	34	Dried samples soaked in water for 12 hours with no significant loss of crystallinity but minor loss in BET surface area.
DUT-51(Zr)	High	34	Dried samples soaked in water for 12 hours with no significant loss of crystallinity but minor loss in BET surface area.
DUT-67(Zr)	High	35	No changes to PXRD after dried powder soaked in water for one day or concentrated HCl for three days. PXRD changes under basic conditions.
		33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
FMOF-1	High	36	No water adsorption or structural changes evidenced from isotherm or IR results structural change after exposure to 100% RH air. No water adsorption or structural changes evidenced from single crystal XRD or IR results after soaking in water for several days.
MIL-100(Al)	High	37	No change in PXRD after 40 hydrothermal isobar stability cycles.
		12	No change in PXRD but slight decrease in BET surface area and water uptake capacity after 40 water isobar cycles between 40 and 140°C at 75% RH in helium.
MIL-100(Fe)	High	4	No change in PXRD after immersion in water at 323 K for one day.
		6	No change in PXRD or BET surface area after soaking in boiling water for one week.
		37	Slight decrease in water capacity after 40 water isobar cycles but no change in PXRD or decrease in subsequent BET surface area.

Table S6: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
MIL-100(Fe)	High	38	No change in BET surface area or pore volume after 6x adsorption/desorption vapor isotherms.
		39	Majority of BET surface area is lost but PXRD maintained after two days in liquid water.
MIL-101-NH_2(Cr)	High	3	Normal adsorption/desorption behavior from vapor isotherm.
		40	No loss of PXRD and only minor loss of BET surface area and micropore volume after 40 adsorption and desorption cycles.
MIL-125-NH_2(Ti)	High	41	No change in PXRD after two days in water. Normal adsorption/desorption behavior from water vapor isotherm.
		42	No change in PXRD but slight decrease in BET surface area and pore volume after 40 water isobar cycles.
		43	No change in FTIR after exposure to water vapor at 373 K.
MIL-127	High	39	No change in PXRD but minor reduction in BET surface area after two days in liquid water.
MIL-53(Al)	High	2	Change in PXRD in 50% steam at 225°C.
		44	Some loss in PXRD intensity and 40% loss of BET surface area after six hours in water at 80°C
		45	PXRD, SEM, TGA, and BET surface area measurements show stability in pH 2 and pH 7 aqueous solutions at 25°C, 50°C, 100°C after one week. Stable for two days in pH 14 solution at 25°C, 50°C, and 100°C.
MIL-53(Cr)	High	44	No change in PXRD or BET surface area after six hours in basic 7E-2 M NaOH, acidic 7.2E-2 M HCl, and neutral water solutions.
MOF-525	High	46	No change in PXRD or BET surface area after activated structures immersed in methanol, water and water:acetic acid (50:50 by vol.) for one day.
MOF-545	High	46	No change in PXRD or BET surface area after activated structures immersed in methanol, water and water:acetic acid (50:50 by vol.) for one day.
MOF-801-P	High	33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.

Table S7: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
MOF-801-SC	High	33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
MOF-802	High	33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
MOF-804	High	33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
MOF-841	High	33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
$Ni_8(OH)_4(H_2O)_2(L_6)_6$	High	47	No change in adsorption behavior or PXRD throughout 3x cyclic vapor adsorption measurements at 298 K.
$Ni_8(OH)_4(H_2O)_2(L_8)_6$	High	47	No change in adsorption behavior or PXRD throughout 3x cyclic vapor adsorption measurements at 298 K.
$Ni_8(OH)_4(H_2O)_2(L_9)_6$	High	47	No change in adsorption behavior or PXRD throughout 3x cyclic vapor adsorption measurements at 298 K.
$Ni_8(OH)_4(H_2O)_2(L_{10})_6$	High	47	No change in adsorption behavior or PXRD throughout 3x cyclic vapor adsorption measurements at 298 K.
$Ni_8(OH)_4(H_2O)_2(L_{10}$-$(CH_3)_2)_6$	High	47	No change in adsorption behavior or PXRD throughout 3x cyclic vapor adsorption measurements at 298 K.
$Ni_8(OH)_4(H_2O)_2(L_{10}$-$(CF_3)_2)_6$	High	47	No change in adsorption behavior or PXRD throughout 3x cyclic vapor adsorption measurements at 298 K.
$Zn_2(BTC)(OH)$-(H_2O)	High	48	No change in PXRD after immersion in boiling water for 18 hours. No change in PXRD after 40 isobar cycles from 40°C to 140°C though slight loss of water sorption capacity is observed.
$Zn(L_{14})(L_{15})$	High	49	No change in PXRD or vapor adsorption behavior throughout four isotherms of water adsorption and desorption.

