Electronic Supplementary Material (ESI) for ChemComm.

Results of the Rietveld refinements of Fe-MIL-59 against PXRD data recorded at different relative humidity values during the sorption and desorption of water.

p/p_0 = 0.007, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.14667(29)
_cell_length_b  19.14667(29)
_cell_length_c  19.14667(29)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7019.07(32)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.76811(22) 0.39982(22) 0.12872(24) 1 3.77(24)
O1 O   0 0.81228(41) 0.49529(59) 0.14285(60) 1 5.61(33)
O2 O   0 0.79280(51) 0.40269(56) 0.02685(44) 1 5.61(33)
O3 O   0 0.72211(46) 0.39560(75) 0.22327(34) 1 5.61(33)
O4 O   0 0.70963(67) 0.31669(31) 0.10599(52) 1 5.61(33)
```

O5 O 0 0.68042(70) 0.45485(70) 0.10461(87) 1 5.61(33)
O6 O 0 0.84645(74) 0.34645(74) 0.15355(74) 1 5.61(33)
C1 C 0 0.51699(47) 0.33084(62) 0.36881(59) 1 12.42(62)
C2 C 0 0.75264(55) 0.38097(87) 0.27929(57) 1 12.42(62)
C3 C 0 0.5933576 0.324478 0.3752813 1 12.42(62)
C4 C 0 0.6229871 0.2939739 0.4337145 1 12.42(62)
C5 C 0 0.6937703 0.299166 0.4450391 1 12.42(62)
C6 C 0 0.7354358 0.3339941 0.3979432 1 12.42(62)
C7 C 0 0.7063247 0.3626704 0.3383728 1 12.42(62)
C8 C 0 0.6351292 0.358563 0.3275014 1 12.42(62)
OW1 O 0 0.54160(75) 0.4825(10) 0.15738(86) 0.791(21) 20.0(19)
OW2 O 0 0.42307(80) 0.48623(70) 0.08558(72) 0.431(17) 20.0(19)

p/p_0 = 0.05, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.17016(25)
_cell_length_b  19.17016(25)
_cell_length_c  19.17016(25)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7044.94(28)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.76545(21) 0.39821(20) 0.13014(24) 1 3.00(23)
O1 O   0 0.80823(39) 0.49215(56) 0.14482(56) 1 4.28(31)
O2 O   0 0.79000(48) 0.39955(53) 0.03091(45) 1 4.28(31)
O3 O   0 0.71935(45) 0.39519(65) 0.22518(31) 1 4.28(31)
O4 O   0 0.70726(60) 0.31330(30) 0.11085(53) 1 4.28(31)
O5 O   0 0.68222(68) 0.45711(57) 0.10287(85) 1 4.28(31)
O6 O   0 0.84750(68) 0.34750(68) 0.15250(68) 1 4.28(31)
C1 C   0 0.51134(44) 0.32888(57) 0.36472(56) 1 10.58(62)
C2 C   0 0.74787(51) 0.38271(74) 0.28367(54) 1 10.58(62)
C3 C   0 0.5867561 0.3262358 0.3759742 1 10.58(62)
C4 C   0 0.6149855 0.2916665 0.4328152 1 10.58(62)
```

C5 C 0 0.6858734 0.2935568 0.4445118 1 10.58(62)
C6 C 0 0.72901 0.3291297 0.3993361 1 10.58(62)
C7 C 0 0.7012329 0.3619132 0.3412664 1 10.58(62)
C8 C 0 0.6299727 0.3610981 0.3300775 1 10.58(62)
OW1 O 0 0.54828(79) 0.49358(97) 0.15946(88) 0.871(20) 20.0(17)
OW2 O 0 0.42631(61) 0.48849(52) 0.08950(58) 0.556(17) 20.0(17)

