IM-17: a new zeolitic material, synthesis and structure elucidation from electron diffraction ADT data and Rietveld analysis

Yannick Lorgouilloux, Mathias Dodin, Enrico Mugnaioli, Claire Marichal, Philippe Caullet, Nicolas Bats, Ute Kolb and Jean-Louis Paillaud*

* e-mail: jean-louis.paillaud@uha.fr

Supporting informations

Tables and Figures

Table S1: Crystal and Rietveld refinement data of calcined and partially rehydrated IM-17 in space group *Cmmm*.

Chemical formula per asymmetric unit	$\|(H_2O)_{0.37}\|[Ge_{2.30}Si_{8.70}O_{22}]$[a]
Space group	*Cmmm*
λ (Å)	1.5406
a (Å)	39.0364(10)
b (Å)	22.2066(6)
c (Å)	12.6737(4)
V (Å^3)	10986.4(6)
Z	16
Temperature (K)	293
Number of data points	5057
Number of observed reflexions	2667
Number of structural parameters	240
Number of profile parameters	15
Number of restraints (bonds, angles)	140 (56, 84)
Number of constraints	65
[b] R_p	0.0574
[b] wR_p	0.0782
[b] wR_{exp}	0.0207
[b] R_F	0.0443
[b] R_F^2	0.0648
[b] χ^2	12.02
Largest difference peak and hole (ē Å^{-3})	0.463, -0.393

[a] The number of water molecules is here the number of refined oxygen atoms without other considerations.
[b] The definition of these residual values are given in the GSAS manual.[1]

[1] A. C. Larson and R. B. Von Dreele, *General Structure Analysis System (GSAS)*, Los Alamos National Laboratory Report LAUR 86-748, 2004.

Table S2: Atomic parameters of IM-17 in space group *Cmmm.* The Si13 and Si14 sites correspond to Si17 and Si18 in Table S5.

Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å^2]
Ge1	16r	1	0.762	0.04099(15)	0.06939(24)	0.3737(6)	0.0765(8)
Si1	16r	1	0.238	0.04099(15)	0.06939(24)	0.3737(6)	0.0765(8)
Si2	16r	1		0.06359(19)	0.15044(33)	0.1911(6)	0.0765(8)
Si3	8p	..m		0.04147(19)	0.0695(4)	0	0.0765(8)
Si4	16r	1	0.854	0.12151(20)	0.2307(4)	0.1266(5)	0.0765(8)
Ge4	16r	1	0.146	0.12151(20)	0.2307(4)	0.1266(5)	0.0765(8)
Si5	16r	1		0.09988(19)	0.36284(34)	0.1954(6)	0.0765(8)
Si6	16r	1	0.539	0.14046(16)	0.42895(26)	0.3761(6)	0.0765(8)
Ge6	16r	1	0.461	0.14046(16)	0.42895(26)	0.3761(6)	0.0765(8)
Si7	8p	..m		0.13702(28)	0.42793(32)	0	0.0765(8)
Si8	16r	1	0.843	0.24213(21)	0.34822(32)	0.1897(6)	0.0765(8)
Ge8	16r	1	0.157	0.24213(21)	0.34822(32)	0.1897(6)	0.0765(8)
Si9	16r	1	0.232	0.22287(16)	0.42828(25)	0.3731(5)	0.0765(8)
Ge9	16r	1	0.768	0.22287(16)	0.42828(25)	0.3731(5)	0.0765(8)
Si10	16r	1		0.19973(22)	0.2408(4)	0.1257(5)	0.0765(8)
Si11	8p	..m		0.21879(29)	0.42840(33)	0	0.0765(8)
Si12	8n	m..		0	0.2335(5)	0.1285(6)	0.0765(8)
Si13	16r	1	0.5	0.02180(21)	0.3670(5)	0.1270(6)	0.0765(8)
Si14	16r	1	0.5	0.03877(21)	0.4296(4)	0.1264(6)	0.0765(8)
O1	8q	..m		0.0430(6)	0.0909(11)	1/2	0.0284(20)
O2	8n	m..		0	0.069(1)	0.3345(17)	0.0284(20)
O3	8o	.m.		0.0581(5)	0	0.3601(26)	0.0284(20)
O4	16r	1		0.06314(31)	0.1201(5)	0.3056(9)	0.0284(20)
O5	16r	1		0.03415(19)	0.2019(5)	0.1787(10)	0.0693(20)
O6	16r	1		0.05730(35)	0.1007(5)	0.1034(5)	0.0693(20)
O7	16r	1		0.10113(26)	0.1756(5)	0.1738(13)	0.0693(20)
O8	4g	2mm		0.0521(10)	0	0	0.0693(20)
O9	4i	m2m		0	0.0757(19)	0	0.0693(20)
O10	16r	1		0.1072(4)	0.2917(4)	0.1796(13)	0.0693(20)
O11	16r	1		0.16127(23)	0.2227(6)	0.1542(14)	0.0693(20)
O12	8p	..m		0.1162(6)	0.2320(11)	0	0.0693(20)
O13	16r	1		0.11483(33)	0.3848(6)	0.3077(9)	0.0693(20)
O14	16r	1		0.11947(32)	0.3985(5)	0.1034(5)	0.0693(20)
O15	16r	1		0.05893(21)	0.3751(4)	0.1873(12)	0.0693(20)
O16	16r	1		0.2108(4)	0.3005(6)	0.1900(12)	0.0693(20)
O17	8p	..m		0.2032(6)	0.2522(10)	0	0.0693(20)
O18	16r	1		0.22323(34)	0.1857(7)	0.1594(13)	0.0693(20)
O19	8q	..m		0.1368(6)	0.4078(12)	1/2	0.0693(20)
O20	8o	.m.		0.1287(5)	1/2	0.3646(26)	0.0693(20)
O21	16r	1		0.18109(19)	0.4208(9)	0.3405(14)	0.0693(20)
O22	8p	..m		0.17794(27)	0.4149(13)	0	0.0693(20)
O23	4g	2mm		0.1308(8)	1/2	0	0.0693(20)
O24	16r	1		0.24664(32)	0.3804(6)	0.3030(9)	0.0693(20)
O25	16r	1		0.23591(33)	0.3994(5)	0.1035(5)	0.0693(20)
O26	8o	.m.		0.2354(5)	1/2	0.3528(26)	0.0693(20)
O27	8q	..m		0.2283(6)	0.4109(13)	1/2	0.0693(20)
O28	4g	2mm		0.2253(9)	1/2	0	0.0693(20)
O29	8n	m..		0	0.3056(5)	0.1576(20)	0.0693(20)
O30	4i	m2m		0	0.2244(14)	0	0.0693(20)
O31	8p	..m	0.5	0.0276(7)	0.3682(15)	0	0.0693(20)
O32	8n	m..	0.5	0	0.4248(6)	0.1612(19)	0.0693(20)
O33	8o	.m.		0.0511(5)	1/2	0.1561(26)	0.0693(20)
O34	8p	..m	0.5	0.0414(8)	0.4182(15)	0	0.0693(20)
Ow1	16r	1	0.374	0.1654(21)	0.0556(27)	0.407(7)	0.1250

Table S3: Selected bond distances (Å) and angles (°) for IM-17 in space group *Cmmm.*

