New members of high-energy-density compounds: YN_5 and YN_8

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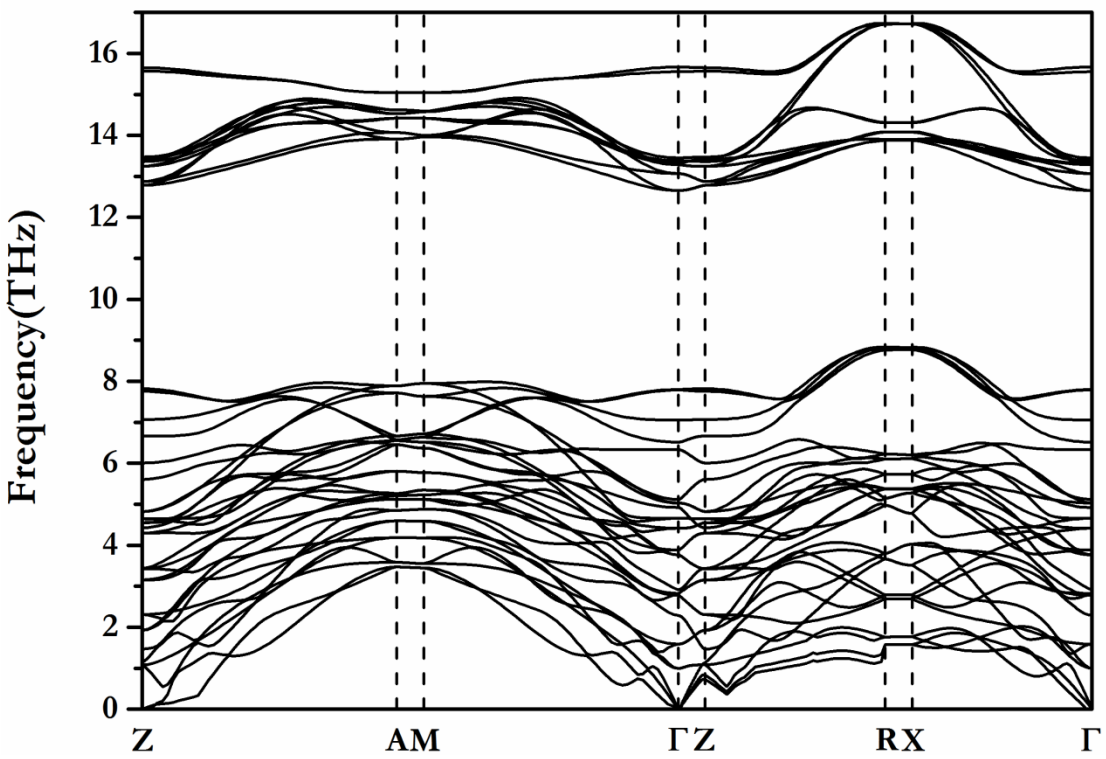

FIG. 1. Phonon dispersion curve of Y_5N_2 in the*P*4/*nmm* phase at 25 GPa

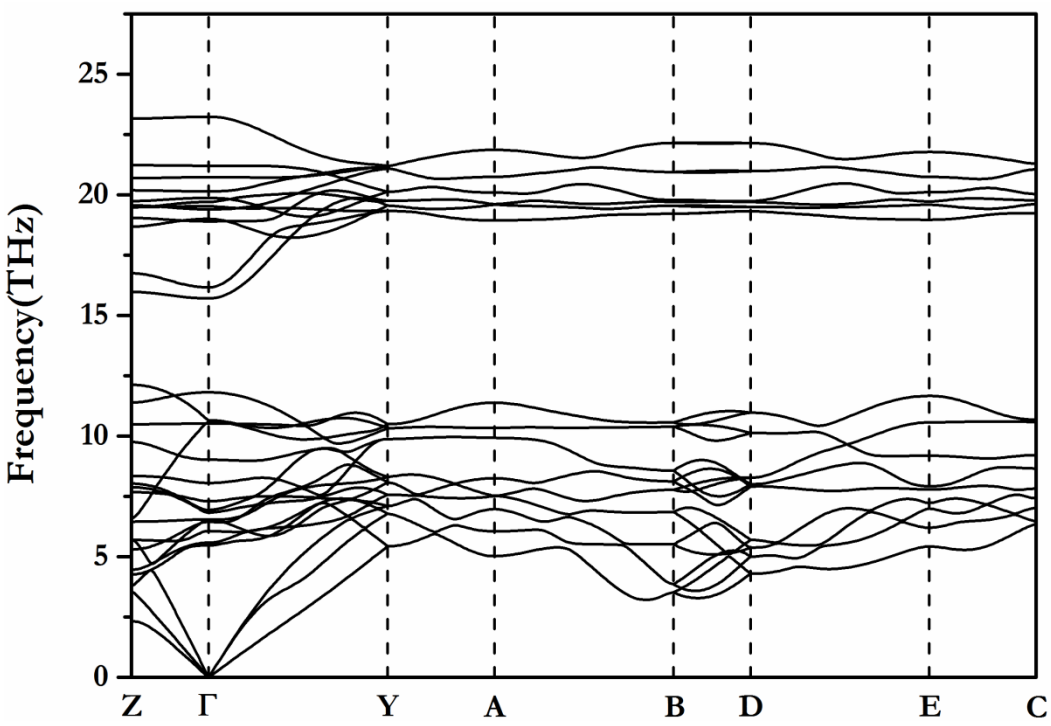

FIG. 2. Phonon dispersion curve of Y_3N_2 in the *C*2/*m* phase at 100 GPa.

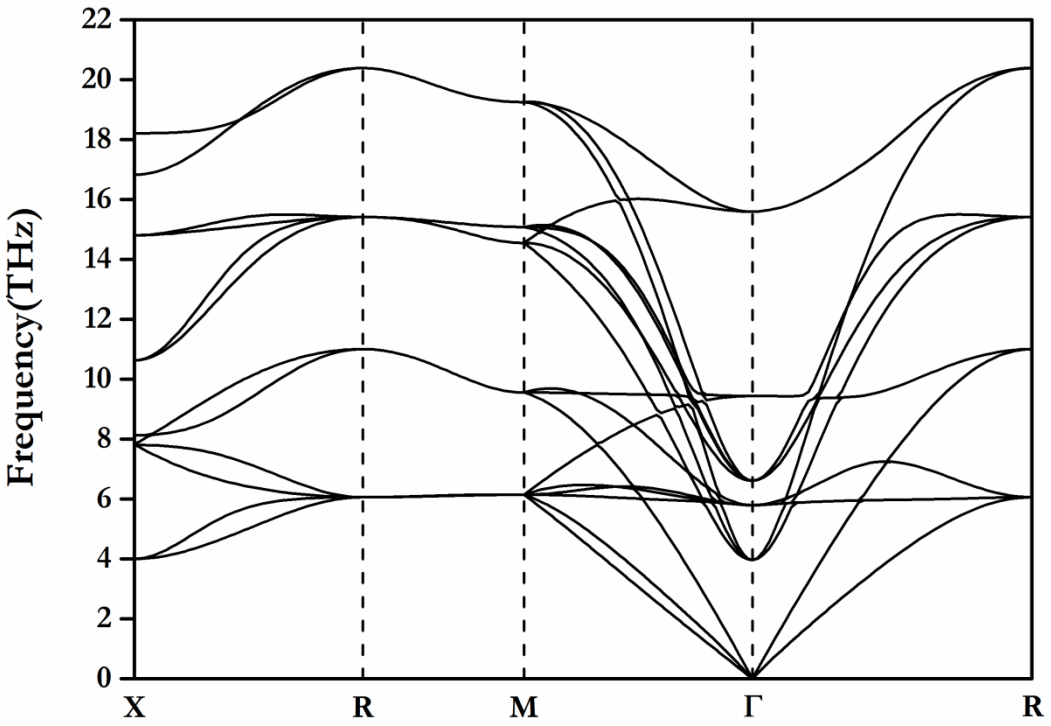

FIG. 3. Phonon dispersion curve of YN in the *Fm*-3*m* phase at 50 GPa.

