Supporting information for

"Single-bonded nitrogen chain and porous nitrogen layer via Ce-N compounds"

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School of Physics and Collaborative Innovation Center of Advanced Microstructures,

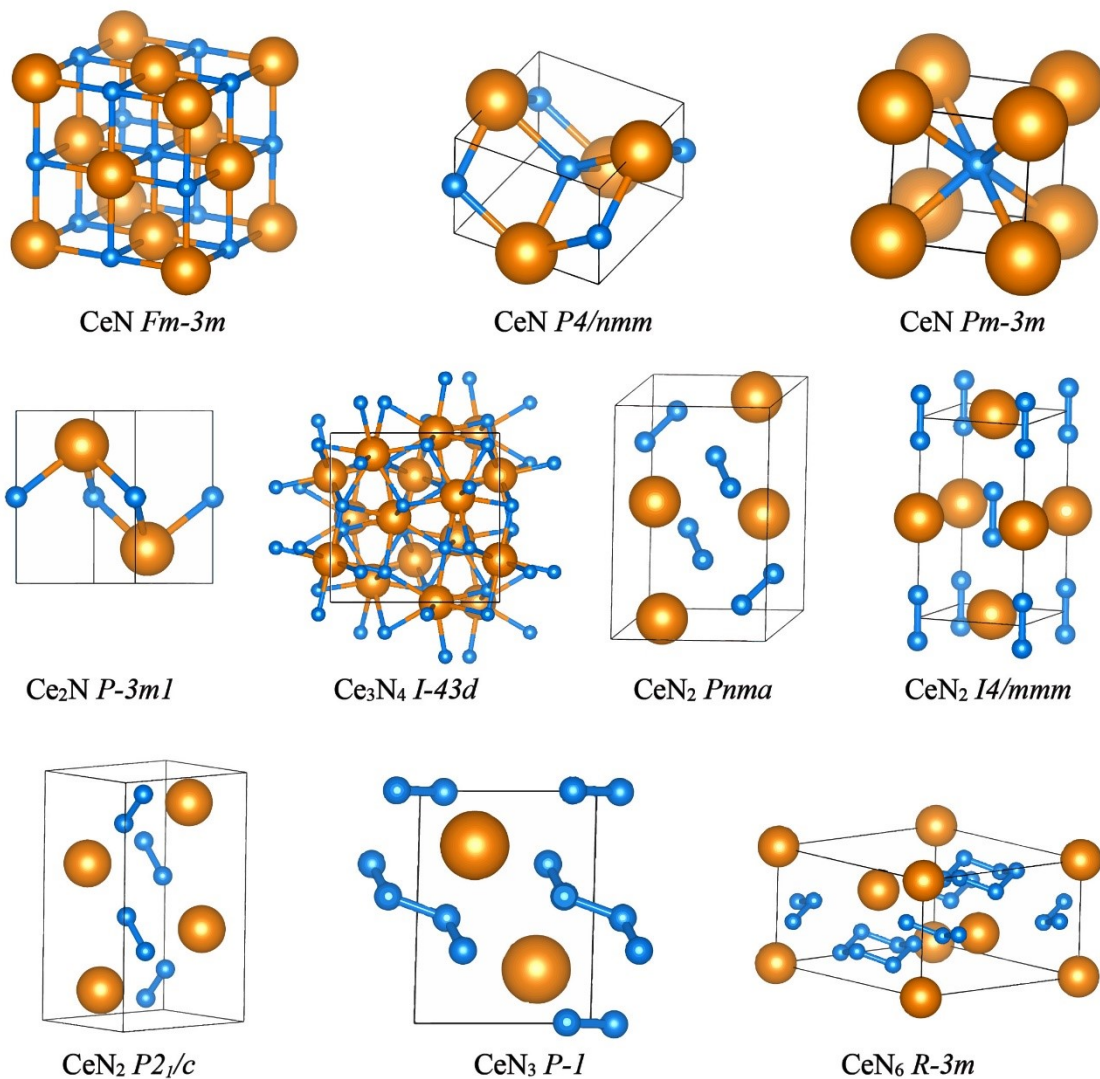*Nanjing University, Nanjing, 210093, China*

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Figure S1. Crystal structures of some dynamically stable Ce-N compounds. The orange and blue balls represent cerium and nitrogen atoms respectively.

Table. S1. The calculated lattice parameters of face-centered cubic (fcc) α-Ce (space group Fm-3m) at zero pressure through a variety of exchange-correlation functionals. Experimental and theoretical results from other works are also presented for comparison.

References	Methods	Lattice constants a
Zachariasen et al.[1]	Exp	4.877
Staun Olsen et al. [2]	Exp	4.877
Amadon et al. [3]	LDA+U	4.52
Casadei et al. [4]	PBE	4.68
This work	PBE	4.726
	PBE+U U=1	4.762
	PBE+U U=2	4.787
	PBE+U U=3	4.822
	PBE+U U=4	4.851
	PBE+U U=5	4.874
	PBE+U U=6	4.943

Table. S2. The calculated lattice parameters (units Å) of B1 CeN (space group *Fm-3m*) at zero pressure and the phase transition pressure point (units GPa) from B1 to B10 (space group *P4/nmm*) through a variety of exchange-correlation functionals. Experimental and theoretical results from other works are also presented for comparison. The experimental values from Olsen et al. and Nielsen et al. should be determined at room temperature (298K).

References	Methods	Lattice constants a	Transition pressure
Staun Olsen et al. [5]	Exp	5.021(2)	65-70
Nielsen et al.[6]	Exp	5.021(3)	65
Staun Olsen et al. [5]	PBE	5.024	68
Nielsen et al.[6]	PBE+U U=6.2 on N-2p	5.016	53
Sahoo et al.[7]	PW91	5.032	53
Zhang et al.[8]	LDA+U U=3.5 J=0.989	5.019	37.5
	PBE	5.045	
This work	PBE	5.049	43.5
	PBE+D3	5.012	40.4
	SCAN+rvv10	5.011	44.4
	PBE+U U=1	5.051	49.0
	PBE+U U=2	5.052	54.5
	PBE+U U=3	5.054	60.0
	PBE+U U=3.5	5.054	63.0
	PBE+U U=4	5.054	65.3
	PBE+U U=5	5.054	70.5
	PBE+U U=6	5.054	75.5

For the elemental cerium phases, Sandalov et al. used the LDA+U method and found that the itinerant electrons become localized 4f states with a Hubbard U above 2.7 eV [9]. Amadon et al. presented the LDA+U study with the values U=6.1 eV and J=0.7 eV (U_{eff} =U-J=5.4).[3] In a recent study, a critical value U_c = 3.29 was found to be necessary to describe the double well potential between α and γ phases.[10] In this study, we present the calculated lattice constants for the α-Ce with several functionals as shown in Table. S1, the PBE functional with a= 4.68Å underestimate the lattice constants. We further employed the DFT+U methods with a series of U values, while keeping the exchange parameters J at 0 eV. The employment of U raises the lattice constants gradually. A large value of U = 5 gives a similar lattice constant a = 4.874Å as the experimental result a=4.877Å. Overall, a large value of U > 3 is needed for the study of elemental cerium phases.

For the cerium nitride phases as presented in Table. S2, the experimentally obtained lattice constants of the B1 phase are near 5.021Å, but the PBE result of 5.049Å overestimates the lattice constants. In addition, the experimentally obtained transition pressure is near 65 GPa, and the previous theoretical works with GGA predicted the transition pressures of about 53 GPa. However, the calculated transition pressure within PBE methods in this work is about 43.5 GPa, which is lower than those experimental and theoretical values. We further employed the DFT+U methods with a series of U values, by which the transition pressure can be improved to a higher value. The DFT+U with U = 4 presents a transition pressure of 65.3 GPa, consistent with the experimental result of 65 GPa. In general, extra pressures are needed to overcome the energy barrier between two phases for structural transition in high-pressure experiments, the practical transition pressure should not be larger than 65 GPa. In another word, the applied U should not be larger than 4 for the cerium nitride phases.

We also take a look at other Ce-based materials, such as the Ce-O systems which are also ionic crystals. Fabris et al found the PBE+U (U=4.5eV) method has a good description of the reduction energy from CeO_2 to Ce_2O_3 and O_2.[11] Da Silva et al. studied the structural and electronic properties of CeO2 and Ce_2O_3 within the LDA, PBE, and HSE functionals.[12] They found PBE+U (U_{eff} =2.0 eV) or LDA+U (Ueff=3-4eV) methods have the best overall description for the energetics, and lattice constants in Ce2O3. They argued that there is no unique U that gives a reasonable account for all the ground properties including the structural parameters, relative energies of different oxides, and spectroscopic properties.

Overall, we think the DFT+U method with U = 3.5 should be a reasonable value for the calculation of Ce-N compounds, but such a unique value should not be the best choice for all the Ce-N systems in different chemical environments within a large pressure range of 0-150 GPa. The results from the PBE functional are also provided for comparison.

Table S3. Structural parameters of the thermodynamically stable and metastable Ce-N compounds at selected pressures within the PBE+U method.

Compounds	Pressure （GPa）	Space group	Lattice constants (distances in Å, angles in °)	Wyckoff position (Fractional coordinates)
			Stable	
Ce_3N_4	0	$R\text{-}3m$	a = 3.775, b =3.775, c = 26.733; α = 90.00, β = 90.00, γ = 120.00	Ce (0.00000, 0.00000, 0.00000), (0.00000, 0.00000,0.77764); N (0.66667, 0.33333, 0.71073), (0.33333, 0.66667, 0.79872)
Ce_3N_4	40	$I\text{-}43d$	a = 6.992, b = 6.992, c = 6.992; α = 90.00, β = 90.00, γ = 90.00	Ce (0.75000, 0.12500, 0.00000); N (0.07333, 0.07333, 0.07333)
CeN_2	5	$P4_32_12$	a = 4.117, b = 4.117, c = 9.595; α = 90.00, β = 90.00, γ = 90.00	Ce (0.53009, 0.53009, 0.50000); N (0.93372, 0.16630, 0.99725)
CeN_2	20	$Pnma$	a=7.656, b = 4.808, c = 3.829; α = 90.00, β = 90.00, γ = 90.00	Ce (0.62565, 0.75000, 0.16149); N (0.43616, 0.75000, 0.65374), (0.30783, 0.75000, 0.89255)
CeN_2	50	$I4/mmm$	a=3.280, b = 3.280, c = 5.873; α = 90.00, β = 90.00, γ = 90.00	Ce (0.50000, 0.50000, 0.00000); N (0.50000, 0.50000, 0.38551)
CeN_2	150	$P2_1/c$	a = 3.5572, b = 4.5468, c = 6.5548; α = 90.00, β = 105.09, γ = 90.00	Ce (0.80250, 0.22006, 0.56394); N (0.58051, 0.55564, 0.73295), (0.20324, 0.20697, 0.87289)
CeN_3	95	$P\text{-}1$	a = 3.6502, b = 3.8362, c = 4.9537; α = 86.35, β = 81.20, γ = 75.45	Ce (0.14876, 0.68404, 0.23297); N (0.45743, 0.16728, 0.45339), (0.24888, 0.73491, 0.68650), (0.64970, -0.13387, 1.00373)
CeN_4	50	$P\text{-}1$	a = 5.208, b = 4.348, c = 4.066; α = 95.70, β = 69.23, γ = 88.76	Ce (0.21348, 0.74710, 0.71533); N (0.28476, 0.22084, 0.43787), (0.02646, 0.25701, 0.68229), (0.51072, 0.63552, 0.09567), (0.70765, 0.80273, 0.91019)
CeN_4	120	$I4_1/a$	a=6.937, b = 6.937, c = 3.032; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.50000); N (0.70362, 0.14531, 0.72808)
CeN_6	140	$R\text{-}3m$	a=6.057, b = 6.057, c = 4.255; α = 90.00, β = 90.00, γ = 120.00	Ce (0.00000, 0.00000, 0.00000); N (0.12057, 0.24115, 0.44898)
CeN_8	60	$P2_1$	a=5.631, b = 4.764, c = 5.644; α = 90.00, β = 119.53, γ = 90.00	Ce (0.21332, 0.87336, 0.74442); N (0.23811, 0.36885, 0.61811), (0.69908, 0.40529, 0.79994), (0.45287, 0.46794, 0.59080),