Ge1|Si1	O4	1.6615(130)	O1	1.6723(103)	106.213(557)
	O4	1.6615(130)	O2	1.6755(88)	110.271(528)
	O4	1.6615(130)	O3	1.6883(100)	111.081(491)
	O1	1.6723(103)	O2	1.6755(88)	109.275(373)
	O1	1.6723(103)	O3	1.6883(100)	109.869(337)
	O2	1.6755(88)	O3	1.6883(100)	110.050(318)
Ge9|Si9	O27	1.6675(97)	O24	1.6676(139)	107.190(523)
	O27	1.6675(97)	O26	1.6858(94)	109.207(328)
	O27	1.6675(97)	O21	1.6906(106)	109.609(578)
	O24	1.6676(139)	O26	1.6858(94)	111.077(556)
	O24	1.6676(139)	O21	1.6906(106)	110.117(633)
	O26	1.6858(94)	O21	1.6906(106)	109.598(524)
Si2	O7	1.5836(128)	O6	1.5861(118)	106.974(769)
	O7	1.5836(128)	O4	1.6000(136)	106.517(791)
	O7	1.5836(128)	O5	1.6283(120)	113.089(635)
	O6	1.5861(118)	O4	1.6000(136)	109.914(647)
	O6	1.5861(118)	O5	1.6283(120)	108.170(724)
	O4	1.6000(136)	O5	1.6283(120)	112.044(727)
Si3	O8	1.5982(134)	O6	1.606(10)	108.464(377)
	O8	1.5982(134)	O6	1.606(10)	108.464(377)
	O8	1.5982(134)	O9	1.6247(82)	109.910(461)
	O6	1.606(10)	O6	1.606(10)	109.369(334)
	O6	1.606(10)	O9	1.6247(82)	110.294(442)
	O6	1.606(10)	O9	1.6247(82)	110.294(442)
Si4|Ge4	O7	1.5773(144)	O11	1.6009(124)	108.666(705)
	O7	1.5773(144)	O10	1.6119(142)	108.607(740)
	O7	1.5773(144)	O12	1.6181(71)	108.983(702)
	O11	1.6009(124)	O10	1.6119(142)	109.767(798)
	O11	1.6009(124)	O12	1.6181(71)	110.050(662)
	O10	1.6119(142)	O12	1.6181(71)	110.722(677)
Si5	O14	1.6036(120)	O13	1.6137(140)	108.639(648)
	O14	1.6036(120)	O10	1.6179(120)	107.938(705)
	O14	1.6036(120)	O15	1.6248(111)	109.907(700)
	O13	1.6137(140)	O10	1.6179(120)	109.900(776)
	O13	1.6137(140)	O15	1.6248(111)	111.155(734)
	O10	1.6179(120)	O15	1.6248(111)	109.242(709)
Si6|Ge6	O19	1.6452(108)	O13	1.6473(142)	106.237(569)
	O19	1.6452(108)	O20	1.6497(85)	109.463(361)
	O19	1.6452(108)	O21	1.6589(109)	108.148(629)
	O13	1.6473(142)	O20	1.6497(85)	110.715(572)
	O13	1.6473(142)	O21	1.6589(109)	111.878(649)
	O20	1.6497(85)	O21	1.6589(109)	110.266(542)

Si7	O14	1.6167(102)	O14	1.6167(102)	108.303(333)
	O14	1.6167(102)	O23	1.6187(86)	109.640(373)
	O14	1.6167(102)	O22	1.6234(159)	110.177(410)
	O14	1.6167(102)	O23	1.6187(86)	109.640(373)
	O14	1.6167(102)	O22	1.6234(159)	110.177(410)
	O23	1.6187(86)	O22	1.6234(159)	108.894(854)
Si8|Ge8	O18	1.5948(161)	O25	1.5950(118)	107.499(828)
	O18	1.5948(161)	O24	1.6136(140)	109.327(851)
	O18	1.5948(161)	O16	1.6182(166)	109.395(875)
	O25	1.5950(118)	O24	1.6136(140)	108.093(651)
	O25	1.5950(118)	O16	1.6182(166)	110.681(766)
	O24	1.6136(140)	O16	1.6182(166)	111.739(815)
Si10	O18	1.5878(172)	O11	1.5956(131)	106.774(784)
	O18	1.5878(172)	O16	1.6151(163)	110.014(905)
	O18	1.5878(172)	O17	1.6188(76)	109.688(719)
	O11	1.5956(131)	O16	1.6151(163)	110.140(849)
	O11	1.5956(131)	O17	1.6188(76)	109.932(682)
	O16	1.6151(163)	O17	1.6188(76)	110.231(662)
Si11	O25	1.6069(103)	O25	1.6069(103)	109.439(333)
	O25	1.6069(103)	O28	1.6102(93)	109.276(375)
	O25	1.6069(103)	O22	1.6226(162)	109.554(424)
	O25	1.6069(103)	O28	1.6102(93)	109.276(375)
	O25	1.6069(103)	O22	1.6226(162)	109.554(424)
	O28	1.6102(93)	O22	1.6226(162)	109.728(856)
Si12	O5	1.6353(107)	O5	1.6353(107)	109.210(381)
	O5	1.6353(107)	O30	1.6411(86)	109.466(422)
	O5	1.6353(107)	O29	1.6430(164)	109.319(377)
	O5	1.6353(107)	O30	1.6411(86)	109.466(422)
	O5	1.6353(107)	O29	1.6430(164)	109.319(377)
	O30	1.6411(86)	O29	1.6430(164)	110.045(849)
Si13	O32	1.5999(161)	O31	1.6256(85)	109.219(477)
	O32	1.5999(161)	O15	1.6484(130)	104.748(564)
	O32	1.5999(161)	O29	1.6534(150)	108.923(637)
	O31	1.6256(85)	O15	1.6484(130)	109.559(680)
	O31	1.6256(85)	O29	1.6534(150)	108.508(473)
	O15	1.6484(130)	O29	1.6534(150)	115.710(597)
Si14	O32	1.5800(106)	O34	1.6251(94)	108.976(455)
	O32	1.5800(106)	O15	1.6370(135)	106.201(554)
	O32	1.5800(106)	O33	1.6785(128)	105.957(475)
	O34	1.6251(94)	O15	1.6370(135)	108.617(688)
	O34	1.6251(94)	O33	1.6785(128)	110.367(462)
	O15	1.6370(135)	O33	1.6785(128)	116.423(605)

Table S4: Details on data collection and structure solution for IM-17 from ADT in *Cm2m* setting of space group *Amm2*.

Diffractometer	Tecnai F30 S-TWIN TEM
λ (Å)	0.01970
Temperature (K)	295(2)
Tilt range (°)	–60 / +60
h, k, l	$-10 \le h \le 10$, $-20 \le k \le 20$, $-35 \le l \le 35$
Measured independent reflections	1866
Completeness (%)	77
Resolution (Å)	1.10
R_{sym} (%)	19.99
Overall U(iso) (Å^2)	0.02405
Structure solution method	Direct methods by SIR2011[2]
R (%)	27.19
Structure refinement method	least-squares refinement on F^2
Independent reflections	1343
Independent reflections (> 4σ)	1121
Refined parameters	35
Constraints / restraints	2 / 21
R indices ($Fo^2 \ge 2\sigma\ (Fo)^2$)	$R_1 = 0.276$, $wR_2 = 0.649$
R indices (all data)	$R1 = 0.290$, $wR_2 = 0.642$
GoF	2.192
Weighting scheme	$w^{-1} = \sigma^2 F_o^2 + (0.2000P)^2$ with $P = (F_o^2 + 2F_c^2)/3$
Max. / min. residual electron density (e Å^{-3})	0.588 / -0.516

[2] M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, M. Mallamo, A. Mazzone, G. Polidori and R. Spagna, *J. Appl. Crystallogr.*, 2012, **45**, 357-361.