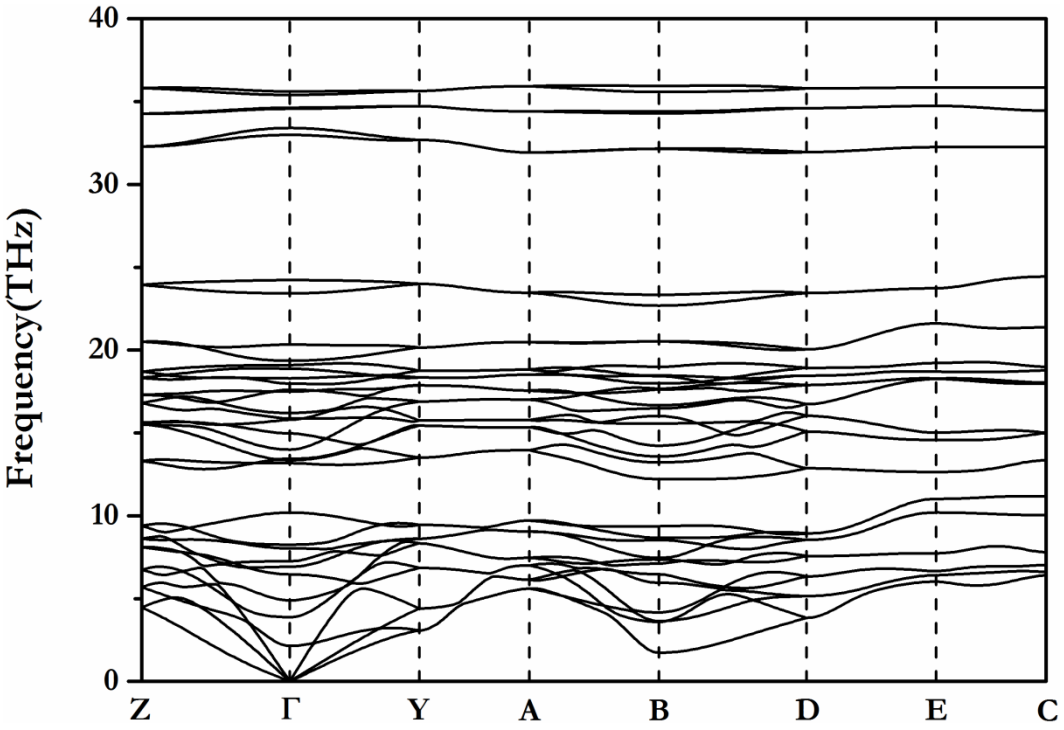

FIG. 4. Phonon dispersion curve of YN_2 in the $P2_1/c$ phase at 100 GPa.

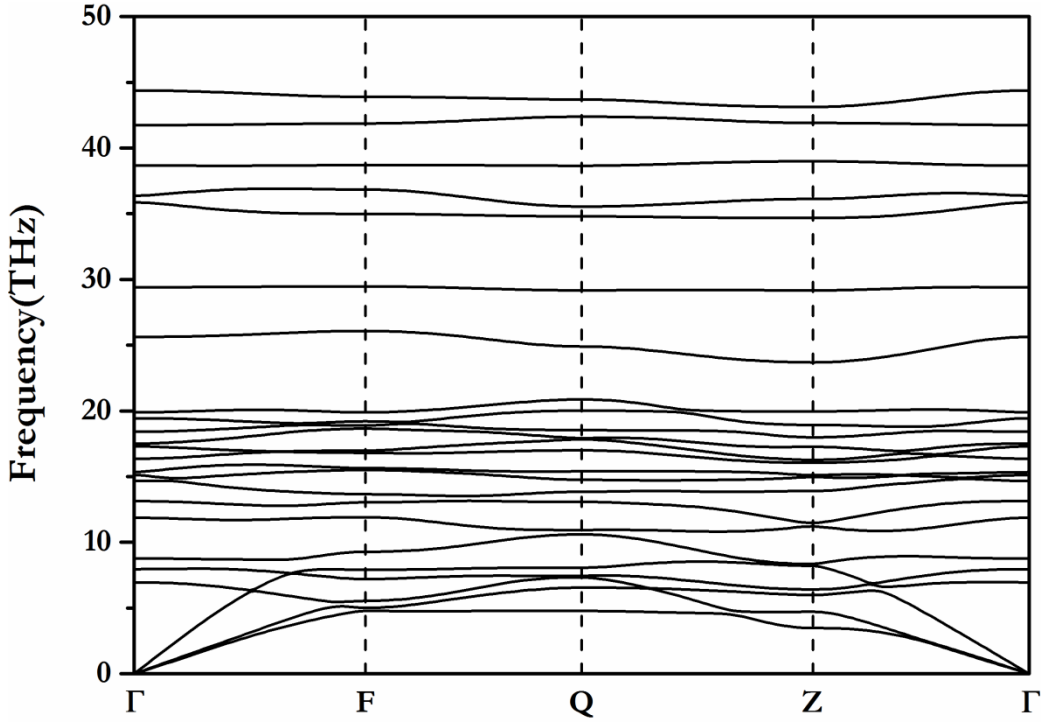

FIG. 5. Phonon dispersion curve of YN_3 in the P-1 phase at 50 GPa.