				(0.16124, 0.39136, 0.17433), (0.66520, 0.84978, 0.10681), (0.12359, 0.86618, 0.28494), (0.87866, 0.95279, 0.07450), (0.58137, 0.94207, 0.65722).
CeN$_{10}$	50	*I4/m*	a=6.669, b = 6.669, c = 7.821; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.78233); N (0.66494, 0.91558, 0.13731), (0.09267, 0.24533, 0.58302), (0.71514, 0.02168, 0.00000)
CeN$_{15}$	35	*C2*	a=11.966, b = 5.084, c = 4.626; α = 90.00, β = 108.05, γ = 90.00	Ce (0.00000, 0.31892, 0.50000); N (0.79056, 0.77123, 0.05943), (0.83766, 0.68593, 0.33929), (0.67916, 0.80631, 0.01859), (0.75786, 0.68599, 0.47866), (0.66193, 0.76511, 0.28399), (0.98762, 0.65221, 0.85400), (0.98010, 0.89642, 0.75869), (0.00000, 0.04379, 0.00000).
CeN$_{15}$	50	*P2$_1$2$_1$2*	a=7.491, b = 7.275, c = 6.636; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.48872); N (0.03315, 0.41927, 0.14721), (0.04539, 0.36483, 0.42497), (0.15424, 0.78224, 0.80571), (0.12203, 0.86170, 0.05335), (0.26915, 0.65204, 0.85452), (0.21892, 0.79002, 0.25758), (0.30604, 0.65581, 0.14288), (0.00000, 0.50000, 0.59693).
Metastable				
Ce$_2$N	50	*P-3m1*	a=3.270, b =3.270, c = 4.507; α = 90.00, β = 90.00, γ = 90.00	Ce (0.33333, 0.66667, 0.78935); N (0.00000, 0.00000, 0.50000)
CeN$_8$	120	*R-3*	a=5.512, b = 5.512, c = 6.636; α = 90.00, β = 90.00, γ = 120.00	Ce (0.00000, 0.00000, 0.00000); N (0.00000, 0.00000, 0.36927), (0.20583, 0.24146, 0.30157).
CeN$_{10}$	20	*Immm*	a=3.758, b = 7.557, c = 7.579; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.00000); N(0.32561, 0.19274, 0.19498), (0.85185, 0.00000, 0.50000).
Quenchable				
CeN$_2$	0	*P4$_3$2$_1$2*	a=4.159, b = 4.159, c = 9.696; α = 90.00, β = 90.00, γ = 90.00	Ce (0.53169, 0.53169, 0.50000); N (0.93431, 0.16507, 0.99745)
CeN$_4$	0	*P-1*	a=4.438, b = 4.626, c = 5.657; α = 86.18, β = 68.91,	Ce (0.61045, 0.74675, 0.19630); N (0.77336, 0.23296, 0.28384),

|				
			$\gamma = 85.32$	(0.77582, 0.25328, 0.03608), (0.88431, 0.60857, 0.53684), (0.90371, 0.78409, 0.70949).
CeN$_4$	0	*I4$_1$/a*	a=7.682, b = 7.682, c = 3.430; $\alpha = 90.00$, $\beta = 90.00$, $\gamma = 90.00$	Ce (0.00000, 0.00000, 0.50000); N (0.70366, 0.15544, 0.68379).

Table. S4. The calculated enthalpy (unit eV/atom), formation enthalpy (unit eV/atom) relative to the Ce and N for the predicted Ce-N compounds at selected pressures with the PBE and PBE+U method; and the calculated zero point energy (ZPE) (unit eV) at the PBE level.

Compounds	Pressure （GPa）	Space group	ZPE (eV/atom)	Enthalpy PBE (eV/atom)	Formation Enthalpy PBE	Enthalpy PBE+U (eV/atom)	Formation enthalpy PBE+U
				Stable			
Ce$_3$N$_4$	0	*R-3m*	0.048	-8.680	-1.379	-8.072	-0.748
Ce$_3$N$_4$	40	*I-43d*	0.056	-5.314	-1.852	-4.692	-1.433
CeN$_2$	5	*P4$_3$2$_1$2*	0.069	-8.201	-1.307	-7.673	-1.270
CeN$_2$	20	*Pnma*	0.073	-7.068	-1.604	-6.513	-1.598
CeN$_2$	50	*I4/mmm*	0.078	-5.008	-1.811	-4.440	-1.889
CeN$_2$	150	*P2$_1$/c*	0.104	0.729	-1.486	1.409	-1.655
CeN$_3$	95	*P-1*	0.108	-2.663	-1.402	-2.212	-1.509
CeN$_4$	50	*P-1*	0.105	-5.145	-1.257	-4.820	-1.319
CeN$_4$	100	*I4$_1$/a*	0.124	-2.664	-1.234	-2.311	-1.333
CeN$_6$	140	*R-3m*	0.136	-1.143	-0.876	-0.880	-0.968
CeN$_8$	60	*P2$_1$*	0.136	-4.623	-0.782	-4.438	-0.821
CeN$_{10}$	50	*I4/m*	0.132	-5.094	-0.639	-4.944	-0.666
CeN$_{15}$	35	*C2*	0.136	-5.808	-0.355	-5.718	-0.377
CeN$_{15}$	50	*P2$_1$2$_1$2*	0.141	-5.070	-0.469	-4.973	-0.492
				Metastable			
Ce$_2$N	50	*P-3m1*	0.053	-2.729	-1.261	-1.452	-1.276
CeN$_8$	120	*R-3*	0.150	-2.057	-0.689	-1.868	-0.753
CeN$_{10}$	20	*Immm*	0.118	-6.683	-0.368	-6.553	-0.388
				Quenchable			
CeN$_2$	0	*P4$_3$2$_1$2*	0.066	-8.619	-1.088	-8.102	-1.044
CeN$_4$	0	*P-1*	0.088	-8.059	-0.205	-7.759	-0.189
CeN$_4$	0	*I4$_1$/a*	0.088	-7.929	-0.074	-7.613	-0.042

Table S5. Structural parameters for the known phases of elemental cerium and cerium nitride at the PBE+U level, and for the elemental nitrogen phase at the PBE level at selected pressures.