p/p_0 = 0.10, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.20555(24)
_cell_length_b  19.20555(24)
_cell_length_c  19.20555(24)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7084.03(27)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.76448(21) 0.39679(20) 0.13160(22) 1 3.00(22)
O1 O   0 0.81100(38) 0.48924(52) 0.14709(60) 1 3.53(29)
O2 O   0 0.78347(44) 0.39844(53) 0.03150(41) 1 3.53(29)
O3 O   0 0.71955(45) 0.39663(64) 0.22637(30) 1 3.53(29)
O4 O   0 0.70560(60) 0.31250(29) 0.11382(54) 1 3.53(29)
O5 O   0 0.67775(66) 0.45163(63) 0.10298(83) 1 3.53(29)
O6 O   0 0.84588(64) 0.34588(64) 0.15412(64) 1 3.53(29)
C1 C   0 0.51085(42) 0.32430(52) 0.36724(54) 1 8.50(56)
C2 C   0 0.74693(48) 0.38259(66) 0.28377(52) 1 8.50(56)
C3 C   0 0.5869887 0.3187757 0.3744242 1 8.50(56)
C4 C   0 0.6164756 0.2884775 0.4330363 1 8.50(56)
```

C5 C 0 0.6872243 0.2937491 0.4445389 1 8.50(56)
C6 C 0 0.7289982 0.3284513 0.3974461 1 8.50(56)
C7 C 0 0.700034 0.3569184 0.3377041 1 8.50(56)
C8 C 0 0.628871 0.3527327 0.3266502 1 8.50(56)
OW1 O 0 0.5617(11) 0.49575(90) 0.17559(86) 0.983(19) 20.0(13)
OW2 O 0 0.41546(68) 0.48726(44) 0.08030(62) 0.742(18) 20.0(13)

p/p_0 = 0.13, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.21997(24)
_cell_length_b  19.21997(24)
_cell_length_c  19.21997(24)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7100.00(26)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.76380(22) 0.39569(19) 0.13256(21) 1 2.96(21)
O1 O   0 0.80822(43) 0.48838(51) 0.14765(59) 1 3.26(28)
O2 O   0 0.78257(51) 0.39908(53) 0.03395(43) 1 3.26(28)
O3 O   0 0.71679(46) 0.39626(52) 0.22458(29) 1 3.26(28)
O4 O   0 0.70719(57) 0.31122(29) 0.11535(56) 1 3.26(28)
O5 O   0 0.67602(70) 0.45259(62) 0.10656(92) 1 3.26(28)
O6 O   0 0.84183(62) 0.34183(62) 0.15817(62) 1 3.26(28)
C1 C   0 0.50633(42) 0.31678(55) 0.36074(53) 1 6.93(53)
C2 C   0 0.74538(47) 0.38301(59) 0.28184(50) 1 6.93(53)
C3 C   0 0.5839994 0.3177682 0.3740928 1 6.93(53)
C4 C   0 0.6134969 0.2872282 0.432574 1 6.93(53)
```

C5 C 0 0.6841904 0.2927764 0.4442835 1 6.93(53)
C6 C 0 0.725903 0.3279992 0.3975241 1 6.93(53)
C7 C 0 0.6969401 0.3567182 0.3379021 1 6.93(53)
C8 C 0 0.6258258 0.3522509 0.3266474 1 6.93(53)
OW1 O 0 0.5669(11) 0.49073(90) 0.17673(89) 1.000(20) 20.0(13)
OW2 O 0 0.39591(59) 0.49597(48) 0.08350(90) 0.760(18) 20.0(13)
A5 O 0 0.5 0.5 0 0.628(36) 20.0(13)