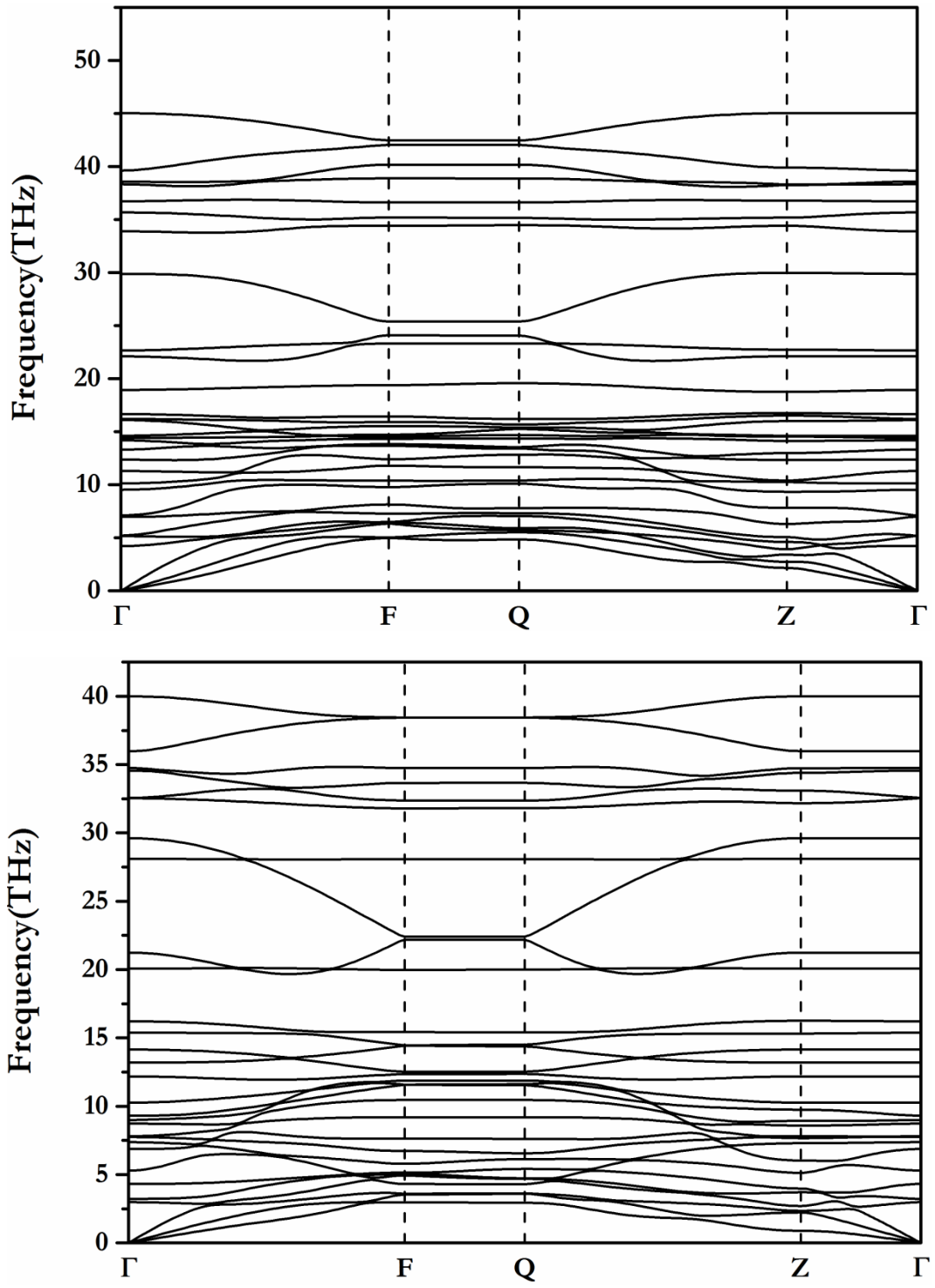

FIG. 6. Phonon dispersion curves of *P*-1 phase YN_4 at 50 GPa (upper panel) and 0 GPa (lower panel).

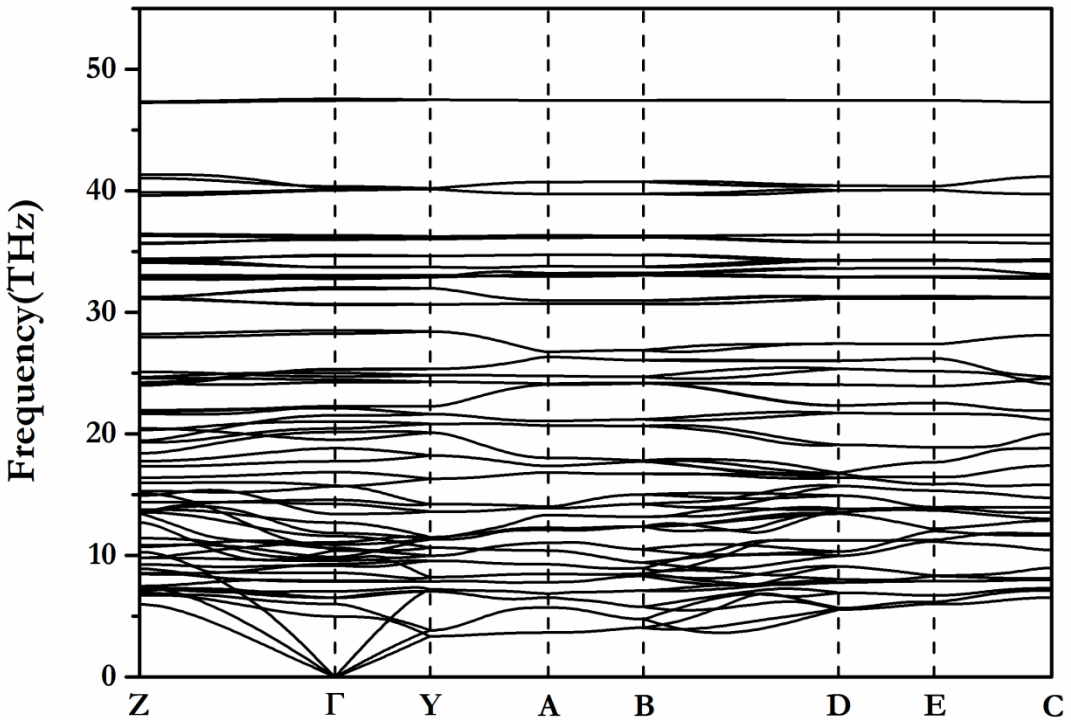

FIG. 7. Phonon dispersion curve of YN_5 in the *C*2/*m* phase at 100 GPa.

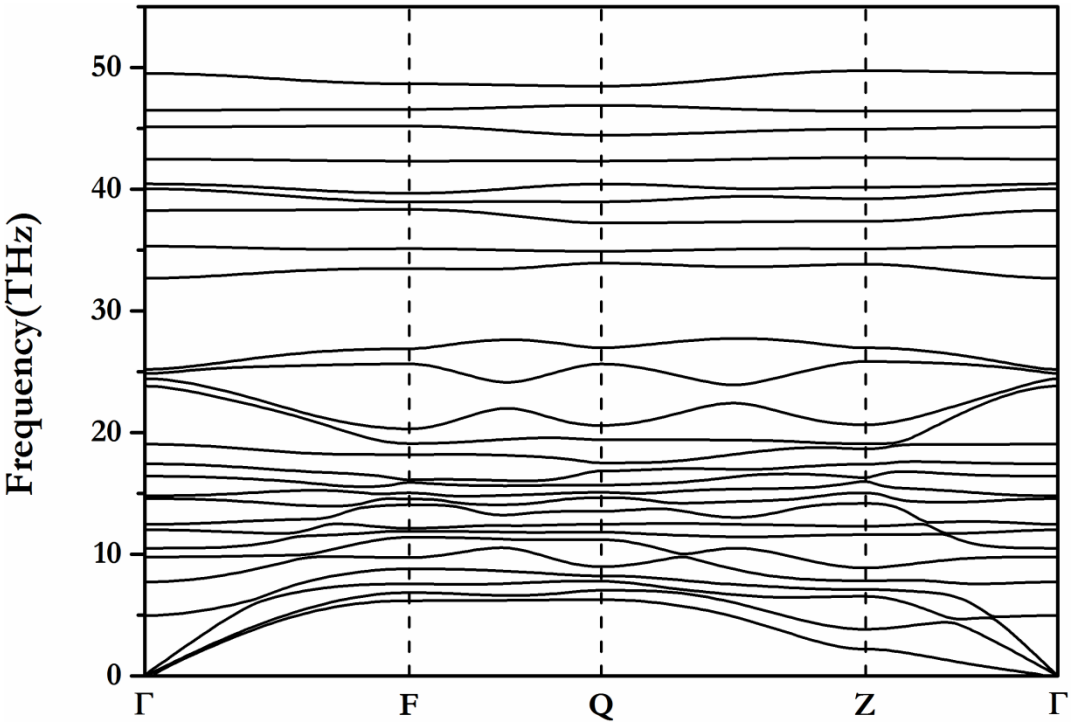

FIG. 8. Phonon dispersion curve of YN_8 in the *P*-1 phase at 75 GPa.