| Compounds	Pressure （GPa）	Space group	Lattice constants (distances in Å, angles in °)	Wyckoff position (Fractional coordinates)
Ce	0	$Fm\text{-}3m$	a=4.828, b =4.828, c = 4.828; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.00000)
Ce	30	$C2m$	a=5.463, b =2.960, c = 2.960; α = 90.00, β = 122.80, γ = 90.00	Ce (0.00000, 0.00000, 0.00000)
Ce	30	$I4/mmm$	a=2.912, b =2.912, c = 4.728; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.00000)
N	0	$Pa\text{-}3$	a=6.150, b =6.150, c = 6.150; α = 90.00, β = 90.00, γ = 90.00	N (0.05221, 0.05221, 0.05221)
N	5	$P2_1/c$	a=4.328, b =4.434, c = 7.511; α = 90.00, β = 126.66, γ = 90.00	N (0.56090, 0.41172, 0.47652)
N	50	$P4_12_12$	a=2.840, b =2.840, c = 8.051; α = 90.00, β = 90.00, γ = 90.00	N (0.44507, 0.29602, 0.72636)
N	100	$I2_13$	a=3.516, b =3.516, c = 3.516; α = 90.00, β = 90.00, γ = 90.00	N (0.17622, 0.17622, 0.17622)
CeN	0	$Fm\text{-}3m$	a=5.054, b =5.054, c = 5.054; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.00000); N (0.50000, 0.00000, 0.00000)
CeN	100	$P4/nmm$	a=3.894, b =3.894, c = 2.773; α = 90.00, β = 90.00, γ = 90.00	Ce (0.50000, 0.00000, 0.94324); N (0.50000, 0.50000, 0.50000)
CeN	150	$Pm\text{-}3m$	a=2.683, b =2.683, c = 2.683; α = 90.00, β = 90.00, γ = 90.00	Ce (0.00000, 0.00000, 0.00000); N (0.50000, 0.50000, 0.50000)