p/p_0 = 0.15, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.21371(18)
_cell_length_b  19.21371(18)
_cell_length_c  19.21371(18)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7093.06(20)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75975(20) 0.39430(20) 0.13938(20) 1 1.40(18)
O1 O   0 0.81152(45) 0.48023(59) 0.15408(60) 1 3.21(27)
O2 O   0 0.77299(49) 0.39912(55) 0.04047(42) 1 3.21(27)
O3 O   0 0.71890(47) 0.39792(44) 0.23054(30) 1 3.21(27)
O4 O   0 0.70031(55) 0.31076(31) 0.12407(59) 1 3.21(27)
O5 O   0 0.67650(79) 0.45455(65) 0.11690(87) 1 3.21(27)
O6 O   0 0.83829(68) 0.33829(68) 0.16171(68) 1 3.21(27)
C1 C   0 0.50074(42) 0.30888(51) 0.36265(55) 1 4.85(50)
C2 C   0 0.74634(49) 0.37395(61) 0.28500(49) 1 4.85(50)
C3 C   0 0.5813796 0.3067528 0.3748029 1 4.85(50)
C4 C   0 0.6097793 0.2755506 0.4334776 1 4.85(50)
```

C5 C 0 0.68046 0.2797345 0.4458145 1 4.85(50)
C6 C 0 0.723241 0.3142457 0.3994917 1 4.85(50)
C7 C 0 0.6953511 0.3436193 0.3396772 1 4.85(50)
C8 C 0 0.6242662 0.3405232 0.3277937 1 4.85(50)
OW1 O 0 0.56488(94) 0.47646(85) 0.20087(83) 1.000(17) 7.62(56)
OW2 O 0 0.38339(96) 0.47135(84) 0.07262(91) 1.000(16) 7.62(56)
OW3 O 0 0.55256(79) 0.55256(79) 0.55256(79) 1.000(26) 7.62(56)
OW4 O 0 0.6448(12) 0.4527(11) 0.4970(11) 0.858(13) 7.62(56)
A5 O 0 0.5 0.5 0 0.608(38) 7.62(56)

p/p_0 = 0.21, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.21269(19)
_cell_length_b  19.21269(19)
_cell_length_c  19.21269(19)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7091.93(21)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75972(20) 0.39487(20) 0.14016(20) 1 1.42(18)

O1 O   0 0.81314(47) 0.47901(60) 0.15241(57) 1 3.56(27)
O2 O   0 0.77198(48) 0.39992(53) 0.04027(42) 1 3.56(27)
O3 O   0 0.71897(46) 0.40021(40) 0.23162(30) 1 3.56(27)
O4 O   0 0.69894(57) 0.31041(31) 0.12419(56) 1 3.56(27)
O5 O   0 0.67702(76) 0.45312(65) 0.11686(85) 1 3.56(27)
O6 O   0 0.83672(69) 0.33672(69) 0.16328(69) 1 3.56(27)
C1 C   0 0.50048(43) 0.30767(50) 0.36169(56) 1 6.11(51)
C2 C   0 0.74674(50) 0.37294(62) 0.28371(50) 1 6.11(51)
C3 C   0 0.5813397 0.307189 0.3738516 1 6.11(51)
```

C4 C 0 0.6094929 0.275607 0.4324418 1 6.11(51)
C5 C 0 0.6801759 0.2793785 0.4448976 1 6.11(51)
C6 C 0 0.7232013 0.3138546 0.3987754 1 6.11(51)
C7 C 0 0.6955503 0.3436099 0.3390388 1 6.11(51)
C8 C 0 0.624468 0.3409264 0.3270401 1 6.11(51)
OW1 O 0 0.56356(82) 0.47540(79) 0.20137(77) 1.000(16) 5.79(47)
OW2 O 0 0.38299(89) 0.46980(76) 0.07432(85) 1.000(16) 5.79(47)
OW3 O 0 0.55288(73) 0.55288(73) 0.55288(73) 1.000(25) 5.79(47)
OW4 O 0 0.64223(96) 0.45417(83) 0.50016(88) 0.992(12) 5.79(47)
A5 O 0 0.5 0.5 0 0.579(35) 5.79(47)

p/p_0 = 0.30, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.21554(19)
_cell_length_b  19.21554(19)
_cell_length_c  19.21554(19)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7095.09(22)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75917(21) 0.39443(21) 0.13990(22) 1 1.18(19)
O1 O   0 0.81262(51) 0.47748(65) 0.15121(61) 1 3.34(28)
O2 O   0 0.77160(50) 0.39971(56) 0.04097(45) 1 3.34(28)
O3 O   0 0.71794(50) 0.40189(42) 0.23074(32) 1 3.34(28)
O4 O   0 0.70033(60) 0.30811(33) 0.12448(59) 1 3.34(28)
O5 O   0 0.67736(77) 0.45086(64) 0.11695(90) 1 3.34(28)
O6 O   0 0.83467(74) 0.33467(74) 0.16533(74) 1 3.34(28)
C1 C   0 0.49785(45) 0.30802(52) 0.36042(59) 1 4.58(51)
C2 C   0 0.74405(53) 0.37419(65) 0.28351(53) 1 4.58(51)
C3 C   0 0.5787629 0.3073095 0.3729142 1 4.58(51)
C4 C   0 0.6067142 0.2752163 0.431323 1 4.58(51)
```

C5 C 0 0.6773737 0.2787566 0.443979 1 4.58(51)
C6 C 0 0.7205756 0.3135117 0.3982327 1 4.58(51)
C7 C 0 0.6931258 0.3437863 0.3386645 1 4.58(51)
C8 C 0 0.622068 0.3413312 0.3264732 1 4.58(51)
OW1 O 0 0.56444(85) 0.47596(81) 0.20224(78) 1.000(17) 4.22(46)
OW2 O 0 0.38370(92) 0.46959(78) 0.07406(87) 1.000(16) 4.22(46)
OW3 O 0 0.55388(76) 0.55388(76) 0.55388(76) 1.000(26) 4.22(46)
OW4 O 0 0.64156(97) 0.45453(85) 0.49947(89) 1.000(13) 4.22(46)
A5 O 0 0.5 0.5 0 0.584(36) 4.22(46)

p/p_0 = 0.37, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.21749(19)
_cell_length_b  19.21749(19)
_cell_length_c  19.21749(19)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7097.25(21)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75914(21) 0.39506(20) 0.14020(21) 1 1.30(18)
O1 O   0 0.81178(49) 0.47871(64) 0.15194(60) 1 3.20(27)
O2 O   0 0.77305(50) 0.39937(55) 0.04153(48) 1 3.20(27)
O3 O   0 0.72037(49) 0.40033(62) 0.23280(32) 1 3.20(27)
O4 O   0 0.69764(61) 0.31163(32) 0.12546(61) 1 3.20(27)
O5 O   0 0.67627(78) 0.45297(67) 0.11688(86) 1 3.20(27)
O6 O   0 0.83548(71) 0.33548(71) 0.16452(71) 1 3.20(27)
C1 C   0 0.49958(44) 0.30794(51) 0.36033(57) 1 4.68(50)
C2 C   0 0.74750(51) 0.37501(62) 0.28639(51) 1 4.68(50)
C3 C   0 0.5804646 0.3080629 0.3733055 1 4.68(50)
C4 C   0 0.607886 0.2740297 0.4308611 1 4.68(50)
```