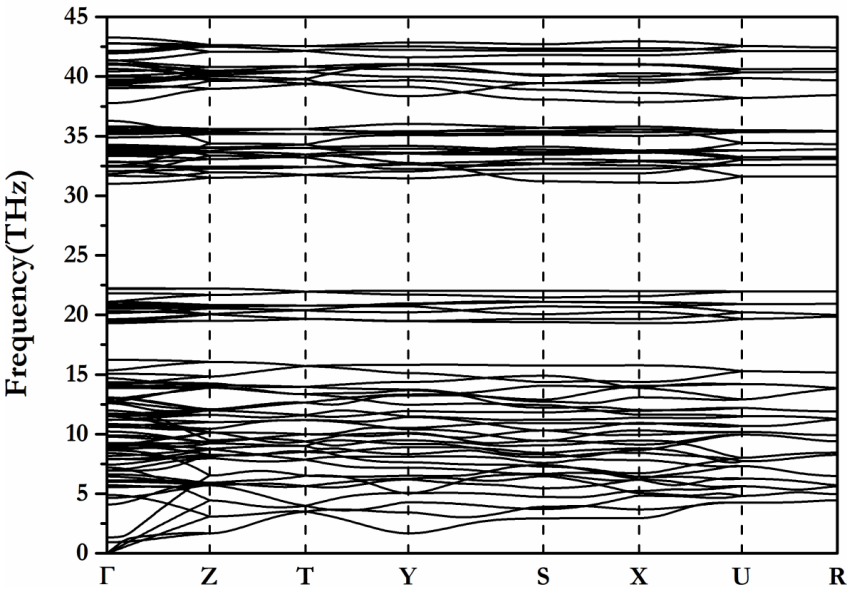

FIG. 9. Phonon dispersion curve of YN_{10} in the *Ibam* phase at 75 GPa.

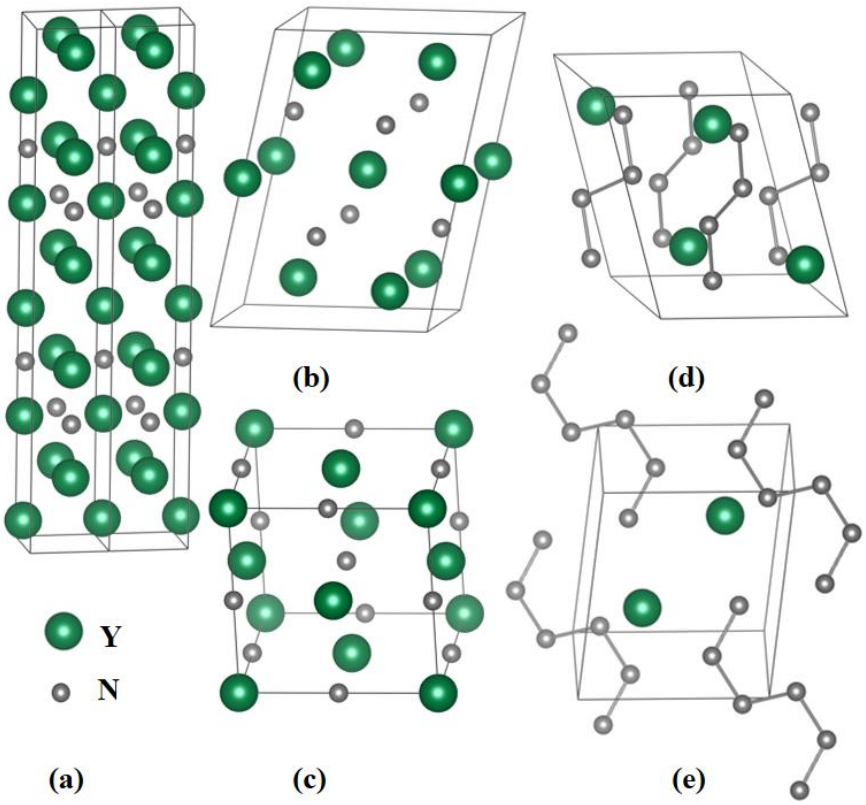

FIG. 10. Crystal structures of polynitrogens for Y-N compounds. (a) *P*4/*nmm* phase for Y_5N_2 at 25 GPa. (b) *C*/2*m* structure for Y_3N_2 at 100 GPa. (c) *Fm*-3*m* structure for YN at 50 GPa. (d) *P*21/*c* phase of YN_2 at 100 GPa. (e) *P*-1 phase of YN_3 at 50 GPa.

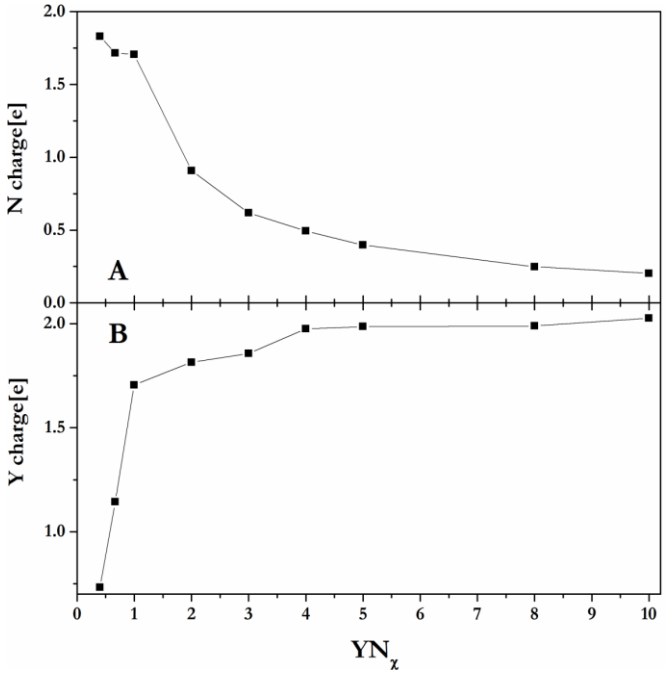

FIG. 11. The calculated cationic and anionic charges of N (A) and Y (B) ions in different YN*x* systems.Bader charge analysis reveals only part of the charges (1.47*e*) of atom transfer to N atom in YN layers and the charges transfer of Y→N are 0.12*e* and 0.31*e* in the double Y layers and quadruple Y layers for Y_5N_2, respectively. Here, we only give the average per atom transfer charges for Y_5N_2.

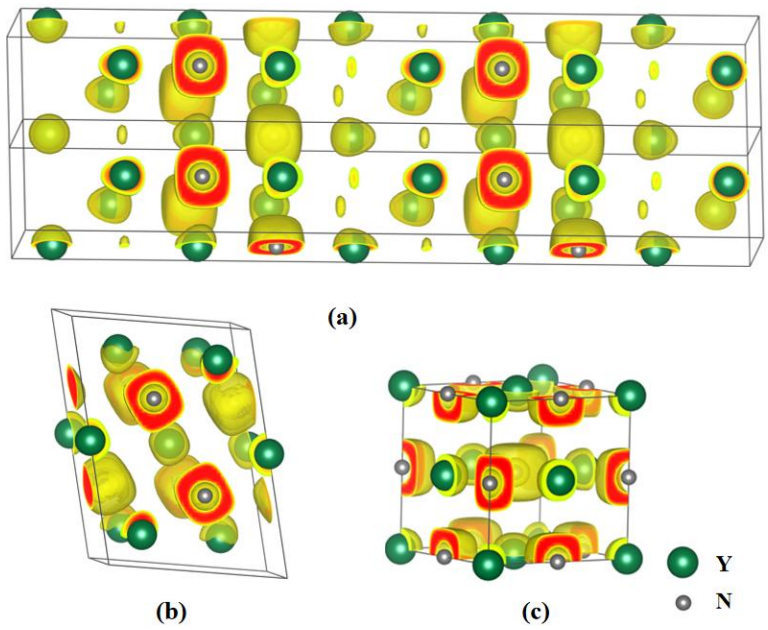

FIG. 12. ELFs for Y-N compounds. (a) *P*4/*nmm* phase for Y_5N_2 at 25 GPa. (b) *C*/2*m* phase for Y_3N_2 at 100 GPa. (c) *Fm*-3*m* phase for YN at 50 GPa.

