Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supporting Information

Low-density nanoporous phases of group-III nitrides built from sodalite cage clusters

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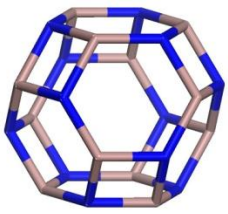
S1. Natural tilings of the new nanoporous phases of MN

SOD-MN $Pm\bar{3}n$

Face symbol: $[4^6.6^8]$

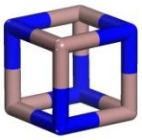
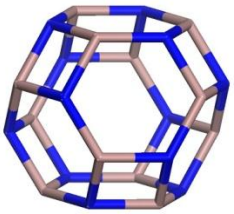
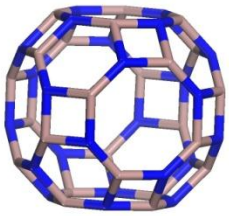


V, E, F: (24, 36, 14)

Symmetry: $m\bar{3}$

LTA-MN $Fm\bar{3}c$

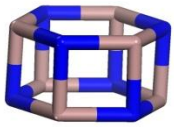
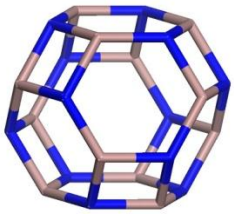
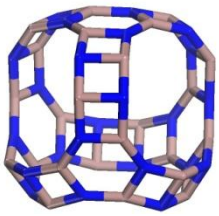
Face symbol: $[4^6]$ $[4^6.6^8]$ $[4^{12}.6^8.8^6]$

V, E, F: (8, 12, 6) (24, 36, 14) (48, 72, 26)
Symmetry: $\bar{4}3m$ $m\bar{3}$ 432

FAU-MN $Fd\bar{3}$

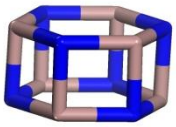
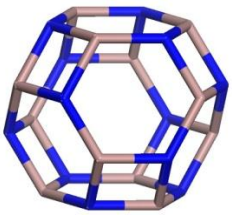
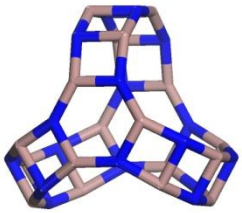
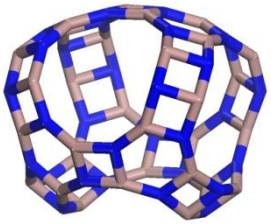
Face symbol: $[4^6.6^2]$ $[4^6.6^8]$ $[4^{18}.6^4.12^4]$

V, E, F: (12, 18, 8) (24, 36, 14) (48, 72, 26)
Symmetry: $\bar{3}m$ $m\bar{3}$ 23

EMT-MN $P\bar{3}1c$

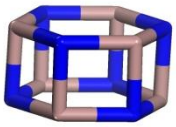
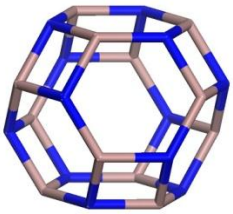
Face symbol: $[4^6.6^2]$ $[4^6.6^8]$ $[4^{15}.6^2.12^3]$ $[4^{21}.6^6.12^5]$

V, E, F: (12, 18, 8) (24, 36, 14) (36, 54, 20) (60, 90, 32)
Symmetry: $\bar{3}m$ $m\bar{3}$ 32 32

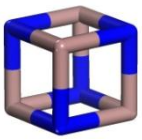
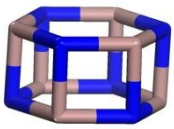
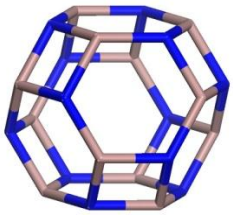
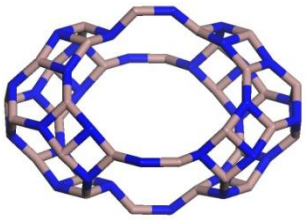
Tri-MN $R\bar{3}$

Face symbol: $[4^6.6^2]$ $[4^6.6^8]$

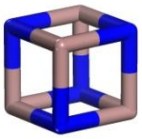
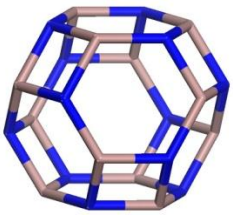
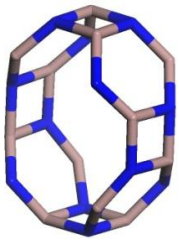
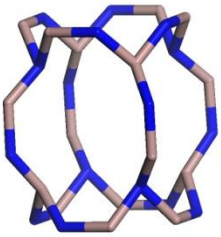



