

Supporting Information for

Ultrastable 3D cage-like metal-organic frameworks constructed by multidentate cyanurate ligand and gas adsorption properties

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Density Functional Theory (DFT) Calculations

Structural optimization was performed by Vienna Ab-initio Simulation Package(VASP)[1] with the projector augmented wave (PAW) method[2]. The exchange-functional was treated using the Perdew-Burke-Ernzerhof (PBE)[3] functional in combination with the DFT-D3 correction[4], to describe the weak interactions between atoms. The cut-off energy of the plane-wave basis was set at 450 eV in structural optimization. For the optimization of both geometry and lattice size, the Brillouin zone integration was performed with a Monkhorst-Pack k -point mesh of 0.04 \AA^{-1} . Partial occupancies of the Kohn–Sham orbitals were allowed using the Gaussian smearing method and a width of 0.05 eV. A geometry optimization was considered convergent when the energy change was smaller than 0.03 eV \AA^{-1} .

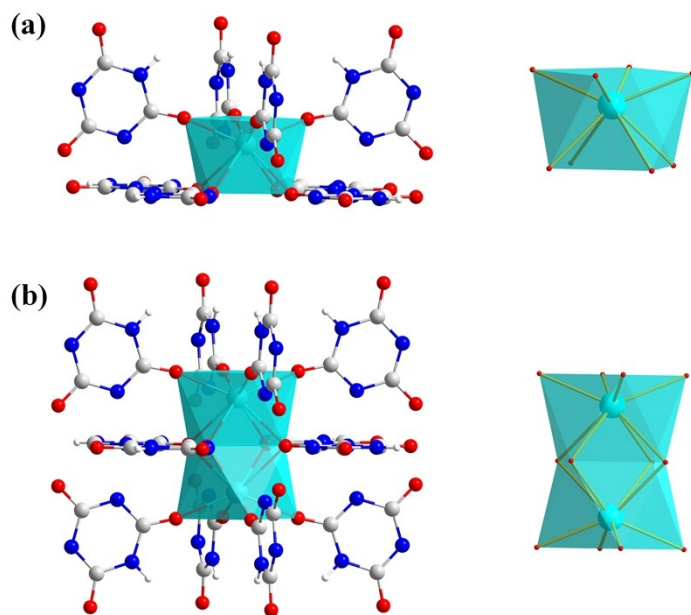


Figure S1. The coordination environment of Sr atom in SrCu(HC₃N₃O₃)₂.

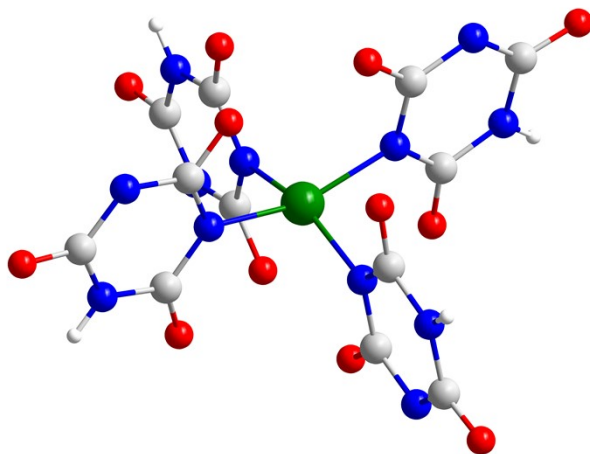


Figure S2. The coordination environment of Cu atom in SrCu(HC₃N₃O₃)₂.