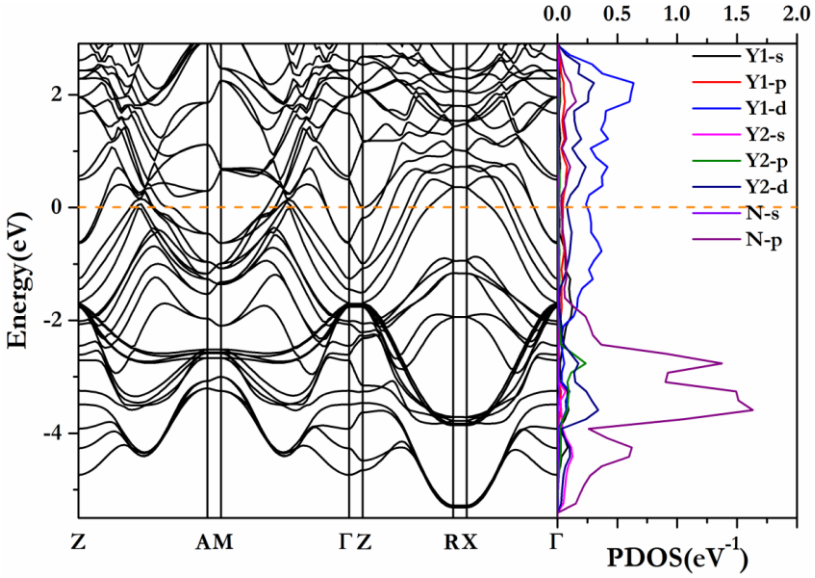

FIG. 13. Electronic band structure and projected DOS per atom of Y1-*s*, Y1-*p*, Y1-*d*, Y2-*s*, Y2-*p*, Y2-*d*, N-*s*, and N-*p* states of P4/*nmm* phase Y_5N_2 at 25 GPa. Y1 is the Y atom in YN layer, and Y2 is the Y atom in Y layer.

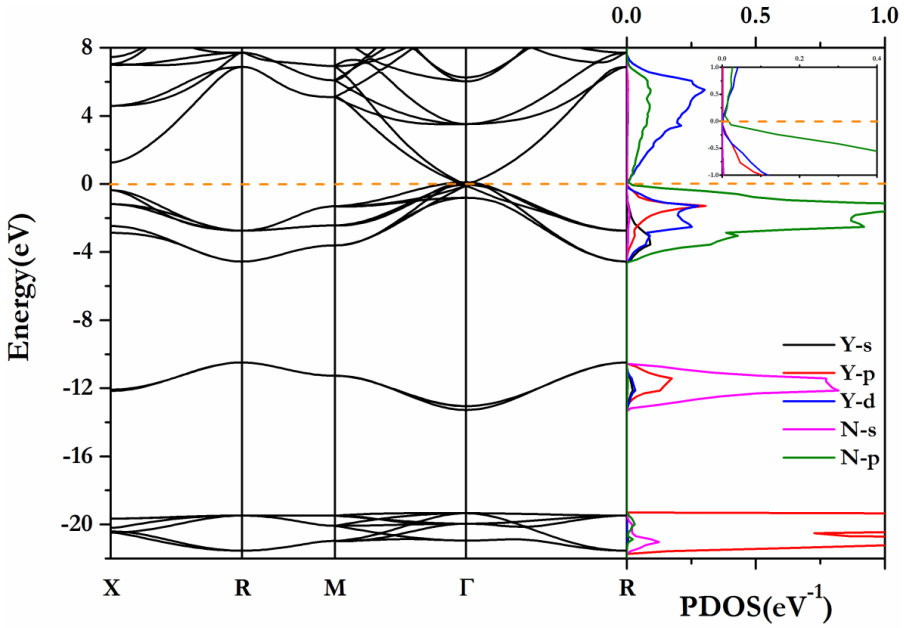

FIG. 14. Electronic band structure and projected DOS per atom of Y-*s*, Y-*p*, Y-*d*, N-*s*, and N-*p* states of *Fm*-3*m* phase YN at 50 GPa. The Y-*d* states at Gamma decompose into e_g and t_{2g} symmetry. The partial DOS also indicates the covalent character due to the fact that Y-*d* and N-*p* PDOS in the occupied parts follow closely with similar weight.

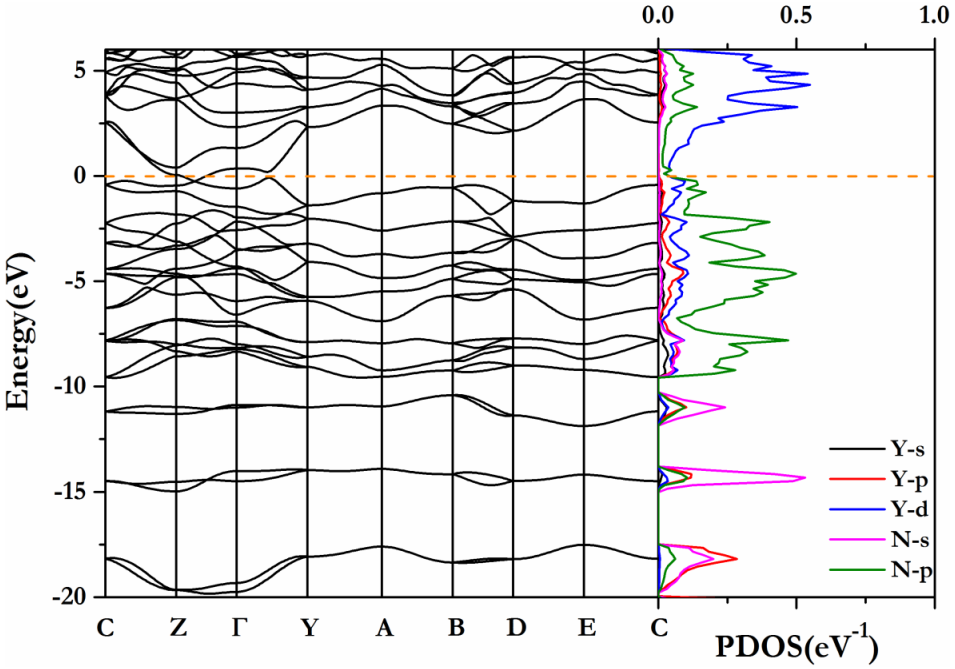

FIG. 15. Electronic band structure and projected DOS per atom of Y-*s*, Y-*p*, Y-*d*, N-*s*, and N-*p* states $P2_1/c$ phase YN_2 at 100 GPa.