V, E, F: (12, 18, 8) (24, 36, 14)
Symmetry: $\bar{3}m$ $m\bar{3}$

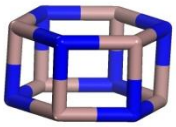
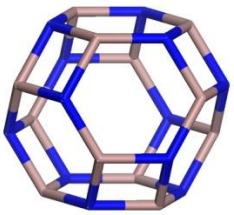
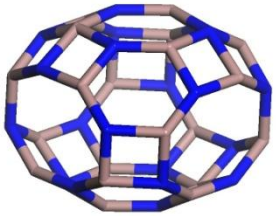
Ort-MN *Pban*

Face symbol:	$[4^6]$	$[4^6.6^2]$	$[4^6.6^8]$	$[4^{18}.6^4.8^4.12^2.16^2]$
				
V, E, F:	(8, 12, 6)	(12, 18, 8)	(24, 36, 14)	(64, 92, 30)
Symmetry:	$\bar{4}3m$	$\bar{3}m$	$m\bar{3}$	

Tet-MN $P4_2/mcm$

Face symbol:	$[4^6]$	$[4^6.6^8]$	$[4^4.6^4.12^2]$	$[12^6]$
				
V, E, F:	(8, 12, 6)	(24, 36, 14)	(24, 32, 10)	(32, 36, 6)
Symmetry:	$\bar{4}3m$	$m\bar{3}$	222	$\bar{4}2m$

Mon-MN $C2/m$

Face symbol:	$[4^6.6^2]$	$[4^6.6^8]$	$[4^{14}.6^6.8^4]$
			
V, E, F:	(12, 18, 8)	(24, 36, 14)	(40, 62, 24)
Symmetry:	$\bar{3}m$	$m\bar{3}$	$2/m$

S2. Estimations of pore volume and specific surface area for the new nanoporous phases

From the natural tilings, one can find that the structure type is “Cage” for all of the eight new nanoporous phases. We believe, therefore, that the volume of a sphere may effectively describe the hollow space of the cage. To choose a rational radius for the sphere of the cage, we use Helium molecules He_n (2-10) to fill the hollow space of $M_{12}N_{12}$. After full optimization without any symmetry constraint, we find that the sodalite cage can be well retained when $n \leq 8$ and $n \leq 6$ for $Ga_{12}N_{12}$ $Al_{12}N_{12}$, respectively. Based on these calculations, the effective radius (R) of the sphere can

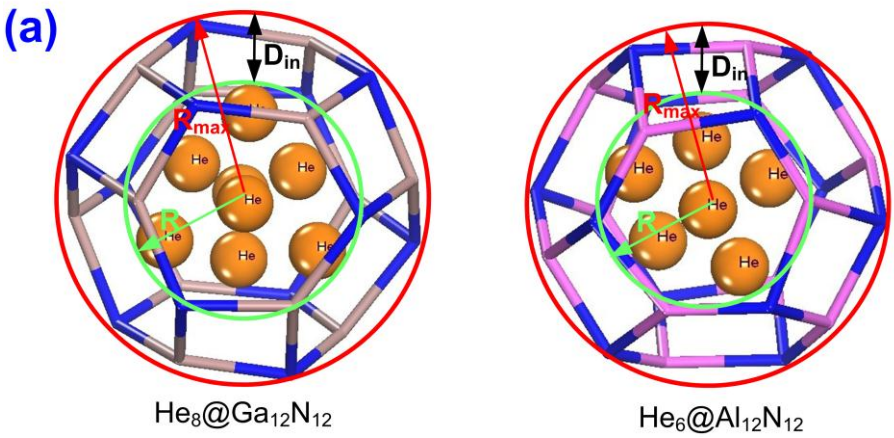
be defined (approximately) as: $R = R_{\max} - D_{in}$ [see Fig. S2(a)]. In Fig. S2(b), we demonstrate how to measure the $R_{\max}$ for the different cages.