Table S8: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
Ni-NIC	High	50	Activated sample exposed to air with 80% RH for three days at room temperature causing an increase in loading and selectivity for CO_2 and N_2 but no change in PXRD. No change in PXRD or adsorption capacities after two days in room temperature water.
NU-1000	High	51	No change in PXRD or BET surface area after one day in liquid water.
PCN-225(M)	High	52	PXRD indicates slight increase in amorphous character, and there is some reduction in BET surface area after soaking in pH 0 to pH 12 aqueous solutions for 12 hours.
SCUTC-18	High	53	No BET surface area loss or change in PXRD after 30 days in humid air.
		54	No change in PXRD after exposure to 40°C water vapor for two weeks.
UiO-66	High	55	No loss in BET surface area or change in PXRD after adsorption isotherm in air at 298 K.
		38	Reproducible isotherm over 6x adsorption/desorption isotherms.
		56	No change in PXRD after 15 hours in boiling water.
		57	No change in PXRD after stirring activated sample in water, acetone, benzene and DMF solutions for one day.
		58	No change in PXRD after one day in 25°C water.
		33	Little change in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
		59	No loss of BET surface area after vapor adsorption. No change in PXRD after one day exposure to water, methanol, isopropanol, acetone, pyridine, chloroform, and 0.1 M HCl. Loss of crystallinity after one day in 0.1 M NaOH. FTIR indicates no change in structure except after NaOH and HCl aqueous exposure.
		39	Majority of BET surface area lost after two days in water. No major changes in PXRD.
UiO-66-MM	High	60	No change in PXRD or loss of BET surface area after vapor adsorption/desorption in air at 298 K.

Table S9: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
UiO-66-NH_2	High	55	No change in PXRD or loss in BET surface area after adsorption/desorption in air at 298 K.
		61	No change in PXRD after vapor exposure and subsequent reactivation.
		59	No loss of BET surface area after vapor adsorption isotherm. No change in PXRD after one day exposure to water, methanol, isopropanol, acetone, pyridine, chloroform, and 0.1 M HCl. Loss of crystallinity after one day in 0.1 M NaOH. FTIR only indicates change in structure after NaOH exposure.
		62	No change in PXRD after exposure to water or 1 M HCl for 2 hours at room temperature. Loss of PXRD after exposure to 1 M basic solution.
		42	No change in PXRD but some loss in BET surface area and pore volume after 40 isobar cycles.
		39	Large loss in BET surface area but no major changes to PXRD after two days in water.
Zn-DMOF-A	High	63	No change in PXRD or loss of BET surface area after vapor adsorption/desorption in air at 298 K.
Zn-DMOF-TM	High	63	No change in PXRD or loss of BET surface area after vapor adsorption/desorption in air at 298 K.
		64	No change in PXRD or loss of BET surface area after 3x vapor adsorption/desorption in air at 298 K or exposure to ambient air for three months.
Zn-MOF-508	High	65	No change in PXRD or loss of BET surface area after vapor adsorption/desorption in air at 298 K.
$ZnPO_3$	High	50	Reduction in PXRD peak intensities but negligible change in capacity and selectivity for CO_2 and N_2 after activated sample exposed to air with 80% RH for 3 days at room temperature.

Table S10: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
CAU-10-CH_3	Med.	66	No change in PXRD or FTIR after soaking in aqueous solutions of pH 2 - 8 for 18 hours or exposure to water at 130°C for three hours.
CAU-10-H	Med.	66	No change in PXRD or FTIR after soaking in aqueous solutions of pH 2 - 8 for 18 hours or exposure to water at 130°C for three hours.
CAU-10-NH_2	Med.	66	No change in PXRD or FTIR after soaking in aqueous solutions of pH 2 - 8 for 18 hours or exposure to water at 130°C for three hours.
CAU-10-NO_2	Med.	66	No change in PXRD or FTIR after soaking in aqueous solutions of pH 2 - 8 for 18 hours or exposure to water at 130°C for three hours.
CAU-10-OCH_3	Med.	66	No change in PXRD or FTIR after soaking in aqueous solutions of pH 2 - 8 for 18 hours or exposure to water at 130°C for three hours.
CAU-10-OH	Med.	66	No change in PXRD or FTIR after soaking in aqueous solutions of pH 2 - 8 for 18 hours or exposure to water at 130°C for three hours.
CdZrSr	Med.	50	Reduction in PXRD intensity but no change in capacity and selectivity for CO_2 and N_2 after activated sample exposed to 80% RH for 3 days at room temperature.
Co-NIC	Med.	18	No decrease in CO_2 or N_2 capacity and selectivity after as-synthesized material exposed to air at 68% RH and 26°C for three days.
Cu-PCN	Med.	18	No decrease in CO_2 or N_2 capacity and selectivity after as-synthesized material exposed to air at 68% RH and 26°C for three days.
Eu-Cu	Med.	50	No change in capacity and selectivity for CO_2 and N_2 after activated sample exposed to 80% RH for 3 days at room temperature.
La-Cu	Med.	50	No change in capacity and selectivity for CO_2 and N_2 after activated sample exposed to 80% RH for 3 days at room temperature.
MIL-53-F(Al)	Med.	67	No change in PXRD or n-hexane adsorption capacity after water vapor adsorption isotherm measurement.
Al(OH)(1,4-NDC)	Med.	68	Normal vapor adsorption/desorption at 298K.