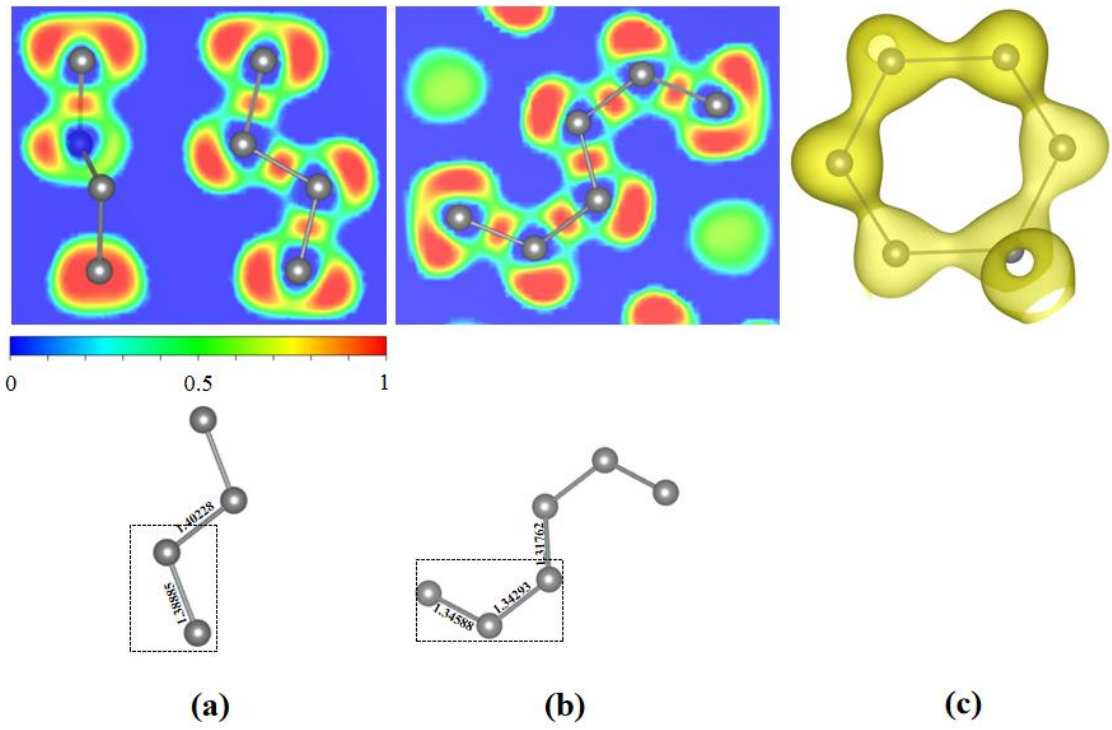

FIG. 16. ELFs and charge densiity of Y-N compounds. (a) *P*21/*c* phase of YN_2 at 100 GPa. The ELF is plotted in (-0.81 -1 0.36) sections for N_4 unit. (b) *P*-1 structure for YN_3 at 50 GPa.The ELF is plotted in (-1 0 -0.68) sections for N_6 unit. (c) The charge densiity of N_6 ring in *C*/2*m* phase of YN_5 at 100 GPa .

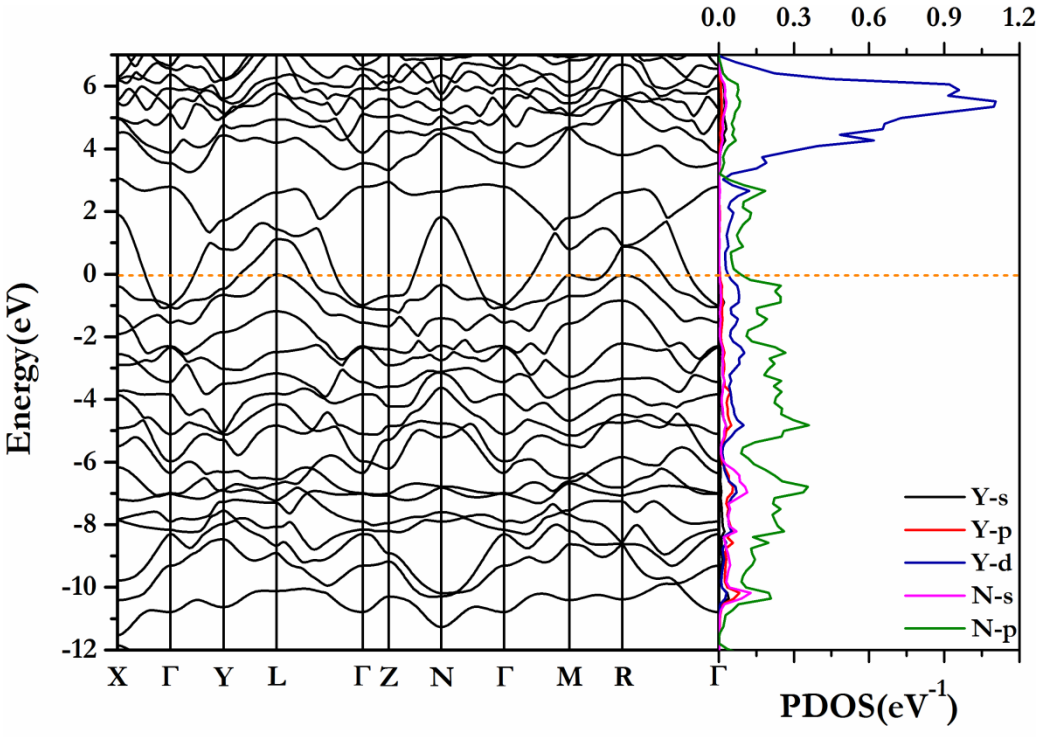

FIG. 17. Electronic band structure and projected DOS per atom of Y-*s*, Y-*p*, Y-*d*, N-*s*, and N-*p* states of *P*-1 phase of YN_4 at 50GPa.

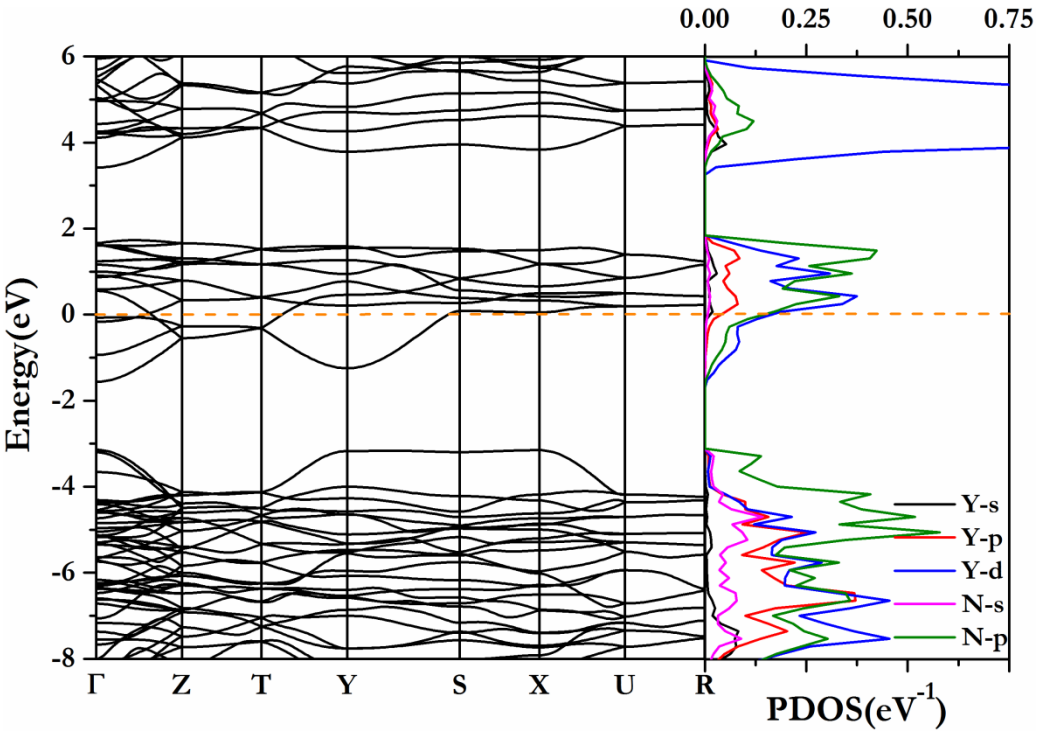

FIG. 18. Electronic band structure and projected DOS per atom of Y-*s*, Y-*p*, Y-*d*, N-*s*, and N-*p* states of the *Ibam* phasee of YN_{10} at 75GPa.