Table S5: The Shelx file produced by Sir2011 for IM-17 from ADT, *Cm2m* setting of space group *Amm2*. The Si17 and Si18 sites correspond to Si13 and Si14 in Table S2.

```
REM
REM  Shelx file produced by Sir2011 on Fri Nov 29  2013 at
16:42:07
REM  Structure name: IM-17
REM
TITL    IM17
CELL   0.01970    22.1420  38.8050  12.6710  90.0000  90.0000
90.0000
ZERR        8    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
LATT -7
SYMM -X,Y,-Z
SYMM -X,Y,Z
SYMM X,Y,-Z
REM  ------ Electron scattering factors ------
REM  SFAC Species a(1) b(1) a(2) b(2) a(3) b(3) =
REM  a(4) b(4) c f' f'' mu cov_radius weight
SFAC O      0.45480  23.78030   0.91730   7.62200   0.47190
2.14400 =
         0.13840   0.29590   0.00000   0.000   0.000   0.000   0.730
15.999
SFAC SI     2.12930  57.77480   2.53330  16.47560   0.83490
2.87960 =
         0.32160   0.38600   0.00000   0.000   0.000   0.000   1.110
28.086
UNIT 352 176
L.S.    30
FMAP      -2
PLAN     25
MERG
BOND
SHEL 99 1.1
WGHT    0.100000
FVAR       0.21039
SI1   2    0.26763    0.56509    0.37949    1.00000   0.03822
SI2   2    0.34651    0.30418    0.29619    1.00000   0.11789
SI3   2    0.34777    0.42928    0.30733    1.00000   0.12333
SI4   2    0.26493    0.24540    0.41569    1.00000   0.14845
SI5   2    0.13257    0.47124    0.32575    1.00000   0.05566
SI6   2    0.43135    0.72418    0.14280    1.00000   0.14638
SI7   2    0.15658    0.13215    0.30614    1.00000   0.12282
SI8   2    0.35632    0.10373    0.32141    1.00000   0.14568
SI9   2    0.12444    0.24666    0.20967    1.00000   0.17464
SI10  2    0.24073    0.65816    0.42598    1.00000   0.15312
SI11  2    0.42815    0.64579    0.08989    1.00000   0.20335
SI12  2    0.27014    0.36285    0.42085    1.00000   0.15960
SI13  2    0.43485    0.32303    0.10524    1.00000   0.27619
SI14  2    0.06380    0.49518    0.07055    1.00000   0.23447
SI15  2    0.42149    0.40291    0.16798    1.00000   0.17896
SI16  2    0.26192    0.48198    0.37997    1.00000   0.13623
O1    1    0.28481    0.65352    0.33050    1.00000   0.14774
O2    1    0.20504    0.47177    0.31349    1.00000   0.04491
O3    1    0.40468    0.72981    0.36862    1.00000   0.13569
O4    1    0.40289    0.41214    0.39886    1.00000   0.22575
O5    1    0.06542    0.18427    0.11670    1.00000   0.16679
O6    1    0.26220    0.19251    0.33767    1.00000   0.13743
O7    1    0.38228    0.08523    0.20513    1.00000   0.25409
O8    1    0.30351    0.46273    0.32898    1.00000   0.08897
O9    1    0.39860    0.63905    0.40623    1.00000   0.16286
O10   1    0.37497    0.30614    0.39932    1.00000   0.18242
Si17  2    0.12178    0.30687    0.34872    1.00000   0.12218
O11   1    0.29675    0.33836    0.26228    1.00000   0.14885
O12   1    0.43439    0.05393    0.09766    1.00000   0.40939
O13   1    0.43893    0.37093    0.11900    1.00000   0.25431
O14   1    0.30262    0.26388    0.28422    1.00000   0.20423
O15   1    0.22288    0.57935    0.36996    1.00000   0.21834
SI18  2    0.06519    0.40378    0.40136    1.00000   0.07418
O16   1    0.28366    0.40855    0.36756    1.00000   0.09974
O17   1    0.27100    0.52700    0.32700    1.00000   0.00000
SI19  2    0.43700    0.09800    0.10700    1.00000   0.00000
SI20  2    0.42866    0.72375    0.50000    0.50000   0.03770
SI21  2    0.43244    0.40518    0.50000    0.50000   0.05789
SI22  2    0.43111    0.32124    0.50000    0.50000   0.09135