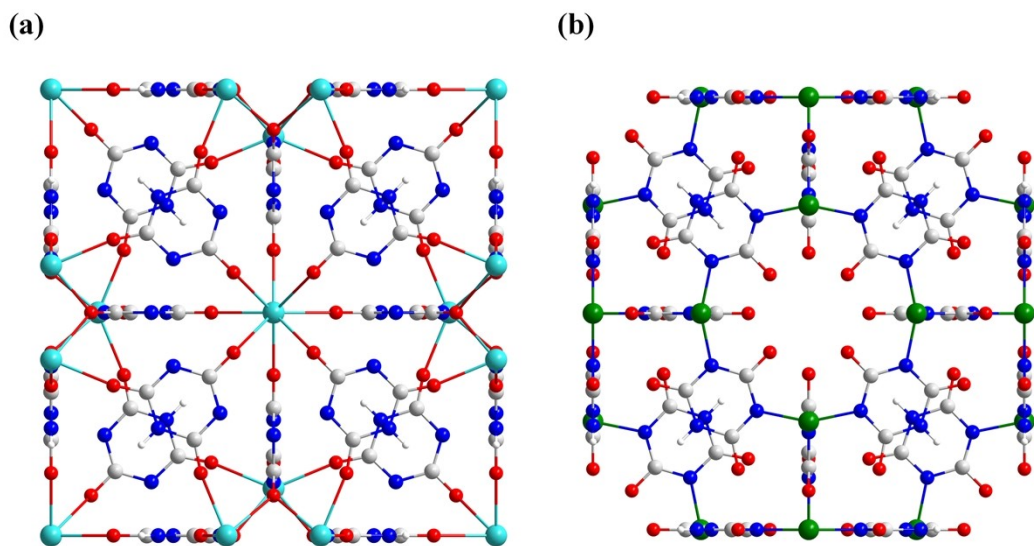


Figure S3. Two set of independent coordination frameworks constructed by (a) Sr and (b) Cu.

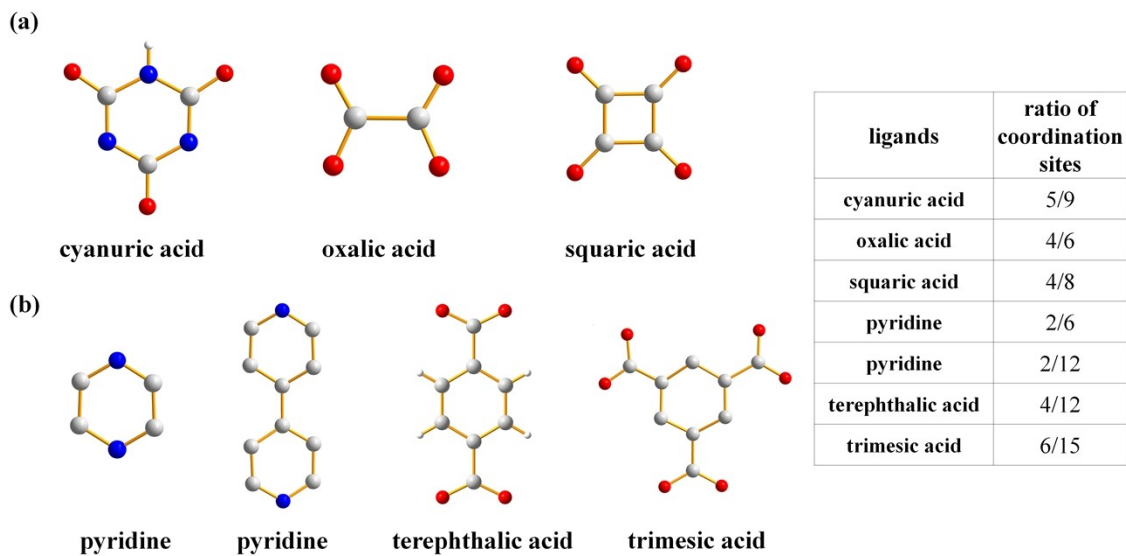


Figure S4. Some organic ligands and ratio of coordination sites.

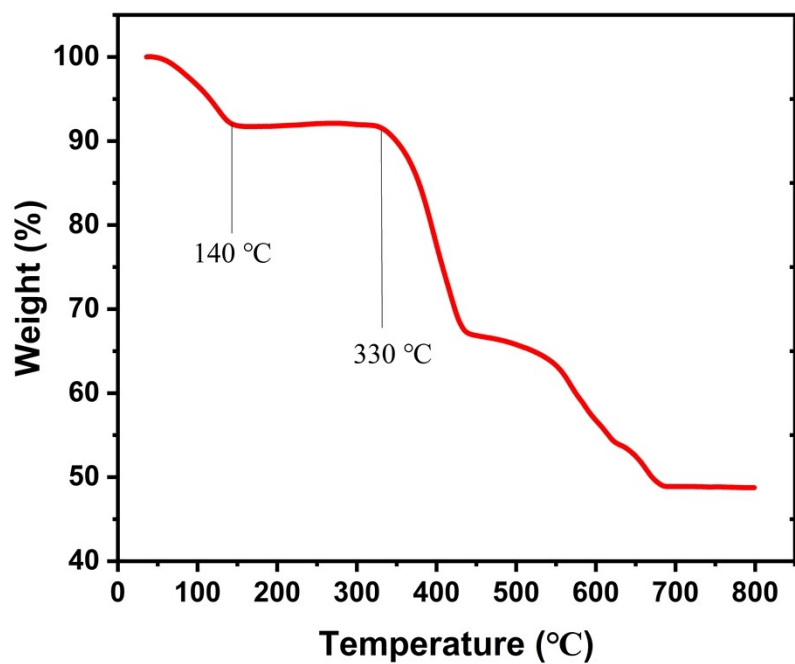


Figure S5. Thermogravimetric analysis curve of $\text{SrCu}(\text{HC}_3\text{N}_3\text{O}_3)_2$.