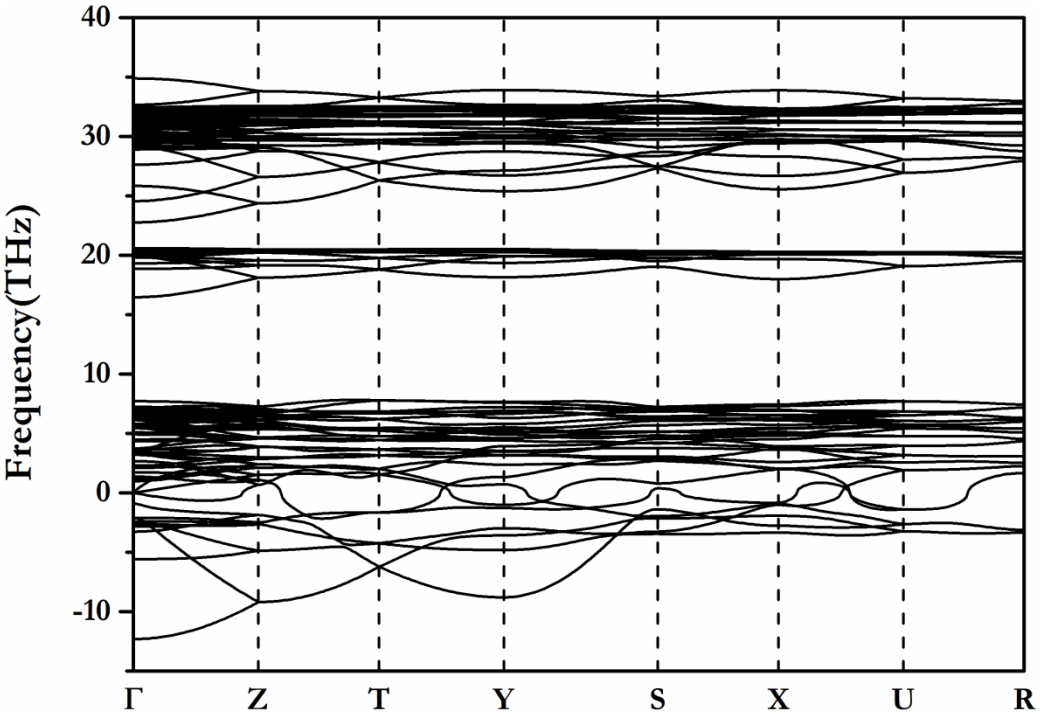

FIG. 19. Phonon dispersion curve of *Ibam* phase YN_{10} at 0 GPa.

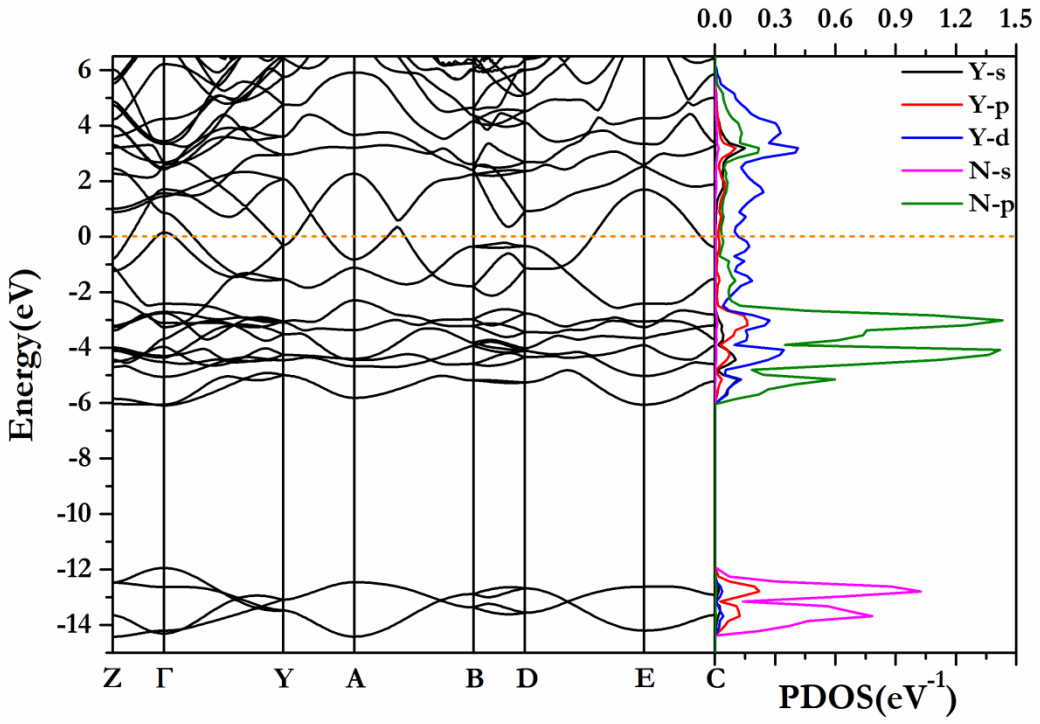

FIG. 20. Electronic band structure and projected DOS per atom of Y-*s*, Y-*p*, Y-*d*, N-*s*, and N-*p* states of *C*/2*m* phase Y_3N_2 at 100GPa.

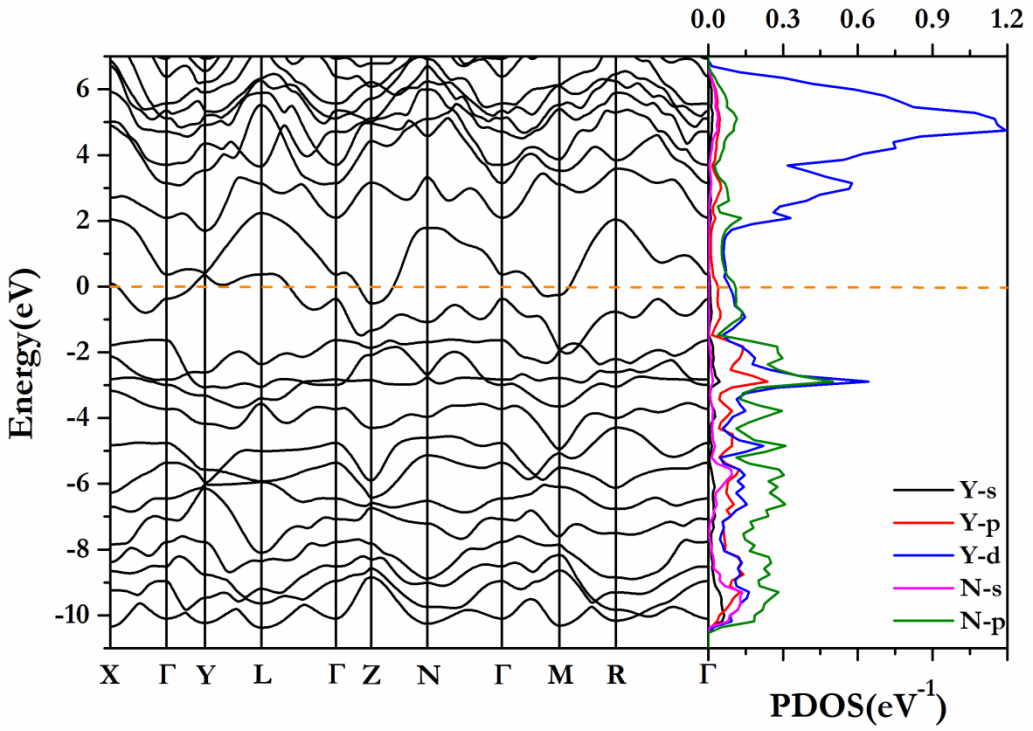

FIG. 21. Electronic band structure and projected DOS per atom of Y-*s*, Y-*p*, Y-*d*, N-*s*, and N-*p* states of *P*-1 phase of YN_3 at 50 GPa.