C5 C 0 0.6784763 0.2768374 0.4440743 1 4.68(50)
C6 C 0 0.7221349 0.3127977 0.3997142 1 4.68(50)
C7 C 0 0.6952144 0.345047 0.3409462 1 4.68(50)
C8 C 0 0.6242276 0.3433113 0.3282287 1 4.68(50)
OW1 O 0 0.56159(83) 0.47430(84) 0.20219(79) 1.000(16) 4.81(46)
OW2 O 0 0.38670(92) 0.47244(76) 0.07582(88) 1.000(16) 4.81(46)
OW3 O 0 0.55367(75) 0.55367(75) 0.55367(75) 1.000(25) 4.81(46)
OW4 O 0 0.64064(97) 0.45303(83) 0.50019(89) 1.000(13) 4.81(46)
A5 O 0 0.5 0.5 0 0.484(36) 4.81(46)

p/p_0 = 0.42, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.21893(19)
_cell_length_b  19.21893(19)
_cell_length_c  19.21893(19)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7098.84(21)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75934(21) 0.39436(21) 0.14047(22) 1 1.76(19)
O1 O   0 0.81112(50) 0.47793(66) 0.15236(63) 1 3.09(27)
O2 O   0 0.77248(50) 0.39980(57) 0.04113(50) 1 3.09(27)
O3 O   0 0.71900(50) 0.39989(44) 0.23253(32) 1 3.09(27)
O4 O   0 0.70018(58) 0.31060(32) 0.12676(63) 1 3.09(27)
O5 O   0 0.67615(80) 0.45186(61) 0.11771(86) 1 3.09(27)
O6 O   0 0.83574(72) 0.33574(72) 0.16426(72) 1 3.09(27)
C1 C   0 0.49849(45) 0.30913(54) 0.36074(59) 1 6.13(55)
C2 C   0 0.74607(54) 0.37254(65) 0.28519(53) 1 6.13(55)
C3 C   0 0.578824 0.3084339 0.3728343 1 6.13(55)
C4 C   0 0.6058666 0.2738836 0.4302608 1 6.13(55)
```

C5 C 0 0.6764053 0.2763499 0.4438136 1 6.13(55)
C6 C 0 0.7203882 0.3124844 0.3999179 1 6.13(55)
C7 C 0 0.6938458 0.3452581 0.341268 1 6.13(55)
C8 C 0 0.6229121 0.3438615 0.3282171 1 6.13(55)
OW1 O 0 0.56276(86) 0.47278(84) 0.20192(80) 1.000(17) 4.95(47)
OW2 O 0 0.38446(93) 0.47289(76) 0.07414(90) 1.000(16) 4.95(47)
OW3 O 0 0.55260(75) 0.55260(75) 0.55260(75) 1.000(26) 4.95(47)
OW4 O 0 0.6417(10) 0.45233(83) 0.50153(88) 1.000(13) 4.95(47)
A5 O 0 0.5 0.5 0 0.508(37) 4.95(47)

p/p_0 = 0.60, adsorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.22287(18)
_cell_length_b  19.22287(18)
_cell_length_c  19.22287(18)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7103.21(20)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75919(21) 0.39448(20) 0.14064(22) 1 1.57(18)
O1 O   0 0.81173(51) 0.47783(64) 0.15050(60) 1 3.03(27)
O2 O   0 0.77337(50) 0.39952(55) 0.04097(48) 1 3.03(27)
O3 O   0 0.71984(50) 0.40064(60) 0.23338(31) 1 3.03(27)
O4 O   0 0.69966(56) 0.31112(32) 0.12614(60) 1 3.03(27)
O5 O   0 0.67355(81) 0.45183(66) 0.11795(86) 1 3.03(27)
O6 O   0 0.83560(71) 0.33560(71) 0.16440(71) 1 3.03(27)
C1 C   0 0.49879(43) 0.30852(51) 0.35899(56) 1 3.83(49)
C2 C   0 0.74641(51) 0.37312(61) 0.28626(51) 1 3.83(49)
C3 C   0 0.5797 0.3074255 0.3737047 1 3.83(49)
C4 C   0 0.6069684 0.2731283 0.4311762 1 3.83(49)
```