Table S11: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
Ni-HF	Med.	18	No decrease in CO_2 or N_2 capacity and selectivity after as-synthesized material exposed to air at 68% RH and 26°C for three days.
UiO-66-Br	Med.	62	No change in PXRD after exposure to water or 1 M HCl for 2 hours at room temperature. Loss of PXRD after exposure to 1 M base.
		39	No significant changes in PXRD but large reduction BET surface area after two days in water.
UiO-67	Med.	51	No change in PXRD or BET surface area after one day in liquid water.
		58	No change in PXRD after one day in 25°C water.
		59	Loss of BET surface area after vapor adsorption. Some change in PXRD after one day in water but no change after methanol, isopropanol, acetone, pyridine, or chloroform. Loss of PXRD after one day in 0.1 M NaOH and 0.1 M HCl. FTIR indicates change in structure only for NaOH and HCl exposure.
		56	Loss of PXRD after 15 hours in boiling water.
UTSA-16	Med.	69	No change in CO_2 uptake after exposure to air for three days before running 4x CO_2 adsorption isotherms at 296 K.
ZIF-7	Med.	18	No decrease in CO_2 or N_2 capacity and selectivity after as-synthesized material exposed to air at 68% RH and 26°C for three days.
ZIF-90	Med.	18	No decrease in CO_2 or N_2 capacity and selectivity after as-synthesized material exposed to air at 68% RH and 26°C for three days.
Zn-TTC	Med.	18	No decrease in CO_2 or N_2 capacity and selectivity after as-synthesized material exposed to air at 68% RH and 26°C for three days.
Zn/Co-BTEC	Med.	18	No decrease in CO_2 or N_2 capacity and selectivity after as-synthesized material exposed to air at 68% RH and 26°C for three days.
Zr-DMBDC	Med.	70	No change in XRD or FTIR after soaking in aqueous $HgCl_2$ solution for 12 hours or exposure to Hg(0) vapor.
AlaZnCl	Low	71	No change in PXRD after six month exposure to 98% RH at room temperature.
AlaZnOAc	Low	71	No change in PXRD after six month exposure to 98% RH at room temperature.

Table S12: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
Bio-MOF-13	Low	1	Minor loss in PXRD after being shaken vigorously in 10 mL of water for one hour.
CUK-1	Low	72	Sample did not need to be changed after long exposures to humid air.
DUT-67(Hf)	Low	35	No changes to PXRD after dried powder soaked in water for one day or concentrated HCl for three days. PXRD changes under basic conditions.
DUT-68(Hf)	Low	35	No changes to PXRD after dried powder soaked in water for one day or concentrated HCl for three days. PXRD changes under basic conditions.
DUT-68(Zr)	Low	35	No changes to PXRD after dried powder soaked in water for one day or concentrated HCl for three days. PXRD changes under basic conditions.
DUT-69(Zr)	Low	35	No changes to PXRD after dried powder soaked in water for one day or concentrated HCl for three days. PXRD changes under basic conditions.
MIL-140 A	Low	56	No change in PXRD after 15 hours in boiling water.
MIL-140 B	Low	56	No change in PXRD after 15 hours in boiling water.
MIL-140 C	Low	56	No change in PXRD after 15 hours in boiling water.
MIL-140 D	Low	56	Minor changes in PXRD after 15 hours in boiling water.
MOFF-2	Low	73	No change in PXRD after water contact angle measurements
MOOFOUR-1-Ni	Low	74	No change in PXRD after one month in air. Some change in PXRD after one month in water. New PXRD peaks after one day in boiling water.
$Zn_6(IDC)_4(OH)_2(HPRZ)_2$	Low	75	No change in PXRD after soaking in ethanol, acetone, tetrahydrofuran, bezene, toluene, and xylene for one day. Partial loss of PXRD intensities after soaking in water.
$Cd(2,6\text{-}NDC)_{0.5}(PCA)$	Low	76	No change in PXRD after exposure to 60°C water vapor for one day or open air for months.
$Zn_2(2,6\text{-}NDC)_2$ (2,2'-dimethyl-BPY)	Low	54	No change in PXRD after exposure to 40°C water vapor for one week.
$Cd(L_1)(Cl)(H_2O)$	Low	77	Normal adsorption/desorption behavior in vapor isotherm.