TABLE I. Calculated structural parameters of various Y-N compounds.

	Space group	lattice parameters *a*, *b*, *c* (Å) *α*, *β*, *γ* (deg)	Atoms	Atomic coordinates (fractional)		
				X	Y	Z
Y_5N_2 (25GPa)	*P4/nmm*	*a*=*b*=3.3154	Y1(2c)	0.50000	0.00000	0.85811
		c=22.1450	Y2(2c)	0.00000	0.50000	0.34819
		α=*β*=*γ*=90.0000	Y3(2c)	0.00000	0.50000	0.54817
			Y4(2c)	0.00000	0.50000	0.95342
			Y5(2c)	0.50000	0.00000	0.24605
			N1(2c)	0.50000	0.00000	0.34982
			N2(2c)	0.50000	0.00000	0.75609
Y_3N_2 (100GPa)	*C*2/*m*	*a*=5.20067	Y1(4i)	0.71138	0.50000	0.13332
		b=3.01959	Y2(2c)	0.00000	0.00000	0.50000
		c=7.20971	N1(4i)	0.60355	0.00000	0.31040
		α=*β*=90.0000				
		γ=103.6652				
YN (50GPa)	*Fm*-3*m*	*a*=*b*=*c*=4.58	Y1(4a)	0.00000	0.00000	0.00000
		α=*β*=*γ*=90.0000	N1(4b)	0.00000	0.50000	0.00000

YN_2	$P2_1/c$	a=5.91050	Y1(4e)	-0.76967	0.47722	-0.11707
(100GPa)		b= 4.42080	N1(4e)	-0.17391	0.02773	0.14925
		c=4.39840	N5(4e)	-0.43333	0.08439	-0.06693
		α=γ=90.0000				
		β=118.4491				
YN_3	P-1	a= 3.11250	Y1(2i)	0.58177	0.69281	0.30482
(50GPa)		b= 4.45580	N1(2i)	0.73189	0.19888	0.36202
		c=4.87550	N2(2i)	0.11071	0.68105	0.83070
		α=99.4988	N3(2i)	0.99749	0.13661	0.96963
		γ=106.3797				
		β= 101.0410				
YN_4	P-1	a= 3.53080	Y1(2i)	0.93742	0.26205	0.72095
(50GPa)		b= 3.60790	N1(2i)	0.36742	0.05172	0.04786
		c=7.10240	N2(2i)	0.35627	0.40938	0.04681
		α=104.1765	N3(2i)	0.72693	0.16915	0.38451
		γ=94.6326	N4(2i)	0.49839	0.40868	0.40707
		β= 106.9361				
YN_5	$C2/m$	a=6.79170	Y1(4h)	0.00000	0.76914	0.50000
(100GPa)		b= 7.04290	N1(8j)	0.88007	0.33681	0.33681
		c= 7.04290	N2(4i)	0.71819	0.00000	0.10381
		α=γ=90.0000	N3(4i)	0.29503	0.00000	0.24716
		β=123.1281	N4(4i)	0.91632	0.00000	0.82301

TABLE II. Calculated structural parameters of various Y-N compounds.

	Space group	**lattice parameters** ***a, b, c* (Å)*α, β, γ* (deg)**	**Atoms**	**Atomic coordinates (fractional)**		
				X	**Y**	**Z**
YN_8	P-1	a= 3.51660	Y1(1d)	0.50000	0.50000	0.00000
(75GPa)		b= 3.71620	N1(2i)	0.19296	0.71884	0.36967
		c=5.09080	N2(2i)	0.62164	0.41220	0.44212
		α=104.0308	N3(2i)	0.82854	0.45677	0.89652
		γ=101.6472	N4(2i)	0.09158	0.11361	0.11361
		β= 100.6977				
YN_{10}	*Ibam*	a= 7.79730	Y1(4a)	0.00000	0.00000	0.25000
(75GPa)		b= 5.51150	N1(16k)	0.88451	0.34289	0.14622
		c=7.25370	N2(8j)	0.52563	0.77617	0.00000
		α=β=γ=90.0000	N3(16k)	0.74878	0.44784	0.91136

TABLE III. Elastic constants C_{ij} (GPa), bulk modulus B(GPa), shear modulus G(GPa), Young's modulus E(GPa), and Possion's ratio v of P-1-YN_4, $C2/m$-YN_5, P-1-YN_8, and $Ibam$-YN_{10} at ambient pressure.

		C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}
YN_4	*P*-1	171	371	259	72	72	29	73	58	19	10	15
YN_8	*P*-1	172	497	239	103	139	148	57	158	22	25	91
		C_{23}	C_{24}	C_{25}	C_{26}	C_{34}	C_{35}	C_{36}	C_{45}	C_{46}	C_{56}	
YN_4	*P*-1	68	71	1	12	10	-1	42	11	4	16	
YN_8	*P*-1	82	60	-49	30	-6	25	135	86	14	10	
		B	*G*	*E*	*v*							
YN_4	*P*-1	113	60	153	0.27							
YN_8	*P*-1	126	77	192	0.25							
		C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{15}	C_{23}	C_{25}
YN_5	*C*2/*m*	353	221	73	52	126	53	36	149	-43	40	15
YN_{10}	*Ibam*	122	61	95	-56	-171	25	56	42		18	
		C_{35}	C_{46}	*B*	*G*	*E*	*v*					
YN_5	*C*2/*m*	-34	11	70	42	105	0.25					
YN_{10}	*Ibam*			51	7	20	0.43					

Note:

For a monoclinic phase, the criteria for mechanical stability are given by the following equation:

$$C_{11}>0,\quad C_{22}>0,\quad C_{33}>0,\quad C_{44}>0,\quad C_{55}>0,$$
$$C_{66}>0,\quad [C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})]>0,$$
$$(C_{33}C_{55}-C_{35}^2)>0,\quad (C_{44}C_{66}-C_{46}^2)>0,$$
$$(C_{22}+C_{33}-2C_{23})>0,$$
$$[C_{22}(C_{33}C_{55}-C_{35}^2)+2C_{23}C_{25}C_{35}-C_{23}^2C_{55}-C_{25}^2C_{33}]>0,$$
$$\{2[C_{15}C_{25}(C_{33}C_{12}-C_{13}C_{23})+C_{15}C_{35}(C_{22}C_{13}-C_{12}C_{23})+C_{25}C_{35}(C_{11}C_{23}-C_{12}C_{13})]-[C_{15}^2(C_{22}C_{33}-C_{23}^2)+C_{25}^2(C_{11}C_{33}-C_{13}^2)+C_{35}^2(C_{11}C_{22}-C_{12}^2)]+C_{55}g\}>0.$$

Here $g=C_{11}C_{22}C_{33}-C_{11}C_{23}^2-C_{22}C_{13}^2-C_{33}C_{12}^2+2C_{12}C_{13}C_{23}$

For an orthorhombic phase, the criteria for mechanical stability are given by the following equation:

$$C_{11}>0,\quad C_{22}>0,\quad C_{33}>0,\quad C_{44}>0,\quad C_{55}>0,$$
$$C_{66}>0,\quad [C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})]>0,$$
$$(C_{11}+C_{22}-2C_{12})>0,\quad (C_{11}+C_{33}-2C_{13})>0,$$
$$(C_{22}+C_{33}-2C_{23})>0.$$