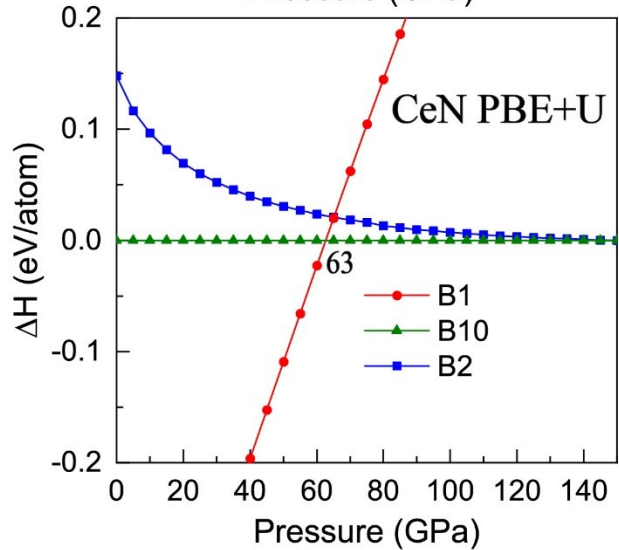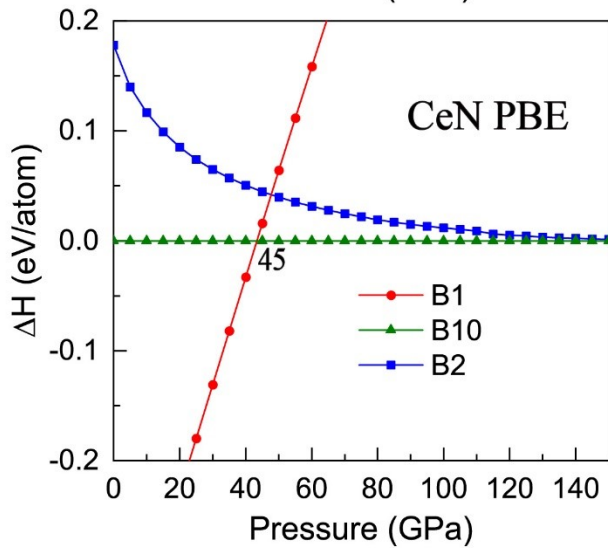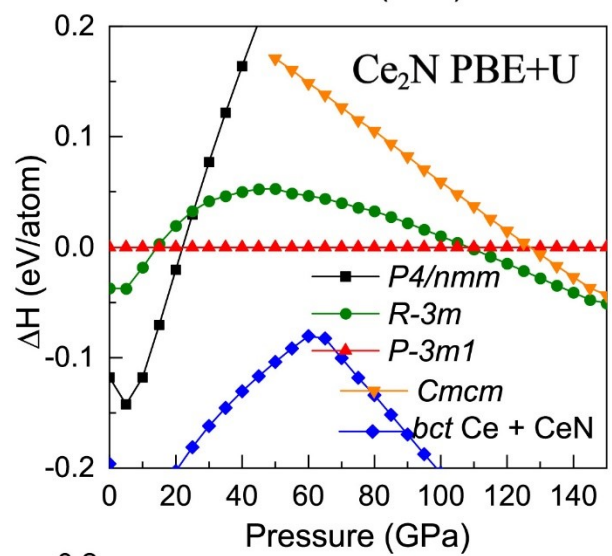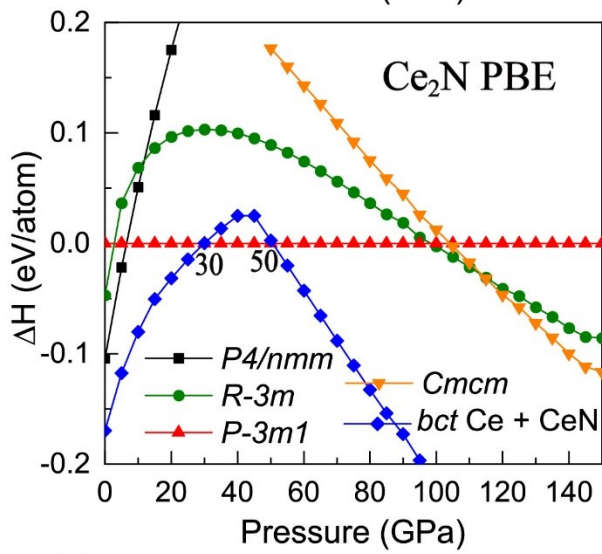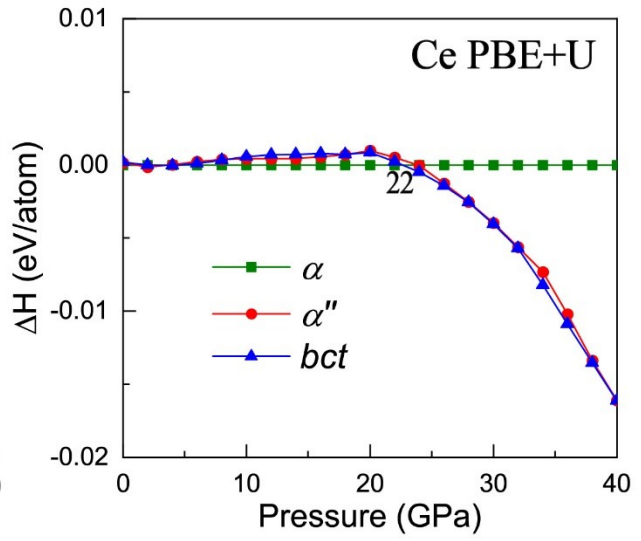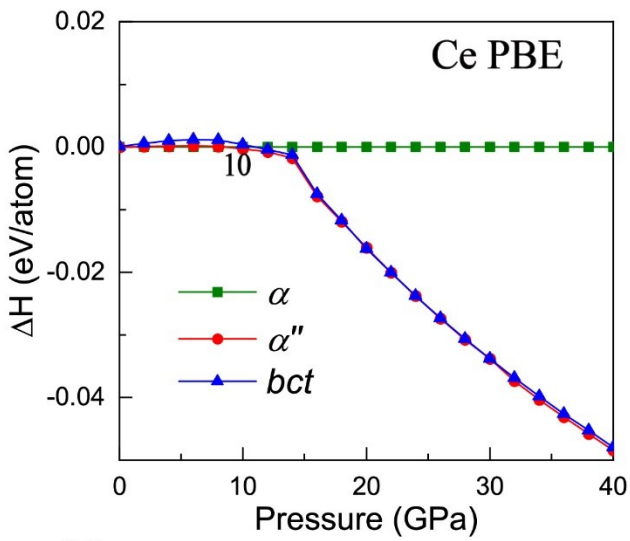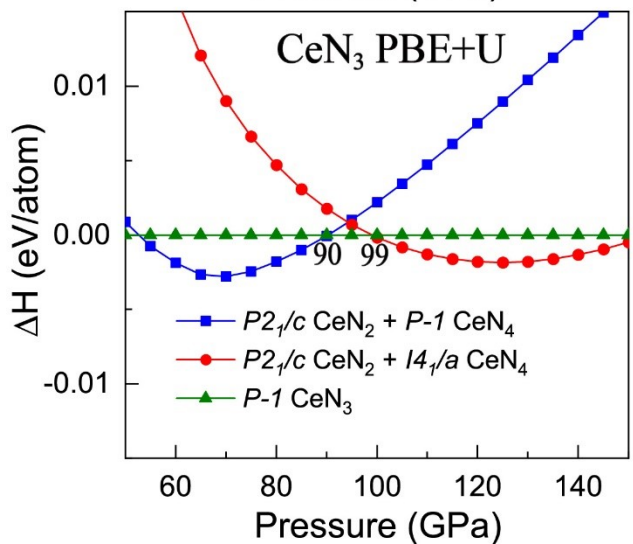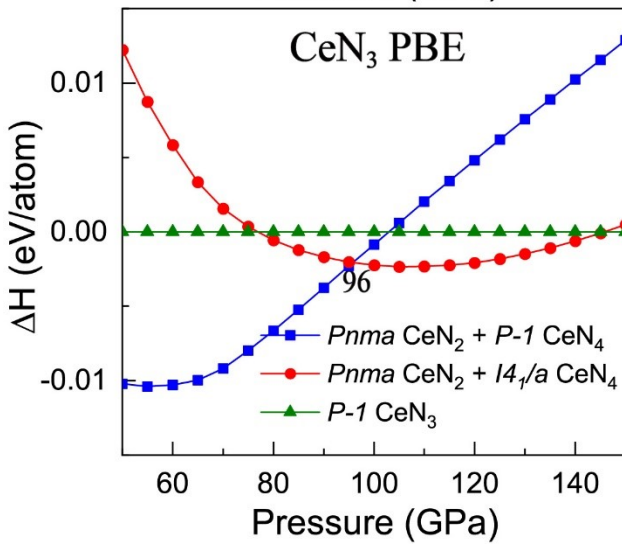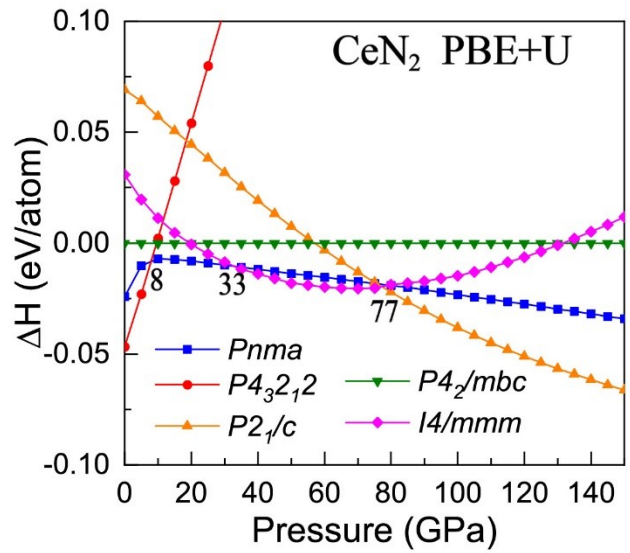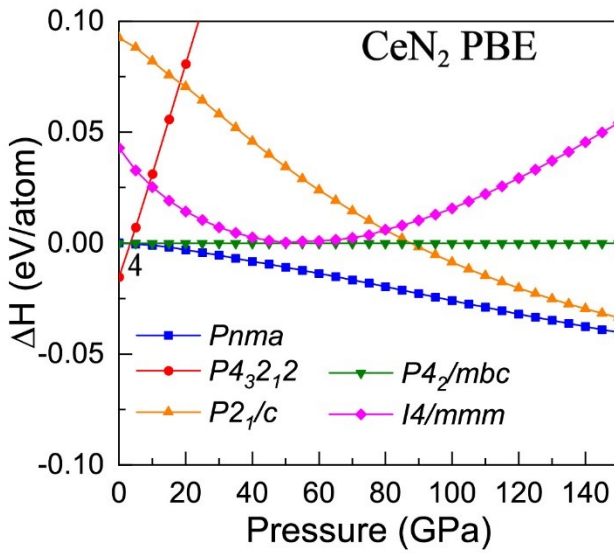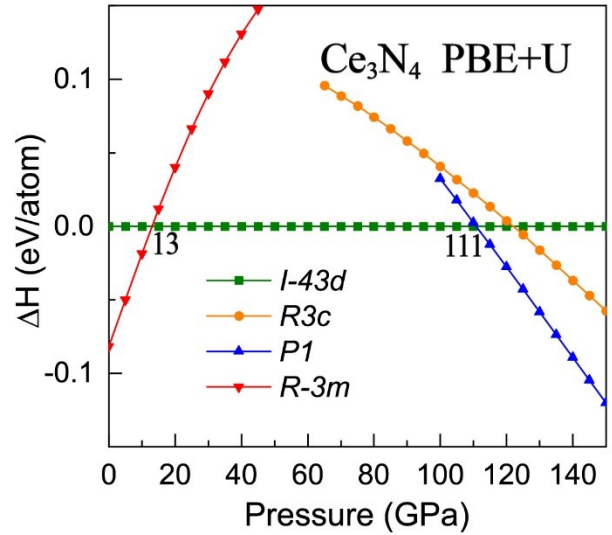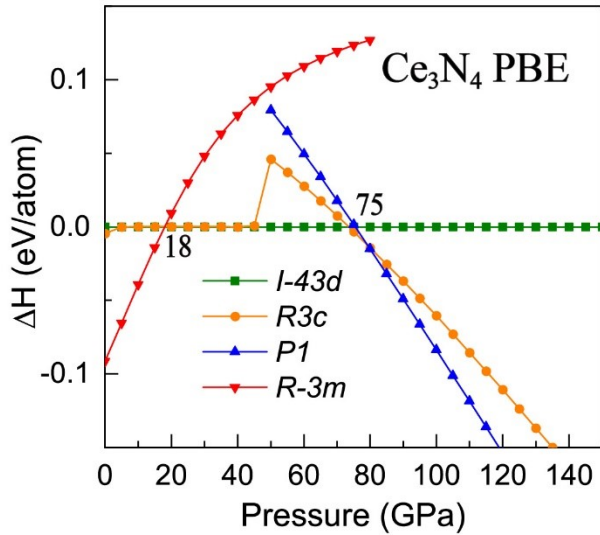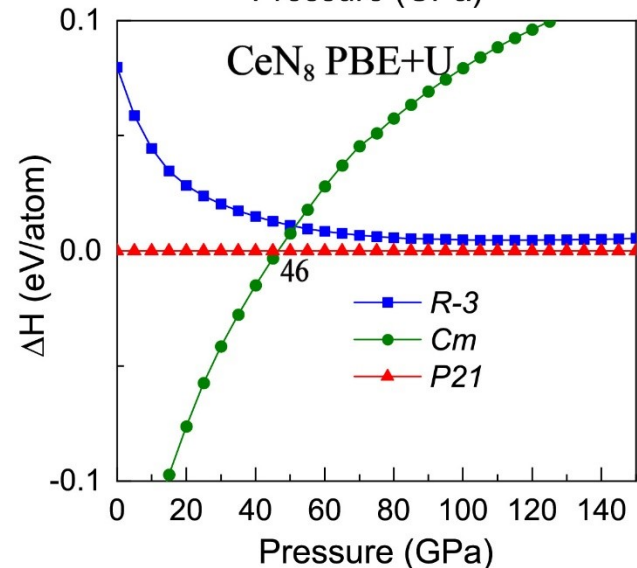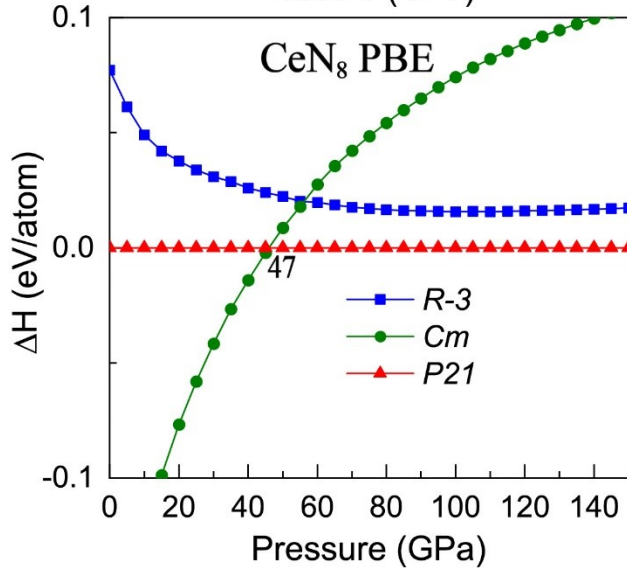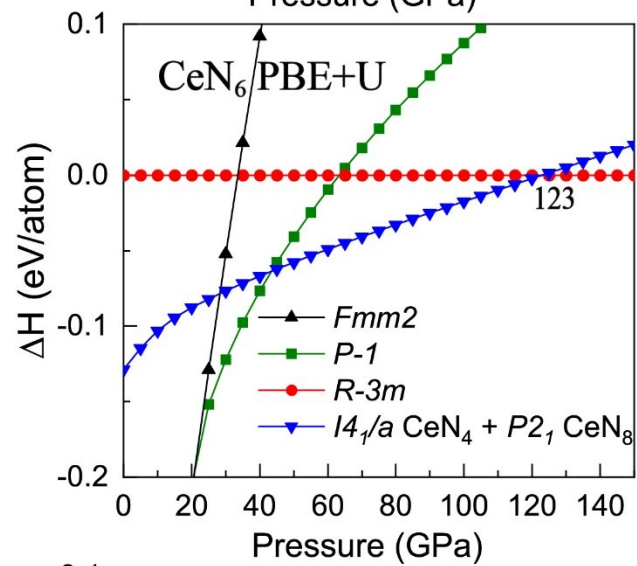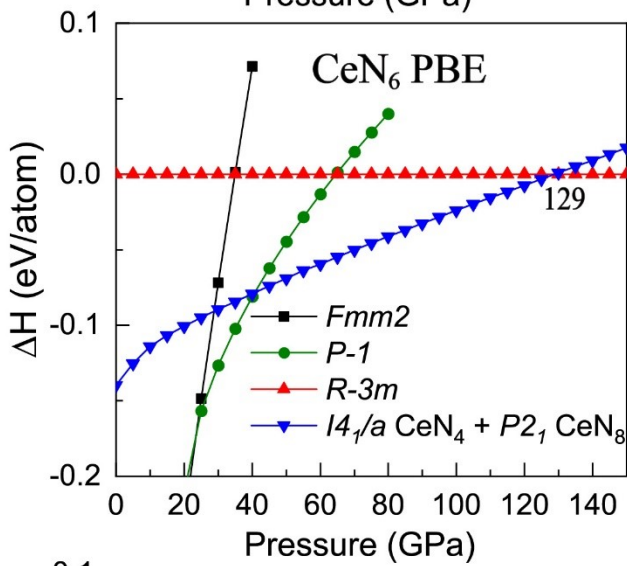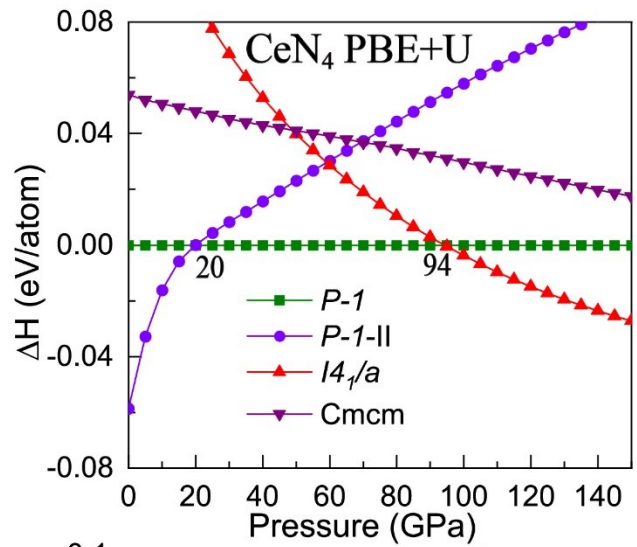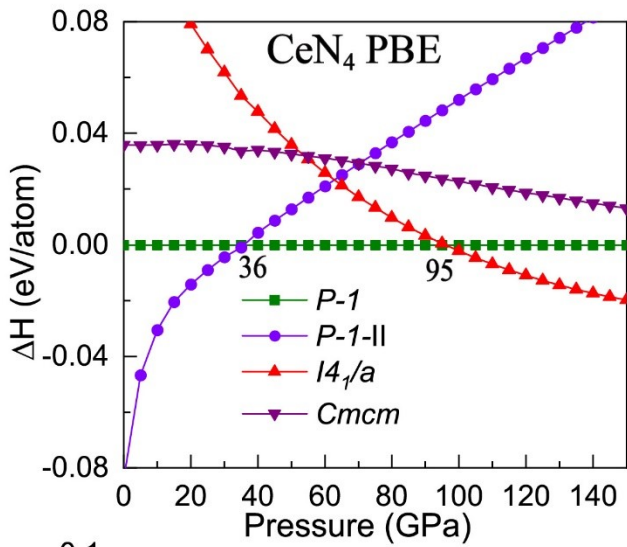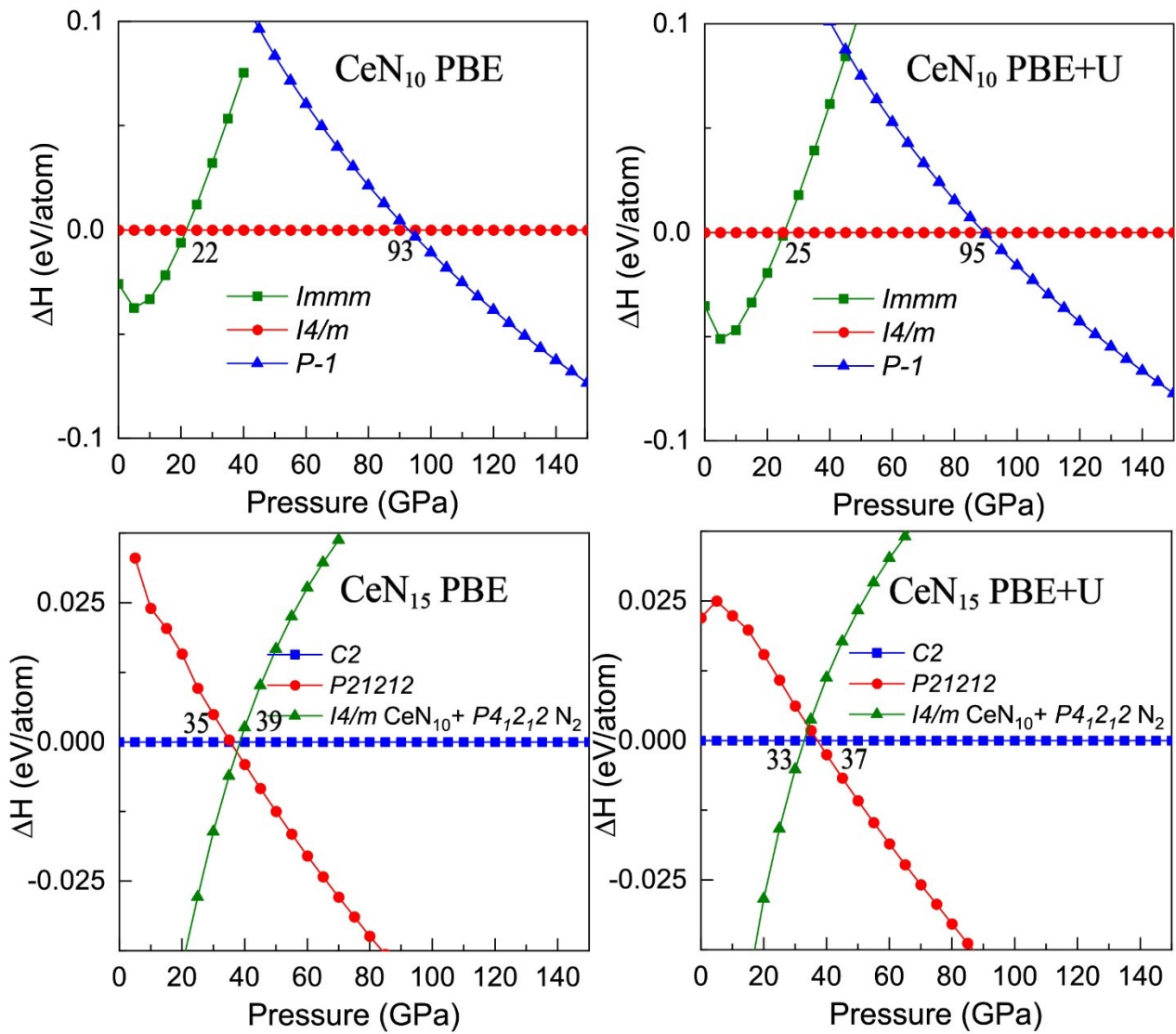
Figure S2. The calculated enthalpy curves with both the PBE and PBE+U method for a variety of Ce-N compositions
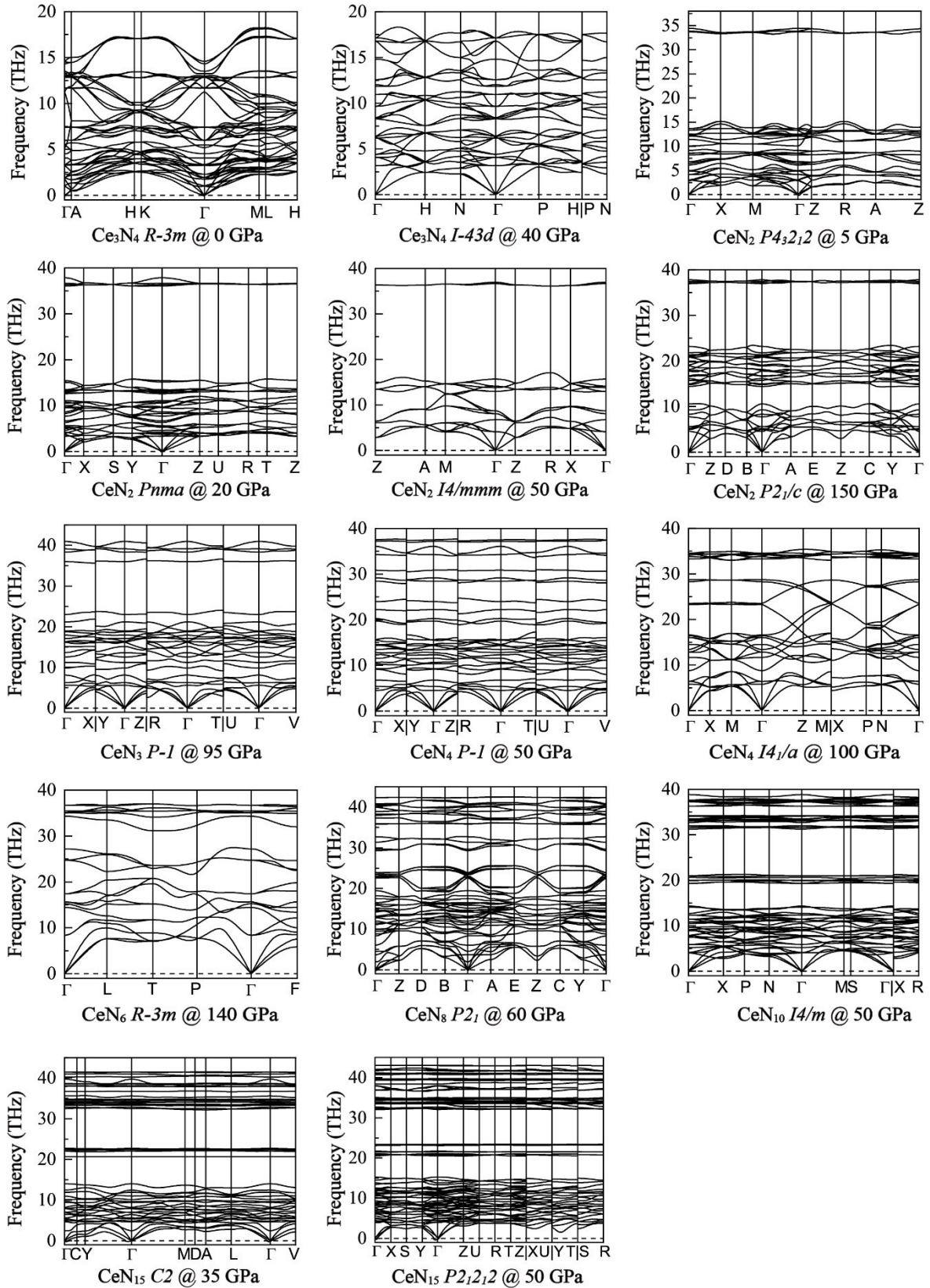
Figure S3. Calculated phonon spectrum for all the thermodynamically stable Ce-N compounds at selected pressures.
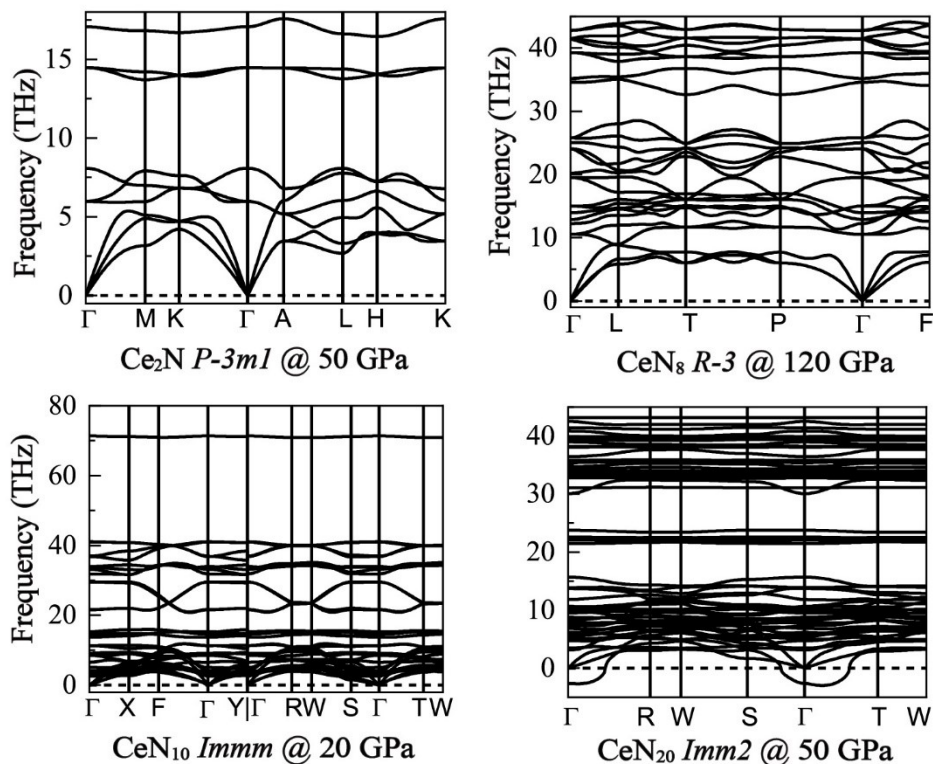
Figure S4. Calculated phonon spectrum for the thermodynamically not stable Ce-N compounds at selected pressures.
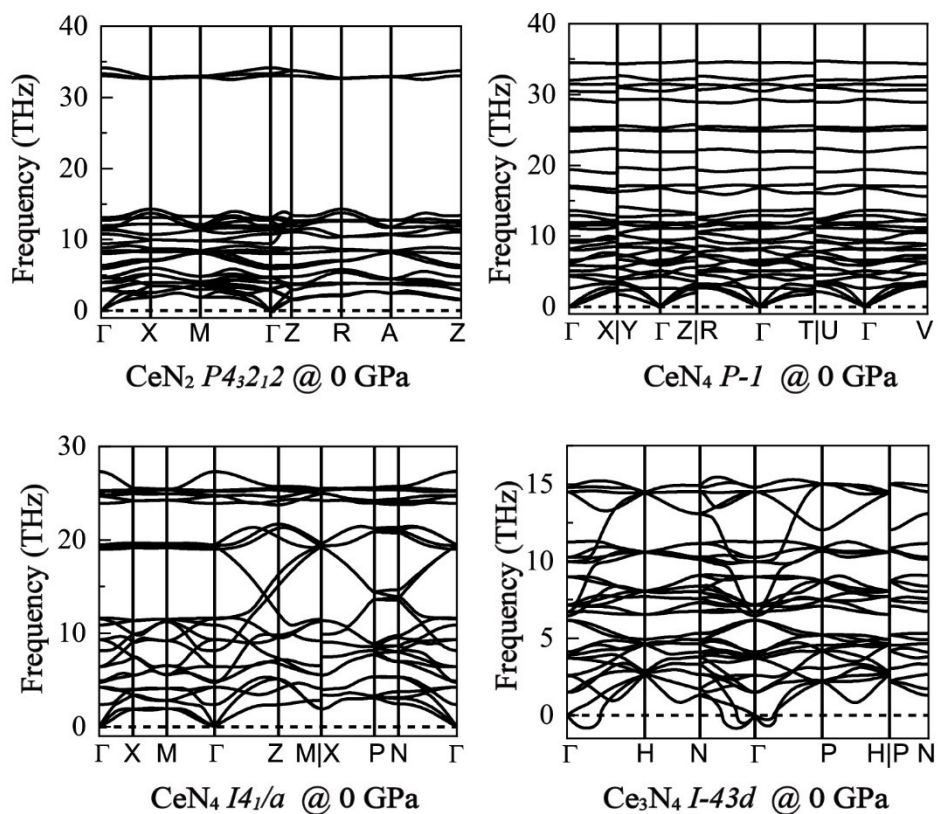