Table S13: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
$Cd(L_2)(Cl)(H_2O)$	Low	77	Normal adsorption/desorption behavior in vapor isotherm.
$Cd_2(L_2)_2(Br)_2(H_2O)_3$	Low	77	Normal adsorption/desorption behavior in vapor isotherm.
$Cd(L_3)(Cl)(H_2O)_2$	Low	77	Normal adsorption/desorption behavior in vapor isotherm.
Zn_2L_4	Low	78	Normal adsorption/desorption behavior in vapor isotherms at 15°C, 25°C, 35°C, and 45°C.
$Ni(HPTZ)_2$	Low	79	Minor changes to PXRD after as-synthesized sample exposed to boiling water, toluene, and ethanol for one week. Minor changes to PXRD after one day in 0.1 M HCl.
$Zn_4O(BFBPDC)_3(BPY)_{0.5}(H_2O)$	Low	80	No change in PXRD after four days in humid conditions
$Ni(L_{13})_2$	Low	81	No change in PXRD after water vapor adsorption isotherm.
$Co(L_{13})_2$	Low	81	No change in PXRD after water vapor adsorption isotherm.
$Ni_2(C_2O_4)(L_{16})_2$	Low	82	Minor changes in PXRD after immersion in room temperature water for one day or 18 hours in 85°C water.
$Zn_3(BPDC)_3$(2,2'-dimethyl-BPY)	Low	83	No change in PXRD after exposure to water vapor for ten days.
NU-1000-SALI-1	Low	84	No change in PXRD after water vapor isotherm.
NU-1000-SALI-3	Low	84	No change in PXRD after water vapor isotherm.
NU-1000-SALI-7	Low	84	No change in PXRD after water vapor isotherm.
NU-1000-SALI-9	Low	84	No change in PXRD after water vapor isotherm.
PCN-56	Low	85	Little change in PXRD after pH 2 HCl for two days and pH 11 NaOH for one day.
PCN-57	Low	85	Little change in PXRD after pH 2 HCl for 4.5 days or pH 2 HCl for one week.
PCN-58	Low	85	Little change in PXRD after pH 2 HCl or water for one day or pH 11 NaOH for 15 hours.
SIFSIX-2-Cu-i	Low	86	No change in PXRD after exposure to 5% - 95% RH under a nitrogen atmosphere.
Tb-FTZB-MOF	Low	87	No change in PXRD after soaking in water for one day or performing a water vapor isotherm.
UiO-1,4-NDC	Low	61	No change in PXRD after exposure to 90% RH and subsequent reactivation.

Table S14: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
UiO-2,6-NDC	Low	56	Some additional peaks in PXRD after 15 hours in boiling water.
		88	No change in PXRD after two hours in 0.1 M NaOH or HCl, one day in H_2S or water, or one week in MeOH, $CHCl_3$, IPA, or Ter-But-OH
UiO-66-$(CO_2H)_2$	Low	89	No change in PXRD after stirring in water, acetic acid, or 1 M HCl for 12 hours. Complete loss of PXRD after 12 hours in 1 M NaOH.
UiO-66-$(OMe)_2$	Low	61	No change to PXRD after vapor exposure and subsequent reactivation
UiO-66-Br_2	Low	89	No change in PXRD after being stirred in water, acetic acid, or 1 M HCl for 12 hours. Complete loss of PXRD after 12 hours in 1 M NaOH.
UiO-66-CF_3	Low	89	No change in PXRD after being stirred in water, acetic acid, or 1 M HCl for 12 hours. Complete loss of PXRD after 12 hours in 1 M NaOH.
UiO-66-Cl_2	Low	89	No change in PXRD after being stirred in water, acetic acid, or 1 M HCl for 12 hours. Complete loss of PXRD after 12 hours in 1 M NaOH.
UiO-66-CO_2H	Low	90	No change in PXRD after being stirred in water, acetic acid, or 1 M HCl for 12 hours. Complete loss of PXRD after 12 hours in 1 M NaOH.
UiO-66-DM	Low	91	No change in PXRD or BET surface area after vapor adsorption. No change in PXRD after exposure to water or 1 N HCl solutions. Complete loss of PXRD in 1 N NaOH solution.
UiO-66-I	Low	90	No change in PXRD after stirring in water, acetic acid, or 1 M HCl for 12 hours. Complete loss of PXRD after 12 hours in 1 M NaOH.
UiO-66-NO_2	Low	61	No change in PXRD after vapor exposure and subsequent reactivation.
		62	No change in PXRD after exposure to water or 1 M HCl for 2 hours at room temperature. Loss of PXRD after exposure to 1 M base.
UiO-66-SO_3H	Low	90	No change in PXRD after being stirred in water, acetic acid, or 1 M HCl for 12 hours. Complete loss of PXRD after 12 hours in 1 M NaOH.