C5 C 0 0.6775421 0.2757622 0.4445136 1 3.83(49)
C6 C 0 0.7213355 0.3118118 0.4003593 1 3.83(49)
C7 C 0 0.6945667 0.3443288 0.3416695 1 3.83(49)
C8 C 0 0.6235976 0.3427658 0.3288312 1 3.83(49)
OW1 O 0 0.56353(83) 0.47515(83) 0.20081(78) 1.000(16) 4.29(44)
OW2 O 0 0.38573(94) 0.47166(76) 0.07361(88) 1.000(16) 4.29(44)
OW3 O 0 0.55238(73) 0.55238(73) 0.55238(73) 1.000(25) 4.29(44)
OW4 O 0 0.63974(95) 0.45476(84) 0.50180(86) 1.000(13) 4.29(44)
A5 O 0 0.5 0.5 0 0.564(36) 4.29(44)

p/p_0 = 0.20, desorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.21277(19)
_cell_length_b  19.21277(19)
_cell_length_c  19.21277(19)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7092.02(21)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75910(21) 0.39472(21) 0.13982(22) 1 1.15(18)
O1 O   0 0.81214(51) 0.47812(65) 0.15119(61) 1 2.82(28)
O2 O   0 0.77312(51) 0.39891(57) 0.04095(45) 1 2.82(28)
O3 O   0 0.71962(50) 0.39971(43) 0.23211(32) 1 2.82(28)
O4 O   0 0.69955(58) 0.31068(32) 0.12589(61) 1 2.82(28)
O5 O   0 0.67404(82) 0.45263(68) 0.11629(88) 1 2.82(28)
O6 O   0 0.83465(73) 0.33465(73) 0.16535(73) 1 2.82(28)
C1 C   0 0.49938(44) 0.30815(52) 0.35972(57) 1 4.20(52)
C2 C   0 0.74678(52) 0.37054(62) 0.28361(51) 1 4.20(52)
C3 C   0 0.5799311 0.3086081 0.3716909 1 4.20(52)
C4 C   0 0.6069754 0.2739862 0.4290735 1 4.20(52)
```

C5 C 0 0.677528 0.2763536 0.4425714 1 4.20(52)
C6 C 0 0.7215219 0.3124602 0.3986638 1 4.20(52)
C7 C 0 0.6949746 0.3453057 0.3400563 1 4.20(52)
C8 C 0 0.6240287 0.3440081 0.3270612 1 4.20(52)
OW1 O 0 0.56381(89) 0.47497(88) 0.20075(83) 1.000(17) 5.38(49)
OW2 O 0 0.3849(10) 0.47373(79) 0.07293(93) 1.000(16) 5.38(49)
OW3 O 0 0.55044(76) 0.55044(76) 0.55044(76) 1.000(26) 5.38(49)
OW4 O 0 0.6425(10) 0.45202(87) 0.50050(91) 1.000(13) 5.38(49)
A5 O 0 0.5 0.5 0 0.590(39) 5.38(49)

p/p_0 = 0.10, desorption branch