Figure S5. Calculated phonon spectrum for some cerium nitrides at ambient pressure.
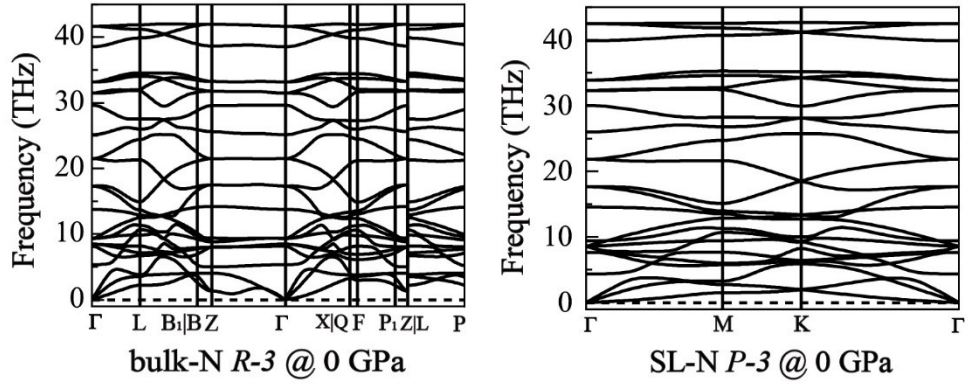
Figure S6. Calculated phonon spectrum for the nitrogen allotrope with the bulk and single layer forms at ambient pressure.
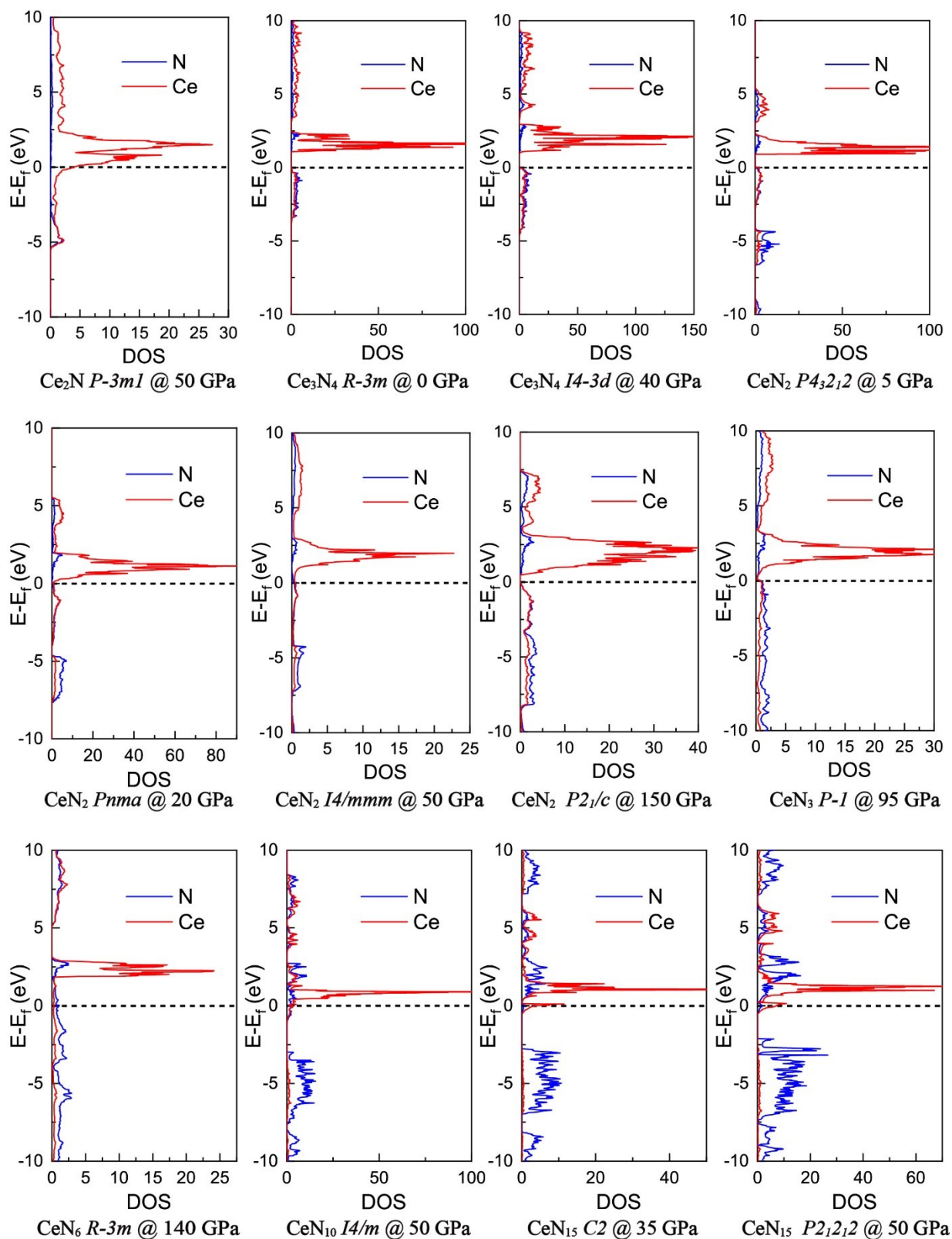
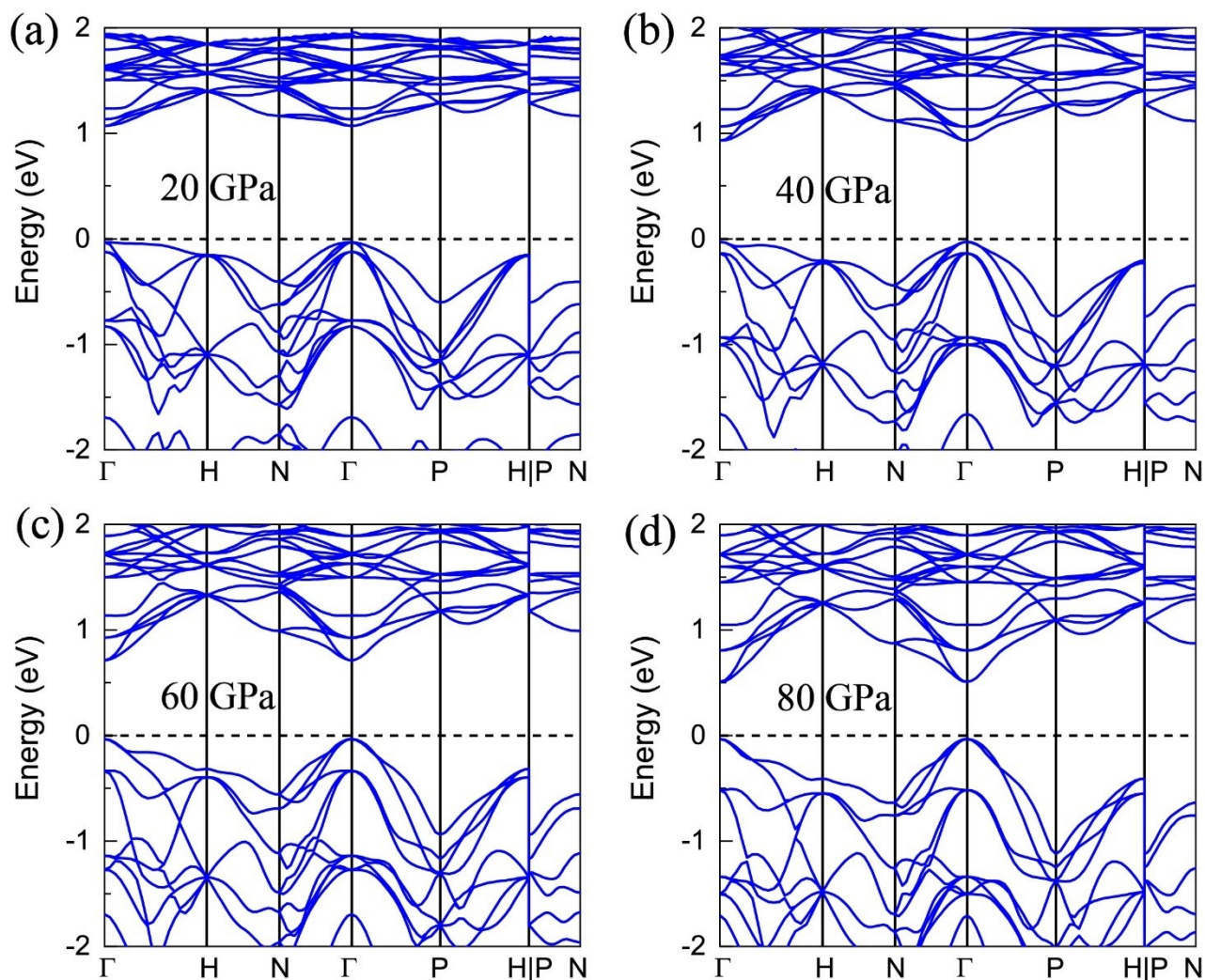**Figure S7.** The calculated projected density of states for some of the Ce-N compounds at selected pressures.