Table S15: Summary of characterization results used in classifying MOFs with high kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
UMCM-150	Low	17	No change in PXRD after placing sample in solutions of various water:dmf ratios.
ValZnCl	Low	71	No change in PXRD after six month exposure to 98% RH at room temperature.
ValZnFor	Low	71	No change in PXRD after six month exposure to 98% RH at room temperature.
Y-FTZB-MOF	Low	87	No change in PXRD after soaking sample in water for one day or performing a water vapor isotherm.
ZIF-11	Low	16	No change in PXRD after one week in 80°C benzene or 65°C methanol. New PXRD peaks after three days in boiling water
Zn-DMOF-$(NO_2)_2$	Low	92	No change in PXRD after vapor adsorption isotherm.
Zn(NDI-H)	Low	93	No significant changes to PXRD after immersing as-synthesized sample in water for one day.
Zr-fum	Low	94	No change in PXRD after stirring in water, physiological NaCl solution, or phosphate buffered saline solution.

Table S16: Summary of characterization results used in classifying MOFs with low kinetic stability.

MOF	Conf.	Ref.	Characterization summary
CAU-6	High	33	Drop in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
Co-MOF-74/ Co-CPO-27/ Co-DOBDC	High	95	85% of initial CO_2 uptake maintained and minor changes to PXRD after exposure to 70% RH at room temperature with subsequent regeneration.
		96	Change in PXRD and propane adsorption behavior after exposure to humidity.
		33	Drop in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
Cu-BTC/HKUST-1	High	2	No change in PXRD but minor loss of BET surface area after exposure to 50 mol% steam at 200°C.
		17	No change in PXRD after placing activated sample water for five hours. Additional PXRD peaks after one day.
		21	Incremental drop in capacity throughout 5x vapor adsorption isotherms.
		55	No change in PXRD but some loss in BET surface area after vapor adsorption isotherm at 298 K.
		38	Incremental drop in capacity throughout 6x vapor adsorption isotherms.
		4	Loss of PXRD after immersion in water at 323 K for one day. Large loss in BET surface area after water vapor adsorption isotherm at 298 K.
		97	15% drop in adsorption uptake after each of four vapor adsorption/desorption cycles at 36°C.
Mg-MOF-74/Mg-CPO-27/Mg-DOBDC	High	98	No change in PXRD but significant loss of BET surface area and low pressure CO_2 capacity loss after two hours in 15 mol% steam conditions at 100°C. 22.8% loss in low pressure CO_2 capacity and some loss of BET surface area after one year in a sealed container.
		95	Minor changes in PXRD and 16% of initial CO_2 uptake maintained after exposure to 70% RH at room temperature with subsequent regeneration.
		55	No change in PXRD but 83% loss of BET surface area after vapor adsorption isotherm in air at 298 K.

Table S17: Summary of characterization results used in classifying MOFs with low kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
Mg-MOF-74/Mg-CPO-27/Mg-DOBDC	High	99	Drop in CO_2 elution time and capacity after 15 CO_2 breakthrough cycles at 313 K with 16.3% RH.
		33	Drop in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
MIL-101-NO_2(Cr)	High	3	Normal adsorption/desorption after vapor isotherm.
		40	No loss of PXRD but some loss of BET surface area and micropore volume after 40 adsorption/desorption cycles.
MIL-47-F(V)	High	67	Loss of PXRD and decreased n-hexane adsorption capacity after water vapor isotherm.
MIL-69(Al)/DUT-4	High	4	Loss of PXRD after immersion in water at 323 K for one day. Desorption falls below the adsorption branch in water adsorption isotherm at 298 K.
MOF-14	High	100	Minor change in PXRD but significant loss of BET surface area after exposure to 90% RH air with subsequent reactivation.
MOF-805	High	33	Drop in high pressure water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
MOF-806	High	33	Drop in high pressure water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
MOF-808	High	33	Drop in high pressure water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
$Ni_8(OH)_4(H_2O)_2(L_7)_6$	High	47	Slight decrease in adsorption behavior after 3x cyclic vapor isotherm measurements at 298 K. No change in PXRD after vapor adsorption
Ni-DMOF	High	101	Normal adsorption/desorption behavior in isotherm until 30% RH at 298K. Additional PXRD peaks and desorption falls below adsorption branch for isotherm run to 60% RH at 298 K.
		102	No bond breakage evidenced by IR or change in PXRD after exposure to 48% RH at 298 K.