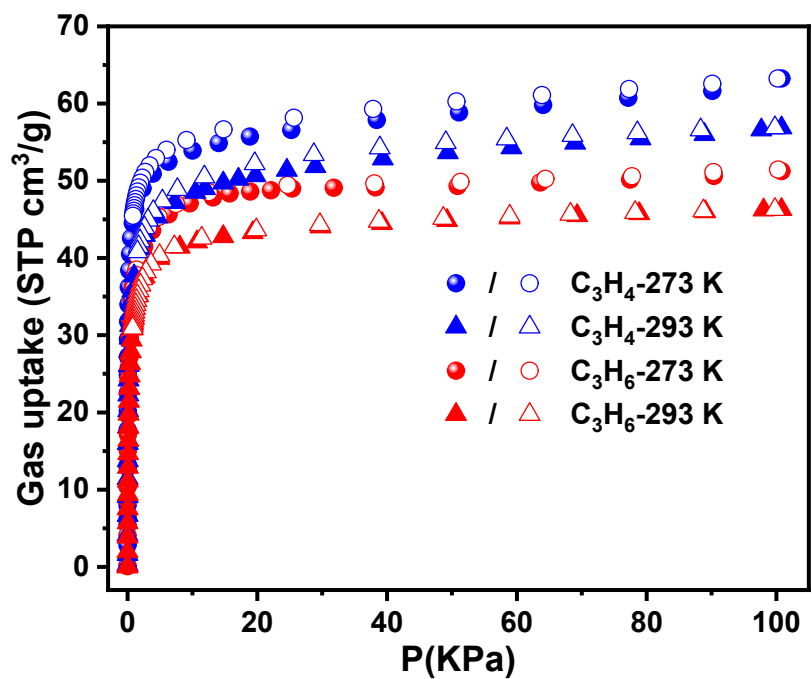


Figure S6. C_3H_4 and C_3H_6 adsorption/desorption isotherms 273 and 293 K for $\text{SrCu}(\text{HC}_3\text{N}_3\text{O}_3)_2$.

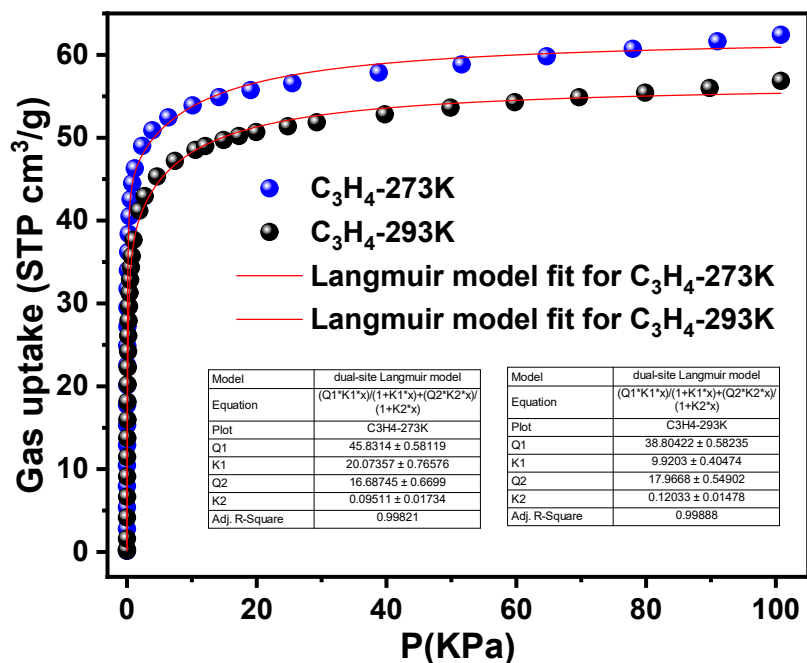


Figure S7. Nonlinear curve fitting of C_3H_4 adsorption isotherms at 273 and 293 K for $SrCu(HC_3N_3O_3)_2$ and using Double-site Langmuir model.

