Supporting information

Table A1. Overview of all existing and seven energetically feasible hypothetical clathrasil structures with six-rings as largest accessible opening.

Structure	Code	Packing [a]	Status	Tiling type [c]	ΔH_f [kJ/mol SiO_2] [d]	Density [kg/m^3]
Afghanite	AFG	$(4^6 6^5)^3(4^6 6^{17})^1$	Existing	ST	12.9	1791
$AlPO_4$-16	AST	$(4^6 6^{12})^1(4^6)^1$	Existing	ST	15.8	1750
Dodecasil 1H	DOH	$(5^{12}6^8)^1(4^3 5^6 6^3)^2(5^{12})^3$	Existing	ST	13.4	1780
Franzinite	FRA	$(4^6 6^{11})^1(4^6 6^5)^1(4^6 6^8)^3$	Existing	ST	13.2	1747
Giuseppettite	GIU	$(4^6 6^{23})^1(4^6 6^8)^2(4^6 6^5)^5$	Existing	ST	12.9	1789
Liottite	LIO	$(4^6 6^{11})^1(4^6 6^{17})^1(4^6 6^5)^4$	Existing	ST	13.7	1743
Losod	LOS	$(4^6 6^5)^1(4^6 6^{11})^1$	Existing	ST	13.1	1785
Linde Type N	LTN [b]	$(4^6 6^8)^3(4^6 6^5)^4(4^{12}6^8 8^6)^1(4^7 6^8 8^1)^6(4^6 6^2)^2$	Existing	ST	14.7	1707
Marinellite	MAR	$(4^6 6^{17})^1(4^6 6^8)^2(4^6 6^5)^3$	Existing	ST	13.0	1786
Melanophlogite	MEP	$(5^{12})^1(5^{12}6^2)^3$	Existing	ST	12.0	1974
MCM-61	MSO	$(6^8)^1(4^6 6^{20})^1(4^6 6^2)^2(4^2 6^4)^3$	Existing	NST	11.8	1858
ZSM-39	MTN	$(5^{12})^2(5^{12}6^4)^1$	Existing	ST	14.9	1795
Nonasil	NON	$(5^4 6^4)^2(4^1 5^8)^2(5^8 6^{12})^1$	Existing	NST	9.9	1932
RUB-10	RUT [b]	$(4^4 5^4 6^2)^1(4^4 5^6 6^5 8^1)^2$	Existing	ST	12.2	1824
Sigma-2	SGT	$(5^{12}6^8)^1(4^3 5^6)^2$	Existing	ST	12.8	1793
Sodalite	SOD	$(4^6 6^8)^1$	Existing	ST	12.9	1777
IM-10	UOZ	$(4^6)^2(4^2 6^4)^1(4^{10}6^{20})^1$	Existing	ST	20.4	1951
-	Dt2_106	$(4^6 6^5)^1(4^6 6^8)^1(4^6 6^{11})^1$	Hypothetical	ST	13.0	1782
-	Dt2_113	$(4^4 5^4 6^6)^1$	Hypothetical	ST	15.4	2106
-	Dt2_117	$(4^2 5^8 6^4)^1$	Hypothetical	ST	10.5	1976
-	Dt3_779	$(4^6 6^2)^6(4^6 6^8)^3(4^6 6^{20})^2$	Hypothetical	ST	26.6	1889
-	Dt3_819	$(4^6 6^2)^6(4^6 6^5)^8(4^6 6^8)^3(4^6 6^{44})^1$	Hypothetical	ST	17.8	1568
-	Dt3_898	$(4^6 6^5)^2(4^6 6^8)^1(4^6 6^{11})^2$	Hypothetical	ST	13.6	1743
-	Dt3_899	$(4^6 6^5)^2(4^6 6^8)^2(4^6 6^{14})^1$	Hypothetical	ST	13.3	1766

[a] Each cage type has its own description in between the brackets and the ratio between the different cage types is given by the superscripts outside the brackets. In between brackets the ring types (normal text) and their occurrence (superscript) in a cage type are given.

[b] The eight-ring in these structures are so-called internal eight-rings, i.e., it is not possible to access the crystals via these rings.

[c] An explanation of tiling type can be found in results and discussion.

[d] The heat of formation is given relative to that of quartz, being -12417.6 kJ/mol SiO_2. See Computational methodology section for calculation details.

Table A2. Overview of the tile volumes of the cages of all existing and hypothetical ST clathrasils.

Existing clathrasils		
Clathrasil	Cage	Volume [Å^3]
AFG	$(4^6 6^5)$	182
AFG	$(4^6 6^{17})$	793
AST	$(4^6 6^{12})$	541
AST	(4^6)	29
DOH	$(5^{12} 6^8)$	674
DOH	$(4^3 5^6 6^3)$	226
DOH	(5^{12})	227
FRA	$(4^6 6^{11})$	488, 493
FRA	$(4^6 6^5)$	182, 185
FRA	$(4^6 6^8)$	334, 335, 336, 339
GIU	$(4^6 6^5)$	181, 182
GIU	$(4^6 6^8)$	334, 335
GIU	$(4^6 6^{23})$	1100
LIO	$(4^6 6^{11})$	500
LIO	$(4^6 6^{17})$	814
LIO	$(4^6 6^5)$	187
LOS	$(4^6 6^5)$	183
LOS	$(4^6 6^{11})$	488
LTN	$(4^6 6^8)$	332
LTN	$(4^6 6^8)$	340
LTN	$(4^6 6^5)$	182
LTN	$(4^{12} 6^8 8^6)$	1206
LTN	$(4^7 6^8 8^1)$	420
LTN	$(4^6 6^2)$	75
MAR	$(4^6 6^5)$	181,182
MAR	$(4^6 6^8)$	335,336
MAR	$(4^6 6^{17})$	795
MEP	(5^{12})	224
MEP	$(5^{12} 6^2)$	315
MTN	(5^{12})	242
MTN	$(5^{12} 6^4)$	461
RUT	$(4^4 5^4 6^2)$	134
RUT	$(4^4 5^6 6^5 8^1)$	425
SGT	$(5^{12} 6^8)$	674
SGT	$(4^3 5^6$	108
SOD	$(4^6 6^8)$	337

Hypothetical clathrasils		
Clathrasil	Cage	Volume [Å^3]
Dt2_106	$(4^6 6^5)$	183
	$(4^6 6^8)$	335
	$(4^6 6^{11})$	490
Dt2_113	$(4^4 5^4 6^6)$	284
Dt2_117	$(4^2 5^8 6^4)$	308
Dt3_779	$(4^6 6^2)$	73
	$(4^6 6^8)$	300, 328
	$(4^6 6^{20})$	902
Dt3_819	$(4^6 6^2)$	73
	$(4^6 6^5)$	180
	$(4^6 6^8)$	343, 345
	$(4^6 6^{44})$	3202
Dt3_898	$(4^6 6^5)$	188
	$(4^6 6^8)$	343
	$(4^6 6^{11})$	500
Dt3_899	$(4^6 6^5)$	182
	$(4^6 6^8)$	339
	$(4^6 6^{14})$	648