```
data_
_chemical_name_mineral Fe-MIL-59
_cell_length_a  19.20148(27)
_cell_length_b  19.20148(27)
_cell_length_c  19.20148(27)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 7079.53(30)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.76354(25) 0.39695(22) 0.13188(24) 1 2.88(27)
O1 O   0 0.80813(46) 0.48758(61) 0.14809(74) 1 3.68(35)
O2 O   0 0.78353(54) 0.40002(60) 0.03250(50) 1 3.68(35)
O3 O   0 0.72150(52) 0.39688(70) 0.22637(34) 1 3.68(35)
O4 O   0 0.70581(61) 0.31423(33) 0.11581(62) 1 3.68(35)
O5 O   0 0.67612(88) 0.45352(68) 0.1027(12) 1 3.68(35)
O6 O   0 0.84519(76) 0.34519(76) 0.15481(76) 1 3.68(35)
C1 C   0 0.50747(47) 0.32233(61) 0.36372(61) 1 8.95(69)
C2 C   0 0.74897(55) 0.37815(68) 0.28327(57) 1 8.95(69)
C3 C   0 0.5850667 0.3212017 0.3726054 1 8.95(69)
C4 C   0 0.6124279 0.2867782 0.4299572 1 8.95(69)
```

C5 C 0 0.6829917 0.2895714 0.4433145 1 8.95(69)
C6 C 0 0.726685 0.3259081 0.3992967 1 8.95(69)
C7 C 0 0.6998289 0.3585573 0.3407203 1 8.95(69)
C8 C 0 0.6288665 0.356832 0.3278659 1 8.95(69)
OW1 O 0 0.5631(16) 0.4871(12) 0.1787(12) 0.963(23) 20.0(15)
OW2 O 0 0.40264(90) 0.49283(76) 0.0712(12) 0.862(23) 20.0(15)

Capillary with Fe-MIL-59, activated for 1 h at 80 °C and 10^{-2} mbar

```
data_
_chemical_name_mineral ??????
_cell_length_a  19.00277(78)
_cell_length_b  19.00277(78)
_cell_length_c  19.00277(78)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 6862.00(84)
_symmetry_space_group_name_H-M Pa-3
loop_
_symmetry_equiv_pos_as_xyz
'-x, -y, -z'
'-x, y+1/2, -z+1/2'
'-x+1/2, -y, z+1/2'
'-x+1/2, y+1/2, z'
'-y, -z, -x'
'-y, z+1/2, -x+1/2'
'-y+1/2, -z, x+1/2'
'-y+1/2, z+1/2, x'
'-z, -x, -y'
'-z, x+1/2, -y+1/2'
'-z+1/2, -x, y+1/2'
'-z+1/2, x+1/2, y'
'z, -x+1/2, y+1/2'
'z, x, y'
'z+1/2, -x+1/2, -y'
'z+1/2, x, -y+1/2'
'y, -z+1/2, x+1/2'
'y, z, x'
'y+1/2, -z+1/2, -x'
'y+1/2, z, -x+1/2'
'x, -y+1/2, z+1/2'
'x, y, z'
'x+1/2, -y+1/2, -z'
'x+1/2, y, -z+1/2'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Fe1 Fe   0 0.75248(59) 0.38703(58) 0.14833(56) 1 6.62(52)
O1 O   0 0.8061(11) 0.4768(15) 0.1613(16) 1 9.1(11)
O2 O   0 0.7697(14) 0.3956(16) 0.04945(96) 1 9.1(11)
O3 O   0 0.7117(10) 0.3971(13) 0.23988(81) 1 9.1(11)
O4 O   0 0.6946(15) 0.29934(80) 0.1303(14) 1 9.1(11)
O5 O   0 0.6619(23) 0.4507(20) 0.1301(28) 1 9.1(11)
O6 O   0 0.8409(20) 0.3409(20) 0.1591(20) 1 9.1(11)
C1 C   0 0.49358(99) 0.3049(15) 0.3616(13) 1 7.2(10)
C2 C   0 0.7335(13) 0.3834(13) 0.3015(11) 1 7.2(10)
C3 C   0 0.5701006 0.3043155 0.3798269 1 7.2(10)
C4 C   0 0.5975801 0.2705402 0.4375066 1 7.2(10)
```

C5 C 0 0.6680549 0.2741531 0.4511344 1 7.2(10)
C6 C 0 0.7115502 0.3106666 0.4070667 1 7.2(10)
C7 C 0 0.6845994 0.3426652 0.3481757 1 7.2(10)
C8 C 0 0.6137128 0.3401191 0.3350424 1 7.2(10)
OW2 O 0 0.4906(84) 0.3787(58) 0.0387(94) 0.391(42) 20(11)