SI23  2    0.43107    0.64750    0.50000    0.50000   0.09233
SI24  2    0.07508    0.50219    0.50000    0.50000   0.12004
SI25  2    0.07087    0.58952    0.50000    0.50000   0.08330
O18   1    0.26212    0.46370    0.50000    0.50000   0.19610
O19   1    0.13328    0.31323    0.50000    0.50000   0.19610
O20   1    0.05322    0.54274    0.50000    0.50000   0.14317
O21   1    0.42300    0.37100    0.50000    0.50000   0.00000
O22   1    0.44566    0.72841    0.00000    0.50000   0.26490
O23   1    0.42477    0.41646    0.00000    0.50000   0.26930
O24   1    0.42300    0.09600    0.00000    0.50000   0.00000
O25   1    0.50000    0.41338    0.50000    0.25000   0.19610
O26   1    0.50000    0.73225    0.50000    0.25000  -0.02822
O27   1    0.50000    0.30700    0.50000    0.25000   0.00000
O28   1    0.50000    0.66641    0.09660    0.50000   0.01688
O29   1    0.50000    0.34689    0.12945    0.50000   0.25991
O30   1    0.00000    0.49500    0.15200    0.50000   0.00000
O31   1    0.00000    0.59788    0.50000    0.25000   0.04522
O32   1    0.00000    0.49327    0.50000    0.25000   0.03906
HKLF 4
END
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Table S6: Atomic parameters of IM-17 after the final Rietveld refinment in space group *Amm2*.

Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å^2]
SI1	4d	m..		0	0.4292(5)	0.8624(9)	0.0711(7)
SI2	4d	m..		0	0.4300(5)	0.9444(9)	0.0711(7)
SI3	8f	1		0.1887(11)	0.3470(6)	0.8396(6)	0.0711(7)
SI4	8f	1	0.762	0.191(1)	0.3520(5)	0.9672(6)	0.0711(7)
SI5	8f	1	0.44	0.3695(10)	0.4305(5)	0.86112	0.0711(7)
SI6	8f	1	0.929	0.1262(8)	0.2705(6)	0.9045(7)	0.0711(7)
SI7	8f	1		0.1232(9)	0.2616(7)	0.7852(6)	0.0711(7)
SI8	8f	1	0.11	0.3764(12)	0.4290(4)	0.94285(34)	0.0711(7)
SI9	8f	1	0.773	0.1258(8)	0.2686(7)	1.0268(6)	0.0711(7)
SI10	8f	1		0.1222(8)	0.1378(7)	0.9298(6)	0.0711(7)
SI11	8f	1		0.1965(9)	0.1328(6)	0.8027(7)	0.0711(7)
SI12	8f	1	0.927	0.1211(9)	0.2547(8)	0.7040(6)	0.0711(7)
SI13	8f	1		0.1936(10)	0.1387(6)	1.0048(6)	0.0711(7)
SI14	8f	1		0.1257(8)	0.2626(8)	1.1047(7)	0.0711(7)
SI15	8f	1		0.1212(10)	0.0712(5)	0.8660(6)	0.0711(7)
SI16	8f	1	0.69	0.3801(12)	0.0714(6)	0.7644(6)	0.0711(7)
SI17	4d	m..		0	0.0691(7)	0.7662(8)	0.0711(7)
SI18	8f	1	0.791	0.1899(10)	0.1505(6)	0.6623(7)	0.0711(7)
SI19	8f	1		0.1848(11)	0.3468(6)	0.6479(7)	0.0711(7)
SI20	8f	1	0.3	0.3716(11)	0.0723(5)	1.0442(6)	0.0711(7)
SI21	4d	m..		0	0.0710(7)	1.0404(8)	0.0711(7)
SI22	8f	1	0.336	0.3741(10)	0.0714(6)	0.6829(6)	0.0711(7)
SI23	4d	m..		0	0.0688(8)	0.6838(8)	0.0711(7)
SI25	4d	m..		0	0.4288(7)	0.6228(8)	0.0711(7)
O1	2a	mm2		0	1/2	0.8540(14)	0.0604(20)
O2	4d	m..		0	0.4192(19)	0.9034(9)	0.0604(20)
O3	8f	1		0.1027(7)	0.3985(7)	0.8461(10)	0.0604(20)
O4	2a	mm2		0	1/2	0.9520(15)	0.0604(20)
O5	8f	1		0.1026(7)	0.4010(7)	0.9613(9)	0.0604(20)
O6	8f	1		0.3034(13)	0.3771(9)	0.8399(6)	0.0604(20)
O7	8f	1		0.1776(26)	0.2945(10)	0.8686(8)	0.0604(20)
O8	8f	1		0.1698(23)	0.3202(9)	0.8024(7)	0.0604(20)
O9	8f	1		0.3036(12)	0.3836(10)	0.9673(5)	0.0604(20)
O10	8f	1		0.1821(25)	0.3038(11)	0.9366(8)	0.0604(20)
O11	8f	1		0.1715(22)	0.3216(10)	1.0038(8)	0.0604(20)
O12	4e	m..		1/2	0.4157(24)	0.8581(8)	0.0604(20)
O13	8f	1		0.3325(18)	0.4284(11)	0.90241(28)	0.0604(20)
O14	4c	.m.		0.345(5)	1/2	0.8444(6)	0.0604(20)
O15	8f	1		0.1466(27)	0.1998(7)	0.9095(8)	0.0604(20)
O16	4d	m..		0	0.2831(17)	0.9047(13)	0.0604(20)
O17	4d	m..		0	0.2564(19)	0.7947(12)	0.0604(20)