Table S18: Summary of characterization results used in classifying MOFs with low kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
Ni-MOF-74/Ni-CPO-27/Ni-DOBDC	High	98	Significant loss of PXRD and BET surface area and some loss of low pressure CO_2 capacity after 2 hours in 5 mol% steam at 100°C conditions. No loss of low pressure CO_2 capacity after 1 year in a sealed container.
		95	Minor changes to PXRD and 61% of initial CO_2 uptake maintained after exposure to 70% RH at room temperature with subsequent regeneration.
		33	Drop in water uptake properties after five adsorption/desorption cycles at 298 K with a two hour activation at 298 K between each cycle.
SCUTC-19	High	53	Loss of PXRD intensity and large BET surface area loss after one week in humid air.
Zn-DMOF	High	101	Normal adsorption/desorption behavior in water isotherm until 30% RH at 298 K. Additional PXRD peaks and desorption falls below adsorption branch for isotherm at 298 K to 60% RH
		55	Change in PXRD and complete loss of BET surface area after water vapor isotherm at 298 K.
		102	Bond breakage evidenced by IR and change in PXRD after exposure to 48% RH at 298 K.
Zn-DMOF-N	High	63	No change in PXRD but some loss in BET surface area after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-$TM_{0.5}$	High	63	No change in PXRD but some loss in BET surface area after vapor adsorption isotherm in air at 298 K.
Zn-MOF-74/ Zn-CPO-27/ Zn-DOBDC	High	2	Change in PXRD in 50% steam at 325°C
		95	Minor change in PXRD and some loss in initial CO_2 uptake after exposure to 70% RH at room temperature with subsequent reactivation.

Table S19: Summary of characterization results used in classifying MOFs with low kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
Zn-NDC	High	50	Activated sample exposed to air with 80% RH for three days at room temperature causing no change in loading and selectivity for CO_2 and N_2 but reduced peak intensities in PXRD. Some change in PXRD and decrease in adsorption capacity for CO_2 after two days in room temperature water.
		54	Some change in PXRD after exposure to 40°C water vapor for one day.
Co-DMOF	Med.	102	Bond breakage and collapse of 3D structure evidenced by IR and PXRD measurements after exposure to 48% RH at 298 K.
Cu-DMOF	Med.	102	Some bond breakage but no collapse of 3D structure evidenced by IR and PXRD measurements after exposure to 48% RH at 298 K.
IRMOF-1-CF_3O/ MOF-5-CF_3O/ Banasorb-22	Med.	103	No change in PXRD but large loss of BET surface area after one week exposure to steam at 100°C
Cu-EBTC	Low	104	Little change in PXRD after water vapor adsorption isotherm.
Cu-HF	Low	50	Activated sample exposed to air with 80% RH for three days at room temperature causing a decrease in loading and selectivity for CO_2 and N_2 and a disappearance of peaks in PXRD. No change in PXRD and change in adsorption capacity for CO_2 after two days in room temperature water.
Cu-MBTC	Low	104	Change in PXRD after water vapor adsorption isotherm.
IRMOF-1-$(CH_3)_2$/ MOF-5-$(CH_3)_2$	Low	105	No PXRD change after four days in ambient air.
IRMOF-1-CH_3/ MOF-5-CH_3	Low	105	No PXRD change after four days in ambient air.
IRMOF-3-AM15	Low	106	No change in PXRD after four days in air.
IRMOF-3/ MOF-5-NH_2	Low	106	Gradual decrease in PXRD intensity throughout four days of exposure to ambient air.
MIL-110 (Al)	Low	2	Change in PXRD after 50% steam at 300°C.
		12	Change in PXRD after 40 isobar cycles between 40 and 140°C at 75% RH in helium.
MIL-125 (Ti)	Low	41	No change in FTIR after exposure to humid air at 373 K.
		43	Loss of PXRD intensity and adsorption falls below adsorption branch in water vapor isotherm.

Table S20: Summary of characterization results used in classifying MOFs with low kinetic stability (continued).