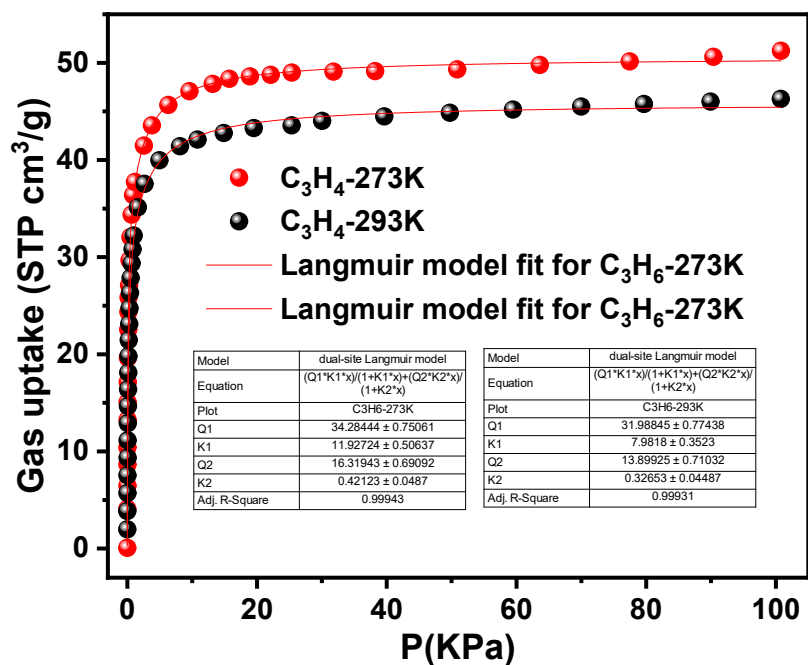


Figure S8. Nonlinear curve fitting of C_3H_6 adsorption isotherms at 273 and 293 K for $SrCu(HC_3N_3O_3)_2$ and using Double-site Langmuir model.

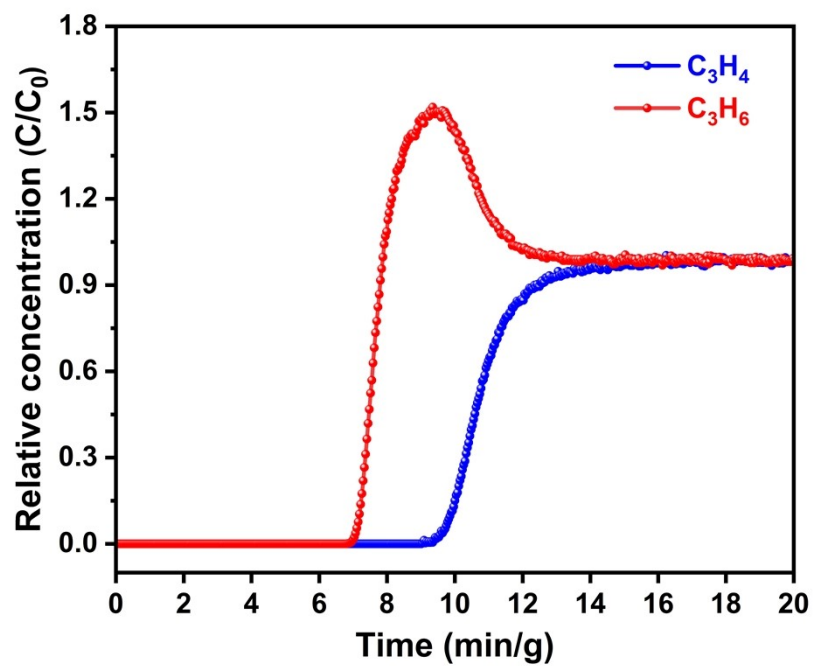


Figure S9. Column breakthrough curve for C₃H₄/C₃H₆ (50:50) at 273 K.

Table S1 Crystallographic data and structure refinement for SrCu(HC₃N₃O₃)₂.

Formula	SrCu(HC ₃ N ₃ O ₃) ₂
CCDC Number	2252835
Formula weight	405.3
Temperature/K	296
Crystal system	cubic
Space group	<i>Im-3m</i>
<i>a</i> /Å	16.2073(10)
Volume/Å ³	4257.28(8)
Z	12
ρ /(g/cm ³)	1.897
μ /mm ⁻¹	7.152
F(000)	2340.0
Radiation	Cu K α (λ = 1.54184)
2 θ range for data collection (°)	7.714 to 153.06
Index ranges	-18 \leq h \leq 19, -15 \leq k \leq 19, -7 \leq l \leq 15
Reflections collected	2976
Independent reflections	450 [Rint = 0.0246, Rsigma = 0.0159]
data/restraints/parameters	450/0/37
GOOF on F ²	1.171
<i>R</i> ₁ , w <i>R</i> ₂ (I > 2 σ (I)) ^a	<i>R</i> ₁ = 0.0212, w <i>R</i> ₂ = 0.0581
<i>R</i> ₁ , w <i>R</i> ₂ [all data]	<i>R</i> ₁ = 0.0230, w <i>R</i> ₂ = 0.0587
Largest diff. peak/hole (e Å ⁻³)	0.50/-0.39

$$^a R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, wR_2 = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right]^{1/2}$$