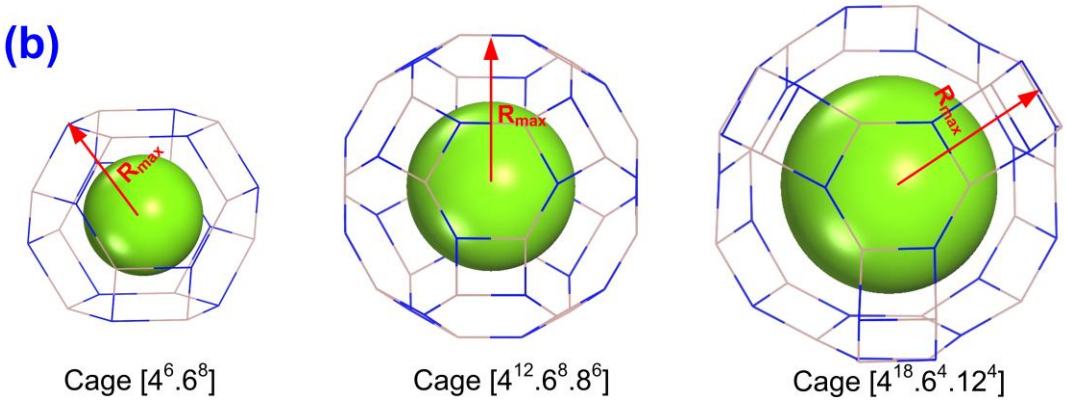
Consequently, pore volume (V_p) and specific surface area (S_a) can be estimated by following equations:

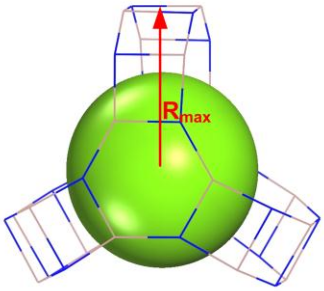
$$V_p = \frac{\frac{4}{3}\pi\sum_i \alpha_i R_i^3}{m} \quad , (1)$$

$$S_a = \frac{4\pi\sum_j \beta_j R_j^2}{m'} \quad . (2)$$

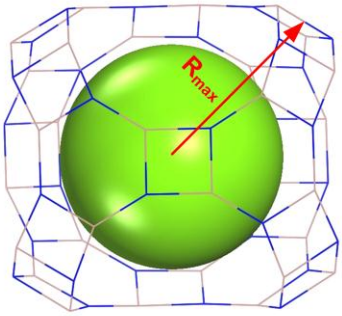
It is important to note that our calculated results are just based on the crystal structure rather than adsorption isotherms which should consider the pressure and temperature. However, it does reflect the porosity of the new nanoporous phases to a certain extent.



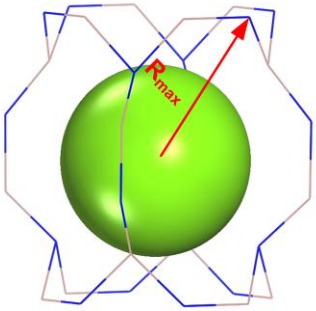




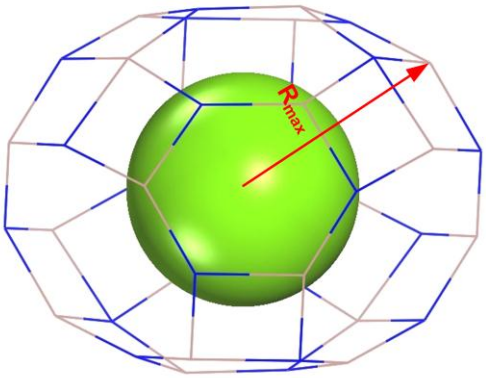
Cage [$4^{15}.6^{2}.12^{3}$]



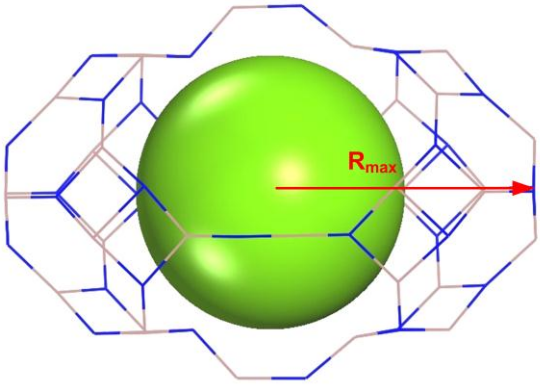
Cage [$4^{21}.6^{6}.12^{5}$]



Cage [12^{6}]



Cage [$4^{14}.6^{6}.8^{4}$]



Cage [$4^{18}.6^{4}.8^{4}.12^{2}.16^{2}$]