Figure S8. The calculated band structure of the *I-43d* Ce₃N₄ at (a) 20 GPa, (b) 40 GPa, (c) 60 GPa, and (d) 80 GPa at the PBE+U level.
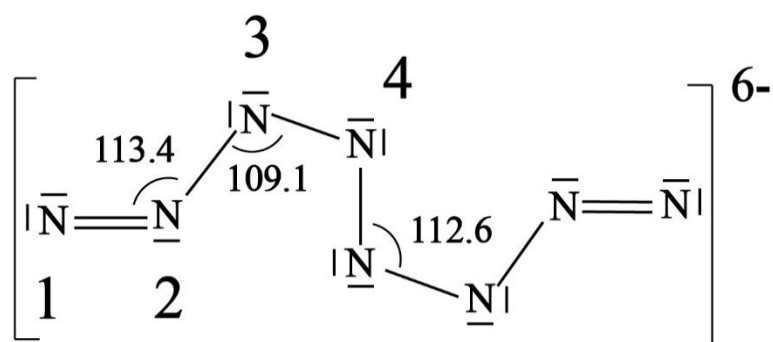

Figure S9. Another possible Lewis structure for the N$_8$ unit in the *P-1* CeN$_4$ at 50 GPa with a formal charge of -6.
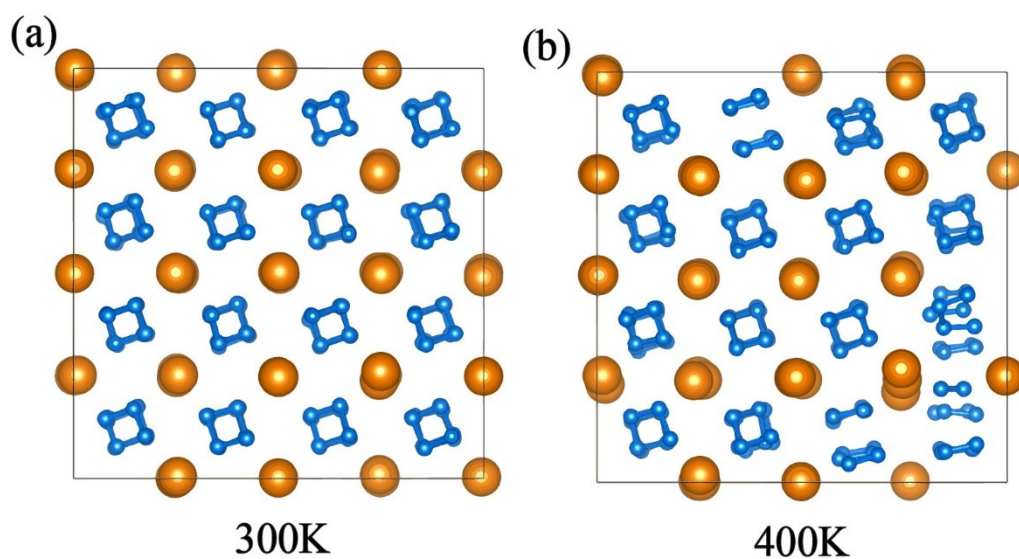
Figure S10. The AIMD simulation results of the $I4_1/a$ CeN$_4$ at (a) 300 K and (b) 400 K at 0 GPa with the PBE method. The infinite helical chain remains stable at 300K, but some chains are decomposed into the nitrogen N$_2$ units at 400 K.
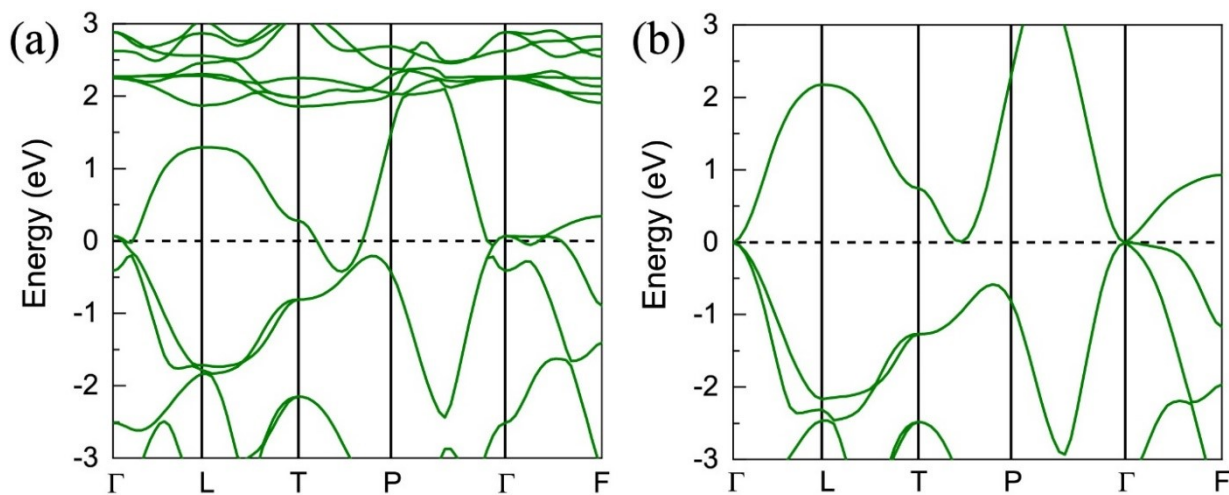