MOF	Conf.	Ref.	Characterization summary
MOFF-1	Low	73	Slight changes in the PXRD pattern after water contact angle measurements .
MOFF-3	Low	73	Slight changes in the PXRD pattern after water contact angle measurements.
Cu_2(TPTC-O-(ethyl))	Low	107	Little change in PXRD after 1 hour exposure to 50% RH air but significant loss of PXRD after 16 days.
Cu_2(TPTC-O-(n-propyl))	Low	107	Little change in PXRD after 1 hour exposure to 50% RH air but significant loss of PXRD after 16 days.
Cu_2(TPTC-O-(n-hexyl))	Low	107	No change in PXRD after 16 days in 50% RH air.
SIFSIX-3-Zn	Low	86	Irreversible change in PXRD after exposure to 5% to 95% RH under a nitrogen atmosphere.
UiO-66-F_2	Low	89	Loss of PXRD after being stirred in water, acetic acid, 1 M NaOH, and 1 M HCl for 12 hours.
UiO-66-F	Low	89	Change in PXRD after being stirred in water, acetic acid, 1 M NaOH, and 1 M HCl for 12 hours.
$Zr_6O_6(ABDC)_{12}$	Low	108	Loss of PXRD after immersion in water for one day.
$Zr_6O_6(ABDC\text{-}Cl_2)_{12}$	Low	56	Significant loss of PXRD peaks after 15 hours in boiling water.
		58	Some additional peaks in PXRD after one day immersion in 25°C water

Table S21: Summary of characterization results used in classifying unstable MOFs.

MOF	Conf.	Ref.	Characterization summary
IRMOF-1/MOF-5	High	2	New PXRD peaks and major loss of BET surface area after exposure to 10mol% water at 40°C.
		17	Change in PXRD after exposure to liquid water.
		103	Complete of BET surface area after minutes and change in PXRD after 2 hours during steam exposure.
		106	Immediate loss of PXRD after exposure to air.
		105	Loss of PXRD and BET surface area as well as large changes to crystal morphology observed via SEM after one hour in liquid water.
		109	New PXRD peaks after one day exposure to ambient air.
MOF-177	High	17	Change in PXRD after exposure to liquid water.
		110	Additional PXRD peaks after one day in 40%RH air. Complete loss of PXRD and BET surface area after three days in 40% RH air.
		111	Significant changes to PXRD after one week in 16% RH air. Complete loss of PXRD and BET surface area after 12 hours in liquid water at 25°C.
MOF-508	High	53	Loss of PXRD peaks after 10 hours in humid air.
		2	Loss of PXRD with 5% steam at 100°C.
		54	Some change in PXRD after exposure to 40°C water vapor for one day.
MOF-69C	High	2	Change in PXRD after 0% steam at ambient temperature.
Zn-DMOF-NO_2	High	92	Additional peaks in PXRD after water vapor isotherm until 60% RH at 298 K.
		63	Change in PXRD and full loss of BET surface area after vapor isotherm in air at 298 K.
UiO-BPY	Med.	59	Complete loss of BET surface area after vapor adsorption. Loss of PXRD after one day exposure to protic solvents (water, methanol, isopropanol) as well as HCl and NaOH but no change in PXRD in acetone, pyridine, or chloroform. FTIR also indicates no change in structure except for NaOH and HCl exposure.
UMCM-1	Med.	55	Full loss of BET surface area and loss of peaks in PXRD after vapor adsorption isotherm in air at 298 K.

Table S22: Summary of characterization results used in classifying unstable MOFs (continued).

MOF	Conf.	Ref.	Characterization summary
Zn-DMOF-Br	Med.	63	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-Cl_2	Med.	63	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-DM	Med.	64	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-$DM_{0.5}$	Med.	64	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-MM	Med.	64	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-$MM_{0.5}$	Med.	64	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-NH_2	Med.	55	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-OH	Med.	63	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-DMOF-TF	Med.	64	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Zn-MOF-508-TM	Med.	65	Full loss of BET surface area and change in PXRD after vapor adsorption isotherm in air at 298 K.
Bio-MOF-11	Low	1	Sample dissolves immediately in water and loses all PXRD peaks after being shaken vigorously in 10 mL water.
Bio-MOF-12	Low	1	Sample partially dissolves immediately in water and loses all PXRD after being shaken vigorously in 10 mL water
MIL-47(V)	Low	44	Full loss of PXRD and BET surface area after exposure for 6 hours in basic (7E-2M NaOH), acidic (7.2E-2 M HCl) and neutral water solutions.
MOF-505	Low	17	Change in PXRD after exposure to liquid water.
Cu_2(TPTC-O-methyl)	Low	107	Change in PXRD peaks after exposure to 50% RH air for 1 hour