O18	8f	1		0.1853(19)	0.2045(7)	0.8001(8)	0.0604(20)
O19	8f	1		0.1372(32)	0.2665(11)	0.7443(6)	0.0604(20)
O20	4c	.m.		0.373(5)	1/2	0.9589(7)	0.0604(20)
O21	4e	m..		1/2	0.4035(20)	0.9433(9)	0.0604(20)
O22	4d	m..		0	0.2657(19)	1.0227(12)	0.0604(20)
O23	8f	1		0.1771(21)	0.2076(7)	1.0142(8)	0.0604(20)
O24	8f	1		0.1557(31)	0.2790(11)	1.0660(7)	0.0604(20)
O25	8f	1		0.1513(22)	0.0835(9)	0.9051(7)	0.0604(20)
O26	4d	m..		0	0.1340(18)	0.9394(10)	0.0604(20)
O27	8f	1		0.1889(18)	0.1314(11)	0.9642(7)	0.0604(20)
O28	8f	1		0.3070(12)	0.1123(11)	0.7877(8)	0.0604(20)
O29	8f	1		0.1035(7)	0.1016(7)	0.7812(9)	0.0604(20)
O30	8f	1		0.1918(18)	0.1129(10)	0.8419(7)	0.0604(20)
O31	4d	m..		0	0.2392(17)	0.6964(12)	0.0604(20)
O32	8f	1		0.1932(17)	0.1991(9)	0.6926(8)	0.0604(20)
O33	8f	1		0.1533(23)	0.3138(10)	0.6828(8)	0.0604(20)
O34	8f	1		0.3056(13)	0.1175(10)	1.0180(7)	0.0604(20)
O35	8f	1		0.1029(7)	0.1007(9)	1.0233(8)	0.0604(20)
O36	4d	m..		0	0.2543(18)	1.1082(13)	0.0604(20)
O37	8f	1		0.1862(20)	0.2022(9)	1.1173(8)	0.0604(20)
O38	8f	1		0.1621(22)	0.3169(10)	1.1277(8)	0.0604(20)

O39	4c	.m.		0.140(4)	0	0.8580(9)	0.0604(20)
O40	4d	m..		0	0.0880(22)	0.8595(10)	0.0604(20)
O41	8f	1		0.3564(35)	0.0862(20)	0.7248(6)	0.0604(20)
O42	4e	m..		1/2	0.0882(28)	0.7728(13)	0.0604(20)
O43	4c	.m.		0.359(5)	0	0.7725(14)	0.0604(20)
O44	4d	m..		0	0.0724(29)	0.7250(8)	0.0604(20)
O45	2a	mm2		0	0	0.7776(17)	0.0604(20)
O46	8f	1		0.3013(13)	0.1176(9)	0.6588(7)	0.0604(20)
O47	8f	1		0.1023(7)	0.1016(7)	0.6693(9)	0.0604(20)
O48	8f	1		0.2968(13)	0.3791(10)	0.6525(7)	0.0604(20)
O49	8f	1		0.1016(7)	0.3980(8)	0.6394(9)	0.0604(20)
O50	4e	m..		1/2	0.0891(26)	1.0408(12)	0.0604(20)
O51	8f	1		0.3334(25)	0.0831(18)	1.0853(6)	0.0604(20)
O52	4c	.m.		0.351(5)	0	1.0326(11)	0.0604(20)
O53	2a	mm2		0	0	1.0326(19)	0.0604(20)
O54	4d	m..		0	0.0814(31)	1.0816(8)	0.0604(20)
O55	4e	m..		1/2	0.0813(23)	0.6726(13)	0.0604(20)
O56	4c	.m.		0.339(4)	0	0.6748(14)	0.0604(20)
O57	2a	mm2		0	0	0.6717(16)	0.0604(20)
O58	4c	.m.		0.361(5)	1/2	0.6393(11)	0.0604(20)
O59	4e	m..		1/2	0.4020(21)	0.6312(11)	0.0604(20)
O60	2a	mm2		0	1/2	0.6312(18)	0.0604(20)
GE4	8f	1	0.238	0.191(1)	0.3520(5)	0.9672(6)	0.0711(7)
GE5	8f	1	0.56	0.3695(10)	0.4305(5)	0.86112	0.0711(7)
GE6	8f	1	0.071	0.1262(8)	0.2705(6)	0.9045(7)	0.0711(7)
GE8	8f	1	0.89	0.3764(12)	0.4290(4)	0.94285(34)	0.0711(7)
GE9	8f	1	0.227	0.1258(8)	0.2686(7)	1.0268(6)	0.0711(7)
GE12	8f	1	0.073	0.1211(9)	0.2547(8)	0.7040(6)	0.0711(7)
GE16	8f	1	0.31	0.3801(12)	0.0714(6)	0.7644(6)	0.0711(7)
GE18	8f	1	0.209	0.1899(10)	0.1505(6)	0.6623(7)	0.0711(7)
GE20	8f	1	0.7	0.3716(11)	0.0723(5)	1.0442(6)	0.0711(7)
GE22	8f	1	0.664	0.3741(10)	0.0714(6)	0.6829(6)	0.0711(7)
GE24	8f	1		0.3717(10)	0.4244(5)	0.6273(6)	0.0711(7)
Ow1	4e	m..	1.16	1/2	0.245(4)	0.2059(21)	0.1250
Ow2	4e	m..	1.17	1/2	0.436(4)	0.0424(18)	0.1250
Ow3	2b	mm2	0.71	1/2	1/2	0.305(5)	0.1250
Ow4	2b	mm2	1.02	1/2	1/2	0.6974(35)	0.1250
Ow5	8f	1	0.8	0.157(7)	0.613(4)	0.7205(18)	0.1250

Table S7: Selected bond distances (Å) and angles (°) for IM-17 in space group *Amm2*.

SI1	O3	1.60(2)	O3	1.60(2)	108.8(5)	SI13	O34	1.58(2)	O23	1.59(2)	109.3(13)
	O3	1.60(2)	O1	1.61(2)	109.6(5)		O34	1.58(2)	O27	1.60(4)	109.1(16)
	O3	1.60(2)	O2	1.62(5)	109.6(10)		O34	1.58(2)	O35	1.60(2)	109.9(10)
	O3	1.60(2)	O1	1.61(2)	109.6(5)		O23	1.59(2)	O27	1.60(4)	108.9(16)
	O3	1.60(2)	O2	1.62(5)	109.6(10)		O23	1.59(2)	O35	1.60(2)	108.0(13)
	O1	1.61(2)	O2	1.62(5)	109.7(17)		O27	1.60(4)	O35	1.60(2)	111.6(17)
