Supporting Information

Stable nitrogen-rich scandium nitrides and their bonding features at Ambient Conditions

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Supplementary Figures

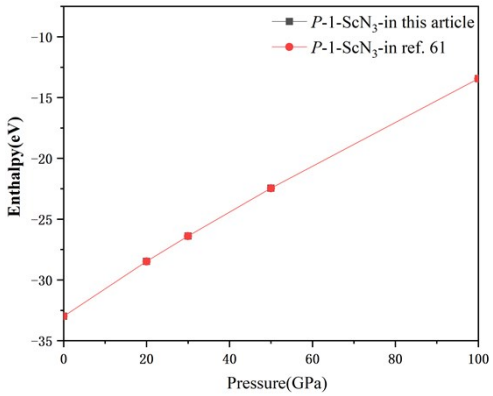


Figure. S1. Calculated enthalpies per formula unit (f.u.) of ScN_3

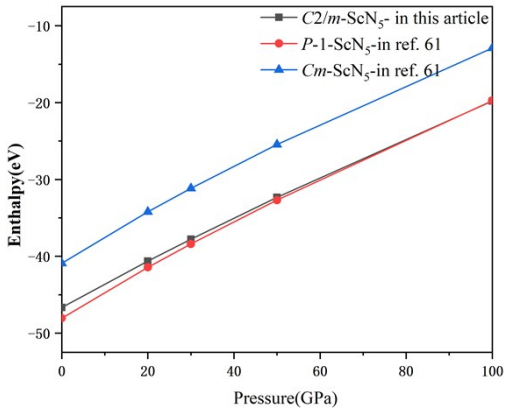
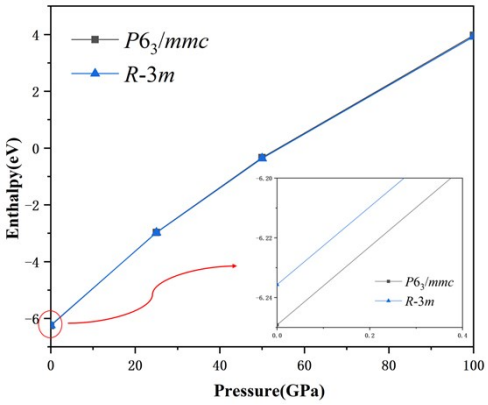


Figure. S2. Calculated enthalpies per formula unit (f.u.) of ScN_5



the Calculated enthalpies per formula unit (f.u.) of Sc at 0GPa	
*P*6$_3$/*mmc*	*R*-3*m*
-6.2491595	-6.23567177

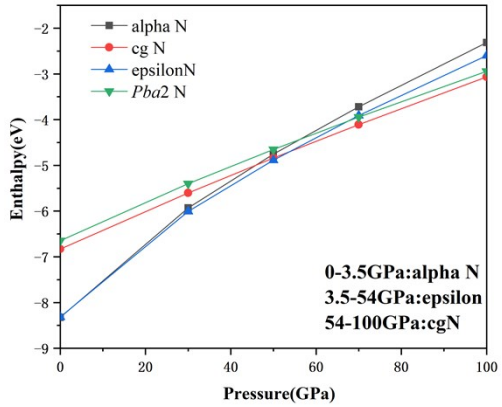


Figure. S3. The phases transition of Sc and N

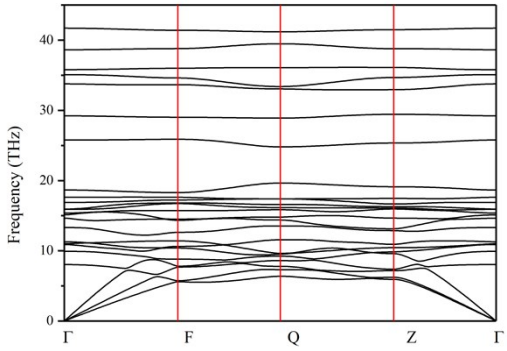


Figure. S4. Phonon dispersion curves of *P*-1-ScN_3 at 50 GPa.