Table S23: Ligand definitions

Abbreviation	**Chemical name**
ALA	Alanine
ABDC	4,4'-azobenzenedicarboxylate
AC	Acetate
AD	Adenine
ADC	Anthracenedicarboxylate
BDC	1,4-benzenedicarboxylate
BDP	Benzenedi(4-pyrazolyl)
BFBPDC	2,2'-bis-trifluoromethyl-biphenyl-4,4'-dicarboxylate
BHTC	Biphenyl-3,4',5-tricarboxylate
BPDC	4,4'-biphenyldicarboxylate
BPE	1,2-bis(4-pyridyl)ethane
BPP	1,3-bis(4-pyridyl)propane
BPTC	Biphenyl-3,3',5,5'-tetracarboxylate
BPY	4,4'-bipyridine
BPZ	3,3',5,5'-tetramethyl-4,4'-bipyrazolate
BTC	1,3,5-benzenetricarboxylate
BTP	1,3,5-tris(1H-pyrazol-4-yl)benzene
BTTRI	1,3,5-tris(1H-1,2,3-triazol-5-yl)benzene
$C_6H_5O_7$	2-hydroxypropane-1,2,3-tricarboxylate
$C_6H_4O_7$	2-oxidopropane-1,2,3-tricarboxylate
DABCO	4-diazabicyclo[2.2.2]-octane
DMBDC	2,5-dimercapto-1,4-benzenedicarboxylate
DOBDC	2,5-dihydroxyterephthalate
DPA	4,4'-dipyridylacetylene
DTTDC	Dithieno[3,2-b;2',3'-d]-thiophene-2,6-dicarboxylate
FOR	Formate
FTZB	3-fluoro-4'-(2H-tetrazol-5-yl)biphenyl-4-carboxylate
FUM	Fumarate
H_2L	Tetraethyl-1,3,6,8-pyrenetetraphosponate
H_2PDA	Phenylenediacetate
H_2PTPTP	2-(5-6-[5-(pyrazin-2-yl)-1H-1,2,4-triazol-3-yl]-pyridin-2-yl-1H-1,2,4-triazol-3-yl)pyrazine
H_4L	Biphenyl-3,3',5,5'-tetracarboxylate
HPTZ	4-(1,2,4- triazol-4-yl)phenylphosphonate)
IDC	Imidazole-4,5-dicarboxylate
ISO	Isophthalate

Table S24: Ligand definitions (continued)

Abbreviation	**Chemical name**
L_1	2-((pyridin-4-yl)methylamino)-4-methylpentanoate
L_2	2-(pyridin-4-yl)methylamino)-3-hydroxypropanoate
L_3	2-((pyridin-4-yl)methylamino)-3-hydroxybutanoate
L_4	4,4'-bipyridine-2,6,2',6'-tetracarboxylate
L_5	1,2,4,5-tetrakisphosphonomethylbenzene
L_6	1H-pyrazole-4-carboxylate
L_7	4-(1H-pyrazole-4-yl)benzoate
L_8	4,4'-benzene-1,4-diylb- is(1H-pyrazole)
L_9	4,4'-buta-1,3-diyne-1,4-diylbis(1H-pyrazole)
L_{10}	4,4'-(benzene-1,4-diyldiethyne-2,1-diyl)bis(1H-pyrazole)
L_{11}	Perfluorinated biphenyl carboxylate
L_{12}	Perfluorinated biphenyl bistetrazole
L_{13}	3,5-di(pyridine-4-yl) benzoate
L_{14}	4,4'-(2,3,5,6-Tetramethoxy-1,4-phenylene)dipyridine
L_{15}	4,4',4",4"'-dibromo-benzene-1,2,4,5-tetrayl-tetrabenzoate
L_{16}	4,2',4",2"-terpyridine-4'-carboxylate
L_{17}	2-methylimidazolate-4-amide-5-imidate
MEIM	2-methylimidazole
MTB	4,4',4",4"'-Methanetetrayltetrabenzoic acid
NDC	Napthalenedicarboxylate
PCP	P,P'-diphenylmethylenediphosphinate
PDC	Pyridine-2,4-dicarboxylate
PHIM	Phenyl benzimidazolate
PRZ	Piperazine
PYR	Pyrazine
PZDC	1H-pyrazole-3,5-dicarboxylic acid
TAZB	3,3',5,5'-azobenzenetetracarboxylate
TBAPY	1,3,6,8-tetrakis(p-benzoate)pyrene
TCMBT	N,N',N"-tris(carboxymethyl)-1,3,5-benzenetricarboxamide
TCPP	Meso-tetra(4-carboxyl-phenyl) porphyrin
TCPP(M)	Tetrakis(4-carboxyphenyl)-porphyrin(M); M =Ni, Co or Fe
TDC	2,5-thiophenedicarboxylate
TEIA	1,3,5,7-tetrakis(4-(2-ethyl-1H-imidazol-1-yl)phenyl)-ane
THIPC	(S)-4,5,6,7-tetrahydro-1H-imidazo[4,5-c]pyridine-6-carboxylate
TPTC-O	2',5'-dialkyloxy-[1,1':4',1"-terphenyl]-3,3",5,5"-tetracarboxylate
TZ	3,5-bis(trifluoromethyl)-1,2,4-triazolate
VAL	Valine

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