SI2	O4	1.58(2)	O5	1.59(2)	108.6(5)	SI14	O38	1.57(3)	O24	1.60(4)	107.2(21)
	O4	1.58(2)	O5	1.59(2)	108.6(5)		O38	1.57(3)	O36	1.61(1)	109.2(12)
	O4	1.58(2)	O2	1.62(5)	109.3(17)		O38	1.57(3)	O37	1.62(3)	108.8(15)
	O5	1.59(2)	O5	1.59(2)	109.3(5)		O24	1.60(4)	O36	1.61(1)	110.0(15)
	O5	1.59(2)	O2	1.62(5)	110.5(9)		O24	1.60(4)	O37	1.62(3)	111.2(18)
	O5	1.59(2)	O2	1.62(5)	110.5(9)		O36	1.61(1)	O37	1.62(3)	110.3(11)
SI3	O8	1.59(3)	O6	1.60(2)	107.5(15)	SI15	O30	1.60(3)	O25	1.60(4)	109.3(18)
	O8	1.59(3)	O3	1.60(2)	108.1(15)		O30	1.60(3)	O40	1.60(2)	108.0(11)
	O8	1.59(3)	O7	1.63(3)	110.7(19)		O30	1.60(3)	O39	1.63(2)	111.6(10)
	O6	1.60(2)	O3	1.60(2)	108.6(10)		O25	1.60(4)	O40	1.60(2)	109.9(13)
	O6	1.60(2)	O7	1.63(3)	111.8(15)		O25	1.60(4)	O39	1.63(2)	108.3(11)
	O3	1.60(2)	O7	1.63(3)	110.0(13)		O40	1.60(2)	O39	1.63(2)	109.6(7)
SI4|GE4	O5	1.58(2)	O9	1.59(2)	109.5(10)	SI16|GE16	O28	1.59(3)	O42	1.60(2)	107.7(10)
	O5	1.58(2)	O11	1.60(4)	108.2(15)		O28	1.59(3)	O41	1.61(3)	109.0(20)
	O5	1.58(2)	O10	1.61(3)	107.5(13)		O28	1.59(3)	O43	1.64(2)	110.4(12)
	O9	1.59(2)	O11	1.60(4)	108.8(14)		O42	1.60(2)	O41	1.61(3)	109.1(17)
	O9	1.59(2)	O10	1.61(3)	111.0(15)		O42	1.60(2)	O43	1.64(2)	110.0(8)
	O11	1.60(4)	O10	1.61(3)	111.8(20)		O41	1.61(3)	O43	1.64(2)	110.6(16)
GE5|SI5	O6	1.67(2)	O13	1.68(1)	108.4(9)	SI17	O45	1.60(3)	O29	1.61(2)	109.3(5)
	O6	1.67(2)	O12	1.69(2)	108.5(6)		O45	1.60(3)	O29	1.61(2)	109.3(5)
	O6	1.67(2)	O14	1.71(2)	111.2(7)		O45	1.60(3)	O44	1.61(4)	108.8(21)
	O13	1.68(1)	O12	1.69(2)	109.6(7)		O29	1.61(2)	O29	1.61(2)	109.4(5)
	O13	1.68(1)	O14	1.71(2)	110.0(5)		O29	1.61(2)	O44	1.61(4)	110.1(9)
	O12	1.69(2)	O14	1.71(2)	109.13(8)		O29	1.61(2)	O44	1.61(4)	110.1(9)
SI6|GE6	O15	1.60(2)	O10	1.62(4)	106.4(14)	SI18|GE18	O38	1.57(4)	O47	1.58(2)	108.0(15)
	O15	1.60(2)	O16	1.62(1)	109.1(11)		O38	1.57(4)	O46	1.60(2)	109.6(15)
	O15	1.60(2)	O7	1.64(4)	111.1(14)		O38	1.57(4)	O32	1.60(3)	109.3(21)
	O10	1.62(4)	O16	1.62(1)	110.4(13)		O47	1.58(2)	O46	1.60(2)	108.8(10)
	O10	1.62(4)	O7	1.64(4)	109.9(21)		O47	1.58(2)	O32	1.60(3)	110.8(13)
	O16	1.62(1)	O7	1.64(4)	109.9(13)		O46	1.60(2)	O32	1.60(4)	110.4(14)
SI7	O8	1.58(3)	O18	1.60(3)	108.3(13)	SI19	O49	1.59(2)	O33	1.60(4)	110.0(16)
	O8	1.58(3)	O17	1.61(2)	108.9(12)		O49	1.59(2)	O48	1.60(2)	107.0(11)
	O8	1.58(3)	O19	1.61(3)	109.0(18)		O49	1.59(2)	O37	1.62(3)	109.6(13)
	O18	1.60(3)	O17	1.61(2)	109.7(11)		O33	1.60(4)	O48	1.60(2)	109.4(15)
	O18	1.60(3)	O19	1.61(3)	111.1(17)		O33	1.60(4)	O37	1.62(3)	108.9(21)
	O17	1.61(2)	O19	1.61(3)	109.9(15)		O48	1.60(2)	O37	1.62(3)	112.0(16)
GE8|SI8	O21	1.67(2)	O9	1.67(2)	108.0(10)	GE20|SI20	O34	1.66(3)	O50	1.68(2)	107.8(10)
	O21	1.67(2)	O13	1.67(2)	108.6(10)		O34	1.66(3)	O52	1.69(2)	109.4(10)
	O21	1.67(2)	O20	1.70(1)	109.6(6)		O34	1.66(3)	O51	1.69(3)	110.8(17
	O9	1.67(2)	O13	1.67(2)	110.6(11)		O50	1.68(2)	O52	1.69(2)	109.9(7)
	O9	1.67(2)	O20	1.70(1)	109.7(9)		O50	1.69(2)	O51	1.69(3)	108.7(14)
	O13	1.67(2)	O20	1.70(1)	110.3(8)		O52	1.69(2)	O51	1.69(3)	110.2(14)
SI9|GE9	O23	1.58(3)	O11	1.59(3)	108.0(14)	SI21	O53	1.61(2)	O35	1.61(2)	108.9(6)
	O23	1.58(3)	O24	1.59(4)	109.0(17)		O53	1.61(2)	O35	1.61(2)	108.9(6)
	O23	1.58(3)	O22	1.60(1)	110.1(11)		O53	1.61(2)	O54	1.63(4)	109.1(22)
	O11	1.59(3)	O24	1.59(4)	110.4(19)		O35	1.61(2)	O35	1.61(2)	108.5(5)
	O11	1.59(3)	O22	1.60(1)	109.6(12)		O35	1.61(2)	O54	1.63(4)	110.7(9)
	O24	1.59(4)	O22	1.60(1)	109.8(15)		O35	1.61(2)	O54	1.63(4)	110.7(9)
SI10	O25	1.59(3)	O27	1.59(3)	108.7(18)	GE22|SI22	O55	1.66(2)	O46	1.67(3)	108.2(9)