Figure S11. The calculated electronic band structure of the *R-3m* CeN$_6$ at 140 GPa at the (a) PBE+U and (b) HSE06 level.
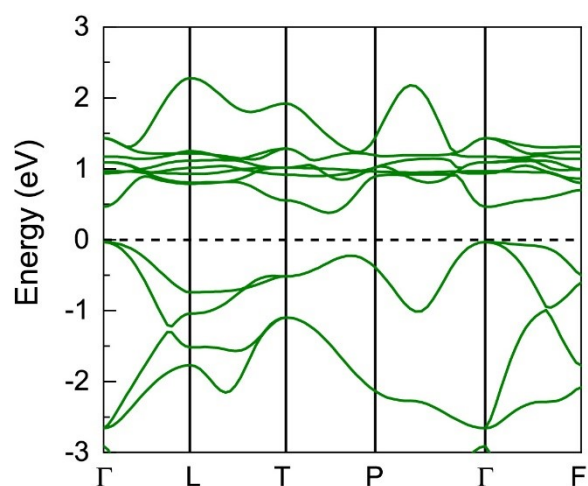
Figure S12. The calculated electronic band structure of the *R-3m* CeN$_6$ at 0 GPa at the PBE+U level.
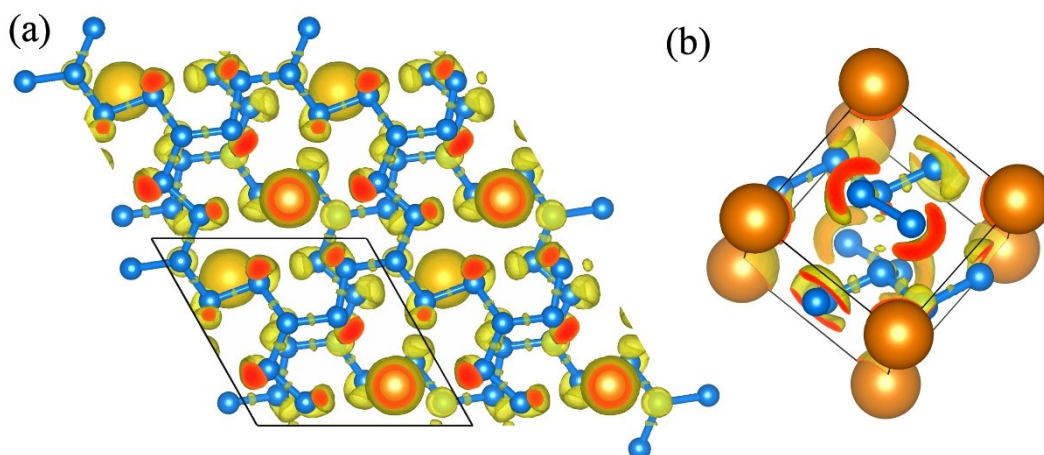

Figure S13. The calculated electron localization function (ELF) for the (a) *P2$_1$* CeN$_8$ at 60 GPa and (a) *R-3* CeN$_8$ at 120 GPa with the isosurface value of 0.85.
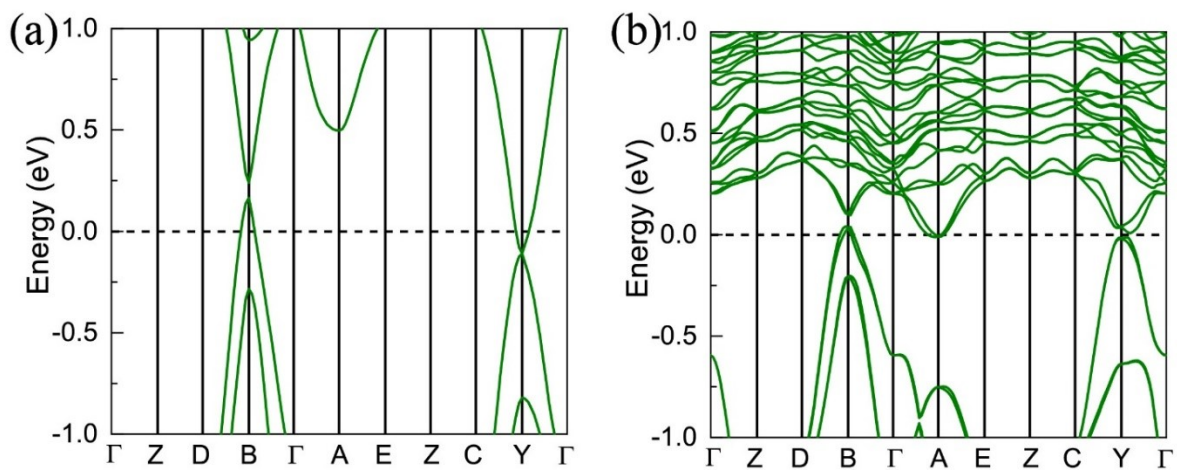
Figure S14. The calculated electronic band structure of the $P2_1$ CeN$_8$ at 60 GPa at the (a) HSE and (b) PBE+U+SOC level.
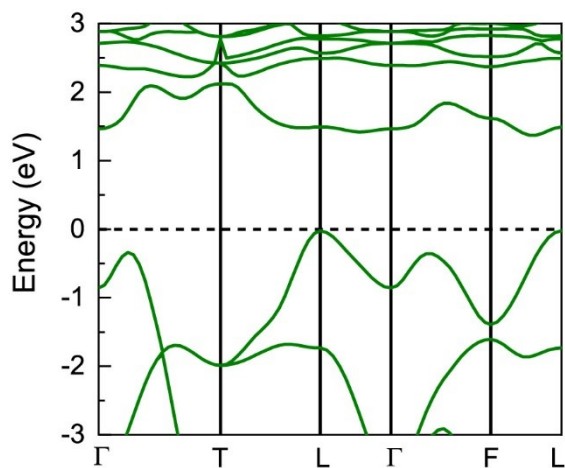

Figure S15. The calculated electronic band structure of the R-3 CeN$_8$ at 60 GPa at the HSE06 level.

Table. S6 The calculated bond orders from Manz' bond order equation with DDEC6 partitioning as employed in the Chargemol program.