Table S2 Atomic coordinates, equivalent isotropic displacement parameters for SrCu(HC₃N₃O₃)₂.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq} (Å ²) ^a
Sr1	0.5000	0.89341 (3)	0.5000	0.0200 (2)
Cu1	0.5000	1.0000	0.2500	0.0165 (2)
O1	0.5000	0.83693 (16)	0.35841 (15)	0.0525 (8)
O2	0.5000	0.91127 (14)	0.08873 (14)	0.0316 (7)
N2	0.5000	0.87922 (15)	0.22478 (16)	0.0229 (5)
N1	0.5000	0.74117 (17)	0.25883 (17)	0.0475 (13)
H1	0.5000	0.7036	0.2964	0.057*
C1	0.5000	0.82169 (19)	0.2837 (2)	0.0327 (7)

^a *U*_{eq} is defined as one-third of the trace of the orthogonalized *U*_{*ij*} tensor.

Table S3 Selected bond distances (Å) and band angles (°) for SrCu(HC₃N₃O₃)₂.

Sr1—O1	2.471 (2)	Cu1—N2 ^{ix}	2.000 (2)
Sr1—O1 ⁱ	2.471 (2)	Cu1—N2 ^x	2.000 (2)
Sr1—O1 ⁱⁱ	2.471 (2)	C1—O1	1.235 (4)
Sr1—O1 ⁱⁱⁱ	2.471 (2)	C1—N1	1.366 (3)
Sr1—O2 ^{iv}	2.668 (2)	C1—N2	1.335 (4)
Sr1—O2 ^v	2.668 (2)	C2—O2	1.252 (5)
Sr1—O2 ^{vi}	2.668 (2)	C2—N2	1.369 (3)
Sr1—O2 ^{vii}	2.668 (2)	C2—N2 ^{xiii}	1.369 (3)
Cu1—N2	2.000 (2)	N1—H1	0.8600
Cu1—N2 ^{viii}	2.000 (2)		
O1—Sr1—O1 ⁱ	82.11 (4)	N2—Cu1—N2 ^{ix}	92.40 (3)
O1—Sr1—O1 ⁱⁱ	136.51 (13)	N2—Cu1—N2 ^{viii}	156.41 (15)
O1—Sr1—O1 ⁱⁱⁱ	82.11 (4)	N2—Cu1—N2 ^x	92.40 (3)
O1—Sr1—O2 ^{iv}	137.77 (4)	N2 ^x —Cu1—N2 ^{viii}	156.40 (15)
O1—Sr1—O2 ^v	137.77 (4)	N2 ^x —Cu1—N2 ^{viii}	92.40 (3)
O1—Sr1—O2 ^{vi}	74.89 (6)	N2 ^{viii} —Cu1—N2 ^{ix}	92.40 (3)
O1—Sr1—O2 ^{vii}	74.89 (6)	C1—N2—C2	120.2 (3)
O2 ^{iv} —Sr1—O2 ^v	65.22 (5)	C1—N1—C1 ^{xiii}	124.4 (4)
O2 ^{iv} —Sr1—O2 ^{vi}	99.31 (9)	N1—C1—O1	118.7 (3)
O2 ^{iv} —Sr1—O2 ^{vii}	65.22 (5)	N1—C1—N2	117.1 (3)
		N2—C1—O1	124.2 (3)

Symmetry codes: (i) $z, y, -x+1$; (ii) $x, y, -z+1$; (iii) $-z+1, y, -x+1$; (iv) $z+1/2, -x+3/2, -y+3/2$;
(v) $-z+1/2, -x+3/2, -y+3/2$; (vi) $-z+1/2, x+1/2, y-1/2$; (vii) $z+1/2, x+1/2, y-1/2$; (viii) $-x+1, -y+2, z$;
(ix) $y-1/2, x+1/2, -z+1/2$; (x) $-y+3/2, -x+3/2, -z+1/2$; (xi) $y-1/2, z+1/2, x-1/2$;
(xii) $-y+3/2, -z+3/2, -x+1/2$; (xiii) $x, -z+1, -y+1$.

References

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2. P. E. Blöchl, *Phys. Rev. B* 1994, 50, 17953.
3. J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 1996, 77, 3865.
4. S. Grimme, *J. Comput. Chem.* 2006, 27, 1787.