	O25	1.59(3)	O26	1.60(1)	109.1(12)		O55	1.66(2)	O56	1.68(2)	109.5(7)
	O25	1.59(3)	O15	1.62(3)	107.7(13)		O55	1.66(2)	O41	1.68(3)	109.7(15)
	O27	1.59(3)	O26	1.60(1)	108.2(10)		O46	1.67(3)	O56	1.68(2)	109.2(10)
	O27	1.59(3)	O15	1.62(3)	112.8(17)		O46	1.67(3)	O41	1.68(3)	110.7(18)
	O26	1.60(1)	O15	1.62(3)	110.2(13)		O56	1.68(2)	O41	1.68(3)	109.4(15)
SI11	O28	1.59(2)	O30	1.59(4)	107.9(17)	SI23	O47	1.59(2)	O47	1.59(2)	109.1(5)
	O28	1.59(2)	O18	1.60(2)	109.9(13)		O47	1.59(2)	O57	1.60(3)	109.4(5)
	O28	1.59(2)	O29	1.61(3)	109.4(9)		O47	1.59(2)	O44	1.61(4)	109.4(9)
	O30	1.59(4)	O18	1.60(2)	109.5(15)		O47	1.59(2)	O57	1.60(3)	109.4(5)
	O30	1.59(4)	O29	1.61(3)	110.8(18)		O47	1.59(2)	O44	1.61(4)	109.4(9)
	O18	1.60(2)	O29	1.61(3)	109.3(12)		O57	1.60(3)	O44	1.61(4)	110.0(21)
SI12|GE12	O32	1.60(3)	O31	1.60(2)	109.3(10)	GE24	O48	1.70(3)	O59	1.71(2)	108.0(9)
	O32	1.60(3)	O33	1.61(3)	110.0(15)		O48	1.70(3)	O51	1.72(3)	109.7(17)
	O32	1.60(3)	O19	1.61(3)	109.0(18)		O48	1.70(3)	O58	1.75(2)	111.7(10)
	O31	1.60(2)	O33	1.61(3)	108.9(13)		O59	1.71(2)	O51	1.72(3)	109.0(13)
	O31	1.60(2)	O19	1.61(3)	109.8(15)		O59	1.71(2)	O58	1.75(2)	109.3(6)
	O33	1.61(3)	O19	1.61(3)	109.8(19)		O51	1.72(3)	O58	1.75(2)	109.1(14)

SI25	O49	1.60(2)	O49	1.60(2)	107.6(5)	O49	1.60(2)	O54	1.63(5)	110.0(9)
	O49	1.60(2)	O60	1.62(2)	109.7(6)	O60	1.62(2)	O54	1.63(5)	109.7(21)
	O49	1.60(2)	O54	1.63(4)	110.0(9)					
	O49	1.60(2)	O60	1.62(2)	109.7(6)					

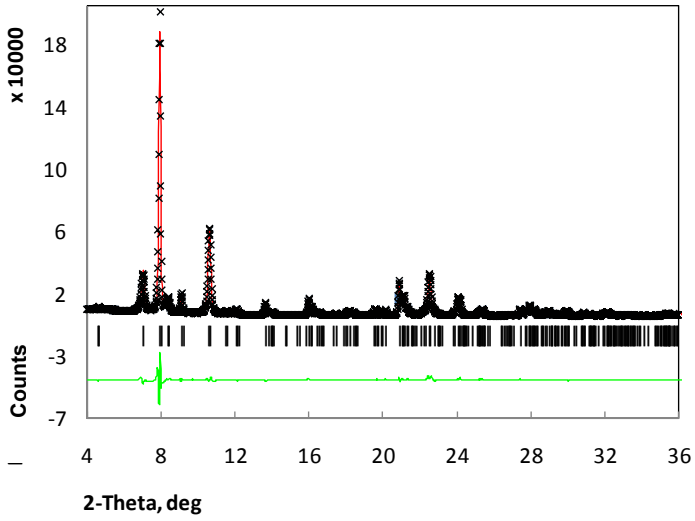
Ow3	O43	2.19(12)
	O43	2.19(12)
	O42	2.33(12)
	O42	2.33(12)
Ow4	O58	2.87(12)
	O58	2.87(12)
Ow5	O33	2.19(85)
	O19	2.84(90)

Table S8: Coordination sequences and vertex symbols calculated for the framework topology of IM-17.[3]

T-atom site	N_1 to N_{12}												Vertex symbol
T_1	4	11	20	29	47	77	103	123	156	211	261	298	$4{\cdot}5_2{\cdot}5{\cdot}6{\cdot}5{\cdot}6$
T_2	4	11	20	29	47	79	105	125	160	210	261	304	$4{\cdot}5_2{\cdot}5{\cdot}6{\cdot}5{\cdot}6$
T_3	4	12	19	33	52	76	105	134	169	208	252	307	$5{\cdot}5{\cdot}5_2{\cdot}10{\cdot}6{\cdot}6$
T_4	4	12	18	31	50	75	104	137	167	203	253	308	$5{\cdot}5{\cdot}5{\cdot}6{\cdot}5_2{\cdot}10$
T_5	4	9	18	33	54	79	104	132	167	206	253	306	$4{\cdot}5{\cdot}4{\cdot}6{\cdot}4{\cdot}10$
T_6	4	11	18	30	47	71	103	136	171	205	249	307	$4{\cdot}5_2{\cdot}5{\cdot}5{\cdot}5{\cdot}6$
T_7	4	11	22	34	51	75	105	142	174	208	256	311	$4{\cdot}6{\cdot}5{\cdot}6_2{\cdot}5{\cdot}12_7$
T_8	4	9	18	33	54	80	106	132	165	208	260	313	$4{\cdot}5{\cdot}4{\cdot}6{\cdot}4{\cdot}10$
T_9	4	11	21	33	52	75	105	140	174	209	255	313	$4{\cdot}5{\cdot}5{\cdot}6_2{\cdot}5{\cdot}12_7$
T_{10}	4	10	21	34	48	68	101	139	178	213	251	314	$4{\cdot}5{\cdot}4{\cdot}8_2{\cdot}5{\cdot}6$
T_{11}	4	12	20	33	52	74	100	136	175	216	263	312	$5{\cdot}6{\cdot}5{\cdot}6{\cdot}6{\cdot}6_2$
T_{12}	4	10	20	35	52	73	106	142	173	204	253	313	$4{\cdot}4{\cdot}5{\cdot}6_2{\cdot}5{\cdot}12_7$
T_{13}	4	12	20	33	52	74	100	135	174	216	262	310	$5{\cdot}6{\cdot}5{\cdot}6_2{\cdot}5{\cdot}8$
T_{14}	4	10	20	34	51	74	103	140	176	208	257	310	$4{\cdot}4{\cdot}5{\cdot}6_2{\cdot}5{\cdot}12_7$
T_{15}	4	10	20	33	47	68	100	137	174	217	262	309	$4{\cdot}6{\cdot}4{\cdot}6_2{\cdot}5{\cdot}8_2$
T_{16}	4	9	18	32	51	76	105	136	169	210	264	316	$4{\cdot}6_2{\cdot}4{\cdot}6_2{\cdot}4{\cdot}10$
T_{17}	4	11	20	27	45	77	105	123	157	216	269	308	$4{\cdot}5_2{\cdot}6_2{\cdot}6_2{\cdot}6_2{\cdot}6_2$
T_{18}	4	11	18	33	53	73	102	135	171	210	253	308	$4{\cdot}6_2{\cdot}5{\cdot}6{\cdot}5{\cdot}10_2$