CeN$_2$ *P4$_3$2$_1$2* @ 5 GPa,

Bond	Bond length	Bond order
N1-N1'	1.36	1.87

CeN$_2$ *Pnma* @ 20 GPa,

Bond	Bond length	Bond order
N1-N1'	1.34	1.86

CeN$_2$ *I4/mmm* @ 50 GPa,

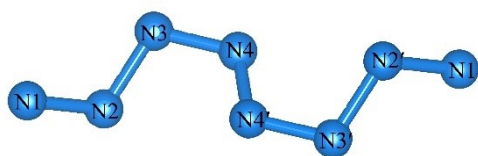| Bond	Bond length	Bond order
N1-N1'	1.34	1.77

CeN$_2$ *P2$_1$/c* @ 150 GPa

Bond	Bond length	Bond order
N1-N1'	1.35	1.43

CeN$_3$ *P-1* @ 95 GPa

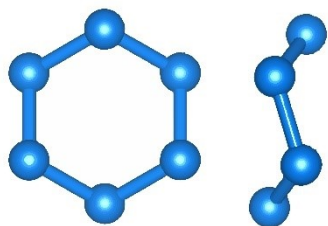| Bond	Bond length	Bond order
N1-N1'	1.30	1.59
N2-N3	1.31	1.46
N3-N3'	1.31	1.25

CeN$_4$ *P-1* @ 50 GPa

Bond	Bond length	Bond order
N1-N2	1.35	1.42
N2-N3	1.40	1.12
N3-N4	1.32	1.34
N4-N4'	1.38	1.16

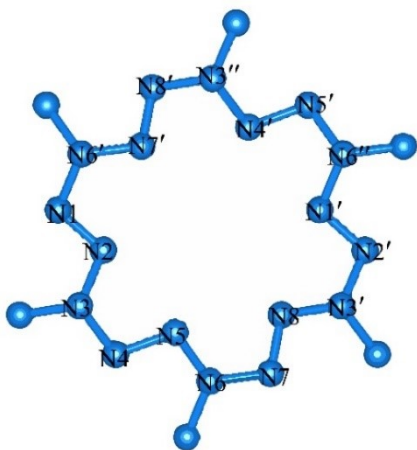CeN$_4$ *I4$_1$/a* @ 120 GPa

Bond	Bond length	Bond order
N1-N1'	1.36	1.16

CeN$_6$ *R-3m* @ 140 GPa

Bond	Bond length	Bond order
N-N	1.34	1.13

CeN$_8$ *P2$_1$* @ 60 GPa

Bond	Bond length	Bond order
N1-N2	1.39	1.32
N2-N3	1.37	1.06
N3-N4	1.39	1.00
N4-N5	1.37	1.21
N5-N6	1.38	1.04
N6-N7	1.32	1.12
N7-N8	1.31	1.27
N8-N3'	1.34	1.09
N1-N6'	1.34	1.09

CeN$_8$ *R-3* @ 120 GPa
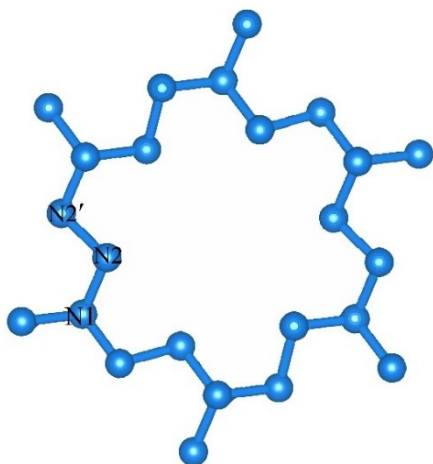
Bond	Bond length	Bond order
N1-N2	1.32	1.04
N2-N2'	1.35	1.15

CeN$_{10}$ *I4/m* @ 50 GPa

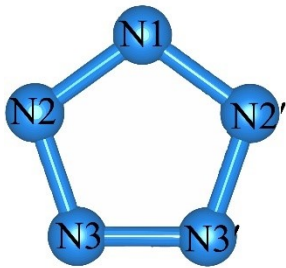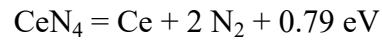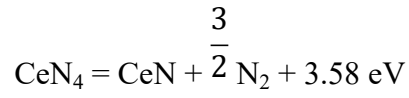| Bond	Bond length	Bond order
N1-N2	1.33	1.26
N2-N3	1.30	1.33
N3-N3'	1.30	1.34

CeN$_{10}$ *Immm* @ 20 GPa
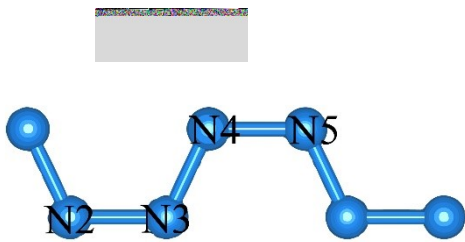
Bond	Bond length	Bond order
N1-N1'	1.11	2.45
N3-N4	1.33	1.35
N2-N3	1.31	1.45
N4-N5	1.31	1.45

Table. S7. The energy density properties of the $I4_1/a$ CeN_4 with different decomposition products including Ce_3N_4, CeN, or Ce at ambient pressure. The energy difference between the crystal α-N_2 and the gaseous nitrogen molecule is taken as 0.25 eV/atom.[13]

$$CeN_4 = \frac{1}{3} Ce_3N_4 + \frac{4}{3} N_2 + 3.67 \text{ eV}$$

$$CeN_4 = CeN + \frac{3}{2} N_2 + 3.58 \text{ eV}$$

$$CeN_4 = Ce + 2 N_2 + 0.79 \text{ eV}$$
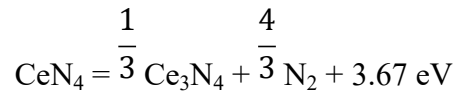
Products	ρ (g/cm³)	E_g (kJ/g)	E_v (kJ/cm³)	V_d (km/s)	P_d (GPa)
$Ce_3N_4 + N_2$	6.43	1.81	11.62	11.69	98.6
$CeN + N_2$	6.43	1.76	11.33	12.33	109.5
$Ce + N_2$	6.43	0.39	2.49	9.75	68.5

Table. S8. The calculated structural parameters and relative energies for a variety of nitrogen element phases at 0 GPa with the SCAN+rvv10 exchange-correlation functional. The energy cutoff for the plane wave basis set is set as 1000 eV. The energy of α-phase (Pa-3) is taken as the reference. The lattice parameters for the P-1 N8 are from ref [14]

Compounds	Space group	Relative Energy (eV/atom)	Lattice constants (distances in Å, angles in °)	Wyckoff position (Fractional coordinates)
α-N$_2$	Pa-3	0	a=5.317, b =5.317, c = 5.317; α = 90.00, β = 90.00, γ = 90.00	N (0.55991, 0.55991, 0.55991)
ε-N2	R-3c	0.0004	a=9.051, b = 9.051, c = 12.436; α = 90.00, β = 90.00, γ = 120.00	N (0.93457, 0.39097, 0.10884), (0.66667, 0.33333, 0.28897)
cg-N	I2$_1$3	1.3850	a=3.770, b =3.770, c = 3.770; α = 90.00, β = 90.00, γ = 90.00	N (0.16597, 0.16597, 0.16597)
Zigzag-N	Cmcm	1.0471	a=3.276, b =5.619, c = 2.148; α = 90.00, β = 90.00, γ = 90.00	N (0.00000, 0.06490, 0.75000)
N$_6$	C2m	0.9701	a=5.799, b =3.459, c = 7.976; α = 90.00, β = 105.39, γ = 90.00	N (0.26830, 0.00000, 0.84241), (0.13695, 0.00000, 0.70781), (0.46135, 0.50000, 0.57833).
SL-N$_8$	P-3	1.1020	a=5.875, b = 5.875, c = 20.000; α = 90.00, β = 90.00, γ = 120.00	N (0.46297, 0.38118, 0.50605), (0.66667, 0.33333, 0.50225).
Bulk-N$_8$	P-1	1.0541	a=4.093, b =4.961, c = 4.208; α = 90.00, β = 105.39, γ = 90.00	N (0.17400, 0.67700, 0.67400), (0.97400, 0.92500, 0.63200), (0.56900, 0.37400, 0.52600), (0.13200, 0.46800, 0.92700).
Bulk-N$_8$	R-3	1.0448	a=5.858, b = 5.858, c = 8,230; α = 90.00, β = 90.00, γ = 120.00	N (0.28634, 0.41493, 0.34791), (0.33333, 0.66667, 0.34393).

Figure S16. The AIMD simulation results of the bulk *R-3* nitrogen at 800K and 900K at ambient pressure. The layered configuration was well maintained at 800K, but some diatomic nitrogen units are dissociated from the nitrogen layers.
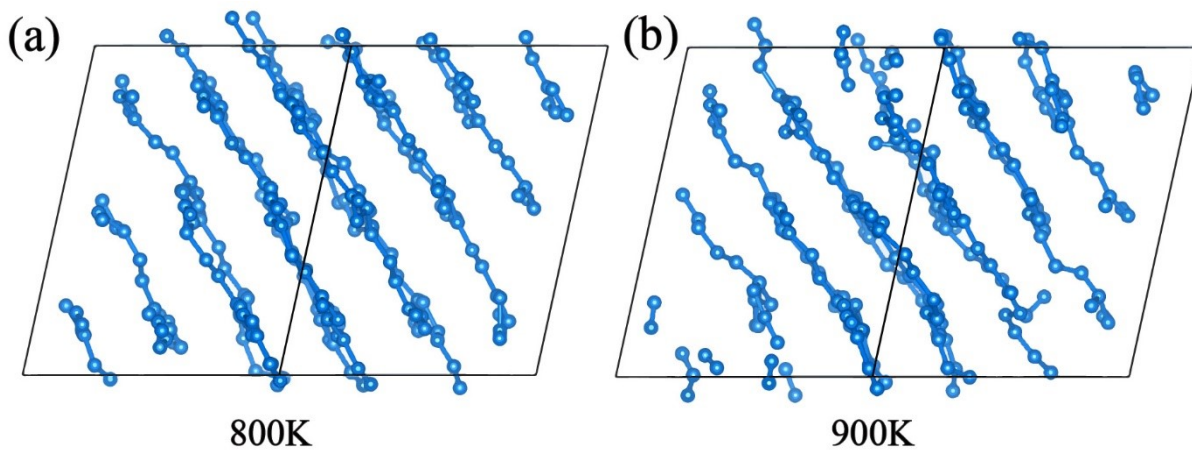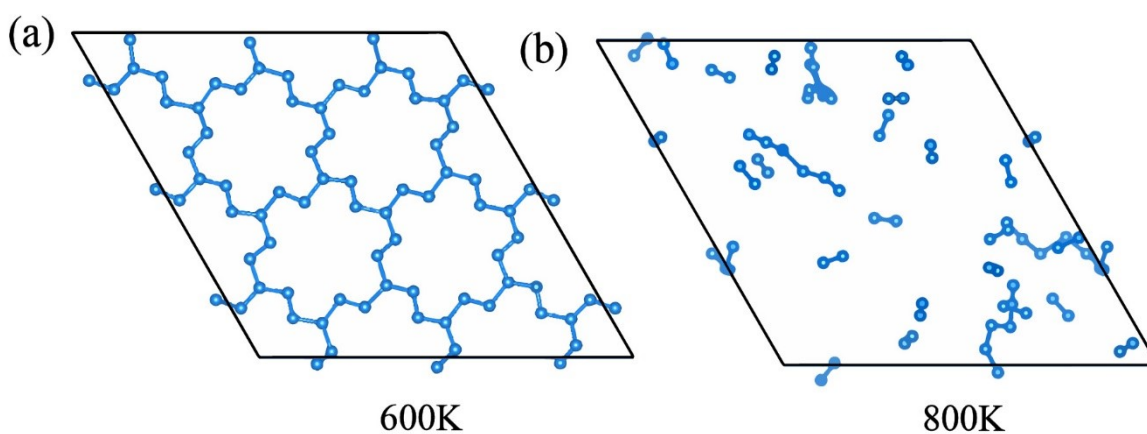

Figure S17. The AIMD simulation results of the monolayer *P-3* nitrogen at 600 K and 800 K at ambient pressure. The layered configuration was well maintained at 600 K, but isolated nitrogen units are formed at 800 K.

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