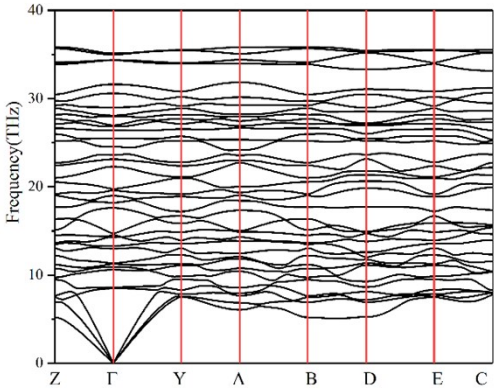


Figure. S5. Phonon dispersion curves of *C*2/*m*-ScN_5 at 50 GPa

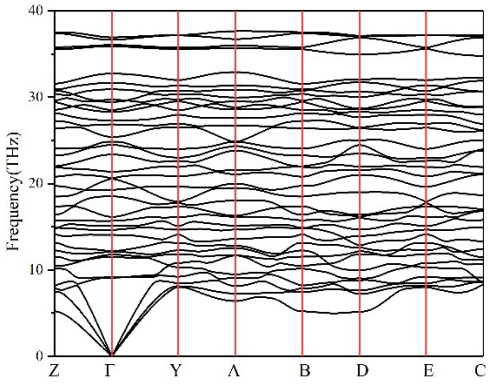


Figure. S6. Phonon dispersion curves of *C*2/*m*-ScN_5 at 100 GPa

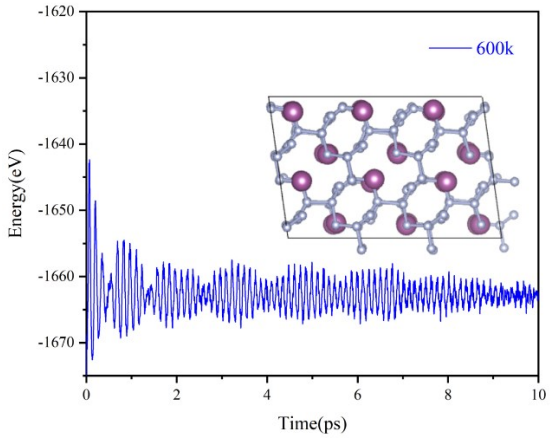


Figure. S7. Images for the equilibrium structures of *C*2/*m*-ScN_5 and fluctuations of the total energies at the end of 10 ps FPMD simulations at the temperatures of 600 K.

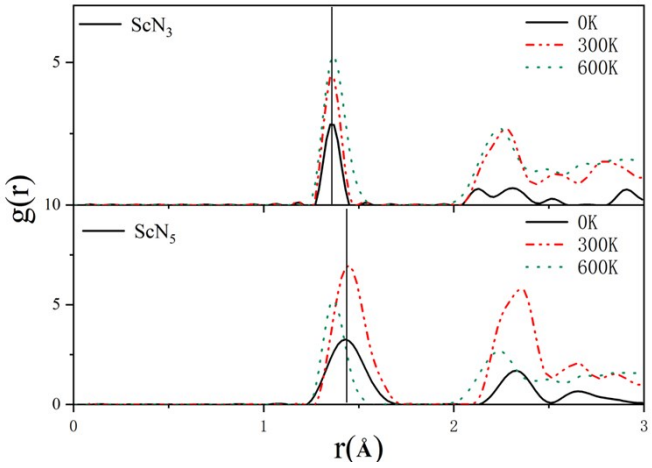


Figure. S8. The Radial Distribution Function curve for N-N separations of ScN_3 and ScN_5 at 0, 300 and 600K.

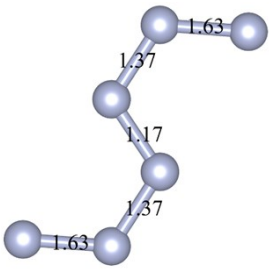


Figure. S9. The calculated bond order of N_6^{2-}.

Supplementary table

Table S1. The unit-cell parameters and atomic positions of ScN_3 at 0 GPa

Space group	Lattice parameter (Å, ^{0})	Atom	Wyckoff position	x	y	z
P-1-ScN_3 in this article	a=4.7339	Sc	2i	0.27171	0.67387	0.83206
	b=5.0811	N1	2i	0.31088	0.15501	0.31762
	c=3.3573	N2	2i	0.13233	0.96986	0.47454
	α=101.1036	N3	2i	0.21088	0.37783	0.22894
	β=91.9075					
	γ=99.7122					
P-1-ScN_3-in ref. 61	a=4.6995	Sc	2i	0.77573	0.18049	0.35575
	b=5.1579	N1	2i	0.81631	0.66513	0.84693
	c=3.2640	N2	2i	0.36492	0.52667	0.01638
	α=100.8608	N3	2i	0.70957	0.87685	0.73754
	β=93.7835					
	γ=99.6239					

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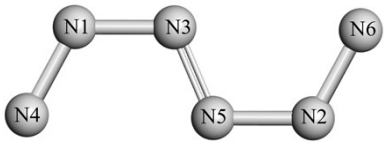
Table S2. The calculated electronic energies, ZPE of predicted structures at 0 GPa.

	electronic energy(meV)	ZPE(meV)
P-1-ScN_3	-32.995	0.3931
*C*2/*m*-ScN_5	-46.669	0.35221

Table S3. The calculated distance, ICOHP and bond order of *P*-1-ScN_3 at 0 GPa.



	distance(Å)	ICOHP (eV/pair)	Bond order
N4-N1 （N2-N6）	1.3769	-12.6981	1.63
N1-N3 （N5-N2）	1.3525	-13.6447	1.37
N3-N5	1.348	-13.3009	1.17

Table S4. Calculated Bader charges for *P*-1-ScN_3 and *C*2/*m*-ScN_5 at 0 GPa

Structure	Atom	Charge value(e)	δ(e)
	Sc1	9.2154	1.79
	Sc2	9.2154	1.79

P-1-ScN_3	N1	5.4579	0.45
	N2	5.4579	0.45
	N3	5.3642	0.36
	N4	5.3642	0.36
	N5	5.9609	0.96
	N6	5.9609	0.96
*C*2/*m*-ScN_5	Sc1	9.1262	1.874
	Sc2	9.1262	1.874
	N1	5.1553	0.1553
	N2	5.5686	0.5686
	N3	5.4965	0.4965
	N4	5.1555	0.1555
	N5	5.4979	0.4979
	N6	5.1558	0.1558
	N7	5.1548	0.1555
	N8	5.5686	0.5686
	N9	5.4965	0.4965
	N10	5.4979	0.4979

The calculation methods for orbitals and bond order

The calculations of orbitals and bond order were carried out with the Gaussian 09 package (G09d01 version) using B3LYP/6-311+(g,d).

Bond order is a measurement of the number of electrons involved in bonds between two atoms in a molecule.