T_{19}	4	11	18	33	54	77	102	136	171	210	254	309	$4{\cdot}6_2{\cdot}5{\cdot}6{\cdot}5{\cdot}10_2$
T_{20}	4	9	19	35	53	74	103	138	171	209	266	321	$4{\cdot}6{\cdot}4{\cdot}6_2{\cdot}4{\cdot}10$
T_{21}	4	11	22	29	43	77	109	125	155	214	270	311	$4{\cdot}5_2{\cdot}6{\cdot}6_2{\cdot}6{\cdot}6_2$
T_{22}	4	9	18	32	51	77	107	137	169	209	258	309	$4{\cdot}6{\cdot}4{\cdot}6_2{\cdot}4{\cdot}10_4$
T_{23}	4	11	20	27	45	79	105	125	159	211	261	301	$4{\cdot}5_2{\cdot}6{\cdot}6_2{\cdot}6{\cdot}6_2$
T_{24}	4	11	20	29	47	79	107	127	159	208	258	304	$4{\cdot}5_2{\cdot}6{\cdot}6_2{\cdot}6{\cdot}6_2$
T_{25}	4	9	18	33	54	80	108	136	167	209	259	309	$4{\cdot}6{\cdot}4{\cdot}6_2{\cdot}4{\cdot}10_4$

[3] M. M. J. Treacy, M. D. Foster and K. H. Randall, *Microporous Mesoporous Mater.*, 2006, **87**, 255-260.

Figure S1: Rietveld plots of calcined and rehydrated IM-17 in space group *Cmmm*) (λ = 1.5406 Å).



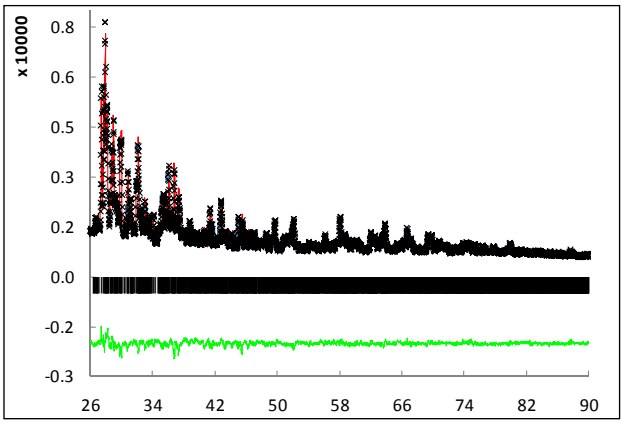


Figure S2: ^{1}H liquid NMR spectrum of IM-17 dissolved in HF and D_2O showing the integrity of the OSDA inside the channels.

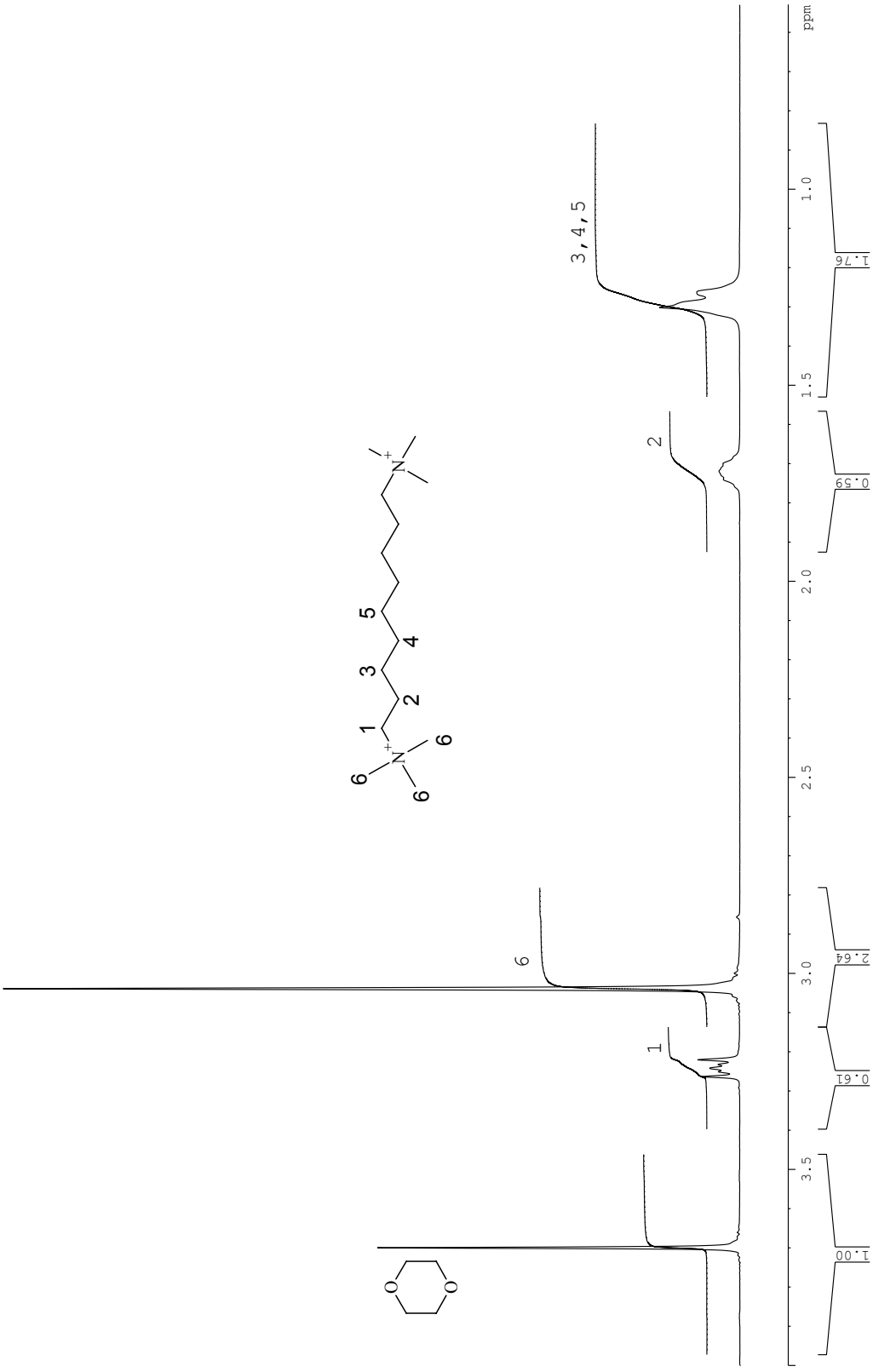
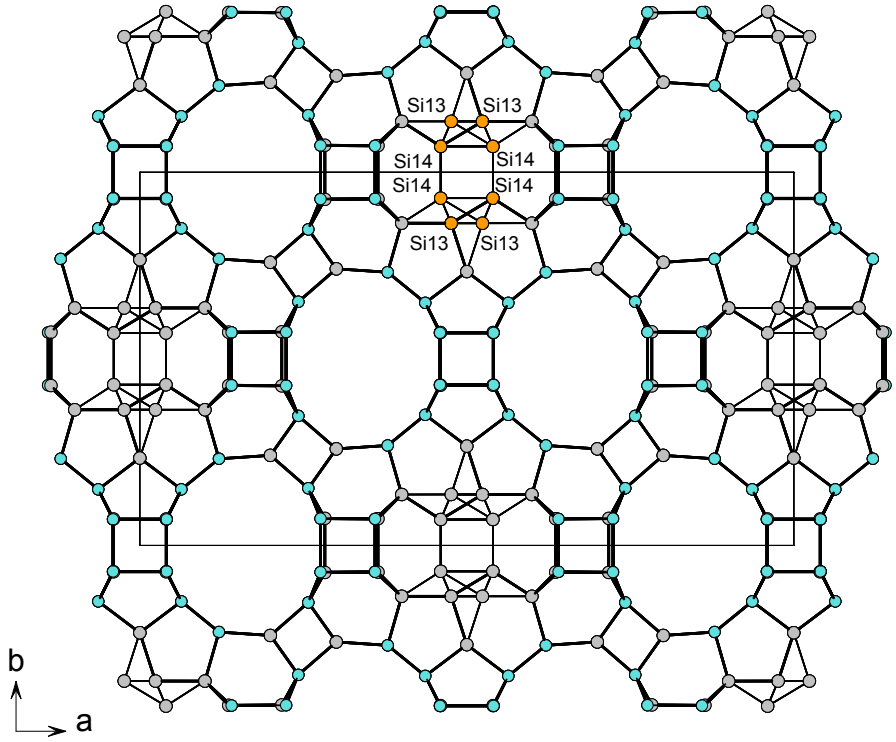
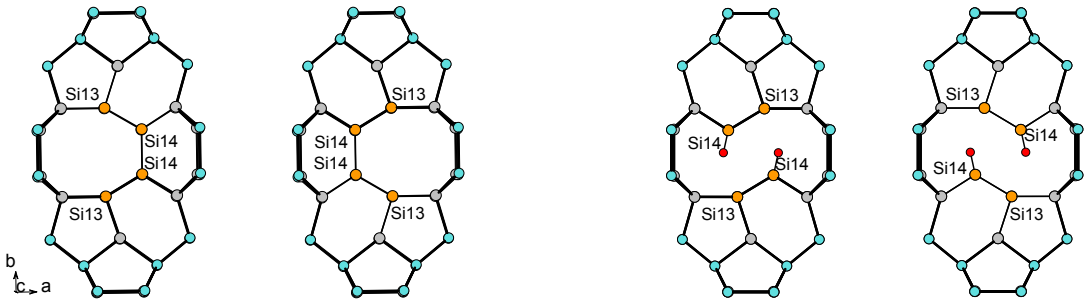


Figure S3: Projection of IM-17 solved in space group *Cmmm* from PXRD along the *c*-axis showing the disorder on the Si13 and Si14 T sites. Oxygen atoms have been removed for clarity.



At this stage, in order to remove the disorder (sites Si13 and Si14), it is possible to lower the symmetry as follow. A super cell is made in space group P1 and 50% of the Si13 and Si14 are removed in different manners as shown on Figure S4 and the occupancy factors of the remaining ones are changed to 1.

Figure S4: The four possibilities to remove disorder in IM-17. Note that the schemes C and D can be eliminated because the ^{29}Si solid state NMR spectrum on the calcined sample shows that no Q3 species are present as it should be the case for interrupted frameworks (on C and D, the red atoms are the OH groups).



A B C D

By taking into account possibilities A and B, we changed the structure in centro- and non centrosymmetric manners. The first one is obtained by alternation of A and B, the second one by using only A or B. On Figure S5 is plotted the projection, after minimisation (Cerius2)[4], of the centric solution in *Pmma* and on Figure S6 the acentric solution in *Amm2* (or *Cm2m* setting after rotation of the axes). In both cases the unit cell content is $T_{176}O_{352}$.

Figure S5: Projection along the *b*-axis of IM-17 in space group *Pmma*.

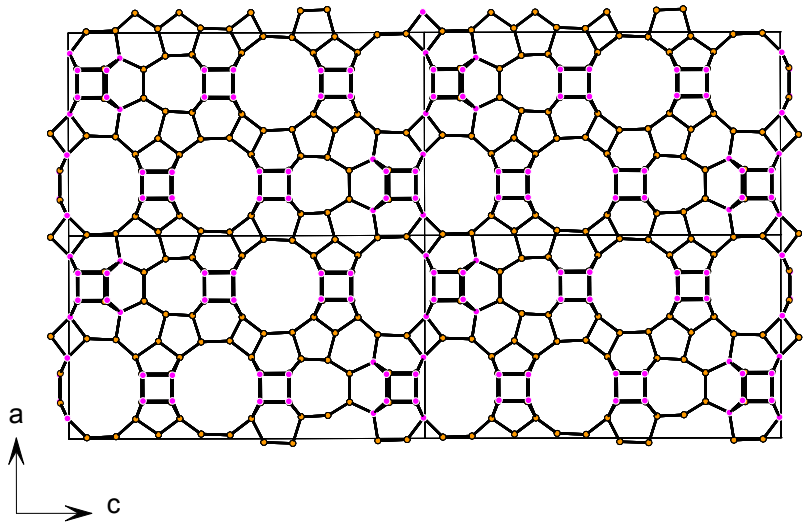
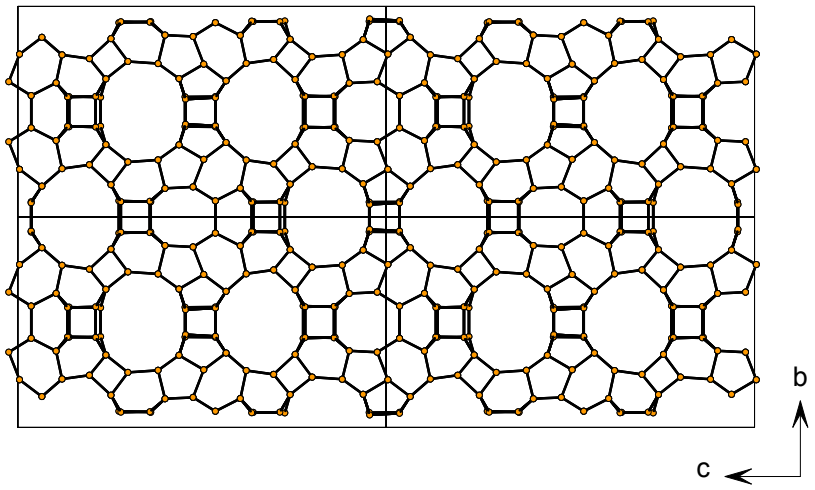


Figure S6: Projection along the *a*-axis of IM-17 in space group *Amm2*.



[4] *Cerius*[2], Molecular Simulations Inc., San Diego, April 2000 version 4.2 MatSci, 2000.

Figure S7: STEM image of a typical crystal of IM-17 used for ADT acquisition. Data were acquired from the right-bottom corner of the crystal.

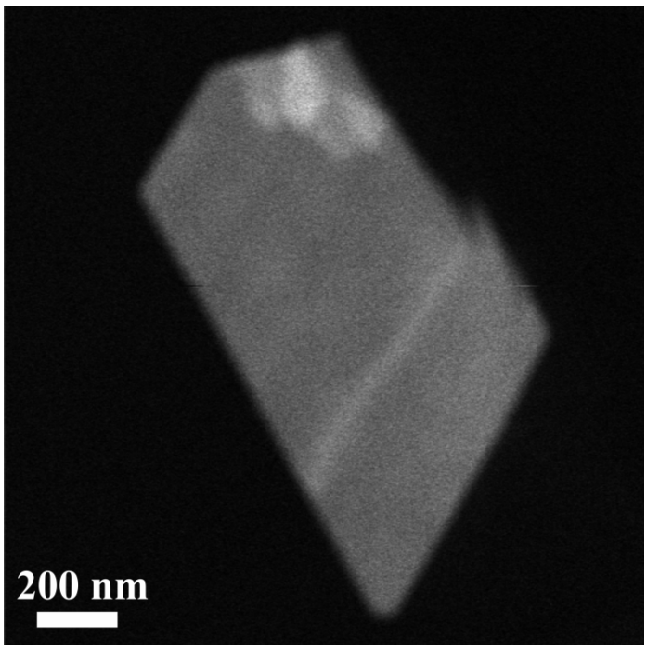


Figure S8: Asymmetric unit of calcined IM-17 after Rietveld refinement in space group *Amm2*, the water molecules have been omitted for clarity.

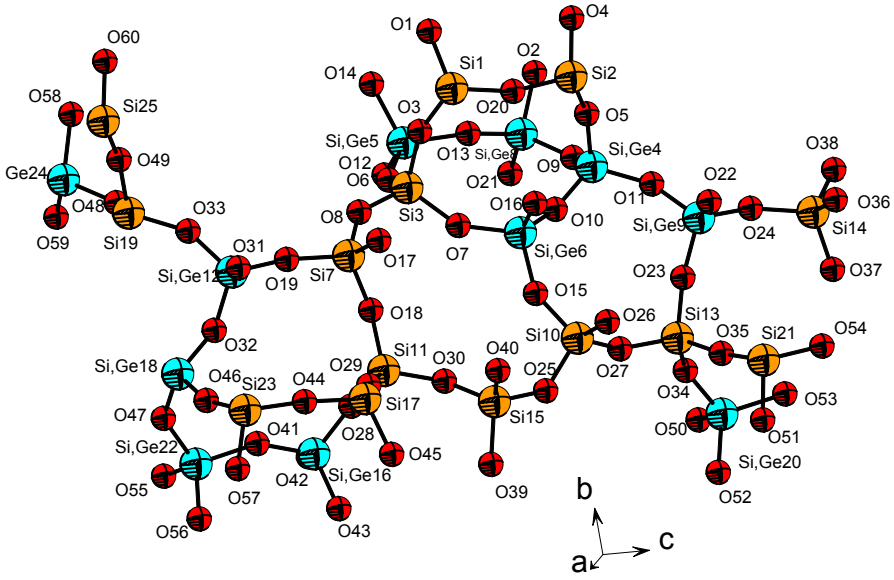


Figure S9: Short contacts between water molecules and the framework oxygen atoms in calcined IM-17 (space group *Amm2*).

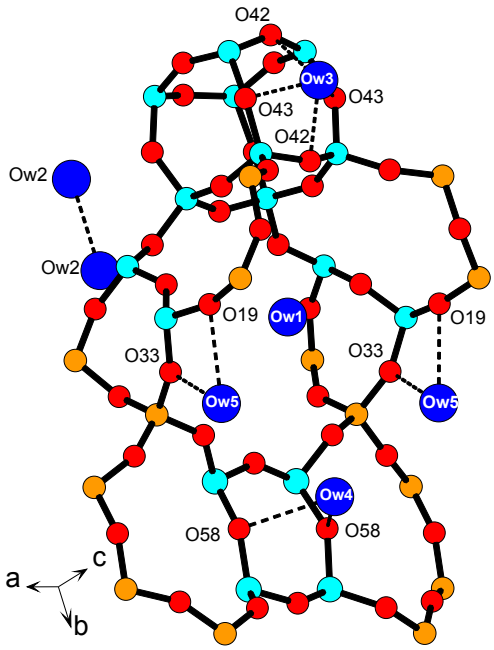


Figure S10: N_2 adsorption–desorption isotherms of calcined IM-17 (sample 14)